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AGRO
CHEMISTRY
for and from
AGRICULTURE

PICOGRAM V. 82

and Abstracts

AMERICAN CHEMICAL SOCIETY

244th National Meeting and Exposition
August 19 – 23, 2012
Philadelphia, Pennsylvania, USA

AGRO

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WATERBORNE ENVIRONMENTAL, INC.

Fall 2012 AGRO Symposia

And Cosponsored Symposia in AGFD and ENVR

Lowes Philadelphia Hotel

POSTER SESSIONS

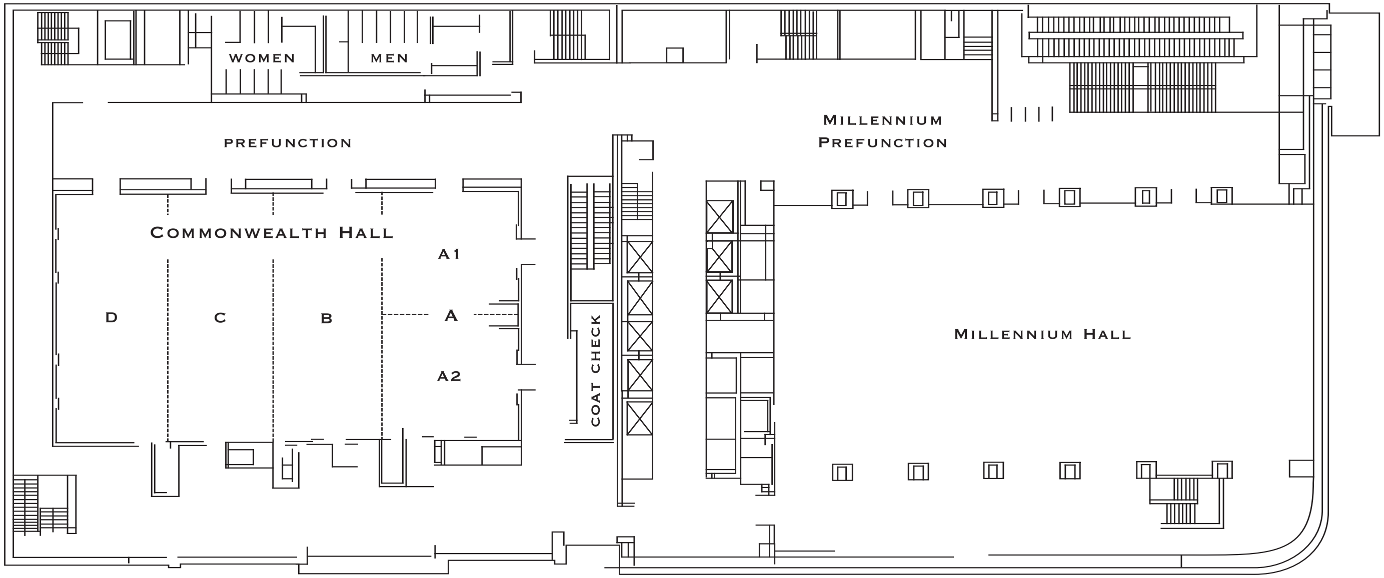
Pennsylvania Convention Center
Mon: 1:00 - 5:00 PM in Hall G; Tues: 1:00 - 5:00 PM in Hall D
Cosponsored in ***ENVR*** Poster Session Wed: 6:00 - 8:00 PM in Hall D

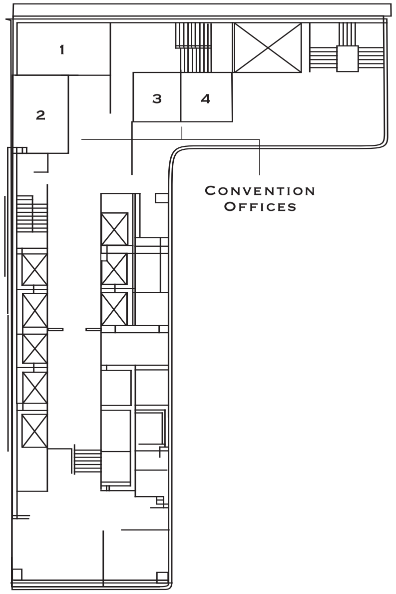
Program: page 61; **Abstracts:** page 86

SYMPOSIUM OR SESSION/SECTION	Room	Sun	Mon	Tue	Wed	Thu
Pesticide Env Fate Properties: Measurement, Predictions, Limitations & Reliability	Commonwealth D	D				
Natural Products for Pest Management	Regency B	D	D			
2012 Kenneth A. Spencer Award Symposium: James Seiber	Regency A	P				
Protection of Agriculture Productivity, Public Health & Environment	Regency C1/C2	P				
AGFD: Neuroactive Compounds from Natural Products	Commonwealth B	D				
ENVR: Materials for Water Sustainability	Washington B/C	D	D		E	
ENVR: Addressing Complex Site: Chemistry, Toxicology & Fate of Mixed Pollutants	Congress A	D			E	
ENVR: Interactions of Nanomaterials with Emerging Environmental Contaminants	Congress B/C	D	A		E	
New Technology & Approaches Applied to the Discovery of Agrochemicals: Symposium in Honor of Thomas Sparks (International Award Symposium)	Regency A		D			
MRLs and Ag Chemicals	Regency C1/C2		D	A		
Pesticides and Fumigant Emissions from Agricultural Systems	Commonwealth D		D			
AGFD: Discovering Bioactive Compounds	Commonwwealth A1/A2		D	D		
ENVR: Green Chemistry and the Environment	Congress A		D	A	E	
AGRO Education Awards: Undergraduate/Graduate Poster Session	PA ConvCtr Hall G		P			
ENVR: Innovative Technology for Green, Grey, Brown, and Black Water Reclamation and Reuse	Congress B/C		P		E	
Integrated Vector and Resistance Management	Commonwealth- D			D		
Environmental Fate, Transport, Modeling/Monitoring of Agricultural Chemicals	Regency B			D	D	
Is Your Analytical Method Good Enough? Innovation Award: Steven Lehotay	Regency A			D	A	
ENVR: Environmental Biotechnology & Sustainability: Applications to Drinking Water, Waste Treatment, Site Remediation	Washington B/C			D	E	
Sterling Hendricks Memorial Lectureship: Eric Block	Howe 33rd Floor			MD		
Reactive Nitrogen (Nr) from Agriculture: Emission, Consequence & Management	Regency C1/C2			P	D	
Protection of Agriculture Productivity, Pub Health & Environment: Poster Session	PA ConvCtr Hall D			P		
AGFD: 2011 Kenneth A. Spencer Award Symposium: Michael Pariza	Commonwealth B			P		
Mechanisms of Insecticidal Action/Resistance: New Compds & Recent Advances	Commonwealth D				D	
Synthesis and Chemistry of Agrochemicals	Lescaze 33rd Floor				D	
ENVR: Nanomaterials in Medicine, Food and the Environment	Congress B/C				D/E	A
Perfecting Communication of Chemical Risk	Regency A				P	
ENVR: Measurements and Methods in Environmental Nanotechnology	Congress A				E	A
Fate/Exposure Urban Applied Pesticides: Human/Ecological Risk Assessments	Commonwealth D					D
Human Health and Transgenic Crops	Commonwealth B					D
Next Generation Biofuels and Bioproducts: Advances & Challenges	Commonwealth C					D
Worker Exposure: Are Your Senses Proper Evaluation of Hazardous Exposure?	Commonwealth A1/A2					A

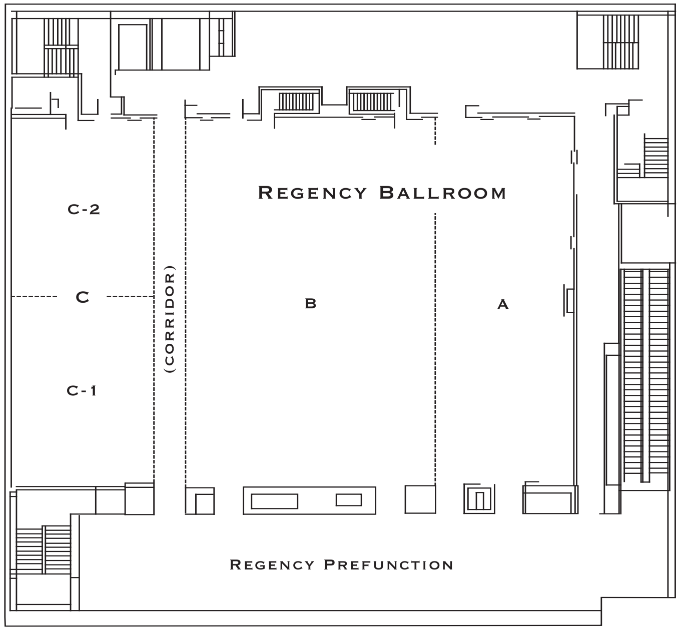
Legend: *A = AM; MD = mid-day; P = PM; D = AM/PM; E = evening*

Second Floor

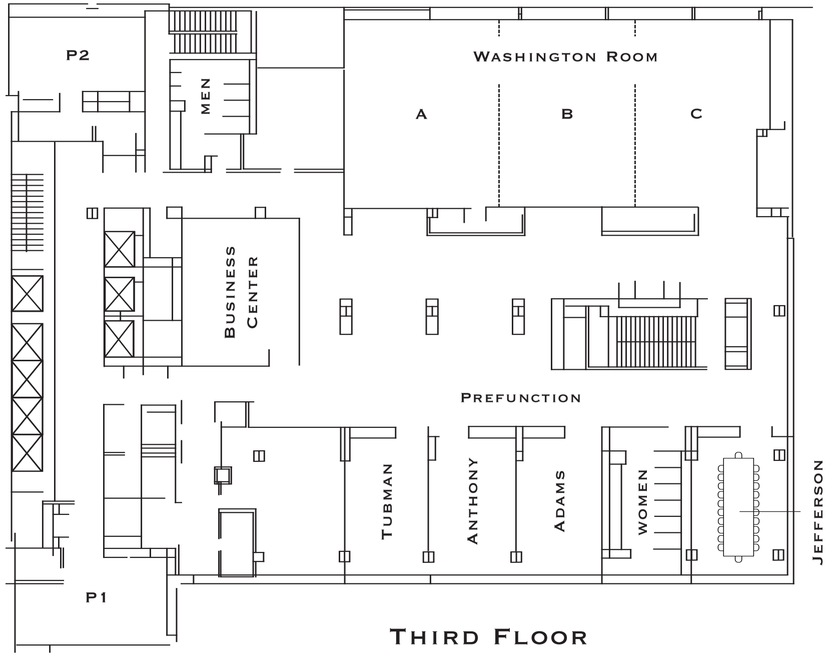




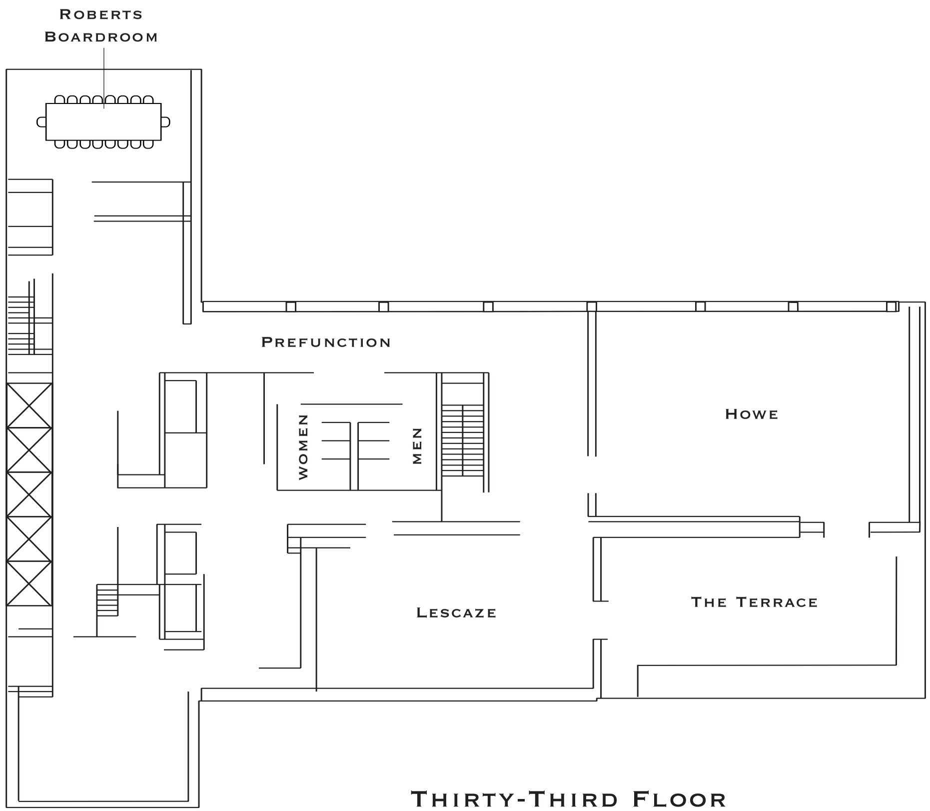
First Floor Mezzanine



Second Floor Mezzanine



THIRD FLOOR



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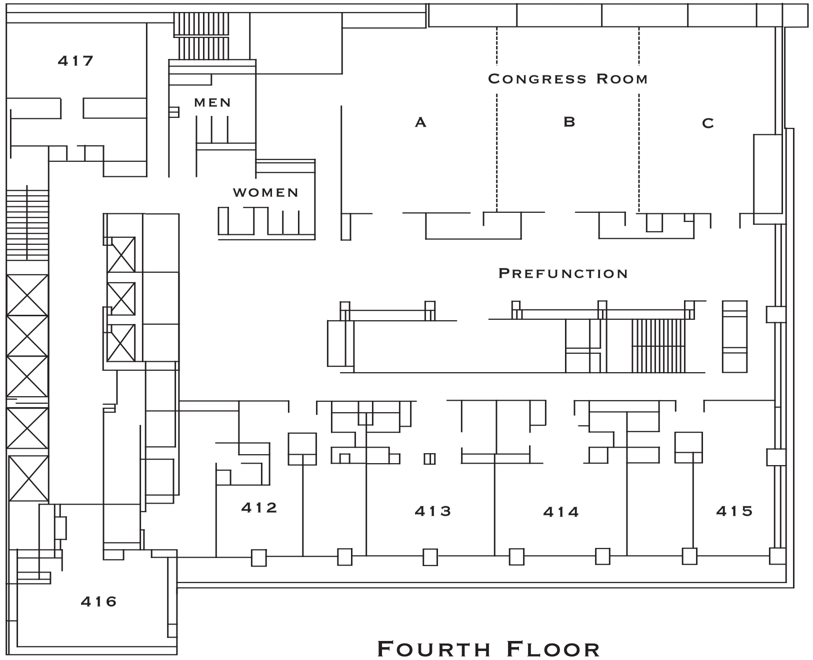

FOURTH FLOOR

LOEWS PHILADELPHIA HOTEL

TABLE OF CONTENTS

FROM THE CHAIR'S DESK

ALDOS BAREFOOT

AGRO's vision of providing a supportive environment for professional growth through innovative programming, services and opportunities for collaboration, and exchange of information continues to drive our activities and has led us to focus on three areas that are critical to our success as a vibrant, professional society.

Programming

The program for Philadelphia will be one of the largest ever organized by AGRO. John Clark's energy and enthusiasm for finding symposium organizers has given us a range of symposia and co-sponsored events that include our core topics in pesticide science, as well as topics of interest to all scientists seeking solutions to protection of agricultural productivity, public health and the environment, such as vector control, nitrogen emissions, health effects of transgenic crops, and risk communication.

John also managed to accomplish a long sought goal of AGRO in having our program in the same venue with AGFD and ENVR. Our interests touch on those of the other divisions in many ways, and we look forward to the opportunities for the members of all three divisions to benefit from the proximity in technical sessions.

As we hoped when we adopted our plan to program at one ACS meeting each year, we have supported programming at several conferences each year. AGRO members are instrumental in the Florida Pesticide Residue Workshop, and we are co-sponsors of the 5th Pan Pacific Pesticide Conference, which will be held in Beijing in conjunction with two conferences organized by IUPAC and the Beijing Pesticide Society. Plans for Indianapolis (Fall, 2013) are underway, and Steve Duke will be looking for more ideas at the Programming Committee meeting and at the Blues and Brews.

Of course the major programming event for 2014 will be the IUPAC Congress in San Francisco. Laura McConnell and Ken Racke are leading the organizing committee and will be looking for your suggestions and help with program topics, social events, presentations, and posters.

Governance

The AGRO Division relies on the Executive Committee for direction and actions that are necessary for a functional organization. We have looked carefully at programming ideas, finances, policies for awards, grants, bylaws and committee structures to ensure that we are meeting the needs of members and using our resources effectively. The Finance Committee is preparing budgets for 2012-2014 to assist our planning for the 2013 and 2014 meetings. Preparations for the IUPAC Congress will require funds this year and next. We expect to recoup those expenses through income derived from the Congress.

The Bylaws committee (Rod Bennett) has prepared changes that we will present at the Annual Meeting on August 19. AGRO has changed, and we need our guiding documents to be current. The Operations Manual, available through the AGRO website was updated last year and is a very useful resource for officers and committees.

The Development Committee has followed up leads for sponsors as we look at new services and provide support for students and speakers to participate in our programs. The support from sponsors is critical to AGRO's awards and programming. Please offer your thanks to our sponsors when you see their representatives in Philadelphia. AGRO has applied for grants from the ACS Division Activities Committee and the International Activities Committee as we develop a webinar series and expand our interactions with professional societies in other countries.

Committee Structure and Leadership

Our restructuring of committees and our need to transition to new leadership have created openings for chairs of several committees and opportunities to serve the Division as a committee member.

Job Openings:

Communications Committee Members – co-ordinate the communication activities of the Division, including e-newsletter, PICOGRAM, Division website, ACS books, and publicity at national meetings. Earlier this year, Yelena Sapozhnikova of USDA-ARS joined the committee as the e-newsletter editor. Please welcome Yelena and thank her for her enthusiasm and service to AGRO in this important role. This is an active committee and more help would be most appreciated.

PICOGRAM Associate Editor – assist the editor in securing input for the PICOGRAM, prepare AGRO program and abstracts for publication, work with sponsors on layout of ads, and work with Vice-chair on Calls for Papers. Please welcome John Beck of USDA-ARS, who has recently joined the editorial team as an associate editor, and we are seeking additional associate editors to ensure strong leadership into the future.

Social Committee Chair – lead and co-ordinate the hospitality events at AGRO meetings. The committee is responsible for the AGRO social, graduate student lunch, and coffee service. The committee works with the Secretary and Program Chair to ensure that food and beverage orders are reviewed with ACS prior to the first technical session of the ACS meeting.

Bylaws Committee Members – revise bylaws and operating manual to reflect current practices and maintain AGRO's guiding documents in accord with ACS requirements. The committee has one member at present, and we are looking for two more members who have the drive and attention to detail needed to keep documents in order.

Early Career Scientist Committee Member, New Investigator Award Coordinator - Administer the annual New Investigator Award program, including publicizing the award, soliciting candidates, evaluating applicants, presenting the award, and organizing a New Investigator Award Competition as part of the AGRO program at the ACS national meeting.

These jobs are critical to the success of the Division and are both a great opportunity to serve AGRO as well as develop professionally. Give them consideration and then get in touch with any member of the Executive Committee.

AGRO DIVISION FELLOWS

1971	Dr. Louis Lykken
	Dr. Tom H. (Bucky) Harris
	Dr. Herman Beckman (Posthumous)
1972	Mr. Wendell F. (Bud) Phillips
	Dr. Don G. Crosby
	Dr. Elvins Y. Spencer
1973	Mr. Roger C. Blinn
	Dr. Philip C. Kearney
	Dr. Julius J. Menn
1974	Dr. Morton Beroza
	Dr. James P. Minyard, Jr.
	Dr. Joe C. Street
1975	Dr. Hank F. Enos
	Dr. Maurice B. Green
	Dr. Charles H. Van Middelem
1976	Dr. Marguerite L. Leng
	Dr. Jack R. Plimmer
	Dr. Gerald G. Still
1977	Dr. Gustave K. (Bob) Kohn
1978	Dr. S. Kris Bandal
	Dr. Paul Hedin
1979	Dr. Rodney D. Moss
1980	Dr. G. Wayne Ivie
	Dr. John B. Siddall (Posthumous)
1981	Dr. Robert M. Hollingsworth
	Dr. Gino J. Marco
1983	Dr. John Harvey, Jr.
1985	Mr. Henry Dishburger
	Dr. Richard C. Honeycutt
1986	Dr. Gunter (Jack) Zweig
1987	Dr. Willa Garner
1988	Dr. Jan Chambers
	Dr. James Seiber
1990	Dr. Joseph Fenyes
1991	Dr. Nancy N. Ragsdale
1992	Dr. Don Baker
	Dr. Joel Coats
	Dr. Guy Paulson
1993	Dr. Larry Ballantine
1994	Dr. James Heitz
	Dr. Ralph Mumma
	Dr. Willis Wheeler
1996	Dr. John Bourke
1998	Dr. Hank Cutler
	Mr. Paul Giesler
2000	Dr. Barry Cross
2001	Dr. Robert Hoagland
2003	Dr. Judd O. Nelson
2005	Dr. Rodney Bennett
2006	Dr. Terry D. Spittler
2007	Dr. John M. Clark
	Dr. Ann T. Lemley
	Dr. R. Don Wauchope
2008	Dr. Allan S. Felsot
2011	Dr. Laura L. McConnell
2012	Dr. Jeffrey J. Jenkins
	Dr. John J. Johnston

AWARDS COMMITTEE REPORT

Dr. Thomas C. Sparks of Dow AgroSciences will receive the International Award at the 244th ACS National Meeting in Philadelphia. Dr. Sparks receives this award, which is sponsored by DuPont Crop Protection, for his research and exceptional accomplishments in applying new technology from a number of disciplines to the discovery of new pest control agents. A full-day symposium in his honor, organized by William Kleschick and B. Clifford Gerwick, will be held on Monday, August 20.

Dr. Steven J. Lehotay of the USDA-Agricultural Research Service is the winner of the first AGRO Award for Innovation in Chemistry of Agriculture. This award, which is sponsored by BASF, is given annually to an active researcher working in North America, who has successfully demonstrated an innovation in the chemistry of agriculture, veterinary science, or public health. Dr. Lehotay will be recognized for his development of QuEChERS, an analytical method streamlining pesticide residue analysis. He will present his work on Tuesday morning, August 21.

Dr. Eric Block of State University of New York at Albany is the winner of the USDA-Agricultural Research Service Sterling Hendricks Lectureship Award for his fascinating and seminal discoveries on sulfur and selenium chemistry in the Allium species. Dr. Block will present his lecture at the 244th ACS National Meeting in Philadelphia which will be hosted by AGFD and cosponsored by AGRO on Tuesday, August 21 at 11:30 AM. Check out his interview on NPR's *Science Friday* http://www.npr.org/templates/story/story.php?storyId=128268496

Dr. Jeffrey J. Jenkins of Oregon State University and **Dr. John J. Johnston** of the USDA Food Safety Inspection Service will receive the Division Fellow Award recognizing dedicated and enthusiastic service to the AGRO Division and the science of agrochemicals. The Awards Committee is accepting new award nominations for the Division Fellow Award. Criteria for the award and what to submit are shown below; nominations must be submitted by May 31, 2013.

Three New Investigator Award finalists, **Dr. Jeremy Conkle** of University of California-Riverside, **Dr. Fan Tong** of University of Florida, and **Dr. Xin Zhang** of Kansas State University, will receive a travel grant and will compete for this award at the 244th ACS National Meeting in Philadelphia. This restructured award now includes judging of their oral presentation at the National meeting by an anonymous panel. The winner will be announced by Thursday, August 23. Eighteen students will also receive travel grants to attend the 244th ACS National Meeting in Philadelphia. Their competition will be held on Monday afternoon and the winners will be announced at the AGRO Social on Tuesday, August 21.

Drs. Michael W. Pariza and **James N. Seiber** and will receive the 2011 and 2012 Kenneth A. Spencer award, which is sponsored by the Kansas City Section of ACS and the Divisions of AGRO and AGFD. Symposia will be held Sunday, August 19 and Tuesday, August 21. Details of the 2013 Spencer award can be found on page 29; nominations must be submitted by November 15, 2012.

The AGRO Division is pleased to announce the selection of **Dr. René Feyereisen** of INRA Centre de Recherche de Sophia Antipolis in France as the recipient of the 2013 International Award for Research in Agrochemicals. A symposium in his honor will be organized by Dr. Jim Ottea for the 246th ACS National Meeting in Indianapolis. Nominations for the 2014 International Award for Research in Agrochemicals are currently being accepted; criteria for the 2014 award can be found on page 23.

Nominations for the 2013 AGRO Award for Innovation in Chemistry of Agriculture and for the 2013 the USDA-Agricultural Research Service Sterling Hendricks Lectureship Award are being solicited by the AGRO Division and USDA-ARS, respectively. Criteria for each of the these awards can be found on pp. 25 and 27; nominations are due September 30, 2012 and November 5, 2012.

Please consider nominating a deserving colleague for the AGRO Division awards.

Respectfully submitted,
James N. Seiber, Chair
Awards Committee

CALL FOR NOMINATIONS
AGRO DIVISION FELLOW AWARD

The AGRO Division has established the ***Division Fellow Award*** to recognize its members whose dedicated and enthusiastic service has kept the Division moving forward.

Criteria shall be –

> *Continued and substantial contributions*
> *of time, talents, and service to the Division of Agrochemicals,*
> *ACS, and agrochemical science*
> *over a period of at least six years.*

Nominations include a letter, noting the contributions to the Division, and a current *curriculum vitae*. Deadline for submitting nominations is May 31 of each year. Contact the Awards Committee for further information. Submit nomination electronically to:

Dr. James N. Seiber
AGRO Awards Committee Chair
530-754-7005
jnseiber@ucdavis.edu

You Are Cordially Invited To:

The AGRO Division
Awards & Social

sponsored by the

JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY
IN CELEBRATION OF ITS 60TH ANNIVERSARY

Meet with Friends Old and New
Celebrate AGRO Member Award Winners

ACS International Award for Research in Agrochemicals
Thomas C. Sparks
AGRO Award for Innovation in Chemistry of Agriculture
Steven J. Lehotay
AGRO Fellow Awards
Jeffrey J. Jenkins & John J. Johnston
USDA-ARS Sterling Hendricks Lecturer
Eric Block
2011 & 2012 ACS Kansas City Section Spencer Award
Michael W. Pariza & James N. Seiber
AGRO New Investigator Award Finalists
AGRO Education Award Winners

Fun, Food, Good Company, Door Prizes, and a Cash Bar
6:00 - 8:00 pm
Tuesday, August 21
Loews Philadelphia Hotel, Millennium Hall

ALL AGRO DIVISION MEMBERS, SPEAKERS, AND
THEIR GUESTS/SPOUSES/SOs ARE INVITED TO JOIN US


DUPONT

ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS

Sponsored by DuPont Crop Protection

Dr. Thomas C. Sparks is the recipient of the 2012 ACS International Award for Research in Agrochemicals. The oldest of five children, Dr. Sparks was born in San Francisco and grew up in a small farming community in California's Central Valley, where growing and packing peaches, plums, nectarines, oranges, grapes, almonds, and other fruit were the mainstay of the local economy. He obtained a B.A. in biology and chemistry minor from Fresno State University(1973) and a Ph.D. in entomology from the University of California, Riverside(1978) under the guidance of Dr. Bruce Hammock. As the first student of Dr. Hammock (now at U.C. Davis and a former winner of the International Award), Dr. Sparks' research focused on insect biochemistry and toxicology. He credits the broad training and inspiration he received in Dr. Hammock's lab as outstanding preparation for his future roles in Academia and Industry.

In 1978, Dr. Sparks joined the faculty of the Department of Entomology at Louisiana State University as the insect toxicologist. Over the next 11 years, his research would cover endocrine regulation of insect metamorphosis, insecticide resistance, and insecticide biochemistry and toxicology. Dr. Sparks also taught introductory and advanced courses in insecticide toxicology. A full Professor, Dr. Sparks left LSU in 1989 and joined the agrochemical research group at Elanco, right at the time of the joint venture between Eli Lilly and The Dow Chemical Company to form DowElanco (now Dow AgroSciences). Shortly after joining DowElanco, Dr. Sparks became leader of a research group that coordinated aspects of spinosad's development along with the exploration of the spinosyn chemistry for the next generation product.

Concerned that available approaches were not leading to spinosyn chemistry nearly as active as the naturally occurring spinosyn A, Dr. Sparks investigated and then applied the radical approach of using artificial neural networks for the analysis of the quantitative structure activity relationships for the spinosyn chemistry. The resulting analysis pointed to new directions for the spinosyn chemistry that directly led to the discovery of new, more highly effective analogs, which in turn led to the next generation spinosyn product, spinetoram.

Spinetoram improves on spinosad by providing an expanded spectrum, improved efficacy and residual activity, while maintaining the excellent toxicological and environmental profile established by spinosad. The novelty and attributes of spinetoram were recognized in 2007 with an EPA Presidential Green Chemistry Challenge Award, and Dr. Sparks' efforts were recognized with R&D Magazine naming him the 2009 Scientist of the Year, the first in the 50 year history of the award for a scientist working in agriculture.

Currently a Dow Research Fellow, during his 23 years at Dow AgroSciences, Dr. Sparks has also led a variety of discovery efforts resulting in the discovery of numerous other insecticidal chemistries, many still active areas for Dow AgroSciences. Dr. Sparks recently led a successful effort to characterize the biochemical basis for lack of resistance to sulfoxaflor, a new sulfoximine insecticide for the control of sap-feeding insect pests. An EPA approval decision is expected in 2012. In addition to his research, Dr. Sparks has been the chair to the Insecticide Resistance Action Committee's Mode of Action Working Group. He currently holds a dozen patents / patent applications and has published extensively in scientific journal and books with 150 referred journal publications, book chapters and other articles. Tom and his wife Sandi have three children, Nicole, Kristina and Janine. He enjoys writing, technology history, and photography.

Please join us in a two part Symposium honoring Dr. Sparks

New Technology and Approaches Applied to the Discovery of Agrochemicals

on Monday, August 20 at 8:30 AM in

Loews Hotel Philadelphia, Regency Ballroom A

The AGRO Division is grateful for the sustained support of the International Award sponsor


Why do we invest more than the industry
average in R&D each year?
Simple — to make this his best year ever.

AGRO AWARD FOR INNOVATION IN CHEMISTRY OF AGRICULTURE

Sponsored by BASF Corporation

Dr. Steven J. Lehotay is the first receipt of the AGRO Award for Innovation in Chemistry of Agriculture. He is a Lead Scientist with USDA-Agricultural Research Service (ARS) at the Eastern Regional Research Center (ERRC) located near Philadelphia, Pennsylvania. Dr. Lehotay grew up in Orlando, Florida, and like many students there, he worked at Disney World - one of his favorite jobs ever was being a street sweeper at EPCOT. He has bled orange and blue since his youth and earned his BS (1987) and PhD (1992) in Chemistry at the University of Florida. Since joining ARS as a post-doc in Beltsville, Maryland, Dr. Lehotay's research has involved improving the analysis of pesticides, veterinary drugs, and other contaminants in food and environmental samples for food safety, regulatory, environmental, economic, and other beneficial purposes. He has authored/co-authored over 110 scientific articles and is the recipient of the 2011 AOAC International Harvey W. Wiley Award.

Dr. Lehotay's most important accomplishment is the co-development with Dr. Michelangelo Anastassiades of the QuEChERS (quick, easy, cheap, effective, rugged, and safe) method for streamlined sample extraction and clean-up, which are typically significant bottle-necks and hazardous waste generators in monitoring labs. QuEChERS reduces sample preparation labor, costs, time, space needs, and waste generation 2-10 fold over traditional methods and has been validated in more labs and for more pesticides and foods than any other residue method.

The practical benefits of QuEChERS are wide in scope. This method simplifies and improves monitoring of chemical residues in food, which leads to increased sampling of agricultural imports/exports and domestic products. Improved detection of contaminated food products encourages farmers to use registered products and good agricultural practices to ensure their products do not contain illegal residues (and potentially maximize yield/profits, too). Better farming practices are better for the environment, and fewer residues (and wider variety of foods year-round) are better for human health. Smoother international trade is better for global economic development. QuEChERS products are being sold by at least 20 different companies.

Most recently, Dr. Lehotay developed, validated, and transferred to the USDA National Residue Program QuEChERS-based methods to screen for over 100 veterinary drug residues in meat, poultry, and egg products. His innovation is not limited to the development of the QuEChERS approach. Other accomplishments with partners include: improvements in qualitative MS identification criteria and validation; efficient analysis of acrylamide in foods; direct sample introduction and analyte protectants for improved GC analysis; solvent-in-silicone tube extraction; development of a ChloroFiltr product; microcystins analysis in fish; monitoring of pesticides in the Chesapeake Bay; investigations of supercritical fluid extraction; and identification of new lipophilic contaminants using GCxGC/ToF analysis.

Dr. Lehotay will be presented this award prior to his paper in the symposium

Is Your Analytical Method Good Enough?

on Tuesday, August 20 at 9:40 AM in
Loews Hotel Philadelphia, Regency Ballroom A

The AGRO Division is grateful for the sustained
support of the AGRO Innovation Award

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- Confined Accumulation Studies on Rotational Crops with C-14 Test Substances
- Animal Metabolism with C-14 Test Substances (i.e. rat, lactating goat, laying hens, cows and pigs)
- Livestock Feeding Studies (i.e. cattle, pigs and poultry)
- Residue Studies: Method Development/Adaptation, Method Validation/ILV, Residue Analysis
- Storage Stability, MRL Calculation

ENVIRONMENTAL SAFETY AND ECOTOXICOLOGY
- Aerobic and Anaerobic Aquatic and Soil Metabolism
- Photo-degradation in Water and Soil
- Aqueous Hydrolysis; Adsorption/Desorption; Column Leaching (Aged); Field Dissipation
- Soil Nitrification Test
- Flow-Through, Semi-Static and Static Acute Fish Toxicity studies (experienced with handling Microencapsulation Formulations as well as conventional formulations)
- Terrestrial Vigor studies / Non-Target Plant Toxicity
- Acute Immobilization Test (i.e. Daphnia Test)

RISK ASSESSMENT
- Preparation of occupational, residential risk assessments/reports for new product registrations or label expansion for submission to U.S. EPA, PMRA, Asia-Pacific and Latin America
- Use of U.S. EPA PHED for occupational handler assessments
- Use of Agricultural Reentry Task Force data for occupational reentry worker risk assessments
- Assistance in design, review, and conduct of human exposure studies requiring review by the EPA Human Studies Review Board

FORMULATION
- HPLC, GC, CE Method Development/Validation and Formulation Analysis
- Product Chemistry (i.e., Physical/Chemical Characterization, Storage Stability Analysis, etc.)
- Cross Contamination Determination
- 5-Batch Analysis

PRODUCT REGISTRATION
- US Federal Registration Services

350 Clark Drive, Mount Olive, NJ 07828; Telephone: (973) 426-9900; Info@symbioticresearch.net
www.SymbioticResearch.com

AGRO DIVISION FELLOW AWARD

For continued and substantial contributions of time, talents, and service to the AGRO Division and agrochemical science

Dr. Jeffrey J. Jenkins received a B.S. in biochemistry from California State Polytechnic University – San Luis Obispo in 1972 and Ph.D. from Michigan State University in 1981. From 1982 to 1985, as a Senior Research Chemist at Merck Sharp & Dohme Agricultural Research and Development, he was part of the team that developed a new class of insecticides – the avermectins. In 1985 he joined the Entomology Department at the University of Massachusetts as an Experiment Station researcher, Extension Specialist, and Associate Director of the Massachusetts Pesticide Analysis Laboratory. He joined the Agricultural Chemistry Department – now the Department of Environmental and Molecular Toxicology – at Oregon State University in 1990.

Dr. Jenkin's current research activities include laboratory and field studies to examine the impact of pesticide use on air and water quality, studies designed to investigate human and wildlife exposure as a result of pesticide use in both agricultural and urban settings, studies to discern the effect of sub-lethal exposures on fitness and survival, and studies that may assist in the development of technologies that mitigate adverse human and environmental impacts. His collaborative research is to examine the impacts of chemical use on individuals, populations, and ecosystems.

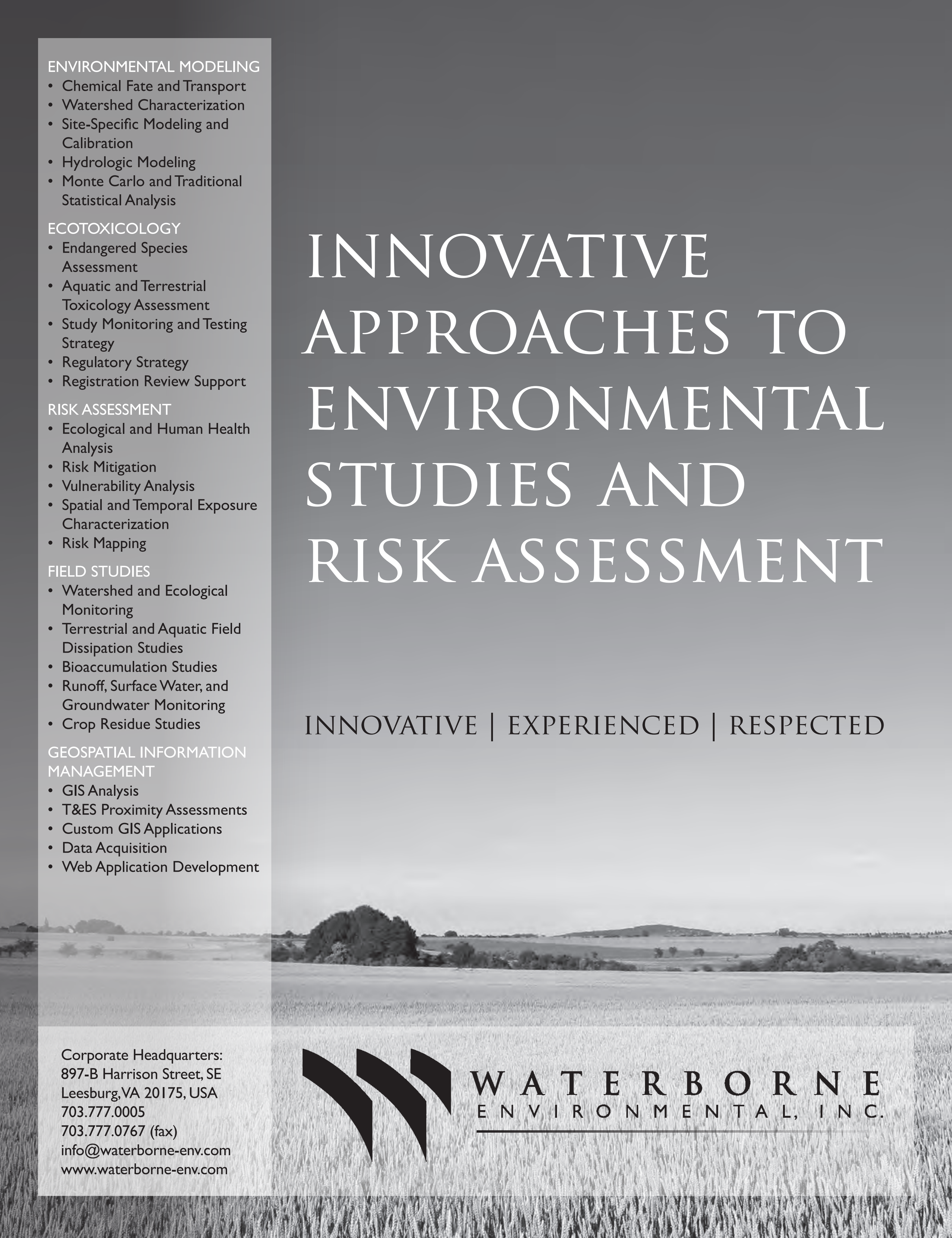
As an stalwart AGRO member of 32 years, Dr. Jenkins has served the Division in the three year Vice Chair, Program Chair, Chair rotation (1999 - 2001), prior to that for nine years as an Executive Committee Member, for the last twelve years as a member on the Hospitality and Public Relations (now Communications) Committees, and he has and continues to organize symposia regularly.

As AGRO Chair, and recognizing that the Division of Fertilizer Chemistry was struggling for survival and that AGRO membership was weakening, Dr. Jenkins initiated and implemented the merger of FERT into the Division of Agrochemicals. His vision of considering not only pesticides but fertilizers as agrochemicals, served as a catalyst to what AGRO is today, "Chemistry for and from Agriculture." Today, AGRO regularly hosts symposium concerning nutrient fate at the National ACS meetings.

Dr. Jenkins is also an educator, not just of undergraduate and graduate students, but of the general public, stakeholders, and policy-makers, both nationally and internationally. These outreach activities include the development of pesticide risk assessment methodology, tools, and materials to communicate risks. He regularly conducts and speaks at workshops for lay and professional audiences and is involved in adult continuing education. A primary goal is to translate scientific methods and findings to a broad and diverse audience. This outcome-driven approach strives to promote transparency and dialogue about risks associated with exposure to pesticides and other environmental agents and to improve use of risk information in individual decision-making and public policy. Dr. Jenkins also serves as Principle Investigator for the National Pesticide Information Center (npic.orst.edu) and Extension Toxicology Network cooperator.

Congratulations Jeff!

Thank you for all your contributions to the Division and agrochemical science and for effectively communicating our science to everyone!



AGRO DIVISION FELLOW AWARD

For continued and substantial contributions of time, talents, and service to the AGRO Division and agrochemical science

Dr. John J. Johnston received his B.S. in Food Science from Rutgers University (1979) and his Ph.D. in Food Toxicology from the University of Florida (1986). After a post-doc with the world-renowned Dr. John Casida in the Pesticide Chemistry and Toxicology Laboratory at the University of California, Berkeley (1986-1987), he joined the Chevron Chemical Company as Metabolism, Environmental Fate, and Residue Chemistry Study Director. His distinguished career in public service began in 1991 when he joined the USDA, Food Safety Inspection Service (FSIS) in Alameda, California as a Mass Spectrometry Specialist. He then served as Chemistry Project Leader at USDA Animal and Plant Health Inspection Service, National Wildlife Research Center in Fort Collins Colorado(1994-2008). During this time he also earned an M.B.A. from Colorado State University.

Dr. Johnson returned to FSIS as Senior Risk Analyst in 2008 where he designed risk assessments to estimate public health risk for chemical hazards in food. He currently serves as the Scientific Liaison for FSIS in Fort Collins, Colorado where he interfaces with government, industry and academic stakeholders, and partners to identify Agency research and data needs and to develop and coordinate solutions.

Dr. Johnston has faithfully served the AGRO Division for more than 10 years. He has exhibited extraordinary creativity, leadership, and scientific excellence, and always with immense enthusiasm. Dr. Johnston has contributed in many ways to the success of the Division, but most substantially, when he chaired the AGRO Education Committee (2002 to 2009). In this demanding role, he served as a primary contact for the dozens of young scientists many of whom remain active in the Division. Dr. Johnston served as Vice Chair, Program Chair, and Division Chair (2006 - 2008) and currently is the Division Treasurer.

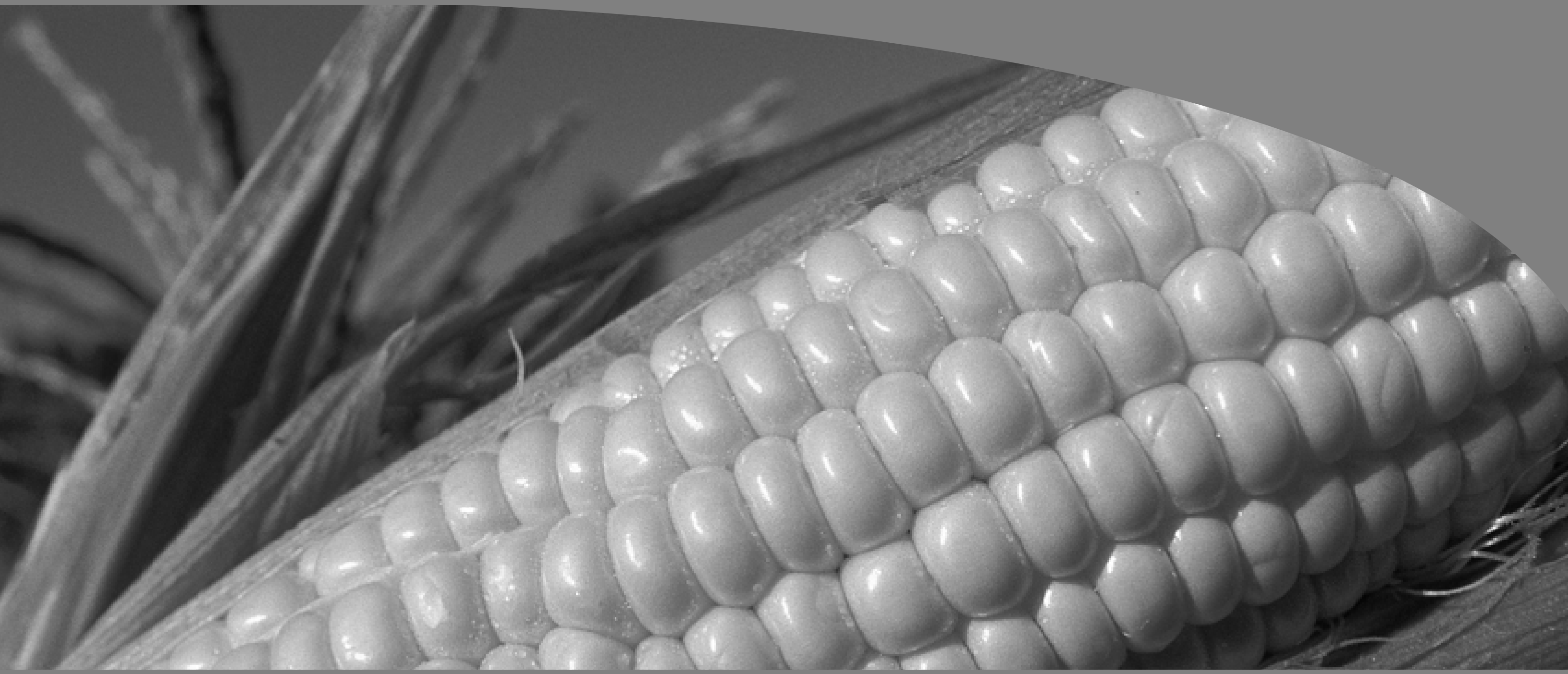
Dr. Johnston has organized and chaired more than 20 technical symposia on a variety of topics. For many years he co-chaired the standing symposium on Residues and Metabolism which has been an important venue for many AGRO scientists to present their work. In 2010, he organized two symposia at the Pacifichem Conference. One of these entitled, “Rodenticide-Based Opportunities for Protection of Agriculture, Ecosystems & Public Health,” was later featured in *Chemical & Engineering News* highlighting the challenges of protecting endangered plant and animal species from rodent infestation in island habitats.

Recognizing that AGRO's strength depended on robust programming and a commitment to long range planning, in 2006 Dr. Johnston initiated the long range planning brainstorming session on Wednesday during Happy Hour at the ACS National Meetings. These sessions are open to all members and interested parties and have become extremely valuable to the Division. What makes these sessions truly unique and enjoyable is the entertainment as Dr. Johnston (aka Johnny Johnston) is not only an accomplished scientist, he is a talented fingerpickin', slide guitarist. Within a year, these sessions became known as the “Blues and Brews”.

In John’s words, “Being active in AGRO has afforded me numerous opportunities which have complemented my scientific career for the past 20+ years. First and foremost, the opportunity to be part of a network of folks that I thoroughly enjoy is clearly the most significant benefit of being an AGRO member. Professionally, AGRO membership affords access to an incredible reservoir of knowledge; knowledge to be tapped during formal symposia or informally, while tapping a keg of beer during happy hour. I greatly appreciate being recognized as an AGRO Fellow.”

Congratulations John!

Thank you for all you have contributed to the Division and agrochemical science and for your commitment to supporting AGRO's students!



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2012 STERLING B. HENDRICKS MEMORIAL LECTURESHIP AWARD

Sponsored by USDA-Agricultural Research Service
Co-Sponsored by AGFD & AGRO Divisions

Fifty years of smelling sulfur: From Allium chemistry to olfactory detection of sulfur compounds.

Dr. Eric Block is a world authority on garlic science and is the Carla Rizzo Delray Distinguished Professor of Chemistry at the University at Albany, State University of New York. The *New York Times* called his 2010 454 page book *Garlic and Other Alliums: The Lore and the Science* (published by the Royal Society of Chemistry) "the definitive word on the alliums." Block, born in New York City, received a B.S. in chemistry from Queens College of the City University of New York, where he was elected to Phi Beta Kappa. He received an M.S. and Ph.D. in chemistry from Harvard University, where he worked with 1990 Nobel Laureate E.J. Corey, and where he held both NSF and NIH pre-doctoral fellowships. Prior to his appointment at the University at Albany in 1981, Block was a faculty member at the University of Missouri-St. Louis.

A member of the Editorial Advisory Board of the *Journal of Agricultural and Food Chemistry* since 1994, Block has been Visiting Professor at Harvard, the Weizmann Institute of Science in Israel and Cambridge University in the UK, and a consultant to numerous major corporations. Eric Block was the 1984 recipient of a John Simon Guggenheim Fellowship, the 1987 recipient of the American Chemical Society's Award for Advancement of Application of Agricultural and Food Chemistry, the 1994 recipient of the International Council on Main Group Chemistry Award for Excellence in Main Group Chemistry Research, the 2003 recipient of the Kenneth C. Spencer Award of the Kansas City Section of the ACS, and was named a Fellow of the Division of Agricultural and Food Chemistry of the ACS in 1993. He is the author of 237 scientific papers, 8 patents, and 4 books, many of which deal with garlic and other alliums, and the chemistry of the elements sulfur and selenium. His current research focuses on the molecular basis of the sense of smell and use of non-natural selenoamino acids in determination of protein structure. Block has trained more than 60 graduate students and postdoctoral fellows during his 45 years in academia.

Selected accomplishments include:

- determination of the structure of the lachrymatory factor of the onion and its dimer;
- demonstration of bird repellent properties of garlic oil;
- identification and synthesis of the garlic anticlotting and anticancer agent ajoene, and bis-sulfine, cepaenes, and zwiebelanes, biologically active flavorants from onion;
- identification of natural trace level organoselenium compounds found in *Allium* volatiles and in human garlic breath;
- a clinical trial on the effectiveness of garlic and garlic supplements as lipid-lowering agents; and
- examination of intact onion cells using synchrotron radiation techniques and direct detection of highly reactive compounds from alliums using DART mass spectrometry.

Recent research by Block and colleagues on olfaction (*PNAS* 2012, *109*, 3492-7) established that copper is required for olfactory detection of (methylthio)methanethiol ("MTMT"), the mouse semiochemical he identified with Duke University colleagues (*Nature* 2005, *434*, 470-7).

Dr. Block will deliver his lecture immediately following presentation of the Sterling Hendricks Award on

on Tuesday, August 21 at 11:30 AM in
Loews Hotel Philadelphia, 33rd Floor - Howe

INTERNATIONAL AWARD FOR ADVANCES IN CROP PROTECTION CHEMISTRY

Sponsored by ***International Union of Pure and Applied Chemistry***
A member of the International Council of Scientific Unions
Advisory Committee on Crop Protection Chemistry

2012 IUPAC International Award for Advances in Harmonized Approaches to Crop Protection

The 2012 *IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry* will be presented to **Lois A. Rossi** of the Office of Pesticide Programs at the US Environmental Protection Agency (EPA). Arrangements are being made for Rossi to receive her award and present an invited lecture as part of the IUPAC-sponsored *5th Pan-Pacific Conference on Pesticide Chemistry* planned for Beijing, China, during 16-19 September 2012.

Rossi has been involved for more than 20 years with international regulatory harmonization efforts. Through her activities with the NAFTA (North American Free Trade Agreement) Technical Working Group she was instrumental in development of harmonized approaches for pesticide evaluation, establishment of maximum residue limits (MRLs) for foods, and pesticide labeling.

Rossi's efforts related to global regulatory harmonization via the OECD Working Group on Pesticides began in 1991 with a workshop held in Washington, DC, and included major contributions to the design and implementation OECD's 10-year vision for "A Global Approach to the Regulation of Agricultural Pesticides" launched in 2004. Rossi has also been active in promoting harmonization efforts involving minor and specialty crops through the OECD Expert Group on Minor Uses, and she served as a lead organizer for the inaugural "Global Minor Use Summit" held in Rome during 2007 with the support of FAO and USDA.

As head of the US Delegation since 2004, Rossi has led efforts via the Codex Committee on Pesticide Residues for development of streamlined international evaluations and accelerated adoption of harmonized MRL standards applicable among the more than 165 Codex member countries.

Rossi has been a tireless advocate for adoption of joint regulatory evaluations of new pesticide active ingredients, whereby the efforts of regulatory authorities in multiple countries are pooled and coordinated for harmonized data reviews. These joint reviews, which began in the NAFTA region and later expanded to a global basis, have resulted in a paradigm shift within both governments and the industry whereby such joint reviews are quickly becoming the norm.

About this Award

The *IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry* is a recently developed award that recognizes individuals in government, intergovernmental organizations, industry, and academia who have exercised personal leadership for outstanding contributions to international harmonization in the regulation of crop protection chemistry.

The award program is administered by the IUPAC Division of Chemistry and the Environment, and was first presented in 2010. Nominations for the award are solicited for receipt by December 1 of odd-numbered years, with the award to be made during even-numbered years in conjunction with an IUPAC-sponsored conference or special symposium. Corporate sponsorship for the award has been arranged with Dow AgroSciences.

Awardees receive an honorarium plus meeting registration, travel, and per diem reimbursement. For further information on the award, please contact IUPAC Committee Chair John Unsworth (UnsworJO@aol.com) or Past-Chair Ken Racke (KRacke@dow.com) or visit the IUPAC website at

www.iupac.org.

Previous Awardee

2010 - Denis J. Hamilton (retired), Queensland Department of Primary Industries, Australia

ACS KANSAS CITY SECTION

2011 KENNETH A. SPENCER AWARD

Co-Sponsored by AGFD & AGRO

Dr. Michael W. Pariza, is an Emeritus Professor of Food Science, and Emeritus Director, Food Research Institute, University of Wisconsin--Madison. He received his B.S. in Bacteriology at the University of Wisconsin--Madison and his M.S. and Ph.D. in Microbiology at Kansas State University. He completed three years of postdoctoral study at the McArdle Laboratory for Cancer Research at the University of Wisconsin--Madison and joined the faculty of the Department of Food Microbiology and Toxicology in 1976. He served as Department Chair from 1982 to 2006 and as Director of the Food Research Institute from 1986 to 2008. He held a Wisconsin Distinguished Professorship from 1993 to 2009.

Dr. Pariza has authored or co-authored over 180 articles and publications, and he holds more than 25 U.S. patents. Dr. Pariza has been recognized by Thompson Scientific as one of the most "Highly Cited Researchers" of the last two decades.

Dr. Pariza has received numerous academic honors and awards including the Marqueta C. Huyck Endowed Lectureship at Wayne State University, the Bruce P. Wasserman Lectureship at Rutgers University, the Bernard L. Oser Food Ingredient Safety Award from the Institute of Food Technologists, the David Kritchevsky Career Achievement Award in Nutrition from the American Society for Nutrition, election as a Fellow of the Institute of Food Technologists, and election as a Fellow of the American Society for Nutrition.

Dr. Pariza is widely recognized as the founder of the modern field of conjugated linoleic acid (CLA) research. The anticancer properties of CLA, and many of the other known biological activities of CLA, were discovered in his laboratory and in the laboratory of his principal UW-Madison collaborator, Professor Mark Cook. Patents on the Pariza-Cook CLA discoveries, assigned to WARF, generate about $2 million annually in royalties (more than $15 million total in the past 10 years).

Dr. Pariza is also an internationally-recognized expert in evaluating food enzyme safety. He developed the principal guidelines for evaluating the safety of microbially-derived food enzymes that are used by government regulators and food enzyme manufacturers throughout the world. Dr. Pariza currently maintains an office and laboratory in the Microbial Sciences Building at UW-Madison.

Please join AGFD in an afternoon Symposium honoring Dr. Pariza

Conjugated Linoleic Acid: A Naturally-Occurring, Anti-obesity, Anti-inflammatory Fatty Acid

on Tuesday, August 21 at 1:30 PM in
Loews Hotel Philadelphia, Commonwealth B

ACS KANSAS CITY SECTION
2012 KENNETH A. SPENCER AWARD
Co-Sponsored by AGRO & AGFD

Dr. James N. Seiber, a native of Missouri, received his degrees in chemistry from Bellarmine College (Louisville, KY), Arizona State University (Tempe, AZ) and Utah State University (Logan, Utah). He has held positions as a research scientist at Dow Chemical Company (Midland MI and Walnut Creek, CA). He was a faculty member at the University of California Davis, Department of Environmental Toxicology, from 1969 to 1992, where he served as Professor and Department Chair, and as Associate Dean for Research in the College of Agricultural and Environmental Sciences. He was founding director of the Center for Environmental Sciences and Engineering at the University of Nevada, Reno in 1992, where he initiated a multidisciplinary program of research and graduate education in Atmospheric Sciences, Hydrology, Conservation Biology, Environmental Health and Environmental Engineering.

He joined the U.S. Department of Agriculture's Agricultural Research Service in 1998 as Director of the Western Regional Research Center (WRRC) in Albany, CA. He oversaw scientists working in eight research units: Exotic and Invasive Weeds, Produce Safety and Health, Bioproduct Chemistry and Engineering, Processed Foods, Crop Improvement and Utilization, Plant Mycotoxins, Genomics and Gene Discovery, and Foodborne Contaminants. He was responsible for the development and implementation of food safety and biobased product initiatives at the WRRC. He also served as Acting Director of the ARS Western Human Nutrition Research Center and Southern Regional Research Center, and earlier in his career worked at the International Rice Research Center in the Philippines.

Dr. Seiber returned to academic life as interim Chair (2009 - 2011) for the Department of Food Science and Technology at the University of California, Davis. He continues his affiliation at UC Davis as an emeritus Professor in the Department of Environmental Toxicology and Editor-in-Chief of the *Journal of Agricultural and Food Chemistry*. In the latter capacity he oversees manuscript flow and decisions regarding acceptance of manuscripts by the 11 person corps of Associate Editors located in North American, Europe, Asia, and Australia.

Dr. Seiber's research recognized in the Spencer Award is in the area of environmental transport and fate of pesticides and other contaminants, where the bulk of his work and that of 40-plus graduate students and research associates he has coordinated resides. A particular area of interest of his has been the role of the atmosphere in contaminant cycling in the environment. Seiber received the AGRO Fellow Award in 1988 and the ACS International Award for Research in Agrochemicals in 1999. In 2010, Dr. Seiber was named an ACS Fellow.

Please join us in an afternoon Symposium honoring Dr. Seiber

Chemical Transport, Fate, and Sustainability

on Sunday, August 19 at 1:30 PM in
Loews Hotel Philadelphia, Regency Ballroom A

Past Awardees of the Burdick & Jackson International Award

1969	Dr. John E. Casida, University of California, Berkley
1970	Dr. Richard D. O'Brien, Cornell University
1971	Dr. Robert L. Metcalf, University of Illinois
1972	Dr. Ralph L. Wain, Wye College, University of London, England
1973	Dr. Hubert Martin, British Crop Protection Council, England
1974	Dr. T. Roy Fukuto, University of California, Riverside
1975	Dr. Michael Elliot, Rothamsted Experiment Station, England
1976	Dr. Morton Beroza, USDA-ARS (retired)
1977	Dr. Francis A. Gunther, University of California, Riverside
1978	Dr. Julius J. Menn, Stauffer Chemical
1979	Mr. Milton S. Schecter, USDA (retired)
1980	Dr. Minuro Nakajima, Kyoto University, Kyoto, Japan
1981	Dr. Philip C. Kearney, USDA-ARS, Beltsville, Maryland
1982	Dr. Jack R. Plimmer, USDA-ARS, Beltsville, Maryland
1983	Dr. Karl Heinz Buechel, Bayer AG, Germany
1984	Dr. Jacques Jean Martel, Roussel Uclaf, Paris
1985	Dr. Junshi Miyamoto, Sumitomo Chemical Co., Japan
1986	Dr. James Tumlinson, USDA-ARS, Gainesville, Florida
1987	Dr. Fumio Matsumura, Michigan State University
1988	Dr. Ernest Hodgson, North Carolina State University
1989	Dr. Toshio Narahashi, Northwestern University
1990	Dr. David Schooley, University of Nevada, Reno
1991	Dr. Stuart Frear, USDA-ARS, Fargo, North Dakota

Past Awardees of the ACS International Award For Research in Agrochemicals

Co-Sponsored by BASF & DuPont Crop Protection

1992	Dr. Bruce Hammock, University of California, Davis
1993	Dr.Morifuso Eto, Kyushu University, Fukoka, Japan
1994	Dr. Toshio Fujita, Kyoto University, Kyoto, Japan
1995	Dr. Mohyee Eldefrawi, University of Maryland, Baltimore Dr. Koji Nakanishi, Columbia University, New York
1996	Dr. Günther Voss, Ciba, Basel, Switzerland Dr. Klaus Naumann, Bayer, Leverkusen, Germany
1997	Dr. Fritz Führ, Jülich, Germany Dr. Izuru Yamamoto, University of Tokyo, Japan
1998	Dr. George Levitt, DuPont, Wilmington, Delaware Dr. Leslie Crombie, University of Nottingham, England
1999	Dr. Don Baker, Zeneca, Richmond, CA Dr. James Seiber, University of Nevada, Reno
2000	Dr. George P. Georghiou, University of California, Riverside Dr. Herbert B. Scher, Zeneca
2001	Dr. Donald Crosby, University of California, Davis Dr. Ralph Mumma, Pennsylvania State University
2002	Dr. Keith Solomon, University of Guelph, Ontario, Canada Dr. Marinus Los, American Cyanamid
2003	Dr. Bob Hollingworth, Michigan State University Dr. Hideo Ohkawa, Kobe University, Japan
2004	Dr. Stephen Duke, USDA-ARS, Oxford, Mississippi Dr. John Marshall Clark, University of Massachusetts
2005	Dr. Robert Krieger, University of California, Riverside Dr. Janice E. Chambers, Mississippi State University
2006	Dr. Joel Coats, Iowa State University Dr. Isamu Yamaguchi, Agricultural Chemicals Inspection Station, Tokyo Japan
2007	Dr. Gerald T. Brooks, West Sussex, UK Dr. Fredrick J. Perlak, Monsanto
2008	Dr. David M. Soderlund, Cornell University
2009	Dr. R. Donald Wauchope, USDA-ARS (retired), Tifton, Georgia
2010	Dr. Shinzo Kagabu, Gifu University, Gifu, Japan
2011	Dr. George P. Lahm, DuPont Crop Science, Newark, Delaware

CALL FOR NOMINATIONS
ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS
Sponsored by DuPont Crop Protection

2014 Fall ACS National Meeting in San Francisco, California

The ACS Award for Innovation in Chemistry of Agriculture is given to an active researcher working in North America for a chemical innovation that significantly enhances agricultural or veterinary pest management and productivity. The awardee will be asked to give an award address at the National ACS meeting.

- The ***nomination letter*** will include the following statement: "I hereby nominate [insert first, middle, last name] as a candidate for the ACS International Award for Research in Agrochemicals." It will also include the ***nominee's birthplace, date of birth, citizenship, business address*** and a **description** (200 – 1000 words) of the reasons why the nominee should receive this award, stressing the individual's major accomplishments.

- Include a current ***curriculum vitae*** of the candidate that includes: places and nature of employment, professional affiliations, honors and awards received, and a list of publications and patents.

- Nominations often include ***one or two letters of support***, although this is optional.

Deadline: Nominations should be received by the committee chair by ***December 31*** of each year. Balloting will be conducted in January/February and results will be announced in the spring of the following year.

The nominating official(s) should be prepared to assist in organizing a symposium at the National ACS meeting in honor of the awardee.

Please email this information to:

Dr. James N. Seiber
AGRO Awards Committee Chair
jnseiber@ucdavis.edu
530-754-7005

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Method development and validation, ILV, clinical sample analysis, analysis of agrochemicals and metabolites in soil, water, air, crops and animal tissues.

FIELD STUDIES

Terrestrial and aquatic dissipation, rotational crops, nature and magnitude of residues in crops, lysimetry and small plot dissipation studies utilizing radiolabels. Volatility and flux determination.

EXPOSURE

Cow and hen feeding studies, dislodgeable foliar and turf residues, mixer/loader and applicator dosimetry. Environmental monitoring (air and water). Tobacco pyrolysis.

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CALL FOR NOMINATIONS

AWARD FOR INNOVATION IN CHEMISTRY OF AGRICULTURE

Sponsored by BASF Corporation

2013 Fall ACS National Meeting in Indianapolis, Indiana

The ACS Award for Innovation in Chemistry of Agriculture is given to an active researcher working in North America for a chemical innovation that significantly enhances agricultural or veterinary pest management and productivity. The awardee will be asked to give an award address at the National ACS meeting.

The Nomination email will include the following as attachments

1. A **formal letter of nomination** that includes
    - Name, business address, phone and email address of the nominator
    - Name, birth date, business address, phone and email address of the nominee
    - A nomination statement (200-1000 words) giving reasons why the nominee should receive this award, stressing the chemical innovation and how it has enhanced agricultural or veterinary pest management and productivity.

2. The nominee's **current curriculum vitae**

3. One or two **letters of support**

4. Reference or e-mail link to 1 or 2 published **manuscripts that report on the work** which supports the award nomination

A single Nomination email, with all attachments listed above should be emailed to:

Dr. James N. Seiber
AGRO Awards Committee Chair
jnseiber@ucdavis.edu
530-754-7005

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CALL FOR NOMINATIONS

2013 STERLING B. HENDRICKS MEMORIAL LECTURESHIP

Sponsored by USDA-Agricultural Research Service

Co-Sponsored by AGFD & AGRO Divisions

The USDA-Agricultural Research Service (ARS) is seeking nominations for the 2013 Sterling B. Hendricks Memorial Lectureship Award. This Lectureship was established in 1981 by ARS to honor the memory of Sterling B. Hendricks and to recognize scientists who have made outstanding contributions to the chemical science of agriculture. Dr. Hendricks contributed to many diverse scientific disciplines, including soil science, mineralogy, agronomy, plant physiology, geology, and chemistry. He is most frequently remembered for discovering phytochrome, the light-activated molecule that regulates many plant processes. The lecture should address a scientific topic, trend, or policy issue related to agriculture. Deadline is **November 2, 2012.**

The AGRO Division and the Agricultural & Food Chemistry Division (AGFD) co-sponsor the Lecture which will be held in a joint session of these divisions. The lectureship is presented at an AGFD symposium in even-numbered years and in an AGRO symposium in odd-numbered years. The award includes an honorarium of $2000, a bronze medallion, and expenses to attend the meeting.

Nominees will be outstanding senior scientists in industry, universities, consulting, or government positions. *Current ARS employees are not eligible.* The Award will be presented during an American Chemical Society National Meeting held in 2013 in Indianapolis, Indiana prior to the Lecture. Giving the presentation is a requirement of the honor.

The **Nomination Package** includes:

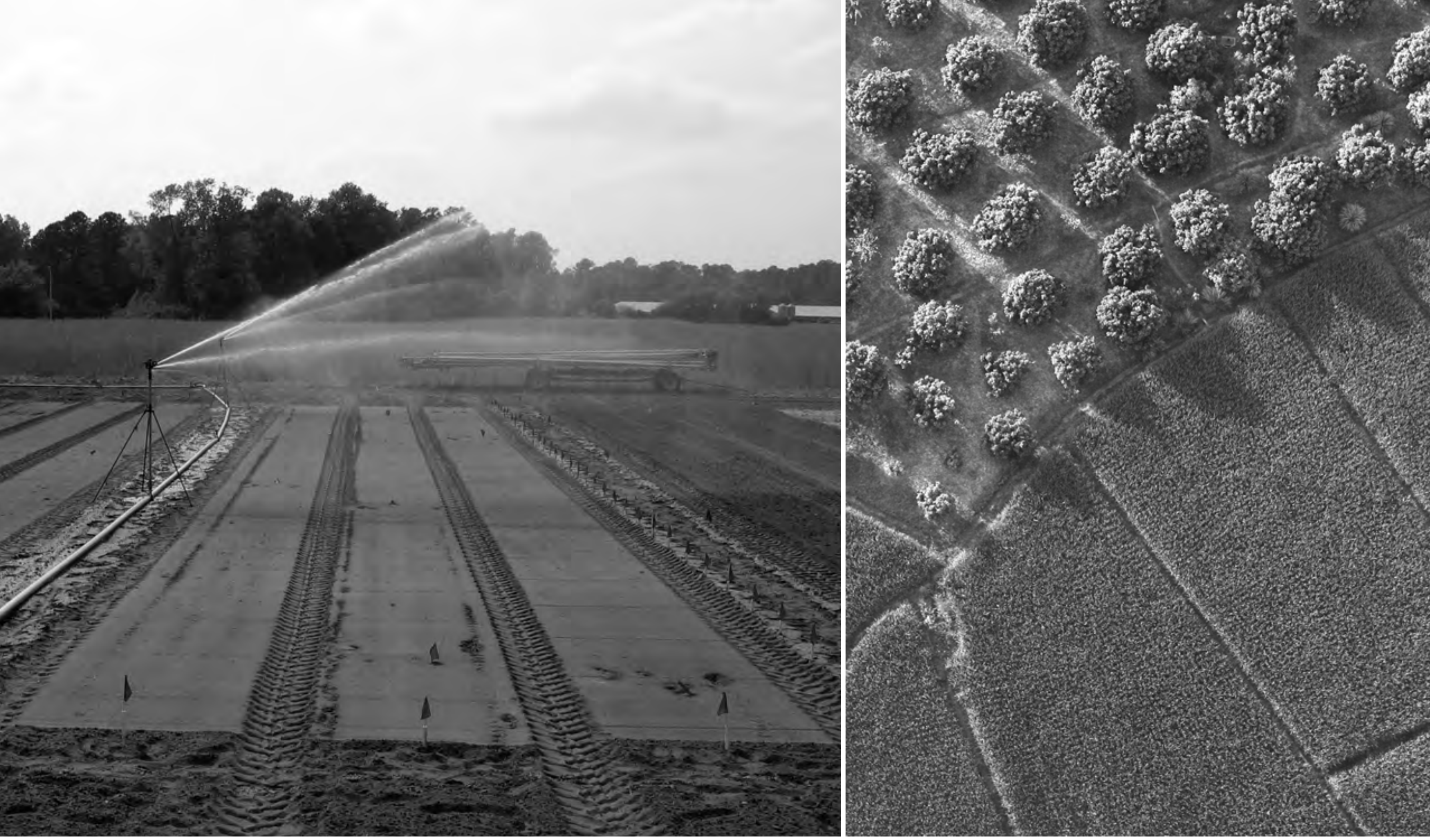
- A letter explaining the nominee's contributions to chemistry and agriculture,
- A current *curriculum vitae* (hard copy only)

Nomination letters may be sent electronically to:
Kim Kaplan, Lecture Coordinator
kim.kaplan@ars.usda.gov

Hard copy nominations and *curriculum vitae* are to be submitted via courier to:
Kim Kaplan, Lecture Coordinator
ARS Information Office
Room 1-2253, Mail Stop #5128
5601 Sunnyside Ave
Beltsville, MD 20705
301-504-1637 – phone

PAST STERLING B. HENDRICKS MEMORIAL LECTURESHIP AWARD WINNERS

1981	Norman E. Borlaug, Nobel Laureate, International Maize and Wheat Improvement Center, Mexico City
1982	Warren L. Butler, University of California, San Diego
1983	Melvin Calvin, Nobel Laureate, University of California, Berkeley
1984	Frederick Ausubel, Harvard Medical School and Massachusetts General Hospital, Boston, MA
1985	Alan Putnam, Michigan State University
1986	Ralph Hardy, Cornell University and BioTechnica International
1987	Mary-Dell Chilton, Ciba-Geigy Corporation, Research Triangle Park, NC
1988	Bruce N. Ames, University of California at Berkeley
1989	Sanford A. Miller, University of Texas Health Science Center at San Antonio
1990	Roy L. Whistle, Purdue University
1991	Peter S. Eagleson, Massachusetts Institute of Technology
1992	John E. Casida, University of California, Berkeley
1993	Philip H. Abelson, Deputy Editor, *Science*, and Scientific Advisor to AAAS
1994	Wendell L. Roelofs, Cornell University
1995	Winslow R. Briggs, Carnegie Institution of Washington
1996	Hugh D. Sisler, University of Maryland
1997	Ernest Hodgson, North Carolina State University
1998	Morton Beroza, USDA-ARS, Maryland (retired)
1999	Bruce D. Hammock, University of California, Davis
2000	William S. Bowers, University of Arizona
2001	Malcolm Thompson, USDA-ARS, Maryland (retired)
2002	Ervin E. Leiner, University of Minnesota
2003	Kriton Kleanthis Hatzios, Virginia Polytechnic Institute and State University
2004	Robert L. Buchanan, Food & Drug Administration
2005	Donald L. Sparks, University of Delaware
2006	Stanley B. Prusiner, Nobel Laureate, University of California, San Francisco
2007	Bruce E. Dale, Michigan State University
2008	Fergus M. Clydesdale, University of Massachusetts, Amherst
2009	Charles J. Arntzen, Arizona State University, Tempe
2010	Chris Somerville, Director of the Energy Biosciences Institute, Berkeley
2011	Deborah P. Delmer, University of California, Davis



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CALL FOR NOMINATIONS

2013 KENNETH A. SPENCER AWARD

Sponsored by ACS KANSAS CITY SECTION

The Kansas City Section of the American Chemical Society is soliciting nominations for the 2013 Kenneth A Spencer Award. The award recognizes meritorious contributions to the field of agricultural and food chemistry. The Kansas City Section presents this award in the hope that it will give added stimulus in research, education, and industry to further progress in agricultural and food chemistry. The award has been awarded annually in Kansas City since 1955 and carries an honorarium of $ 6,000. At this meeting the recipient will deliver an address, preferably upon the subject of the work for which they have been recognized. Subsequently, that address will be published, if possible, in an appropriate journal. The Kansas City Section will reimburse the recipient and spouse for round-trip travel expenses to Kansas City for the presentation.

To be eligible for the award, a candidate must be a citizen of the United States and must have done the work for which he or she qualifies as a candidate within the United States. The candidate need not be a member of the American Chemical Society. A candidate's work, whether it be done in education, industry or research, should have meritoriously contributed to the advancement of agricultural and food chemistry.

The nomination shall include a biographical sketch of the nominee containing minimum vital statistics, parents' names, education and professional experience; a list of published papers and patents; a specific identifying statement of the work on which the nomination is based; and an evaluation and appraisal of the nominee's accomplishments with special emphasis on the work to be recognized by the award. The nomination form can be found at http://cas.umkc.edu/chemistry/kcacs/spencer/AwardLogistics/spencer_nomination.pdf

Send nomination by November 15, 2012 to:

Kenneth A. Spencer Award
Kansas City Section of ACS
c/o Dr. Eckhard Hellmuth
Department of Chemistry
University of Missouri- Kansas City
5100 Rockhill Road
Kansas City, MO 64110
816-235-2290 - phone

PAST KENNETH A. SPENCER AWARD WINNERS

1955	Ralph M Hixon, Iowa State University
1956	Conrad A Elvehjem, University of Wisconsin
1957	William C Rose, University of Wisconsin
1958	EV McCollum, Johns Hopkins University
1959	Karl Folkers, Merck, Sharpe & Dohme Res. Labs.
1960	CH Bailey, University of Minnesota
1961	HL Haller, USDA-Agricultural Research Service
1962	AK Balls, USDA-Agricultural Research Service
1963	CC King, Rockefeller Foundation
1964	Daniel Swern, Temple University
1965	Aaron M. Altschul, USDA-Agricultural Research Service
1966	Robert L. Metcalf University of California, Riverside
1967	Melville L. Wolfrom, The Ohio State University
1968	Herbert E. Carter, University of Illinois
1969	Edwin T. Mertz, Purdue University
1970	Lyle D. Goodhue, Phillips Petroleum Company
1971	William J. Darby, Vanderbilt University
1972	Emil M. Mrak, University of California, Davis
1973	Esmond E. Snell, University of California, Berkeley
1974	Roy L. Whistler, Purdue University
1975	Thomas H. Jukes, University of California, Berkeley
1976	E. Irvine Liener, University of Minnesota
1977	N. Edward Tolbert, Michigan State University
1978	John E. Casida, University of California, Berkley
1979	Charles W. Gehrke, University of Missouri-Columbia
1980	George K. Davis, University of Florida, Gainesville
1981	John Speziale, Monsanto Agricultural Products Co.
1982	Howard Bachrach, USDA-Agricultural Research Service
1983	Peter Albersheim, University of Colorado
1984	Richard H. Hageman, University of Illinois
1985	Bruce N. Ames, University of California, Berkeley
1986	John M. Brenner, Iowa State University
1987	Hector F. DeLuca, University of Wisconsin, Madison
1988	Boyd L. O'Dell, University of Missouri-Columbia
1989	Robert H. Burris, University of Wisconsin
1990	John E. Kinsella, University of California, Davis
1991	George Levitt, DuPont Experimental Station
1992	Clarence A. Ryan, Jr., Washington State University
1993	Bruce Hammock, University of California, Davis
1994	William S. Bowers, University of Arizona
1995	Robert T. Fraley, Ceregen, A Unit of Monsanto Co.
1996	James N. BeMiller, Purdue University
1997	William M. Doane, USDA-Agricultural Research Service
1998	Mendel Friedman USDA-Agricultural Research Service
1999	James A. Sikorski, Monsanto Co.
2000	Wendell L. Roelofs, Cornell University
2001	James Tumlinson USDA-Agricultural Research Service
2002	Daniel W. Armstrong, Iowa State University
2003	Eric Block, University at Albany, State Univ. New York
2004	Steven D. Aust, Utah State University
2005	Don R. Baker, Berkeley Discovery Inc.
2006	Russel Molyneux USDA-Agricultural Research Service
2007	David A. Schooley, University of Nevada, Reno
2008	Ron G. Buttery, USDA-Agricultural Research Service
2009	George P. Lahm, DuPont Crop Protection
2010	Clive A. Henrick, Trece, Inc.


INNOVATION

AGRO DIVISION

2012 NEW INVESTIGATOR AWARD FINALISTS

Sponsored by Dow AgroSciences

Jeremy Conkle, Fan Tong, Xin Zhang

Please plan to attend presentations by our Three NIA Finalists

All talks will be in Loews Hotel Philadelphia - Commonwealth D

SUNDAY
Pesticide Environmental Fate Properties: Measurement, Prediction, Limitations, and Reliability

3:50 – 37. Forty years later: A reconnaissance of DDT in sediments of two southern California lakes. **Jeremy L. Conkle**, W. Wang, L. Delgado-Moreno, M. Anderson, J. Gan

WEDNESDAY
Mechanisms of Insecticidal Action and Resistance: New Compounds and Recent Advances

9:00 – 209. Fluorescent assay of acetylcholinesterase ligand interactions for design of insecticides targeting the mosquito vector of malaria, *Anopheles gambiae*. **Fan Tong**, P. R. Carlier, J. Li, M. Totrov, J. R. Bloomquist

9:25 – 210. Explore new insecticidal site targeting on chitin synthesis enzymes in *Anopheles gambiae*. **Xin Zhang**, K. Michel, K. Y. Zhu

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CALL FOR APPLICANTS

2013 Fall ACS National Meeting in Indianapolis, Indiana

The AGRO Division seeks nominations for the New Investigator Award to be awarded at the ACS meeting in Philadelphia in August 2012. The purpose of the New Investigator Award is to recognize scientists who have obtained a doctoral degree and are actively conducting academic, industrial, consulting, or regulatory studies.

The Division is interested in work on all aspects of agrochemicals which are broadly defined to mean pesticides of all kinds (e.g., chemical pesticides, biopesticides, pheromones, chemical attractants, fumigants, plant incorporated protectants, disinfectants) as well as biotechnology-derived crops (e.g., Bt crops, Roundup Ready crops, etc.). The categorical areas of study related to agrochemicals are very broad and encompass environmental chemistry, toxicology, exposure assessment, risk characterization, risk management, and science policy.

Studies of veterinary pharmaceuticals and antibiotics are included in the Division's mission. The Division especially encourages submissions related to public health protection as well as crop, livestock, aquaculture, and wildlife protection.

AGRO is also interested in the environmental chemistry and effects resulting from agricultural production (e.g., soil processes, water/air quality) and in chemical products made from agricultural commodities and byproducts. This includes biofuels and bioproducts and the issues surrounding their production and use.

The Process:

- To be eligible for the award, the scientist must have obtained his or her doctorate no more than five years before the time of the Fall ACS National Meeting. Thus, for 2013, applications will be considered from ***scientists who have obtained their doctorates no earlier than the year 2008***
- A panel consisting of at least three AGRO members will chose up to three finalists based on their extended abstracts and letter(s) of recommendation
- ***Each finalist will receive up to $1000 for travel and meeting expenses***
- Each finalist will deliver an oral presentation (which will be judged by the panel) in one of the AGRO Program symposia. The winner, who will receive a plaque, will be chosen after all finalists have presented their papers

To Apply for the New Investigator Award:

1. Submit a **150-word abstract** to a symposium in the AGRO Division using ACS PACS abstract submission at *http://abstracts.acs.org/*
2. Submit an **extended abstract (maximum 2 pages) describing the candidate's research/studies**. Include the impact (or potential impact) of the results as it pertains to issues of concern to the AGRO
3. Submit least **one letter of recommendation** from a current supervisory scientist (e.g., post-doctoral mentor a business manager, departmental chair).
4. Deliver an oral presentation in AGRO at Division
5. For consideration of an award at the 2013 Fall ACS National Meeting, both the extended abstract and letter of recommendation must be received by the new coordinator of the New Investigator Award **no later than March 1, 2013**

The AGRO Division is grateful for the sustained support of the AGRO New Investigator Award

Dow AgroSciences

2012 AGRO EDUCATION AWARDS
FOR STUDENT TRAVEL
Sponsored by Bayer Cropscience

Congratulations to all our travel grant winners

First, Second, and Third Place Winners will be announced at the
AGRO Awards & Social on Tuesday evening.

Vurtice Albright, III. Phytoremediation of atrazine from simulated surface water runoff using switchgrass. *Joel Coats, Iowa State U.* **AGRO 115**

Fnu Astha. Five-membered ring heterocyclic carbamates and carboxamides: The quest for resistance-breaking, species-selective acetylcholinesterase inhibitors against the malaria mosquito. *Jeffrey Bloomquist, U Florida.* **AGRO 97**

Joseph Felix. Investigating ammonia emission sources and transport using stable nitrogen isotopes. *Emily Elliott, University of Pittsburgh.* **AGRO 106**

Aaron Gross. Monoterpenoid binding at the house fly (*Musca domestica*) nicotinic acetylcholine receptor. *Joel Coats, Iowa State U.* **AGRO 101**

Lacey Jenson. High throughput screening technique for detecting the presence of insecticide target site proteins expressed in non-engineered insect cell lines. *Jeffrey Bloomquist, U Florida.* **AGRO 103**

Fang Jia. Isotope exchange method (IEM) to study the bioavailability of DDTs in sediment. *Jay Gan, U California-Riverside.* **AGRO 112**

Nicholas Larson. Evaluation of novel insecticidal compounds as new mosquitocides for control of *Aedes aegypti* and *Anopheles gambiae*. *Jeffrey Bloomquist, U Florida.* **AGRO 98.**

Juying Li. Degradation of the pharmaceuticals acetaminophen and carbamazepine in soils. *Jay Gan, U California-Riverside.* **AGRO 108**

Zhijiang Lu. Oxidation of nonylphenol and octylphenol by manganese dioxide: Kinetics and pathway. *Jay Gan, U California-Riverside.* **AGRO 109**

Katherine Neafsey Engler. Development of an *in vitro* method to determine the bioavailability of xeno-estrogens in soil. *Ann Lemley*, *Cornell U.* **AGRO 99**

Laishram Nirpen. Risk assessment of groundwater contamination of chlorpyrifos in neutral and alkali soil through lysimetric studies. *Tanu Jindal, Amity University, Uttar Pradesh, India.* **AGRO 116**

Ngoc Pham. Evidence for P-glycoprotein modification of insecticide toxicity in vector mosquitoes. *Troy Anderson, Virginia Tech.* **AGRO 100**

Alison Reeves. Multifactorial assessment of nutrition and immunity in honey bees exposed to in-hive pesticides. *Troy Anderson, Virginia Tech.* **AGRO 96**

Gayatri Sankaran. During the dissipation of dislodgeable foliar residues a transfer coefficient does not predict potential dermal exposure of hand harvesters. *Robert Krieger, U California-Riverside.* **AGRO 114**

Daniel Swale. Design of novel carbamate insecticides with superior selectivity for the control of cattle tick (*Boophilus microplus*) and sandfly (*Phlebotomus papatasi*) populations. **AGRO 102**

Lijuan Su. Quantification and identification of biodegradation products of sulfamethoxazole in wastewater. Diana Aga, **AGRO 113**

Jennifer Williams. Toxicological effects of in-hive pesticides to honey bees. *Troy Anderson, Virginia Tech.* **AGRO 95**

Xiao Xiao. Degradation of emerging contaminants by biogenic manganese (III/IV) oxides. *Ann Lemley, Cornell U.* **AGRO 110**

All Graduate Students and Post-Docs

You Are Cordially Invited To Attend

AGRO Graduate Student Box Luncheon

We will host a panel of professionals in academia, industry, and government to participate in an open discussion with the students on career opportunities in the AGRO sector.

Monday, August 20 at 11:30 am – 1:00 pm
Loews Hotel Philadelphia - Tubman

CONTACT: JULIE EBLE (Julie.Eble@criticalpathservices.com)
TROY ANDERSON (anderst@vt.edu)
RESERVATIONS ARE REQUIRED
Reservations made after by July 31 are on a space available basis.

THE FOOD IS FREE!

>

CALL FOR APPLICANTS
2013 AGRO EDUCATION AWARDS
Sponsored by Bayer Cropscience

UNDERGRADUATE & GRADUATE STUDENT RESEARCH

Support for Poster Presentations
At the 2013 Fall ACS National Meeting in Indianapolis, Indiana

The AGRO Division has established an endowment fund in collaboration with Bayer CropScience that will be used to promote an understanding of the role of chemistry in agriculture. To address this goal, awards will be made through the Division's Education Committee.

Proposals are sought for the 2013 awards. Selected undergraduate and graduate students will be awarded up to $600 each to help defray costs of attendance to give poster presentations at the ACS 2013 Fall Meeting, which will be held September 8 - 12, 2013 in Indianapolis, Indiana. Posters will be displayed in a special poster session of the ACS AGRO Division. First, Second, and Third place winners will receive an additional cash award.

The subject of the presentation should pertain to the chemistry of the AGRO Division. Topics should relate to pest management chemistry including synthesis, metabolism, regulatory, biotechnology, delivery, risk assessment, resistance, residues, mode of action, fate/behavior/transport, and agronomic practices. The AGRO Division is also interested in chemical products made from agricultural commodities and byproducts, including biofuels and the issues surrounding their production.

To apply, a graduate student should submit the following to be received no later than March 1, 2013 (PACS deadline):

1. An abstract formatted according to the directions given on the ACS website. Be sure to include name (of applicant), address, and e-mail address.
2. A two page extended abstract giving more detail of the research/presentation.
3. A short letter of nomination from the faculty advisor.

Submit item 1 to the ACS OASYS abstract submission website.
http://abstracts.acs.org/

Submit item 2 and 3 as a Word or pdf file to
Dr. Diana Aga
dianaaga@buffalo.edu
or
Dr. Marja Koivunen
marjakoivunen@eurofins.com

For more information, please contact the co-organizers:

Dr. Marja Koivunen
Eurofins Agroscience Services, Inc.
328 N. Bethel Ave
Sanger, CA 93657
tel: 559-399-4510
email: marjakoivunen@eurofins.com

Dr. Diana Aga
Chemistry Department, NSC 611
University of Buffalo
Buffalo, NY 14260
tel: 716-645-4220
email: dianaaga@buffalo.edu

Abstracts will be reviewed by the Education Committee.
Submitters will be notified of their selection status in May 2013.

Special thanks to our sponsor for their generous contribution!

Bayer CropScience

NOTES FROM THE PROGRAM CHAIR

JOHN M. CLARK

The AGRO program for the 244th National Meeting in Philadelphia on August 19-23, 2012 has been finalized and should have something for everyone. There will be 18 technical symposia, including 5 award presentations, encompassing 41 half-day sessions. We will be presenting 5 concurrent sessions Monday through Wednesday, with 4 concurrent sessions on Sunday and Thursday. This will be a busy program so come early, stay late, and bring your PICOGRAM so you don't miss anything.

Of the 15 technical topics for which we actively program, we will have symposia that address 13 of these topics, with a good number that address the theme of this meeting *Materials for Health and Medicine*. These *thematic* offerings include symposia on *Human Health and Transgenic Crops*, *Integrated Vector and Resistance Management*, *Mechanisms of Insecticidal Action and Resistance: New Compounds and Recent Advances*, and *Natural Products for Pest Management*.

Related to these *thematic* symposia, we have a number of linked symposia on human and ecological risk assessments and risk communication including: *Fate and Exposure of Urban Applied Pesticides in their Context of Human and Ecological Rick, Perfecting Risk Communications,* and *Pesticides: Bridging the Gaps between Chemistry, Exposure Science, Epidemiology and Health Risks.*

In keeping with AGRO's Strategic Plan, we have a couple of new topics being covered, Regulatory Harmonization and MRLs (*Maximum Residue Levels of Agrochemicals on Food*) and Bioenergy, Bioproducts, and Biochars: Advances in Production and Use (*Next Generation Biofuels and Bioproducts: Advances and Challenges*). As always, the strength of AGRO's programming has been agrochemical synthesis, analysis, and environmental fate, and this year's program is no exception with applied symposia such as, *Is your Analytical Method Good Enough*?, *Pesticide Environmental Fate Properties: Measurement, Prediction, Limitations and Reliability,* and *Synthesis and Chemistry of Agrochemicals,* to name only a few.

We will, of course, honor the achievements of our colleagues in agrochemical research through our five award symposia. This year, we honor Dr. Thomas C. Sparks, Dow AgroSciences, with the International Award for Research in Agrochemicals. Dr. James N. Seiber is the recipient of the 2012 Kenneth A. Spencer Award. Dr. Stephen J. Lehotay is the recipient of the 2012 AGRO Award for Innovation in Chemistry of Agriculture. The two-day symposium *Natural Products for Pest Management*, will be dedicated to the lifetime contributions of Dr. Horace Cutler. AGRO and AGFD will co-host the Sterling B. Hendricks Memorial Lecture, *Fifty years of smelling sulfur: From Allium chemistry to olfactory detection of sulfur compounds*, given this year by Dr. Eric Block. Please make every effort to attend these symposia and celebrate our award winners' achievements.

Diana Aga and Marja Koivunen will organize the AGRO Education Awards and students' poster session. Cathleen Hapeman is again in charge of the New Investigator Award which has a new structure. Three finalists will be judged by their oral presentation and the winner will be announced Wednesday afternoon after all have presented. The New Investigator Awards (NIA) Finalists and the Student Poster Presenters will be recognized with awards and grants for travel. Make plans to attend the poster session and the NIA presentations and encourage these new scientists.

Although our poster sessions will be in the Pennsylvania Convention Center along with all the posters from all the other divisions, AGRO, AGFD, and ENVR will all be in the Lowes Hotel Philadelphia. AGRO will have extensive co-programming with both the AGFD and ENVR Divisions, 3 symposia in AGFD and 7 in ENVR. AGFD will also co-program in 7 AGRO and in 5 ENVR symposia. ENVR will co-program in 4 AGFD and in 10 AGRO symposia. Bring your PICOGRAM for listings!

We look forward to an exciting five days of science, meeting old friends, and making new colleagues.

See you all in Philly!

COMMENTS FROM THE VICE CHAIR

STEPHEN O. DUKE

Long-term programming was identified as a critical need in the current AGRO 3-year strategic plan. The Division currently programs technical symposia in approximately 15 standing topics. An ad hoc steering committee for the Programming Committee was formed to direct the revitalization of long-term (2 – 3 years in advance) programming of technical symposia.

The steering committee felt that no single individual could be an expert on all topics, considering the breadth of our symposia topic areas. Individual experts in each topic area were identified from our membership to act as 'Champions' of that topic.

The champions serve as liaisons to the current Vice Chair and Program Chair, providing ideas for new and timely symposia within their topic areas and to assist in identifying possible organizers. The champions thereby provide the Vice Chair and Program Chair with a long-term institutional memory of the Division's programming efforts as officers rotate into and out of office.

The Vice Chair is responsible for contacting them as necessary and organizing a conference call or two each year.

We have already identified Champions for most topics, but still need more. Please let me know if you would like to volunteer for this valuable activity (sduke@olemiss.edu). Also consider proposing a symposium for the 2013 Fall ACS National Meeting (the Call for Symposia is on the next pages). I welcome your comments and ideas.

Program Committee Member Meeting

August 20, Monday 5:00 pm

Loews Hotel Philadelphia - Washington A

You Are Cordially Invited To:

AGRO Brainstorming, Blues & Brews

Happy Hour

August 23, Wednesday 5:00 - 7:00 pm

Loews Hotel Philadelphia - Millennium

- Share your ideas about AGRO programming
- Learn more about organizing a symposium
- Let us know what topics are the most important to you
- Meet scientists with mutual interests

Free refreshments will be served

ALL ARE WELCOME

Call for Symposia Proposals
For 2013 Programming

246th ACS National Meeting & Exposition
ACS Theme: Chemistry in Motion

AGRO anticipates an exciting and diverse technical program
in Indianapolis, Indiana

Suggestions and proposals for
additional symposia and organizers are most welcome.

Please contact AGRO Program Chair for 2013:
Stephen Duke, USDA-Agricultural Research Service
662-915-1036, sduke@olemiss.edu

Symposium proposal template can be found at:
www.agrodiv.org

Proposal deadline is November 15, 2012

Award Symposia, Lectures, Platform & Poster Presentations

ACS International Award for Research in Agrochemicals
René Feyereisen Awardee
Sponsored by DuPont
Organizer: Jim Ottea, jottea@agctr.lsu.edu

Sterling B. Hendricks Memorial Award Lecture
Awardee TBA Spring 2013
Sponsored by USDA-ARS
Organizer: Stephen Duke, sduke@olemiss.edu

Innovation in Chemistry of Agriculture
Awardee TBA Spring 2013
Sponsored by BASF
Scott Jackson, BASF
919-547-2349, scott.jackson@basf.com

AGRO New Investigator Award
Finalists TBA Spring 2013
Sponsored by Dow AgroSciences
Cathleen Hapeman, USDA-ARS
301-504-6451, cathleen.hapeman@ars.usda.gov

AGRO Education Awards for
Undergraduate and Graduate Student Travel
Research Poster Presentations
Awardees TBA Spring 2013
Sponsored by Bayer CropScience
Diana Aga, University of Buffalo
716-645-4220, dianaaga@buffalo.edu
Marja Koivunen, Marrone Bio Innovations
530-750-2880, mkoivunen@marroneorganics.com

Call for Symposia Proposals
For 2013 Programming

Standing Programming & Champions

Protection of Agricultural Productivity, Public Health and the Environment – General Session
Stephen Duke, sduke@olemiss.edu

Advances in Agrochemical Residue, Analytical and Metabolism Chemistry & Metabolomics
Kevin Armbrust, armbrust@msci.msstate.edu
Steve Lehotay, steven.lehotay@ars.usda.gov
Michael Krolski, mike.krolski@bayercropscience.com
Rod Bennet, rodney@bennett@jframerica.com
Chad Wujcik, chad.e.wujcik@monsanto.com
Teresa Wehner, teresa.wehner@merial.com

Air Quality and Agriculture
Laura McConnell, laura.mcconnell@ars.usda.edu
Jim Seiber, jnseiber@ucdavis.edu
Amrith Gunasekaram, amrith.gunasekara@cdph.ca.gov
Scott Yates, scott.yates@ars.usda.gov

Agrochemical Toxicology and Mode of Action
John Clark, jclark@vasci.umass.edu
Tom Sparks, tcsparcks@dow.com
Dave Soderlund, dms6@cornell.edu

Bioenergy, Bioproducts, and Biochars: Advances in Production and Use
Cathleen Hapeman, cathleen.hapeman@ars.usda.gov
Chris Peterson, cjpeterson@fs.fed.us

Biorationale Pesticides, Natural Products, Pheromones, and Chemical Signaling in Agriculture
Steve Duke, stephen.duke@ars.usda.gov
Joel Coats, jcoats@iastate.edu
Marja Koivunen, mkoivunen@marroneorganics.com

Development of Value-added Products from Agricultural Crops and Byproducts
Jim Seiber, jnseiber@ucdavis.edu

Developments in Integrated Pest Management and Resistance Management
Jeff Bloomqiust, jbquist@epi.ufl.edu
Tory Anderson, anderst@vt.edu
Si Hyeock Lee, shlee22@snu.ac.kr

Environmental Fate, Transport, and Modeling of Agriculturally-related Chemicals
Tom Potter, tom.potter@ars.usda.gov
Pam Rice, pamela.rice@ars.usda.gov
Jay Gan, jgan@ucr.edu

Human and Animal Health Protection: Vector Control, Veterinary Pharmaceutical, Antimicrobial and Worker Protection Products
George Cobb, george.cobb@tiehh.ttu.edu
Laura McConnell, laura.mcconnell@ars.usda.gov
Jay Gan, jgan@ucr.edu
Teresa Wehner, teresa.wehner@merial.com

Human Exposure and Risk Assessment
Bob Krieger, bob.krieger@ucr.edu
Kurt Lunchick, kurt.lunchick@bayer.com
Dan Stout, stout.dan@epa.gov

Regulatory Harmonization and MRLs
Ken Racke, kracke@dow.com
Philip Brindle, philip.brindle@basf.com
Heidi Irrig, heidi.irrig@syngenta.com

Synthesis of Bioactive Compounds
Thomas Stevenson, thomas.m.stevenson@usa.dupont.com
Wenming Zhang, wenming.zhang@usa.dupont.com

Technological Advances and Applications in Agricultural Science (e.g., Nanotechnology, Genetically-modified Organisms and Biocontrol Agents)
John Clark, jclark@vasci.umass.edu
Daniel Goldstein, daniel.a.goldstein@monsanto.com

Urban Agriculture- Turf, Ornamentals, Household Products, and Water-Re-Use
John Clark, jclark@vasci.umass.edu

JRF GLOBAL

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jrfa@jrfamerica.com

www.gclabs.com
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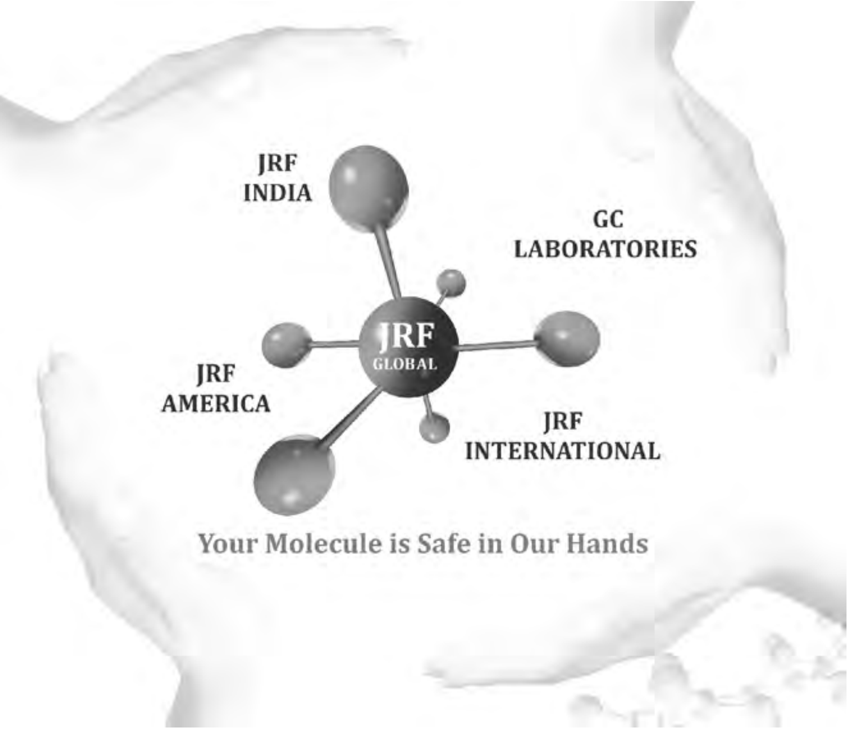
JRF Global is a non-clinical Contract Research Organization, with its multinational presence in India (Jai Research Foundation, Gujarat), the USA (JRF America, PA) and the UK (GC Laboratories, Stotfold).

JRF Global offers integrated services in Toxicology, Ecotoxicology, Chemistry, Environmental Fate, Metabolism and Regulatory Affairs. One of the most important strengths of JRF Global is cost effective safety data generation, in compliance with Good Laboratory Practice (GLP). Studies are conducted in accordance with global regulatory guidelines. Studies conducted by JRF Global are well received by global regulatory authorities.

JRF Global has professional experience exceeding three decades as well as multi-site expertise. This expertise gives JRF Global, a competitive edge over other CROs to establish it as a highly revered multinational brand. The client list exceeds 800 companies, including several leading multinationals from the Pharmaceutical, Biopharmaceutical, Agrochemical, Biocidal and Chemical industries.



Your Molecule is Safe in Our Hands

Endorsements & Accreditations

- Good Laboratory Practice (GLP) – Government of The Netherlands
- Good Laboratory Practice (GLP) – Government of India
- AAALAC accreditation
- US-EPA inspection – JRF America
- MHRA GLP – G C Laboratories

Programming & Outreach Activities
2012 – 2015

Activity/Event	Leaders Champions	Status	Actions Required
5th Pan-Pacific Conference on Pesticide Science Beijing, China September 15-20, 2012	Hiroshi Matsumoto Steve Duke Jim Seiber John Clark Hisashi Miyagawa Xinling Yang	Combined with 4th International Symposium on Pesticide & Environmental Safety and 8th International Workshop on Crop Protection Chemistry & Regulatory Harmonization	
Activities 2013 – 2015			
50th North American Chemical Residue Workshop July 2013 St Pete Beach, Florida	Kevin Armbrust Steve Lehotay	• Program under development	
246th ACS National Meeting Indianapolis, Indiana September 8-12, 2013	Steve Duke	• Symposia planning at Blues and Brews on Wednesday, August 22, 2012	• Submit symposia proposals (in Call for Papers format) to Steve Duke by November 15, 2012 for inclusion in Spring 2013 PICOGRAM
248th ACS National Meeting & 13th IUPAC Pesticide Congress San Francisco, CA August 10-14, 2014	Cathleen Hapeman Laura McConnell Ken Racke	• Follow progress on website www.iupac2014.org	• Sign up for email updates at website www.iupac2014.org
250th ACS National Meeting August 16-20, 2015 Boston, Massachusetts	2014 Vice Chair		

Thinking about organizing a symposium for a future National Meeting?
It's really not that difficult. Here's how.

7 Easy Steps for Organizing a Symposium

1. Propose, adopt or borrow a symposium topic *(e.g., Chemistry for and from Agriculture*)
2. Inform the AGRO program chair, who will add to the list and arrange for Program Committee endorsement
3. Develop a paragraph summary of the symposium scope and potential lecture topics (template is on the website)
4. Identify one or more co-organizers if desired
5. Recruit speakers and invite abstracts (Half-day = 5-8 speakers; 1 day = 12-15 speakers)
6. Review and accept abstracts, order your speakers/sessions
7. Chair the symposium session

Division Support for Symposium Organizers

- Assistance with developing a symposium summary and Call for Papers
- Help with identifying co-organizers
- Funding to help with travel, non-member registrations ($500 each ½ session)
- Promotion and publicity of the symposium to attract speakers and attendees (Call for Papers, announcement via *PICOGRAM*, website, and AGRO e-newsletter)
- Advice from veteran symposia organizers

5th Pan-Pacific Conference on Pesticide Chemistry

4th International Symposium on Pesticides and Environmental Safety

8th IUPAC Workshop on Crop Protection Chemistry and Regulatory Harmonization

Beijing International Convention Center
Beijing, China
September 15-20, 2012

Background

The scientific study, evaluation, and regulation of crop protection chemistry are rapidly developing in China and nearby Asian countries, particularly with respect to product quality, risk assessment, environmental impacts, and food residues. There is a growing desire on the part of scientists, regulators, and industry leaders throughout the region to consider the applicability of international approaches for management of crop protection chemistry in support of a safe and abundant food supply. Increased participation of countries in the region with world trade in both agrochemicals and foods has also brought new challenges related to compliance with import standards to seek applicability of internationally harmonized approached to crop protection chemistry within the contest of regional agricultural and world trade needs.

Scientific Main Topics

- Global views and harmonized approaches to pesticide regulation
- Pesticide residues in food and international trade standards
- Environmental fate, exposure modeling, and risk assessment of pesticides
- Pesticide quality, formulation, and application techniques
- New pesticide discovery and synthesis
- Pesticide mode of action, metabolism, and resistance mechanisms

Organizers and Sponsors

- Beijing Pesticide Society (BPS)
- International Union of Pure and Applied Chemistry (IUPAC)
- Pesticide Science Society of Japan (PSSJ)
- China Agricultural University (CAU)
- Institute for the Control of Agrochemicals, Ministry of Agriculture, China (ICAMA)
- AGRO Division of the American Chemical Society

For Additional Information

Workshop Secretariat: Zhang Jing (zj810515@163.com)
Conference Website: www.2012iupac.com

IUPAC website: www.iupac.org/web/act/Beijing_2012-10-08

AGRO Coordinators:
Steve Duke (sduke@olemiss.edu)
Jim Seiber (jnseiber@ucdavis.edu)


How do we feed a growing world population?
☐ Farm new land
☐ Get more from existing farmland

IUPAC 2014
SAN FRANCISCO

13TH IUPAC CONGRESS OF PESTICIDE CHEMISTRY CROP, ENVIRONMENT, AND PUBLIC HEALTH PROTECTION: TECHNOLOGIES FOR A CHANGING WORLD

Co-sponsored by IUPAC and ACS-AGRO

The Congress will be held concurrently with the 248th American Chemical Society National Meeting & Exposition. Sign up for email updates at our website www.iupac2014.org

MAJOR TOPIC AREAS WILL INCLUDE:

- Discovery, Mode of Action, Resistance Management
- Biotechnology
- Non-Crop Uses
- Environmental Fate and Ecological Effects
- Food Residues and Human Exposure
- Regulation, Stewardship, and Delivery Systems

AUGUST 10-14, 2014
San Francisco, California USA
www.iupac2014.org

AGRO
ACS
Chemistry for Life®

Come Celebrate the 50th Anniversary of the Florida Pesticide Residue Workshop (FPRW) as it changes its name to the North American Chemical Residue Workshop (NACRW)

July 21-24, 2013

St. Pete Beach, Florida

NACRW

North American Chemical Residue Workshop

The name change is being made to better reflect the broadened scope and international nature of topics covered by its scientific program. Issues of interest include pesticides, veterinary drugs, environmental contaminants, toxins, and other chemicals of concern in food, environmental, and related applications. The workshop has grown 5 years in a row, and we welcome your participation!

Please find additional information at:
www.nacrw.org

Expected Submission Deadlines:
Oral presentations: April 15
Poster presentations: June 1

Manuscripts related to the meeting will be considered for publication in a special section of ***Journal of Agricultural and Food Chemistry***

Sponsored by FLAG Works, Inc., a non-profit organization, which has an agreement with ACS (via the AGRO Division) to help plan and coordinate the event.

Future ACS National Meetings & Expositions

244th ACS National Meeting & Exposition
August 19-23, 2012
Philadelphia, Pennsylvania
Program Theme: *Materials for Health & Medicine*

245th ACS National Meeting & Exposition
April 7-11, 2013
New Orleans, Louisiana
Program Theme: *Chemistry of Energy & Food*

246th ACS National Meeting & Exposition
September 8-12, 2013
Indianapolis, Indiana
Program Theme: *Chemistry in Motion*

247th ACS National Meeting & Exposition
March 16-20, 2014
Dallas, Texas

248th ACS National Meeting & Exposition
August 10-14, 2014
San Francisco, California

249th ACS National Meeting & Exposition
March 22-26, 2015
Denver, Colorado

250th ACS National Meeting & Exposition
August 16-20, 2015
Boston, Massachusetts

251st ACS National Meeting & Exposition
March 13-17, 2016
San Diego, California

252nd ACS National Meeting & Exposition
August 21-25, 2016
Philadelphia, Pennsylvania

253rd ACS National Meeting & Exposition
April 2-6, 2017
San Francisco, California

254th ACS National Meeting & Exposition
September 10-14, 2017
St. Louis, Missouri

255th ACS National Meeting & Exposition
March 18-22, 2018
New Orleans, Louisiana

256th ACS National Meeting & Exposition
August 19-23, 2018
Boston, Massachusetts

257th ACS National Meeting & Exposition
March 31-April 4, 2019
Orlando, Florida

258th ACS National Meeting & Exposition
August 25-29, 2019
San Diego, California

AGRO 2012 Election Results

Congratulations to our new 2013 Officers and Executive Committee Members!

Cathleen Hapeman has been elected Vice-Chair to a 1-year term beginning August 24, 2012

Del Koch has been elected Treasurer to a 1-year term beginning January 1, 2013

Sharon Papiernik has been elected Secretary to a 1-year term beginning January 1, 2013

John J. Johnston, Michael Barrett, Troy D. Anderson, Steven Lehotay, and Wenlin Chen
have been elected as the at-large members of the Executive Committee
to 3-year terms beginning January 1, 2013

2012 AGRO Division Officers

Dr. Aldos C. Barefoot
Division Chair

Dr. John M. Clark
Program Chair

Dr. Stephen O. Duke
Vice Chair

Dr. John J. Johnston
Treasurer

Dr. Sharon K. Papiernik
Secretary

AGRO Division Past Chairs

1969	Donald G. Crosby
1970	Elvins Y. Spencer
1971	Wendell Phillips
1972	Philip C. Kearney
1973	Roger C. Blinn
1974	Charles H. Van Middelem
1975	Henry F. Enos
1976	Julius J. Menn
1977	James P. Minyard
1978	Gerald G. Still
1979	S.K. Bandal
1980	Jack R. Plimmer
1981	Marguerite L. Leng
1982	Gino J. Marco
1983	G. Wayne Ivie
1984	Robert M. Hollingsworth
1985	John Harvey, Jr.
1986	Henry J. Dishburger
1987	James N. Seiber
1988	Paul A. Hedin
1989	Gustave K. Kohn
1990	Willa Garner
1991	Guy Paulson
1992	Joel Coats
1993	Larry Ballantine
1994	Nancy N. Ragsdale
1995	Don Baker
1996	Barry Cross
1997	Willis Wheeler
1998	Judd O. Nelson
1999	Richard Honeycutt
2000	Ann T. Lemley
2001	Jeffery Jenkins
2002	Terry D. Spittler
2003	Jeanette Van Emon
2004	Rodney Bennett
2005	Allan Felsot
2006	R. Donald Wauchope
2007	Laura L. McConnell
2008	John J. Johnston
2009	Kevin L. Armbrust
2010	Ellen L. Arthur
2011	Kenneth D. Racke

Officers and Committees of the AGRO Division

AGRO HAS PUBLISHED AN UPDATED VERSION OF THEIR OPERATIONS MANUAL TO REFLECT THE NEW COMMITTEE STRUCTURE ADOPTED IN 2011 AS PART OF THE NEW STRATEGIC PLAN. SEE AGRODIV.ORG UNDER ABOUT US FOR MORE DETAILS.

AGRO DIVISION OFFICERS 2012

Division Chair , Aldos C. Barefoot
302-451-5856, aldos.c.barefoot@usa.dupont.com
Program Chair, John M. Clark
413-545-1052, jclark@vasci.umass.edu
Vice Chair, Stephen O. Duke
662-915-1036, stephen.duke@ars.usda.gov
Secretary, Sharon K. Papiernik,
605-693-5201, sharon.papiernik@ars.usda.gov
Treasurer, John J. Johnston
202-365-7175, john.johnston@fsis.usda.gov

EXECUTIVE COMMITTEE MEMBERS

2010 – 2012
Todd Anderson, todd.anderson@tiehh.ttu.edu
Rodney Bennett, rodney.bennett@jframerica.com
Allan Felsot, afelsot@tricity.wsu.edu
Laura McConnell, laura.mcconnell@ars.usda.gov
Sharon Papiernik, sharon.papiernik@ars.usda.gov

2011 – 2013
Julie Eble, julie.eble@criticalpathservices.com
Scott Jackson, Scott.jackson@basf.com
Pamela Rice, pamela.rice@ars.usda.gov
Jim Seiber, jnseiber@ucdavis.edu
Keith Solomon, ksolomon@uoguelph.ca

2012 – 2014
Jay Gan, jgan@ucr.edu
Cathleen Hapeman, cathleen.hapeman@ars.usda.gov
Mike Krolski, mike.krolski@bayer.com
Patricia Rice, patricia.rice@basf.com
Liliana Schwartz, Liliana.Schwartz@usa.dupont.com

COUNCILORS 2012 – 2015

Rodney Bennett, rodney.bennett@jrfamerica.com
Jeanette Van Emon, vanemon.jeanette@epa.gov
Kevin Armbrust, Alternate
Barry Cross, Alternate

AWARDS COMMITTEE

James Seiber, Chair
530-752-1465, jnseiber@ucdavis.edu
John Casida
Janice Chambers
John Marshall Clark
Joel Coats
Steve Duke
Bruce Hammock
Ernest Hodgson
Robert Hollingworth
Robert Krieger
Ralph Mumma
Hideo Ohkawa
Sharon Papiernik
Nancy Ragsdale
Will Ridley
David Soderlund
Don Wauchope
Willis Wheeler
Izuru Yamamoto

BYLAWS COMMITTEE

Rodney Bennett, rodney.bennett@jrfamerica.com

COMMUNICATIONS COMMITTEE

Cathleen Hapeman, Chair
301-504-6451, cathleen.hapeman@ars.usda.gov
Tim Ballard – email newsletter
Laura McConnell – Ads/Website Coordinator
Jay Gan – Abstracts Editor
Chris Peterson - Abstracts Editor
Sharon Papiernik – Awards Coordinator
Yelena Sapozhnikova – eNewsletter Editor
Jeff Jenkins, Public Relations

COMMITTEE ON COMMITTEES

Steve Duke, Chair
662-915-1036, stephen.duke@ars.usda.gov
Al Barefoot
Rod Bennett
John Clark
John Johnston
Ken Racke

DEVELOPMENT COMMITTEE

Scott Jackson, Co-Chair, 919-547-2349
scott.jackson@basf.com
Del Koch, Co-Chair, 573-443-9003
kochd@abclabs.com
Laura McConnell, 301-504-6298
laura.mcconnell@ars.usda.gov

Officers and Committees of the AGRO Division

(con't)

EARLY CAREER SCIENTIST COMMITTEE

Diana Aga, Co-Chair
716-645-4220, dianaaga@buffalo.edu
Marja Koivunen, Co-Chair
530-750-2800, mkoivunen@marroneorganics.com
John Bourke, Investment Coordinator
Cathleen Hapeman, New Investigator Award Coordinator
301-504-6451, cathleen.hapeman@ars.usda.gov
David Barnekow
John M. Clark
David Barnekow
John M. Clark
Joel Coats
Barry Cross
Vincent Hebert
Ann Lemley
Glenn Miller
Judd O. Nelson
William Ridley

FINANCE COMMITTEE

Joel Coats, Chair, jcoats@iastate.edu
John J. Johnston, Ex Officio, john.johnston@fsis.usda.gov
Kevin Armbrust
Al Barefoot
Barry Cross
Scott Jackson
Terry Spittler

INTERNATIONAL ACTIVITIES COMMITTEE

Ken Racke, Co-chair
317-337-4654, kracke@dow.com
Jay Gan, Co-chair
951-827-2712, jgan@ucr.edu
Michele Arienzo
Paul Hendley
Rai Kookana
Steven Lehotay
Weiping Liu
Laura McConnell
Jim Seiber
Keith Solomon
John Unsworth

MEMBERSHIP COMMITTEE

Dan Stout, Chair
919-541-5767, stout.dan@epa.gov
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NOMINATING COMMITTEE

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Kevin L. Armbrust, armbrust@mscl.msstate.edu

PROGRAMMING COMMITTEE

Stephen Duke, Chair, stephen.duke@ars.usda.gov
See page 41 for more information

SOCIAL COMMITTEE

Coffee Hour

Patricia Rice, 919-547-2668
patricia.rice@basf.com
Jim Brady, 336-643-1158, Cell: 336-708-0097
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Julie Eble, 610-558-3001
Julie_eble@criticalpathservices.com
Joe Massey, 662-325-4725
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Social Hour

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Jeff Jenkins, 541-737-5993
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STRATEGIC PLANNING COMMITTEE

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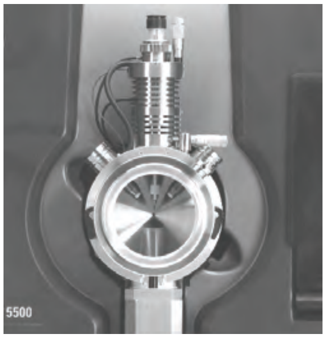
Ellen Arthur
Al Barefoot
Ashli Brown
Keri Carstens
John Clark
Steve Duke
Jay Gan
Amrith Gunasekara
Marja Koivunen
Ken Racke
Will Ridley
Jeanette Van Emon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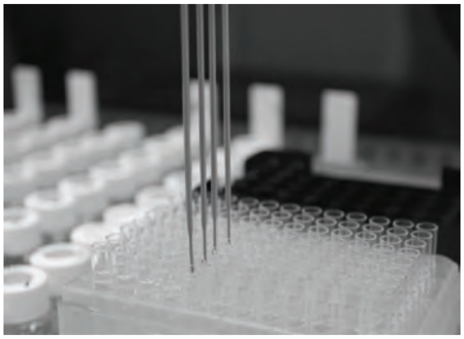

American Chemical Society
AGRO Division Strategic Plan
Progress Report

Mission Statement

AGRO, a Division of the American Chemical Society, brings together a worldwide community of scientists and stakeholders to advance knowledge and promote innovative solutions for the protection of agricultural productivity, public health, and the environment.

Vision

AGRO will provide its members an interactive and supportive environment for professional growth, based on innovative programming and services that meet member needs. It will also serve as a community where collaboration and exchange of information will advance innovative solutions for a sustainable supply of food and fiber and protection of the environment and public health.

Goal 1

AGRO will enhance the membership experience by providing an interactive and supportive environment for professional growth.
Leader: Laura McConnell, laura.mcconnell@ars.usda.gov

Accomplishments in 2011

- A member survey was conducted on the new strategic plan and information is being utilized to recruit new members for committee assignments
- The committee structure of the division was re-organized to support the priorities of the division
- The operations manual for the division was updated to reflect the new committee structure and was posted on the AGRO website
- Email newsletter was initiated
- Presentations and recordings from a number of AGRO symposia at the 2011 Fall National Meeting are now posted on the website.

Activities in 2012

- Post presentations from the 2012 Fall National Meeting on the AGRO website
- Begin to fill all vacant positions within new committee structure with an emphasis on including early career scientists.
- One symposium will be webcast at the Fall National Meeting.

Indications of success:

New email newsletter editor
New organizers for Graduate Student Luncheon

Goal 2

AGRO will develop the infrastructure for innovative, long range program planning to meet the needs of members and the scientific community.
Leaders: Aldos Barefoot, aldos.c.barefoot@usa.dupont.com
John Clark, jclark@vasci.umass.edu

Accomplishments in 2011

- *ad hoc* steering committee for the standing Programming Committee was formed to direct the revitalization of long-term programming of technical symposia
- Champions were identified for major programming topics to guide the development of symposia and to recruit symposia organizers

Activities for 2012

- Co-locate with ENVR and AGFD at the 2012 Fall National Meeting
- Developed grant proposal to develop scientific programming in emerging area of Biopesticides

Indications of success:

Largest program every presented by AGRO including co-sponsored symposia.

Goal 3

AGRO will be a global platform for collaboration and information exchange to advance innovative solutions for a sustainable food supply and the protection of the environment and public health.
Leaders: Ken Racke, kracke@dow.com
Jay Gan, jgan@ucr.edu

Accomplishments in 2011

- International Activities Committee established
- Website established for 13th IUPAC Congress of Crop Protection Chemistry to be held in San Francisco in 2014

Activities for 2012

- Co-sponsoring 5th Pan Pacific Conference of Pesticide Chemistry to be held in Beijing, September, 2012
- Initiated organizing committee for 13th IUPAC Congress of Crop Protection Chemistry.
- Submitted grant proposal to ACS Committee on International Activities to support participation in Pan Pacific Conference

Indications of success:

Strengthened ties established with IUPAC, Pesticide Science Society of Japan, and Beijing Pesticide Society

AGRO Executive Committee Phone Conference Meeting

April 3, 2012

1:00 – 3:00 pm EDT

Chair – Al Barefoot

Participants

Officers: Al Barefoot (Chair), John Clark (Program Chair), Steve Duke (Vice Chair), Sharon Papiernik (Secretary)
Past Chair: Ken Racke
Councilors: Rod Bennett, Jeanette Van Emon
Executive Committee: Julie Eble, Cathleen Hapeman, Laura McConnell, Scott Jackson, Ann Lemley, Pam Rice, Pat Rice, Jim Seiber

1. Final Plans for Philadelphia (John Clark)

- AGRO is planning 20 symposia (2 are 2-day; 2 are ½-day; rest are 1-day) with 322 accepted abstracts.
- The Education Committee is reviewing 18 complete abstracts for graduate student poster session.

2. Al Barefoot led a discussion of the budget for 2012

- Barefoot had distributed a detailed spreadsheet on March 14 for Executive Committee review. He thanked Johnston and Finance Committee for making budget information more clear.
- 2012 allocations include income (2 years) and expenses (webinars broadcast during Philadelphia meeting only) for ACS Innovation Award Grant, which has not been awarded yet.
- Budgeted income is lower than 2011, although ACS allocation will be slightly higher than budgeted.
- Total expenses are slightly less than last year, but AGRO would still be committing more funding than we are projecting to receive. Difference comes out of Education Fund. Value of Education fund is about $344K as of 2/29/12.
- Already reduced coffee, budgeted for smaller number of sessions, increased funding for student posters.

ACTION: International Award winner is from Dow. Seiber will check with winner (Tom Sparks) regarding his ability to receive honorarium and travel stipend, and notify him of AGRO's policy on awards.

Things to consider:

- Maybe could save money on social if move that to a location away from the convention center.
- Contribution to Pan Pacific (in China) meeting is quite large ($25,000) and was intended to be used primarily to support travel for AGRO members to participate in the meeting, especially co-organizers (Seiber, Duke). When the meeting got moved from Japan to China, Executive Committee decided to keep the $25,000 commitment. AGRO will not be liable for meeting expenses other than $25,000, and will receive no income from this meeting. May want to look for other funding sources in the future: ACS International Activities Committee or Innovative Project Grants.
- Regarding Innovative Project Grants: Each division can request up to $12,500 per year. AGRO already requested $7500 for webinars, so AGRO is able to apply for another $4-$5 in funding requests (due in July). May want to request Innovative Projects funding for activities to be undertaken in part at Beijing meeting: publicity and delegate boosting for IUPAC Congress.

MOTION: Revise commitment to Pan Pacific to $15,000 to support AGRO travel to Beijing meeting. Understanding is that co-organizer (Seiber and Duke) travel will be first priority with remainder supporting additional AGRO-related expenses. Motion passed.
ACTION: International committee (Gan and Racke) will write Innovative Project Grant for $5000 to support AGRO activities at the Pan Pacific meeting.

- Other large expenses are in Communications, especially the *PICOGRAM*. Ad prices will be increased in 2013 to $300 (1/2 page) and $500 (full page), which will bring in another ~$1000. Because *PICOGRAM* is only tangible product that all AGRO members receive, Executive Committee members expressed support for continuing the *PICOGRAM* as a printed document that includes abstracts and award announcements. If ACS eliminates printed abstracts, perhaps ACS would give support to Divisions to print abstracts in Division publications. Look for opportunities to enhance *PICOGRAM* content. Look for members to take on new features to be added to *PICOGRAM*.
- Each ½-day symposium is allocated $500 for speaker travel. ($15,000 for registrations and travel for Philadelphia.) How much is used? Consider having organizers propose expenses or have program chair prioritize expenses. Clark has not received requests for funding yet, nor does he know if organizers have made promises to speakers.
- Budget should be driven by strategic plan; budget discussion should be in the context of the strategic plan.

ACTION: Finance Committee (Coats) will present budget for following year at the annual meeting.
MOTION: Accept revised budget (commitment to Pan Pacific max $15,000; apply for another $5,000 for international activities). Motion passed with Barefoot objecting.

3. McConnell led a discussion of proposed Innovative Projects activities.

- Current plan is to produce live webinars during Philadelphia meeting (Communicating Risk symposium) so members can hear talks in real time and have capability of asking questions; these will also be recorded and available on our website after the meeting. ACS will also record some presentations.
- Would like to have "lunch and learn" seminars available during the year as distance learning. Consider funding sources (advertising or small fee for attending) to continue beyond Innovation Grant. Challenge is to come up with good-quality learning topics. Group will be asking membership for proposed topics.

4. By-Laws Committee

- Barefoot reminded the Bylaws Committee that they are tasked with updating the AGRO bylaws.

ACTION: Bylaws Committee will submit proposed changes to Executive Committee by 60 days before the fall meeting (June). Includes changes to committee structure, election process, other items.

5. Nominations

- Racke asked for the Executive Committee's input on nominations.
- Nominating Committee is trying to get ballot assembled earlier than usual because person elected Chair will be Program Chair in 2014 (including IUPAC Congress).
- Racke has received excellent suggestions for most positions but is having no luck identifying nominees for Treasurer. Suggestions are welcome.

6. Awards Committee

- Seiber provided an update from the Awards Committee.
- Rene Feyereisen will receive 2013 International Award (He lives in France; consider this as possible expense in 2013)
- Jim Seiber will receive 2012 Spencer Award. Congratulations!
- Deadline for AGRO fellowship awards is May 31. Consider nominating a worthy colleague.

COUNCILORS' REPORT

Jeanette Van Emon & Rodney Bennett

SAN DIEGO, CALIFORNIA - MARCH 28, 2012

The Spring ACS Meeting was very successful with 16,921 registrants (8,974 regular attendees and 5,742 students). The following is an abbreviated list of items of general interest and web addresses from the Council meeting.

- Candidates for President-Elect, 2013 for the Fall election are Thomas J. Barton, and Luis A. Echegoyen (William A. Lester, Jr., and Barry M. Trost were also on the Council ballot).

- ACS generated strong operating results in 2011 with total revenue of $472.0 million, up +1.8% over 2010. The Net from Operations was $20.9 million, or $7.7 million favorable to budget. This result was attributable to better-than-expected performance by the ACS Publications Division and the Society's careful expense management. The Unrestricted Net Assets declined from $130.5 million to $102 million primarily due to a sizable accounting charge related to the Society's closed postretirement benefit plans.

- To keep the Society financially sound, member dues for 2013 are now set at the fully escalated rate of $151.00 based on an inflation-adjustment formula devised by the Society.

- Membership recruitment and retention efforts were very successful last year. The Society ended 2011 with 164,215 members – the highest number in Society history. 24,249 new members were elected into the Society – 16,092 Regular Members and 8,157 Undergraduate Members.

- The Council voted to approve a Chemical Professional's Code of Conduct. This document offers guidance for Society members in various professional dealings, especially those involving conflicts of interest. We will let you know when this is available.

- ACS President Shakhashiri's working group on ACS Climate Science is developing a web-based toolkit as a resource for understanding and communicating basic climate science.

- The Ohio Supreme Court heard oral arguments in the appeal of the *ACS vs. Leadscope* case. A link to the arguments can be found on acs.org.

Web addresses for material presented at the Council meeting:

Safety
safety@acs.org – email address for sharing ideas on *How can ACS best cultivate a culture of safety in US universities and colleges?*
www.acs.org/safety - information on the Committee on Chemical Safety including *Creating Safety Cultures in Academic Institutions*

Employment/Careers
www.acs.org/careers - information on ACS career resources
www.acs.org/ei - information on the ACS Entrepreneurial Initiative (Training and Resources)

Local Section Resources
www.acs.org/getinvolved : grant information, important deadlines, officer resources
www.acs.org/forms: submit annual reports, record meetings, activities and events year round
speakers@acs.org: nominate speakers for the Online Speaker Directory

Other
www.acs.org/strategicplan - information on the new ACS Strategic Plan for 2012 and Beyond
www.acs.org/bulletin5: location of the Society's governing documents and unit bylaws, and information on the petition process to amend the Society's governing documents
bylaws@acs.org: email address for questions to the Committee on Constitution and Bylaws
www.acs.org/climatescience: information on the Climate Science Toolkit

Bylaws of the AGRO Division
of the
American Chemical Society *

** Effective October 27, 2000. Approved, as amended, by the Committee on Constitution and Bylaws, acting for the Council of the American Chemical Society.*

Bylaw I. Name and Objects

Section 1. The name of this organization shall be the Division of Agrochemicals (hereinafter referred to as "the Division") of the AMERICAN CHEMICAL SOCIETY (hereinafter referred to as "the SOCIETY").

Section 2. The objects of the Division shall be to bring together persons particularly interested in agrochemicals, to consider all scientific aspects of chemistry relevant to the control of pests of agricultural or public health significance and to other methods for enhancing or modifying agricultural productivity, to develop and improve the professional stature of chemists with these interests, and to render whatever service it may to the scientific and lay communities on the topic of agrochemicals.

Bylaw II. Members and Affiliates

Section 1. Membership in the Division shall be open to all members of the SOCIETY. Application for membership shall be made in writing to the Secretary of the Division and shall be accompanied by one year's dues.

Section 2. A National Affiliate of the SOCIETY may apply to the Secretary to become a National Affiliate of the Division. Provided that Division dues established for National Affiliates are paid, a National Affiliate shall have all the privileges of membership in the Division except those of voting for or holding an elective position of the Division, voting on articles of incorporation or bylaws of the Division, or serving as a voting member of its Executive Committee.

Section 3. The Division may accept Division Affiliates who are not members or National Affiliates of the SOCIETY but who wish to participate in the activities of the Division. Such affiliates shall be entitled to all the privileges of membership in the Division save those withheld by the Bylaws of the SOCIETY.

Section 4. Members may resign their membership in the Division by submitting their resignation, in writing, to the Secretary during the year for which their dues are paid.

Section 5. The name of any member of the Division who is in arrears in payment of dues by as much as two years shall be stricken from the rolls. A member dropped for nonpayment of dues may be reinstated upon payment of arrearages.

Section 6. Affiliates shall retain affiliate status only so long as payment is made of Division dues. An affiliate's name is to be stricken from the rolls as soon as the affiliate is in arrears in the payment of dues.

Section 7. The anniversary dates of Division members and National Affiliates of the Division shall coincide with their anniversary dates in the SOCIETY.

Bylaw III. Officers and Councilors

Section 1. The officers of the Division shall be a Chair, a Chair-Elect, a Vice-Chair, a Secretary, and a Treasurer. The Chair-Elect shall automatically succeed to the office of Chair upon expiration of the latter's term of office or if this office becomes vacant. The Vice-Chair shall automatically succeed to the office of Chair-Elect upon expiration of the latter's term of office or if this office becomes vacant. The offices of Secretary and of Treasurer may be held by one individual. Only MEMBERS are eligible to hold elective positions.

Section 2. The duties of the Chair shall be to preside at meetings of the Executive Committee, to carry into effect the decisions and recommendations of the Committee, to preside at stated meetings of the Division, and to appoint all committees except as otherwise provided.

Section 3. The duties of the Chair-Elect shall be to serve in the absence of the Chair of the Division and to act as Chair of the Program Committee.

Section 4. The duties of the Vice-Chair shall be to serve in the absence of the Chair-Elect and to act as Assistant Chair of the Program Committee, with particular emphasis on planning and developing technical programs.

Section 5. The duties of the Secretary shall be to keep minutes of all meetings of the Division and of the Executive Committee; to keep a roll of Division members and affiliates and to submit the same annually to the Executive Director of the SOCIETY for verification as provided in the Bylaws of the SOCIETY; to conduct the business correspondence of the Division as assigned to the Secretary by the Chair or by the Executive Committee; to prepare and submit an annual report of Division activities to the SOCIETY as required in the SOCIETY's Bylaws; to perform such other duties as may, from time to time, be assigned by the Chair or Executive Committee or required by the SOCIETY's Bylaws. The Secretary shall send to each member, at least two weeks before the regular meetings of the Division, abstracts of papers to be presented at said meetings.

Section 6. The Treasurer shall act as custodian of the funds of the Division, collect dues and other revenues, and pay the bills of the Division after the same have been authorized by the Executive Committee. The Treasurer shall maintain accurate records of receipts and disbursements and shall submit a report of the financial condition of the Division at the annual meeting of the Division. The Treasurer shall furnish a surety bond, the premium for which shall be paid from Division funds.

Section 7. Councilors and Alternate Councilors shall represent the Division on the Council of the SOCIETY as provided in the Constitution and Bylaws of the SOCIETY.

Section 8. The Division shall have an Executive Committee, which shall consist of the officers of the Division; the Immediate Past Chair of the Division; the Councilors and Alternate Councilors; the Chairs, Chairs-Elect, Vice-Chairs, and Immediate Past Chairs of Subdivisions, if any; and fifteen (15) Members-at-Large. The Chair of the Division shall serve as Chair of the Executive Committee.

Section 9. The officers of the Division other than the Chair and the Chair-Elect shall be elected by mail ballot as described elsewhere in these bylaws.

Section 10. At the annual meeting of the Division, the Executive Committee shall appoint a Nominating Committee consisting of at least three members, one of whom shall be the Immediate Past Chair of the Division, who shall serve as Chair of this Committee. This Committee shall nominate two candidates for the office of Vice-Chair and at least ten (10) candidates for the positions as Members-at-Large to be filled on the Executive Committee. This Committee shall nominate candidates for each of the following offices to be filled: Councilor, Alternate Councilor, Secretary, and Treasurer. This Committee shall submit a report in writing to the Chair of the Division for preparation of the ballot to be mailed to the membership. Additional nominations may be made in writing by any group of at least five members and presented to the Chair of the Division not less than three months prior to the fall meeting.

Section 11. Officers and Members-at-Large shall be elected by the members and Division Affiliates of the Division. Only members of the Division may vote for Councilors and Alternate Councilors. The Secretary or other designated officer of the Division shall prepare an election ballot, on which shall appear the names in order chosen by lot of all candidates nominated and found willing to serve. In all Division balloting conducted by mail, the ballot voted shall be sealed, without voter identification, in a special ballot envelope. The special ballot envelope, bearing no voter identification, shall be enclosed in a larger envelope upon which—or within which, on a separate slip—shall be hand-inscribed the name of the member voting; the larger envelope shall then be sealed and forwarded to the Chair of the Tellers Committee. The Tellers shall count the ballots thus received, using the list of members provided by the Secretary to verify the eligibility of all those voting. Any ballot envelope not validated by the voter's accompanying hand-inscribed name shall be rejected. The Secretary shall set and announce in advance of the neither balloting the interval during which ballots must be received to be counted; this interval shall not be less than four nor more than seven weeks following the ballot mailing. The Tellers Committee, appointed by the Chair of the Division, shall be responsible for counting all valid ballots received within the interval and shall certify the results to the Secretary, who shall in turn certify the results to the SOCIETY, the elected officials, and the Division. Elections are to be by plurality, should there be more than two candidates for an office. Resolution of a tie vote shall be made by the Executive Committee.

Section 12. The Chair, the Chair-Elect, the Vice-Chair, the Secretary, and the Treasurer of the Division shall serve for one year or until their successors are elected.

Section 13. The terms of office of the Members-at-Large of the Executive Committee shall be three years. Five Members-at-Large shall be elected each year.

Section 14. The terms of Councilors, Alternate Councilors, and all officers excluding the Chair, Chair-Elect, and Vice-Chair shall begin on January 1 following their election. The terms for Chair, Chair-Elect, and Vice-Chair shall begin at the conclusion of the fall meeting of the SOCIETY.

Section 15. Vacancies in offices other than Chair and Chair-Elect shall be filled by the Executive Committee. Incumbents so selected shall serve until the next regular election.

Bylaw IV. Councilors

The Division shall have Councilors and Alternate Councilors whose terms of office shall be three years. Alternate Councilors shall serve only for specific meetings of the Council when a Councilor is not able to attend.

Bylaw V. Committees

Section 1. There shall be a Program Committee, consisting of three or more members, one of whom shall be the Chair-Elect of the Division, who shall serve as Chair of the Committee. A second member of the Committee shall be the Vice-Chair. The Program Committee shall have the entire responsibility for organizing the program of papers for all Division meetings. It shall work cooperatively with other Divisions of the SOCIETY and other bodies in planning joint sessions and symposia of mutual and timely interest.

Section 2. There shall be a Membership Committee of three or more members. This Committee shall aggressively promote membership in the Division by members of the SOCIETY.

Section 3. There shall be a Finance Committee of two or more members. This Committee shall audit the accounts of the Treasurer prior to the business meeting of the Division and report its findings at the annual meeting. This Committee shall advise the Executive Committee on financial resources.

Section 4. There shall be an Awards Committee of at least six members. This Committee shall maintain and develop the Division and International Awards Programs.

Section 5. There shall be a Hospitality Committee of at least two members. This Committee shall direct social events in coordination with other committees and maintain a hospitality table at Division meetings.

Section 6. There shall be a Publication Committee of at least three members. This Committee shall be responsible for publication of the Division newsletter, PICOGRAM, and other Division publications.

Section 7. Special committees may be appointed to consider, conduct, and report upon such special matters as may be delegated to them.

Section 8. Except where otherwise provided, committee appointments shall be made by the Chair, with the advice and approval of the Executive Committee.

Bylaw VI. Dues

Section 1. Members of the Division shall pay annual dues, the exact amount to be decided by the Executive Committee. Dues are payable in advance. Members who have been granted emeritus status by the SOCIETY and who are interested in the work of the Division shall be granted all privileges of Division membership without the payment of annual dues.

Section 2. Affiliates shall pay annual dues of $2.00 more than members; except that Division Affiliates who are regularly matriculated students specializing in a chemical science shall pay annual dues of an amount to be decided by the Executive Committee.

Bylaw VII. Subdivisions

Section 1. Composition. The Division may sponsor Subdivisions devoted to specialized fields within the area of Division interest. Membership in the Division shall be a requirement for membership in a Subdivision.

Section 2. Formation. Formation or discontinuance of a Subdivision shall be at the discretion of the Executive Committee of the Division. Steps to initiate a Subdivision may be made by petition of a group of Division members to the Executive Committee or by the action of the Executive Committee. The scope of the activities of any Subdivision shall be defined by the Executive Committee.

Section 3. Officers. Upon approval of the formation of a Subdivision, the Executive Committee of the Division shall appoint a Chair, Chair-Elect, Vice-Chair, and Secretary for the Subdivision. The Chair-Elect shall assume the office of Chair after one year. In succeeding years the Subdivision shall elect at the annual meeting a Chair-Elect and a Secretary. The Chair, a Chair-Elect, and Secretary shall constitute a Steering Committee for the Subdivision. This Steering Committee shall report through the Chair of the Subdivision and be responsible to the Executive Committee of the Division, of which Subdivision Chairs shall be members ex officio.

Section 4. Funds. The necessary expenses for each Subdivision shall be authorized by the Executive Committee of the Division from Division funds and shall be paid by the Treasurer of the Davison upon the usual authentication.

Bylaw VIII. Meetings

Section 1. There shall be a meeting of the Division at each national meeting of the SOCIETY unless the Executive Committee votes otherwise, provided the requirements for a minimum number of meetings as specified in the SOCIETY Bylaws shall be met.

Section 2. The annual meeting of the Division shall be held at the fall meeting of the SOCIETY. Division business requiring vote of the membership shall be conducted only at this meeting, except as provided elsewhere in these bylaws. However, voting by the membership may be conducted by mail or as directed by the Executive Committee.

Section 3. Special meetings of the Division may be called by the Executive Committee, provided notice is given to the membership in writing or by publication in Chemical & Engineering News at least two months in advance. Special meetings may not be held within one month before or after a national meeting.

Section 4. Fifteen (15) members of the Division shall constitute a quorum for the conduct of business.

Section 5. The fee for registration at any special meeting shall be decided by the Executive Committee in accordance with the Bylaws of the SOCIETY.

Section 6. The rules of order in the conduct of Division meetings not specifically provided in these bylaws or in the SOCIETY's documents shall be the most recent edition of Robert's Rules of Order, Newly Revised.

Bylaw IX. Papers

Section 1. The Program Committee may approve or reject papers submitted for presentation before any meeting of the Division.

Section 2. The rules for papers presented before meetings of the SOCIETY as outlined in the Bylaws and Regulations of the SOCIETY shall govern the Division.

Bylaw X. Amendments

Section 1. These bylaws may be amended at any annual meeting of the Division by a two-thirds (2/3) vote of the members present. All amendments shall be submitted in writing to the Secretary at least sixty (60) days prior to the meeting. Upon approval of the Executive Committee, the Secretary shall send the text of the proposed amendment to the members of the Division at least thirty (30) days prior to the annual meeting.

Section 2. Amendments shall become effective upon approval by the Committee on Constitution and Bylaws, acting for the Council, unless a later date is specified.

Bylaw XI. Dissolution

Upon dissolution of the Division, any assets of the Division remaining thereafter shall be conveyed to such organization then existent as is dedicated to objects similar to those of the Division and the AMERICAN CHEMICAL SOCIETY, or to the AMERICAN CHEMICAL SOCIETY, so long as whichever organization is selected by the governing body of the Division at the time of dissolution shall be exempt under Section 501(c)(3) of the Internal Revenue Code of 1954 as amended or under such successor provision of the Code as may be in effect at the time of the Division's dissolution.

American Chemical Society
AGRO Division

244th ACS National Meeting
August 19 - 23, 2012
Philadelphia, Pennsylvania USA
J. Clark, *Program Chair* and A. Barefoot, *Division Chair*

PROGRAM

DIVISION BUSINESS

AGRO Business Meeting
Sunday 5:00 – 10 :00 PM
Loews Philadelphia Hotel, 33rd floor, Howe
All Members Welcome
AGRO Long-Range Program Meeting
Monday 5:00 – 7:00 PM
Loews Philadelphia Hotel, Washington A
All Members Welcome; see page 39

SOCIAL EVENTS

2012 Kenneth A. Spencer Award Reception
Sunday during & after symposium 1:30 – 5:00 PM
Loews Philadelphia Hotel, Regency Ballroom A
Graduate Student Luncheon
Monday 11:30 – 1:00 PM
Loews Philadelphia Hotel, 3rd floor, Tubman
Reservations Required; see page 34
Sterling B. Hendricks Award Lecture Reception
Tuesday following the 11:30 AM lecture
Loews Philadelphia Hotel, 33rd floor, Howe
AGRO Awards Social
Tuesday 6:00 – 8:00 PM
Loews Philadelphia Hotel, Millennium Hall
Members/Guests welcomed; see page 7
Blues & Brews – Program Planning Social
Wednesday 5:00 – 7:00 PM
Loews Philadelphia Hotel, Millennium Hall
Members/Speakers welcomed; see page 39

SUNDAY MORNING

Pesticide Environmental Fate Properties: Measurement, Prediction, Limitations, and Reliability
Cosponsored by ENVR
T. Potter, R. Parker, S. Senseman, *Organizers, Presiding*

Section C
Loews Hotel Philadelphia - Commonwealth D

8:30 Introductory Remarks.

8:40 – 1. Pesticide K_d values: How valuable are they? **S. Senseman**, E. Camargo, J. Krutz

9:00 – 2. Development of an adsorption window for pesticides: A potential alternative to comparing soil adsorption values. **E. Camargo**, S. Senseman

9:20 – 3. Modeling pesticide sorption in the surface and subsurface soils of an agricultural catchment. **A. Ghafoor**, J. Stenström, N. J. Jarvis

9:40 – 4. How constant are pesticide K_d values during a rainfall event? **C. Truman**, T. Potter

10:00 – 5. Quantifying the effect of sorption and moisture content on biodegradability of organic compounds in soil. **W. Chen**

10:20 Intermission.

10:40 – 6. Spatial variation in sorption and dissipation is herbicide dependent. **S. K. Papiernik**, R. S. Oliveira, A. Cabrera, W. C. Koskinen

11:00 – 7. Effect of soil wetting and drying cycles on metolachlor fate when applied as commercial and as controlled-release formulations. O. Goldreich, Y. Goldwasser, **Y. G. Mishael**

11:20 – 8. Interpreting kinetic data during adapted degradation. **T. Potter**

11:40 – 9. Soil dissipation of fomesafen in vegetable production systems. **T. Grey**, T. Potter

Natural Products for Pest Management
Natural Products: Dedication to Horace Cutler
-- see page 173 --
Cosponsored by AGFD and ENVR
J. J. Beck, S. Duke, *Organizers*
M. Koivunen, J. Coats, *Organizers, Presiding*

Section D
Loews Hotel Philadelphia, Regency Ballroom B

8:00 Introductory Remarks.

8:10 – 10. From the rainforest to your grocery store and medicine cabinet: A review of the recent 50 years of natural products research. **S. J. Cutler**

8:35 – 11. Natural products as sources for new pesticides. **C. L. Cantrell**, S. O. Duke, F. Dayan

9:00 – 12. Discovery and development of natural products for pest management. **R. N. Asolkar**, A. Córdova-Kreylos, R. Lam, P. Himmel, P. Marrone

9:25 – 13. Product stewardship: Discovery to commercialization. **D. Sesin**, D. C. Manker, T. Meragelman, J. Margolis

9:50 Intermission.

10:15 – 14. Natural product options for repelling ticks of medical importance. **J. F. Carroll**

10:40 – 15. *Streptomyces lydicus*: Natural chemical factories for integrated crop pest management. **G. Stallings**

11:05 – 16. Manipulation of insect behavior with Specialized Pheromone & Lure Application Technology (SPLAT®). **A. Mafra-Neto**, L. E. Mafra, R. Borges, C. Bernardi, L. P. Silva, D. Zeni, L. Stoltman

11:30 – 17. Development of effective extended-release delivery systems with the biopesticide spinosad for mosquito larvae control. **M. Willis**, M. Saunders

11:55 Concluding Remarks.

AGFD Division

Neuroactive Compounds from Natural Products

Cosponsored by AGRO and ENVR
A. M. Rimando, B. Shukitt-Hale, *Organizers, Presiding*

Section B
Loews Hotel Philadelphia - Commonwealth B

8:30 Introductory Remarks.

8:35 – AGFD 7. Reversal of age-related motor deficits following stilbene dietary supplementation. **J. E. Cavanaugh**, E. Allen, A. M. Rimando, C. S. Mizuno

9:05 – AGFD 8. Systemic and neuronal cross-talk: Effects of nature's products. **B. Burton-Freeman**, B. Shukkit-Hale

9:35 – AGFD 9. Diverse cellular mechanisms underlying the neuroprotective effects of dietary polyphenols in ischemic injury in vitro. **K. S. Panickar**

10:05 Intermission.

10:20 – AGFD 10. Use of cannabinoid receptors in the identification of biologically active secondary metabolites as immunestimulants from foods. **S. J. Cutler**

11:00 – AGFD 11. Exploring nature against depression, anxiety, and opioid withdrawal. **A. T. El-Alfy**

11:30 – AGFD 12. Anthocyanin effects in cognition and dementia: Probable mechanisms and future directions. **P. E. Milbury**

12:00 Concluding Remarks.

ENVR Division

Materials for Water Sustainability Sensors and Adsorbents

Cosponsored by AGFD and AGRO
B. Chaplin, D. Cwiertny, *Organizers*
D. Ladner, *Organizer, Presiding*

Section A
Loews Philadelphia Hotel, Washington B/C

8:30 Introductory Remarks

8:35 – ENVR 1. Lab–on-a-chip devices for microbial monitoring and detection in water. **W. Liu**

9:15 – ENVR 2. Nitrogen-anchored granular activated carbon to remove perchlorate from groundwater. **P. Hou**, T. Byrne, X. Gu, F. S. Cannon, N. R. Brown

9:35 – ENVR 3. Novel tailoring activated carbons for enhanced removal of natural organic matter. **L. Yan**, G. A. Sorial

9:55 – ENVR 4. Synthesis and application of granular mesoporous carbon materials for removal of pharmaceuticals. **Y. Kim**, H. Choi

10:15 Intermission

10:30 – ENVR 5. Development of novel cyclodextrin adsorbents for the removal of emerging contaminants from water. **B. Bhattarai**, M. Manickavachagam, R. Suri

10:50 – ENVR 6. Removal of antibiotics from water using sewage sludge derived composite material. **R. Ding**, P. Zhang, M. Seredych, T. J. Bandosz

11:10 – ENVR 7. Utilization of biowaste as a potential adsorbent for various pollutants in water. **M. Ramakrishna**, V. Suresh

Addressing the Complex Site: Chemistry, Toxicology, and Fate of Mixed Pollutants Across Environmental Media

Cosponsored by AGFD and AGRO
J. Rice, J. Goldfarb, *Organizers, Presiding*

Section B
Loews Hotel Philadelphia - Congress A

8:15 Introductory Remarks

8:20 – ENVR 8. Roles of black carbon on the fate of heavy metals and agrochemicals in soil. **M. Uchimiya**

8:45 – ENVR 9. Integrating field, lab, and modeling to assess the distribution of PCBs in a stream ecosystem. **C. M. Lee**, V. D. Dang, D. L. Delach, D. C. Hahn

9:10 – ENVR 10. Organic chemical composition of $PM_{2.5}$ in vehicular exhaust: Gasoline and diesel light duty vehicles. **M. Li**, S. Tang, R. Whitby, M. Mazurek, C. Belisle, M. Ullah

9:35 – ENVR 11. Moisture-filled porosity as a key parameter for accurate prediction of vapor intrusion rates. **P. Indeglia**, K. G. Pennell

10:00 Intermission

10:15 – ENVR 12. Carbamazepine accumulation in soil and plants following land application of wastewater. **B. Hosseini Amoli**, **C. Fedler**

10:40 – ENVR 13. Efficacy of in situ bioremediation of industrial wastes in Canada: Applications in PHC bioremediation and industrial soil fabrication. **P. A. Boyd**

11:05 – ENVR 14. Ionic strength effects on the sorption of tylosin on clay minerals. Q. Zhang, **C. Yang**

11:30 – ENVR 15. Equilibria of bisolute sorption on soil. **B. Xiao**, Q. Li, W. Huang

Interactions of Nanomaterials with Emerging Environmental Contaminants

Cosponsored by AGFD and AGRO
R. Doong, V. Sharma, S. Chang, Y. Huang, *Organizers*
C. Huang, *Presiding*

Section C
Loews Philadelphia Hotel - Congress B/C

8:30 Introductory Remarks

8:35 – ENVR 16. Photocatalytic degradation of microcystin-YR using size-controlled monodisperse TiO_2 films. **C. Han**, N. H. Koralegedara, M. Pelaez, R. Luque, P. S. Dunlop, J. Byrne, K. O'Shea, D. D. Dionysiou

9:05 – ENVR 17. Visible light-sensitive Cu-grafted TiO_2 photocatalysts. **L. Chiang**, R. Doong

9:30 – ENVR 18. Oxidation of arsenite to arsenate on birnessite in the presence of light. **S. Singireddy**, R. J. Reeder, D. R. Strongin

9:55 – ENVR 19. Application of potassium ferrite to remove contaminants: Role of nanomaterials. L. Machala, J. Philip, R. Prucek, J. Tucek, J. Frydrych, **V. K. Sharma**, R. Zboril

10:20 Intermission

10:35 – ENVR 20. Nanoscale zerovalent iron (nZVI): Toggling between oxidative and reductive pathways for contaminant sequestration. **W. Yan**

11:00 – ENVR 21. Dual redox functionality of nanoscale zerovalent iron: Fundamentals and applications in environment. **H. L. Lien**

11:25 – ENVR 22. Degradation of pentachlorophenol by well-suspended zerovalent iron nanoparticles. **C. Tso**, Y. Shih

11:50 Concluding Remarks

SUNDAY AFTERNOON

2012 Kenneth A. Spencer Award

Symposium in Honor of Dr. James N. Seiber Chemical Transport, Fate, and Sustainability

Cosponsored by AGFD
E. Hellmuth, *Organizer*
R. Molyneux, *Organizer, Presiding*

Section A
Loews Hotel Philadelphia - Regency Ballroom A

1:30 Introductory Remarks.

1:35 – 18. Prospective approach to understanding transport and fate of bioactive environmental contaminants. **J. N. Seiber**

2:10 – 19. Natural products chemistry and its applications to real-world agricultural problems. **J. J. Beck**

2:35 – 20. Immunoassay approaches for environmental and exposure monitoring. **J. M. Van Emon**

3:00 Intermission & Reception.

3:15 – 21. Developing novel approaches to characterize emissions from agricultural operations. Q. Huang, **L. L. McConnell**, E. Razote, W. F. Schmidt, B. Vinyard, A. Torrents, C. J. Hapeman, R. Maghirang, S. Trabue

3:40 – 22. New plants for sustainable fuels and chemicals. **G. C. Miller**, B. Neupane

4:05 – 23. Environmental contaminants in wildlife intended for human consumption. K. Horak, R. Chipman, L. Murphy, **J. J. Johnston**

4:30 – 24. Designer low-calorie and weight-loss or weight-maintenance ingredients. **J. W. Finley**

4:55 Concluding Remarks & Reception.

Protection of Agricultural Productivity, Public Health and the Environment

J. Clark, *Organizer*
D. Tessier, *Presiding*

Section B
Loews Hotel Philadelphia - Regency Ballroom C1/C2

1:30 Introductory Remarks.

1:35 – 25. VOC emission from silage: Compounds, processes, and implications. **S. D. Hafner**, F. Montes, P. Green, C. J. Howard, R. B. Franco, F. Mitloehner, C. Rotz

2:00 – 26. Comparative metabolism of [^{14}C]α-, β-, and γ-hexabromocyclododecane (HBCD) in rats. **H. Hakk**, J. K. Huwe

2:25 – 27. Multiclass, multiresidue method for analysis of pesticides, polychlorinated biphenyls, flame retardants and polyaromatic hydrocarbons in catfish using fast, low-pressure gas chromatography-tandem mass spectrometry. **Y. Sapozhnikova**

2:50 Intermission.

3:15 – 28. Absorption and distribution of perfluorooctane sulfonate (PFOS) in beef cattle. **S. J. Lupton**, J. Huwe, D. J. Smith, K. Dearfield, J. J. Johnston

3:40 – 29. Strategies for countering herbicide resistance. **D. R. Sammons**, D. Wang, P. Morris, B. Duncan, G. Griffith, D. Findley

4:05 – 30. Community-based approach to indirect effects assessments for terrestrial plants. **J. W. Perine**, J. Bang, R. Brain, K. A. Kabler, J. P. Overmyer, N. Peranginangin

4:30 Concluding Remarks.

Pesticide Environmental Fate Properties: Measurement, Prediction, Limitations, and Reliability

T. Potter, R. Parker, S. Senseman, *Organizers, Presiding*

Section C
Loews Hotel Philadelphia - Commonwealth D

1:30 – 31. Effect of bioavailability testing of soil residues using 0.01 M $CaCl_2$(aq) equilibration on the subsequent extractability of the residues. **R. A. Weintraub**, P. Z. Lian, S. R. Connor, M. M. Steadman, K. Malekani

1:50 – 32. Use of passive sampling devices to estimate the bioavailability of pyrethroids. **K. O'Neal**, D. Shea

2:10 – 33. Fate and transport of glyphosate and AMPA into surface waters of agricultural watersheds. **R. H. Coupe**, P. D. Capel, S. J. Kalkhoff, C. Gregoire

2:30 – 34. Transport and loading of herbicides and their degradates during mega-floods in the upper Mississippi River basin. **M. T. Meyer**, D. W. Kolpin, W. A. Battaglin

2:50 Intermission.

3:10 – 35. Chiral separation of metolachlor ethane sulfonic acid as a groundwater dating tool. **C. P. Rice**, K. Bialek-Kalinski, G. W. McCarty

3:30 – 36. Holistic assessment of the occurrence of metolachlor and two of its degradates across various environmental compartments in seven environmental settings. **C. E. Rose**, H. L. Welch, R. H. Coupe, P. D. Capel

3:50 – 37. AGRO New Investigator Finalist: Forty years later: A reconnaissance of DDT in sediments of two southern California lakes. **J. L. Conkle**, W. Wang, L. Delgado-Moreno, M. Anderson, J. Gan

4:10 Concluding Remarks.

Natural Products for Pest Management
Insect Management and Team Innovation Award
J. J. Beck, M. Koivunen, *Organizers*
S. Duke, J. Coats, *Organizers, Presiding*

Section D
Loews Hotel Philadelphia - Regency Ballroom B

1:30 Introductory Remarks.

1:35 – 38. Repellent activity of orange peel essential oils against *Tetranychus urticae* in laboratory and greenhouse bioassays. C. A. da Camara, **Y. Akhtar**, R. Seffrin, M. B. Isman

2:00 – 39. Determination of repellent efficacy of natural compounds. **U. Bernier**, N. Tabanca, I. A. Khan, E. K. Blythe, B. Demirci, M. Tsikolia, N. M. Agramonte, D. E. Wedge

2:25 – 40. Spinosad toxicity and resistance in stored-product insects. **D. Boina**, B. Subramanyam, K. Zhu

2:50 – 41. Volatile natural products for monitoring a California tree nut insect pest. **J. J. Beck**, B. S. Higbee, D. M. Light, W. S. Gee, J. M. Hayashi

3:15 Intermission.

3:20 Introductory Award Remarks.

3:30 – 42. Award Address (*ACS Award for Team Innovation sponsored by ACS Corporation Associates*). Spinetoram: Health and environmental assessments supporting an accelerated registration pathway. R. Boucher, J. E. Dripps, D. E. Kelley, **N. D. Simmons**

4:00 – 43. Award Address *(ACS Award for Team Innovation sponsored by ACS Corporation Associates*).Spinetoram: Accelerating the technical and commercial development of a new, semi-synthetic natural product insecticide. **R. Boucher**, J. E. Dripps, D. E. Kelley, N. D. Simmons

4:30 Concluding Remarks.

AGFD Division

Neuroactive Compounds from Natural Products
Cosponsored by AGRO and ENVR
A. M. Rimando, B. Shukitt-Hale, *Organizers, Presiding*

Section B
Loews Hotel Philadelphia - Commonwealth B

1:30 Introductory Remarks.

1:35 – AGFD 29. Effectiveness of the botanical drug candidate PBI-05204 derived from Nerium oleander in ex vivo and in vivo models of ischemic stroke. **R. A. Newman**, D. E. Dunn, D. He, M. Johansen, P. Yang, D. C. Lo

2:15 – AGFD 30. Attenuation of stress/age associated toxic protein accrual and tau-hyperphosphorylation in brain by berries and walnuts. **S. M. Poulose**, D. F. Bielinski, S. M. Gomes, K. Carrihill-Knoll, B. M. Rabin, B. Shukitt-Hale

2:45 – AGFD 31. Novel tetrameric galectin from a marine sponge potentiates mammalian glutamate receptor function. T. Ueda, Y. Nakamura, P. J. Focia, C. Smith, A. Inoue, T. Ojima, S. Matsunaga, D. M. Freymann, R. Sakai, **G. T. Swanson**

3:15 Intermission.

3:30 – AGFD 32. Novel neuroactive compounds from aqueous extract of marine sponges. **R. Sakai**, S. Matsunaga, M. Jimbo, M. B. Gill, L. Lash-Van Wyhe, G. T. Swanson

4:00 – AGFD 33. Neuroactive natural products from mollusks and their associated bacteria. **Z. Lin**, G. P. Concepcion, M. G. Haygood, A. R. Light, R. Teichert, B. Olivera, E. W. Schmidt

4:30 – AGFD 34. Potential agents to enhance the expression of neurotrophins in the brain. **N. S. Murthy**

5:00 Concluding Remarks.

ENVR Division

Materials for Water Sustainability
Sensors and Adsorbents
Cosponsored by AGFD and AGRO
B. Chaplin, D. Cwiertny, *Organizers*
D. Ladner, *Organizer, Presiding*

Section A
Loews Philadelphia Hotel - Washington B/C

1:30 Introductory Remarks

1:35 – ENVR 23. Rapid detection of waterborne parasites in complex matrixes using piezoelectric-excited millimeter-sized cantilever (PEMC) sensors. **R. Mutharasan**, S. Xu

2:15 – ENVR 24. X-ray photoelectron spectroscopy investigation of soluble manganese removal by MnO_x(s)-coated media. **J. M. Cerrato**, W. R. Knocke, M. F. Hochella, A. M. Dietrich, A. Jones, T. F. Cromer

2:35 – ENVR 25. Magnetically activated charcoal (MAC): Synthesis from natural products, characterization, and green application in arsenic remediation. **J. A. Zavaleta**, M. G. Nunez, T. M. Trad

2:55 Intermission

3:10 – ENVR 26. Urine source-separation and treatment: Novel applications of ion exchange materials.**T. H. Boyer**

3:30 – ENVR 27. Effects of iron amended, naturally aerated soil on dissolved phosphorus retention within surface-flow constructed stormwater wetlands. **K. Vacca**, B. M. Wadzuk

3:50 – ENVR 28. Hybrid hematite/multiwalled carbon nanotube (α-Fe_2O_3/MWCNT) nanostructures as sorbents for metal contaminants in water. **E. M. Verdugo**, Y. Xie, D. Cwiertny

4:10 – ENVR 29. Effects of surface functional groups on boron-doped diamond electrodes on organic compound oxidation and perchlorate formation. **W. Jawando**, B. Chaplin

4:30 – ENVR 30. Activated carbon nanofiber anodes for microbial fuel cells. **S. S. Manickam**, U. Karra, L. Huang, N. Bui, B. Li, J. R. McCutcheon

Addressing the Complex Site: Chemistry, Toxicology, and Fate of Mixed Pollutants Across Environmental Media

Cosponsored by AGFD and AGRO
J. Rice, J. Goldfarb, *Organizers, Presiding*

Section B
Loews Hotel Philadelphia - Congress A

1:30 Introductory Remarks

1:35 – ENVR 31. Estimating the polyethylene-water partition coefficients of organic chemicals using comprehensive 2D gas chromatography. **A. Tcaciuc**, R. K. Nelson, C. M. Reddy, P. M. Gschwend

2:00 – ENVR 32. Partitioning of polybrominated diphenyl ethers to dissolved organic matter. **M. L. Wei-Haas**, Y. Chin, K. J. Hageman

2:25 – ENVR 33. Tidal effects on PAH concentration in the water column of an urban stream. **K. L. Francisco**, W. Huang, L. A. Rodenburg, G. A. Burlingame

2:50 – ENVR 34. Classifying landfill leachates using major ions. **D. J. Tonjes**

3:15 Intermission

3:30 – ENVR 35. Discarded plastics and priority pollutants: A multiple stressor in marine habitats. **C. M. Rochman**, E. Hoh, B. Hentschel, S. Teh

3:55 – ENVR 36. FSIS activities regarding dioxin. **M. O'Keefe**, K. Dearfield, S. Edwards, N. Abdelmajid, A. Blanchard, D. LaBarre, P. Bennett

4:20 – ENVR 37. Chemical dispersant synergy the Deepwater Horizon oil spill's toxicity on the growth, reproduction, and gene expression of Caenorhabditis elegans. **Y. Zhang**, X. Pan

4:45 – ENVR 38. Effects of Marcellus Shale gas drilling wastewater discharge on trihalomethane formation. **N. Rossi**, M. Spear, Y. Xie

5:10 Concluding Remarks

Interactions of Nanomaterials with Emerging Environmental Contaminants

Cosponsored by AGFD and AGRO
R. Doong, V. Sharma, Y. Huang, S. Chang, *Organizers*
W. Yan, *Presiding*

Section C
Loews Philadelphia Hotel - Congress B/C

1:30 Introductory Remarks

1:35 – ENVR 39. Fluorescence detection of lead(II) ions through their induced catalytic activity of DNAzymes. **H. Chang**, C. Li

2:05 – ENVR 40. New double shell zero-valent iron nanoparticles with high potential of halogenated organic compounds removal.**K. Siskova**, L. Machala, E. Otyepkova, R. Zboril

2:30 – ENVR 41. Integrated decomposition of perfluorooctane sulfonate on nanoscale zerovalent iron. **W. A. Lawal**, H. Choi

2:55 – ENVR 42. Interactions of amines with activated carbons and potential catalyzed nitrosamine formation. **C. Huang**

3:20 Intermission

3:35 – ENVR 43. Black carbon-mediated reduction of 2,4-dinitrotoluene: The role of electrical conductivity. **S. Oh**, P. C. Chiu, J. Son

4:00 – ENVR 44. Comparative study for the adsorption of Cu(II) on functionalized nano graphene platelets and multiwall carbon nanotubes: Effect of size and morphology. **S. Rosenzweig**, G. Sorial, E. Demessie

4:25 – ENVR 45. Characterization of natural organic matter from Ohio River and investigation of their influence on stability and transport of engineered nanoparticles in water filtration system. **Z. Li**, E. Sahle-Demessie, A. Aly Hassan, G. A. Sorial

4:50 – ENVR 46. Mass loading effect of different lengths of polyethylene glycols on the enhancement of tetrachloroethylene dechlorination by zerovalent silicon. **C. Lee**, R. Doong

5:15 Concluding Remarks

MONDAY MORNING

International Award for Research in Agrochemicals

Symposium in Honor of Dr. Thomas C. Sparks New Technology and Approaches Applied to the Discovery of Agrochemicals

Financially supported by
DuPont Crop Protection
B. Gerwick, W. Kleschick, *Organizers, Presiding*

Section A
Loews Hotel Philadelphia - Regency Ballroom A

8:30 Introductory Remarks.

8:40 – 44. "What if" approaches to agrochemical discovery. **T. C. Sparks**

9:30 – 45. Crop protection market trends and opportunities for new active ingredients. **M. W. Phillips**, J. McDougall

10:05 Intermission.

10:20 – 46. High throughput screening in the agrochemical discovery process. **M. Drewes**

10:55 – 47. Potassium channels as insecticidal targets. **J. Dickhaut**, C. Beyer, F. Braun, J. A. Dorsch, N. B. Rankl, B. Wedel

MRLs and Ag Chemicals
Maximum Residue Levels of Agricultural Chemicals on Food

Cosponsored by AGFD and ENVR
P. Brindle, *Organizer*
H. Irrig, J. Huang, *Organizers, Presiding*

Section B
Loews Philadelphia Hotel - Regency Ballroom C1/C2

8:00 Introductory Remarks.

8:05 – 48. Production of export crops depends on the worldwide annual use of pesticides. **L. P. Gianessi**

8:30 – 49. Foreign Agricultural Service: Linking US agriculture to the world. **N. Mikulski**

8:55 – 50. Incentives to encourage specialty crop registration: A grower's perspective. **D. A. Botts**

9:20 – 51. US EPA advances in international harmonization and cooperation. **L. Rossi**

9:45 Panel Discussion.

10:05 Intermission.

10:20 – 52. Grower issues with the Codex process. **M. Goodwin**

10:45 – 53. Canadian initiatives for addressing MRL differences. **P. Chan**

11:10 – 54. Global joint data generation project. **J. Sandahl**

11:35 Panel Discussion.

11:55 Concluding Remarks.

Pesticides and Fumigant Emissions from Agricultural Systems
Pesticide Emissions and Transport

Cosponsored by ENVR
C. Hapeman, L. McConnell, J. Seiber, *Organizers*
S. Yates, *Organizer, Presiding*; D. Ashworth, *Presiding*

Section C
Loews Hotel Philadelphia - Commonwealth D

8:25 Introductory Remarks.

8:30 – 55. Modeling pesticide volatilization for complex soil and environmental conditions. **S. R. Yates**, T. Gish, L. Luo

9:15 – 56. Development of intelligent spraying systems to reduce airborne spray drift. **H. Zhu**

9:40 – 57. Improved indirect procedure for estimating pesticide volatility flux from neighboring area sources. **S. A. Cryer**, P. L. Havens, D. E. Hillger

10:05 – 58. Thirteen-year summary of field-scale herbicide volatilization. **T. Gish**, J. Prueger, W. Kustas, L. McKee, A. Russ, J. Hatfield

10:30 Intermission.

10:45 – 59. Atmospheric transport of endosulfan to Everglades and Biscayne National Parks. C. J. Hapeman, **L. L. McConnell**, T. L. Potter, J. A. Harman-Fetcho, W. F. Schmidt, C. P. Rice, B. A. Schaffer, R. Curry

11:10 – 60. Assessing natural isothiocyanate air emissions after field incorporation of a mustard cover crop. **V. R. Hebert**, D. Trott, J. LePage

11:35 – 61. Pesticides exposure assessment of Kettleman City residential area in September 2006 - December 2009 using ISCST3 model. **J. Tao**, T. Barry, R. Segawa, R. Neal, A. Tuli

12:00 Concluding Remarks.

Natural Products for Pest Management
Insect Management

J. Coats, M. Koivunen, S. Duke, *Organizers*
J. J. Beck, *Organizer, Presiding*

Section D
Loews Hotel Philadelphia - Regency Ballroom B

8:30 Introductory Remarks.

8:35 – 62. Multiple insecticidal mechanisms of action of monoterpenes. **J. R. Coats**, A. D. Gross, F. Tong, J. Anderson

9:00 – 63. Volatile organic compound profiling using differential mobility spectrometry (DMS). **W. Cheung**

9:25 – 64. Attracting carnivorous arthropods with plant volatiles: The future of biocontrol or playing with fire? **I. Kaplan**

9:50 – 65. Role of terpenes and other stimuli in host-plant assessment by Asian citrus psyllid, vector of citrus greening disease. **P. M. Joseph**

10:15 Intermission.

10:40 – 66. Highly irregular terpenoids as mealybug pheromones: Chemistry and applications. **Y. Zou**, J. G. Millar, S. Chinta

11:05 – 67. Personalized pesticides: A new paradigm. **S. Miresmailli**

11:30 – 68. Natural products from plants and their synthetic analogs against pests. **K. M. Meepagala**, W. Osbrink, U. Bernier, C. Burandt, A. Lax, J. Becnel, G. Sturtz, S. O. Duke

11:55 Concluding Remarks.

AGFD Division

Discovering Bioactive Compounds

Cosponsored by AGRO and ENVR

N. P. Seeram, J. Finley, *Organizers, Presiding*

Section A
Loews Philadelphia Hotel - Commonwealth Hall A1/A2

8:30 Introductory Remarks.

8:35 – AGFD 42. Bioactive potential of resveratrol oligomers of the *Carex* genus. **G. E. Henry**

9:05 – AGFD 43. Anthocyanin content and percent polymeric color of commercial berry products. **L. R. Howard**, R. L. Prior, R.Liyanage, J. O. Lay

9:35 – AGFD 44. Whey protein hydrolysates inhibits hydrogen peroxide induced oxidative stress. **M. Jin**, Y. Lin, J. Li, R. Lu

10:05 – AGFD 45. Curcumin inhibits metastasis of thyroid cancer cells. **C. Zhang**, L. Zhang, H. Yu, C. Tan, R. Lu

10:35 Intermission.

10:50 – AGFD 46. Cytotoxic polymeric proanthocyanidins from Pourouma cecropiifolia fruit. **C. Osorio**, J. Barrios, C. Cordero, S.Morantes, F. Aristizabal, A. Morales

11:20 – AGFD 47. Potential of coffee and coffee constituents for promoting body weight-maintenance in healthy subjects. **V.Somoza**, A. Riedel

11:50 – AGFD 48. Anthocyanins as xenobiotic medicines. **P. E. Milbury**

ENVR Division

Materials for Water Sustainability
Oxidative and Reductive Treatment Technologies

Cosponsored by AGFD and AGRO

D. Ladner, D. Cwiertny, *Organizers*
B. Chaplin, *Organizer, Presiding*

Section A
Loews Philadelphia Hotel - Washington B/C

8:00 Introductory Remarks

8:05 – ENVR 47. First principles simulation of intermediate steps in nitrate reduction on metal catalysts. **W. F. Schneider**, D. F. McCalman

8:45 – ENVR 48. Structure sensitivity study of hydrogenation for waterborne contaminants using shape- and size- controlled Pd nanoparticles. **D. Shuai**, J. Shapley, C. Werth

9:05 – ENVR 49. Treatment of perchlorate in waste ion-exchange regenerant brine with a Re-Pd catalyst. **J. Liu**, J. Choe, Z. D. Sasnow, C. J. Werth, J. R. Shapley, T. J. Strathmann

9:25 – ENVR 50. Zero-valent Fe/Al bimetal for water sustainability. **H. Lien**, S. Lin

9:45 Intermission

10:00 – ENVR 51. Two approaches to achieve visible light upconversion for environmental application. **J. Kim**

10:40 – ENVR 52. Assessing long-term photocatalyst activity, inhibition, and deactivation by non-target water constituents when treating trace micropollutants. **T. J. Strathmann**, S. Carbonaro

11:00 – ENVR 53. Synthesis and optimization of photocatalytic TiO_2 nanofibers for treatment of impaired water supplies. **M. J. Nalbandian**, D. M. Cwiertny, N. V. Myung

11:20 – ENVR 54. Computational methods in the interpretation of reactivity of emerging contaminants by ozone-based technologies: Combined DFT QSAR approach. **R. Suri**, T. Singh, E. Rokhina

11:40 – ENVR 55. Effect of organics on perchlorate byproduct formation during electrochemical oxidation of chloride-containing waters. **A. G. Donaghue**

Green Chemistry and the Environment
Biomass and Waste Valorisation Practices

Cosponsored by AGFD and AGRO

S. Obare, *Organizer;* R. Luque, *Organizer, Presiding*

Section B
Loews Hotel Philadelphia - Congress A

8:00 Introductory Remarks

8:05 – ENVR 56. From waste to wealth using green chemistry. **J. H. Clark**

8:50 – ENVR 57. Valorisation of coffee grinds and unconsumed bakery waste from Starbucks Hong Kong for the sustainable production of chemical and materials. **C. S. Lin**, C. J. Leung, A. Y. Zhang, W. Han

9:20 – ENVR 58. Integrated, catalytic strategy to enable production of cellulosic jet fuels. **J. Q. Bond**, D. Martin Alonso, S. Wettstein, D. J. Braden, J. A. Dumesic

9:50 – ENVR 59. Catalytic hydrothermal processing for hydrocarbon production from waste lipid feedstocks using renewable hydrogenation agents. **D. R. Vardon**, T. J. Strathmann, B. K. Sharma

10:20 Intermission

10:30 – ENVR 60. Integrated catalytic conversion of lignocellulosic biomass to chemicals and fuels. **D. M. Martin Alonso**, S. G. Wettstein, E. I. Gürbüz, J. A. Dumesic

11:00 – ENVR 61. Biomass gasification and gas conversion process for the recovery of useful gases.**K. Kawamoto**, B. Lu

11:30 – ENVR 62. Photocatalysis and biomass: An effective combination for the conversion of solar energy into chemical energy. **J. C. Colmenares Quintero**

12:00 Concluding Remarks

Interactions of Nanomaterials with Emerging Environmental Contaminants
Novel Materials

Cosponsored by AGFD and AGRO
R. Doong, V. Sharma, *Organizers*
Y. Huang, S. Chang, *Organizers, Presiding*

Section C
Loews Philadelphia Hotel - Congress B/C

8:30 Introductory Remarks

8:35 – ENVR 63. SERS analysis of arsenic species in water. **X. Meng**, Z. Xu, J. Hao

9:00 – ENVR 64. Degradation of pentachlorophenol by surfactant stabilized Ni/Fe nanoparticles. **C. Lin**, Y. Shih

9:25 – ENVR 65. Identification of the amount of binding sites and dissociation constants of an ligand-receptor complex using AlGaN/GaN high electron mobility transistors. **C. Huang**, G. Lee, J. Chyi, H. Cheng, **C. Hsu**, **Y. Hsu**, **Y. Huang**,**Y. Wang**

9:50 Intermission

10:05 – ENVR 66. DNAzyme based lead (II) ions biosensor development on a portable optic fiber sensing platform. **N. Yildirim**, F. Long, C. Gao, A. Gu

10:30 – ENVR 67. Multilayered microspheres as a signal amplification mode for sandwich immunoassays. **H. Lin**, Y. W. Chu, B. Y. Wang, S. Lin, H. Chou, C. Chen, **J. R. Carey**

10:55 – ENVR 68. Visual detection of copper(II) ions in blood samples by controlling the leaching of protein-capped gold nanoparticles. **Y. F. Huang**, Y. F. Lee, T. W. Deng, W. J. Chiu, T. Y. Wei, P. Roy, C. C. Huang

11:20 – ENVR 69. Adsorption of pharmaceuticals onto carbon nanotubes. Y. Hwang, **H. Kim**

11:45 Concluding Remarks

MONDAY AFTERNOON

AGRO International Research Award: Symposium in Honor of Dr. Thomas C. Sparks
New Technology and Approaches Applied to the Discovery of Agrochemicals

Financially supported by DuPont Crop Protection
B. Gerwick, *Organizer, Presiding*
W. Kleschick, *Presiding*

Section A
Loews Hotel Philadelphia - Regency Ballroom A

1:30 – 69. Discovery of veterinary antiparasitic agents. **D. J. Woods**, J. Wendt, C. S. Knauer, V. Vaillancourt, N. Chubb, P. Meeus

2:05 – 70. Significance of heterocycles for agrochemicals: Current examples from fungicide research. **C. Lamberth**

2:40 – 71. New herbicides and herbicide solutions to combat weed resistance. **B. C. Gerwick**

3:15 Intermission.

3:30 – 72. Approaches towards the discovery of novel insecticides from practically inactive hits/leads: Pyridalyl and others. **N. Sakamoto**

4:05 – 73. Pharmacophore inversion as a tactic for the discovery of new biologically active substances. **T. M. Stevenson**

4:40 Concluding Remarks.

MRLs and Ag Chemicals
Global Challenges and Efforts in MRL Issues

Cosponsored by AGFD and ENVR
P. Brindle, *Organizer*
H. Irrig, J. Huang, *Organizers, Presiding*

Section B
Loews Philadelphia Hotel Regency Ballroom C1/C2

1:30 Introductory Remarks.

1:35 – 74. Challenges of global residue programs. **M. G. Cole**

2:00 – 75. Impact of OECD MRL Calculator on global harmonization of MRLs. **J. Stewart**

2:25 – 76. Residue data: Addressing extrapolation between global regions. **C. Tiu**

2:50 Panel Discussion.

3:05 Intermission.

3:20 – 77. USDA IR-4 Project: Global partnerships in support of US trade. **J. J. Baron**, D. L. Kunkel, M. Braverman

3:45 – 78. IR-4 Project's international collaborations for global harmonization. **D. L. Kunkel**, J. J. Baron, M. Braverman

4:10 – 79. Role of USDA-FAS in addressing MRL challenges in foreign markets. **M. A. Rasmussen**

4:35 Panel Discussion.

4:55 Concluding Remarks.

Pesticides and Fumigant Emissions from Agricultural Systems
Fumigant Measurement, Modeling, and Mitigation

C. Hapeman, L. McConnell, *Organizers*
J. Seiber, S. Yates, *Organizers, Presiding*
L. Luo, *Presiding*

Section C
Loews Hotel Philadelphia - Commonwealth D

1:30 Introductory Remarks.

1:35 – 80. Interlaboratory validation of standardized method to determine permeability of plastic films. **S. K. Papiernik**, S. R. Yates, Y. Qian, H. Ajwa, S. Gao, R. Qin, F. Sances, K. A. Spokas

2:00 – 81. Fate and transport of methyl iodide in raised beds under field conditions. **D. J. Ashworth**, S. R. Yates, L. Luo, S. Lee, R. Xuan

2:25 – 82. Predicting emission and distribution of fumigants applied via drip irrigation to raised beds. **L. Luo**, S. Yates, D. Ashworth, J. Šimunek

2:50 – 83. Validation of a regional air dispersion modeling system (SOFEA) with long-term continuous measurements of air concentrations of 1,3-dichloropropene. **I. J. van Wesenbeeck**, S. A. Cryer, N. Zhang

3:15 Intermission.

3:30 – 84. Contribution of good agricultural practices (GAPs) to soil fumigant emission reduction. **D. O. Chellemi**, H. A. Ajwa

3:55 – 85. Airborne flux of 1,3-dichloropropene and chloropicrin applied under totally impermeable film as a function of tarp cutting time. **H. Ajwa**, D. Sullivan, S. Gao, M. Stanghellini, R. Sullivan

4:20 – 86. Emission and movement of 1,3-dichloropropene and chloropicrin in a large field tarped with low permeability film. **S. Gao**, R. Qin, H. Ajwa, D. A. Sullivan, M. S. Stanghellini

4:45 – 87. Depleting methyl iodide emissions from fumigated soils. **R. Xuan**, D. J. Ashworth, S. R. Yates

Natural Products for Pest Management
Weed and Pathogen Management

J. Coats, M. Koivunen, *Organizers*
J. J. Beck, S. Duke, *Organizers, Presiding*

Section D
Loews Hotel Philadelphia - Regency Ballroom B

1:30 Introductory Remarks.

1:35 – 88. Microbial and plant metabolites as potential herbicides for the control of parasitic plants. **A. Evidente**

2:00 – 89. Guaianolides for multipurpose molecular design. **F. A. Macias**, A. Santana, A. G. Duran, A. Cala, J. G. Galindo, J. G. Molinillo

2:25 – 90. Advancing *Phoma macrostoma* selective bioherbicide to commercialization. **S. Falk**, K. Bailey

2:50 – 91. Investigating the roles of rice diterpenoid natural products. **R. J. Peters**

3:15 Intermission.

3:40 – 92. Metabolic response of *Arabidopsis* to co-cultivation with white clover (*Trifolium repens* L.) suggests a herbicide-like mode of action. **H. A. Pedersen**, P. Kudsk, O. Fiehn, I. S. Fomsgaard

4:05 – 93. Clues to new herbicide modes of action from natural compounds. **S. O. Duke**

4:30 – 94. Induction of cryptic natural product fungicides from actinomycetes. **D. R. Hahn**, S. Fotso, S. Oilar, N. Russell, G. Davis, C. Avila-Adame, Q. Xiong

4:55 Concluding Remarks.

AGRO Education Award Poster Session

Financially supported by Bayer CropScience
D. Aga, M. Koivunen, *Organizers*

1:00 - 5:00 pm

Section E
Pennsylvania Convention Center - Hall G

95. Toxicological effects of in-hive pesticides to honey bees. **J. R. Williams**, R. D. Fell, T. D. Anderson

96. Multifactorial assessment of nutrition and immunity in honey bees exposed to in-hive pesticides. **A. M. Reeves**, J. R. Williams, B. E. Traver, C. C. Brewster, R. D. Fell, T. D. Anderson

97. Five-membered ring heterocyclic carbamates and carboxamides: The quest for resistance-breaking, species-selective acetylcholinesterase inhibitors against the malaria mosquito. **F. Astha**, Q. Chen, D. M. Wong, J. M. Mutunga, J. Li, P. C. Lam, M. M. Totrov, J. R. Bloomquist, P. R. Carlier

98. Evaluation of novel insecticidal compounds as new mosquitocides for control of *Aedes aegypti* and *Anopheles gambiae*. **N. R. Larson**, R. Islam, P. R. Carlier, M. Ma, J. R. Bloomquist

99. Development of an in vitro method to determine the bioavailability of xenoestrogens in soil. **K. Neafsey Engler**, A. T. Lemley

100. Evidence for P-glycoprotein modification of insecticide toxicity in vector mosquitoes. **N. N. Pham**, S. S. Scates, T. L. Carpenetti, T. D. Anderson

101. Monoterpenoid binding at the house fly (*Musca domestica*) nicotinic acetylcholine receptor. **A. D. Gross**, F. Tong, M. J. Kimber, J. R. Coats

102. Design of novel carbamate insecticides with superior selectivity for the control of cattle tick (*Boophilus microplus*) and sandfly (*Phlebotomus papatasi*) populations. **D. R. Swale**, P. R. Carlier, J. A. Hartsel, M. M. Totrov, K. B. Temeyer, J. R. Bloomquist

103. High throughput screening technique for detecting the presence of insecticide target site proteins expressed in non-engineered insect cell lines. **L. J. Jenson**, C. S. Knauer, D. J. Woods, A. Townley, P. Meeus, J. R. Bloomquist

104. Withdrawn

105. Novel pyrazolone fungicide: Applications of byproducts in agrochemicals. **B. Chai**, C. Liu

106. Investigating ammonia emission sources and transport using stable nitrogen isotopes. **J. D. Felix**, E. M. Elliott

107. Quantification of organic phosphate in soil samples by electrospray ionization mass spectroscopy. **L. P. Heighton**, E. E. Codling, C. P. Rice, W. F. Schmidt

108. Degradation of the pharmaceuticals acetaminophen and carbamazepine in soils. **J. Li**, J. Gan

109. Oxidation of nonylphenol and octylphenol by manganese dioxide: Kinetics and pathway. **Z. Lu**, J. Gan

110. Degradation of emerging contaminants by biogenic manganese (III/IV) oxides. **X. Xiao**, C. Xu, A. G. Hay, A. T. Lemley

111. Gas-phase reaction of methyl isothiocyanate with hydroxyl radicals under static relative-rate conditions. **Z. Lu**, V. R. Hebert, G. C. Miller

112. Isotope exchange method (IEM) to study the bioavailability of DDTs in sediment. **F. Jia**, L. D. Moreno, G. Jay

113. Quantification and identification of biodegradation products of sulfamethoxazole in wastewater. **L. Su**, D. Aga

114. During the dissipation of dislodgeable foliar residues a transfer coefficient does not predict potential dermal exposure of hand harvesters. **G. Sankaran**, T. Ahuja, L. Chen, Z. Chen, A. Krieger, W. Krieger, Y. Liu, T. Lopez, L. Tang, H. Vega, R. I. Krieger

115. Phytoremediation of atrazine from simulated surface water runoff using switchgrass. **V. C. Albright, III**, I. J. Murphy, J. Anderson, J. R. Coats

116. Risk assessment of groundwater contamination of chlorpyrifos in neutral and alkali soil through lysimetric studies. **L. Nirpen**, T. Jindal, K. Gulati, S. Thakur

117 - 119. Withdrawn

AGFD Division

Discovering Bioactive Compounds
Cosponsored by AGRO and ENVR
N. P. Seeram, J. Finley, *Organizers, Presiding*

Section A
Loews Philadelphia Hotel - Commonwealth Hall A1/A2

1:30 Introductory Remarks.

1:35 – AGFD 64. Comparison of antithrombotic activity and protective activities on alcohol gastric ulcer and immune system ofdifferent Fucoidan from Laminaria japonica. **X. Zhao**, B. Li, A. Chen, S. Dong, F. Li, J. Wang, S. Yuan

2:05 – AGFD 65. Effect of blueberry anthocyanidin extract on plasma cholesterol in hamsters fed a high cholesterol diet. **Z. Chen**, Y.Liang

2:35 – AGFD 66. Dietary flavonoids: Red-ox ingredients or just simple "travellers" of plant foods? **M. Serafini**

3:05 – AGFD 67. Plum fruit polyphenols differentially inhibit inflammation, and fat accumulation in cell models (adipocytes, macrophages, and HUVEC) associated to metabolic syndrome. P. Castillo, F. Ibanez, C. Cao, P. Simons, **L. Cisneros-Zevallos**

3:35 Intermission.

3:50 – AGFD 68. Effects of raspberry supplementation on measures of motor and cognitive function in aged rats. **R. L. Galli**, B. Shukitt-Hale, D. Bielinski

4:20 – AGFD 69. Colonic fermentation of dietary fibers is altered by background diet. **J. W. Finley**, M. Janes, M. Goita

4:50 – AGFD 70. Stone fruit extracts revert insulin resistance and glucose insensitivity in cell models (muscle, hepatic, and pancreatic ß cells) associated to type 2 diabetes. F. Ibanez, P. Castillo, C. Cao, P. Simons, **L. Cisneros-Zevallos**

5:20 Concluding Remarks.

ENVR Division

Materials for Water Sustainability
Membranes
Cosponsored by AGFD and AGRO
D. Ladner, D. Cwiertny, *Organizers*
B. Chaplin, *Organizer, Presiding*

Section A
Loews Philadelphia Hotel - Washington B/C

1:30 – ENVR 80. Comparison of silver- and copper-charged polypropylene feed spacers for biofouling control. **I. C. Escobar**, R. Hausman

2:10 – ENVR 81. Antiadhesive and antibacterial coatings for biofouling control. **C. S. Marambio Jones**, F. Peng, E. M. Hoek, R. Damoiseaux

2:30 – ENVR 82. Understanding the relationship between osmotic membrane structure, chemistry, and performance. **M. C. Wong**, E. M. Hoek

2:50 – ENVR 83. Development of antifouling reactive electrochemical membranes for water treatment and water reuse. **A. M. Zaky**, B. P. Chaplin

3:10 Intermission

3:25 – ENVR 84. Biomimetic membranes for water purification. **M. Kumar**, Y. Shen, P. O. Saboe

4:05 – ENVR 85. Dendritic polymers, carbonaceous nanomaterials, and composite inorganic/organic nanoparticles as regenerable membrane coatings for trace contaminant removal and fouling control. **D. A. Ladner**, M. Smith, C. Richards, D. L. Baker, J. Ellerie, T. Karanfil

4:25 – ENVR 86. Poly ethylene terephthalate electrospun nanofibrous membranes for water purification. **J. Bae**, H. Choi

4:45 – ENVR 87. Application of spray layer-by-layer assembled composite polyelectrolyte-clay thin films as selective layers in reverse osmosis membranes. **J. R. Kovacs**, P. T. Hammond

Green Chemistry and the Environment
Benign By Design: Greener Catalytic Protocols
Cosponsored by AGFD and AGRO
R. Luque, S. Obare, *Organizers*
J. Clark, R. Varma, *Presiding*

Section B
Loews Hotel Philadelphia - Congress A

1:00 Introductory Remarks

1:05 – ENVR 88. Benign synthesis of N-aryl sulfoximines and unnatural amino acids with dithiocarbamate side chain. **J. Leazer**, R. S. Varma, B. Vaddula, A. Saha, N. R. Baig

1:50 – ENVR 89. Green synthesis of glycerol carbonate: Biocatalytic alternative for glycerol industry. M.

Tudorache, A. Negoi, A. Nae, L. Protesescu, **V. I. Parvulescu**

2:20 – ENVR 90. Tuneable bifunctional water-compatible heterogeneous catalyst for the selective aqueous hydrogenation of phenols. **Y. Li**

2:50 – ENVR 91. Design of ionic liquids for green lignin extraction from woods. **T. Itoh**, K. Ohira, Y. Hamada

3:20 Intermission

3:35 – ENVR 92. Fe/Al bimetal: A solid-phase hydrogen peroxide generator for effective mineralization of dye wastewater. S. Lin, **H. Lien**

4:05 – ENVR 93. Pd(II)-catalyzed cycloisomerization of alkynoic acids in water: New tandem cycloisomerization/click chemistry reactions. **J. García-Álvarez**, J. Gimeno, J. Díez, C. Vidal

4:35 – ENVR 94. UpScaling Microwave-assisted chemical reactions. **S. Barry**, R. W. Wagner, H. Brownell

5:05 Concluding Remarks

Innovative Technologies for Green, Grey, Brown, and Black Water Reclamation and Reuse

Cosponsored by AGRO
S. Ahuja, *Organizer*
N. Savage, K. Hristovski, *Organizers, Presiding*

Section C
Loews Philadelphia Hotel - Congress B/C

1:30 Introductory Remarks

1:40 – ENVR 95. Integrating water reuse systems in a self-sustaining outpost. **K. D. Hristovski**, A. Warner, D. Teague, B. L. Ruddell, M. Stinson, A. McKenna

2:00 – ENVR 96. Modified polanyi-based model for mechanistic understanding of adsorption of phenolic compounds onto polymeric adsorbents. B. Pan, **H. Zhang**

2:20 – ENVR 97. Nitrate assisted UV advanced oxidation in wastewater effluent. **O. Keen**, K. Linden

2:40 – ENVR 98. Drying of wastewater sludge through a hydrophobic membrane: A novel approach to water protection and reclamation. **S. Marzooghi**, S. K. Dentel

3:00 Intermission

3:15 – ENVR 99. Water quality assessments using hydroxyl radical probes in gamma irradiations. **J. Peller**, S. Mezyk

3:35 – ENVR 100. Thermodynamic studies of wastewater treatment from rubber processing factory using snail shell. **I. O. Asia**, E. O. Jatto, F. Egharevba

3:55 – ENVR 101. Air-based membrane biofilm reactor (MBfR) for energy efficient wastewater treatment. **R. Nerenbegr**, M. Aybar, G. Pizarro, K. J. Martin

4:15 – ENVR 102. Water reclamation and reuse. **S. Ahuja**

4:35 Concluding Remarks

MONDAY EVENING

8:00 - 10:00 Sci-Mix

J. Clark, *Organizer*

Section A
Pennsylvania Convention Center - Hall D

95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116,. See previous listings.
162, 181, 185, 189, 191, 203, 204, 205, 326. See subsequent listings.

TUESDAY MORNING

Integrated Vector and Resistance Management

J. Bloomquist, T. D. Anderson, *Organizers, Presiding*

Section A
Loews Hotel Philadelphia - Commonwealth D

8:00 Introductory Remarks.

8:05 – 120. Bed nets and insecticide resistance: The way forward. **J. Lucas**, Y. Shono, T. Ishiwatari, P. Guillet

8:30 – 121. Health impacts of product development partnerships. **J. Hemingway**

8:55 – 122. Mosquito P-glycoproteins and their emerging role in insecticide resistance. **T. D. Anderson**

9:20 – 123. Field studies of rodent baits for sand fly control. **L. Foil**, T. Mascari

9:45 Intermission.

10:00 – 124. Acetylcholinesterases of *Rhipicephalus (Boophilus) microplus* and *Phlebotomus papatasi*: Gene identification, expression, and biochemical properties of recombinant proteins. **K. B. Temeyer**, P. U. Olafson, D. K. Brake, A. P. Tuckow, A. Y. Li, A. A. Pérez de León

10:25 – 125. Designing anticholinesterase insecticides to achieve high selectivity for the malaria mosquito, *Anopheles gambiae*, and potency against known resistance mutations. **P. R. Carlier**, J. R. Bloomquist, J. Li, M. Totrov

10:50 – 126. Developing novel small molecule agonists and antagonists of arthropod G protein-coupled receptors as next gen insecticides for vector control. J. M. Meyer, K. F. Ejendal, L. V. Avramova, E. E. Garland-Kuntz, G. I. Giraldo-Calderon, T. F. Brust, V. J. Watts, **C. A. Hill**

11:15 Concluding Remarks.

MRLs and Ag Chemicals
Real World Impact of MRLs

Cosponsored by AGFD and ENVR
J. Huang, *Organizer*
H. Irrig, P. Brindle, *Organizers, Presiding*

Section B
Loews Philadelphia Hotel - Regency Ballroom C1/C2

8:00 Introductory Remarks.

8:05 – 127. US Food and Drug Administration pesticide MRL enforcement program. **R. R. Roy**

8:30 – 128. Monitoring pesticides in foods: Responding to global market changes. **M. N. Lamont**

8:55 – 129. Practical challenges of monitoring trace residues in the US food supply: Limits of detection and quantitation. **M. M. Bogner**

9:20 Panel Discussion.

9:40 Intermission.

9:55 – 130. Retailer pesticide secondary standards in the food chain. **C. J. Willetts**

10:20 – 131. Maximum residue limits (MRLs): Challenges of a global business. **M. M. Hampton**

10:45 – 132. Effect of adjuvants on residues in relation to routine residue trial variability. **P. A. Brindle**, J. M. Stewart

11:10 – 133. Kenya major and minor crops in international trade. **G. N. Maina**

11:35 Panel Discussion.

11:55 Concluding Remarks.

Environmental Fate, Transport and Modeling/Monitoring of Agricultural Chemicals
General Modeling

Financially supported by Waterborne Environmental Inc.
S. Jackson, *Organizer*
P. Hendley, N. Peranginangin, *Organizers, Presiding*

Section C
Loews Hotel Philadelphia - Regency Ballroom B

8:30 Introductory Remarks.

8:40 – 134. Comparing different modeling approaches of pH-dependent sorption with FOCUS-PEARL. **M. Anyusheva**, W. Reiher

9:00 – 135. Setting groundwater monitoring sites in a European wide spatial context. **T. Haering**, B. Erzgraeber, B. Gottesbueren

9:20 – 136. Modeling herbicide metabolite concentrations in groundwater at shallow karst monitoring sites in France. **B. Miles**, L. Garcia, B. Gottesbueren, H. Shbaita

9:40 – 137. Monitoring and predictive modelling of leaching and transport of a pesticide metabolite from a field to a drinking water abstraction point. **R. Sur**, T. Oertel, M. Himml, G. Goerlitz

10:00 Intermission.

10:20 – 138. Multidimensional modeling of pesticide placement and fate in the soil-root-plant system. **P. Sweeney**, K. Travis, R. Whalley, A. Whitmore, G. Dailey, L. Wu, W. van Beinum, C. Brown

10:40 – 139. Development and evaluation of the Pesticide Root Zone Model (PRZM) for estimating pesticide concentrations in groundwater. R. Baris, M. R. Barrett, **R. F. Bohaty**, M. Echeverria, I. Kennedy, G. P. Malis, J. K. Wolf, D. Young

11:00 – 140. Validation and refinement of PRZM-GW predicted soil-pore water concentrations using terrestrial field dissipation data. **T. L. Negley**, A. C. Newcombe, K. L. Gehl, P. L. Havens, I. J. van Wesenbeeck

11:20 – 141. Enhancement of a pesticide leaching assessment tool in Hawaii for screening volatile agrochemicals. S. Ki, P. Das, **C. Ray**

11:40 Questions .

Is Your Analytical Method Good Enough?

Cosponsored by AGFD and ENVR
J. Eble, S. J. Lehotay, *Organizers, Presiding*

Section D
Loews Hotel Philadelphia - Regency Ballroom A

8:00 Introductory Remarks.

8:05 – 142. How good is good enough? An instrument vendor's perspective on method development. **P. L. Wylie**

8:30 – 143. Tools for contract testing labs: Incorporating new technologies for routine testing workflows. **L. Bailey**, A. Schreiber

8:55 – 144. Mass spectrometry-based methods for trace-level analysis in industrial and agrochemical research. **S. C. Nanita**

9:20 Intermission.

AGRO Award for Innovation in Chemistry of Agriculture

Dr. Steven J. Lehotay

Financially supported by
BASF Corporation
J. Eble, S. J. Lehotay, Organizers, Presiding

Section D
Loews Hotel Philadelphia - Regency Ballroom A

9:40 Introductory Remarks.

9:45 – 145. What is good enough? **S. J. Lehotay**

10:10 – 146. Validation and analytical quality control in pesticide residue analysis: An EU perspective. **H. Mol**

10:35 – 147. Method validation criteria: US EPA Office of Pesticide Programs. **T. Nguyen**

11:00 – 148. Method acceptability standards: A perspective from a state FIFRA laboratory. **Y. S. Johnson**

11:25 Concluding Remarks.

AGFD Division

Discovering Bioactive Compounds

Cosponsored by AGRO and ENVR
N. P. Seeram, J. Finley, *Organizers, Presiding*

Section A
Loews Philadelphia Hotel - Commonwealth Hall A1/A2

8:30 Introductory Remarks.

8:35 – AGFD 85. Mechanism of inhibition of advanced glycation end products by bioactive compounds present in okra seed extracts: A comparison with the well known inhibitor aminoguanidine. **B. Dayal**, R. George, M. Lea

9:05 – AGFD 86. Portable nanoparticle-based sensor for the discovery of food antioxidants. **E. M. Sharpe**, S. Andreescu

9:35 – AGFD 87. Alkylresorcinol as the major active components in wheat bran for colon cancer prevention. **Y. Zhu**, D. Soroka, S. Sang

10:05 – AGFD 88. Activity-guided discovery of antioxidative and antidiarrheal components in bark extract of *Garcinia buchananii*. **T. Stark**, O. B. Balemba, T. Matsutomo, S. Lösch, T. Hofmann

10:35 Intermission.

10:50 – AGFD 89. Cranberry fruit and leaves (*Vaccinium macrocarpon*) as a source of antimicrobial natural products. **C. C. Neto**, A. R. Dovell, R. C. Boddeti, S. Kwasny, T. J. Opperman, F. J. Scarano

11:20 – AGFD 90. Protective effect of steryl ferulate from bamboo shoot on experimental nonbacterial prostatitis in rats. **L. Xiong**, B. Lu, W. Huang, H. Cai, Y. Luo, Y. Hu

11:50 – AGFD 91. Effect of dietary tocopherol isomers on inflammatory response of adult- and infant-derived intestinal cell lines. **I. Elisia**, D. D. Kitts

12:20 Concluding Remarks.

ENVR Division

Green Chemistry and the Environment Nanomaterials

Cosponsored by AGFD and AGRO
R. Luque, *Organizer*; S. Obare, *Organizer, Presiding*

Section B
Loews Hotel Philadelphia - Congress A

7:55 Introductory Remarks

8:00 – ENVR 110. Natural and nature-inspired materials for environmentally-friendly, green organic electronics. **M. Irimia-Vladu**, E. D. Glowacki, U. Monikowius, L. Leonat, G. Schwabegger, Z. Bozkurt, H. Sitter, S. Bauer, S. Sariciftci

8:30 – ENVR 111. Environmental applications of iron oxide nanomagnets. **A. S. Samia**

9:00 – ENVR 112. Biodegradable and biocompatible functional nanomaterials. **R. R. Ozer**, P. Hari, U. Butt, T. J. Athauda

9:30 – ENVR 113. Green synthetic routes toward shape-controlled nanoscale materials. S. O. Obare, **C. P. Adams**

10:00 Intermission

10:15 – ENVR 114. Organic synthesis via magnetic attraction: Benign and sustainable protocols using magnetic nanocatalysts. **R. S. Varma**, R. Baig

10:45 – ENVR 115. Synthesis and characterization of nanoscaled doped titanium dioxide with high nitrogen concentration for visible light catalysis. **C. Burda**

11:15 – ENVR 116. Multi-electron transfer catalysts for conversion of biorenewables into commodity chemicals. **S. O. Obare**

11:45 – ENVR 117. Facile hydrogenation of carbon-carbon double bonds using catalytic noble nanoparticles immobilized in microfluidic reactors. **R. Y. Ofoli**, R. Lin, X. Ma

12:15 Concluding Remarks

Environmental Biotechnology and Sustainability: Applications to Drinking Water, Industrial Waste Treatment, and Site Remediation

Cosponsored by AGFD and AGRO
E. Sahle-Demessie, A. Aly Hassan, *Organizers, Presiding*

Section D
Loews Philadelphia Hotel - Washington B/C

8:00 Introductory Remarks

8:05 – ENVR 126. Abiotic transformations in the removal of estrogens during wastewater treatment: Effects of operating conditions. **M. T. Suidan**, R. Marfil-Vega

8:45 – ENVR 127. Chemotaxis of pollutant-degrading bacteria to toluene droplets retained within the low permeable region in a heterogeneous porous microfluidic device. **X. Wang**, J. Atencia, R. M. Ford

9:05 – ENVR 128. Bioregeneration of spent anion exchange resin produced in treatment of nitrate. **X. Meng**, X. Meng

9:25 – ENVR 129. Anaerobic bioreactor system for treatment of groundwater contaminated with chlorinated volatile organic compounds. **M. M. Lorah**, C. Walker, A. Baker

9:45 – ENVR 130. Biological removal of chloroform by using biotrickling filter (BTF). **B. Mezgebe**, G. Sorial, A. Aly Hassan, S. Demessie

10:05 Intermission

10:15 – ENVR 131. Treatment of mixtures of hydrophobic and hydrophilic volatile organic compounds in trickling bed air biofilters. **A. Zehraoui**, G. A. Sorial

10:35 – ENVR 132. Remediation of metal-contaminated drinking water using electrospun alginate nanofibers. **M. Bradley**, M. D. Cathell

10:55 – ENVR 133. Sustainable approach for simultaneous wastewater treatment and bio-energy production in mediator-less microbial fuel cell. **Z. Z. Ismail**, A. J. Jaeel

11:15 – ENVR 134. Feasibility of laccases for the removal of pharmaceutical compounds. **L. Lloret**, G. Eibes, **M. Moreira**, **G. Feijoo**, J. Lema

11:35 – ENVR 135. Oxidation of bisphenol A and triclosan by laccase from *Trametes versicolor* and *Myceliophtora thermophila*. A. Arca-Ramos, J. Martínez-Patiño, G. Eibes, **M. Moreira**, G. Feijoo, J. Lema

11:55 Concluding Remarks

TUESDAY MIDDAY

Sterling Hendricks Memorial Lectureship

Sponsored by USDA-Agricultural Research Service
Cosponsored by AGFD & AGRO
Hosted by AGFD

Dr. Eric Block

M. H. Tunick, S. Duke, K. Kaplan,
Organizers, Presiding

Section A
Loews Hotel Philadelphia - 33rd Floor - Howe

11:30 Award Presentation.

11:40 – AGFD 97. Fifty years of smelling sulfur: From Allium chemistry to olfactory detection of sulfur compounds. **E. Block**

12:30 Award Reception.

TUESDAY AFTERNOON

Integrated Vector and Resistance Management

J. Bloomquist, T. D. Anderson, *Organizers, Presiding*

Section A
Loews Hotel Philadelphia - Commonwealth D

1:30 – 149. Imitating insecticidal spider peptides: In silico screening and optimization of a new heterocyclic family of mosquitocides. **R. M. Kennedy**, H. W. Tedford, L. Bao, B. A. Steinbaugh, A. Tempczyk-Russell, C. A. Hendrickson, B. D. Tait

1:55 – 150. Renal potassium channels of mosquitoes as potential new insecticidal targets. **P. M. Piermarini**, J. S. Denton, K. W. Beyenbach

2:20 – 151. Development of acylpiperidine and carboxamide repellents using structure-activity models. **U. R. Bernier**, M. Tsikolia, N. M. Agramonte

2:45 Intermission.

3:00 – 152. Mosquito biting deterrence: Structure-activity relationship of saturated and unsaturated fatty acids. **C. L. Cantrell**, A. Ali, U. R. Bernier

3:25 – 153. Mode of action of insect repellents. **J. C. Dickens**

3:50 – 154. Neurotoxicology of N,N-diethyl-*meta*-toluamide (DEET). **J. Bloomquist**, D. Swale

4:15 Concluding Remarks.

Reactive Nitrogen (Nr) from Agriculture: Emission, Consequence, and Management

Overview, Emissions and Modeling

B. Schichtel, L. McConnell, P. Silva, *Organizers*
S. Trabue, V. Aneja, *Organizers, Presiding*

Section B
Loews Philadelphia Hotel - Regency Ballroom C1/C2

1:30 Introductory Remarks.

1:35 – 155. Management of excess reactive nitrogen in the environment. **T. Theis**, J. Galloway, O. Doering

2:05 – 156. Trends in emissions of reactive nitrogen from US agriculture. **R. Knighton**

2:30 – 157. Agriculture and nitrogen: A view of 80 years of maize production. **J. Gaffney**, J. Shanahan, D. Warner, B. Weer, T. Greene

2:55 – 158. Estimation of national-scale bidirectional ammonia flux using a coupled air quality and farm management modeling system. **E. Cooter**, J. O. Bash, V. Benson, L. Ran

3:20 Intermission.

3:35 – 159. Predicting the reactive nitrogen footprint of milk production systems. **C. A. Rotz**, S. D. Hafner

4:00 – 160. Estimation of ammonia emissions from beef cattle feedyards in the southern High Plains with process-based modeling. **H. M. Waldrip**, R. W. Todd, N. Cole, C. Li, W. Salas

4:25 – 161. Ammonia emissions from beef cattle feedyards: A summary of seven years of research. **R. W. Todd**, N. Cole

4:50 – 162. Nitrous oxide emissions from biofuel crops and its parameterization in the EPIC biogeochemical model. **P. R. Pillai**, V. P. Aneja, J. T. Walker, A. Njegovan

5:15 Concluding Remarks.

Environmental Fate, Transport and Modeling/Monitoring of Agricultural Chemicals

Surface Water Monitoring, Watershed Characterization, and Modeling

Financially supported by Waterborne Environmental Inc.
S. Jackson, *Organizer*
P. Hendley, N. Peranginangin, *Organizers, Presiding*

Section C
Loews Hotel Philadelphia - Regency Ballroom B

1:30 – 163. Survey sampling approach for estimating upper centile pesticide concentrations from surface water monitoring. **W. Chen**, P. Mosquin, P. Hendley, R. W. Whitmore

1:50 – 164. Watershed characterization: An overview of how watersheds can be classified and compared in terms of their environmental characteristics, their potential vulnerability to runoff from agricultural fields, and the presence of existing agricultural structural mitigation features. **P. Hendley**, C. M. Harbourt, P. S. Miller, M. Andrus, W. Northcott, J. Prenger

2:10 – 165. Watershed characterization: Multivariate approaches for identifying key factors contributing to potential vulnerabilities for agrochemical runoff in small headwater Midwest watersheds. **P. Miller**, C. M. Harbourt, M. Andrus, W. Northcott, J. Prenger, P. Hendley

2:30 – 166. Watershed characterization: Approaches to characterizing agricultural stewardship practices and best management related structural features in small headwater Midwest watersheds and an assessment of their potential significance in determining the potential for agrochemical runoff. **C. M. Harbourt**, J. D. Davis, P.

S. Miller, J. Prenger, S. Zelonis, G. Hoogeweg, P. Hendley

2:50 Intermission.

3:10 – 167. Integration of SWAT modeling and pesticide monitoring to assess aquatic life exposure in an Oregon watershed. **P. Janney**, J. Jenkins

3:30 – 168. Refined application of the SWAT model for endangered species effects determination. **M. F. Winchell**, S. Folle, R. Breton

3:50 – 169. Evaluation of a simplified SWAT model approach for prediction of insecticide concentrations in a small watershed in northwestern Oregon. **N. Peranginangin**, M. F. Winchell, S. Folle

4:10 – 170. Withdrawn

4:30 Questions.

Is Your Analytical Method Good Enough?

Cosponsored by AGFD and ENVR
J. Eble, S. J. Lehotay, *Organizers, Presiding*

Section D
Loews Hotel Philadelphia - Regency Ballroom A

1:30 – 171. High-throughput LC-MS/MS analysis of acetochlor residues in raw agricultural commodities. **L. S. Riter**, N. R. Smith, J. Allan, C. E. Wujcik

1:55 – 172. Cost effective analytical methods for the determination of TRIAZOLE residues in plant matrices using LC-MS/MS. **M. Saha**, R. Gooding, J. Jones

2:20 – 173. Use of SRMs in method development and validation. **K. Lippa**, M. Schantz

2:45 – 174. Ruggedness testing and validation of a practical method for more than 100 veterinary drug residues in bovine muscle by UHPLC-MS/MS. **L. Geis-Asteggiante**, S. J. Lehotay, A. R. Lightfield

3:10 Intermission.

3:30 – 175. GC-MS method for determination of pesticides residues in vegetables, fruits, and cereals: Validation and uncertainty estimation following the Eurachem guides. **M. Nocentini**, C. Focardi, M. Fortini, C. Pacciani, G. Biancalani

3:55 – 176. Sample preparation strategies for multiresidue screening, targeted, and confirmatory analysis: Is your sample preparation good enough? **M. S. Young**, K. Tran, J. C. Shia

4:20 – 177. Analysis of pesticides by QuEChERS in fatty samples: Application of Z-Sep+ sorbent. K. Stenerson, E. Barrey, O. Shimelis, **M. Ye**, J. Claus

4:45 Concluding Remarks.

Protection of Agricultural Productivity, Public Health and the Environment - AGRO Poster Session

J. Clark, *Organizer*

Section E
Pennsylvania Convention Center - Hall D

1:00 - 5:00

178. Insectidical azetidines. **D. A. Clark**, S. Bolgunas, G. Lahm, R. Vallinayagam

179. Synthesis and herbicidal activity of novel substituted pyridazin-3(*2H*)-one methanesulfonylisoxazolines. **D. Travis**, T. P. Selby

180. Insecticidal alkylsulfur compounds. **M. Xu**, T. Wagerle, T. M. Stevenson, D. Cordova, M. Schroeder

181. Synthesis of fluorinated diphenylmethane derivatives as insecticides. **T. Briddell**, M. Xu, T. Wagerle, T. M. Stevenson, D. Cordova

182. Insecticidal heteroaromatic tetrazoles. **T. M. Stevenson**, E. A. Marshall, D. Cordova

183. Fungicidal pyridazinone carboxanilides. **T. M. Stevenson**, E. A. Marshall

184. Ortho-Heterocyclic substituted phenyl anthranilic diamide insecticides. **T. M. Stevenson**, R. Husted, G. P. Lahm, T. P. Selby

185. Pyrazole-N-acetamides as starting points for herbicide discovery. **T. M. Stevenson**, T. V. Thieu, D. L. Piotrowski, A. L. Casalnuovo, T. P. Selby

186. Fungicidal pyrazinone-2-carboxamides. **T. M. Stevenson**, J. F. Bereznak, A. E. Taggi, L. Geist, C. M. Dubas-Cordery

187. Insecticidal 4-piperazinyl pyridazinones. **T. M. Stevenson**, P. L. Sharpe, T. C. Tiscione, J. F. Bereznak

188. 4-(2-Pyridinyl)-5-halo-imidazoles as powdery mildewicides. **T. M. Stevenson**, E. A. Marshall

189. Phenyl substituted thiazoles as fungicides. **R. Vallinayagam**, S. F. McCann

190. PI3 kinase inhibitors as fungicides. **G. R. Cherukupalli**, S. Bathini

191. Modeling of herbicide binding in the inhibition of acetyl-CoA carboxylase. **D. W. Boerth**, A. Arvanites

192. Allelopathic potential of *Rhododendron formosanum* Hemsl in Taiwan. **S. Chou**, C. Huang, T. Hsu, C. Wu, C. Chou

193. Allelopathic effects of biochanin A on selected weed species. M. I. Shajib, A. G. Mortensen, **H. A. Pedersen**, P. Kudsk, I. S. Fomsgaard

194. Establishing acceptability criteria for assessing the homogeneity and stability of test substances in artificial arthropod diets. **C. Davis**, A. Unger, B. Stolte, J. Anderson

195. Herbicide washoff from forest canopy through-fall depends on rainfall dynamics. **K. Bialek-Kalinski**, C. P. Rice, G. W. McCarty

196. Exploring the association of the metolachlor metabolite MESA and agricultural nitrate-N fate and transport in the Choptank River Watershed. **C. J. Hapeman**, G. W. McCarty, C. P. Rice, W. Hively, L. L. McConnell, A. M. Sadeghi, M. W. Lang, D. R. Whitall, K. Bialek, P. Downey

197. Potential arsenic sources in a Choptank River subwatershed and the influence of land use and watershed characteristics. **G. T. Nino de Guzman**, E. E. Codling, K. Prabhakara, C. J. Hapeman, W. Hively, G. W. McCarty, M. W. Lang, A. Torrents

198. Endosulfan wet depostion in southern Florida. **T. L. Potter**, C. J. Hapeman, L. L. McConnell, W. F. Schmidt, C. P. Rice, B. A. Schaffer

199 - 200. Withdrawn

201. Developing a web-based system for computing pre-harvest residue limits (PHRLs). **H. Chang**, H. Bae, Y. Son, I. Song, C. Lee, N. Choi, Y. Lee

202. Analysis for oxytetracycline in soils using solid-phase extraction and liquid chromatography tandem mass spectrometry. S. Seal, **D. Robaugh**

203. Comparison of LC/MS/MS and ELISA methodology for a typical allergen. **C. Cunningham**, L. Mallis, C. Miller, J. Eble

204. Discovery of a novel glucuronide metabolite of methyltestosterone in tilapia bile by liquid chromatography/quadrupole-time of flight mass spectrometry. **H. Jayasuriya**, K. Amarasinghe, P. S. Chu, R. Reimschuessel, N. Hasbrouck, E. Evans, C. Chattopadhaya

205. Identification and quantification of organosiloxane and nonylphenol polyethoxylate surfactants in honey bee hive samples by LC-ESI-MS. **J. Chen**, C. A. Mullin

206. Micro-analysis of soil total and mineral nitrogen under different nitrogen fertilization levels. **A. Jurisic**, M. Mesic, Z. Zgorelec, I. Sestak

207. pH-based method for measuring gaseous ammonia. **S. D. Hafner**, J. J. Meisinger, W. Mulbry, S. K. Ingram

AGFD Division

Discovering Bioactive Compounds

Cosponsored by AGRO and ENVR
N. P. Seeram, J. Finley, *Organizers, Presiding*

Section A
Loews Philadelphia Hotel - Commonwealth Hall A1/A2

1:30 Introductory Remarks.

1:35 – AGFD 98. Where have all the polyphenols gone? **J. Vinson**, C. A. Peters, Jr., V. Chopra

2:05 – AGFD 99. Health benefits of fruit polyphenols: Clinical evidence of fruit-derived polyphenol action in the postprandial state,and effects on blood pressure. **B. Burton-Freeman**

2:35 – AGFD 100. Chardonnay grape seed flour reduces plasma lipids and increases expression of hepatic genes for cholesterol and fat synthesis in hamsters fed a high fat diet. **R. Lipson**, T. Arvik, G. Bartley, H. Kim, W. Yokoyama

3:05 – AGFD 101. Transplacental chemoprevention by dietary indole-3-carbinol (I3C) in a mouse model of T-cell lymphoblastic leukemia/lymphoma (T-ALL). **A. D. Benninghoff**, D. P. Larson, B. C. Packard, T. J. Fish, A. M. Hagman, S. M. Frauen, M. S. Gebre, K. J. Hintze, D. E. Williams

3:35 Intermission.

3:50 – AGFD 102. Chardonnay grape seed flour, not red grapes, reduce plasma cholesterol and body weight gain in hamsters on high fat diets. **T. Arvik**, R. Lipson, G. Bartley, H. Kim, W. Yokoyama

4:20 – AGFD 103. Nutritional and pharmaceutical applications of bioactive compounds of some edible berries and tropical fruits. **S. Gorinstein**, S. Flis, Z. Jastrzebski, H. Leontowicz, M. Leontowicz, Z. Tashma, P. Arancibia-Avila, S. Poorvarodom, M. Suhaj,S. Trakhtenberg

4:50 – AGFD 104. Total Western Diet (TWD) increases azoxymethane induced aberrant crypt foci (ACF) compared to the AIN93G diet. **K. J. Hintze**, A. D. Benninghoff, R. E. Ward

5:20 Concluding Remarks.

2011 Kenneth A. Spencer Award

Symposium in Honor of Michael W. Pariza
Conjugated Linoleic Acid: A Naturally-Occurring, Anti-obesity, Anti-inflammatory Fatty Acid

Cosponsored by AGFD
E. Hellmuth, *Organizer*
M. Cook, *Organizer, Presiding;* L. Jackson, *Presiding*

Section B
Loews Hotel Philadelphia - Commonwealth B

1:30 Introductory Remarks.

1:35 – AGFD 105. Synthesis of CLA isomers and their effect on milk fat production. **D. E. Bauman**

1:55 – AGFD 106. CLA and its effect on dairy cow fertility with emphasis on low level inflammatory processes. **G. Bertoni**, P.Grossi, E. Trevisi

2:15 – AGFD 107. Isomers of conjugated linoleic acid as important nutrients in the dairy cow. **K. J. Shingfield**

2:35 – AGFD 108. CLA's role in biochemical processes. **Y. Park**, Y. Park, J. H. Kim, J. Kim, H. Lee

2:55 Panel Discussion.

3:05 Intermission.

3:15 – AGFD 109. Dietary CLA reduces clinical signs of acute and chronic inflammatory disease. **M. E. Cook**

3:35 – AGFD 110. CLA in obesity. **L. D. Whigham**

3:55 – AGFD 111. CLA in cardiovascular disease. **R. J. Nicolosi**

4:15 – AGFD 112. Perspectives on CLA. **M. W. Pariza**

4:35 Panel Discussion

ENVR Division

Environmental Biotechnology and Sustainability: Applications to Drinking Water, Industrial Waste Treatment, and Site Remediation

Cosponsored by AGFD and AGRO
E. Sahle-Demessie, A. Aly Hassan, *Organizers, Presiding*

Section D
Loews Philadelphia Hotel - Washington B/C

1:30 Introductory Remarks

1:35 – ENVR 161. Investigations into water quality indicators along southern Lake Michigan beaches. **J. Peller**, R. Whitman, M. Byappanahalli, D. Shively

1:55 – ENVR 162. Determining indicator compounds representative of pharmaceuticals and personal health care products (PPHCPs) in water cycle. **S. Zhang**, S. Gitungo, L. Axe, J. E. Dyksen, R. F. Raczko

2:15 – ENVR 163. Pilot plant study on indicator compounds representative of pharmaceuticals and personal health care products (PPHCPs) in the water cycle. **S. W. Gitungo**, S. Zhang, L. Axe, J. E. Dyksen, R. F. Raczko

2:35 – ENVR 164. Degradation of iodinated carboxylic acid compounds in water. **L. M. Olson**, K. A. Rickman, S. P. Mezyk, M. P. Schramm, S. Smith, J. A. LaVerne

2:55 – ENVR 165. Reactivity of the hydroxyl radical with International Humic Substances Society natural organic matter isolates. **G. McKay**, F. Rosario-Ortiz, S. P. Mezyk

3:15 Intermission

3:30 – ENVR 166. Evaluation of the hydroxyl radical based degradation efficiency for antibiotics in water. **S. Otto**, S. P. Mezyk, R. Acey

3:50 – ENVR 167. Removal of antibiotics from water using the advanced oxidation/reduction process with sulfate radicals. **D. K. Asamoto**, S. P. Mezyk

4:10 – ENVR 168. Emerging contaminants in water containing nitrogen-nitrogen single bonds: An examination of their degradation chemistry, reactivity, and products. **J. J. Kiddle**, S. P. Mezyk

4:30 – ENVR 169. Investigation of the dark reaction between hydrogen peroxide and chloramines. **M. Chagnon**, G. McKay, B. L. Sjelin, S. P. Mezyk

4:50 Concluding Remarks

WEDNESDAY MORNING

Mechanisms of Insecticidal Action and Resistance: New Compounds and Recent Advances
Mechanism of Action

D. Soderlund, J. Clark, *Organizers*
B. Pittendrigh, T. D. Anderson, *Presiding*

Section A
Loews Hotel Philadelphia - Commonwealth D

8:30 Introductory Remarks.

8:35 – 208. Diamide insecticides: Global efforts to address stewardship challenges. **L. A. Teixeira**, J. T. Andaloro

9:00 – 209. AGRO New Investigator Finalist: Fluorescent assay of acetylcholinesterase ligand interactions for design of insecticides targeting the mosquito vector of malaria, *Anopheles gambiae*. **F. Tong**, P. R. Carlier, J. Li, M. Totrov, J. R. Bloomquist

9:25 – 210. AGRO New Investigator Finalist: Explore new insecticidal site targeting on chitin synthesis enzymes in *Anopheles gambiae*. **X. Zhang**, K. Michel, K. Y. Zhu

9:50 – 211. Selective actions of insecticides on nicotinic receptor subtypes. **V. L. Salgado**, B. London, R. Paulini, N. B. Rankl, X. Zhao

10:10 Intermission.

10:25 – 212. Identification of a novel pyrethroid receptor site on a mosquito sodium channel. Y. Du, Y. Nomura, G. Satar, Z. Hu, B. S. Zhorov, **K. Dong**

10:50 – 213. Sodium channel inhibitor insecticides: Blurring the line between insecticides and drugs. **D. M. Soderlund**

11:15 – 214. Mode of action of metaflumizone on voltage-gated sodium channels. **R. T. von Stein**, D. M. Soderlund

11:40 Discussion.

Reactive Nitrogen (Nr) from Agriculture: Emission, Consequence, and Management
Transport, Transformation, and Deposition

S. Trabue, P. Silva, V. Aneja, *Organizers*
L. McConnell, B. Schichtel, *Organizers, Presiding*

Section B
Loews Philadelphia Hotel - Regency Ballroom C1/C2

8:00 Introductory Remarks.

8:05 – 215. Characterization of ammonia emissions from agricultural sources in California and their implications for ammonium nitrate formation. **J. B. Nowak**, J. A. Neuman, R. Bahreini, A. M. Middlebrook, J. S. Holloway, S. A. McKeen, T. B. Ryerson, M. Trainer, D. D. Parrish

8:30 – 216. Environmental and ecological effects of atmospheric nitrogen deposition. **M. E. Fenn**

8:55 – 217. Emissions of ozone precursors from a central California dairy facility. **A. S. Hasson**, S. O. Ogunjemiyo, S. Trabue, S. Ashkan, C. Olea, S. Middala, K. Vu, A. Scruggs, L. R. Addala, L. Nana, J. Steele, T. Shelton

9:20 – 218. Nitrogen enrichment and species change in shortgrass prairie adjacent to a cattle feedyard. **R. W. Todd**, N. Cole

9:45 Intermission.

10:00 – 219. Atmospheric reactivity studies of aliphatic amines. D. R. Cocker, **P. J. Silva**, K. Purvis-Roberts, D. J. Price, X. Tang, Q. Malloy, M. E. Erupe, R. S. Brown

10:25 – 220. Organic nitrogen speciation in aerosols, precipitation, and cloudwater. **Y. Desyaterik**, Y. Sun, K. B. Benedict, J. L. Collett, Jr., B. A. Schichtel

10:50 – 221. Reactive nitrogen composition and origin in the United States Rocky Mountains. **B. A. Schichtel**, K. Benedict, A. J. Prenni, M. G. Barna, K. A. Gebhart, M. A. Rodriguez, D. Day, E. Levin, C. M. Carrico, W. C. Malm, J. L. Collett, S. M. Kreidenweis

11:15 – 222. Examining the sources and transport of agricultural reactive N emissions using stable isotope techniques. **J. D. Felix**, E. M. Elliott

11:40 Concluding Remarks.

Environmental Fate, Transport and Modeling/Monitoring of Agricultural Chemicals
Drift and Environmental Fate

Financially supported by Waterborne Environmental Inc.
P. Hendley, *Organizer*
S. Jackson, N. Peranginangin, *Organizers, Presiding*

Section C
Loews Hotel Philadelphia - Regency Ballroom B

8:30 Introductory Remarks.

8:40 – 223. Applying methods to elucidate non-target organism impact using conventional lab, field, and modeling observations. **S. A. Cryer**, D. G. Ouse, P. L. Havens, J. M. Gifford, K. Qin, D. E. Hillger

9:00 – 224. Comparison of multiple source ground spray deposition curves for determination of buffers in simulation models. **S. H. Jackson**

9:20 – 225. Kresoxim methyl drift and related runoff in a vineyard catchment. **M. Lefrancq**, G. Imfeld, S. Payraudeau, M. Millet

9:40 – 226. Modeling the vapor drift potential of current-use pesticides. **C. L. Davie-Martin**, K. J. Hageman, Y. Chin

10:00 Intermission.

10:20 – 227. Conduct of aquatic herbicide fate and transport studies on moving water bodies. **D. K. Moore**, A. C. Newcombe, P. L. Havens

10:40 – 228. Colloid facilitated transport of veterinary pharmaceutical florfenicol in saturated sand and soil columns. **Y. Zou**, W. Zheng, S. Bradford

11:00 – 229. Sorption of organophosphate and triazine agrochemicals on biochars and soils. **M. Uchimiya**

11:20 – 230. Trapping and analysis of large quantities of volatile gases in an anaerobic aquatic metabolism study: A case study using [*S*-methyl-^{14}C]methamidophos. **S. Mislankar**, K. Dallstream

11:40 Questions.

Is Your Analytical Method Good Enough?

Cosponsored by AGFD and ENVR
J. Eble, S. J. Lehotay, *Organizers, Presiding*

Section D
Loews Hotel Philadelphia - Regency Ballroom A

8:30 Introductory Remarks.

8:35 – 231. Determination of nine *N*-nitrosamines in drinking water by fast solid phase extraction and GC/MS. S. Qin, **G. Lu**, J. Liu

9:00 – 232. Determination of triazines and degradates in water using LC-MS/MS and stable isotope analogs as internal standard. **S. Chen**, A. Merritt, S. Huang, L. Mayer

9:25 – 233. Analysis of environmental samples for pyrethroid insecticides using multianalyte methods and stable isotope internal standards. **K. Clark**, D. A. Koch, D. M. Tessier

9:50 Intermission.

10:10 – 234. Tell-"tail" indicator: Quantifying iophenoxic acids in deer serum via LC/MS/MS analysis. **D. A. Goldade**, G. E. Phillips

10:35 – 235. Immunochemistry-based protein detection in genetically engineered crops. **G. Shan**

11:00 – 236. Second generation technology for transgenic protein quantitation in stacked traits. **C. Kramer**

11:25 – 237. Validating enzyme-linked immunosorbent assay (ELISA) methods for protein quantification from environmental matrices. **A. Unger**, J. Anderson, C. Davis, B. Stolte

11:50 Concluding Remarks.

Synthesis and Chemistry of Agrochemicals

V. Hegde, T. Stevenson, *Organizers*
J. Long, *Presiding*

Section E
Loews Hotel Philadelphia 33rd Floor - Lescaze

9:00 Introductory Remarks.

9:10 – 238. Formation of fungicidal tricyclic isoquinolines via a modified Ritter reaction. **S. F. McCann**, A. Crews

9:30 – 239. Synthesis and SAR studies of fungicidal 3-aryl-1,2,4-triazin-6-ones. **M. R. Loso**, J. Owen, K. G. Meyer, M. T. Sullenberger, M. C. Yap, C. Yao, T. Mathieson, Y. A. Adelfinskaya, P. Graupner, S. Shaber, F. D. Smith

9:50 Intermission.

10:05 – 240. Synthesis and SAR studies on the aryl component of the aminosulfone fungicides. **M. Sullenberger**, J. Phillips, W. C. Lo, A. Buysse, M. Iamauti, C. Klittich, T. Mathieson, M. Olson, M. J. Ricks, I. Morrison, B. Rieder

10:30 – 241. Identification of novel fungal acetyl-coenzyme A carboxylase inhibitors via fragment-based design approach. W. K. Brewster, D. P. Cudworth, S. C. Fields, M. L. Foster, F. P. Hollinger, **J. E. Hunter**, Z. Konteatis, C. T. Lowe, J. L. Ludington, A. Owens Merlo, D. J. Pernich, K. G. Meyer, S. Rong, C. L. Schmidt, M. E. Stumpf, J. D. Webster

10:50 – 242. From target-based research to herbicidal activity in the field. **M. C. Witschel**

ENVR Division

Nanomaterials in Medicine, Food and the Environment
Cosponsored by AGFD and AGRO
D. Bello, *Organizer*
A. Keller, J. Gardea-Torresdey, *Organizers, Presiding*

Section C
Loews Philadelphia Hotel - Congress B/C

8:30 Introductory Remarks

8:35 – ENVR 188. Nanomaterial contamination of agricultural crop species. **J. C. White**

9:05 – ENVR 189. Synchrotron imaging of the uptake and speciation of ZnO and CeO_2 in soil cultivated soybean (Glycine max). **J. A. Hernandez-Viezcas**, J. Andrews, H. Castillo-Michel, C. Rico, Y. Ge, J. H. Priester, R. Mielke, A. M. Horst, S. C. Moritz, Y. An, L. Zhao, K. Espinosa, R. Palmer, J. Gardea-Torresdey, P. A. Holden, S. L. Walker, J. Schimel, R. Nisbet

9:35 – ENVR 190. Phytotoxicity and biotransformation of Yb_2O_3 nanoparticles in cucumber plants. **Z. Zhang**, Y. Ma, X. He, P. Zhang, Y. Zhao, W. Feng

9:55 – ENVR 191. Impact of cerium oxide nanoparticles on Kidney beans (*Phaseolus vulgaris*). **S. Majumdar**, J. R. Peralta-Videa, J. L. Gardea-Torresdey

10:15 Intermission

10:30 – ENVR 192. Comparative toxicity assessment of CeO_2 and ZnO nanoparticles towards nitrogen fixing gram negative species *Sinorhizobium meliloti*. **S. Bandyopadhyay**, J. R. Peralta-Videa, G. P. Villa, J. L. Gardea-Torresdey

10:50 – ENVR 193. TiO_2 NPs can be taken up by roots and translocated to leaves in cucumber (*Cucumis sativus*) plants. **A. D. Servin**, J. A. Hernandez, H. Castillo-Michel, J. Peralta-Videa, J. Gardea-Torresdey

11:10 – ENVR 194. Uptake of fullerene (C60) induced catalase (CAT) activity in *Lumbriculus variegatus*. **J. Wang**, J. D. Maul, G. D. Mayer, G. P. Cobb

11:30 – ENVR 195. Nanomaterials in food packaging and water: Addressing safety concerns. **A. J. Whelton**

WEDNESDAY AFTERNOON

Mechanisms of Insecticidal Action and Resistance: New Compounds and Recent Advances
Insecticide Resistance
J. Clark, *Organizer;* D. Soderlund, *Organizer, Presiding*
J. Bloomquist, *Presiding*

Section A
Loews Hotel Philadelphia - Commonwealth D

1:30 Introductory Remarks.

1:35 – 243. Human lice: Past, present, and future control. **J. M. Clark**

1:55 – 244. Body and head lice as a model system for understanding xenobiotic responses. **B. R. Pittendrigh**, K. S. Yoon, W. Sun, B. Olds, S. H. Lee, J. M. Clark

2:15 – 245. Brief exposure of human body and head lice to sub-lethal amounts of ivermectin over transcribes detoxification genes involved in tolerance. **K. S. Yoon**, J. P. Strycharz, J. H. Baek, W. Sun, J. H. Kim, J. S. Kang, B. R. Pittendrigh, S. H. Lee, J. M. Clark

2:35 – 246. Comparison of the immune responses between body and head lice following bacterial challenge. **J. Kim**, J. Min, J. Kang, D. Kwon, K. Yoon, J. Strycharz, Y. Koh, B. R. Pittendrigh, J. M. Clark, S. Lee

2:55 – 247. MRSA transmission by human lice and bed bugs: Is more effective control necessary? **K. S. Yoon**, D. J. Previte, J. J. Song, G. Xu, S. H. Lee, N. Balaban, S. M. Rich, J. M. Clark

3:15 Intermission.

3:30 – 248. Extent of the bed bug problem: Past, present, and future control. **R. Koganemaru**

3:50 – 249. Molecular genetic characterization of bed bug populations: From local infestations to global patterns. **E. L. Vargo**, W. Booth, V. Saenz, R. G. Santangelo, C. Schal

4:10 – 250. Deep sequencing of pyrethroid-resistant bed bugs reveals multiple mechanisms of resistance within a single population. **Z. N. Adelman**, K. A. Kilcullen, R. Koganemaru, M. A. Anderson, T. D. Anderson, D. M. Miller

4:30 – 251. Evidence of CYP397A1-mediated pyrethroid resistance in bed bugs. **T. D. Anderson**, T. L. Carpenetti, Z. N. Adelman, R. Koganemaru, D. M. Miller

4:50 Concluding Remarks.

Reactive Nitrogen (Nr) from Agriculture: Emission, Consequence, and Management
Mitigation and Analytical Methods
B. Schichtel, L. McConnell, V. Aneja, *Organizers*
S. Trabue, P. Silva, *Organizers, Presiding*

Section B
Loews Philadelphia Hotel - Regency Ballroom C1/C2

1:30 Introductory Remarks.

1:35 – 252. Ammonia emissions from poultry operation affected by dietary modification and litter amendment. **H. Li**

2:00 – 253. Optimizing nitrogen fertilizer use on small landholder farms in India and Vietnam. **J. Rudek**, K. Kritee, R. Ahuja

2:25 – 254. Impact of animal diet on ammonia and greenhouse gas emissions. **S. L. Trabue**, B. J. Kerr

2:50 – 255. Adaptation of an ambient ion monitor for detection of amines in gas and particulate agricultural emissions. **P. J. Silva**

3:15 – 256. New soil sampling technique for increased accuracy of total soil nitrogen determination. **M. Mesic**, A. Jurisic, Z. Zgorelec, I. Sestak

Environmental Fate, Transport and Modeling/Monitoring of Agricultural Chemicals
Pyrethroids and Aquatic Exposure

Financially supported by Waterborne Environmental Inc.
N. Peranginangin, *Organizer*
S. Jackson, P. Hendley, *Organizers, Presiding*

Section C
Loews Hotel Philadelphia - Regency Ballroom B

1:30 – 257. Identification of important pathways for residential runoff transport of pyrethroids: Facility design. **P. C. Davidson**, C. M. Harbourt, R. L. Jones, P. Hendley

1:50 – 258. Identification of important pathways for residential runoff transport of pyrethroids: Preliminary experimental results. **R. L. Jones**, P. C. Davidson, C. M. Harbourt, P. Hendley

2:10 – 259. Laboratory degradation rates of eleven pyrethroids under aerobic and anaerobic conditions. **B. N. Meyer**, C. Lam, S. Moore, R. L. Jones

2:30 – 260. Assessment of the potential influence of physical habitat, pyrethroids, and metals on benthic communities in urban California streams in 2009-2011. **L. Hall, Jr.**, W. Killen, R. Anderson, R. Alden III

2:50 Intermission.

3:10 – 261. Fate of pyrethroid insecticides in wastewater treatment processes. **D. Tessier**, J. McGrath, J. Cleary

3:30 – 262. Aquatic exposure model parameterization using outdoor simulated pond study. **Z. Tang**, T. Ramanarayanan, L. Ortego, R. Allen

3:50 – 263. Predicting the bioconcentration of herbicides, insecticides, and fungicides in fish with partitioning and biotransformation. **D. T. Kuo**, D. M. Di Toro

4:10 – 264. Assessing exposure of the California Red-Legged Frog to an insecticide in irrigation pond habitat. **B. Toth**, J. Hanzas, T. Estes, R. Breton

4:30 Questions.

Perfecting Communication of Chemical Risk

Cosponsored by AGFD and ENVR
J. Seiber, J. Johnston, I. Kennedy, *Organizers*
K. Armbrust, T. Potter, K. Solomon, *Organizers, Presiding*

Section D
Loews Hotel Philadelphia - Regency Ballroom A

1:00 Introductory Remarks.

1:05 – 265. Communicating science-based assessment of risks and benefits of agricultural biotechnology. **D. A. Fischhoff**

1:25 – 266. Communicating risks and benefits of soil fumigant use. **J. N. Seiber**

1:45 – 267. Inter-agency risk communication: Inorganic arsenic residues in poultry. **J. J. Johnston**, T. Zhou

2:05 – 268. Communicating the risk of polycyclic aromatic hydrocarbons (PAHs) measured in seafood in Mississippi following the Gulf oil spill. **K. L. Armbrust**, A. Brown, G. Hagood, J. Jewell, D. Diaz, N. Gatian, H. Folmer, K. Xia

2:25 – 269. POPs on the cusp: The case of endosulfan. **K. Solomon**

2:45 Intermission.

3:00 – 270. Using local community-protection values to provide evidence of reduced catchment-scale risk from pesticides. **M. Burns**, A. N. Crossan, G. Hoogeweg, I. R. Kennedy

3:20 – 271. Real world exposure and biomonitoring are not part of the alarmist agenda. **L. E. Hammond**

3:40 – 272. Lessons from the endosulfan case for achieving rational risk assessment in the face of chemical paranoia. **I. R. Kennedy**, M. T. Rose, A. N. Crossan

4:00 – 273. Achieving rational regulatory action for the management of risk from diuron in catchments with outfalls to the Great Barrier Reef. **A. N. Crossan**, M. T. Rose, M. Burns, I. R. Kennedy

4:20 Panel Discussion.

Synthesis and Chemistry of Agrochemicals
Tubulin Modulators as Fungicides

T. Stevenson, V. Hegde, *Organizers*
S. McCann, *Presiding*

Section E
Loews Hotel Philadelphia -33rd Floor - Lescaze

1:30 – 274. Synthesis and fungicidal activity of mono- and biheterocyclic tubulin polymerisation promoters. **C. Lamberth**

2:00 – 275. 3,4-Diarylpyridines as broad-spectrum fungicides. **B. L. Finkelstein**, R. J. Crosswicks, A. E. Trivellas

2:30 – 276. Fungicidal 2- and 4-pyridones. **T. M. Stevenson**, P. L. Sharpe, T. P. Selby

2:50 Intermission.

3:10 – 277. Synthesis and biological activity of di- and tri-aryl pyridazines as broad spectrum fungicides. **P. L. Sharpe**, T. M. Stevenson

3:40 – 278. Fungicidal carbonyl-containing heterocycles. **T. M. Stevenson**, T. C. Tiscione

4:10 – 279. Diaryl-imidazoles as tubulin-inhibiting fungicides. **A. E. Taggi**, T. P. Selby, J. F. Bereznak, J. J. Bisaha, L. Geist, M. Hanagan, P. R. Kovacs, C. E. Liberato, E. A. Marshall

4:30 Concluding Remarks.

ENVR Division

Nanomaterials in Medicine, Food and the Environment
Life Cycle Considerations

Cosponsored by AGFD and AGRO
A. Keller, *Organizer*
D. Bello, J. Gardea-Torresdey, *Organizers, Presiding*

Section C
Loews Philadelphia Hotel - Congress B/C

1:30 – ENVR 215. Nanosilver markets and global regulatory concerns. **J. R. Ellis**

2:00 – ENVR 216. Emerging trends in nanoparticle fate and transport. **A. A. Keller**, D. C. Zhou

2:30 – ENVR 217. Environmental releases of engineered nanomaterial resulting from biosolids disposal to land and air. **K. D. Hristovski**, Y. Wang, N. Buck, P. Westerhoff, J. E. McLane

2:50 – ENVR 218. Multimedia environmental distribution of nanomaterials. **H. Liu**, Y. Cohen

3:10 – ENVR 219. Fate and occurrence of fullerenes in airborne particulate, combustion particles, contaminated soils and wastewater samples. **D. Barcelo**, J. Sanchis, M. Farré, N. Al-Harbi, L. Silva

3:30 Intermission

3:45 – ENVR 220. Effect of short-chain organic acids on the removal of pentachlorophenol with zerovalent iron in soil. **O. Yu-heng**, S. Yang-hsin

4:05 – ENVR 221. Clay particles destabilize engineered nanoparticles in aqueous environments. **D. Zhou**, S. Tjan, A. I. Abdel-Fattah, A. Keller

4:25 – ENVR 222. Stability of the coating in TiO_2-based sunscreens: Potential implications. **J. Virkutyte**, S. Al-Abed, D. D. Dionysiou

4:45 – ENVR 223. Influence of light on the formation of silver nanoparticles in aquatic environment. **V. K. Sharma**, N. Adegboyega, K. Siskova, M. Sohn

WEDNESDAY EVENING

ENVR Division Poster Session

Cosponsored by AGFD and AGRO

Section A
Pennsylvania Convention Center - Hall D

6:00 - 8:00

Addressing the Complex Site: Chemistry, Toxicology & Fate of Mixed Pollutants Across Environmental Media

ENVR 224. Impact of dry-wet cycles on the release of PAHs from wetland sediments in South Texas. **Z. Wang**, Z. Liu

ENVR 225. Examination of the diverse environmental impacts of long-term acid mine drainage on a Virginia stream ecosystem.**M. Szulczewski**

ENVR 226. Investigating of the levels, trends, and fate of pollutants in street dust in the Long Creek Watershed, South Portland ME. **L. A. Benedict**, K. McDonald, J. Barilone, N. Chouinard

ENVR 227. Sorption of the chemical warfare agent VX to clay minerals. **K. M. Morrissey**, A. M. Schenning, R. L. Cheicante, K. B. Sumpter

ENVR 228. Uncertainty analysis of vapor intrusion models using stochastic response surface method. **A. Gharehtapeh**, M. Tootkaboni, K. G. Pennell

ENVR 229. Reactions of dehydropyrrolizidine alkaloids with valine and hemoglobin. **S. Wang**, Y. Zhao, Q. Xia, A. G. da Costa, L. Cai, P. P. Fu

ENVR 230. Debromination of HBCD-isomers by reduced sulfur species. J. H. Wilson, K. W. Lo, **U. Jans**

ENVR 231. Contamination profiles of PCB congeners, chlorinated pesticides, and PBDEs in sediment and fish samples from riverine and brackish waters of Savannah, Georgia, USA. **K. S. Sajwan**, **B. Cassidy**, P. Chakraborty, J. P. Richardson, B. G. Loganathan

ENVR 232. Trace elements and PCB congener concentrations in annual growth rings of pine trees from western Kentucky. **B. G. Loganathan**, B. Patibandla

Environmental Biotechnology and Sustainability: Applications to Drinking Water, Industrial Waste Treatment, and Site Remediation

ENVR 233. Effects of ozonation and UV radiation on the molecular and optical properties of natural water and wastewater effluent dissolved organic matter. **A. L. Paul**, W. T. Cooper

ENVR 234. Coking wastewater treatment plant as sources of polycyclic aromatic hydrocarbons to the atmosphere. **W. Zhang**, C. Wei, W. Huang

ENVR 235. Determination of haloacetic acids by 2D matrix elimination ion chromatography. **P. R. Perati**, R. Lin, K. Srinivasan, B. De Borba, J. Rohrer

ENVR 236. Preparation and characterization of polyamide-polyetheramide (PAPEA) copolymer membranes for reverse osmosis and nanofiltration. N. Arnett, **M. Gayle**, J. Adediga

ENVR 237. Effects of environmental variables on coastal fecal indicator bacteria concentrations in Orange County, California. **Y. Jeong**, S. Y. Choi, S. Chung

ENVR 238. Overview of the remediation of cyanotoxins from water using physicochemical processes. **D. D. Dionysiou**

Green Chemistry and the Environment

ENVR 289. Towards a new organocatalyzed microwave-assisted isocyanate-free synthesis of [*n*]-oligourea: A new energy-saving, eco-friendly method generating oligourea using green chemistry approaches. **A. K. Qaroush**, A. S. Al-Hamayda, Y. K. Khasman, V. D'Elia, S. Vagin, C. Troll, B. Rieger

ENVR 290. Performance of multilevel antimicrobials in clinical environment. H. Leung, Y. Li, **W. Han**, K. Yeung, J. K. Kwan

ENVR 291. Efficiently Starbons® based catalysts for biomass valorisation. A. Negoi, L. Zala, J. H. Clark, R. Luque, S. M. Coman, **V. I. Parvulescu**

ENVR 292. Waste valorisation practises: Changing problems into solutions. A. M. Balu, **R. Luque**, J. C. Serrano-Ruiz, M. Ojeda, A. Pineda, A. A. Romero, J. M. Campelo

Innovative Technologies for Green, Grey, Brown, and Black Water Reclamation and Reuse

ENVR 300. Catalytic hydrodechlorination of dioxins over palladium nanoparticles in supercritical CO_2 swollen microcellular polymers. **K. Chiu**, W. Liao

ENVR 301. Performance evaluation of CDI system based on electrode capacitance. **S. Kim**, J. Yoon

Interactions of Nanomaterials with Emerging Environmental Contaminants

ENVR 302. Effect of pH on aqueous phase Hg(II) removal by nanoscale zero-valent iron. **S. Lee**, S. Han

ENVR 303. Modification of silica nanoparticles surface via "click" chemistry and their adjuvant effects. **Q. Zhang**, W. Chen, B. L. Kaplan, N. E. Kaminski, G. L. Baker

ENVR 304. Degradation of cylindrospermopsin using brookite titanium dioxide under simulated solar light. G. Zhang, M. Nadagouda, M. Pelaez, K. O'Shea, A. Ismail, **D. D. Dionysiou**

ENVR 305. Stabilizing acetylcholinesterase on carbon electrodes to produce effective biosensors. T. J. Stevens, D. Kim, S. R. Kanel, **M. N. Goltz**

Materials for Water Sustainability

ENVR 311. Adsorption of cationic and anionic dyes from aqueous solutions on KOH-activated multiwalled carbon nanotubes. **J. Ma**

ENVR 312. Selective removal of Cu^{2+} and CrO_4^{2-} from natural waters by nanoporous sorbents modified by mono-/di- /tri- amino-organoalkoxysilanes. X. Chen, T. Ng, **W. Han**, K. Yeung

ENVR 313. Removal of cesium ion by zeolite modified carbon electrode. **J. Lee**, C. Kim, J. Yoon

ENVR 314. Removal and recovery of phosphorous from contaminated waters using renewable resource-based magnetic nanocomposites. **S. N. Ramasahayam**, G. N. Gunawan, T. K. Viswanathan

ENVR 315. Removal of antibiotics from contaminated waters using natural zeolite. B. Lee,**P. Zhang**

Measurements and Methods in Environmental Nanotechnology

ENVR 316. Environmental safety of nanocomposites: Assessing degradation of nanocomposites under environmental condition. **G. Ramakrishnan**, J. Ging, P. Feka, A. Hubert, C. S. Korach, A. Orlov

ENVR 317. Applications for fluorescence and zeta potential measurements via nanoparticle tracking analysis. **S. S. Capracotta**, A. Malloy, P. Hole

Nanomaterials in Medicine, Food and the Environment

ENVR 318. Competitive adsorption of toluene, ethylbenzene, and xylene isomers and heavy metal onto multiwalled carbon nanotubes in multisolute system. **F. Yu**, J. Ma, Y. Wu

ENVR 319. Uptake and effects of multiwalled carbon nanotubes on germination and growth of various plant species. **B. Shrestha**, P. Payton, F. Irin, M. Green, J. Cañas

ENVR 320. Reduction of hydroxylated C_{60} (fullerenol) by Zn (0) in water: Reaction kinetics and product characterization.**J. Wu**, W. Li, L. Petrie, Y. Jiang, J. Fortner

ENVR 322. Persistence of commercial nanoscale zero-valent iron (nZVI) and its by-products. **A. Adeleye**, A. Keller, R. Miller, H. Lenihan

ENVR 323. Influence of morphology and phase on TiO2 photoactivity in natural waters. **S. Bennett**, A. Keller

ENVR 324. Interaction between biofilms and nanoparticles. **H. Jing**, B. Mezgebe, **A. A. Hassan**, E. Sahle-Demessie, G. Sorial

ENVR 325. High contrast two-photon fluorescence in vitro imaging using novel fluorescent polymeric nanoparticles. **A. K. Pal**, S. Satapathi, L. Li, J. Kumar, D. Bello

ENVR 326. Toxicity of nZVI to freshwater and marine organisms. **K. Garner**

THURSDAY MORNING

Fate and Exposure of Urban Applied Pesticides in the Context of Human and Ecological Risk Assessments

Cosponsored by AGFD and ENVR
S. Cohen, P. Rice, J. Clark, *Organizers, Presiding*

Section A
Loews Hotel Philadelphia - Commonwealth D

8:25 Introductory Remarks.

8:30 – 280. Movement of soil and trunk injected imidacloprid through the hardwood *Acer rubrum*. **J. Pettis**, J. Johnson

8:50 – 281. Survey of imidacloprid levels in water sources frequented by honey bees (*Apis mellifera*) in Maryland. **J. Johnson**, J. Pettis

9:10 – 282. Impacts of modern pesticide formulation technologies on honey bee health. **C. A. Mullin**, J. Chen, T. J. Ciarlo, W. Zhu, M. T. Frazier, J. L. Frazier

9:30 Discussion.

9:40 Intermission.

9:50 – 283. Insecticides on concrete: Role of particles in offsite transport. **J. Gan**, W. Jiang, F. Ernst, D. Haver

10:10 – 284. Insecticide runoff from simulated lawn and driveway surfaces. **R. Williamson**, J. C. Stier, A. Walston, S. Hong

10:30 – 285. Offsite transport of fungicides with snowmelt and rainfall runoff from golf course fairway turf. **P. J. Rice**, B. P. Horgan, J. L. Rittenhouse

10:50 – 286. Optimization of vegetative filter strips for the treatment of pesticide-laden runoff from turf. **J. J. Doherty**, R. Putnam, B. DeFlorio, J. M. Clark

11:10 Discussion.

Human Health and Transgenic Crops

Cosponsored by AGFD
A. M. Rimando, S. Duke, *Organizers, Presiding*

Section B
Loews Hotel Philadelphia - Commonwealth B

9:00 Introductory Remarks.

9:05 – 287. Unintended effects of transgene insertion in crop plants: What are the unique food-safety risks compared with non-transgenic breeding methods? **R. A. Herman**

9:25 – 288. Crop composition: A key component in the safety assessment of a new plant variety. **J. Srinivasan**

9:45 289. Influence of transgenic crops on pesticide use. **C. A. Abel**

10:05 Intermission.

10:20 – 290. Environmental risk assessment and release of flower-color modified transgenic plants. **Y. Tanaka**, S. Chandler

10:40 – 291. Review of mutational breeding and genetic engineering approaches to the development of high protein content in the grain. **I. Wenefrida**, H. S. Utomo, S. D. Linscombe

11:00 – 292. Creating a plant-based source of essential long-chain omega-3 fatty acids. **J. R. Petrie**, S. P. Singh, P. D. Nichols

11:20 – 293. Enhancing desirable nutrients in fruits and vegetables by transgenic approaches. **A. K. Mattoo**

11:40 Concluding Remarks.

Next Generation Biofuels and Bioproducts: Advances and Challenges

Cosponsored by CELL and ENVR
A. Gunasekara, A. Hotchkiss, C. Hapeman, D. Sparks, *Organizers*
A. Brown, *Organizer, Presiding*

Section C
Loews Hotel Philadelphia - Commonwealth C

9:00 Introductory Remarks.

9:05 – 294. Deconstructing nature's structural material for biofuels. **S. Gnanakaran**

9:25 – 295. Investigation of structural changes in Cel7A cellulase when bound to cellulose substrates. **H. O'Neill**, J. He, S. Pingali, L. Petridis, V. Urban, W. Heller, B. Evans, P. Langan, J. Smith, B. Davison

9:45 – 296. Developing the biorefinery: Production of value-added products and fuel from lignocellulosic feedstocks. **N. P. Nghiem**, K. B. Hicks, D. B. Johnston

10:05 – 297. Electrospun core-shell Nafion/enzyme membranes for biofuel production. **D. Tran**, K. J. Balkus

10:25 Intermission.

10:40 – 298. Corn oil as a co-product of fuel ethanol production. **R. A. Moreau**, D. B. Johnston, K. B. Hicks

11:00 – 299. Characterization of biomass fast pyrolysis oils using NMR and chemometrics. **C. A. Mullen**, G. D. Strahan, A. A. Boateng

11:20 – 300. Sophorolipid biosurfactant synthesis and value-added derivatization. **D. K. Solaimin**, R. D. Ashby, J. A. Zerkowski

11:40 – 301. Catalytic and process development for glycerol-free biofuel from acylglyceride lipids. **T. J. Benson**, M. R. Islam, Y. M. Kurle

Worker Exposure: Are Your Senses a Proper Evaluation of Hazardous Exposure?

R. Bennett, *Organizer, Presiding*
D. Sullivan, *Presiding*

Section D
Loews Philadelphia Hotel - Commonwealth Hall A1/A2

8:30 Introductory Remarks.

8:35 – 302. Evaluation of odor perception of a fumigant using in-field volunteers. **R. M. Bennett**

9:00 – 303. Field trial results for Bayfilm tarp material. **D. Sullivan**, H. Ajwa, R. Sullivan

9:25 – 304. Science and technology of odor measurement. **M. A. McGinley**

9:50 Intermission.

10:05 – 305. Sensory irritation from volatile chemicals. **P. Wise**

10:30 – 306. Metam sodium shank compaction applications as a case study in mitigating airborne flux. **D. Sullivan**, H. Ajwa, M. Holdsworth, R. Sullivan

10:55 – 307. Factors affecting the ability to detect and respond to environmental odors. **C. J. Wysocki**

11:20 Panel Discussion.

11:40 Concluding Remarks.

ENVR Division

Measurements and Methods in Environmental Nanotechnology

Cosponsored by AGRO
B.Nelson, E. Petersen, *Organizers, Presiding*

Section B
Loews Hotel Philadelphia - Congress A

8:00 Introductory Remarks

8:05 – ENVR 341. Detection of carbon nanotubes in environmental and biological matrices using programmed thermal analysis. **P. Westerhoff**, K. Doudrick, P. Herckes

8:25 – ENVR 342. Surface analysis of carbon nanotubes and its application to understanding particle and nanocomposite properties in the environment. **H. Fairbrother**, B. Smith, J. Yang, J. Bitter, D. Goodwin, K. Marsh, E. Bouwer, B. Ball

8:45 – ENVR 343. Development of a new detection method for carbon nanotube contamination in water. L. C. Mota, E. E. Urena-Benavides, X. Wang, Y. Yoon, **A. Son**

9:05 – ENVR 344. Measuring black carbon in geosorbents by elemental mapping. **D. T. Kuo**, J. B. Vander Sande, P. M. Gschwend

9:25 – ENVR 345. Measuring particle interactions using total internal reflection microscopy. **J. L. Bitter**, G. A. Duncan, D. H. Fairbrother, M. A. Bevan

9:45 – ENVR 346. Donnan membrane technique: Separating nanoparticles from ions. **R. D. Holbrook**, B. Yezer, R. MacCuspie, J. Gorham

10:05 Intermission

10:15 – ENVR 347. Environmentally relevant nanoparticle surfaces studied by vibrational sum frequency generation and second harmonic generation. **F. M. Geiger**

10:35 – ENVR 348. Use of single particle – inductively coupled plasma – mass spectrometry for analysis of engineered nanoparticle stability in varied media. R. B. Reed, D. M. Mitrano, E. P. Gray, C. P. Higgins, **J. F. Ranville**

10:55 – ENVR 349. Test protocols and results for the nanosilver containing pesticide AGS-20. **J. Costanza**

11:15 – ENVR 350. Tools and approaches for the assessment of nanomaterial induced oxidative DNA damage. **E. J. Petersen**, B. J. Marquis, P. Jaruga, M. Dizdaroglu, B. C. Nelson

11:35 – ENVR 351. Lipid oxidation for measuring bioreactivity of iron nanomaterials. **A. M. Dietrich**, S. Mirlohi, K. Phetxumphou

11:55 – ENVR 352. Nanomaterial Registry: Minimal information standards for well-characterized nanomaterials in environmental studies. **M. L. Ostraat**, K. Mills, D. Murry, K. Guzan

Nanomaterials in Medicine, Food and the Environment Toxicity Mechanisms

Cosponsored by AGFD and AGRO
D. Bello, J. Gardea-Torresdey, *Organizers*
A. Keller, *Organizer, Presiding*
J. Hernandez-Viezcas, *Presiding*

Section C
Loews Philadelphia Hotel - Congress B/C

8:00 – ENVR 353. Thin nanorods and nanowires induce inflammasome activation at lower aspect ratios. **Z. Ji**, X. Wang, H. Zhang, S. Lin, H. Meng, B. Sun, S. George, T. Xia, A. E. Nel, J. I. Zink

8:30 – ENVR 354. Surfactant driven surface changes on single-walled carbon nanotubes: Toxicological implications. **J. G. Clar**, J. Bonzongo, K. J. Ziegler

8:50 – ENVR 355. Screening for oxidative damage by engineered nanomaterials: A comparative evaluation of FRAS and DCFH.**A. K. Pal**, D. Bello, S. Hsieh, D. Schmidt, M. Khatri, P. Gaines, E. Rogers

9:10 – ENVR 356. Evaluation of cytotoxic, genotoxic, and inflammatory responses of nanoparticles from photocopiers in three human cell lines. **M. Khatri**, D. Bello, A. Pal, P. Gaines

9:30 Intermission

9:45 – ENVR 357. Biosynthesis of noble metal nanoparticles by diatoms and their catalytic and antimicrobial properties. **A. Schröfel**, L. M. Shor

10:05 – ENVR 358. Transcriptional-level response of cyanobacterial nitrogen status to titanium dioxide nanomaterials exposure.**C. Cherchi**, A. Z. Gu

10:25 – ENVR 359. In-solution characterization of nanomaterials for in-vitro studies based on Scanning Ion Occlusion Sensing (SIOS). **A. K. Pal**, I. Aalaei, Y. Ganor, D. Bello

10:45 – ENVR 360. Nano-SAR development with application to regulatory decision making. **R. Liu**, R. Rallo, S. Shaw, Y. Cohen

11:15 Concluding Remarks

THURSDAY AFTERNOON

Fate and Exposure of Urban Applied Pesticides in the Context of Human and Ecological Risk Assessments

S. Cohen, P. Rice, J. Clark, *Organizers, Presiding*

Section A
Loews Hotel Philadelphia - Commonwealth D

1:25 Introductory Remarks.

1:30 – 308. Modeling pesticide runoff from urban areas to assess impacts on threatened and endangered species in California. **W. Williams**, D. Denton, R. Breuer, G. Hoogeweg

1:50 – 309. Evaluation of an approach for modeling the transport of residential pyrethroid applications. **M. F. Winchell**, S. Folle, S. Jackson, B. Toth, J. Hanzas, G. Mitchell

2:10 – 310. Urban stressors for pesticide endangered species assessments: Should recent nutrient TMDLs and laws be considered? **S. Z. Cohen**, N. L. Barnes

2:30 Intermission.

2:45 – 311. Post-application irrigation reduces golfer exposure to the insecticide cyfluthrin. **R. Putnam**, J. Doherty, J. Clark

3:05 – 312. Design of an observational pest control operator worker exposure study. **M. E. Krolski**, S. Moore, C. Lunchick, J. Panara

3:25 – 313. Epidemiology in public health risk assessments: A case study of 2,4-D. **C. J. Burns**

3:45 Discussion.

Human Health and Transgenic Crops

A. M. Rimando, S. Duke, *Organizers, Presiding*

Section B
Loews Hotel Philadelphia - Commonwealth B

1:30 Introductory Remarks.

1:35 – 314. Elicitation and metabolic engineering strategies to increase the levels of health-related polyphenols in root cultures. **F. Medina-Bolivar**, C. Balmaceda, R. L. Atwill, T. Yang, Z. Marsh, C. Nopo-Olazabal, L. Nopo-Olazabal, N. Joshee

1:55 – 315. Metabolic engineering of lignan biosynthesis in *Forsythia*. **H. Satake**

2:15 – 316. Production of pterostilbene in *Nicotiana* species and *Arabidopsis thaliana* via co-expression of peanut stilbene synthase and sorghum *O*-methyltransferase. **A. M. Rimando**, S. R. Baerson, Z. Pan, J. J. Polashock, F. E. Dayan, C. S. Mizuno, C. Liu, M. E. Snook

2:35 Intermission.

2:50 – 317. Quantification of allergenic lipid transfer proteins in maize kernels by liquid chromatography with ultraviolet and mass spectrometric detection. **S. A. Young**, K. Kuppanan, S. Julka, B. Schafer, D. Albers, D. Dielman

3:10 – 318. Assessment of the natural variation of soybean protein expression through proteomics. **S. Natarajan**

3:30 – 319. Comparison of aflatoxin and fumonisin levels in corn from Bt and conventional hybrids. **H. K. Abbas**, A. Bruns, M. A. Weaver, W. T. Shier

3:50 – 320. Lactoferrin imparts resistance against fungal pathogens in transgenic plants. **D. K. Lakshman**, A. Mitra

4:10 Concluding Remarks.

Next Generation Biofuels and Bioproducts: Advances and Challenges

Cosponsored by CELL
A. Hotchkiss, A. Gunasekara, C. Hapeman, *Organizers*
A. Brown, D. Sparks, *Organizers, Presiding*

Section C
Loews Hotel Philadelphia - Commonwealth C

1:25 Introductory Remarks.

1:30 – 321. Evaluating the economic benefits of the advanced biofuels targets under the RFS2. **G. Oladosu**, K. Kline, P. Leiby, R. Uria-Martinez, M. Davis, V. Dale, M. Downing, L. Eaton

1:50 – 322. Towards model-based identification of next generation biofuels: Aspects of product and process design. **J. J. Victoria Villeda**, M. Dahmen, M. Hechinger, A. Voll, W. Marquardt

2:10 – 323. Efficient production of light olefins from biomass. **A. Goyal**, L. Turner

2:30 – 324. Alternative processes for the bioconversion of waste into fuels and chemicals. **R. Hernandez**, T. French, A. Mondala, P. Pham, E. Revellame, W. Holmes

2:50 Intermission.

3:05 – 325. Developing an industrial sugar-feedstock platform in the Mid-South for renewable chemicals and biobased products. **B. J. Savary**, J. Xu, V. S. Green, P. Nelson, R. W. Powell

3:25 326. Giant panda intestinal microbes: Biofuels and conservation. **C. Williams**, I. Johnston, A. Kouba, S. Willard, D. Sparks, A. Brown

3:45 327. Fuel production from cellulose by subterranean termites. **J. M. Rodriguez**

4:05 Concluding Remarks.

AGRO

CHEMISTRY
for and from
AGRICULTURE

AGRO DIVISION

AGRO 1

Pesticide K_d values: How valuable are they?

Scott Senseman[1], *s-senseman@tamu.edu, Edinalvo Camargo*[1,2]*, Jason Krutz*[3]*. (1) Department of Soil and Crop Sciences, Texas A&M University, Texas AgriLife Research, College Station, TX 77843-2474, United States (2) Conselho Nacional de Desenvolvimento Científico e Tecnológico, Brasília, DF, Brazil (3) Agricultural Research Service, United States Department of Agriculture, Stoneville, MS 38776, United States*

K_d (distribution coefficient) values have been calculated for pesticides for over forty years. The seminal work was done by Talbert and Fletchall in the 1965 when they studied the adsorption of several s-triazine herbicides using the K_d value for comparative purposes. During the next forty years, this value has lost meaning through variations in adsorption methodology, adjustments for organic carbon, and averaging of adsorption values among others. These values must be calculated prior to pesticide registration and have theoretical ramifications related to leaching as well as plant availability. Values that have been summarized, corrected, and averaged have been used in environmental fate computer models that can and have been used to dictate policy on the practical use of such materials. The author will discuss historical development and use of adsorption coefficients and a possible alternative to the K_d study such that comparisons between compounds can be more adequately made.

AGRO 2

Development of an adsorption window for pesticides: A potential alternative to comparing soil adsorption values

Edinalvo Camargo[1,2], *edinalvo_camargo@yahoo.com.br, Scott Senseman*[1]*. (1) Department of Soil and Crop Sciences, Texas A&M University, Texas AgriLife Research, College Station, TX 77843-2474, United States (2) Conselho Nacional de Desenvolvimento Científico e Tecnológico, Brasília, DF, Brazil*

The objective of this research was to investigate the use of reference compounds (minimum and maximum K_d values) during the determination of pesticide adsorption with different soil to solution ratios. Ten soils, five herbicides (2,4-D, atrazine, clomazone, *S*-metolachlor, and saflufenacil) and three soil:solution ratios (1:3, 1:5, and 1:10) were selected to conduct the study. Ultrapure water without $CaCl_2$ was used to perform the batch equilibrium. Furthermore, aqueous solution containing $CaCl_2$ (0.01 M) was used for an additional study using the 1:5 ratio. Results indicated that $CaCl_2$ decreased pH of soils affecting adsorption results of weak acid herbicides such as 2,4-D. Soil to solution ratios affected K_d values, but responses were dependent of the soil-pesticide interaction. The use of reference compounds during K_d estimation allowed for calculation of a conceptual adsorption window (AW) generating a more comprehensive set of data with alternatives for comparison of soils and methods.

AGRO 3

Modeling pesticide sorption in the surface and subsurface soils of an agricultural catchment

Abdul Ghafoor[1], *abdul.ghafoor@slu.se, John Stenström*[2]*, Nicholas J. Jarvis*[1]*. (1) Department of Soil and Environment, Swedish University of Agricultural Sciences, Uppsala, Sweden (2) Department of Microbiology, Swedish University of Agricultural Sciences, Uppsala, Sweden*

Sorption models that improve upon the K_{oc} concept are needed, especially for spatial modeling applications. Sorption of three test compounds (glyphosate, bentazone, and isoproturon) was measured in the topsoil and sub-surface soils of an agricultural catchment. The Freundlich sorption coefficients K_f showed considerable differences between soils with coefficients of variation ranging from 22 to 84% for the three compounds. The inorganic sorbents, clay and aluminum and iron oxides, clearly dominated sorption of all three compounds in sub-surface soils and their effects were only masked by organic matter in surface soils with organic carbon contents larger than about 2%. A simple empirical 'extended' partitioning model for pesticide sorption that also accounts for the influence of inorganic sorbents and pH is proposed. Results showed that a consideration of interactions between organic and inorganic sorbents was needed to adequately describe glyphosate sorption, but not bentazone or isoproturon. The analyses further suggest that information on clay and iron and aluminum oxide contents and soil pH, in addition to organic carbon, would be generally needed for reliable spatial modeling of pesticide leaching. We emphasize the need to measure and report contents of oxides of Al and Fe in soil survey databases because small variations in their concentrations might contribute significantly to large variations in sorption, especially of ionizable pesticides.

AGRO 4

How constant are pesticide K_d values during a rainfall event?

Clint Truman, *clint.truman@ars.usda.gov, Tom Potter.Southeast Watershed Research Laboratory, USDA-Agricultural Research Service, Tifton, GA 31793, United States*

Pesticide partitioning between water and sediment (K_d) and surface processes controlling runoff and sediment production determine the magnitude of pesticide losses associated with infiltration, runoff and/or, sediment from agricultural fields during a rainfall event. Pesticide K_d values have traditionally been calculated from slurries in lab settings and assumed constant. However, under non-equilibrium field conditions, soil and rainfall characteristics and management practices (tillage, irrigation) affect erosional processes and effective K_d's during rainfall events by altering the soil surface, antecedent water content, and how soil surface water content changes at the onset of a rainfall event. We will present experimental results that show the range in K_d values for multiple pesticides (K_d's) during a rainfall event under conventional-till, seedbed conditions. Implications of variable K_d on model predictions will be discussed.

AGRO 5

Quantifying the effect of sorption and moisture content on biodegradability of organic compounds in soil

***Wenlin Chen**, wenlin.chen@syngenta.com.Environmental Safety, Syngenta Crop Protection LLC, Greensboro, NC 27409, United States*

The spatial distribution of organic compounds in the microscopic soil/pore-water system due to sorption has fundamental implications on assessing biodegradability. If only the fraction of the organic compounds in the microbe-accessible region (e.g., soil pore water) is directly subject to intracellular transformation, sorption into microbe-absent regions (e.g., intra-particle/intra-aggregate micro-pores/interstitial spaces) might become rate-limiting to biodegradation. In this paper, several data sets with direct measurements of soil pore water concentrations are used to elucidate the effect of sorption/desorption on biodegradation. A bioavailability factor defining the proportion of the degradable mass under the condition of sorption/desorption is explored for estimating the intrinsic biodegradability in soil pore water. Potential linear free energy relationships of compound biodegradability with molecular properties are also discussed.

AGRO 6

Spatial variation in sorption and dissipation is herbicide dependent

***Sharon K. Papiernik**[1], Sharon.Papiernik@ars.usda.gov, Rubem S. Oliveira[2], Alegria Cabrera[3], William C. Koskinen[4]. (1) North Central Agricultural Research Laboratory, USDA-Agricultural Research Service, Brookings, SD 57006, United States (2) Department of Agronomy, Universidade Estadual de Maringá, Maringá, PR 87020-900, Brazil (3) Department of Soil, Water, and Climate, University of Minnesota, St. Paul, MN 55108, United States (4) Soil and Water Management Unit, USDA-Agricultural Research Service, St. Paul, MN 55108, United States*

In eroded landforms, soil properties that influence herbicide fate are highly variable with landscape position. Understanding the variation in herbicide sorption and dissipation is essential to characterize weed control efficacy and availability for off-site transport. We evaluated the sorption and/or dissipation of four herbicides in surface soils from an eroded prairie landform. Soil organic carbon in the eroded upper slope was about half that in the depositional lower slope. Sorption of saflufenacil, aminocyclopyrachlor, and picloram was on average 3-5 times higher in the lower slope than in the upper slope. For these herbicides, sorption coefficients were less variable when normalized to the fraction of organic carbon. Metolachlor showed the same sorption in soils from these landscape positions, despite the large difference in soil properties. Dissipation proceeded at approximately the same rate in both soils. Results emphasize the need for compound- and soil-specific information to enable accurate predictions of pesticide fate.

AGRO 7

Effect of soil wetting and drying cycles on metolachlor fate when applied as commercial and as controlled-release formulations

*Osnat Goldreich, Yaacov Goldwasser, **Yael G Mishael**, mishael@agri.huji.ac.il.Soil and Water, Hebrew University, Rehovot, Israel*

We have developed metolachlor controlled-release formulations (CRF) based on its solubilization in micelles and adsorption to clay. This study aims to test the effect of soil wetting and drying cycles (WDCs) on metolachlor fate applied as commercial and as CRFs. Surprisingly, metolachlor release from the soil subjected to WDCs was higher than its release from the untreated soil. This was attributed to soil aggregation, higher in untreated soils, which trapped the herbicide and reduced its release. Metolachlor leaching from the commercial product through a thin soil layer was high and increased with WDCs while its leaching from the CRF was moderate, even when subject to WDCs. A bioassay in soil columns demonstrated good weed control and reduced leaching for the CRF in comparison with the commercial formulation, even after four WDCs. These results emphasize the advantage of the CRF over the commercial formulation even when the soil is subjected to WDCs.

AGRO 8

Interpreting kinetic data during adapted degradation

***Thomas Potter**, tom.potter@ars.usda.gov.Southeast Watershed Research Laboratory, USDA-Agricultural Research Service, Tifton, GA 31794, United States*

Dissipation and degradation are fundamental processes governing pesticide environmental fate. It has become standard practice to describe rates using single first-order kinetic equations (SFO). In SFO the time for a decrease of a certain fraction of the compound remains constant; thus dissipation rate data can be conveniently described by the compound's soil half-life ($t_{1/2}$). SFO equations are simple to use, inherently conservative, and are used almost exclusively in regulatory pesticide assessments. However, there are numerous published studies that demonstrate that SFO might not be the most appropriate kinetic model to describe pesticide dissipation kinetics. In this presentation, we will describe some of our experiences in using SFOs and alternate models. Model use when adapted degradation conditions develop in soils will be highlighted. In almost all cases biphasic models that incorporate dissipation rates that change with time provide better fits to the data.

AGRO 9

Soil dissipation of fomesafen in vegetable production systems

***Timothy Grey**[1], tgrey@uga.edu, Thomas Potter[2]. (1) Crop and Soil Sciences, University of Georgia, Tifton, GA 31793, United States (2) Southeast Watershed Laboratory, USDA-Agricultural Research Service, Tifton, GA 31793, United States*

Field studies were conducted to evaluate dissipation of fomesafen for bare-soil compared to soil under low-density polyethylene (LDPE). Laboratory experiments evaluated dissipation over time at 10 and 30 °C. For field studies, fomesafen dissipation was rapid for bare-soil with $t_{1/2}$ of 14 days. However, fomesafen dissipation in soil under LDPE $t_{1/2}$ was 61 days. For laboratory studies, $t_{1/2}$ for fomesafen at 30 °C was 120 days, in contrast to 10 °C at 220 days. Data from these experiments indicate that dissipation can be extended at colder soil temperatures and covered with LDPE. A bioassay was conducted infield where fomesafen was applied to bare soil or under LDPE in a spring crop. After crop removal, an autumn cabbage crop was planted. There was carryover under the LDPE resulting in significant injury, but no injury for bare soil plots. These data indicate that fomesafen applied to soil under LDPE could carryover in rotations.

AGRO 10

From the rainforest to your grocery store and medicine cabinet: A review of the recent 50 years of natural products research

Stephen J Cutler, *cutler@olemiss.edu.Department of Medicinal Chemistry, University of Mississippi, University, MS 38677, United States*

Over the past 50 years, many biologically active natural products have been discovered and have utility in agriculture and pharmaceuticals industry. It is interesting to find there is a certain pleasure that comes from migrating across scientific disciplines. In this transition it happens that chemical structures and their derivatives turn up like old friends. Perhaps another metaphor exists between the chemistry of agrochemicals and pharmaceuticals with the common thread being chemistry. Of course, modern civilization is built upon the pillars of agrochemicals and pharmaceuticals, with the first giving rise to an abundance of food and the latter keeping the mind and body healthy. This paper will interweave examples of agrochemicals that possess pharmaceutical effects and, conversely, medicinal agents that have agrochemical properties. Included in these examples are biologically active natural products discovered by Horace “Hank” Cutler during his 50 years as a natural products chemist.

AGRO 11

Natural products as sources for new pesticides

Charles L. Cantrell, *clcantr1@olemiss.edu, Stephen O. Duke, Franck Dayan.Natural Products Utilization Research Unit, USDA-Agricultural Research Service, University, MS 38677, United States*

Natural products as pesticides have been reviewed from several perspectives in the past, however no review has examined the impact of natural product and natural product-based pesticides as a function of new active ingredient registrations with the Environmental Protection Agency (EPA) on the US market. EPA registration details of new active ingredients for all conventional pesticide registrations and biopesticide registrations were compiled from the years 1997-2010. Conventional pesticide registrations and biopesticide registrations were examined both collectively and independently for all 277 new active ingredients (NAI) and subsequently categorized and sorted into four types: biological (B), natural product (NP), synthetic (S), and synthetic natural derived (SND). When examining conventional pesticides alone, S accounted for the majority of NAI registrations with 78.0% followed by SND with 14.7%, NP with 6.4%, and B with 0.9%. Biopesticides alone were dominated by NPs with 54.8% followed by B with 44.6%, SND with 0.6%, and 0% for S. When examining conventional pesticides and biopesticides combined, NP accounted for the majority of NAI registrations with 35.7% followed by S with 30.7%, B with 27.4%, and SND with 6.1%. Despite the common perception that natural products might not be the best source for NAIs as pesticides, when you look at both conventional and biopesticides collectively, and consider that NP, SND, and B all have origins from natural product research, one could argue that their combined impact on NAI registrations with the EPA from 1997 to 2010 account for 69.3% of said NAIs.

AGRO 12

Discovery and development of natural products for pest management

Ratnakar N. Asolkar, *rasolkar@marronebio.com, Ana Lucía Córdova-Kreylos, Ray Lam, Phyllis Himmel, Pamela Marrone.Marrone Bio Innovations, Davis, California 95618, United States*

Natural products from microbial sources have been successfully used for the development of new biopesticides for pest management. Interesting chemical structures and novel modes of action make these secondary metabolites very attractive due to improved efficacy, environmental and non-target safety, and resistance management. As part of a search for new leads for biopesticides, microbes isolated from various sources are screened for activities against various pests such as insects, plant pathogens, nematodes and weeds. The examples of promising molecules obtained as a result of bioassay guided isolation work from the various microbial hits will be discussed in detail.

AGRO 13

Product stewardship: Discovery to commercialization

David Sesin, *dsesin@agraquest.com, Denise C. Manker, Tamara Meragelman, Jonathan Margolis.AgraQuest, Inc., Davis, CA 95618, United States*

Product stewardship is the responsibility to reduce the environmental, health, and safety impact of a product. Biopesticides are becoming an integral part of the agricultural industry. The biological activity elicited by biopesticides results from the microbe and the metabolites produced. Therefore, good product stewardship for biopesticides requires comprehension of the biology and chemistry of the microbe. Knowledge of both attributes assists in clear understanding of mode of action and formulation of the final product. Applying conventional chemical, biological, and QA methodologies improve product efficacy and consistency and eliminate many of the failures that have tarnished the promise of biopesticides. Additionally, full understanding of the biopesticide provides safety to consumer, beneficial organisms, and the environment. A series of case studies will be presented highlighting strategies for securing good product stewardship.

AGRO 14

Natural product options for repelling ticks of medical importance

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Tick-borne diseases pose a serious threat throughout much of the habitable world, with tens of thousands of new human cases of tick-borne disease reported annually in the US. There is considerable public interest in arthropod repellents based on natural products, which is reflected in the number of contemporary studies evaluating the efficacy of plant extracts and constituent compounds. Although natural products have a long history of use as repellents, in recent years laboratory evaluations have found additional compounds and essential oils that have potential for commercialization. In behavioral bioassays with ticks, direct comparisons of natural products with the widely used synthetic repellent deet show that the efficacies of several are similar to that of deet. Repellent phytochemicals cannot automatically be assumed to be safe for application to human skin and require toxicological testing.

AGRO 15

Streptomyces lydicus: Natural chemical factories for integrated crop pest management

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Global crop production is challenged by many significant issues, including chemical resistance, environmental protection, food safety, consumer safety, invasive pests, and shifting environmental conditions. Durable, forward-leaning integrated pest management (IPM) strategies designed for the modern global food crop market are coming of age and moving beyond single mode of action (MOA) petrochemical-based pesticides. Modern IPM programs now have available effective, naturally occurring, multiple MOA tools that address current crop protection challenges with sustainable outcomes. One of these new tools is the naturally occurring, environmentally durable *Streptomyces lydicus* strain WYEC 108, which presents multiple solutions for effective crop IPM strategies including chemical resistance alternatives, chitinase-siderophore antibiotic(s) production, and deploying physical disease control mechanisms of exclusion and mycoparisitism.

AGRO 16

Manipulation of insect behavior with Specialized Pheromone & Lure Application Technology (SPLAT)

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SPLAT (ISCA Technologies, www.iscatech.com) is a biologically-inert matrix for the sustained release of insect semiochemicals, phagostimulants, plant volatiles, biological control agents, insecticides, and countless other compounds used for pest management in agricultural, urban, and forest ecosystems. SPLAT formulations can be tailored to deliver species-specific control through a variety of mechanisms including attract & kill, mating disruption, repellency, and mass trapping. The amorphous and flowable quality of the SPLAT matrix allows for flexible methods of application including disposable syringes, electric and pneumatic grease guns, tractor and gator-driven systems, and aerial applications. Another benefit is the ability to vary the placement, density, and size of chemical-emitting point sources in the field to optimize control of the insect target. Point sources can be applied to almost any application surface and will remain in place, releasing active ingredient over a period of weeks to months. Most formulations become rain-fast after three hours of drying, forming a protective skin that maintains the shape of the point source and offers protection of the active ingredients from UV rays. Numerous studies have shown that SPLAT is non-phytotoxic and safe for the environment. A US EPA science review has certified all inert ingredients in SPLAT to be "suitable for food use," with several formulations labeled as organic. We will discuss the use of SPLAT formulations in the management of several insect pests of vegetable crops.

AGRO 17

Development of effective extended-release delivery systems with the biopesticide spinosad for mosquito larvae control

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Spinosad is a fermentation product of the actinomycete bacteria *Sacharopolyspora spinosad* that exhibits excellent control of mosquito larvae. The physical and chemical properties of spinosad presented unique challenges in developing effective delivery systems for control of mosquito larvae. The desire to develop formulations that would qualify and be approved for use in organic farming presented additional challenges and limitations in the selection of inert ingredients that could be used in the end-use formulations. To meet the extended-release properties desired in the end-use formulations, a solid matrix was developed that permitted tableting production while converting to a slow-release matrix when exposed to water, thus providing mosquito larvae control for up to 180 days.

AGRO 18

Prospective approach to understanding transport and fate of bioactive environmental contaminants

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Developing the ability to predict environmental transport and fate of toxicants, including exposures and effects for people and wildlife, has been a significant undertaking from the late 1900s to the present. Examples of collaborative contributions in the areas of contaminant transport and fate, with emphasis on atmospheric processes and deposition, will be discussed for fumigants and other pesticides, hydrocarbon fuel components, fire retardants, fluoroacetic acids, and other environmental contaminants. Developments in analytical methods have been critical to providing data upon which today's predictive tools are based, as have developments in structure-property-function relationships. Research conducted with a number of students and collaborators will be summarized, along with thoughts about needs and opportunities in assuring future environmental safety and sustainability.

AGRO 19

Natural products chemistry and its applications to real-world agricultural problems

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Agricultural commodities are exposed to many biotic and abiotic stressors over the course of the growing season as well as during storage or transit. In particular, feeding damage by insect pests or contamination with fungi play large roles in the problems often faced by growers or shippers of many agricultural products. Scientists typically involved in addressing these problems can be entomologists, plant pathologists, microbiologists, and biochemists. Natural products chemists can also play a role in helping solve these problems faced by the agricultural industry. Two projects involving natural products from almonds and pistachios and their role in the monitoring of an insect pest and fungal contamination will be discussed.

AGRO 20

Immunoassay approaches for environmental and exposure monitoring

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Environmental monitoring and exposure studies can be hampered by high analytical costs, limiting the number and types of samples that can be analyzed within time and budget constraints. Biomonitoring surveys can be particularly challenging as they often necessitate the generation of data for target analytes within specified timeframes, pathways, and routes of exposure. Single-analyte immunoassays have been incorporated into monitoring studies to determine exposures to environmental pollutants in a wide variety of matrices and exposure scenarios. Multiplexed immunoassays, developed for proteomic analyses, can determine protein expression signatures in plants and animals generated in response to exposures to environmental pollutants. The application of these methods for the analysis of multiple environmental and biological matrices is needed to determine linkages between exposure sources and health effects. Examples of immunoassays for environmental and biological monitoring will be given to illustrate this approach. [Notice: This is an abstract of a proposed presentation and does not necessarily reflect the US EPA policy. The actual presentation has not been peer reviewed by EPA. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.]

AGRO 21

Developing novel approaches to characterize emissions from agricultural operations

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Large-scale animal feeding operations (AFOs) are sources of both gaseous and particulate pollutants to the atmosphere. Current efforts to characterize particulate matter (PM) emissions from AFOs do not provide information on the emission sources. Raman microscopy was employed to characterize the distribution of sources present in PM_{10} emitted from a large cattle feedlot. Spectra from potential source materials were compiled to create a spectral library. A multivariate statistical analysis approach was developed to identify the source of particles collected on PM_{10} sample filters. Source characterization results from samples collected at a cattle feedlot over a typical summer two-day period indicates that materials from the cattle pen surface contributed more than 50% of the total PM_{10} particles captured, followed by unpaved roads at approximately 20% and then feed materials. Results indicate this approach could be used in a number of different agricultural emission characterization scenarios.

AGRO 22

New plants for sustainable fuels and chemicals

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Grindelia squarrosa, commonly known as gumweed, is a biennial flowering plant common to Nevada and other areas of the arid western United States, particularly along roadsides where increased precipitation is available from road runoff. A preliminary analysis of numerous desert plants has singled out gumweed as a strong candidate for fuel production, and potentially as a substitute for rosin. Processed gumweed has provided an average of 12-23% crude oil by dry weight, primarily consisting of a diterpene hydrocarbon acid, grindelic acid, depending on the plant stand collected and the method of sample drying. While the majority of hydrocarbons present in the acetone extracts are at the heavy end of diesel fuel, a methylated B20 blended biodiesel was shown to meet ASTM standards for flash point, kinematic viscosity, and sulfur content. Direct catalytic thermal conversion of grindelic acid to a lower molecular weight neutral hydrocarbon has also been demonstrated. Production of a biocrude from *Grindelia squarrosa* is estimated to be 60-100 gallons/acre-year.

AGRO 23

Environmental contaminants in wildlife intended for human consumption

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The USDA Food Safety and Inspection Service and the US Food and Drug Administration monitor commercially produced poultry for chemical contaminants. Various groups, including hunters (and their families), patrons of community services that receive donated wildlife from wildlife management agencies, and patrons of retail outlets that specialize in game meats consume wildlife. As no public health entity routinely monitors contaminants in wildlife tissues, the public health risk to consumers of wildlife tissues is not well characterized. To address this knowledge gap, we: 1) assayed environmental contaminants (pesticides, metals, PCBs) in harvested Canada geese, and 2) assessed public health risk of wild-harvested poultry by comparing Canada geese contaminant concentrations to contaminant concentrations in commercially produced poultry and regulatory guidance levels. Potential contaminants of concern were further evaluated via a probabilistic risk assessment. Risk estimates and potential risk management strategies will be presented.

AGRO 24

Designer low-calorie and weight-loss or weight-maintenance ingredients

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Obesity continues to be a major public health concern in most parts of the world. Efforts to convince consumers to alter food choices and exercise have not been successful. The concept of escalating calories and reduced exercise combine to fuel the obesity epidemic. Possible interventions are to replace existing ingredients with lower calorie ingredients that do not substantially change the organoleptic qualities of the food. Reduced-calorie ingredients can range from dilution of calorically dense foods, to low-calorie lipids (including structured lipids that modify fat deposition), to modified proteins that prevent growth, to polyphenolic ingredients that alter fat deposition in adipocytes. The chemistry and physiological effects of structured lipids, chemically modified proteins, type 4 resistant starch, and polyphenolics will be discussed. The impact on the quality of conventional food products will be discussed.

AGRO 25

VOC emission from silage: Compounds, processes, and implications

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Recent studies have identified silage on dairy farms as a source of volatile organic compounds (VOCs) in the troposphere. Although reliable means of estimating emissions have not been developed, measurements strongly suggest that silage is a significant source of VOCs, a regulated ozone precursor, in central California. We compiled data on the concentrations of VOCs in silage and measured emission rates, and identified important processes for VOC production and emission. Our results suggest that alcohols make the largest contribution to ozone formation, when concentration, volatility, and reactivity are taken into consideration. Concentrations of alcohols and other VOCs are highly variable in silage, which suggests that significant reductions in VOC concentrations are possible. High variability also means that development of accurate emission estimates may require farm-specific measurements or predictions. We will discuss bounds on silage VOC emissions based on concentrations, and potential approaches for reducing VOC production and emission.

AGRO 26

Comparative metabolism of [^{14}C]α-, β-, and γ-hexabromocyclododecane (HBCD) in rats

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Hexabromocyclododecane (HBCD) is a persistent flame retardant manufactured as a mixture of *α*-, *β*-, and *γ*-stereoisomers. *γ*-HBCD dominates the commercial product, while *α*-HBCD dominates biotic residues. Differential metabolism of *α*- and *γ*-HBCD is thought to influence *α*-HBCD bioaccumulation, but the contribution of *β*-HBCD is unknown. The goal of this research was to measure the fate of radiolabeled HBCD stereoisomers in rats. Each isomer was eliminated in feces and urine, with elimination of $\beta > \gamma > \alpha$. Oxidation, stereoisomerization, and conjugation were evident. Adipose tissue, GI tract, skin, and liver contained the greatest concentration of residues, and bound residues were significant in liver and feces. *α*-HBCD exceeded the concentrations of the *β*- and *γ*-HBCD in brain by 5-20 times. Persistence of HBCD stereoisomers was generally low and was isomer specific. Differences in isomer fate were due to metabolism and isomerization, and are consistent with the observed stereoisomer profiles in biota.

AGRO 27

Multiclass, multiresidue method for analysis of pesticides, polychlorinated biphenyls, flame retardants and polyaromatic hydrocarbons in catfish using fast, low-pressure gas chromatography-tandem mass spectrometry

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We developed a multi-class, multi-residue method for analysis of 14 novel flame retardants, 18 representative pesticides, 14 PCB congeners, 14 PAHs, and 7 PBDE congeners in catfish muscle using fast low-pressure gas chromatography triple-quadrupole tandem mass spectrometry LP-GC/MS-MS. The method is based on a QuEChERs extraction with acetonitrile, dispersive solid phase extraction (d-SPE) clean-up with C18 and PSA sorbents, and LP-GC/MS-MS analysis. Comparison of d-SPE clean-up using C18/PSA and other SPE sorbents: Z-sep and Z-sep+ from Supelco will be presented. Sample preparation for a batch of 10 homogenized samples takes less than 2 hours. Fast LP-GC/MS-MS allows for a chromatographic run of 9 min. In preliminary tests, the recoveries of most target analytes were acceptable, ranging between 70 and 120% with relative standard deviations less than 20%. Monitoring results of fish samples using the developed technique will be discussed.

AGRO 28

Absorption and distribution of perfluorooctane sulfonate (PFOS) in beef cattle

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Perfluorooctane sulfonate (PFOS) is an industrial chemical that is found in biosolids, and the application of these biosolids to pastures has raised concerns about human exposure through the accumulation of PFOS in edible tissues of these animals. The United States Department of Agriculture (USDA) has undertaken a study to determine the absorption and distribution of PFOS in beef. Two Angus steers were given single oral bolus doses containing PFOS at 0.1 mg/kg and four Angus heifers were given single bolus doses containing PFOS at 10 mg/kg. Plasma was collected from each animal prior to and at various intervals after dosing through 11 months. PFOS concentrations were determined by liquid chromatography-quadrupole time of flight mass spectrometry (LC-QToF). The average maximum concentrations of PFOS in plasma for the steers and heifers were 0.77 ± 0.05 µg/mL and 65 ± 12 µg/mL, respectively. Half-life determinations for the two PFOS levels administered will be done using plasma concentrations.

AGRO 29

Strategies for countering herbicide resistance

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Herbicide resistance has travelled a well-trod path laid by antibiotics, chemotherapy agents, insecticides, fungicides, etc. Herbicide metabolism and target-site mechanisms

accounted for most of the resistance, but not for glyphosate. Recently horseweed (*C. canadensis*) and ryegrass (*L. multiflorum*) were the first species to show active sequestration of glyphosate into the vacuole. Additionally, Palmer amaranth (*A. palmeri*) has an unusual MOA with extensive gene duplication of 5-enolypyruvyl shikimate 3-phosphate (EPSPS). Herbicide resistance has been managed by changing or combining active compounds with different modes of action (MOA) to control weeds and reduce selection pressure. However, the paucity of new herbicide MOAs and multiple MOA-resistant weedy species is threatening economical weed control in some row crops. A review of current strategies and discussion of new strategies to control herbicide-resistant weeds will be presented as a means to create a weed management system with sustainable weed control.

AGRO 30

Community-based approach to indirect effects assessments for terrestrial plants

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In pesticide registrations, terrestrial plant risk assessments are inherently conservative. The pesticide's lowest EC_{25} value among ≥ 10 test species is compared to the highest exposure estimate for a given crop use. For protection of threatened and endangered plant species, the lowest NOAEC or EC_{05} value is used. This coupling of worst-case exposure and hazard estimates is used for the assessment of both direct effects to plants and indirect effects to species relying on plants for food or habitat. However, indirect effects to listed species are typically associated with community-based estimates rather than individual species effects, as in the case of aquatic species relying on ecosystem services provided by riparian vegetation. In this presentation, a higher tier, statistically based risk assessment method, built on community-based estimates of relevant toxic effects, is described. This allows for refinement of the screening level risk assessment, taking into account the complexity associated with community level effects.

AGRO 31

Effect of bioavailability testing of soil residues using 0.01 M $CaCl_2$(aq) equilibration on the subsequent extractability of the residues

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Bound residues most generally are known as residues unavailable and therefore depleted from the system. It follows that there must be a link with the extraction techniques and mechanisms of binding. Residues desorbed or extracted from soil with 0.01 M $CaCl_2$(aq) provide an assessment of bioavailability and might be used in an aerobic soil metabolism study to assess aged bioavailability of the residues. We evaluated the extraction or release of residues in soils using 0.01 M $CaCl_2$(aq) followed by extraction using a wide variety of solvent systems, and compared these to extraction using the solvent systems without the initial 0.01 M $CaCl_2$(aq) treatment. A range of soil types and organic contents were tested with representative test compounds. The initial 0.01 M $CaCl_2$(aq) treatment can have substantial effects, decreasing the apparent extractability of the residues from the soil.

AGRO 32

Use of passive sampling devices to estimate the bioavailability of pyrethroids

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Following the withdrawal of organophosphates, there has been a significant shift towards the use of pyrethroid insecticides. With this increased usage, there has been increased concern about the risks pyrethroids might pose to aquatic ecosystems, especially with measured concentrations in surface waters often exceeding toxicity thresholds for aquatic invertebrates. However, we and others have found that these apparently toxic concentrations of pyrethroids often do not exhibit toxicity in the field. We will report on laboratory and field experiments demonstrating that one reason for this overestimation of field toxicity is the decreased bioavailability of pyrethroids. Our results also show that sorptive passive sampling devices (PSDs) provide a good estimate of the bioavailable fraction of cypermethrin and permethrin under most conditions. We will present a quantitative model of pyrethroid-organic carbon partitioning and its effect on bioavailability, and how PSDs can be used in the field to estimate chronic exposure to bioavailable pyrethroids.

AGRO 33

Fate and transport of glyphosate and AMPA into surface waters of agricultural watersheds

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The agricultural use of glyphosate [*N*-(phosphonomethyl)glycine] has increased from less than 10,000 Mg in 1992 to more than 80,000 Mg in 2007. The greatest aerial use is in the Midwest, where glyphosate is applied on transgenic corn and soybeans. Yet the characterization of the transport of glyphosate on a watershed scale is lacking. Glyphosate and its degradate AMPA were frequently detected in the surface waters of four agricultural watersheds. The load as a percent of use ranged from 0.009 to 0.86 percent and could be related to three factors: source strength, hydrology, and flowpath. Glyphosate use in a watershed results in some occurrence in surface water at the part per billion level, however, those watersheds most at risk for the offsite transport of glyphosate are those with high application rates, rainfall that results in overland runoff, and a flowpath that does not include transport through the soil.

AGRO 34

Transport and loading of herbicides and their degradates during mega-floods in the upper Mississippi River basin

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Herbicides are primarily transported to streams during storm events that occur around their time of application. When fields are inundated due to mega-flooding, sediments are wetted for longer periods of time and transported from larger tracts of land than are impacted during typical runoff events. During the 1993, 2008, and 2011 floods in the

Midwestern US, water samples were collected from select stream sites in the Midwest and along the Mississippi River and analyzed for 15 and 61 herbicides and degradates in 1993 and 2008-2011, respectively. During the 2008 flood 30 herbicides and degradates were detected in the Mississippi River at Thebes, IL. During the 1993 and 2008 floods, about 4.8 (3.1 ug/L) and 0.22 kg/min (0.18 ug/L) of atrazine and two degradates, respectively, were transported in the Mississippi River at Thebes, IL near peak flow. Further comparison of the herbicide loads for the three floods will be presented.

AGRO 35

Chiral separation of metolachlor ethane sulfonic acid as a groundwater dating tool

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We have studied the hydrologic fate of metolachlor and its two predominant metabolites, metolachlor ethane sulfonic acid (MESA) and metolachlor oxanilic acid, in groundwater and base flows of streams for several years. These two metabolites are excellent markers for groundwater processes related to agriculture and they appear to have extended retention in aquifers. Chiral separations were carried out on selected archived samples from these sites extending from 2000 to 2005. Enantiomeric excess values for the *S* and *R* racemic forms show a clear signal for increasing levels of the *S*-enriched form of MESA over this time interval. This shift in chiral abundance agrees with the change in usage patterns for metolachlor were the *S*-enriched form was introduced in 1997, replacing the less effective racemic product used prior to that date. Hydrologic dating with this very specific agricultural marker appears to be a promising application for this information.

AGRO 36

Holistic assessment of the occurrence of metolachlor and two of its degradates across various environmental compartments in seven environmental settings

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Metolachlor is frequently detected in surface water and groundwater throughout the United States. The US Geological Survey conducted a study to assess the controlling factors in the transport and fate of metolachlor across seven watersheds during 1997-2007. The occurrence of metolachlor, metolachlor ethane-sulfonic acid, and metolachlor oxanilic acid was examined, and its degradates primarily are affected by a number of factors including use, management, environmental setting, and physical and chemical properties of the compounds. The fate of metolachlor can be generalized: 90% of metolachlor is taken up by plants, degraded in the soil, or adsorbed to soil. About 10% of applied metolachlor is volatilized into the atmosphere, and about 0.3% returns by rainfall, 0.4% metolachlor reaches surface water, while an equal amount is infiltrated into the unsaturated zone and might move downward. Generally, groundwater stores less than 0.02% and does not serve as a metolachlor source to receiving waters.

AGRO 37

Forty years later: A reconnaissance of DDT in sediments of two southern California lakes

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The use of DDT was banned in 1972, and despite 40 years without application in the US, DDT residues are still easily detected in sediments of impacted water bodies. The Salton Sea, a large man-made lake, and McGrath Lake were surveyed for the distribution of DDT and its derivatives. Sediment samples were collected along the southern rim of the Salton Sea and throughout the extent of McGrath Lake. Soil cores were sectioned at various depths to examine the distribution and concentrations of DDT derivatives. Total DDT concentrations reached 108 and 2914 ng g^{-1} in Salton Sea and McGrath Lake sediments, respectively. DDE was the most common form of DDT detected, above the effect threshold value in 85 and 100% of Salton Sea and McGrath Lake samples, respectively. The distribution of DDT residues also displayed unique patterns both vertically and horizontally in these lakes.

AGRO 38

Repellent activity of orange peel essential oils against *Tetranychus urticae* in laboratory and greenhouse bioassays

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Repellent effects of the essential oils from fruit peels of *Citrus sinensis* var. pera ('pera') and *C. aurantium* ('lima'), and their major constituents, were evaluated against two-spotted spider mite, *Tetranychus urticae,* in laboratory and greenhouse bioassays. Both of the natural oils and an artificial mixture of mono- and sesquiterpenes intended to mimic one of the oils showed similar repellent effects to eugenol (positive control) for up to 3 h in laboratory bioassays. Both major and minor constituents of the two oils were responsible for the repellent effects after 3 h. Although both the oils showed similar repellent effects, the repellent effect of lima oil was significantly greater than that of pera oil in residual bioassays after 24 h. Comparing the repellent activity of the two oils in greenhouse experiments, lima oil prevented the movement of mites between plants across oil-treated strings for one week. Lima oil has potential for development as a commercial repellent against spider mites and could prevent their spread in commercial greenhouses.

AGRO 39

Determination of repellent efficacy of natural compounds

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Since 1942, USDA has performed repellent testing, initially for the US military. In recent years, there has been a collaborative effort to evaluate a number of natural extracts and compounds for their repellent efficacy. Plant-produced compounds are usually more volatile than synthetic repellents and therefore will not persist as long on the skin. Formulation might extend the lifetime of natural repellents, therefore we currently assess the minimum effective dosage (MED) of compounds rather than the complete protection time (CPT). The MED is an estimation of the threshold surface concentration at which a repellent fails or drops below the effective dose for 100% bite prevention (ED_{100}). Extracts of plants have been evaluated and some found to be repellent. Individual compounds from these extracts as well as compounds from citrus have been evaluated for their MED and will be presented in this talk.

AGRO 40

Spinosad toxicity and resistance in stored-product insects

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Spinosad, an organic pesticide containing fermentation products from the soil actinomycete *Saccharopolyspora spinosa* has been registered for use as a grain protectant in 2005 by the US Environmental Protection Agency at a maximum labeled rate of 1 mg (a.i.) kg^{-1} of grain. In this paper, results from a series of investigations conducted to determine the various factors affecting the toxicity of spinosad to stored-product insects are presented. Also, results from a study conducted to determine the potential risk of resistance development to spinosad with associated fitness costs and stability of resistance in selected stored-product insect species are presented.

AGRO 41

Volatile natural products for monitoring a California tree nut insect pest

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The navel orangeworm (NOW) is a major insect pest to California tree nuts and inflicts serious economic damage. Feeding by NOW larvae causes physical damage that lowers kernel quality, but more importantly the larvae are purported to introduce aflatoxigenic fungi. Aflatoxins are toxic metabolites produced by aspergilli and are a grave food safety problem. A blend of volatiles derived from in situ emissions of almonds undergoing hull split was compared to the current female monitoring standard, almond meal, in NOW field trapping studies. The volatile blend attracted both male and female NOW throughout several two-week trapping experiments in commercial almond orchards. The blend demonstrated greater captures for adult NOW than almond meal. Results from the field trapping studies highlight important progress toward a host plant volatile blend for NOW, which presently lacks an adequate monitoring lure, particularly during mating disruption treatments.

AGRO 42

Award Address (ACS Award for Team Innovation sponsored by ACS Corporation Associates). Spinetoram: Health and environmental assessments supporting an accelerated registration pathway

Raymond Boucher, James E. Dripps, Donald E. Kelley, ***Nick D. Simmons****, nsimmons2@dow.com.Dow AgroScienecs LLC, Indianapolis, IN 46268, United States*

Spinetoram represents the next generation of naturally derived spinosyn insecticides. Spinetoram is a chemically modified analog of spinosad that offers a broader spectrum of insect control than spinosad at generally lower use rates, while retaining the same favorable characteristics as spinosad. Low mammalian toxicity and favorable environmental profile are key attributes for modern insecticides and these characteristics secured a Reduced Risk determination from US-EPA, leading to accelerated reviews and registrations across the NAFTA region.

AGRO 43

Award Address (ACS Award for Team Innovation sponsored by ACS Corporation Associates).Spinetoram: Accelerating the technical and commercial development of a new, semi-synthetic natural product insecticide

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Spinosad is a novel, fermentation-derived insecticide produced by the actinomycete *Saccharopolyspora spinosa*. It was registered under EPA's Reduced Risk Pesticide Initiative and received a Presidential Green Chemistry Award. Spinosad is highly compatible with IPM and controls many major insect pests across a wide range of crops. Given spinosad's many positive attributes, Dow AgroSciences sought a significantly better spinosyn insecticide. Spinetoram is a semi-synthetic spinosyn with chemical modifications making it more potent, faster-acting, and longer-acting than spinosad. Spinetoram controls a wider range of insect pests than spinosad yet maintains very favorable toxicological and environmental fate profiles. Spinetoram was also registered under EPA's Reduced Risk Pesticide Initiative and also received a Presidential Green Chemistry Award. Developing natural products into commercial insecticides is more complex than synthetic chemicals, requiring ever closer coordination of many technical and commercial disciplines. However, we were able to accelerate spinetoram's development by applying lessons learned from developing spinosad.

AGRO 44

"What if" approaches to agrochemical discovery

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The need for new agrochemicals remains constant due to the ever-changing composition of crop pests, increasing environmental requirements, and the development of resistance to existing crop protection agents, coupled with the need to provide adequate food supply for an expanding world population. There is a diverse and evolving set of approaches to the discovery of new agrochemicals including natural products, combinatorial chemistry and high throughput screening, exploring novel chemistry and bioactive scaffolds, QSAR and pharmacophore modeling, and structure-based design. Examples of different approaches, current and historical, relating to the discovery of new agrochemicals will be discussed.

AGRO 45

Crop protection market trends and opportunities for new active ingredients

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This paper will analyse the current position and future prospects for the global crop protection market and investigate trends in R&D for both agrochemical products and genetic solutions for crop protection. Crop protection market development by region, crop, and chemistry sector will be described, tracking the influence of herbicide-tolerant and insect-resistant crops on agrochemical usage. The cost of R&D will be reviewed for both new agrochemicals and traits, whilst the shift in company R&D expenditure will also be analysed. Alterations in the rate of new product introduction and the number of products in development will be presented, along with the change in focus of many of the leading companies in the industry. The paper will conclude with a forecast for the crop protection market and an outlook for the future.

AGRO 46

High throughput screening in the agrochemical discovery process

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Target-based high throughput screening was established in the late 1990s in the pharmaceutical industry. To identify new targets, functional genomic programs were initiated. BayerCropScience followed the trend with genomic projects involving biotech partners and chemistry driven cooperations. This led to 100 new screening assays. Ultimately, this approach didn´t deliver the desired output. In BCS, early research was reorganised. A complementary in vivo and in vitro screening platform was established. The new direction has led to improved follow-up with indication biochemistry to ensure better starting points for chemistry, cleansing of the screening library to increase the sample quality and the chemical diversity, and screening of new, validated modes of action to help innovative areas such as plant stress or malaria. The above measures have significantly increased the proportion of true hits. This approach is now delivering well characterized classes which help to decrease the attrition rate in research.

AGRO 47

Potassium channels as insecticidal targets

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Historically, ion channels have been the most successful insecticidal targets, and therefore have been the focus of our target-based approach for novel insecticidal entities. From the roughly 15000 insect genes, 150 are ion channels, and from this we identified a subset of potential insecticidal targets. Several potassium channels were identified as potentially lethal targets and were selected for cloning and expression in mammalian cell lines. High throughput screens on an internal library yielded a number of hits in the micromolar activity range. This approach was exemplified by our work on the calcium-activated potassium channels Sk and Slack. A chemical synthesis program allowed us to optimize the identified hit series, resulting in compounds with activity in the low nanomolar range. We will discuss our screening process, the chemical optimization of this hit class, and the value of potassium channels as insecticidal targets.

AGRO 48

Production of export crops depends on the worldwide annual use of pesticides

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In the United States and Europe, widespread pesticide use began over 100 years ago as a result of consumer demands for insect-free fruit and vegetables. Today, consumers all around the world have similar expectations: produce free of pest damage. As a result, most of the world's fruit and vegetables are treated with insecticides and fungicides. Pesticides are widely used in growing export crops in the Tropics. Production of coffee, bananas, cocoa, mangoes, and tea would decline significantly without regular use of insecticides and fungicides to prevent losses to insects and diseases. Hazelnuts from Turkey and kiwi from New Zealand are just two examples of crops for which export markets are dependent on the regular use of pesticides for production.

AGRO 49

Foreign Agricultural Service: Linking US agriculture to the world

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The US agricultural industry faces tough challenges in exporting products abroad. Over the last few decades we have seen a strong increase in the technical hurdles that our agricultural community must overcome to maintain markets and to expand opportunities for US commodities. The USDA-Foreign Agricultural Service is responsible for linking US agriculture to the world to enhance export opportunities. Our mission is to expand and to preserve access to foreign markets for US agricultural products by removing trade barriers and enforcing US rights under existing trade agreements. We work in collaboration with US regulatory agencies, foreign governments, and international organizations to establish international standards and science-based rules to improve accountability and predictability for agricultural trade. FAS utilizes tools to address Sanitary and Phytosanitary and Technical Barriers to

Trade. FAS Embassy Attaches, trade databases, and market development programs are essential instruments for ensuring a level playing field for US agricultural trade.

AGRO 50

Incentives to encourage specialty crop registration: A grower's perspective

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Growers of specialty crops are directly impacted by MRLs. In today's world, a farmer cannot simply grow a crop, but they must also be engaged in the legislative and regulatory process to have access to worldwide markets. The Minor Crop Farmer Alliance is dedicated to providing coordinated legislative, regulatory, technical, and educational support to address MRLs issues impacting farmers ability to trade in the market place. There are many incentives for countries to harmonize MRLs across the world. Governments, registrants, and growers working together can provide farmers with support to address MRL issues. We have every reason to expect an optimistic outcome from all these efforts.

AGRO 51

US EPA advances in international harmonization and cooperation

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The US EPA, Office of Pesticide Programs is responsible for registering the use of pesticide products on agricultural crops and establishing a tolerance or maximum residue limit. The importance of setting MRLs that are aligned with those of other national authorities, Codex, and coordinating pesticide regulatory decisions is increasing as global trade of food commodities increases. Several initiatives are underway to advance the coordination and alignment of pesticide regulatory decisions. The progress made on the registration of pesticide products for minor use/specialty crops was discussed at the recently held 2nd Global Minor Use Summit along with recommendations for a five-year strategy. The Regulatory Cooperation Council between Canada and the United States focuses on near and long term strategies to remove regulatory barriers with regard to pesticide registration and MRL setting. The global joint review program for new pesticide active ingredients has expanded to include more countries and manufacturing companies.

AGRO 52

Grower issues with the Codex process

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The countries that rely on Codex trade huge volumes of food under the regulatory references provided by Codex. Many are becoming wealthier and import significant quantities of food to feed growing populations. As an example, of the top 10 export destinations for Canadian grain, six rely on Codex as the primary means of MRL setting. The lack of Codex MRL levels for many commonly-used products generates a potential technical barrier for trade. Many countries defer to Codex levels as their national MRL. In the absence of an MRL, huge trade flows are left in a limbo where there is no guidance on pesticide residues, and thus the whole area is left to interpretation on a subjective or transitory basis. All of these issues add up to a grower community around the world that is increasingly anxious to see the Codex process undergo reform.

AGRO 53

Canadian initiatives for addressing MRL differences

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While Health Canada's (HC) regulatory process for setting MRLs is consistent with that of the US Environmental Protection Agency (US EPA), the Organisation for Economic Co-operation and Development (OECD), and Codex, MRL differences exist between the various jurisdictions for several reasons. HC is currently participating in several initiatives to address these discrepancies, such as, Crop Groups, OECD MRL Calculator, NAFTA and Global Joint Reviews, and Regulatory Cooperation Council projects to find efficiencies in the overall MRL setting process. The status of these initiatives will be presented. On a moving-forward basis, NAFTA and OECD countries will continue to look for areas of cooperation for new chemicals and for new uses of currently-registered products. The various international regulatory bodies will also continue to encourage industry to submit pesticide registration applications simultaneously in the various countries to reduce trade barriers and provide pesticide users equal access to safer pesticide products.

AGRO 54

Global joint data generation project

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Pesticide residues on agricultural products are regulated in international trade. Most developing countries utilize Codex maximum residue limits (MRLs - established under the United Nation's Food and Agriculture Organization - FAO) as their national trade standards, and many of the pesticides registered for use in the United States for specialty crops do not have Codex MRLs established. This lack of Codex MRLs has become a significant trade problem for US specialty crops. In order to bring more countries into the international standard-setting process, and to help ensure that US agricultural products are not turned back at foreign ports, the USDA Foreign Agricultural Service is leading a global data generation project to establish a process in which global priorities are considered, data are collaboratively generated across multiple countries, and data packages are submitted jointly for review into the Codex system.

AGRO 55

Modeling pesticide volatilization for complex soil and environmental conditions

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Pesticide use has led to increased crop yields and more abundant food supplies. However, pesticide emissions to the atmosphere can adversely affect ecosystem and human health. Pesticide fate and transport are affected by many complex soil and environmental processes. An improved understanding is needed so that optimal methods to control pesticide emissions can be developed. Recent field and laboratory studies have provided a wealth of information that can be used to elucidate factors affecting pesticide emissions. Advanced numerical models have been developed to simulate pesticide fate, transport and volatilization, and can also be used to evaluate our current understanding of processes. This presentation will describe a research effort to improve prediction of pesticide fate and transport with the goal of increasing the accuracy of predicted short-term volatilization rates. As researchers improve their understanding of the relationships between anthropogenic activities and environmental systems, methods can be developed that enable increased agricultural production while reducing adverse consequences on the environment and public health.

AGRO 56

Development of intelligent spraying systems to reduce airborne spray drift

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Precision pesticide application technologies are needed to achieve efficient and effective spray deposition on target areas and minimize airborne spray drift. Two variable-rate sprayers were developed as an introduction of new generation sprayers for tree crop applications. The first sprayer was a hydraulic vertical boom spraying system using ultrasonic sensors to detect tree size and volume, and the second sprayer was an air-assisted spraying system using a laser scanning sensor to measure the entire tree structure quickly. The automatic controllers consisted of a computer program, a signal generation and amplification unit, and pulse width modulated solenoid valves. The controllers provided variable flows to nozzles based on tree characteristics and plant occurrence. Laboratory and field tests demonstrated that both sprayers had the capability to control spray outputs that continuously matched canopy characteristics in real time and that significantly reduced chemical off-target losses to the air and ground.

AGRO 57

Improved indirect procedure for estimating pesticide volatility flux from neighboring area sources

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A back calculation method (BCM) exists for estimating volatility loss from a single field. However, spatial and temporal variability often mask differences when different pesticide formulations are evaluated under field conditions. To minimize such uncertainty, different fields should be in close proximity and treated at the same time. Multiple sources dictate that a new methodology be applied for proper interpretation of field observations. BCM is expanded using a downhill simplex optimization procedure (BBCM). The transient volatility rates for each field are consecutively adjusted using dispersion model iterations such that the sum of the squared residuals between predicted and measured air concentrations is minimized**.** The BBCM is used with observations from two herbicide field trials, each having multiple treated fields, to deduce differences in volatility between different formulations. The BBCM is an advanced alternative to the original BCM and provides better correlation between measured and observed concentrations in air, inferring a closer approximation of the actual flux.

AGRO 58

Thirteen-year summary of field-scale herbicide volatilization

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Once lost to the atmosphere, herbicide transport can result in unintended re-deposition to inhabited areas, streams, rivers, and lakes. To understand better the factors governing herbicide volatilization and to determine its impact relative to other loss pathways, field-scale turbulent volatilization fluxes of two herbicides have been conducted annually since 1998. This represents perhaps the most detailed and longest herbicide volatilization database in existence. Herbicide runoff and turbulent vapor fluxes were simultaneously monitored on the same site located at the OPE3 Field site in Beltsville, Maryland. Site location, herbicide formulations, and agricultural management have remained unchanged during the 13 years. Metolachlor and atrazine were co-applied as a surface broadcast spray. Herbicide runoff was monitored a month before application through harvest using H-flumes. For the first 10 years, flux gradient technique was used to compute volatilization fluxes for only the first 5 days after application using herbicide concentration profiles and turbulent fluxes of heat and water vapor as determined from eddy covariance measurements. For the last three years, herbicide volatilization has been monitored for the first 10 days after application. Various results and future research will be discussed. For example, when averaged over all years and both herbicides, off-site transport was at least 25 times larger for volatilization than surface runoff. Additionally, herbicide volatilization losses were strongly influenced by soil moisture. Temperature increased herbicide volatilization when soils were moist, but had little impact on herbicide volatilization when soils were dry. This research confirms that vapor losses for some commonly-used herbicides far exceeds runoff losses and that herbicide vapor losses will need to be quantified and evaluated if management practice and formulations are to be developed which reduce herbicide loads on surrounding environments.

AGRO 59

Atmospheric transport of endosulfan to Everglades and Biscayne National Parks

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Urban encroachment and agricultural activities have been implicated in contributing to the environmental health decline and loss of organism diversity of South Florida ecosystems. Intensive agricultural pesticide use on vegetable and horticultural crops in the region may have a negative effect on sensitive organisms. One possible transport mechanism is pesticide release to the atmosphere after application. We examined the atmospheric fate of the widely-used insecticide endosulfan. Air samples were collected over a five-year period at a site within the agricultural community and at sites located in nearby Biscayne and Everglades National Parks. Endosulfan emissions from agricultural areas around Homestead appeared to influence air concentration observations at the NP sites. The physio-chemical properties of the two endosulfan isomers were used to examine contributions from pesticide drift and volatilization to the receptor sites.

AGRO 60

Assessing natural isothiocyanate air emissions after field incorporation of a mustard cover crop

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A regional air assessment was performed to characterize volatile natural isothiocyanate (NITC) compounds in air during soil incorporation of mustard cover crops in Washington State. Field air sampling and analytical methods were developed specific to three NITCs known to be present in air at appreciable concentrations during/after field incorporation. The maximum observed concentrations in air for the allyl, benzyl, and phenethyl isothiocyanates were 188, 6.1, and 0.7 µg m-3, respectively, during mustard incorporation. Based on limited inhalation toxicity information, airborne NITC concentrations did not appear to pose an acute human inhalation exposure concern to field operators and bystanders. The findings of this single field inhalation exposure assessment should be viewed as preliminary since NITC air concentrations may vary appreciably in different mustard growing regions and under varying seasonal growing conditions.

AGRO 61

Pesticides exposure assessment of Kettleman City residential area in September 2006 - December 2009 using ISCST3 model

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Kettleman City reported a higher than expected number of infants born with birth defects between 2007 and March 2010. Nineteen pesticides possibly causing birth defects were investigated to evaluate the potential resident exposure during September 2006 – December 2009. The ISCST3 was used to model off-site air concentrations associated with pesticide applications within 8 km of the community. The health screening levels were designed to indicate potential health effects and used for health evaluations. The pesticide use database of CDPR provided application information. Weather input data were summarized from the measurements of a local weather station of CIMIS. The ISCST3 modeling results indicate that during the period of more than three years, only two application days of one pesticide (MITC) could have produced air concentrations at the boundary of Kettleman City above the screen level for developmental effects. Therefore, the risk of birth defects from pesticide exposure was low.

AGRO 62

Multiple insecticidal mechanisms of action of monoterpenes

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Terpenoid insecticides based on plant essential oils, including peppermint, thyme, clove, and rosemary, can kill insects rapidly, which suggests a neurotoxic mechanism of action in insects and ticks. We have studied individual monoterpenoids, including camphor, menthol, carvacrol, and eugenol, to determine their effects at three types of receptors in the insect nervous system and one enzyme in the insect nervous system. Certain monoterpenoids have activity at GABA receptors from house fly and American cockroach, as positive or negative modulators, while others have no effect. Some monoterpenoids have activity at an octopamine receptor cloned from American cockroach brain, as positive allosteric modulators or inverse agonists. One monoterpenoid (carvacrol) inhibits binding of ^{14}C-nicotine at the nicotinic acetylcholine receptor from house fly head. Investigation of many monoterpenes in GABA and octopamine in vitro systems is allowing development of quantitative structure-activity relationships and a better understanding of the physicochemical properties required for potency.

AGRO 63

Volatile organic compound profiling using differential mobility spectrometry (DMS)

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Differential mobility spectrometry (DMS) is a novel analytical technique able to operate at atmospheric pressure and temperature. The DMS system is small, compact, portable, and is able to operate on site with minimal lab support. DMS might offer an attractive alternative for high throughput VOCs profiling. One of the major advantages of DMS is its ability to operate in field and its rapid analysis time (near real time for high temporal resolution VOCs analysis). I will present some of the research that is currently on going within our group, specifically the early detection of asymptomatic pathogenic infection in economically important citrus crops. The project involves the use of multiple orthogonal analytical profiling techniques such as GC/MS and GC/DMS based methods for in field and lab based profiling.

AGRO 64

Attracting carnivorous arthropods with plant volatiles: The future of biocontrol or playing with fire?

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Herbivore-induced plant volatiles (HIPVs) are potent attractants for entomophagous arthropods, and researchers have long speculated that HIPVs can be used to lure natural enemies into crops, reestablishing predator-prey relationships that become decoupled in disturbed agricultural habitats. This speculation has since become reality as the number of field trials investigating HIPV-mediated attraction and the consequences for pest suppression has risen dramatically over the past 10 years. Here, I provide an overview of recent field efforts to augment natural enemy populations using HIPVs and present my own field work testing: (i) the consequences of phytochemical diversity for natural enemy recruitment, focusing on the ubiquitous HIPVs methyl salicylate, 2-phenylethanol, and cis-3-hexen-1-ol; and (ii) the spatial effects of attraction in field crops (corn and soybean) and the impact of using volatiles to 'pull' arthropods into a focal area from adjacent areas.

AGRO 65

Role of terpenes and other stimuli in host-plant assessment by Asian citrus psyllid, vector of citrus greening disease

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Asian citrus psyllid transmits citrus greening, a devastating disease of citrus trees. To evaluate the importance of terpenes and other stimuli in host-plant assessment and location, behavioral responses to combinations of visual, olfactory, and gustatory stimuli were measured in test arenas with no-choice tests. Psyllids were placed on a piece of plastic laboratory film that mimicked a leaf surface. Color and scent stimuli were presented via two 'midribs' made from lines of an emulsified wax formulation. Probing levels were measured as a function of color saturation, scent composition, and scent concentration. Test scents were based on qualitatively major volatiles emitted by attractive host-plants. Results indicate that there are interactive effects between different sensory modalities in directing host-plant assessment behavior in Asian citrus psyllid. This information will be used to design more effective traps and attractants to improve detection and monitoring of this important pest insect.

AGRO 66

Highly irregular terpenoids as mealybug pheromones: Chemistry and applications

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Mealybugs are widely distributed pests of numerous agricultural crops and ornamental plants. In addition to causing direct damages, they transmit important plant diseases. The identification and several alternate syntheses of the irregular terpenoid pheromones of two important mealybug species (obscure and passionvine mealybugs) will be described, along with the development of practical applications of the pheromones for detection and monitoring of these major pests. Identification of the sex pheromone of a closely related species, the invasive scale *Acutaspis albopicta*, will also be described.

AGRO 67

Personalized pesticides: A new paradigm

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Botanical pesticides are generally considered as safer alternatives for conventional chemical pesticides. Unlike conventional pesticides, botanical pesticides consist of several components that might play an active role in the toxicity of the mixture. These components not only can chemically interact with each other and synergize or suppress each other's effects, but they also can affect the physical properties of the mixture, such as volatilization rate. Our objective in this project was to study volatilization of a commercial botanical insect repellent on human skin. We analyzed a sample of an insect repellent on human skin with an ultra-fast gas chromatograph (zNose) and noticed that different constituents are released from the mixture at different times in human subjects. We found significant differences in volatilization patterns based on our subjects' gender, ethnicity, skin color, and condition. The results of this study not only create a foundation for more detailed studies in the future, but also can help the industry to promote the concept of personalized pesticides as an alternative for generic formulation.

AGRO 68

Natural products from plants and their synthetic analogs against pests

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As USDA efforts to search for effective, environmentally friendly pest control agents, natural products isolated from plant extracts belonging to various families were evaluated for activity against pests. The compounds were tested against algae, snails, termites, fire ants, and *Ae. egypti* for activity as larvicides and repellents. These active compounds were isolated from plants in Asteraceae, Piperaceae, Rutaceae, and Apiaceae plant families. Amides isolated from Piperaceae family have shown activity against larvae of *Ae. egypti.* Analogs of these natural products were synthesized and found to be more effective as larvicides than indoxacarb, but less effective as repellents. These amides were effective as termiticides against Formosan subterranean termites. A moderately active chromene amide isolated from a member of the Rutaceae family has been modified to obtain highly potent termiticides. Two natural products were found to be effective as molluscicides against ram's horn snail (*Planorbella trivolvis)* and golden apple snails (*Pomacea canaliculata*). Isolation, synthesis of analogs, and biological activities of these compounds will be discussed.

AGRO 69

Discovery of veterinary antiparasitic agents

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There are strong similarities between the aims and objectives of the agrochemical and animal health industries when approaching the discovery of novel insecticides and nematicides; clearly demonstrated by the presence of similar (and in some cases identical) molecules being marketed by both industries. In this presentation I will discuss the challenges of antiparasitic drug discovery for veterinary medicine and in the process highlight similarities and differences between pesticide and antiparasitic discovery.

AGRO 70

Significance of heterocycles for agrochemicals: Current examples from fungicide research

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There are two major reasons for the fundamental value of heterocycles for the lead optimisation of agrochemicals. The heterocyclic scaffold of an agrochemical often has a positive impact on its synthetic accessibility and its physicochemical properties, determining uptake and bioavailability. In addition, heterocycles seem to be perfect bioisosteres of other isocyclic or heterocyclic rings as well as of several

different functional groups, leading in many cases to better biological activity. Recently, some unique heterocyclic ring closure reactions have been found to be valuable tools for the synthesis of examples from the modern fungicide classes of succinate dehydrogenase inhibitors and tubulin polymerisation promoters. Such applications of heterocyclisations to current crop protection chemistry will be reported in the lecture.

AGRO 71

New herbicides and herbicide solutions to combat weed resistance

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The emergence of glyphosate resistant weeds has renewed investment and focus on weed control technologies, including new herbicides with new modes of action. A look at the numbers of issued US patents covering herbicide innovations indicates a steep drop following the introduction of glyphosate resistance crops in the late 1990s, a trend that has only recently been reversed. A review of these new patents indicates few describe materials with unknown modes of action, reflecting both the challenge of identifying such materials and an industry-wide effort to fully leverage existing modes of action. A number of herbicide-tolerance traits are to be released in the next 2-5 years and stacked on top of glyphosate tolerance to broaden the weed control spectrum and incorporate underexploited modes of action into herbicide-tolerant cropping systems. The durability of these systems will depend on whether they are utilized as part of broader weed control programs.

AGRO 72

Approaches towards the discovery of novel insecticides from practically inactive hits/leads: Pyridalyl and others

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Major conventional insecticides have been widely used and played an important role in crop protection. Despite this fact, some conventional insecticides were found to be toxic not only to the target pests, but also to beneficial insects. In addition, most of the pests are continually developing resistance to insecticides in use over long periods. Thus, it is necessary to discover new and safer insecticidal agents with different modes of action. Usually, the discovery of new products begins with generating suitable hit/lead compounds. These molecules are structurally modified to other compounds with higher activity. Although a variety of approaches might be used for creating appropriate hits/leads, we have focused on the discovery of novel insecticides from very weakly active hits/leads, which are dropped off during primary screening. In holding pyridalyl and others up as an example, our unique approaches will be discussed.

AGRO 73

Pharmacophore inversion as a tactic for the discovery of new biologically active substances

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The term pharmacophore describes the structural features inherent in a biologically active molecule that are responsible for its binding to a receptor. Scientists in crop protection and pharmaceutical research try to determine these important features and interactions during the optimization of any new class of biologically active molecules. In many classes of chemistry it has proven possible to move seemingly key structural elements in rings and chains without losing biological efficacy at the target being investigated. This talk will highlight examples of several different kinds of successful inversion of pharmacophoric elements in biologically active molecules.

AGRO 74

Challenges of global residue programs

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Field crop residue data are required to set maximum residue limits (MRL's). Historically, individual countries have established their own procedures for such trials, leading to disparate MRLs thus hindering global trade. Much thought has been given to harmonized residue programs. However differing use patterns, pest pressures, and commercial requirements make this a complex topic. Some regional harmonization, e.g., NAFTA and EU, has emerged but true harmonized global residue programs remain difficult to design and implement. The recently adopted OECD guideline offers a path forward, but it requires some global standardization of use patterns by the petitioning companies. Increasing regulatory acceptance of proportionality principals might help to alleviate some of the complexities of such programs.

AGRO 75

Impact of OECD MRL Calculator on global harmonization of MRLs

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The OECD MRL Calculator was published on the OECD website March 3, 2011. Encouraged by both authorities and industry groups, such as Crop Life International, regulatory authorities in both OECD and many non-OECD countries and groups have started using the OECD Calculator to set new MRLs and re-establish existing MRLs for many crops and commodities. The OECD MRL Calculator provides a single global procedure for setting MRLs, which is one important element in achieving global harmonization of pesticide standards. More than one year after its adoption, the honeymoon is over, and the reviews are in. How has the OECD MRL Calculator performed in the real World? How has the use of the OECD Calculator impacted policy and procedure internationally? It is time to read the first report card.

AGRO 76

Residue data: Addressing extrapolation between global regions

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Comparative assessment proved crop residue datasets homogeneity and low variability across experiments from different geographical regions (zones) to support global residue programs and harmonized MRLs. This project has confirmed that variability across different regions is not greater than within any region. The concept also known as Global Zoning has been developed since 2000 based on analysis of Joint FAO/WHO Meeting on Pesticide Residues (JMPR) data and published by the OECD/FAO Zoning Project (May 2003). Since data reported at JMPR has rarely been generated at consistent Good Agricultural Practices (GAP) in different regions, Dow AgroSciences used internal data to validate the concept. Data from five active ingredients on six main crops were generated in global field experiments in more than two regions at the same/similar GAP's (application rate, pre-harvest interval-PHI) across geographical regions. Variables included in this study were geographical zone, trial, and replicate within trial in a nested multi-linear approach by using JMP statistical software.

AGRO 77

USDA IR-4 Project: Global partnerships in support of US trade

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For nearly fifty years, the IR-4 Project has been the primary resource in the US for facilitating specialty crop registrations of conventional pesticides, pesticides for organic production, and biopesticides. As US trade markets grow, IR-4's participation and data are needed to reduce or to remove pesticide residues as a potential trade barrier for specialty commodities especially for the newer products. IR-4 has actively partnered with US EPA, the crop protection industry, and foreign governments to assist in removing pesticide residues as a barrier to trade. IR-4 serves as a member of the US delegations to the NAFTA Technical Working Group on Pesticides, OECD, and Codex Committee on Pesticide Residues and has co-sponsored the Global Minor Use Summits. Minor uses have also been identified as a key object of the US/Canada Regulatory Cooperation Council.

AGRO 78

IR-4 Project's international collaborations for global harmonization

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This paper will cover many of the areas of global collaborations that assist with international harmonization of pesticide uses as well as residue levels that may limit agricultural commodities in trade. Areas of work developed during the second Global Minor Use Summit will be presented. Activities of the OECD, especially with regard to the Expert Group on Minor Uses working group activities, will be discussed. An update will be provided on the many actions taking place in Codex, including the Codex Electronic working group on Minor Uses and progress with Codex crop groups or extrapolation using representative commodities. Exploring prospects and examples for global residue data generation and gathering of existing data as a means of providing robust data sets to regulators will be covered. Other collaborations and contributions through capacity development will be covered as well.

AGRO 79

Role of USDA-FAS in addressing MRL challenges in foreign markets

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The USDA Foreign Agricultural Service (FAS) represents US agricultural trade interests overseas. The expansion and retention of market access of US agricultural products to foreign markets is a primary goal of the agency. One of the significant challenges to US agricultural producers in today's market place is the regulation of maximum residue limits (MRLs) for pesticides on agricultural products by trading partners. Due to increased awareness among consumers of food safety issues, many important trading partners are devoting greater resources in establishing and in monitoring pesticide MRLs in food. FAS is working with US agricultural industries and US regulatory agencies in various ways to meet these challenges.

AGRO 80

Interlaboratory validation of standardized method to determine permeability of plastic films

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To support regulations controlling soil fumigation, we are standardizing the laboratory method we developed to measure the permeability of plastic films to fumigant vapors. The method was validated using an inter-laboratory comparison with 7 participants. Each participant evaluated the mass transfer coefficient (h) of multiple fumigant compounds through 4 films of varying permeability. Standard methods were used to determine outliers, usually 1 value per analysis. For film-chemical combinations with $h>1\ \text{cm h}^{-1}$ (relatively high permeability), the coefficient of variation of h values reported by individual participants was 0.05 (for methyl bromide) to 0.3 (for trans-1,3-D). For a film with at least 100 times lower permeability, the coefficient of variation of h values ranged from 0.1 to 1.1. Results of the round-robin test show that h values can be measured with precision, even for low-permeability films, indicating that this method is robust.

AGRO 81

Fate and transport of methyl iodide in raised beds under field conditions

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Despite the increasing potential for significant methyl iodide (MeI) use, very little work has been reported concerning the soil fate and transport of MeI under field conditions, particularly its emission potential. In Summer 2011, we conducted a field study in which the soil-air emission of MeI from raised beds covered with virtually impermeable film (VIF) was quantified using dynamic flux chambers. Following drip application of the MeI, emission flux rates and total emission losses were determined over time. Measurements focused on the relative contribution of the top, sidewall, and furrow regions of the beds to the emission loss. In addition, the distribution of MeI gas within the bed and the potential for MeI residues to remain in soil post-fumigation were assessed. Results will be reported that demonstrate the importance of soil moisture, length of environmental exposure of the VIF, and region of the bed system (top, sidewall, or furrow) to MeI fate and transport.

AGRO 82

Predicting emission and distribution of fumigants applied via drip irrigation to raised beds

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Reducing atmospheric emission of agricultural fumigants is increasingly important to protect both human and environmental health. Drip application has been proposed as an alternative of the conventional shank injection to reduce atmospheric emissions from the agricultural use of highly volatile pesticides. In this study, the effects of plastic films, application depth, bed width, and furrow treatment on emission reduction and pest control efficacy were assessed using a process-based mathematical model. The simulations were carried out using Hydrus-2D, modified to include various fumigant-related processes, such as temperature dependent properties of the surface tarp and a removal of tarp at a specified time, and different surface conditions. Validation comparison between the simulated and experimentally measured results was made for fumigant period-averaged emission rates and cumulative emissions under high-density polyethylene film (HDPE) and virtually impermeable film (VIF). Then the model was extended to simulate other scenarios incuding different application depths (5, 10, 15, and 20 cm), bed widths (50, 100, and 150 cm), and furrow treatments (buried film depth at the edge (5, 10, 15, and 20 cm), with and without a reagent). Beside emissions, the concentration-time values were also calculated for assessing pest control efficacy. These findings will be helpful for optimizing fumigant application and minimizing negative environmental effects, while maintaining efficient pest control.

AGRO 83

Validation of a regional air dispersion modeling system (SOFEA) with long-term continuous measurements of air concentrations of 1,3-dichloropropene

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Soil injected fumigants are quite volatile which enhances their ability to diffuse through soil and control pests, but also results in the potential for evaporation from the soil and subsequent off-site movement via air dispersion. A stochastic/deterministic numerical system (SOil Fumigant Exposure Assessment system [SOFEA]) was developed using the US EPA air dispersion model ISCST3, field observed 1,3-D flux, and links to Geographic Information Systems (GIS). SOFEA was used retrospectively to simulate concentrations of 1,3-D in air for direct comparison with continuously monitored concentrations of 1,3-D at 9 locations within 9 contiguous high use townships in Merced County, CA. All 1,3-D applications, including field size, application rate, application depth, and exact field location in the 9 Merced townships have been tracked for a period of 14 months. The general approach to the model validation is described, including the georeferencing of 1,3-D application inputs and model output at specific receptor locations.

AGRO 84

Contribution of good agricultural practices (GAPs) to soil fumigant emission reduction

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Soil fumigant emission critically impacts air quality, regulatory restrictions, and pest control efficacy. Advances in application technology and improved knowledge regarding the impacts of edaphic and environmental variables on fumigant soil persistence create opportunities to develop good agricultural practices (GAPs) to reduce fumigant emission. Replicated field trials and flux studies involving multiple soil fumigants were conducted to quantify the interactive effects of low rate and low disturbance application technology, plastic films with resistance to fumigant diffusion, soil moisture, and tillage on soil fumigant retention and atmospheric flux. The results demonstrated that atmospheric flux rates of chloropicrin, 1,3-dichloropropene, and methyl isothiocyanate were reduced to less than 10 $\mu g\ m^{-2}\ s^{-1}$ using various combinations of GAPs during fumigant application. In particular, low disturbance technology, virtually impermeable films, soil moisture above field capacity, and the creation of a soil surface seal prior to application all affected fumigant emission.

AGRO 85

Airborne flux of 1,3-dichloropropene and chloropicrin applied under totally impermeable film as a function of tarp cutting time

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The most promising emission reduction technique for soil fumigants is the use of totally impermeable film (TIF). This

study was conducted to accurately determine the waiting time before cutting and removing TIF from fumigated soils. Four fields were established in CA to identify optimal times to cut TIF in order to control flux peaks of chloropicrin (CP) and 1,3-dichloropropene (1,3-D). The primary difference between fields was the duration of the tarp covering period (5, 10, or 16 days). A mixture of CP and 1,3-D (Pic-Clor 60) was shank applied at a rate of 659 kg/ha. Fumigant emission rates were determined by measuring air concentrations around the four fields. The results of this study demonstrated that peak and total emissions of CP and 1,3-D under TIF are significantly low when tarp cutting is extended from five to 10 days. Differences in total emissions between 10 and 16 days were very small.

AGRO 86

Emission and movement of 1,3-dichloropropene and chloropicrin in a large field tarped with low permeability film

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Tarping fumigated fields with low permeability films (LPF) can effectively minimize the emission peak and reduce total emission loss, but increases fumigant retention that would require prolonged tarping duration to reduce exposure risk during tarp cutting and removal. In June 2011, the commercial LPF product, VaporSafe^{TM}, was evaluated for fumigant emission reduction and movement in the field and at tarp edges in an 8-acre field fumigated with Pic-Clore 60 (40/60 mixture of 1,3-dichloropropene and chloropicrin) at 659 kg/ha. Over 16 days, <10% emission loss for both fumigants was measured from the tarped field. Although substantially higher near the tarp edges, the flux reduced to below detection limits in 2 m distance from the tarp edge with a total emission loss <1% of total applied. With the proper use and handling of LPF tarp, soil fumigation can be improved for greater efficiency, lower chemical input, and reduced environmental impact.

AGRO 87

Depleting methyl iodide emissions from fumigated soils

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Methyl iodide (MeI), an alternative to methyl bromide, has been registered as a soil fumigant in 48 States of the USA. Though not harmful to stratospheric ozone, MeI is a highly hazardous chemical to humans. Two main concerns of its use are (1) its high emissions into the atmosphere; and (2) the leaching of its breakdown product iodide anion (I^-) into ground water. Ammonia aqueous solution (NH_4OH) can accelerate MeI transformation. Sealed under HDPE (high density polyethylene film) and VIF (virtually impermeable film) in permeability cells, MeI was quickly transformed by NH_4OH. As a consequence, low MeI emissions were achieved. In this experiment, a novel plastic bag was designed, which was filled with NH_4OH and placed on the fumigated soil surface under VIF. Based on the applied mass, it reduced MeI emission through VIF to 0.4%, and retained 96.9% in the form of I^-.

AGRO 88

Microbial and plant metabolites as potential herbicides for the control of parasitic plants

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Broomrapes (*Orobanche* and *Phelipanche* spp.) and dodder (*Cuscuta campestris* Yuncker.) attack strategic food crops and their continuous spread limits the choice of rotational crops and often force farmers to give up growing the most profitable host crops. Annual food crop losses due to broomrape infestation was estimated at about $1.3 to 2.6 billion. Difficulties in the control of parasitic plants arise from their physiological traits and life cycle. Environmentally friendly strategies for their control are based on the use of phytopathogenic fungi and/or the phytotoxic metabolites they produce. Plant phytotoxins might also contribute to competition and invasiveness by suppressing the growth of neighbouring plant species. An alternative green solution is suicidal germination based on the use of fungi or plant root exudates metabolites. This communication will illustrate the isolation, chemical and biological characterization, and potential activity of some fungi and plant metabolites to control broomrapes and dodder.

AGRO 89

Guaianolides for multipurpose molecular design

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Guaianolides constitute a large and diverse group of biologically active plant sesquiterpenes mainly belonging to the Asteraceae family that highlight phytotoxic activity, but have also reported antifungal, bactericide, anticancer, and anti-inflammatory properties. We have carried out the preparation of a secoguaianolide isolated from *Artemisia gorgonum*. This compound has shown high activity in the wheat coleoptile bioassay, as well as in STS phytotoxicity bioassay. Additionally, this compound was tested on human cell cultures, showing apoptosis induction on ovarian cancer cells. These findings show that the same compound could be used for inhibition of plant growth or as a pharmaceutical. Other guaianolides could be used as germination stimulators, with a clear agronomic utility to control parasitc weeds such as witchweeds (*Striga* spp.) and broomrapes (*Orobanche* spp.). With this purpose a collection of new compounds which have been named guaianestrigolactones were synthesized and tested using the natural guaianolide dehydrocostuslactone as the starting material.

AGRO 90

Advancing *Phoma macrostoma* selective bioherbicide to commercialization

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The Scotts Company entered into a collaborative research and development agreement with Agriculture & Agri-Food Canada (AAFC) in 2003 to commercialize *Phoma macrostoma* as a selective broadleaf herbicide. Since then AAFC has published on the genetic variation among isolates of *P. macrostoma*, environmental fate of the fungus and its phyotoxic macrocidins, host range, and on the rhizosphere interaction with hosts. This research has advanced the science of weed biocontrol but also provided information critical for registration. Numerous efficacy trials were conducted in North America to fulfill registration requirements in Canada. In June 2011 and January 2012, registration was received by PMRA and EPA, respectively. Commercialization is still a few years away as development of large scale fermentation continues to present challenges. We are currently working with an external partner to adapt an existing commercial fermentation process for the launch of a granular end product for selective control of broadleaf weeds in lawns.

AGRO 91

Investigating the roles of rice diterpenoid natural products

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Rice produces a number of labdane-related diterpenoids. These include not only the ubiquitous gibberellin plant hormones, but also derived alternative, more specialized natural products. Using a functional genomics approach, my group has made significant progress towards elucidating the underlying biosynthetic network. In turn, this has enabled a reverse genetic approach through which we have now begun to investigate the physiological/ecological roles of the resulting labdane-related diterpenoids. Our results provide the first genetic evidence for natural-product mediated plant-plant allelopathy, and are consistent with a role for the momilactones as allelochemicals, as well as a role for other labdane-related diterpenoids in defense against microbial pathogens.

AGRO 92

Metabolic response of *Arabidopsis* to co-cultivation with white clover (*Trifolium repens* L.) suggests a herbicide-like mode of action

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Allelopathy contributes to competition between plants and has potential use for weed suppression in agriculture. A co-cultivation system for *Arabidopsis thaliana* and *Trifolium repens* was used to study allelopathic effects. Plants were cultivated for up to two weeks to provide a timeline. Growth was modeled using Gompertz curves, and including the co-cultivation factor significantly affected the model (for *Arabidopsis*, $P < 0.001$; *Trifolium*, $P < 0.05$). Harvested plants were extracted and analyzed by GC-TOF-MS. In total 163 metabolites were identified using the online database BinBase. Co-cultivation altered the metabolic profile of both species. Overall 34 *A. thaliana* metabolites increased while 54 decreased and in *T. repens* 20 increased while 33 decreased. To our knowledge, no in vitro allelopathic studies have used untargeted library-based metabolomics. The decreases in *A. thaliana* of aromatic and branched-chain amino acids suggest a herbicide-like suppressant effect by *T. repens* because of the similarity with effects expected from glyphosate or sulfonylurea herbicide treatment.

AGRO 93

Clues to new herbicide modes of action from natural compounds

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The last commercial herbicides with a new mode of action were the HPPD inhibitors more than 20 years ago. There is a growing need for new modes of action because of the increasing evolution of target site resistance in weeds. Natural compounds have been and continue to be good sources of new herbicide molecular target sites. In the past, glufosinate and the triketone herbicides were derived from natural compounds and introduced new modes of action. The modes of action of natural product phytotoxins, such as tentoxin, ascaulitoxin aglycone, the natural product derivative cinmethylin, and other natural product or natural product derivatives will be discussed.

AGRO 94

Induction of cryptic natural product fungicides from actinomycetes

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It is known from genomic sequencing that actinomycetes have many cryptic biosynthetic pathways which are not expressed under normal fermentation conditions. The ability to induce these cryptic biosynthetic pathways would provide a means to discover novel bioactive metabolites from actinomycetes. It has been demonstrated that sub-inhibitory concentrations of antibiotics can induce gene expression in bacteria, however, this technique has not been extensively evaluated in actinomycetes. We tested a wide range of antibiotics for their ability to induce novel metabolites in a variety of actinomycete isolates. The metabolites produced were assessed by LC-MS based chemical fingerprinting. In our hands, sub-inhibitory concentrations of antibiotics were able to over express metabolites as well as induce cryptic metabolites in a variety of actinomycetes. Methods used and implications for novel metabolite discovery will be discussed.

AGRO 95

Toxicological effects of in-hive pesticides to honey bees

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Pollinators are a critical component of the plant health and production of agricultural landscapes. Pesticide exposures to honey bees, *Apis mellifera* L., are implicated in the decline of these pollinators and their ecosystem services. Knowledge of the toxicological consequences of these pesticide exposures, alone and in combination, to bees and their decline is limited. In the present study, we will show the: 1) acute toxicities of in-hive pesticides to bees, 2) binary interactions of in-hive pesticides to bees, and 3) metabolic activities of bees towards in-hive pesticides. The use of this information for the development of ecologically and chemically based strategies to improve pollinator health and reduce pesticides exposures to bee colonies will be discussed.

AGRO 96

Multifactorial assessment of nutrition and immunity in honey bees exposed to in-hive pesticides

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The decline of honey bees, *Apis mellifera* L., is a nationally recognized problem that demands attention from both the scientific community and the beekeeping industry. The pesticides *tau*-fluvalinate (pyrethroid miticide), coumaphos (organophosphate miticide), and chlorothalonil (organochlorine fungicide) are commonly found in bee hives throughout the United States. These pesticides are implicated in bee decline, however knowledge of the consequences of these pesticides and their relationship to bee health is limited. In this study, we will: 1) assess the nutrition and immune status of bees exposed to *tau*-fluvalinate, coumaphos, and chlorothalonil, 2) determine the presence and prevalence of *Nosema* disease for bees exposed to these pesticides, and 3) develop predictive models of bee health thresholds that will improve management practices for colony health and reduce colony losses for the beekeeping industry.

AGRO 97

Five-membered ring heterocyclic carbamates and carboxamides: The quest for resistance-breaking, species-selective acetylcholinesterase inhibitors against the malaria mosquito

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Malaria causes nearly one million deaths every year, of which 91% are in Africa. Insecticide-treated nets (ITNs) provide the first line of defense against malaria transmission in malaria-endemic countries. At present only pyrethroid insecticides are approved by WHOPES for use on ITNs, but the emergence of pyrethroid resistant strains of *Anopheles gambiae* has jeopardized this disease control method. Our goal is to identify a new class of insecticides that will be safe to be deployed on ITNs. An additional design goal is to inhibit the G119S resistant mutant of the mosquito enzyme and at the same time to achieve selectivity for inhibition of *An. gambiae* acetycholinesterase (*Ag*AChE) over the human acetycholinesterase (*h*AChE). We have discovered that selected five-membered ring heterocyclic carbamates and carboxamides show good contact toxicity to both wild-type and G119S resistant malaria mosquitoes. Variation in the ring substituent can lead to good selectivity for *Ag*AChE over *h*AChE.

AGRO 98

Evaluation of novel insecticidal compounds as new mosquitocides for control of *Aedes aegypti* and *Anopheles gambiae*

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We developed an assay using headless *Aedes aegypti* larvae to bypass cuticular penetration. Headless control larvae, when stimulated with a probe, show vigorous lateral contractile movement and are responsive for up to five hours. Larvae exposed to toxicants display sluggish movement or no movement at all. The LC_{50} of many of the known potassium channel blockers in this assay were high (> 100 ppm), whereas tetraethylammonium chloride and 4-aminopyridine (4-AP) had LC_{50} values in the low ppm range. Force transducer measurements of electrically evoked *A. aegypti* muscle contraction showed that a catechol, PRC 725, increased the amplitude of evoked contractions and the baseline tension, similar to 4-AP. In addition, an intact larval bioassay showed blackening of the larvae and 100% mortality at 100 ppm PRC725, suggesting that catechol oxidation was involved. It was also toxic to adult *Anopheles gambiae* by contact. The implications of these results for insecticide development are discussed.

AGRO 99

Development of an in vitro method to determine the bioavailability of xenoestrogens in soil

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Biosolids applied to agricultural fields, parks, and other areas represent significant sources of estrogen-like endocrine disrupting compound (EEDC) inputs to soil. It is important to determine the bioavailability of EEDCs in soil to inform risk assessment concerning their environmental presence. The development of an in vitro bioavailability method that is as effective as a traditional in vivo method will decrease time, expenses, and use of solvents in future analyses. A thin-film solid-phase microextraction (TF-SPME) method for determining the bioavailability of several EEDCs detected in biosolids was developed and compared with a traditional method employing *Eisenia fetida*. TF-SPME effectively measures equilibrium pore-water concentrations of diethylhexyl phthalate, bisphenol A, and benzophenone in soil at environmentally relevant concentrations within 60, 20, and 60 minutes, respectively. The relationship between TF-SPME-predicted concentrations of EEDCs and those extracted from *E. fetida* will be presented, indicating the ability of TF-SPME to predict concentrations in terrestrial organisms.

AGRO 100

Evidence for P-glycoprotein modification of insecticide toxicity in vector mosquitoes

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Mosquitoes affect human health worldwide as a result of their ability to vector multiple diseases. Widespread resistance is a serious public health challenge that limits the use of high efficacy insecticides to reduce the risk of mosquito-vectored diseases. P-glycoproteins (P-gps) are efflux transporters that assist in maintaining the blood-brain barrier interface of insects and might serve as a first line of defense to insecticide exposures. Our previous studies have demonstrated the blood-brain barrier of mosquitoes interferes with the target-site action of established and experimental insecticides. However, the interaction of P-gps toward these chemistries is unclear. In this study, we will provide a: 1) toxicological analysis of select anticholinesterases for mosquitoes alone and in combination with inhibitory ligands of P-gps, 2) biochemical analysis of acetylcholinesterase for mosquitoes exposed to these compounds, and 3) molecular analysis of P-gps expressed in mosquitoes.

AGRO 101

Monoterpenoid binding at the house fly (*Musca domestica*) nicotinic acetylcholine receptor

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Essential oils are a hydrophobic liquid obtained from plant materials and contain volatile aroma compounds, in particular various monoterpenoids. Botanical compounds, including essential oils and terpenoids, have gained interest as alternatives to synthetic insecticides because of their safety and decreased non-target toxicity. Several aromatic and aliphatic monoterpenoids have been shown to be toxic to insects. Their precise mechanism of toxic action is not known, and several mechanisms have been suggested. The nicotinic acetylcholine receptor (nAChR) is an important insecticide target. The nAChR is the target of natural nicotinoids (nicotine, epibatidine), as well as spinosad and synthetic insecticides (neonicotinoids). Recently, we have demonstrated in house fly nAChR that a naturally occurring aromatic monoterpenoid, carvacrol, inhibits the binding of ^{14}C-nicotine in a concentration-dependent manner. Further characterization of the binding of ^{14}C-nicotine in the presence of nicotinoids (nicotine and epibatidine) and neonicotinoids (imidacloprid, dinotefuran, and thiamethoxam) will also be presented.

AGRO 102

Design of novel carbamate insecticides with superior selectivity for the control of cattle tick (*Boophilus microplus*) and sandfly (*Phlebotomus papatasi*) populations

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The cattle tick, *Boophilus microplus* (*Bm*), and the sandfly, *Phlebotomus papatasi (Pp),* are disease vectors to cattle and humans, respectively. The purpose of this study was to characterize the inhibitor profile of acetylcholinesterases from *Bm* (*Bm*AChE1) and *Pp* (*Pp*AChE) compared with human and bovine AChE in order to identify divergent pharmacology that might lead to selective inhibitors. Results indicate that *Bm*AChE1 has uniquely low sensitivity (IC_{50} = 220 µM) toward tacrine, an inhibitor with nanomolar blocking potency in all previous species tested, including *Pp*. In addition, *Bm*AChE1 and *Pp*AChE have low-nanomolar sensitivity to a variety of carbamate anticholinesterases. One experimental compound, 2-((2-ethylbutyl)thio)phenyl methylcarbamate, possesses > 300-fold selectivity for *Bm*AChE1 and *Pp*AChE over human AChE, and a mouse oral LD_{50} of > 1500 mg/kg, thus providing an excellent new lead for vector control.

AGRO 103

High throughput screening technique for detecting the presence of insecticide target site proteins expressed in non-engineered insect cell lines

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The need for new, novel chemicals and chemical insecticides is imperative for the control of increasingly resistant agricultural, medical, and veterinary relevant pest species. This research evaluated the presence of insecticide target proteins from insect cell lines, which could lead to new high throughput screening methods. We used cultures of *Anopheles gambiae* (Sua1B), *Aedes albopictus* (CRL-1660), and *Spodoptera frugiperda* (Sf21) insect cells treated with 20-hydroxyecdysone, which was previously shown to induce cell outgrowths structurally similar to axons in Sf21 cells. We evaluated established pharmacological agents for the ability to depolarize the cell membrane by using fluorescence imaging. Significant, concentration-dependent responses were observed with the chloride channel blocker DIDS, among others. The presence of ion channels and receptors in these cells will potentially accelerate high throughput screening for new insecticides.

AGRO 104 - withdrawn

AGRO 105

Novel pyrazolone fungicide: Applications of byproducts in agrochemicals

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SYP-8448, methyl 3'-(4-chlorophenyl)-1'-methyl-5'-oxo-1',5'-dihydro-1H-spiro[naphthalene-2,4'-pyrazole]-4-carboxylate, is a novel pyrazolone fungicide, and provides potent activity against cucumber downy mildew. SYP-8448 is the byproduct of the preparation of pyraoxystrobin (SYP-3343). The structure was comfirmed by X-ray single crystal diffraction. The possible reaction mechanism is also introduced.

AGRO 106

Investigating ammonia emission sources and transport using stable nitrogen isotopes

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Ammonia (NH_3) emissions are generally unregulated in the US although wet and dry atmospheric deposition of NH_3 and ammonium (NH_4^+) can be a substantial source of nitrogen pollution to sensitive terrestrial, aquatic, and marine ecosystems. Identifying NH_3 emission sources and quantifying NH_3 source contributions are important initial steps for reducing nitrogen inputs to the environment. The stable isotopic composition of NH_3 may be a valuable tool for characterizing NH_3 sources, transport, and fate. Here, we use N-NH_3 isotopes to: 1) create an isotopic inventory of NH_3 sources, 2) trace NH_3 emissions across landscapes, 3) provide first approximations of NH_3 source apportionment, and 4) trace the fate of regional NH_3 emissions in collaboration with the Ammonia Monitoring Network (AMoN) of the National Atmospheric Deposition Program (NADP).

AGRO 107

Quantification of organic phosphate in soil samples by electrospray ionization mass spectroscopy

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Electrospray ionization mass spectroscopy (ESI-MS) was used to quantify inositol-hex-*kis* phosphate–iron metal adducts in two soil samples using a quadrupole mass analyzer. ESI-MS of inositol-hex-*kis* phosphate (IHP) does not generate robust mass spectra. The addition of a transition metal (Fe) to the IHP solution generates pH-dependent adducts that are quantifiable by mass spectroscopy. Structural identification of stoichiometric IHP-Fe complexes was made based on the acid dissociation constants of IHP (pKa). A standard curve was developed for the IHP-Fe adduct at pH 6.5 using (m/z) 198. The correlation coefficient for the standard curve was 0.998. The IHP-Fe adduct was than quantified in two Maryland Matapeake silt loam soils and in Evesboro sand following an aqueous, neutral pH extraction and an extraction using EDTA. Quantification of IHP-Fe complexes could be accomplished at ppb concentration levels. This method can be used to quantify phosphate from IHP in the presence of inorganic phosphate in environmental samples.

AGRO 108

Degradation of the pharmaceuticals acetaminophen and carbamazepine in soils

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Pharmaceuticals and personal care products (PPCPs) are emerging contaminants in the environment. This study was performed using ^{14}C-acetaminophen and ^{14}C-carbamazepine to assess their fate and degradation pathways in soils. When incubated at room temperature, there was a gradual dissipation of both compounds. After 105 d, 1.07% of ^{14}C-carbamazepine or 16.25% of ^{14}C-acetaminophen in a sandy clay loam soil was mineralized to $^{14}CO_2$. Enhanced mineralization was seen in sandy clay loam or silty clay soils than in a medium loam soil. Soil sterilization significantly decreased the mineralization rate of acetaminophen and carbamazepine, implying microbes played an important role in the degradation. Application of biosolids significantly retarded their transformation. For instance, only 1.94% of ^{14}C-acetaminophen was mineralized to $^{14}CO_2$ in the biosolid amended soil, compared to 16.25% in the soil without amendment.

AGRO 109

Oxidation of nonylphenol and octylphenol by manganese dioxide: Kinetics and pathway

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Nonylphenol and octylphenol are raw materials for nonylphenol ethoxylates and octylphenol ethoxylates, which are non-ionic surfactants widely used in agricultural, industrial, and domestic products. They are known as environmental estrogens and are frequently detected in soil, water, and sediment. This study investigated the kinetics, influencing factors, and pathways of the oxidation of these pollutants by manganese dioxide. At pH 5.5, with 100 mg/L MnO_2, the half lives of 1 mg/L technical nonylphenol mixture, 4-*n*-nonylphenol and 4-*tert*-octylphenol were 45, 23, and 36 min, respectively. The reaction was pH dependent, following an order of pH 4.5 > pH 5.5 > pH 6.5 > pH 7.5 > pH 8.6. Addition of metal ions suppressed the reactions, following the order $Mn^{2+} > Ca^{2+} > Mg^{2+}$. However, addition of humic acid accelerated the reactions. Multiple reaction products, including hydroxylated products, dimers, and trimers, were identified by GC-MS/MS and UPLC-MS/MS. Tentative pathways were proposed based on these products.

AGRO 110

Degradation of emerging contaminants by biogenic manganese (III/IV) oxides

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Natural Mn (III/IV) oxides are recognized as important oxidants in the environment, affecting the environmental fate of many micropollutants. A biological Mn (II) oxidation process is believed to be the predominant pathway for natural Mn (III/IV) oxide formation. In this study, *Leptothrix discophora SS-1*, a Mn (II) oxidizing bacterium, is used to produce biogenic manganese oxides ($BioMnO_{x)}$. The structure of $BioMnO_x$ is characterized by XRD, SEM, XPS, N_2-BET, TGA, FTIR, and Raman. XRD results indicate $BioMnO_x$ is poorly crystallized, similar to δ-MnO_2. Degradation of the emerging contaminants ciprofloxacin and bisphenol A in presence of $BioMnO_x$ is investigated. The oxidative reactivity of $BioMnO_x$ is compared with that of its synthetic analog δ-MnO_2. The effects of organic content in $BioMnO_x$ and the solution conditions (pH, presence of co-solutes) on the reaction kinetics are also discussed. Degradation products will be identified and discussed.

AGRO 111

Gas-phase reaction of methyl isothiocyanate with hydroxyl radicals under static relative-rate conditions

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Gaseous methyl isothiocyanate (MITC), the principal breakdown product of the soil fumigant metam sodium (sodium methyl-dithiocarbamate), is an inhalation exposure concern to bystanders, especially in residential communities near large production acreages. Inhalation exposure might not be limited to MITC but might also include methyl isocyanate (MIC), a tropospheric oxidative transformation product of MITC. Under controlled laboratory conditions, the gas-phase reaction of hydroxyl (OH) radicals with MITC was examined using static relative-rate techniques in 10 L Tedlar air sampling bags over a 1 hr period. Gas phase MITC, MIC, and OH reference compounds were quantified by solid phase microextraction-GC/MS. In this work an MITC OH rate constant of 25×10^{-12} cm^3 $molecule^{-1}$ s^{-1} was estimated. The MITC atmospheric lifetime would be ca. 0.6 days under tropospheric OH radical concentrations of 8.0×10^5 molecules cm^{-3} over a period of 24 hrs. MIC was observed to be the primary transformation product in the gas phase.

AGRO 112

Isotope exchange method (IEM) to study the bioavailability of DDTs in sediment

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DDT is an organochlorine insecticide that was banned in the US in the 1970s. However, DDT and its main metabolite DDE are still widely detected in sediments. Given their strong hydrophobicity, bioavailability plays a critical role in the actual risk of DDT derivatives to aquatic organisms. Chemically based approaches have been explored for predicting the bioavailability of organic compounds due to

their reproducibility, simplicity, and low cost. In this study, a stable isotope exchange method (IEM) was developed to measure the exchangeable pool (*E*) of both *p,p'*-DDT and *p,p'*-DDE in sediments as an indicator of bioavailability. The measured *E* values showed a decreasing trend with an increase in sediment organic carbon (OC) content. The capability of IEM to estimate bioavailability was validated by comparing with other methods, including solid phase microextraction (SPME) and Tenax-aided desorption. There was generally a good agreement among these biomimetic methods.

AGRO 113

Quantification and identification of biodegradation products of sulfamethoxazole in wastewater

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Sulfamethoxazole (SMX) is an antibiotic used on both human and animals, and has been detected in wastewater and surface water worldwide. SMX can be introduced into agricultural croplands through irrigation using recycled water. Therefore, it is essential to monitor the concentrations of SMX at low levels to determine their removal efficiencies in wastewater treatment plants (WWTPs). In addition, knowledge on the degradation products is also valuable to assure that the transformation products are not a threat to the environment. This study focuses on quantifying SMX in wastewater by high performance liquid chromatography coupled with tandem mass spectrometry (HPLC/MS/MS) using isotope dilution for accurate quantification. Furthermore, this study will identify the degradation products of SMX formed during biological treatment using Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS). Bioreactors seeded with wastewater from a municipal WWTP were run under anaerobic, microaerobic, and aerobic environments to produce samples for this project.

AGRO 114

During the dissipation of dislodgeable foliar residues a transfer coefficient does not predict potential dermal exposure of hand harvesters

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Potential dermal harvester pesticide exposures (PDE; µg/d) may be represented by an empirical relationship: Dislodgeable Foliar Residue (DFR; µg/cm^2) x Transfer Coefficient$_{\text{strawberry harvester}}$ (3000 cm^2/h) x hours/d. Pesticide glove residues (PGR$_{\text{day}}$) represent potential dermal hand exposure by accumulation of foliar residues on gloves since harvester hand exposure represents the major route of worker exposure. Glove transfer coefficients (TC$_{\text{glove}}$; cm^2/hr) may be expressed as: PGR$_{\text{day}}$ (µg/pair) = DFR (µg/cm^2) x TC$_{\text{glove}}$ (cm^2/hr) x hours/day. Our studies show that TC$_{\text{glove}}$ increased (malathion: +500% and fenpropathrin: +112%) as the DFRs dissipated (malathion: -99% and fenpropathrin: -87%) between the pre-harvest interval (PHI = 3 days) and at the end of 15 days. Since TC$_{\text{glove}}$ is not constant for all study periods, estimating PDE using a single empirical value for TC$_{\text{glove}}$ seems improper. A lower TC$_{\text{glove}}$ at a given study period may be related to more residues being transferred relative to a higher TC$_{\text{glove}}$.

AGRO 115

Phytoremediation of atrazine from simulated surface water runoff using switchgrass

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Atrazine is one of the most widely used herbicides in the agricultural industry today and is commonly found in many bodies of water in the Midwest. Atrazine and its metabolites have many adverse effects on plants and animals within an ecosystem. Previous research has shown that switchgrass can take up and degrade atrazine into its less toxic metabolites. The current research project has two objectives: (1) determine the degradation of atrazine using radiolabeled ^{14}*C*-atrazine to allow for more sensitivity than previous studies and (2) determine the possible exudation of atrazine metabolites from switchgrass after uptake and degradation. The research presented here shows that atrazine was taken up and degraded into the metabolites deethylatrazine, deisopropylatrazine, didealkylatrazine, and cyanuric acid. Contrary to published research, the metabolite hydroxyatrazine was not detected. Additionally, we showed that switchgrass did not exude metabolites of atrazine into soil following uptake and degradation.

AGRO 116

Risk assessment of groundwater contamination of chlorpyrifos in neutral and alkali soil through lysimetric studies

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Chlorpyrifos, an organophosphate insecticide used extensively for termite control, has been banned in India. Chlorpyrifos is used indiscriminately by pest controllers in foundations of buildings above the recommended dosages of 1 L/m^2 of 20% EC formulation. It is used around buildings, yards, wooden objects, crevices through drilling, spraying, etc. It is also used in agricultural practices by farmers as a broad-spectrum pesticide. Farmers use more than the recommended dosages out of their ignorance, and chlorpyrifos residues in soil and groundwater have been reported. Indian soil is mainly neutral or alkali in nature. Therefore, lysimeter studies were conducted in soils of neutral and alkaline pH for leachability of chlorpyrifos to assess groundwater contamination. Leaching of chlorpyrifos was lower in alkali soil as compared to neutral soil as chlorpyrifos is an organophosphorous insecticide. The possibility of groundwater contamination is much higher in neutral soil compared to alkali soil.

AGRO 117 - 119 - Withdrawn

AGRO 120

Bed nets and insecticide resistance: The way forward

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Long-lasting, insecticide-impregnated bed nets (LNs) and indoor residual sprays (IRS) form the mainstay of malaria vector control interventions, reducing the number of cases and deaths across Africa and other disease endemic countries. In recent years, large numbers of LNs were distributed to meet universal coverage targets, and IRS programs have treated many millions of homes each year. A few classes of chemistry with different modes of action are available for IRS, while all currently available LNs are based on pyrethroids. This heavy reliance on a few classes of chemistry is at least partly responsible for the insecticide resistance that is now being detected in mosquito populations in many parts of the world. The spread of resistance is threatening the effectiveness of vector control. Innovative tools and new chemistry will be required if we are to sustain recent gains against malaria. The development of such innovative tools is discussed.

AGRO 121

Health impacts of product development partnerships

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Over 40 Product Development Partnerships (PDPs) have been established in the last 20 years to stimulate industry to accelerate the development of new drugs, vaccines, insecticides, and diagnostics for a range of tropical diseases. The products supported by these PDPs are now being used to affect decreases in disease transmission and prevalence. The Innovative Vector Control Consortium (IVCC) is the only vector control PDP supporting the development of public health pesticides and diagnostics for malaria, dengue, and other insect-borne disease prevention. The impact on policy and practice of IVCC-supported products 7 years after the PDP's inception will be discussed. These include implementation of a diagnostic for pesticide quantification at the point of use, insecticide resistance detection kits that can differentiate operationally-significant pyrethroid resistance, and new, longer-lasting insecticide formulations for indoor residual spraying.

AGRO 122

Mosquito P-glycoproteins and their emerging role in insecticide resistance

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Widespread resistance is a serious public health challenge that limits the use of high efficacy insecticides to reduce the risk of mosquito-vectored diseases. P-glycoprotein (P-gp) is a multi-specific drug efflux transporter that assists in maintaining the blood-brain barrier interface of mosquitoes and, in turn, can limit the target-site action of insecticidal chemistries for their control. In this presentation, we will show the: 1) molecular analysis of P-gp subfamilies that confer the multi-drug resistant phenotype; 2) toxicological modification of established and experimental insecticides alone and in combination with P-gp inhibitors; and 3) P-gp-mediated transport and target-site action of these insecticides in vector mosquitoes.

AGRO 123

Field studies of rodent baits for sand fly control

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Rodent baits containing a systemic insecticide are a potential tool to control sand fly vectors that feed on rodent reservoir hosts, interrupting the cycle of transmission of *Leishmania major*. Baits incorporating systemic bio-indicators have also been developed for use as control-efficacy diagnostic tools to demonstrate that these insecticide treatments are reaching bloodfeeding sand flies in a population. An objective of our studies was to use baits containing bio-indicators to determine the level of blood feeding by sand flies on targeted rodents and to demonstrate the effect of rodent baits containing ivermectin on sand fly populations. A study was conducted in Kenya and Morocco which have different sand fly vectors and rodent reservoirs of *L. major*. In both locations, female sand flies collected at sites treated with rodent baits containing bio-indicators were marked, while no marked female sand flies were collected at sites treated with baits containing the bio-indicators plus ivermectin. The results of this study constitute proof of concept for the targeted control of an epidemiologically-significant portion of the population of the sand fly vector of *L. major* (sand flies that take bloodmeals from rodent reservoirs of *L. major*), and demonstrate the potential for the interruption of the transmission of *L. major* using rodent baits containing a systemic insecticide.

AGRO 124

Acetylcholinesterases of *Rhipicephalus (Boophilus) microplus* and *Phlebotomus papatasi*: Gene identification, expression, and biochemical properties of recombinant proteins

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Rhipicephalus (Boophilus) microplus (*Bm*) is a vector of bovine babesiosis and anaplasmosis. Tick resistance to organophosphate (OP) acaricide involves acetylcholinesterase (AChE) insensitivity to OP and metabolic detoxification. *In vitro* expression of *Bm* genes encoding AChE allowed biochemical characterization of three BmAChEs expressed in tick synganglion. BmAChE1, BmAChE2, and BmAChE3 exhibited substrate preference for acetylthiocholine, high substrate inhibition, and sensitivity to AChE-specific inhibitors. OP-insensitivity mutations were found in *BmAChE1* and *BmAChE3*. Gene silencing suggested functional complementation of BmAChEs *in vivo*. BmAChE genes had amplified copy number and multiple transcript polymorphisms were expressed in individual tick synganglia for each of the *BmAChE*s, suggesting allelic diversity within individuals. Studies identified a cDNA encoding AChE of the sand fly, *Phlebotomus papatasi*, a vector of leishmaniasis in humans and animals. Expression of recombinant *P. papatasi* AChE (PpAChE) enabled biochemical characterization and identification of inhibitors selectively targeting PpAChE.

AGRO 125

Designing anticholinesterase insecticides to achieve high selectivity for the malaria mosquito, *Anopheles gambiae*, and potency against known resistance mutations

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Currently available insecticide-treated nets (ITNs) are losing efficacy due to emerging resistance of *Anopheline* mosquitoes to the pyrethroid insecticides impregnated on these nets. Anticholinesterase inhibitors that are highly selective for *An. gambiae* acetylcholinesterase (AChE) could replace or supplement pyrethroids on ITNs if low mammalian toxicity could be demonstrated. In addition, new anticholinesterases that show toxicity to G119S AChE carbamate-resistant mosquitoes could be very useful for ITNs or indoor residual spraying. In this presentation we will review the structural determinants of inhibition selectivity and potency of a wide series of carbamates to wild-type (WT) and G119S *An. gambiae* AChE. A ligand-based *in silico* model that offers good predictive power for *An. gambiae*/human inhibition selectivity will be presented. Current efforts to combine high *An. gambiae*/human selectivity with good contact toxicity towards WT and G119S-bearing mosquitoes will be reviewed, as will preliminary mouse oral toxicity of promising candidates.

AGRO 126

Developing novel small molecule agonists and antagonists of arthropod G protein-coupled receptors as next gen insecticides for vector control

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New mode-of-action chemistries are needed to control arthropod vectors, especially where vector populations have acquired resistance to insecticides. We describe a genome-to-lead approach for discovery of novel small molecule chemistries that disrupt arthropod G protein-coupled receptor (GPCR) targets and that have potential for development as next gen insecticides. We demonstrated the utility of this approach by determining the molecular and pharmacological properties of two dopamine receptors (AaDOP1 and AaDOP2) identified from the genome sequence of the dengue vector, *Aedes aegypti*. We performed screens for small molecule agonists and antagonists of AaDOP2 and demonstrated that several hit chemistries are selective for the mosquito over the human dopamine receptor *in vitro*. These chemistries cause significant mortality of mosquito larvae 24 hours after exposure, identifying them as possible leads for insecticide development. This research demonstrates the potential of target-specific approaches that could accelerate discovery of new classes of insecticides for vector control.

AGRO 127

US Food and Drug Administration pesticide MRL enforcement program

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US FDA conducts a pesticide monitoring program to enforce US tolerances (MRLs) on all foods except meat and poultry, primarily targeting high consumption and children's foods. FDA analyzes several thousand samples annually using state of the art multi-residue procedures. Most pesticide violations found by FDA are for residues in foods for which there are no US tolerances. Imported foods have shown a higher violation rate than domestic foods. Available intelligence helps FDA target its import monitoring. When an import violation is detected, the grower and commodity can be placed on FDA Import Alert, and admission of future entries will require the importer to demonstrate compliance. The Food Safety and Modernization Act (FSMA), passed early in 2011, will put added responsibility on food importers to implement supplier verification activities to ensure compliance with US MRLs.

AGRO 128

Monitoring pesticides in foods: Responding to global market changes

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The USDA Pesticide Data Program (PDP) has been collecting data on pesticide residues in foods available to the American consumer since 1991. The data are provided to the US Environmental Protection Agency to evaluate dietary risk posed by pesticide residues in foods. Over the 21 years of the program's existence, the number of pesticides tested by PDP has increased to capture changes in pesticide usage driven by the Food Quality Protection Act. To date, PDP has primarily focused on pesticides registered for use in the US; however, the significant increase of imported foods in the US market is forcing PDP to incorporate additional pesticides. PDP plans to add pesticides used overseas in production of imported foods with special emphasis on children's high consumption foods.

AGRO 129

Practical challenges of monitoring trace residues in the US food supply: Limits of detection and quantitation

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Defining limits of detection (LODs) and limits of quantitation (LOQs) is critical for the use of data in a program where a majority of the data is "none detected" or below LOQ. LODs and LOQs, or some fraction of the them, are often used in statistical manipulation of the data making these values just as relevant as residues. In monitoring trace residues in our food supply, the demand is to set LODs as low as possible. This presentation will discuss challenges of establishing LODs and LOQs in pesticide residue analysis, working with analytes with multiple peaks, specific challenges of MS/MS instruments, and the relationship of EPA food pesticide tolerances to food pesticide residue LODs.

AGRO 130

Retailer pesticide secondary standards in the food chain

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Often of EU origin, secondary standards are aimed at controlling the levels of pesticide residues in food. They play an increasingly important role in international trade, particularly of fresh fruit and vegetables. They are based on established regulatory levels, but go beyond the legal requirements, e.g., they may be a percent of the Maximum Residue Level (MRL) or the Acute Reference Dose (ARfD), a value used to set acceptable short-term dietary levels. Secondary standards are both increasing in number and becoming more complex, e.g., for certain crops, some retailers combine both a percent of MRL and/or ARfD with a limit on the numbers of pesticides allowed. This presentation will examine the circumstances that lead to the development of these food chain standards, briefly review current standards and their impacts, and consider how such standards may develop in the future.

AGRO 131

Maximum residue limits (MRLs): Challenges of a global business

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Differences in pesticide maximum residue limits (MRLs) between regions of the world are prevalent and create commodity trade barriers. Such differences ultimately impact the development and commercial viability of these chemicals, which are essential to production agriculture. Disease and pest pressure varies between global regions. This fact, combined with regionally-specific regulatory and/or efficacy requirements, can lead to significant differences in regional MRLs. MRL differences may also occur as a result of new use patterns for existing products with established MRLs, e.g., the addition of a post-harvest treatment to an existing product label. Definition of the residue of concern (DoR) can also vary regionally, resulting in different MRLs for commodities with identical treatment regimes. One common strategy to harmonize MRLs is through the establishment of import tolerances (ITs) between regions. However, the impact on risk assessments, balancing of regional vs. global business priorities, and regulatory timelines and processes must be considered.

AGRO 132

Effect of adjuvants on residues in relation to routine residue trial variability

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Adjuvants added to farmers' spray tanks may increase residues in crops, which could have implications for setting Maximum Residue Levels (MRLs). CropLife America's Residue Expert Work Group analyzed a significant quantity of data to investigate the effect of adjuvants in side-by-side residue trials conducted with or without adjuvants. Residue data sets and methodologies used in development of the OECD MRL Calculator were applied in this work.

Results showed there is a tendency for adjuvants to increase residues in certain crops; however, the observed increase should not be applied as a general rule. Any potential magnitude of increase due to adjuvants was shown to be well within the variability found in routine residue work, as well as the variability in estimating the corresponding MRLs.

AGRO 133

Kenya major and minor crops in international trade

Gladys N. Maina, *pcpboard@todays.co.ke.Pest Control Products Board, Kenya Government, Nairobi, Kenya*

Horticulture contributes significantly to the Kenyan economy by being the second foreign exchange earner, providing employment, and increasing food security and self-sufficiency. There are many challenges related to residues encountered by horticultural crop farmers exporting to key markets. The main problem for growers is the lack of available approved pesticides for specific crops. The second major challenge for Kenyan growers is non-compliance of MRLs in some export markets. Finally, the lack of harmonized MRLs in the international market is an obstacle for growers. Kenya is addressing these challenges in a number of ways.

AGRO 134

Comparing different modeling approaches of pH-dependent sorption with FOCUS-PEARL

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pH-dependent sorption behaviour of pesticides and metabolites can be handled in various ways in environmental exposure modelling within the regulatory procedure of pesticide registration in the European Union. In the groundwater model FOCUS-PEARL 4.4.4, pH-dependent sorption can either be addressed by parameterising a sigmoidal function based on $K_{fom,ac}$, $K_{fom,bas}$ (Freundlich adsorption coefficient of the protonated ($K_{fom,ac}$) and deprotonated ($K_{fom,bas}$) form of a substance normalised for organic matter content) and pK_a-value or by entering directly horizon-specific K_f-values that again can be calculated externally in different ways. The presentation will introduce both approaches, discuss sorption representation in detail based on: sigmoidal relationship between K_{fom} and soil pH (pK_a-value necessary); sigmoidal relationship between K_f and soil pH (pK_a-value necessary); linear relationship between K_f and soil pH (pK_a-value not necessary); and horizon specific sorption versus K_f-values employed in modelling based on top-soil pH-value (pK_a-value not necessary), and then compare the effects in view of the Predicted Environmental Concentration (PEC$_{gw}$) at different locations of the European FOCUS scenarios. These options addressing pH-dependent sorption will be compared with other (national) approaches such as separately deriving appropriate K_{foc}-values from studies conducted with alkaline and acidic soils and neglecting scenario specific pH-conditions.

AGRO 135

Setting groundwater monitoring sites in a European wide spatial context

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Groundwater monitoring (GWM) is considered as the highest tier of assessment of pesticide leaching in regulatory evaluation in the European Union. To determine the representativeness of sites for a country with regard to the vulnerability of groundwater to pesticide leaching, the locations should be set into context, taking into account agronomical, pedoclimatical, and hydrogeological conditions.However, current approaches are limited, because more or less rough and discrete ecoregions are used, e.g., a specific soil texture class, the amount of rainfall, or a combination of soil and climatic conditions. We present a method to define the represented area of a GWM site based on the spatially-distributed groundwater leaching model MetaPEARL. We generate maps of leaching concentrations on a European scale and compare these maps with concentrations calculated on the GWM site. Thereby, we are able to account for wide set of environmental characteristics and therefore a more realistic estimation of representativeness.

AGRO 136

Modeling herbicide metabolite concentrations in groundwater at shallow karst monitoring sites in France

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Concentrations of metabolites of an agricultural herbicide were monitored in wells supplying drinking water from captured groundwater springs in areas with shallow fractured and karst aquifers and known to have widespread application of the product. For two sites sufficient hydrological, hydrogeological, and pedological data were available to provide a reasonable basis for a pragmatic modeling approach to address the question of whether the measured concentrations could be regarded as representative for documented applications of the product in the area of the well. Leaching simulations were carried out for relevant fields using the PEARL leaching model. A mass balance based model considering simple groundwater flow was developed and implemented in a spreadsheet to calculate time-dependent concentrations at the monitoring wells resulting from the simulated leachate solute mass fluxes in the catchment area. The results indicate that the measured concentrations can be considered as representative for the documented product usage and local conditions.

AGRO 137

Monitoring and predictive modelling of leaching and transport of a pesticide metabolite from a field to a drinking water abstraction point

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The duration and extent of future drinking water exposure was investigated for a pesticide metabolite caused by long-term application of a plant protection product in an orchard within the catchment area of a water works from 1993 to 2006. The leaching of the metabolite into groundwater under the orchard was calculated with the 1-dimensional model PEARL based on the actual pesticide use history and using local soil and weather data for model parameterization. The further dilution during transport in the aquifer to the drinking water abstraction point was simulated using a 2-dimensional modelling approach applying HYDRUS-(2D/3D). Horizontal hydraulic conductivities in the aquifer for model input were experimentally determined across the catchment. The modelling work was accompanied by extensive monitoring programmes confirming the results of the simulations. In summary, a transfer factor of ca. 20 between the concentration of the metabolite in groundwater recharge and in raw water for drinking water production was calculated. The drinking water exposure is predicted to remain constant until 2015 and to terminate by 2025.

AGRO 138

Multidimensional modeling of pesticide placement and fate in the soil-root-plant system

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Many pesticides are soil applied, including residual herbicides, soil insecticides, and seed treatments incorporating fungicides and/or insecticides. Regulation within Europe is becoming increasingly stringent with regard to water contamination which is driving registrants to pursue novel means of application to reduce off-site movement of active ingredients. Simulation models are the primary basis for regulating pesticides against EU ground and surface water protection standards, but the current models cannot explicitly represent plants or their roots or the effects of formulations and formulation placement strategies (e.g., slow-release microcapsules and seed treatments). We present a new model of the soil/plant system to enable the environmental benefit of advanced formulations and placement strategies to be quantified in a cost-effective way for the first time.

AGRO 139

Development and evaluation of the Pesticide Root Zone Model (PRZM) for estimating pesticide concentrations in groundwater

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The Pesticide Root Zone Model Groundwater (PRZM-GW) was developed as a regulatory model to estimate pesticide concentrations in vulnerable groundwater supplies. Input parameters include pesticide fate properties, environmental factors, such as soil type, aquifer depth and weather, and agronomic practices including application method, timing, and frequency of application. PRZM-GW output data include peak and time weighted concentrations. Evaluation of PRZM-GW was completed by comparing simulated pesticide concentrations to available targeted and non-targeted monitoring data. PRZM-GW predicted pesticide concentrations represent upper-bound estimates of groundwater concentrations when conservative input parameters are used (e.g., maximum application rates, annual applications, and conservative degradation assumptions). Physical processes such as preferential flow or particle transport into the aquifer are not accounted for in PRZM-GW; therefore, some pesticide detections in the monitoring data are not represented in the model output. When site specific adjustments (e.g., environmental factors and agronomic practices) are made to the input parameters, PRZM-GW estimated pesticide concentrations compare well to monitoring data. These results show that PRZM-GW is a versatile exposure model that can be used as a risk assessment tool for estimating pesticide concentrations in groundwater.

AGRO 140

Validation and refinement of PRZM-GW predicted soil-pore water concentrations using terrestrial field dissipation data

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The United States Environmental Protection Agency in collaboration with Canada's Pest Management Regulatory Agency has developed a draft Tier II modeling approach to predict pesticide transport to groundwater. This approach uses a modified version of the Pesticide Root Zone Model (PRZM) to predict groundwater concentrations (PRZM-GW) at a desired depth. Evaluation of the sensitivity of predicted pesticide concentrations in groundwater on PRZM-GW inputs is ongoing. This presentation summarizes PRZM-GW modeling using custom scenario inputs derived from site-specific environmental monitoring and laboratory data. Predicted soil-pore water residues are compared to observed data obtained from suction-cup lysimeters that were installed as part of a deep leaching module of a terrestrial field dissipation study. Several key factors that improved the agreement between monitoring data and model predictions are discussed, including the influence of soil maximum water content.

AGRO 141

Enhancement of a pesticide leaching assessment tool in Hawaii for screening volatile agrochemicals

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Complex simulation models generally provide an accurate assessment of subsurface behavior of contaminants. However, they are limited to situations where adequate data are available. In reality, such data are not available for national and regional scale assessments. Due to these reasons, a GIS-aided screening tool is being used for the islands of Hawaii for a qualitative evaluation of pesticide leaching based on soil and chemical benchmark properties since mid-1990's. In this study, an attempt has been made to update the tool that allows additional agrochemicals, i.e., volatile organic compounds (VOCs), to be assessed. As convective mobility implemented alone as a screening indicator of pesticide leaching is not adequate for substances with high volatile loss, i.e., vapor-phase transport, the current tool is not suitable to screen the leaching behavior of VOCs. To account for loss by volatilization, the previous version of the tool is further expanded to include additional terms such as liquid-vapor partitioning for the retardation factor (RF) and vapor loss at the soil surface for the attenuation factor (AF) estimations, respectively. From the results, it is shown that the leaching potential of selected VOCs is assessed well by the ranking scheme provided by the extended screening tool. In addition, the modified tool is in fairly good agreement with closed-form models that describe VOC leaching potential in soils, as long as leaching is dominant and there is little water to evaporate. Therefore, the simple mobility indices, i.e., RF and AF, extended in this study not only assist decision makers determine priority VOCs responsible for groundwater contamination, but can be still used as a first-tier screening tool on the islands of Hawaii.

AGRO 142

How good is good enough? An instrument vendor's perspective on method development

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Many analysts turn to the manufacturer of their laboratory instrumentation for methods to solve a particular analytical problem. Methods are generally developed by an applications chemist who is familiar with customer needs and the limitations of existing methods. Our company supplies everything from a simple chromatogram run on a standard to analyzers that are built and tested at the factory to perform a specific analysis. For example, we offer several different pesticide analyzers based on GC with single and triple quadrupole mass spectrometers. These analyzers are built at the factory with the appropriate columns, liners, and retention-time-locked methods. A sample containing 17 pesticides is run at the factory and again when the instrument is installed to verify that the analyzer is functioning properly. While these methods have not undergone a formal multi-lab validation, we have a lot of experience with customers who have implemented the methods.

AGRO 143

Tools for contract testing labs: Incorporating new technologies for routine testing workflows

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Contract food-testing labs face analytical challenges every day. Not only are these laboratories tasked with testing a huge variety of foods, ingredients, and consumer products for a number of different chemical contaminants using analytical methods that are targeted and validated, but to add to that challenge, they also carry the responsibility of ensuring that food products are, in general, safe and contaminant-free – covering both the compounds they are targeting as well as anything else that could unexpectedly be present. In an effort to screen for unlimited potential contaminants in food products (in essence, to collect all-of-the-data, all-of-the-time), while still ensuring the utmost in data accuracy and quality, new technology, equipment, software, and methods are essential tools for growing contract food testing labs. Here we will highlight some of these new tools, how they can be easily implemented into the workflows of routine testing labs, and the processes that can be used to support method validation and data verification.

AGRO 144

Mass spectrometry-based methods for trace-level analysis in industrial and agrochemical research

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Mass spectrometry is widely used by industry in research and development efforts that lead to novel agricultural chemicals. The requirements and acceptability of mass spectrometry-based analytical methods are variable. Several examples of DuPont analytical methods will be presented: from early agrochemical discovery research, to regulatory studies for product registration, and post-registration product support. These diverse methods are based on chromatography/tandem mass spectrometry and high-throughput flow injection/tandem mass spectrometry to analyze active ingredients, such as sulfonylureas, anthranilic diamides, and carbamates at part-per-billion levels in complex environmental and food matrices. The challenges of optimizing quantitative analysis quality (i.e., accuracy and precision), sample analysis throughput, and sensitivity to meet the objectives of agrochemical research and comply with regulatory guidelines will be highlighted. In addition, current collaborative research programs that pursue the development of novel methods of analysis and the improvement of analytical technology at DuPont will be briefly discussed.

AGRO 145

What is good enough?

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A young Winston Churchill was once asked by his boss to write a report. When Churchill handed in the report, his boss asked, “Is this the best you could do?” and Churchill replied, “No.” “Do it again!” the boss demanded. When Churchill returned with the revised version, he was asked again, “Is this the best you could do?” Churchill was ready with his response, “No, but it is equal to the task.” Although Churchill was not an analytical chemist, he captured the essence of the fit-for-purpose concept well. Usually, the purpose of analysis involves a purely objective measurement to arrive at the correct answer. However, analytical chemists must also address the purely subjective question, “What is good enough?” This presentation is intended to meet the dual purpose as an award lecture for Innovation in Chemistry of Agriculture and to open the symposium, “Is your analytical method good enough?"

AGRO 146

Validation and analytical quality control in pesticide residue analysis: An EU perspective

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Pesticide residue analysis is a challenging task for the analytical chemist due the high number of analytes and the enormous variation in food and feed commodities. The establishment of criteria for quantitative and qualitative validation and analytical quality control is even more challenging, especially since new instrumental technologies offer us new possibilities to do the analysis. Since 1997 in the EU, a guidance document has been established for validation and analytical quality control for the analysis of pesticide residues in food and feed. This document is biannually updated to take into account advancing insights and application of new technologies. In this contribution, the current version of the guidance document, SANCO/12495/2011 (http://ec.europa.eu/food/plant/protection/pesticides/docs/qualcontrol_en.pdf) and its recent modifications will be presented. This will include validation of quantitative methods, qualitative screening methods, and requirements for identification. The importance of having a guidance rather than a regulation will be illustrated by examples from practice.

AGRO 147

Method validation criteria: US EPA Office of Pesticide Programs

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The US EPA Office of Pesticide Programs (OPP) reviews and evaluates scientific data submitted by pesticide manufacturers to ensure that products registered in the US are safe and effective. Many of the scientific studies required to make these decisions are based upon analytical measurement, i.e., determination of pesticide residues in a variety of matrices including soil, water, plant and animal commodities, and commercial pesticide products. Analytical data submitted to OPP in support of pesticide registrations must be generated following EPA Good Laboratory Practices and published OPP Residue Chemistry Test Guidelines. This presentation will discuss some of the various requirements for environmental methods, food tolerance enforcement methods, and product enforcement analytical methods.

AGRO 148

Method acceptability standards: A perspective from a state FIFRA laboratory

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In support of the state's pesticide regulatory activities, the laboratory division of the Minnesota Department of Agriculture analyzes a variety of pesticide residue samples for monitoring, enforcement, and forensic purposes. Each type of sample is analyzed by different analytical methods that were developed under different method acceptability standards. Some examples are analyte identification criteria, use of internal standards, use of matrix matched standards, and detection limit determination procedure. Method acceptability criteria also vary depending on the regulatory authority under which the lab is working. In addition, pesticide misuse/incident response samples are often requested for quick turn around and are analyzed by non-standard methods. For this type of analyses, we continue to search for method acceptability criteria that can be met within minimum amount of time, yet produce legally defensible data.

AGRO 149

Imitating insecticidal spider peptides: In silico screening and optimization of a new heterocyclic family of mosquitocides

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Scanning alanine mutagenesis of hexatoxins when combined with the 3D structure yielded information about the structural features which crucially contribute to the insecticidal activities of these peptides. These structure features were digested into a 3D search term for mining commercially available compound databases. Screening the resultant hits by insect bioassay yielded insecticidal leads. One family of leads, triazines, was optimized with guidance from SAR and the 3D search term. This led to a class of aryl triazines and pyrimidines with greatly increased mosquitocidal activity as well as lepidopteran activity.

AGRO 150

Renal potassium channels of mosquitoes as potential new insecticidal targets

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Malpighian tubules play vital roles in the excretory functions of mosquitoes. The tubules generate urine by active transepithelial secretion of potassium, sodium, chloride, and water from the hemolymph to the tubule lumen. Previous physiological studies by our laboratory on isolated mosquito Malpighian tubules have demonstrated that barium-sensitive potassium channels are critical to urine production, but the molecular identities of these channels have not been resolved. In the present study, we show that: 1) mosquito Malpighian tubules express at least 3 putative inward-rectifying potassium (Kir) channel genes; 2) one of these genes indeed encodes a barium-sensitive potassium channel when expressed heterologously in *Xenopus* oocytes; and 3) a novel small molecule antagonist of a mosquito Kir channel inhibits urine production in isolated Malpighian tubules and elicits desirable sub-lethal effects in intact mosquitoes when injected into the hemolymph. Funded by a grant from the Foundation for the NIH, VCTR program.

AGRO 151

Development of acylpiperidine and carboxamide repellents using structure-activity models

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The US Department of Agriculture (USDA) has developed repellents and insecticides for the US Military since 1942. Data for over 30,000 compounds are contained within the USDA archive. Repellency data from similarly structured compounds were used to develop artificial neural network (ANN) models to predict new compounds for testing. Compounds were synthesized and evaluated for their repellency against *Aedes aegypti* mosquitoes. The complete protection time (CPT) of compounds was used to develop Quantitative Structure Activity Relationship (QSAR) models to predict repellency. Successful prediction of novel acylpiperidine structures by ANN models resulted in the discovery of compounds that provided protection over three times longer than DEET. The acylpiperidine QSAR models employed 4 descriptors to describe the relationship between structure and repellent duration. The ANN model of the carboxamides did not predict compound structures with exceptional CPTs as accurately; however, several carboxamide candidates did perform equal to or better than DEET.

AGRO 152

Mosquito biting deterrence: Structure-activity relationship of saturated and unsaturated fatty acids

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We systematically evaluated, for the first time, the biting deterrent effects of a series of saturated and unsaturated fatty acids against *Aedes aegypti* using the K & D bioassay system. The saturated fatty acids ($C_{6:0}$ to $C_{16:0}$ and $C_{18:0}$) and unsaturated fatty acids ($C_{11:1}$ to $C_{14:1}$, $C_{16:1}$, $C_{18:1}$, and $C_{18:2}$) showed Biting Deterrence Index (BDI) values significantly greater than ethanol, the negative control. Among the saturated fatty acids, mid-chain length acids ($C_{10:0}$ to $C_{13:0}$) showed the highest biting deterrent activity against *Ae. aegypti* as compared to short chain length acids ($C_{6:}$ to $C_{9:0}$) and long chain length acids ($C_{14:0}$ to $C_{18:0}$) except $C_{8:0}$ and $C_{16:0}$ where the activity was significantly higher than the other short and long chain acids. The *in vivo* treated-cloth-patch assay system results will also be discussed.

AGRO 153

Mode of action of insect repellents

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The mode of action of DEET and other insect repellents has been a topic of interest since the discovery of DEET in the mid-twentieth century. Nearly 60 years have passed since DEET applied topically to the skin was shown to be effective in preventing mosquito bites. With the discovery and characterization of odorant receptors in insects, modern technology has provided the tools necessary to characterize the effects of insect repellents at the molecular level. Now DEET has been shown to modulate responses of odorant receptors to chemical signals, thus scrambling messages sent to the brain of the insect leading to disruption of behavior. Taste receptor neurons have also been shown to detect DEET resulting in inhibition of feeding. These studies and other recent results provide a better understanding of how insect repellents exert their effects and insight into strategies for discovery of chemicals with enhanced repellent activity.

AGRO 154

Neurotoxicology of N,N-diethyl-*meta*-toluamide (DEET)

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There are still questions regarding the mode of action of biting insect repellents, such as DEET, upon odorant receptors and related ion channels. Recent studies have also raised the possibility that DEET is an anticholinesterase and that this action may contribute to its effects in insects and cause risk of toxicity in exposed humans. We have confirmed that DEET is lethal to *Aedes aegypti* mosquitoes at topical doses in the microgram range, but observed that DEET is an extremely poor anticholinesterase (<10% inhibition of *Aedes* enzyme), even at a concentration of 10 mM, whereas human, *Drosophila melanogaster*, and *Musca domestica* enzymes are more sensitive (IC_{50}'s of ca. 10 mM). Thus, while DEET shows excitatory signs of intoxication in mosquitoes, it seems unlikely that anticholinesterase action would be the major determinant of acute effects. Results of additional mode of action analyses will be discussed in the context of DEET neurotoxicity.

AGRO 155

Management of excess reactive nitrogen in the environment

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Managing the impacts of excessive reactive nitrogen (Nr) in the environment is a complex problem that begins with the recognition of the dietary need for Nr by all living populations. The human solution to this need has been to devise ways to bring Nr into the biosphere (via the Haber-Bosch process) where it can be used to grow sufficient food to support our population. Other Nr is created as a by-product through human-devised combustion processes for generating power. The net result is the introduction of more than five times the Nr created by natural processes in the US, only a fraction of which is converted back to diatomic nitrogen through denitrification. This presentation summarizes findings and recommendations of the US EPA Science Advisory Board's Integrated Nitrogen Committee report, *Reactive Nitrogen in the United States: An Analysis of Flows, Consequences, and Management Options*, that deal specifically with approaches for solving the excess Nr problem.

AGRO 156

Trends in emissions of reactive nitrogen from US agriculture

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The use of synthetic forms of nitrogen in US agriculture has had dramatic impacts on agricultural productivity over the last 50-60 years. However, agriculture is viewed as an inefficient and leaky system for utilizing nitrogen. Gains in nitrogen use efficiency in both plant and animal productivity have been slow compared to improvements in yield. Reactive nitrogen losses to the environment from US agriculture continue to be problematic. Atmospheric transport of reactive nitrogen will be used as a case study to illustrate the difficulty in reducing reactive nitrogen emissions from agriculture. Trends in emissions of reactive nitrogen will be discussed along with the most recent advances in science that can alter the trends in emissions. Science strategies for reducing reactive nitrogen in US agriculture will be highlighted.

AGRO 157

Agriculture and nitrogen: A view of 80 years of maize production

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The Haber-Bosch process earned Nobel prizes for the inventors, created inexpensive nitrogen for crop production, and dispelled Malthus' prediction of catastrophic human population decline. The eventual commercialization of hybrid maize in the 1920s by Henry A Wallace and concomitant management practices have created a crop-production system with consistent annual maize yield improvements. More options are needed for growers around the world to improve and maintain crop production sustainably, which includes improved nitrogen utilization. Solutions for intensifying global maize production while simultaneously improving nitrogen utilization will require a more comprehensive strategy for nitrogen management. This will include use of sound agronomics and manure management practices as well as adoption of innovative technologies like crop sensors, better nitrogen formulations (i.e., inhibitors, stabilizers, and slow-release products), and improved maize hybrids and biotech traits. Delivery of these solutions to developing countries will require investment in infrastructure, extension, and market access.

AGRO 158

Estimation of national-scale bidirectional ammonia flux using a coupled air quality and farm management modeling system

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Measurements of ammonia fluxes from agricultural soils receiving supplemental fertilizer applications have demonstrated that agricultural management practices influence the magnitude, direction, and temporal patterns of emission and deposition. The 2012 release of the Community Multiscale Air Quality (CMAQ) model version 5.0 captures these observations by including an option for coupling national simulations of agricultural practices using the USDA's Environment Policy Integrated Climate (EPIC) model with CMAQ to estimate NH_3 emissions from fertilizer application and to improve parameterization of the bidirectional air-surface exchange of NH_3. This coupled modeling system results in improved evaluations against reduced nitrogen wet deposition and ammonium aerosol observations. Bidirectional NH_3 exchange reduced the continental US annual total N deposition estimates in CMAQ by 5%, but resulted in much larger regional deposition changes. The coupled model continues to be refined and updated, and recent enhancements and updated results will be presented.

AGRO 159

Predicting the reactive nitrogen footprint of milk production systems

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On dairy farms, nitrogen is required to grow the crops that supply feed protein to maintain animals, and much of this nitrogen is recycled back to the crops through manure application. This recycling forms a closed system, but there are many leaks to the environment including ammonia emission from manure sources, nitrous oxide emission from soil and manure, and runoff and leaching of dissolved nitrogen to surface and ground waters. In addition, secondary losses of nitrogen-containing compounds occur during the production of resources used on the farm including fuel, electricity, machinery, fertilizer, and purchased feed or animals. A new component was incorporated in the Integrated Farm System Model that sums these primary and secondary sources to give the total reactive nitrogen loss from the production system per unit of milk produced. This new tool is used to evaluate and compare the effects of alternative production strategies on this reactive nitrogen footprint of milk production.

AGRO 160

Estimation of ammonia emissions from beef cattle feedyards in the southern High Plains with process-based modeling

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Ammonia (NH_3) emissions from beef cattle feedyards represent N loss and can have negative environmental consequences. Models have been developed to estimate NH_3 emissions from various livestock production systems, however little work has been conducted to assess their accuracy for large open-lot feedyards. To validate Manure-DNDC, a process-based biogeochemical model, simulated NH_3 flux was compared to emissions data collected from two commercial feedyards in the Texas High Plains. Model predictions were in good agreement with measured observations from both feedyards ($p < 0.001$), and reflected high sensitivity to variations in air temperature and dietary crude protein level. Predicted mean daily NH_3 flux densities for the two feedyards were 43.6 and 55.7 kg NH_3-N ha^{-1} d^{-1}, and were not significantly different from observed data. This indicates that Manure-DNDC can assist with NH_3 emissions reporting for commercial feedyards, and can be used to evaluate the effects of management practices on N loss.

AGRO 161

Ammonia emissions from beef cattle feedyards: A summary of seven years of research

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Beef cattle feedyards in the US annually emit about 400 Gg of ammonia-N to the atmosphere. We summarize seven years of field and laboratory research on ammonia emissions from beef cattle feedyards on the southern High Plains. Daily and annual ammonia emission patterns depended strongly on temperature, with summer emissions consistently twice those during winter. Ammonia emissions were also sensitive to crude protein content of cattle diets. Ammonia emissions increased from 25-50% when crude protein increased above requirements of cattle. Annually, ammonia emissions averaged from 80 to 130 g NH_3-N $head^{-1}$ d^{-1}, which was 52 to 59% of fed N. We tested strategies to reduce ammonia emission, including reducing N intake, urease inhibitors, and ammonium binders. Reducing N intake was the most economically and operationally feasible strategy, but a feeding environment that includes higher protein ethanol byproducts like distillers grains challenges efforts to reduce ammonia emissions.

AGRO 162

Nitrous oxide emissions from biofuel crops and its parameterization in the EPIC biogeochemical model

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Soil nitrous oxide (N_2O) emissions from agricultural crop production for biofuels offset greenhouse gas reductions accomplished by replacing fossil fuels with biofuels. Crops with potentially lower nitrogen demand, such as grasses (e.g., switchgrass), might exhibit lower N_2O emissions from soil relative to other biofuel crops, leading to lesser climate impacts. In North Carolina, switchgrass has the potential to become a bio-energy feedstock. However, its N_2O emission rate is not yet fully characterized. In this study we compare soil emissions of N_2O and nitric oxide (NO) from switchgrass and corn fields for different fertilizer (ammonium sulfate granular, $(NH_4)_2SO_4$) application rates at a site in the southeast US for the purpose of calibrating and testing for the Erosion Productivity Impact Calculator (EPIC) biogeochemical model.

AGRO 163

Survey sampling approach for estimating upper centile pesticide concentrations from surface water monitoring

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A survey sampling approach is presented for estimating upper centiles of aggregate distributions of surface water pesticide concentrations obtained from water monitoring programs with large sample sizes but variable sampling frequency. It is applied to three atrazine monitoring programs of Community Water Systems (CWS) that used surface water as their drinking water source: 1. The nationwide Safe Drinking Water Act (SDWA) data, 2. The Syngenta Voluntary Monitoring Program (VMP), and 3. The Atrazine Monitoring Program (AMP). Requisite sample sizes are determined using statistical tolerance limits, relative standard error, and the Woodruff interval sample size criterion. These analyses provide 99.9% confidence that the existing data include the 99.9th centile atrazine concentration for CWS raw and finished drinking water in the Midwest atrazine use areas and in the nationwide SDWA dataset, assuming no bias due to nonrandom selection of CWS and monitored days during these years. The general validity of these approaches is established by a simulation that shows estimates to be close to target quantities for weights based on sampling probabilities or time intervals between samples.

AGRO 164

Watershed characterization: An overview of how watersheds can be classified and compared in terms of their environmental characteristics, their potential vulnerability to runoff from agricultural fields, and the presence of existing agricultural structural mitigation features

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Several approaches exist for understanding and comparing the potential vulnerability of watersheds to surface water runoff. However, these current approaches are typically limited by the quality/quantity of environmental data for model development and lack sufficient high quality monitoring data for validation. This new approach is based on a program with over 180 site years of monitoring data across ~70 small headwater watersheds combined with high resolution spatial analyses to characterize key drivers for watershed-scale agrochemical runoff. Multivariate analyses indicated how field-by-field scale agricultural operations aggregate to contribute to overall watershed behaviour. The resulting predictions, modified by an understanding of the presence of structural best management practices, can predict, classify, compare and contrast watershed runoff potential. Four key contributing factors to watershed-scale agrochemical runoff were identified: field-scale environmental vulnerability, presence of structural and behavioural best management practices as well as stochastic factors associated with application timing relative to rainfall intensity/timing.

AGRO 165

Watershed characterization: Multivariate approaches for identifying key factors contributing to potential vulnerabilities for agrochemical runoff in small headwater Midwest watersheds

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An earlier paper provided an overview of the use of monitoring and environmental spatial data from ~70 small headwater watersheds to characterize key contributing factors leading to watershed-scale agrochemical runoff potential. This paper provides more detail on the multivariate analysis and visualization approaches. Data included daily monitoring across several seasons accompanied by weather, flow measurements, and crop observations. Numerous spatial environmental variables as well as combined and derived data (e.g., measures such as co-occurrence of shallow clay pan depth ranges with slopes in agricultural fields and over 200 PRZM model runoff model outputs) were aggregated at both watershed and individual field scales. Multivariate analysis involved identifying key response variables followed by correspondence analyses, non-metric multi-dimensional scaling, and various principal components techniques. Principal component 1 derived from field-by-field data overlaid closely with exposure metrics. A process was developed for visualizing and quantifying aggregated watershed results, enabling simple watershed-to-watershed comparisons.

AGRO 166

Watershed characterization: Approaches to characterizing agricultural stewardship practices and best management related structural features in small headwater Midwest watersheds and an assessment of their potential significance in determining the potential for agrochemical runoff

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Earlier papers provided an overview of the use of monitoring and environmental data from ~70 small headwater watersheds to characterize key factors contributing to watershed-scale agrochemical runoff potential and detailed the multivariate analyses and visualization approaches used. This paper describes how these monitored watersheds have also been characterized on a field-by-field basis in terms of agricultural stewardship practices. Careful interpretation of high resolution photographic imagery (occasionally enhanced by techniques such as LiDAR) allowed field-by-field categorization of the presence of various agricultural stewardship practices and BMP's. We identified a critical subset of structural stewardship practices including terracing categories, filter strips, and grassed waterways. The occurrence of these permanent landscape changes was used to modify field-by-field estimates of potential runoff vulnerability based on spatial/environmental factors. Preliminary evaluation of this approach suggests runoff vulnerability models based solely on environmental factors may be misleading since effective farmer stewardship may outweigh intrinsic vulnerability estimates.

AGRO 167

Integration of SWAT modeling and pesticide monitoring to assess aquatic life exposure in an Oregon watershed

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Pesticide loading into surface water is a complex process influenced by pesticide physiochemical properties, agronomic practices, climatic variables, landscape characteristics, and hydrology. Dynamic ecohydrologic models have become useful tools in developing an understanding between agronomic practices and pesticide occurrence in surface waters. The Soil & Water Assessment Tool (SWAT), a watershed scale hydrologic and environmental fate model was used to evaluate pesticide loading in the Zollner Creek watershed, located in Oregon's Willamette Valley. To maximize the utility of SWAT in assessing aquatic life exposure patterns, measurements of stream flow and pesticide concentration are necessary to parameterize the model. Pesticide surface water monitoring data collected between 1993 and 2005 were used to calibrate SWAT. Using the calibrated model simulation results were compared to pesticide surface water monitoring data collected between 2007 and 2011.

AGRO 168

Refined application of the SWAT model for endangered species effects determination

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The Soil and Water Assessment Tool (SWAT) model was applied to assess estimated environmental concentrations (EECs) in the Watsonville Slough (WVS) watershed near Salinas California as part of an endangered species effects determination. The WVS watershed has historically-high pesticide use and contains California Red-Legged Frog (CRLF) critical habitat coinciding with streams, agricultural ditches, and shallow impoundments (sloughs). The SWAT model was constructed to incorporate pesticide application patterns based upon historical use extracted from the California Pesticide Use Reporting (PUR) database. In addition, the SWAT model was modified to include the input of pesticide spray drift to water bodies within the watershed. A Monte Carlo simulation approach was employed to account for uncertainty in the spatial and temporal distribution of pesticide applications, hydrologic characteristics of the sloughs, and spray drift inputs. The modeling results at multiple locations across the watershed allowed for a more robust, probabilistic set of EECs and eventual effects determination.

AGRO 169

Evaluation of a simplified SWAT model approach for prediction of insecticide concentrations in a small watershed in northwestern Oregon

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The need for a modeling approach to estimate pesticide concentrations in flowing water bodies has become increasingly important due to the endangered species assessment process. To address this need, a modeling approach using the Soil and Water Assessment Tool (SWAT) was developed and tested for a widely used corn herbicide on 30 watersheds across the corn belt and southern US. The assessment evaluated the ability of SWAT to predict pesticide concentration distributions using a simplified parameterization approach. The encouraging results from this study led to the application of the methodology to an insecticide in a different geographic region, Northwest Oregon. In stark contrast to the original watersheds studied, the Oregon watershed modeled included heterogeneous cropping patterns with a more variable pesticide use pattern. Simulation results from the Northwest Oregon watershed will be presented and the potential for transferring of the herbicide-based modeling approach to other classes of pesticides will be discussed.

AGRO 170 - Withdrawn

AGRO 171

High-throughput LC-MS/MS analysis of acetochlor residues in raw agricultural commodities

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The throughput for quantitation of acetochlor residues in various raw agricultural commodities (RACs) has been increased 5-10 fold over existing methodologies by leveraging process improvements in our laboratory. Production of uniform and consistent sub-samples by secondary cryogenic milling has enabled the direct scale-down of sample size to a liquid-handler compatible 96-well format. This format allows subsequent extractions and cleanup procedures to be performed in parallel. These modifications have led to improved consistency and robustness of the method while simultaneously reducing cost and ergonomic risks associated with sample processing. The key components that dramatically increased the net sample throughput will be addressed in the presentation.

AGRO 172

Cost effective analytical methods for the determination of TRIAZOLE residues in plant matrices using LC-MS/MS

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The triazole classes of fungicides are systemic and control wide ranges of fungal diseases on crops. There are many triazoles with U.S. crop tolerances and a number of others with or pending import tolerances. The triazole fungicides have four common metabolites: 1,2,4-triazole (T), triazolylalanine (TA), triazolylacetic acid (TAA) and triazolyllactic acid (TLA), which are regulated by the USEPA for cumulative risk assessments.

For the registration of these fungicides and tolerance establishment, a residue analytical method for these four analytes was developed using LC-MS/MS by BASF with a limit of quantitation ranging from 0.01 to 0.05 mg/kg. The method development was challenging due to the diverse chemical nature of these analytes. This cost effective method was a shake and shoot approach which produced rapid analysis with high sample throughput (30-40 samples/day/analyst). In this presentation, the method description, results with accuracy and precision will be discussed.

AGRO 173

Use of SRMs in method development and validation

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The National Institute of Standards and Technology (NIST) has developed a variety of solution and natural-matrix Standard Reference Materials (SRMs) characterized for pesticides, polycyclic aromatic hydrocarbons, and other organic contaminants. Solution SRMs, such as SRM 2261 Chlorinated Pesticides in Hexane (Nominal Concentration 2 µg/g), are useful in spiking samples and for evaluating analyte recoveries, in addition to validating chromatographic separations and determining response factors of individual organic constituents. Natural-matrix SRMs, such as SRM 1941b Organics in Marine Sediment, are intended for use in analytical method validation and as quality control materials for the determination of contaminants. NIST has also coordinated a number of intercomparison quality assurance exercises for contaminants in tissue and sediment samples. These activites are invaluable for assessing interlaboratory, analytical comparability among the environmental measurement community. This talk will focus on the use of certified reference materials in method development and validation including examples from quality assurance exercises.

AGRO 174

Ruggedness testing and validation of a practical method for more than 100 veterinary drug residues in bovine muscle by UHPLC-MS/MS

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Motivated by the necessity of the USDA's Food Safety and Inspection Service (FSIS) for a screening method to monitor veterinary drug in bovine tissues, and in continuation of our previous research on bovine kidney, our research group has investigated the ruggedness testing and validation of a simple and reliable method for bovine muscle. This ruggedness study consisted of testing different clean-up sorbents, calculating amount of co-extractives, evaluating matrix effects using post-column infusion of representative analytes and determining recoveries and reproducibility. Also, the effect of 2- and 4-fold dilutions before injection was measured. As part of the optimization process, we evaluated different mobile phases and ultimately chose to use post-column infusion of ammonium formate as an ionization enhancer for the late eluting anthelmintics. The results obtained from multi-day validation showed good qualitative performance demonstrating that the method is suitable for FSIS screening purposes at or below US regulatory tolerance levels.

AGRO 175

GC-MS method for determination of pesticides residues in vegetables, fruits, and cereals: Validation and uncertainty estimation following the Eurachem guides

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The AOAC official method 2007.01 has been used for the determination of pesticides belonging to different classes, in vegatables, fruits, and cereals. The extraction and purification of the samples has been performed using QuEChERS (Quick, Easy, Cheap Effective, Rugged, Safe) methodology. The analysis is done using Gas Chromatography-Mass Spectrometry with single ion monitoring. The method is single laboratory validated following the Eurachem guide (Eurachem/Citac Guides 2000 Quantifying Uncertainty in Analytical Measurement and 1998 The Fitness for Purpose for Analytical Chemistry) and the Document SANCO12495/2011, and using fortified samples with reference materials at three different concentration levels. The limit of detection (LOD) has been calculated from the calibration curve performed in matrix; the accuracy, expressed in terms of trueness and precision, was verified by performing repeated analysis of fortified samples. Another common expression of accuracy is the measurements of uncertainty; it has been estimated following the bottom-up approach.

AGRO 176

Sample preparation strategies for multiresidue screening, targeted, and confirmatory analysis: Is your sample preparation good enough?

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Typically, an analytical screening method is performed to identify and to quantify many possible residues using a single and simple sample preparation method. Depending on the selectivity of the screening method and the sensitivity of the analytical instruments available, a targeted or confirmatory analysis may be required for residues initially detected with the screening method. Recently, a non-registered fungicide residue, carbendazim, was detected in orange juice. In this presentation, we will discuss sample preparation strategies for determination of multiresidue pesticides, including carbendazim. We will focus on the requirements for the initial screening method using a standard screening protocol (QuEChеRS) and LC-MS/MS with low ppb limits of detection. We will then discuss sample preparation strategies for targeted confirmatory analysis of carbendazim using LC/MS and also LC/UV with sub-ppb detection limits. A similar approach will be discussed for screening and targeted analysis of veterinary drug residues.

AGRO 177

Analysis of pesticides by QuEChERS in fatty samples: Application of Z-Sep+ sorbent

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The concept of dispersive solid phase extraction (dSPE) cleanup (otherwise known as QuEChERS method) for the analysis of contaminants in food samples is an example of just enough cleanup before the end-analysis is performed. The current SPE phases for QuEChERS include: C18 for the removal of lipid components, primary-secondary amine (PSA) for the removal of acids, polar pigments and sugars, and graphitized carbon black (GCB) for the removal of pigments such as chlorophyll. Here we introduce the use of a new SPE phase, Z-Sep+, and compare it to the most common sorbents used for cleanup. The first application that will be discussed is analysis of pesticides with detection by LC-MS. The cleanup and the recovery of pesticides was evaluated from a number of foods (olives, nuts) when Z-Sep+ cleanup or conventional sorbent cleanup were used. The second application is analysis of pesticides in high-fat fruit (avocado) by GC-MS. We have found that Z-Sep+ sorbent is performing better then C18 for the removal of fats in model solutions including glycerides and phospholipids. It was applied to the cleanup of the avocado extracts in combination with and without the PSA sorbent. The recoveries and the method ruggedness by both methodologies will be discussed

AGRO 178

Insectidical azetidines

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The chemistry and insecticidal activity of certain 4-aryloxy azetidines will be presented.

AGRO 179

Synthesis and herbicidal activity of novel substituted pyridazin-3(*2H*)-one methanesulfonylisoxazolines

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Discovered at Kumiai, pyroxasulfone is a substituted pyrazolyl methanesulfonylisoxazoline herbicide in development for preemergent weed control in corn, soybeans, and cereals. The compound is representative of a new class of potent very long chain fatty acid (VLCFA) biosynthesis inhibitors that have a much lower use rate and broader activity spectrum than older acetanilide-based products with this mode of action. In our search for a novel chemotype from this area of chemistry, we recently reported that pyrimidinone substituted methylsulfonylisoxazolines such as **1** also expressed very high levels of herbicidal activity with crop safety. Potent inhibition of VLCFA biosynthesis was also observed for **1** . This work demonstrated that a “carbonyl-containing” heterocycle could serve as an effective surrogate to a traditional heteroaryl ring and, in the case of **1** , the pyrimidinone carbonyl group also served as a critical *ortho* substituent to the methanesulfonyl bridge. In the substantial optimization effort that followed, a number of carbonyl-containing heterocyclic variations were explored. Here, we report on the synthesis and herbicidal activity of a series of pyridazin-3(*2H*)-one methylsulfonylisoxazolines as represented by **2** .

AGRO 180

Insecticidal alkylsulfur compounds

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A series of haloalkylthio derivatives were prepared to investigate their insecticidal activity. We have found that compounds such as those of Formula 1 show strong potency on several important insect species of Lepidoptera and Hemiptera. The chemical synthesis, biological activity, structure-activity relationships, and studies on the mode of action will be presented.

AGRO 181

Synthesis of fluorinated diphenylmethane derivatives as insecticides

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Tetrazoles of Formula 1 were reported to have strong insecticidal activity. We were interested in exploring activity of the carbon-linked analogs of Formula 2. In this poster we will present the chemical synthesis, biological activity, and results of studies on the mode of action.

AGRO 182

Insecticidal heteroaromatic tetrazoles

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In the 1980s ICI reported that a class of diarylsubstituted tetrazoles possessed good levels of insecticidal activity. A replacement strategy for the aromatic rings with heterocycles was undertaken. These compounds also showed potent activity against insects such as the diamondback moth. Synthetic methods used to prepare this class of compounds will be presented along with a summary of the biological activity and structure-activity relationships.

AGRO 183

Fungicidal pyridazinone carboxanilides

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Pyridazinones have proved to be a good ring scaffold for the discovery of crop protection products. We have found that pyridazinone 4-carboxanilides and their heterocyclic equivalents have fungicidal activity against *Puccinia recondita* and other economically important pathogens. Methods to synthesize these compounds will be presented along with a summary of the biological activity and structure-activity relationships of this class.

AGRO 184

Ortho-Heterocyclic substituted phenyl anthranilic diamide insecticides

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Anthranilic diamides were prepared from *ortho*-heterocyclic aromatic carboxylic acids. Both *C*-linked and *N*-linked heterocycles were prepared. These compounds proved to have good levels of insecticidal activity on Lepidopteran insects. Synthetic methods to prepare these compounds will be presented along with a summary of the biological activity and structure-activity relationships of this class.

AGRO 185

Pyrazole-N-acetamides as starting points for herbicide discovery

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Pyrazole acetamides represent an active class of herbicides which have been known for over 30 years. We have investigated a number of approaches to modify the core structure to design novel active herbicides. Among these were amide replacement by heterocycles, constraining the aromatic ring in a ring and replacing the pyrazole with a 1,2,3-triazole. Synthetic methods to prepare these compounds will be presented along with a summary of the biological activity and structure-activity relationships of this class.

AGRO 186

Fungicidal pyrazinone-2-carboxamides

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Pyrazinones with a variety of heteroatom-containing substituents at the 2-position exhibit potent fungicidal activity. Amides which are bonded to the ring through either nitrogen or carbon retain high levels of broad-spectrum activity. Methods to synthesize these compounds will be presented along with a summary of the biological activity and structure-activity relationships of this class.

AGRO 187

Insecticidal 4-piperazinyl pyridazinones

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The pyridazinone ring system has proved to be a rich source of leads for the discovery of crop protection products. We have found that 4-piperazinyl and 4-piperidinyl substituted pyridazinones have insecticidal activity against *Lepidopteran* insects. Synthetic methods to prepare these compounds will be presented along with a summary of the biological activity and structure-activity relationships of this class.

AGRO 188

4-(2-Pyridinyl)-5-halo-imidazoles as powdery mildewicides

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As an attempt to explore the effect of ring contraction in an area of pyrazinone fungicides, 4-(2-Pyridinyl)imidazoles were synthesized. These compounds showed fungicidal activity on powdery mildews in greenhouse testing. Synthetic methods used to synthesize this ring system will be presented along with a summary of the biological activity and structure-activity relationships.

AGRO 189

Phenyl substituted thiazoles as fungicides

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Combining our in-house fungicide hit **1** (4,5-diphenyl substituted thiazole analog) and Bayer's recent (WO2010/069494) thiazole analog **2** (4-phenyl 5-pyridyl substituted thiazole), led to the discovery of a novel fungicide analog **3** with good activity. Optimization of different substituents on the phenyl ring, pyridine ring, and at the C2 position of the thiazole was studied to find lower application rate fungicide. Synthesis and structure-activity relationships of these substituted thiazoles will be presented.

AGRO 190

PI3 kinase inhibitors as fungicides

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Scouting around Pfizer's PI3 kinase inhibitor **1** (WO2010/038165), led to the discovery of imidazonapthyridine **2** with good fungicidal activity. A substantial optimization effort followed with many substitutions on the pyridine ring and imidazolone ring were explored for better fungicidal activity at lower application rates. Synthesis, biology, and structure activity relationships of imidazonapthyridines as well as the bicyclic quinoline central core **3** will be detailed.

AGRO 191

Modeling of herbicide binding in the inhibition of acetyl-CoA carboxylase

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Inhibition of the biosynthesis of fatty acids is an important mode of action for a variety of postemergence herbicides. These include the aryloxypropionic acid derivatives and substituted cyclohexanediones, used to control annual and perennial grasses. In grasses these herbicides block fatty acid biosynthesis by inhibiting the transcarboxylation step in the transformation of acetyl Co-A into malonyl Co-A by the enzyme acetyl Co-A carboxylase. Broadleaf crop plants in weed-treated fields are not affected. Two enzymatic steps are involved: 1) the carboxylation of biotin linked to a carrier protein and 2) the transfer of this biotin activated carboxyl group to acetyl Co-A. Although the transcarboxylation domain is the binding region, both classes of herbicides interact with different sets of residues in the protein and bind at slightly different, overlapping zones. In this study, binding by congeners of these herbicide classes was modeling by molecular docking of these herbicide molecules with carboxylase and compared with known structures. Binding affinities in the protein were computed and compared for aryloxypropionic acids and cyclohexanediones using ab initio and density functional methods.

AGRO 192

Allelopathic potential of *Rhododendron formosanum* Hemsl in Taiwan

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Bidens pilosa was used as a test species in greenhouse and laboratory experiments. The powdered leaves of *R. formosanum*, when mixed in soil at 1% concentration, moderately suppressed the growth of *B. pilosa* seedlings. Aqueous leachates of *R. formosanum* flowers, leaves, litter, and organic matter inhibited the radicle growth of *Ageratum houstonianum*, *Amaranthus inamoenus*, *Brassica chinensis*, *Bidens pilosa*, *Lactuca sativa*, and *Ocimum basilicum*. The aqueous leaf extract contained the phytotoxins *p*-hydroxybenzoic acid, trans *p*-coumaric acid, syringic acid, vanillic acid, *cis* ferulic acid, methyl ferulate, coumarin, protocatechuic acid, and (-)-catechin. These findings and identification of phytotoxins suggests that the lack of understory species beneath an *R. formosanum* canopy was due to allelopathic effects.

AGRO 193

Allelopathic effects of biochanin A on selected weed species

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The uptake and allelopathic effects of biochanin A on monocot and dicot weed species were evaluated in agar medium bioassays with concentrations up to 400 μmol L^{-1}. The monocot *Echinochloa crus-galli,* the dicot *Geranium molle,* and the dicot *Silene noctiflora* were non-susceptible, susceptible, and very susceptible, respectively. Biochanin A and its known transformation products genistein, dihydrobiochanin A, pratensein, and coumaric acid were found and quantified in all tested weed species using LC-MS and pure reference standards. Concentrations of all compounds were higher in roots than in shoots. The uptake of biochanin A was highest in *G. molle*. For identification of unknown compounds principal component analysis was performed using the peaks observed during LC-MS. An unknown compound displaced along the first principal component was identified as biochanin A 7-*O*-β-D-glucopyranoside (sissotrin). Glucosylation thus appears to be a mechanism for detoxification of biochanin A.

AGRO 194

Establishing acceptability criteria for assessing the homogeneity and stability of test substances in artificial arthropod diets

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Regulatory agencies require thorough environmental risk assessments (ERAs) of genetically modified (GM) crops such as those expressing insecticidal proteins. ERAs typically follow a tiered approach for evaluating the potential adverse effects GM crops might have on the agroecosystems in which they will be cultivated. Laboratory testing requires incorporation of test substances such as purified protein or GM plant material into artificial diets in order to evaluate their effects on non-target organisms relevant to the ERA. Good laboratory practice (GLP) guidelines require homogeneity and stability of the test substance in the diet be established; however acceptability criteria are not well-defined. Factors to consider for homogeneity and stability assessment of artificial diets—such as the need for validated analytical methods—as well as recommendations for establishing acceptability criteria, are discussed.

AGRO 195

Herbicide washoff from forest canopy through-fall depends on rainfall dynamics

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Fate of the herbicides atrazine and metolachlor, released to the atmosphere and deposited in rain, was studied following their field application in a small agricultural watershed located in Maryland. We monitored delivery of herbicides in the rain in both open and closed canopy areas of a forested riparian buffer at different distances from the field. We observed a direct linear relationship between precipitation amounts and decreases in the volume of rain collected under a tree canopy, as compared to the volume of rain collected in the tree-free areas. For the lowest range precipitation, the rain volume collected under the tree canopy was around 60% of the rain collected in the open area; however, for precipitations above 30 mm, it was around 90%. We utilized an established relationship to calculate atmospheric deposition of herbicides to the riparian buffer during rain based on monitored precipitation and herbicides analyses of the rain.

AGRO 196

Exploring the association of the metolachlor metabolite MESA and agricultural nitrate-N fate and transport in the Choptank River Watershed

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Nearly half of US water bodies and waterways are deemed impaired by Clean Water Act criteria with nonpoint source pollution from croplands a major contributor. Innovative monitoring and modeling strategies are needed to account for pollutant-matrix interactions, climatic conditions, and landscape complexity, especially for nitrate-N. MESA {2-[(2-ethyl-6-methylphenyl) (2-methoxy-1-methylethyl)amino]-2-oxoethanesulfonic acid}, a metabolite of the extensively used herbicide metolachlor, is an ideal nitrate-N tracer because MESA is highly stable and soluble, has a low K_{oc} value, and is formed in the unsaturated zone where nitrate-N is transported to groundwater. Here, we use MESA to track nitrate-N concentrations within the watershed of the Choptank River, a Chesapeake Bay tributary, and to identify critical nitrate-N source areas. Exploiting this fortuitous MESA-nitrate-N correlation in this and other intensive agricultural areas will allow policy makers and land managers greater ability in identifying areas where conservation and mitigation practices will be most effective at curbing agricultural nitrate-N pollution.

AGRO 197

Potential arsenic sources in a Choptank River subwatershed and the influence of land use and watershed characteristics

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Row-crop and poultry production have been implicated as water pollution sources along the Choptank River, an estuary and tributary of the Chesapeake Bay. Arsenic, found in a poultry feed additive, is a possible poultry facility marker. This study examined land use, subwatershed characteristics, and climatic condition effects on total arsenic concentrations in a Choptank River subwatershed. Catchments within the subwatershed were defined using advanced remotely sensed data and current geographic information system processing techniques. Water samples were collected May – October 2009 and April – June 2010 under mostly baseflow conditions. A negative correlation of arsenic concentration with percent forest was found and explained by head water signals and overland flow of particulate phase inputs. Service roadways at some poultry facilities were found to redirect runoff to neighboring catchments, affecting water

quality parameters. Results suggest possible arsenic point source signatures for poultry production facilities in this subwatershed compared to catchments without these facilities.

AGRO 198

Endosulfan wet depostion in southern Florida

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Vegetable and other crops are produced on about 25000 ha in southern Florida in an area adjacent to the Everglades and Biscayne Bay National Parks (NP). High pest pressures require high pesticide use rates. We recently reported that one mechanism for transport of the insecticide endosulfan from treated fields was volatilization after application and movement with prevailing winds to the NPs. Here we describe companion wet deposition measurements. Rain samples were collected continuously for 5 years (2002 to 2006) at sites within the agricultural community of Homestead, Florida and in the NPs. Wet deposition tracked endosulfan atmospheric measurements and seasonal use patterns. The highest deposition, ca. 90 ug m^{-2} yr^{-1}, was observed within Homestead's crop-production area with most deposition occurring during winter months when vegetables were grown. At NP stations, wet deposition had the same seasonal pattern but annual rates were about 50-fold less.

AGRO 199 - Withdrawn

AGRO 201

Developing a web-based system for computing pre-harvest residue limits (PHRLs)

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This study describes the development of a web-based system that collects all data generated in research conducted to set pre-harvest residue limits (PHRLs) for agricultural product safety control. These data, including concentrations of pesticide residues, limit of detection, limit of quantitation, recoveries, weather charts, and growth rates, are incorporated into a database. A regression analysis of the data is performed using statistical techniques, and the PHRL for an agricultural product is automatically computed. The development and establishment of this system increased the efficiency and improved the reliability of the research in this area by standardizing the data and maintaining data accuracy without temporal or spatial limitations. The system permits automatic computation of the PHRL and a quick review of the goodness of fit of the regression model

AGRO 202

Analysis for oxytetracycline in soils using solid-phase extraction and liquid chromatography tandem mass spectrometry

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Antibiotics have been widely used in agriculture for many years. Concerns have been mounting regarding public health issues over the occurrence of antibiotics in the environment as well as indications of increased bacterial resistance in agricultural wastes. Hence there is a need for rapid and sensitive analytical methods to measure low-level concentrations of antibiotics in agricultural and environmental samples that may be impacted by exposure. Methods have been developed and validated for the trace level detection of Oxytetracycline (OTC) and its metabolite EPI-Oxytetracycline (EPI) in soil matrices using solid-phase extraction and liquid chromatography tandem mass spectrometry. OTC and EPI were extracted from two soil sample types using a 90/10 mixture of methanol/water (v/v) saturated with oxalic and citric acid. Aliquots are then removed and cleaned up using a polymeric C18 SPE method. Large concentrations of citric and oxalate buffers were required to improve extraction efficiency and improve precision. Method quantification limit in soils for OTC was demonstrated at 10 ng/g (LOQ) with recoveries that averaged 87% ± 4%. In addition, recoveries at 10XLOQ averaged 87% ± 4%. Method quantification limit in soils for EPI was demonstrated at 10 ng/g (LOQ) with recoveries that averaged 93% ± 14%. In addition, recoveries at 10XLOQ averaged 99% ± 7%. Calibration curves were linear over the range of 5 ng/g to 500 ng/g with correction coefficients of 0.995 or better. Supporting data are presented to address the challenges of analyzing OTC in soil. These analytes are particularly difficult because of the low detection limits required, the complexity of the samples, and difficult separations from interferences. OTC and EPI also readily form metal chelates in matrix and in the HPLC system, and they interact with silanol groupgs on columns causing peak tailing. These issues results in limited detection limits and higher variability. The final results will be discussed in terms of example environmental fate and terrestrial field dissipation studies.

AGRO 203

Comparison of LC/MS/MS and ELISA methodology for a typical allergen

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Allergic reactions are caused by an immune response to a substance not otherwise pathogenic. The quantity of allergen required to produce anaphylaxis varies greatly between individuals. Managing, identifying, and preventing trace allergen levels are therefore primary concerns for all food manufacturers. The most typical approach to quantifying proteins are ELISA-based methods; however, this methodology has limitations including high variability, a limited sensitivity range, and issues with antibody specificity. This paper compares the accuracy and sensitivity of LC-MS-MS methodology to an ELISA-based method for *Gly m Bd 30k* , a typical allergen in soybeans.

AGRO 204

Discovery of a novel glucuronide metabolite of methyltestosterone in tilapia bile by liquid chromatography/quadrupole-time of flight mass spectrometry

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In the United States, methyltestosterone (MT) is not approved for use in fish. However fish farmers may use MT for sex reversal, to produce fast growing all male population for economic gains. Therefore there is a need to develop methods for the detection of MT and its metabolite residues in fish tissue for monitoring its use for regulatory purposes. Previously, our laboratory had developed a liquid chromatography/quadrupole time of flight (LC/Q-TOF) method for the characterization of 17-*O*-glucuronide metabolite in bile of tilapia dosed with MT. The system used was an Agilent 6530 Q-TOF with a jet stream electrospray ionization interface. Utilization of the molecular feature extraction algorithm of the Agilent mass hunter software to screen against an in-house library of possible MT-metabolites in dosed tilapia bile has resulted in the discovery of a novel, major glucuronide metabolite of MT. Preliminary MS data indicate it to be a glucuronide of a hydroxylated MT. The novel glucuronide persists in tilapia bile for several days after dosing. We are presenting a rapid and sensitive LC/MS/MS method for the detection and characterization of the novel glucuronide metabolite in tilapia bile, which can serve as a marker to monitor the illegal use of MT in tilapia culture.

AGRO 205

Identification and quantification of organosiloxane and nonylphenol polyethoxylate surfactants in honey bee hive samples by LC-ESI-MS

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Organosiloxane and nonylphenol polyethoxylates are widely used as nonionic surfactants around honey bee hives or in their foraging areas as spray adjuvants or additives in agrochemical formulations. Our previous work on commercial adjuvants showed that trisiloxane polyethoxylates like Silwet L-77 and, less potently, the nonylphenol polyethoxylate Activator 90 reduced the learning performance of forager honey bees at 20 µg per bee, and Silwet L-77 at 1% oral dose was highly lethal to adult bees. Here, a method for the analysis of organosiloxane and nonylphenol polyethoxylate surfactants was developed. A combined liquid-liquid extraction and solid-phase extraction method was used. Identification and quantification were accomplished employing liquid chromatography coupled to electrospray ionization mass spectrometry (LC-ESI-MS). Both organosiloxane and nonylphenol polyethoxylate surfactants were found in honey and frequently in pollen samples. The possibility of recent bee declines being associated with these surfactants will be discussed.

AGRO 206

Micro-analysis of soil total and mineral nitrogen under different nitrogen fertilization levels

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Agricultural contamination by reactive nitrogen from nitrogenous fertilizers is a worldwide concern. In order to determine micro-spatial analysis of mineral (N-NO_3^- and N-NH_4^+) and total nitrogen (TN), surface soil samples (0-0.25 m) were collected during maize vegetation (June 2007) from a long-term experimental field in central Croatia (Popovaca). This study was carried out on drained Stagnosols in an area characterized by a continental climate where mean annual temperature is 10.7 °C and annual average rainfall is 865 mm. A 1 x 1 m sampling grid was established at treatments with four different nitrogen fertilization levels (0, 100, 200, 300 kg N ha^{-1}) and 16 samples were taken at every 0.25 m along a 1 m grid length. Mineral nitrogen was determined by ion chromatography and total nitrogen by the dry combustion method. The coefficients of variation (CV) for nitrate-nitrogen were 31.1-58.9%, for ammonium-nitrogen 27.7-53.8%, and for total nitrogen 6.9-10.0%. Variability described by variance indicate that variance increased with applied fertilization levels and average values for all treatments were 492 mg kg^{-1}, 77.5 mg kg^{-1} and 27,400 mg kg^{-1} for N-NO_3^-, N-$NH_4^{+,}$ and TN, respectively.

AGRO 207

pH-based method for measuring gaseous ammonia

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Gaseous ammonia concentration is often measured using an “acid trap” method, where ammonia is captured in an acidic solution that is later analyzed for total ammonia. This method is accurate, and depending on the technique used for analysis, can be inexpensive. However, it is labor intensive and difficult to apply at a high sampling frequency. In this work we describe a new acid trap method in which captured ammonia is determined from the pH of a citric acid solution using a speciation model. With this method, multiple measurements can be made with a single solution, and the sampling frequency is limited only by the sensitivity of the method. We tested this citric acid-pH (CA-pH) method through titrations, emission measurements, and measurement of gaseous ammonia on a dairy farm. Results showed that the CA-pH method is accurate, but has a higher quantitation limit than some other methods. It is best suited for measuring gaseous ammonia above about 0.5 ppm.

AGRO 208

Diamide insecticides: Global efforts to address stewardship challenges

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The diamide insecticides chlorantraniliprole, cyantraniliprole, and flubendiamide are ryanodine receptor modulators (IRAC Group 28) that are active on insects through the uncontrolled release of internal calcium from the cell. The diamides have become very successful in the marketplace with multiple offerings from different companies. However, with widespread adoption comes the risk of insect resistance. DuPont is taking a two-pronged approach to prevent or delay the evolution of resistance: 1) investing in a comprehensive baseline susceptibility survey and 2) working with other diamide-producing companies and interested stakeholders to develop and to implement resistance management strategies. The baseline susceptibility survey helps determine if any shifts in resistance are occurring. Joint initiatives by the diamide companies are helping disseminate the importance of resistance management to company sales teams and extension services.

AGRO 209

Fluorescent assay of acetylcholinesterase ligand interactions for design of insecticides targeting the mosquito vector of malaria, *Anopheles gambiae*

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There is an urgent demand to discover and to develop alternatives to conventional insecticides used in mosquito control due to their high toxicities to non-target organisms and development of resistance. Here we present fluorescence data on the interactions between various acetylcholinesterase (AChE) inhibitors and the AChE peripheral anionic site, which is considered to be a potential target for new insecticides acting on this enzyme. The assay uses thioflavin-t (TFT) as a probe, which binds to the peripheral anionic site of AChE and yields an increase in fluorescent signal. In the present study, we screened effects of AChE inhibitors on *Anopheles gambiae* AChE and human recombinant AChE to compare and to contrast changes of peripheral site conformation and catalytic ability responding to various inhibitors. Our results showed that all the inhibitors reduced TFT fluorescence with human recombinant AChE. With mosquito AChE, all the peripheral site inhibitors, two bivalent inhibitors, and one catalytic site inhibitor showed inhibitory effects on the TFT fluorescence. However, all the carbamates and two bivalent tacrine dimers potentiated the TFT fluorescent signal, suggesting a different mechanism for catalytic site ligands modulating the conformation of the peripheral site of mosquito AChE. This finding may provide insights into the structural differences between mosquito AChE and human AChE, which is a key point for the design of novel, selective insecticides.

AGRO 210

Explore new insecticidal site targeting on chitin synthesis enzymes in *Anopheles gambiae*

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Chitin biosynthesis represents an attractive target site for combating insect pests as this process is absent in humans and other vertebrates. However, current understanding of this process is rather limited in insects. The exact mechanisms of the chitin synthesis inhibitor insecticide benzylphenolureas, such as diflubenzuron, are still elusive. To explore the mechanisms of diflubenzuron, a high-throughput method was adapted and optimized to examine the chitin synthase activity and its inhibition by diflubenzuron, polyoxin D, and nikkomycin Z in mosquitoes. A chitosan/dsRNA nanoparticle-based RNA interference through larval feeding was developed to analyze the functions of chitin synthase genes. Mosquito larvae fed on the nanoparticles assembled *AgCHS1* and *AgCHS2* dsRNA increased larval susceptibilities to diflubenzuron, and calcofluor white or dithiothreitol, respectively. These results suggest a great potential for using such a nanoparticle-based RNAi technology for high-throughput screening of gene functions and for developing novel strategies for pest management.

AGRO 211

Selective actions of insecticides on nicotinic receptor subtypes

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Nicotinic acetylcholine receptors (nAChRs) are the major receptors for fast excitatory neurotransmission in the insect central nervous system and are among the most valuable insecticide target sites. There is a clear distinction between desensitizing and nondesensitizing nAChR subtypes, and it is well established that spinosyns act selectively on nondesensitizing nAChR subtypes. Neonicotinoids act on desensitizing nAChRs, of which at least two subtypes can be distinguished in many insects, based on differential sensitivity to neonicotinoids and desensitization kinetics. The commonly-used probe for insect nAChRs, [^3H]-imidacloprid, labels different populations of subtypes depending on concentration. Misleading results can be obtained if attention is not paid to the subtype being measured in binding assays. Our results using [^3H]-imidacloprid and voltage-clamp studies on native insect nAChRs provide an improved understanding of the selective actions on nicotinic receptor subtypes of novel subclasses of neonicotinoids recently launched or under development.

AGRO 212

Identification of a novel pyrethroid receptor site on a mosquito sodium channel

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Pyrethroids are a large class of structurally diverse, synthetic analogues of natural pyrethrins from the flower extracts of *Chrysanthemum* spp. The primary target site of pyrethroids is voltage-gated sodium channels, which are essential for the initiation and propagation of action potentials in the nervous system. Currently, pyrethroid insecticide-treated nets (ITNs) are the most powerful control measure to reduce malaria morbidity and mortality. A major threat to the sustained use of pyrethroids is the emergence of mosquito resistance to pyrethroids. Due to the lack of a functional expression system for mosquito sodium channels, the pyrethroid-receptor site in mosquitoes has remained elusive. Here, we report the establishment of a functional expression system for the *Aedes aegypti* sodium channel in *Xenopus* oocytes and identification of molecular determinants that are critical for the binding and action of pyrethroids. Our study provides critical information for monitoring sodium channel mutation-mediated pyrethroid-resistance in mosquito populations.

AGRO 213

Sodium channel inhibitor insecticides: Blurring the line between insecticides and drugs

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Sodium channel inhibitor (SCI) insecticides were discovered almost four decades ago, but have only recently yielded important commercial products (e.g., indoxacarb and metaflumizone). SCI insecticides inhibit sodium channel function by binding selectively to slow-inactivated (non-conducting) sodium channel states. Characterization of the action of SCI insecticides on mammalian sodium channels using both biochemical and electrophysiological approaches demonstrates that they bind at or near a drug receptor site, the local anesthetic receptor. This mechanism and site of action on sodium channels differentiates SCI insecticides from pyrethroids, lipid amides, and other insecticidal agents that act on sodium channels. However, SCI share a common mode of action with drugs currently under investigation as anticonvulsants and treatments for neuropathic pain. The properties that distinguish therapeutic and toxic state-dependent SCIs remain to be identified.

AGRO 214

Mode of action of metaflumizone on voltage-gated sodium channels

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Sodium channel inhibitor (SCI) insecticides are an emerging class of neurotoxic insect control agents that inhibit nerve function by stabilizing voltage-gated sodium channels in the slow-inactivated state. Metaflumizone is a newly-commercialized insecticide for the treatment of fleas on domesticated pets and is reported to inhibit slow-inactivated insect sodium channels selectively, thereby implying that it is also a member of the SCI class. Using the *Xenopus* oocyte expression system, we show that although metaflumizone preferentially inhibits rat $Na_v1.4$ sodium channels under experimental conditions that promote slow inactivation. It also appears to interact with channels in other states in a manner distinct from other compounds in the SCI class. We used site-directed mutagenesis to show that metaflumizone shares similar domain IV segment 6 (DIV-S6) binding determinants on $Na_v1.4$ channels with other SCI insecticides and therapeutic drugs. However, additional mutations made at V787 in DII-S6, which modulate slow inactivation, selectively reduced metaflumizone sensitivity in a residue-specific manner that was better correlated with side chain hydrophobicity rather than changes in slow inactivation gating. Together, these data provide useful insight into the mechanism of metaflumizone action on non-target related sodium channels.

AGRO 215

Characterization of ammonia emissions from agricultural sources in California and their implications for ammonium nitrate formation

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Ammonia (NH_3) is the dominant gas-phase base in the troposphere. Two major NH_3 sources from agricultural activity are animal waste and crop fertilization. Anthropogenic emissions of NH_3 and NO_x ($NO + NO_2$), which can be oxidized in sunlight to form nitric acid (HNO_3), can react to form atmospheric ammonium nitrate (NH_4NO_3) particles. Agricultural activity (e.g., dairy farms), and urban centers (e.g., Fresno, Los Angeles) are sources of ammonium nitrate gas-phase precursors in both the South Coast Air Basin and the San Joaquin Valley of California. Airborne measurements of NH_3, HNO_3, and particle composition made aboard the NOAA WP-3D aircraft as part of the CalNex 2010 field campaign are used to quantify NH_3 emissions from agricultural sources, describe the vertical structure and transport of NH_3 from these sources, examine its impact on ammonium nitrate formation, and contrast sources in the South Coast Air Basin to those in the San Joaquin Valley.

AGRO 216

Environmental and ecological effects of atmospheric nitrogen deposition

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Nitrogen emissions from agriculture, transportation, and industry result in elevated atmospheric nitrogen deposition, thus contributing to eutrophication and acidification effects in terrestrial and aquatic ecosystems. Such ecological and environmental impacts include: diversity loss in plant communities, acidification of soils and surface waters and associated effects on forest health and aquatic communities, N enrichment of remote lakes and changes in diatom assemblages, coastal eutrophication and dead zones, and harmful algal blooms. Additional impacts include elevated nitrate concentrations in water from forested watersheds, climate change effects, impaired visibility, and human health effects. Health effects from N depostiion occur by way of degraded air and water quality. As emissions of nitrogen oxides have decreased, deposition of reduced N forms (e.g., ammonium) have become an increasingly large fraction of total N deposition. Recently, critical loads of atmospheric N deposition have been established in the US for a variety of ecological effects.

AGRO 217

Emissions of ozone precursors from a central California dairy facility

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Dairy facilities are recognized to be significant sources of volatile organic compounds (VOCs), which contribute to high summertime ozone concentrations in central California. They are generally not considered to be an important source of NO_x, but a few studies reported in the literature suggest that silage can produce NO. Concentrations of VOCs, NO_x, and ozone were measured at a central California dairy using a combination of online and offline techniques. Summertime ozone levels were found to be lower and NO concentrations higher at the dairy compared with levels at an air district monitoring site located approximately two miles away. Flux chamber measurements of NO_x emissions from silage samples in the laboratory indicate that emissions from silage might account for the high NO concentrations observed at the dairy. Implications of these results will be discussed.

AGRO 218

Nitrogen enrichment and species change in shortgrass prairie adjacent to a cattle feedyard

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Excessive reactive nitrogen negatively impacts N-sensitive ecosystems when invasive nitrophilic species outcompete native species adapted to low N. Part of a shortgrass prairie pasture directly downwind from a cattle feedyard in the Texas Panhandle degraded to annual weeds during thirty years of feedyard operation. Published studies from 1966 to 1972 and anecdotal observations and photos from the 1940s were used as benchmarks to compare historic plant composition with contemporary (2000) plant composition. Soil N and P and dust deposition gradients with distance downwind from the feedyard were also measured during 2000 and 2004. Annual weeds dominated within 150 m of the feedyard, with almost total exclusion of desirable native perennials. Manure dust deposition and soil N and P were greatest within 150 m, decreasing with distance from the feedyard. Evidence indicated that N enrichment initiated a cascade of negative ecological change, with effects limited to less than 500 m from the feedyard.

AGRO 219

Atmospheric reactivity studies of aliphatic amines

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Ambient studies of particulate matter have shown that alkyl amines are often present in particles in areas impacted by agricultural emissions. These locations include California's Central Valley and Inland Empire and Utah's Cache Valley. These compounds are not typically observed in airsheds that solely contain urban/suburban sources, leading to speculation that agricultural influences might be important sources. Our research team has conducted a number of experiments using an environmental smog chamber to understand the fate of amines in the atmosphere. Atmospheric reactions of amines are a competitive process between acid-base interactions (similar to ammonia) and photochemical radical reactions (similar to other organic compounds). Primary, secondary, and tertiary amines appear to have divergent chemical mechanisms and product formation, but resulting in surprising amounts of aerosol formation despite the small sizes of the molecules.

AGRO 220

Organic nitrogen speciation in aerosols, precipitation, and cloudwater

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The atmospheric transport of fixed nitrogen (N) is a critical component of the global N cycle. It has been shown that organic N is an important contributor to atmospheric N, but its sources and composition are largely unknown. In an effort to better understand the sources of organic nitrogen we analyzed aerosol and precipitation samples collected in Rocky Mountain National Park and Grand Teton National Park, fresh smoke collected from the burning of various biomass fuels, and cloud water collected during the agricultural waste burning season that occurs in the eastern plains of China. The samples were analyzed using liquid chromatography/mass spectrometry (LC/MS), complemented by a range of other measurements. High resolution mass spectrometry allowed unambiguous determination of the elemental formula of the detected species. LC/MS analysis indicates that nitro-compounds are the most abundant N-containing organic species found in the aerosol and precipitation samples collected in the national parks. Compounds with reduced nitrogen were abundant in fresh biomass burning samples.

AGRO 221

Reactive nitrogen composition and origin in the United States Rocky Mountains

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Excess reactive nitrogen (Nr) deposition in some high alpine lakes in the Rocky Mountains has passed critical thresholds and is causing biogeochemical changes. Nr is a rich mix of inorganic and organic oxidized and reduced N compounds originating from an array of sources. Routine monitoring programs measure half of the Nr deposition, missing dry-deposited ammonia and dry- and wet-deposited organic N (ON). To better understand the Nr composition and origin, field studies in Rocky Mountain NP (RMNP) were conducted in 2006 and 2009 as well as in Grand Teton in the summer of 2011. In RMNP, large contributions of wet-deposited ON (~20%) and dry-deposited ammonia (~15%) occurred during all seasons. The Nr originated from sources throughout the western US, though sources in northeastern Colorado were the largest contributors. Measurements of ambient ON compounds are still problematic, though the water-soluble particulate ON fraction was found to be significant. In addition, limited measurements suggest that during biomass burning events reduced ON gases are equal to or greater than ammonia concentrations.

AGRO 222

Examining the sources and transport of agricultural reactive N emissions using stable isotope techniques

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Reactive nitrogen (Nr) emissions (i.e., NO_x, HNO_3, and NH_3) from the transportation and electricity-generating sectors are declining due to increasingly stringent air quality regulations and development of new emission reduction technologies. In comparison, Nr emissions from the agricultural sector are increasing and are largely unregulated in the US. Identifying Nr emission sources and quantifying Nr source contributions are important initial steps for reducing nitrogen inputs to the environment and have become of particular concern to air quality managers, modelers, and epidemiologists. The stable isotopic composition of Nr may be a valuable tool for characterizing Nr sources, transport, and fate. Here we demonstrate, using several examples, how stable isotopes can be used to: 1) differentiate industrial and agricultural Nr sources, 2) trace Nr across agricultural landscapes, and 3) investigate the transport of Nr emissions across regions.

AGRO 223

Applying methods to elucidate non-target organism impact using conventional lab, field, and modeling observations

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Individual studies are performed with an endpoint in mind but under unique discipline bias. For example, lab studies performed to quantify the relative differences between formulation volatility do provide input to standard, temperature dependent, chemical kinetic analysis. Field observations provide a snapshot of the near infinite parameter combinations but are useful in model validation. Conventional transport modeling can deduce areas of exposure under a variety of different conditions, with 1-D drift models predicting 2-D impact areas for deposition and potential source terms for volatility. Finally, observations of organism injury can be converted to an appropriate dose-response curve, and then modeling/programming approaches can join all the information gleaned from these stand-alone studies in a unified fashion. An example of risk to non-target plants from herbicide drift and volatility is provided where laboratory and field observations are used with numerical modeling to garner insight into appropriate mechanisms, thus maximizing the understanding from a limited amount of observational data.

AGRO 224

Comparison of multiple source ground spray deposition curves for determination of buffers in simulation models

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Spray drift models typically rely on field-developed, spray deposition data in order to estimate buffer distances. This presentation is an analysis and comparison of deposition data sets used to support several commonly used spray drift models. The goal of this analysis is to assess commonality between datasets as well as assess their usefulness for predicting off field deposition. Initial work indicates that while the development of spray nozzles has continued in evolution as a large contributor for reducing off field deposition, this development has precluded the use of many older field generated deposition curves. Findings suggest the use of older deposition curves in simulation models can be useful, but only to reflect currently-used older spray nozzle technology.

AGRO 225

Kresoxim methyl drift and related runoff in a vineyard catchment

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Pesticide spray drift and runoff represent major pathways of pesticide loss from agricultural land to aquatic ecosystems. Knowledge on pesticide drift in agricultural catchments and its contribution to runoff contamination is scarce. Here we characterisedthe spatial variability of drift from the fungicide kresoxim methyl (KM) in a vineyard catchment, and we quantified its export *via* runoff. Surface deposits were monitored at 54 locations during air assisted spraying to evaluate direct ground-exposure. Pesticide deposits ranged from 0 to 1.5 mg m^{-2}. Our results indicate that KM deposition on soil varied largely at both temporal and spatial scales, and depended mainly on the vegetation characteristics and climatic factors. The load of deposited KM that can be mobilised via runoff was 375 times larger than the mass exported at the catchment outlet, which suggests large KM attenuation within the catchment. Spray drift and runoff require thorough characterisation for better predicting the runoff-related loads of KM.

AGRO 226

Modeling the vapor drift potential of current-use pesticides

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Vapor drift occurs following application, when pesticides volatilize from agricultural fields and are transported off-site by the wind. Volatilization can account for up to 99% of pesticide losses from fields, leading to reduced efficacy and unintentional harm to non-target ecosystems. We present a visual screening technique for predicting the volatilization and vapor drift potential of pesticides from bare agricultural soils. A flux approach based on environmentally-relevant partition coefficients and the mass-balance distribution of pesticides between soil, air, and water was used to calculate 24-h cumulative volatilization losses. These were displayed on chemical space diagrams for sets of hypothetical chemicals and used to identify the pesticides and environmental conditions under which the greatest risk of vapor drift occurred. Vapor drift potential increased with increasing temperature and relative humidity and decreased with increasing soil organic carbon content. This approach could be used to aid future decision-making regarding pesticide selection and use.

AGRO 227

Conduct of aquatic herbicide fate and transport studies on moving water bodies

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Two aquatic dissipation studies were conducted to determine the aquatic fate of a broadcast-applied herbicide in moving water bodies located in the northwestern and southeastern United States. These studies were conducted on water bodies of differing flow rate, with the objective to determine the environmental fate of the test substance in water, sediment, and soil (stream banks). Detailed depth gauging and flow velocity measurements of the water bodies were conducted using Acoustic Doppler Current Profiler (ADCP) instruments. Stream velocity measurements were also collected at regular sampling intervals. Each study was performed over an approximately 120-d time period and involved treating an approximate 250 foot (length) by 15 foot (width) swath with the herbicide and Rhodamine WT dye (conservative tracer). Post-application water samples within the treated area were collected at designated sampling stations via peristaltic low-flow sampling pumps. Three automated ISCO® type samplers were placed at known distances downstream of the treated area to collect water samples at pre-determined time intervals. Additionally, roving water sampling stations were established beyond the location of the automated samplers where grab samples were collected throughout the day of application. The objectives of both studies were achieved. The water bodies were characterized in detail and the rapid dispersion and dissipation of the test substance in each water body was well defined.

AGRO 228

Colloid facilitated transport of veterinary pharmaceutical florfenicol in saturated sand and soil columns

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Veterinary pharmaceuticals are widely used in concentrated animal feeding operations (CAFOs). The potential loading of pharmaceutical residues into the environment from animal wastes associated with land application is receiving attention due to the fact that colloids derived from manure could affect transport of soil contaminants. This study revealed that florfenicol, a veterinary antibiotic, was recalcitrant in the manure-amended soils and that manure colloids could facilitate its transport. The colloid-facilitated transport of this antibiotic was further investigated using saturated sand and soil columns. A modified numerical advection-dispersion model using finite difference scheme was developed to fit the observed transport processes. The lumped effect of straining and sorption in the model on the transport process of florfenicol was also evaluated. The sorption coefficient of florfenicol in soils was obtained from its batch sorption experiment. The straining coefficient was estimated by subtracting the sorption from the lumped effect which was estimated from the modified model.

AGRO 229

Sorption of organophosphate and triazine agrochemicals on biochars and soils

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Biochars are known to strongly sorb polar and nonpolar organic compounds; biochar soil amendment can have counteracting effects on the efficacy of and runoff contamination by agrochemicals. This study investigated the sorption-desorption isotherms and kinetics of triazine (deisopropylatrazine) and organophosphorus (malathion, parathion, diazinon) pesticides on various soil types ranging from sandy acidic to clayey alkaline, as well as unactivated and activated biochars having a wide range of BET surface areas. Regardless of feedstock and pyrolysis condition, an increase in Freundlich distribution coefficient and isotherm nonlinearity was observed for deisopropylatrazine as a function of BET surface area at low surface coverage. Sorption of deisopropylatrazine was strongly hysteric on biochars and soils and competition was observed with Cu^{2+} in binary-solute experiments. Fate of organophosphate pesticides were strongly influenced by their stability. A general increasing trend was observed for the sorption on different soil samples: deisopropylatrazine < malathion < diazinon < parathion.

AGRO 230

Trapping and analysis of large quantities of volatile gases in an anaerobic aquatic metabolism study: A case study using [*S*-methyl-^{14}C]methamidophos

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Previous anaerobic aquatic metabolism studies of methamidophos resulted in low recoveries of applied radioactivity due to poor volatile trapping efficiencies of large quantities of volatile gas arising from the degradation of this compound. To correct the problem, a new trapping and analytical procedure was developed. A special combustion chamber was constructed which was equipped with a copper oxide, silver vanadate, and platinum catalyst for combustion of volatile gases. The trapping efficiency of this unit was tested by combusting methane gas and afforded an efficiency of >95%. The combustion chamber was then used to trap volatile gas from an anaerobic aquatic test system by flushing the headspace first through traps containing 2N KOH traps and then through the combustion chamber. Identity of the volatile components were confirmed by gas chromatography / RAGA (RadioActive Gas Analyzer) and by their co-elution with a ^{14}C standards. These techniques gave rise to much better overall recoveries of the applied activity. The paper will present the trapping, analysis, and identification of the volatile gases produced in the study.

AGRO 231

Determination of nine *N*-nitrosamines in drinking water by fast solid phase extraction and GC/MS

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N-Nitrosomines, a group of probable human carcinogens, has been detected as a disinfection by-products (DBPs) in drinking water. To investigate the occurrence of possible nitrosamines in drinking water, we developed a determination method with SPE-GC/MS. Cleanert LDC 521 SPE cartridge with 40 mm internal diameter was applied to allow fast loading of the water sample. The method had been evaluated and the results were acceptable.

AGRO 232

Determination of triazines and degradates in water using LC-MS/MS and stable isotope analogs as internal standard

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Our laboratories have been analyzing water samples for triazines since the 1980's using constantly-improving analytical technology. New methodological advances have recently been incorporated for routine analysis of residues of atrazine and simazine and their degradates in water from small streams and in raw and finished drinking water monitoring programs. This method uses stable isotope labeled internal standards for each analyte to minimize potential matrix effects and improve accuracy of residue quantification. This is especially important since the method uses direct injection without sample cleanup. This method has been successfully used to analyze thousands of water samples in multiple laboratories. Our history of method improvement, current analytical procedures, method performance, data acceptance criteria, and QC/QA process will be presented.

AGRO 233

Analysis of environmental samples for pyrethroid insecticides using multianalyte methods and stable isotope internal standards

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Over the last decade, analytical method requirements for agrochemicals in a range of environmental matrices have become increasingly-more demanding in terms of ruggedness, breadth of applicability, and sensitivity, with methods for pyrethroid insecticides being a notable example of this trend. The Pyrethroid Working Group (PWG) has developed methodology that monitors for eight different pyrethroids at low (ca. 0.5 – 5.0 ng/L) concentrations in difficult aquatic based matrices. The current approach utilizes negative chemical ionization gas chromatography with mass selective detection (NCI-GC-MSD), which provides embedded confirmatory information via the capability of the GC to provide separation of characteristic pyrethroid stereoisomers (and thus a fingerprint) and by the monitoring of confirmatory ions. The presentation will highlight the benefits of employing stable isotope internal standards in conjunction with a multi-analyte method for analysis of surface waters, sediments, and other matrices of interest, such as wastewater treatment influent/effluent water and biosolids. It will also discuss other key learnings on practical constraints that make quantifying this class of chemistry a challenge.

AGRO 234

Tell-"tail" indicator: Quantifying iophenoxic acids in deer serum via LC/MS/MS analysis

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Chemical biomarkers are often used to identify animals that have consumed baits used to deliver pharmaceuticals to wildlife species. Iophenoxic acids (IOPAs) have been used as bait markers in a variety of wildlife species. Traditionally, quantification of IOPA was accomplished by measurement of serum iodine levels. However, this method can often be confounded by dietary intake of iodine. We investigated various extraction and clean-up approaches for direct quantification of IOPAs in serum of white-tailed deer. Performance of the direct quantification method was explored through the use of various techniques, including the Bradford protein assay, post-column infusion, and quantitation of selected phospholipids. Ion suppression and enhancement of the analytes in the MS source were taken into account as well as removal of selected phospholipids which contribute to this effect. The final method employed a solid-phase extraction clean-up with recoveries averaging 95% at serum levels from 0.25 to 100,000 ng/mL.

AGRO 235

Immunochemistry-based protein detection in genetically engineered crops

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Since the introduction of genetically engineered (GE) crops in the mid-1990s, immunochemistry-based protein detection methods have played an important role in various areas across the agricultural biotechnology industry. This technology is widely used in trait discovery research, product development, registration, seed production, commercialization, and numerous post-launch activities. The primary use of immunoassays is to quantify the amount of GE protein present in a product or to verify the presence or absence of GE material in a product. Lately this technology has been developed to meet high-throughput needs for handling large quantities of samples, and for analyzing growing multi-trait stack products. A good quality method should be specific, sensitive, accurate, and reproducible which requires a rigorous method validation prior to its application in GE crops. The immunoassay method validation requirement and the challenges of its applications in GE products will be presented. In addition, emerging new technologies for protein detection in agricultural biotechnology will be discussed in detail.

AGRO 236

Second generation technology for transgenic protein quantitation in stacked traits

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Since the first genetically modified (GM) crops were commercialized in the US in 1996 with the introduction of insect resistance mediated by expression of Bt genes, there has been continuous and rapid adoption of the technology. By 2008, 125 million ha were planted globally with GM crops in 25 countries. Additional insect control options as well as tolerance to herbicides have become standard trait offerings for GM maize. In 2010, 86% of corn and 93% of cotton and soybean planted in the US contained at least one biotech trait, and almost half of GM corn and cotton products sold in 2010 contained stacked traits combined by conventional breeding of GM crops. Recently the industry has moved towards providing two or more modes of action to reduce development of resistance in target pests. For regulatory approval of GM crops, the level of each transgenic protein needs to be determined in a variety of plant tissues and products to estimate exposure to the environment as well as food and feed. Enzyme-linked immunosorbent assays (ELISAs) have been the industry standard for quantitation of transgenic proteins in GM crops, but with the increasing number of proteins in the stacked GM products, methods that allow multiple proteins to be quantitated simultaneously provide a clear advantage. An overview of various multi-plexing platforms will be presented as well as their potential for use in generating data for registration of GM crops.

AGRO 237

Validating enzyme-linked immunosorbent assay (ELISA) methods for protein quantification from environmental matrices

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Protein quantification from different environmental matrices using ELISA methods can be difficult due to the buffer requirements to extract immunoreactive protein and potential matrix interference, both of which may affect accurate protein concentration determination. Comprehensive validation experiments are necessary to ensure that an ELISA method can accurately and reproducibly detect and quantify a specific protein. Central to this validation are experiments to characterize matrix interference and the protein recovery from the matrix. Additional validation to determine accurate interpolation of the protein concentration at multiple dilutions, applicability of extraction buffers, and cross-reactivity with other proteins, as well as using well-characterized quality controls and applying acceptability limits to the standard curve help ensure the ELISA method is robust and reliable. Validated methods for protein quantification are necessary for accurate reporting and analyses.

AGRO 238

Formation of fungicidal tricyclic isoquinolines via a modified Ritter reaction

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1-Phenyl cylcoalkanols **1** react with nitriles **2** in the presence of triflic acid to give tricyclic isoquinolines **3** via a Ritter-type process. The products **3** arise via Wagner-Meerwein migration of a methyl or hydride of the initially formed cycloalkyl carbonium ion. The scope and mechanism of this novel variation of the Ritter reaction will be discussed. The tricyclic isoquinolines **3** were found to possess antifungal activity, which will also be discussed.

AGRO 239

Synthesis and SAR studies of fungicidal 3-aryl-1,2,4-triazin-6-ones

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3-Aryl-1,2,4-triazin-6-ones are a class of fungicides that exhibit activity against a broad spectrum of agriculturally relevant pathogens, including *Septoria tritici*. Initial efforts to probe the SAR resulted in analogs with demonstrated curative activity but limited residual activity. A more comprehensive effort was undertaken to better understand the SAR and enhance potency and spectrum. Several directed approaches were taken to enhance the residual protectant activity of these molecules. The design, synthesis, and biological evaluation of these targeted molecules will be discussed.

AGRO 240

Synthesis and SAR studies on the aryl component of the aminosulfone fungicides

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The aminosulfone fungicides, discovered at Dow AgroSciences, demonstrate excellent curative and protectant activity against *Plasmopara viticola* (PLASVI) in grapevine and *Phytophthora infestans* (PHYTIN) in potato and tomato. The key difference between the aminosulfones and structurally related valinamide carbamate fungicides (e.g., iprovalicarb and benthiavalicarb) is that the amide moiety is replaced with a methylenesulfone as shown below. A program of investigation was conducted to optimize the activity of the aminosulfones by probing different portions of the molecule. This presentation focuses on the structure-activity relationships (SAR) of the aryl component. The synthesis and biological evaluation of these materials will be discussed.

AGRO 241

Identification of novel fungal acetyl-coenzyme A carboxylase inhibitors via fragment-based design approach

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Acetyl-coenzyme A carboxylase (ACCase) is a commercially unexploited fungicidal mode of action. Leveraging literature and proprietary ligand-bound protein crystal structures, a research effort was conducted to identify novel inhibitors of the ACCase carboxyl transferase domain using a fragment-based design approach. The fragments were combined to form six synthetically actionable scaffolds. The subsequent targeted libraries prepared were influenced by an additional round of fragment-based design. The scaffold identification, synthesis of the elaborated scaffold libraries, and their optimization as fungal ACCase inhibitors will be discussed.

AGRO 242

From target-based research to herbicidal activity in the field

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Based on a novel herbicidal target, that has been identified and validated by an antisense screening approach, a high throughput screening has been performed and several micromolar hits were identified. Around one of the hits a cluster could be developed and a first cocrystal structure with the plant enzyme was achieved. Also some herbicidal activity could be observed with these early leads. Using metabolite profiling techniques this activity could also be correlated to the presumed target of this class. Using the information revealed by several further cocrystal structures, further optimization to sub-nanomolar target activity was achieved. With several of these highly target-active compounds significant greenhouse activity was observed and after further finetuning of the physicochemical properties interesting activity in the field could be shown.

AGRO 243

Human lice: Past, present, and future control

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Human head and body lice are obligate ectoparasites, and their occurrence is increasing due to control failures driven by the evolution of resistance to commercially-available pediculicides, principally the pyrethroids (*kdr* mutation) and malathion (enhanced carboxylesterases). Although head and body lice are ecotypes, only body lice transmit several bacterial diseases that have killed millions. Given the small, well annotated and validate genomes (108 Mb), which are virtually identical, the availability of functional RNA interference (RNAi) methods for gene knockdown, and an *in vitro* rearing system allowing the maintenance of louse strains without the use of a human host, human lice provide an efficient model in which to study xenobiotic metabolism and resistance (1/3 to 1/2 as many detoxification genes compared to other sequenced insect genomes) and the evolution of vector competence, which is assumed to be due to their different cellular and humoral immune responses.

AGRO 244

Body and head lice as a model system for understanding xenobiotic responses

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Body and head lice have the smallest insect genomes sequenced to date. These genomes have a much-reduced number of xenobiotic response genes as compared to many other insect systems. Additionally, assay systems are now in place to expose head and body lice to a diversity of chemical and bacterial challenges. Assays to expose lice to sub-lethal amounts of pesticides, coupled with transcriptional profiling, have revealed both the induction of pesticide tolerance and genes potentially underlying this phenomenon. Bacterial challenge assays and transcriptional profiling have also revealed important insights into why body lice vector diseases and head lice do not.

AGRO 245

Brief exposure of human body and head lice to sub-lethal amounts of ivermectin over transcribes detoxification genes involved in tolerance

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In this study, we investigated whether the optimization of dose, the timing of exposure, and the assessment of transcript levels during tolerance can be used to identify detoxification genes that metabolize ivermectin (IVM). Using a non-invasive induction assay (brief exposure to sub-lethal levels of IVM administered in a stress reducing fashion) and qPCR, our transcriptional profiling results identified IVM-induced detoxification genes. *CYP6CJ1, CYP9AG1, CYP9AG2*, and *phABCC4* were most significantly induced, had high basal expression levels, and were most closely related to genes from other organisms that metabolized insecticides, including IVM. Lice injected with dsRNAs against either *CYP9AG2* or *PhABCC4* exhibited significant reduction of their respective transcript level and showed increased IVM sensitivity, indicating that *CYP9AG2* and *phABCC4* are involved in the IVM metabolism and in the production of tolerance. Functional expression of these candidate genes will establish the actual metabolism of ivermectin and identify the metabolites formed.

AGRO 246

Comparison of the immune responses between body and head lice following bacterial challenge

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The differences in the immune responses between body lice, *Pediculus humanus humanus*, and head lice, *Pediculus humanus capitis*, were investigated by measuring the proliferation rates of model bacteria in their hemocoels and gut tissues. Head lice suppressed the proliferation of both *Staphylococcus aureus* and *Escherichia coli* more effectively than body lice. Annotation of the body and head louse genomes revealed that there are no differences in the genetic components for major immune responses between them. Nevertheless, the basal transcription levels of three important genes, PGRP as a recognition gene and defensin 1 and 2 as effector genes, were higher in the gut tissues of head lice than in those of body lice. In addition, head lice exhibited a higher phagocytotic activity. These findings suggest that head lice have more sensitive immune responses to invading bacteria than body lice, which could determine the difference in vector competence between the louse subspecies.

AGRO 247

MRSA transmission by human lice and bed bugs: Is more effective control necessary?

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Using the *in vitro* rearing system, the possibility of mechanical transmission of MRSA by human lice following a biofilm-based exposure scenario was tested. Both body and head louse females mechanically transmitted viable MRSA to their external surfaces and into their alimentary track (gut) following MRSA exposure. Using surface-disinfected lice, both body and head lice internally harbored viable MRSA, most likely in their gut. Body lice were, however, statistically more-rapidly infected by MRSA and at a higher frequency than head lice. Transmission of internalized MRSA was also tested. The substantially-increased number of MRSA-contaminated blood samples and the MRSA contamination in excrement in body lice suggest that body lice may be evolved to decrease innate immune response allowing more MRSA proliferation in body lice compared with head lice, particularly in their excrement. MRSA transmission by bed bug under the similar exposure conditions is currently being investigated.

AGRO 248

Extent of the bed bug problem: Past, present, and future control

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The worldwide resurgence of bed bugs has resulted in infestations being reported in countries where bed bugs have been largely absent for decades. The recent resurgence of bed bugs in the US has us living in the past with regard to bed bug control. The turn of century, when bed bugs were a common problem in the US, most people had a certain level of bed bug awareness. They were conscious of the fact that they might encounter bed bugs during daily activities and altered their behavior to avoid them. When an infestation did develop in housing facilities, fumigants were typically used to eradicate infestations. The widespread use of DDT in the 1940s and 1950s essentially eliminated bed bugs from the US. However, bed bug populations still existed in other nations where organophosphates, carbamates, and later pyrethroids were used for their control. The current resurgence of highly-resistant bed bugs in the US is likely due to their long history of exposure to multiple chemical classes. Current bed bug populations in the US are highly resistant to the pyrethroid class. Due to this resistance, and the fact that OPs and carbamates are no longer registered for the control of indoor pests, the use of non-chemical methods and enhanced bed bug awareness may prove to be our best defense against bed bugs in the future.

AGRO 249

Molecular genetic characterization of bed bug populations: From local infestations to global patterns

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A large gap in our understanding of resurgent bed bug populations concerns their geographic origins and their patterns of spread into new areas. To address this gap, we conducted a population genetic analysis of bed bug infestations in the US, Canada, and Europe using microsatellite markers. We found that infestations within a building have low genetic diversity, suggesting they are generally started by a small number of individuals, possibly a single inseminated female. We found that heavily infested apartment buildings are comprised of closely related individuals and are likely colonized by a single introduction event which spreads through the building. At the continent level, there is a high genetic diversity with no clear structure at the scale of the city or state. Finally, there is a lack of strong genetic differentiation between populations in North America and Europe suggesting a common global source of bed bugs on the two continents.

AGRO 250

Deep sequencing of pyrethroid-resistant bed bugs reveals multiple mechanisms of resistance within a single population

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A frightening resurgence of bed bug infestations has occurred over the last 10 years in the US, and current chemical methods have been inadequate for controlling this pest due to widespread insecticide resistance. We have identified bed bugs collected in Richmond, VA which exhibit both *kdr*-type (L925I) and metabolic resistance to pyrethroid insecticides. To identify metabolic genes potentially involved in the detoxification of pyrethroids, we performed deep-sequencing of the adult bed bug transcriptome, obtaining more than 2.5 million reads on the 454 titanium platform. Analysis of assembled transcripts in both Harlan (susceptible) and Richmond (resistant) bed bugs revealed several candidate cytochrome P450 and carboxylesterase genes which were significantly over-expressed in the resistant strain, consistent with the idea of increased metabolic resistance. These data will accelerate efforts to understand the biochemical basis for insecticide resistance in bed bugs and will provide molecular markers to assist in the surveillance of metabolic resistance.

AGRO 251

Evidence of CYP397A1-mediated pyrethroid resistance in bed bugs

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The common bed bug, *Cimex lectularius* L., a hematophagous ectoparasite of humans, is a serious public health challenge across the US. The rapid resurgence of this pest is attributed to widespread insecticide resistance; however, there is minimal information regarding these mechanisms of resistance. Our previous studies provide biochemical and genetic evidence for the over-expression of cytochrome P450 monooxygenase genes that are consistent with increased metabolic activities in pyrethroid-resistant bed bugs. Knowledge of the *in vivo* metabolism and *in vitro* substrate specificities of these P450s towards pyrethroids and other insecticide chemistries used for bed bug control is limited. In the present study, we will show the: 1) *in vivo* and *in vitro* metabolism of select pyrethroid insecticides for bed bugs; 2) heterologous expression of bed bug CYP397A1; and 3) molecular modeling and substrate recognition of bed bug CYP397A1 for select pyrethroid insecticides.

AGRO 252

Ammonia emissions from poultry operation affected by dietary modification and litter amendment

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Dietary manipulation and litter amendments can substantially lower ammonia (NH_3) emissions from poultry houses or manure storage. Recent lab and field studies involving laying hen and broiler manure from control or experimental diets showed a decrease (30-60%) in ammonia emissions for the experimental diets containing corn dried distillers grains with solubles (DDGS), a mixture of zeolite and gypsum (EcoCal), and enzyme production. A study to evaluate the effects of feeding diets containing different feed additives on NH_3 emissions, laying-hen production performance, and economic returns has been conducted at the farm scale. In addition to dietary manipulation, repeated application of litter amendments provides a means to reduce ammonia production from broiler litter, thus improving air quality and reducing ammonia emissions. A study to evaluate the effects of repeated PLT application on NH_3 emission from broiler chickens is being conducted using environmentally controlled chambers. Two different application rates and schedules are evaluated.

AGRO 253

Optimizing nitrogen fertilizer use on small landholder farms in India and Vietnam

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Like many developing nations, the agriculture of India and Vietnam is characterized by small farms (> 2 hectares) and inefficient fertilizer use. Working with non-governmental organizations in India and a university in Vietnam, we are encouraging more sustainable agricultural practices by assisting in the establishment of scientifically rigorous monitoring programs to determine the effects of alternate farming practice on yields, fertilizer use, water management, and GHG emissions. In India, the partnerships are establishing laboratories in rural villages and training local teams to run monitoring programs. In Vietnam, we are working with Can Tho University to establish robust measurement and sampling protocols. In both countries, we are working towards establishing verifiable GHG credits for CH_4 and N_2O emissions reductions through selection and calibration of models. If successful, GHG credit sales will provide the incentives to encourage farmers to continue to use more environmentally benign farming practices as part of programs to increase crop yields.

AGRO 254

Impact of animal diet on ammonia and greenhouse gas emissions

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Crude protein (CP) in animal diets is the main source for ammonia emissions from animal feeding operations (AFO). Lower CP and alternative biofuel production co-product diets were formulated and tested on swine. Emission of both ammonia and greenhouse gases were intensely monitored during the six-week trial. Animals fed lower CP diets had significantly lower ammonia emissions than animals fed control diets and CP source had a significant effect on ammonia emissions. There was no effect on GHG emissions levels between animals fed the control diet and alternative diets, but there was a significant increase in levels of nitrous oxide emissions associated with lower CP diets.

AGRO 255

Adaptation of an ambient ion monitor for detection of amines in gas and particulate agricultural emissions

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Volatile amines are emitted from many sources, including agricultural facilities. Recent work has shown that amines might be important players in secondary aerosol formation. Because amine emissions are significantly lower than ammonia, previous measurements and emission studies at agricultural facilities have often not detected them and information in the literature is sparse and sometimes contradictory. It is not clear whether the presence or absence of amines in previous studies represents instrumentation limits, atmospheric conditions controlling their reactivity, effects of different management practices, or other issues. Because of these issues we have adapted the ambient ion monitor (AIM) for detecting gaseous and particulate forms of amines at the low concentrations reported in previous studies. The AIM has previously been used for detection of common particulate ions and precursor gases in studies of urban air quality. The method can currently detect amines at facilities with a sampling time of one hour.

AGRO 256

New soil sampling technique for increased accuracy of total soil nitrogen determination

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After construction of newly designed circular soil sampling apparatus with possibility for collection of 16 soil samples in a radius of 50 cm from the central point, we have analyzed 4 composite samples and 56 single samples taken from the agricultural field. After comparison of the coefficient of variation for total nitrogen content in soil from single samples, we have concluded that it is better to use the new sampling probe, especially when precise information is needed. In a radius of 50 cm, total soil nitrogen in 16 single samples varied between 0.149 and 0.247% (average 0.190%, standard deviation 0.03, and coefficient of variation 16%). By this way of soil sampling it is possible to increase the volume of sampled soil 16 times compared to classical sampling methods. In the case of total nitrogen content in soil, we have found that this is superior way of soil sampling.

AGRO 257

Identification of important pathways for residential runoff transport of pyrethroids: Facility design

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Full scale runoff collection studies provide many challenges due to design constraints and environmental factors. Developing a proper study design matched with proper site construction and instrumentation are crucial for achieving the desired objectives. This study involved the design and implementation of a full scale test facility for replicated measurement of insecticide transport in runoff following residential applications. This presentation describes the design of a facility constructed in central California, including house lot and wall construction, sloping lawns and water management (residential lawn sprinklers, natural rainfall, and simulated rainfall), and pesticide applications. Runoff collection systems for measuring and sampling widely-varying runoff-volumes were implemented. Wireless, remote communication systems were utilized for real-time monitoring and collection of study data that allowed for the ability to diagnose and often correct problems from nearly 2,000 miles away. The facility has been operated successfully for one year and preliminary experimental results are presented in a second paper.

AGRO 258

Identification of important pathways for residential runoff transport of pyrethroids: Preliminary experimental results

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Replicated runoff studies to determine the major pathways for transport of pyrethroids applied to suburban residences were conducted at a full scale test facility in central California (described in an earlier presentation). Transport occurred in runoff from lawn irrigation (mostly from water landing on hard surfaces) and natural and simulated rainfall events. Under typical application practices the washoff from the driveway and garage door and wall directly above the driveway resulted in the largest masses of pyrethroids leaving the plot, with losses from applications to the vertical wall above grass, the grass next to the wall, and the lawn being an order of magnitude less. With recently adopted label practices, the washoff from the driveway decreased by more than a factor of ten and the washoff from the garage door and the walls above the driveway were reduced by a factor of five.

AGRO 259

Laboratory degradation rates of eleven pyrethroids under aerobic and anaerobic conditions

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Degradation of eleven pyrethoids was measured over approximately 100 days in three sediment/water systems under aerobic and anaerobic conditions at 25°C in the dark. The three California sediments represented a range of textures and organic matter. Test compounds were bifenthrin, cypermethrin, zeta-cypermethrin, cyfluthrin, beta-cyfluthrin, deltamethrin, esfenvalerate, fenpropathrin, gamma-cyhalothrin, lambda-cyhalothrin, and permethrin. The test compounds were applied as two test mixtures (six active ingredients per mixture, with bifenthrin common to both) at approximately 50 µg of test compound per kg of sediment (dry weight). Extracts of sediment/water were cleaned up by SPE, concentrated, and analyzed by GC/MS (except deltamethrin) against matrix-matched standards with cyfluthrin-d_6 as internal standard. Deltamethrin was analyzed by LC/MS/MS using deltamethrin-phenoxy-$^{13}C_6$ as internal standard. The study was fully replicated and, for the same sediments, results from the two test mixtures indicate general agreement between degradation rates measured for bifenthrin in both mixtures and for related isomeric products (e.g., cyfluthrin and beta-cyfluthrin). Degradation was generally faster under aerobic conditions compared to anaerobic.

AGRO 260

Assessment of the potential influence of physical habitat, pyrethroids, and metals on benthic communities in urban California streams in 2009-2011

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The objectives of this study were to measure benthic community conditions, physical habitat, basic water quality parameters, pyrethroids, sediment total organic carbon, grain size, and metals annually in two urban California streams (Arcade Creek and Salinas streams) from 2009 to 2011. Univariate and stepwise multiple regression techniques were used to determine the relationship between 14 benthic community metrics and physical habitat, pyrethroids, and metals. Tolerant benthic taxa, poor habitat, and potentially toxic metals and pyrethroids were reported in both study areas, but were more apparent in Salinas streams. Analysis of the three year data sets for Arcade Creek showed more significant and consistent relationships with benthic metrics and habitat metrics than with metals or pyrethroids. The three year data sets for Salinas streams showed that habitat, and not metals or pyrethroids, was the only stressor to show a significant relationship with benthic metrics.

AGRO 261

Fate of pyrethroid insecticides in wastewater treatment processes

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A laboratory investigation determined the fate of eight pyrethroids through four wastewater treatment processes: primary sedimentation, biological treatment (aerobic and anaerobic), and ultra-filtration. Pyrethroid concentrations were monitored before and after each treatment process. Primary sedimentation, anaerobic biological treatment, and ultrafiltration were performed on a batch basis. Aerobic biological treatment was simulated via a continuous-flow system for approximately 30 days. Low adsorption of pyrethroids in primary sedimentation was attributed to limited contact time and high dissolved organic carbon in the primary supernatant. Pyrethroid removal ranged from 34.2 to 81.6% via aerobic treatment and ranged from 31.9 to 81.2% via anaerobic digestion. Adsorption to aeration solids was limited to 4.4 to 14.4% of pyrethroid mass. The aeration system effluent retained 13 to 51% of initial concentrations of pyrethroids; however, ultra-filtration was effective in removing the residual pyrethroids in the aeration

system effluent, achieving greater than 90% removal of the residual pyrethroids.

AGRO 262

Aquatic exposure model parameterization using outdoor simulated pond study

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Standard aquatic exposure assessments conducted by US EPA for pesticides have been based on environmental fate data derived from laboratory studies. However, the behavior of chemicals in the environment is different because of simultaneous processes occurring in real world conditions that are not captured by controlled laboratory studies. This study demonstrates the value of using available field studies to parameterize environmental fate models in higher-tier refined exposure assessments. A water monitoring study was conducted to measure residues of fipronil and its metabolites in an on-site pond of an established golf course following fipronil applications on turf adjacent to the pond. In addition, an outdoor simulated pond study was conducted to characterize the fate of fipronil and its metabolites in aquatic environments. The PRZM and EXAMS models were used to simulate the fate and transport of fipronil and its major fiprole metabolites observed in the study. The models were parameterized using the data from the outdoor simulated pond study and some parameters were calibrated within their recommended limits. The simulation results from PRZM and EXAMS models showed good correspondence to observed data from the water monitoring study. The calibrated models were then run with long-term weather records to predict temporal distribution of fipronil and the total fiprole exposure concentrations. The results show that the aquatic exposure modeling parameterized using field studies can better represent the complex behavior of a chemical in environment and should be considered in higher-tier risk assessment.

AGRO 263

Predicting the bioconcentration of herbicides, insecticides, and fungicides in fish with partitioning and biotransformation

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A new approach for modeling bioconcentration factors (BCF) of herbicides, insecticides, and fungicides in fish is presented. Bioconcentration is modeled as a product of thermodynamic and depuration kinetic factors. The thermodynamic component, which considers partitioning to various phases, can be determined *a priori* from the chemical properties and the biota composition. The depuration kinetic factor, which represents the total contribution of depuration processes to BCF, is primarily dominated by respiratory elimination and biotransformation. A new biotransformation model based on the Abraham solvation parameters was constructed while the conventional model for respiratory elimination was adopted. The final BCF model was tested using a compiled BCF database consisting of measurements for 276 agrochemicals. The performance of the new model was found to be comparable to those of the major BCF models developed for the various environmental agencies.

AGRO 264

Assessing exposure of the California Red-Legged Frog to an insecticide in irrigation pond habitat

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A spatial analysis of California Red-Legged Frog (CRLF) critical habitats and core areas concluded that there were four types of aquatic habitat vulnerable to the use of pesticides: streams, drainage ditches, natural ponds, and irrigation ponds. Irrigation ponds are constructed for the purpose of providing water to crops grown in the adjacent fields, but they also provide habitat for aquatic organisms. One hundred and ten irrigation ponds were identified in two CRLF core areas that were found to be vulnerable to insecticide applications. Because these ponds are constructed with a berm around the perimeter, potential exposure due to runoff is not possible. Exposure may occur through drift of pesticide applications only. Observed pond dimensions, setback distances to fields, use rates, and a drift exposure model were used to estimate exposure to all identified ponds. A risk assessment was then conducted, and setbacks were determined that would be protective for direct and indirect effects to the CRLF.

AGRO 265

Communicating science-based assessment of risks and benefits of agricultural biotechnology

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The first generation of agricultural biotechnology crop products resulted in the successful development of new systems for insect and weed control that replaced or reduced alternative pest management methods with higher risk profiles. Significant scientific efforts were undertaken globally to assess whether the use of transgenic technology presented new benefits and/or risks to food, feed and environmental safety in the crops and in food and feed products compared to conventional counterparts. Scientific data has continued to demonstrate that biotechnology offers substantial benefits to the environment, consumers and farmers using these new tools to control pests compared to traditional methods. However, opponents of this science platform continue to challenge its safety generating doubt while its supporters use science as the proof of its safety. Communicating the results of science-based risk and benefit assessments is a continuing challenge for agricultural biotechnology. Lessons learned and new insights into improving communications will be shared.

AGRO 266

Communicating risks and benefits of soil fumigant use

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Soil fumigants continue to be needed for the production of a number of valuable food commodities ranging from carrots and grapes to strawberries. One preplant application of soil fumigant chemicals or mixtures can control nematodes, weeds, and plant pathogens and protects the crop from planting to harvest. But the use of fumigants entails risks to the applicators and other farm workers as well as those residing or working in the vicinity of fumigated fields. Research data can provide information that addresses risks and assists in the communication of these risks to the public. Examples will be given for risks from airborne exposure to

methyl bromide and chloropicrin, including the use of buffer zones, barriers, and other tools to minimize exposure. Risk communication associated with methyl bromide alternatives, and the potential for reduced risk approaches to control of soil pests in strawberry fields, will be discussed from a 'lessons learned' perspective.

AGRO 267

Inter-agency risk communication: Inorganic arsenic residues in poultry

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Roxarsone was used as a coccidiostat in poultry for 50 years. Using recent advances in instrumentation, FDA detected very low concentrations of carcinogenic inorganic arsenic in the livers of Roxarsone treated chickens. By combining these residue data with a prospective risk assessment, FDA concluded that the future cancer risk to consumers of Roxarsone-treated poultry was very low yet avoidable. The manufacturer initiated actions to suspend Roxarsone use in the United States. Anticipating public concern, USDA conducted a risk assessment based on historic poultry consumption and arsenic residue data to estimate the magnitude of cancer induced by consumption of inorganic arsenic residues in poultry meat prior to the termination of Roxarsone. USDA concluded that historic use of Roxarsone resulted in negligible public health risk. This presentation discusses the risk communication challenges associated with this situation and the inter-agency coordination that resulted in successful risk communication to the public.

AGRO 268

Communicating the risk of polycyclic aromatic hydrocarbons (PAHs) measured in seafood in Mississippi following the Gulf oil spill

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Following the sinking of the Deepwater Horizon, the state of Mississippi began sampling and monitoring crabs, shrimp, oysters, and several species of fish from numerous locations within Mississippi state waters. From the end of May 2010 to date, over 400 samples have been analyzed by the State for polycyclic aromatic hydrocarbons (PAHs) as listed in the NOAA method for analysis of PAHs in seafood. Additional samples were also collected and submitted to the NOAA laboratory in Pascagoula, MS to support the reopening of state waters in accordance with the protocol jointly developed by the gulf coast states, FDA and NOAA. PAHs have not been detected in any sample collected to date at levels above the level of concern (LOC) as established in the reopening protocol. PAHs were routinely detected in most samples at low part-per-billion levels and are consistent with values commonly detected in samples measured in other studies unrelated to the oil spill. However, to allay consumer concerns about low detections of PAHs in seafood and to best communicate the risk of these levels to consumers, concentrations of PAHs were also evaluated in common meat products (smoked turkey, ham, chicken, catfish, and barbecued pork) purchased at local restaurants and super markets. The levels of PAHs measured in seafood were consistent with or below levels of PAHs detected in these food items.

AGRO 269

POPs on the cusp: The case of endosulfan

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Criteria for the identification of POPs were developed from the properties of the so-called “dirty dozen” (DDT, etc.) that had been observed to be persistent (P), bioacumulative (B), toxic (T), and transported over long distances (LRAT). The quantitative criteria for identification of POPs are deterministic values for P and B and qualitative for T and LRAT. The objective of these regulations is to avoid the use of chemicals that, over time, will increase in concentration in environmental compartments to the extent that they cause harm to organisms, including humans. Thus, the combined properties that drive P, B, and T must have, or will, result in accumulation to harmful levels. This was the case for some of the legacy POPs, but not necessarily for compounds that have properties close to the criterion values. These compounds are “on the cusp” and present scientific challenges that will be discussed using endosulfan as a case example.

AGRO 270

Using local community-protection values to provide evidence of reduced catchment-scale risk from pesticides

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River concentrations of pesticides result from practices undertaken by individual farmers over an entire catchment. This might contain environments of different ecological value, for example irrigation channels vs. a protected wetland. Subsequently, ecological risk assessments (ERA), when applied at the catchment-scale, could use assessment endpoints that reflect the ecological significance of the different environments according to the local environmental protection goals, such as those defined by the local catchment management agency. Advances in spatial information techniques, applied to ERA, have provided the capability for distinguishing and estimating ecological impacts of pesticides in the different environments of a catchment. This paper presents an Australian case study that evaluates the ecological risk of diuron in an agricultural catchment. In this study a set of assessment endpoints formed in consultation are used to distinguish different environments and a refinement of the current management scale is suggested.

AGRO 271

Real world exposure and biomonitoring are not part of the alarmist agenda

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Toxicological data has been misrepresented to express alarm and multiple health effects. Detection does not mean health concerns. To a large segment of the public and environmentalists, exposure to pesticides means harm. EPA guideline testing requires determining toxicological limits of

a pesticide called hazard, thus those values are the focus of the alarmists. The NOAEL, nor the 100X lower RfD, nor real-world biomonitoring exposure is considered. Selected old publications and adverse findings are highlighted. In contrast there is a huge difference in the recent 2,4-D one-gen reproduction study; the male systemic toxicity NOAEL is ~13,000-fold higher than 2,4-D exposures reported in human biomonitoring studies. Also, there is a huge difference between the Agency's 2,4-D reference dose and the CDC NHANES biomonitoring. After rigorous analysis of the relevant scientific data, expert panels and government agencies all reach the same conclusion: 2,4-D is acceptable for use according to label directions.

AGRO 272

Lessons from the endosulfan case for achieving rational risk assessment in the face of chemical paranoia

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On April 21, 2011, COP5 of the UNEP's Stockholm Convention ratified POPRC's recommendation to list the insecticide endosulfan as a persistent organic pollutant (POP) and be added to the “dirty dozen.” A case has been made that the Convention exceeded its brief in declaring endosulfan a POP, as there is little environmental evidence to support the conclusion that it is persistent. Only by choosing apparent outliers for degradation rates was POPRC able to support its case for the listing. Furthermore, little or no input was sought from experts in insect control or food security. The decision might therefore be regarded more as an act of eco-politics rather than one based on rational science. This case raises important issues related to the regulation of agrochemicals and how stewardship is best achieved. Feeding 10 billion humans in the foreseeable future in the face of climate change might require continued access to a range of chemicals.

AGRO 273

Achieving rational regulatory action for the management of risk from diuron in catchments with outfalls to the Great Barrier Reef

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Activists often advance unbalanced views of risks or benefits of pesticides, for political or social influence, making rational action difficult to achieve. A relevant case is that of the herbicide diuron, with potential for runoff to the Great Barrier Reef (GBR). In a recent review, the Australian environmental agency (DSEWPaC) concluded that low concentrations of diuron in the GBR lagoon (0.1-17 ng L^{-1}) did not present an acute or a chronic risk, although during floods levels can reach levels of concern (0.1-1 µg L^{-1}) near ocean outfalls. DSEWPaC was more concerned about risks from runoff to algae and aquatic plants in primary and secondary streams. As a result, the Australian Pesticides and Veterinary Medicines Authority suspended the registration of diuron products nationwide. This presentation will discuss the responses from registrants, government agencies, farmers' organisations and environmentalists. However, following an interactive process a rational regulatory approach might be emerging.

AGRO 274

Synthesis and fungicidal activity of mono- and biheterocyclic tubulin polymerisation promoters

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Pyrido[2,3-b]pyrazines and pyrido[3,2-e][1,2,4]triazines, in which the pyridine moiety is persubstituted, as well as similar substituted monocyclic pyridazines and imidazoles, are highly active against a broad range of phytopathogens, such as *Mycosphaerella graminicola* (wheat leaf blotch), *Alternaria solani* (potato and tomato early blight), and *Magnaporthe grisea* (rice blast) by disrupting their microtubule dynamics. Synthesis and structure-activity relationship data of this class of experimental fungicides will be presented.

AGRO 275

3,4-Diarylpyridines as broad-spectrum fungicides

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A series of 3,4-diarylpyridines were prepared and shown to possess broad-spectrum fungicidal activity. This talk will focus on the discovery, chemistry, biology and structure-activity relationships of these compounds.

AGRO 276

Fungicidal 2- and 4-pyridones

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2- and 4-pyridones containing vicinally di- and tri-substituted aromatic substituents exhibit activity on a broad range of commercially important fungi. Synthetic methods to synthesize these three distinct ring systems will be presented along with a summary of the biological activity and structure-activity relationships.

AGRO 277

Synthesis and biological activity of di- and tri-aryl pyridazines as broad spectrum fungicides

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Kumiai first examined fungicidal triaryl-4-pyridones as tubulin inhibitors in 1987. Sumitomo disclosed diaryl pyridazines as tubulin-inhibiting fungicides in 2005. At DuPont we have examined both di- and tri-aryl pyridazines, as well as the related di-aryl-4-pyridones as tubulin-inhibiting fungicides. We will present the synthesis and structure activity relationships of the di- and tri-aryl-substituted pyridazines and the diaryl-4-pyridones, as well as their fungicidal evaluation.

AGRO 278

Fungicidal carbonyl-containing heterocycles

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Oxazinones and pyranones containing substituted aromatic substituents exhibit activity on a broad range of commercially important fungi. Methods to synthesize these distinct heterocyclic ring systems will be presented along with a summary of the biological activity and structure-activity relationships of the class.

AGRO 279

Diaryl-imidazoles as tubulin-inhibiting fungicides

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The world's population is expected to reach 9 billion people by 2050. In order to support this population, there will need to be a 70% increase in global food production over current levels. In order to achieve this, new fungicides will need to be developed to combat an ever-changing disease landscape. In this presentation, we will describe the design and synthesis of the diaryl-imidazole class of tubulin-inhibiting fungicides.

AGRO 280

Movement of soil and trunk injected imidacloprid through the hardwood *Acer rubrum*

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Animal and Plant Health Inspection Service (APHIS) has undertaken an insect eradication program using the neonicotinoid imidacloprid to prevent the further spread of *Anoplophora Glabripennis,* the Asian Longhorned Beetle in New York City (NYC). Trunk injections were applied in the high water table soils of Staten Island whereas soil injections were applied to the drier soils in Queens and Brooklyn. Imidacloprid levels were followed for six treatment years. Of the twenty+ susceptible species of trees treated, red maple, *Acer rubrum*, was chosen for study because it is highly attractive to honey bees (*Apis mellifera*) as a nectar and pollen source and it is plentiful in NYC. Imidacloprid partitioned mostly to the leaves (max = 10^4 ppb), moderately to flowers (max = 10^3 ppb), and least to pollen (max = 10^1 ppb). Imidacloprid expression in plant tissue varied with application method, tree sex, and treatment year. The presence of six metabolites was followed.

AGRO 281

Survey of imidacloprid levels in water sources frequented by honey bees (*Apis mellifera*) in Maryland

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Detrimental sublethal effects of imidacloprid, a water soluble pesticide, have been noted in honey bees. To determine the presence of this neoniocotinoid in water sources frequented by bees in urban, suburban, and rural environments across Maryland, eighteen sites (6 samples/site) including golf courses, various farms, residential neighborhoods, and cityscapes were monitored. Imidacloprid was quantifiable in 8% of the samples at sublethal levels (7-131 ppb) by ELISA while 13% of the samples were at the detection threshold (LOD = 0.07 ppb). After initial sampling, all positive sites were sampled again in six months and analyzed by LC/MS/MS to compare seasonal variation and methodology. Imidacloprid was found to be transiently present over a season; some samples that had no imidacloprid in June had quantifiable levels in October, while some quantifiable June samples showed no detection in October. Imidacloprid was found in many terrains but most often at the golf course and nursery sites.

AGRO 282

Impacts of modern pesticide formulation technologies on honey bee health

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Modern pesticide formulations, particularly when multiple active ingredients are blended, require proprietary adjuvants and inerts to achieve high efficacy for targeted pests. Although numerous pesticides have been found in beehive samples, no individual pesticide amount correlates with recent bee declines. Here we examine the potential involvement of more generic formulation additives that co-occur across classes of pesticides and that are used where bees forage. Since formulations of chlorothalonil and amitraz were four times more toxic to honey bees than respective active ingredients, we focused on recent technologies including organosilicone surfactants and co-solvents like N-methylpyrrolidone (NMP) of unknown bee ecotoxicity. NMP was more orally toxic to larvae than adults. Organosilicones such as Silwet L-77 above 5 µg/bee impaired learning more than other nonionic adjuvants in the proboscis extension reflex assay. Monitoring methods are needed for major adjuvant residues so risks of formulation additives and their pesticide synergisms for pollinators can be assessed.

AGRO 283

Insecticides on concrete: Role of particles in offsite transport

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In residential areas, insecticides may be directly applied on concrete or they may be indirectly transferred from surrounding areas by wind or water. Surface runoff as facilitated by urban hardscapes is perceived as a significant source of pesticide contamination in urban watersheds. However, little is known about how such offsite transport takes place. We evaluated the role of loose particles as the carrier for pesticide residues in surface runoff. We observed a close correlation between the amount of pesticides in particles (recovered on a sponge wipe) and that in runoff for permethrin, bifenthrin, and fipronil. Using a simple vacuum method to collect dislodgeable particles, we further found many insecticides, often at high levels, on the concrete surface of driveway, walkway, and street around single family houses in Riverside. These results suggest that loose particles are the main form by which pesticides are moved in urban surface runoff.

AGRO 284

Insecticide runoff from simulated lawn and driveway surfaces

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Several studies suggest that turf unlikely contributes to pesticide runoff. Pesticides inadvertently applied to impervious surfaces may be a significant source. We compared the potential for insecticides to contaminate runoff from concrete and from turf surfaces. Insecticides were applied over a two-year period to concrete and to turf field plots on a 6% slope. Pesticide residue from collected runoff samples was measured by HPLC analysis. A significant main effect between surface type and a significant interaction between surface type and insecticide treatment occurred. Diazinon was detected (0.629 µg ml^{-1}) from the homeowner concrete surface. Imidacloprid was detected on the concrete surfaces (0.318 µg ml^{-1} and 0.348 µg ml^{-1}) and was detected at a low level (0.003 µg ml^{-1}) on the homeowner turf surface. Chlorpyrifos was detected on the professional concrete surface (0.206 µg ml^{-1}), but was undetectable on all other surfaces. Our results suggest that insecticides applied to turf surfaces result in negligible amounts of insecticide runoff.

AGRO 285

Offsite transport of fungicides with snowmelt and rainfall runoff from golf course fairway turf

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Pesticides associated with the turfgrass industry have been detected in storm runoff and surface waters of urban watersheds, inferring contaminant contributions from residential, urban, and recreational sources. Golf course turf often requires multiple applications of pesticides at rates that exceed those typically found in agricultural or home environments. The objective of this study was to quantify concentrations of fungicides transported in snowmelt and rainfall runoff from creeping bentgrass turf managed as a golf course fairway. Chemographs from rainfall runoff occurring within days of fungicide application showed fungicides in the initial runoff and throughout the runoff event. Snowmelt collected nearly four months after fungicide application contained fungicides and a degradation product. Loads of fungicides measured in the edge-of-turf runoff were used to calculate estimated environmental concentrations of fungicides anticipated to occur in surface waters receiving the snowmelt and rainfall runoff. Concentrations were compared to known toxicological endpoints to evaluate environmental risk.

AGRO 286

Optimization of vegetative filter strips for the treatment of pesticide-laden runoff from turf

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Pesticides in runoff can degrade water quality and has led to mitigation strategies, including the use of vegetative filter strips (VFS). Five plant species that degraded turf pesticides were planted in VFS with a 5% slope. Three replicated VFS were planted in either successions (shortest to tallest) or random mixtures and compared to unvegetated and turfgrass plots. Runoff volume was reduced in mixture (23X), succession (6X), and turfgrass (23X) VFS vs. unvegetated plots. All six pesticides were detected in the runoff from unvegetated plots, ranging from 0.4% (imidacloprid) to 61% (pendimethalin) of the total pesticide applied. For succession plots, four pesticides were detected, ranging for 0.008% (imidacloprid) to 1.0% (chlorothalonil); chlorpyrifos and pendimethalin were not detected. Only chlorothalonil was detected at one time point in one replicate for the mixture (0.016%) and turf (0.0002%) VFS. These data suggest that the turfgrass and mixture treatments attenuated water and pesticide movement in VFS.

AGRO 287

Unintended effects of transgene insertion in crop plants: What are the unique food-safety risks compared with non-transgenic breeding methods?

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Government safety regulation of transgenic crops often requires an experimental assessment of the unintended effects of gene insertion on crop composition. Composition study costs to meet global regulatory requirements commonly exceed $1M. Several phenomena associated with gene insertion have been postulated to create risks, including insertional mutagenesis, creation of cryptic reading frames, and upregulation of endogenous allergens. The theoretical risks of these events occurring via transgenic breeding are reviewed and shown to be lower than these same risks in traditionally-bred crops. Extensive empirical evidence is also presented verifying this theory. For crops where endogenous metabolic processes are intentionally altered, targeted compositional analyses are recommended as prudent, although equivalent perturbations caused by traditional breeding are rarely investigated. Where compositional safety risks are suspected, it is suggested that compositional analyses may be less useful in predicting safety risks compared with animal feeding studies that measure general health and growth.

AGRO 288

Crop composition: A key component in the safety assessment of a new plant variety

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The policy statement developed by the US Food and Drug Administration in 1992 provides guidance on relevant scientific and regulatory issues related to safety of food and feed from new plant varieties. An important component of this safety assessment is compositional analysis of the food and feed from the new plant varieties. In such an effort, the composition of the new plant variety is compared to its

conventional counterpart. This comparison is made for key nutrients (e.g., proteins, fatty acids, carbohydrates); key antinutrients (e.g., phytic acid, glucosinolates), and any naturally occurring toxicants (e.g., solanine in potato) in the plant. Data from scientific literature and compositional databases are used to view the results in the context of nutritional and biological relevance. This talk will discuss aspects of compositional analysis as it relates to safety of food and feed from new plant varieties; a few examples will also be examined.

AGRO 289

Influence of transgenic crops on pesticide use

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Commercial production of *Bt* crops genetically modified to produce insecticidal toxins from the soil bacterium, *Bacillus thuriengiensis,* began in 1996. Since then, the technology has been widely adopted in the US and several other countries. This presentation will assess the impact of the technology on the environment and human health from reduced pesticide usage. Overall, pesticide use has been reduced, however, this benefit varies by country, region, and crop.

AGRO 290

Environmental risk assessment and release of flower-color modified transgenic plants

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Flower color is genetically determined, mainly by the structures of anthocyanins. These flavonoid classes are largely responsible for orange, red, violet, and blue flower colors. Engineering the anthocyanin biosynthetic pathway leads to novel flower colors in transgenic plants. Flavonoid 3', 5'-hydroxylase is critical for plants to accumulate the delphinidin-based anthocyanins that most blue/violet flowers contain. Carnation and rose plants expressing this gene produce blue/violet color flowers accumulating delphinidin-based anthocyanins. Through the extensive regulatory approval processes that must occur for the commercialization of transgenic carnation and rose, we have obtained experimental and trial data to show commercial release poses no environmental risk. Though not required to be regulated as a food, it is relevant that delphinidin-related anthocyanins are also found in common foods like blueberry, eggplant, and red bean. Experimental and literature studies suggest that no potentially negative health impacts could be associated with consumption of the transgenic flowers.

Reference: Int. J. Mol. Sci. 2009, 10, 5350-5369

AGRO 291

Review of mutational breeding and genetic engineering approaches to the development of high protein content in the grain

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Most plant foods contain lower quality proteins because of one or more essential amino acids being low. Efforts to improve the protein and the content of essential amino acids in the grain used a variety of approaches from a basic breeding technique to genetic engineering. In genetic engineering research, seed-specific promoters are typically used to target the expression of the trait in the seed, i.e., in the case of high lysine corn cultivar LY038. In the past 5 years, mutational breeding has been focused on improving both lysine and crude protein content in the rice grain. The line with the most improved lysine content (05PWLS100115) has a moderate yield of 5,685 lb/A. However, the line with a moderate increase in lysine content (07PCC201570; 32.21%) has an excellent yield of 8,029 lbs. /A. The mutational breeding technique used will be discussed, together with genetic engineering approaches previously done by others.

AGRO 292

Creating a plant-based source of essential long-chain omega-3 fatty acids

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Long-chain polyunsaturated fatty acids (LC-PUFA) have a carbon backbone of at least twenty carbons in length and contain multiple double-bond desaturations. LC-PUFA can be grouped into either an omega-3 or omega-6 category based on the position of the first double-bond from the methyl (omega) fatty acid terminus. LC-PUFA omega-3 fatty acids, like EPA and DHA, have critical roles in human health and development. Studies indicate that deficiencies in these fatty acids can increase the risk or severity of cardiovascular disease, inflammatory diseases and rheumatoid arthritis, hypertension, and neuropsychiatric disorders such as depression or dementia. This talk will discuss the production of EPA and DHA in plant oils through the use of metabolic engineering. Currently, these fatty acids are predominantly sourced from fish and algal oils. Wild-harvest marine fish stocks are widely recognised to be under threat. In order to be able to meet the increasing demand for these oils there is an urgent need for an alternative and sustainable source of EPA and DHA. Oilseed plants producing high yields of EPA and DHA are, therefore, an attractive alternative to fish oils. This talk will describe the efforts under way in CSIRO to create an oilseed with significant amounts of EPA and DHA in its oil and how these plant oils will be able to meet the growing demand for these fatty acids. The development of a leaf-based vegetative source of EPA and DHA will also be described.

AGRO 293

Enhancing desirable nutrients in fruits and vegetables by transgenic approaches

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Malnutrition and food security are two major concerns confronting the world as we move forward in the third millennium. Fruits and vegetables are dietary sources of vitamins, antioxidants, fiber, and minerals. Nutritionally-enriched diets have shown promise in decreasing incidences of diseases, with interactions among fruit nutrients enabling anti-cancerous activity. There is a paucity of information on the variation in specific nutrient levels in different edible crops and their potential as pro-health factors. We employ precision-based genetic manipulation for increasing nutrient levels and shelf-life using tomato as a model. Cellular metabolome was defined in transgenic lines that accumulated either antioxidants, increased shelf-life, or enhanced texture. Increasing shelf-life of tomato by reducing production of the ripening hormone ethylene caused major effects on the metabolome. This was reversed by back-crossing these lines with transgenics that accumulated cancer-fighting lycopene. Double-triple transgenic events, therefore, affected nutrient levels and fruit quality in a powerful manner.

AGRO 294

Deconstructing nature's structural material for biofuels

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This talk will highlight results from recent multiscale modeling studies of lignocellulosic biomass structure, recalcitrance, and pretreatment. Challenges encountered during the conversion of biomass to biofuels are critically linked to the uncertainties of the physical properties of the feedstock. In particular, a better understanding of lignocellulose and its biodegradation will allow one to address the factors preventing an efficient fuel economy based on cellulosic biomass conversion. One of the major challenges is how cellulose, an assembly of polymers of glucose, can be effectively isolated and disassembled to its basic building block, glucose. We have quantified the relative interplay between stacking and hydrogen bonding interactions that give rise to the underlying stability of cellulose. Additionally, experiments and computations under various pretreatment conditions provide valuable clues on rational procedure for the efficient degradation of cellulose. Another challenge is the intimate association of cellulose with lignin, a recalcitrant structural component of the plant cell wall. Our calculations have now revealed several details of how lignin can be attacked and cleaved. Also, we make predictions on dissociation energies of different lignin linkages. This should provide insights into the selection and design of plants that have the types of lignin structures that could lead to optimal delignification. Research done in collaboration with USDA, University of New Mexico, and Great Lakes Bioenergy Research Center.

AGRO 295

Investigation of structural changes in Cel7A cellulase when bound to cellulose substrates

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A deeper mechanistic understanding of the saccharification of cellulosic biomass, which is recognized as a bottleneck in biorefining applications, could enhance the efficiency of biofuel development. Cellobiohydrolase I (Cel7A) is a major component of the cellulytic enzyme cocktail secreted by the fungus *Trichoderma reesei*. Our progress in investigating the structure of Cel7A conformation when free in solution and when bound to cellulose substrates will be discussed. Using small-angle neutron scattering it was possible to distinguish the scattering contributions of different components in a complex system to gain new insight into the mechanism of action of protein. Approaches for producing deuterated crystalline cellulose substrates were developed as part of these studies. This research approach is broadly applicable to investigating solution structures of proteins under a wide range of environmental conditions and can provide structural information on complex systems that is not attainable by other means.

AGRO 296

Developing the biorefinery: Production of value-added products and fuel from lignocellulosic feedstocks

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Traditionally in a lignocellulosic ethanol process all available C5 and C6 sugars are used for ethanol production. However, none of the organisms developed for conversion of both C5 and C6 sugars to ethanol is as efficient or robust as the yeast *Saccharomyces cerevisiae,* which readily converts C6 sugars to high titers of ethanol. In addition, having ethanol as the only main product may not be an economically attractive option considering the high capital costs of lignocellulosic processing plants. In our proposed new approach, the pretreated biomass is first hydrolyzed by hemicellulase to produce a stream rich in C5 sugars, which is subsequently used for production of value-added co-products instead of ethanol. The solid residue is then hydrolyzed with cellulase to produce a glucose-rich stream, which is used for ethanol production with *S. cerevisiae*. This approach creates many opportunities but also presents many challenges. These opportunities and challenges will be discussed.

AGRO 297

Electrospun core-shell Nafion/enzyme membranes for biofuel production

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Cellulase enzymes were successfully fabricated through core-shell electrospinning. These fibers remained active and retained 24% of the free enzyme for the hydrolysis of cellulose. To improve the activity further, we have electrospun β-glucosidase and cellulase fibers with a Nafion outer shell. Fibers provide a higher surface area when compared to protein immobilized on films, translating to higher active site accessibility and activity. The outer shell Nafion helps to hydrolyze cellulose which then is broken down to glucose by enzymes in the inner core. These fibers can potentially be incorporated as reactive membranes for the production of biofuels using solid substrates under mild conditions.

AGRO 298

Corn oil as a co-product of fuel ethanol production

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Due to the loss of subsidies, the fuel ethanol industry must find new ways to generate income. Production of value-added coproducts is one way to achieve this. Corn kernels contain only 4% by weight of oil, but that oil has value. Before 2011, few of the ~180 dry grind corn ethanol plants in the US recovered that oil. Today, in about 25% of those plants, a new type of non-edible corn oil is being produced at the back end of the plant. We have analyzed that oil and found it contains valuable components not present in commercial corn oil. We and others have also developed green processes to extract corn oil from ground corn using ethanol instead of hexane. We have also developed an enzymatic, solvent-free aqueous process for oil extraction from pre-fractionated corn germ. These technologies provide new green opportunities for fuel ethanol plants to produce more green assets.

AGRO 299

Characterization of biomass fast pyrolysis oils using NMR and chemometrics

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Biomass fast pyrolysis oils and other biofules can have very complex compositions, which makes their characterization challenging. Pyrolysis oils, their upgraded products and other biofuels produced from a variety of feedstocks were characterized by ^{1}H, ^{13}C and DEPT NMR analyses. The NMR spectra provided information on the chemical compositions of the fuels, but were found to oversimplify the information, resulting in a loss of important details. Hence, a chemometric method based on principle component analysis (PCA) was used to extract more from the NMR spectra. Comparison of the PCA scores and loadings plots enabled a determination of the chemical shifts and functional groups that were most important in discriminating amongst the samples. The clustering of the fuel samples based on PCA results were shown to track with their properties including energy content. Therefore NMR PCA analysis was shown to be a powerful and facile technique for classifying biofuels.

AGRO 300

Sophorolipid biosurfactant synthesis and value-added derivatization

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Sophorolipid (SL) is a glycolipid produced by yeast *Candida bombicola*. Research activities abound to develop applications of SL in commercial products because of its fine surfactant and antimicrobial properties. To help achieve lower overall production cost, we studied the use of surplus industrial coproducts as feedstocks in the fermentation process. We showed that glycerol and soy molasses, both coproducts generated respectively from biodiesel production and soy-protein isolation, could support production of SL at a volumetric yield of 60-75 g/L-culture under lab-scale fermentation conditions. To add value to SL, we concentrated on its 17-hydroxyoleate moiety as a starting material to generate “building-block” chemicals that are potentially useful for manufacture of new polymers and lubricants.

AGRO 301

Catalytic and process development for glycerol-free biofuel from acylglyceride lipids

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Biofuels, especially biodiesel, have become commonplace over the last couple of decades. The transesterification process used for biodiesel production leaves manufacturers with a byproduct, glycerol, that is of low value. Dimethyl carbonate has been studied as an alternate methylating agent to methanol and alters the chemistry such that glycerol is not formed. In our earlier studies, triazabicyclodecene (TBD) was chosen as an intial catalyst due to its ability to easily ionize the dimethyl carbonate and relative ease of separation post reaction. Additional advances have led to the implantation of TBD onto a solid hydrotalcite material via ligand binding to create a truly heterogeneous catalytic scenario. Manipulation of the d-spacing between the hydrotalcite double hydroxide layers made it an excellent support material. We will report on the developments of this novel catalyst (XRD, SEM-EDX, and *in situ* FTIR/Raman spectroscopies), reaction kinetics, and the chemical process development using Aspen 7.1 simulation software.

AGRO 302

Evaluation of odor perception of a fumigant using in-field volunteers

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Odor perseption of a fumigant was evaluated using local subjects. Various application rates (low and high) onto various soil types (sandy loam to clay loam) were evaluted. The subjects were driven in golf carts to specific locations at measured distances from the treated plots. Each subject was asked to rate the presence of an odor, the type of odor, and the intensity and characteristics (pleasant, offensive, etc.) for each marked location. The actual concentration was determined for each location as well. Control plots were evaluated along with actual treated plots.

AGRO 303

Field trial results for Bayfilm tarp material

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The objective of this research was to obtain comparative flux data for several alternative versions of Bayfilm in comparison to TIF tarp material. The test medium of this study was four agricultural test plots, of which tarp type was the primary test variable. All four fields were adequately separated, prepared similarly, and applied with PIC Chlor 60 EC® fumigant (~60% chloropicrin and ~40% 1,3-dichloropropene). Air and soil sampling was conducted on each of the four fields from the date of the application. Sonic meteorological sensors were established at pre-determined heights on each field to establish a vertical flow profile representative of field-specific meteorological conditions. This vertical profile, in conjunction with the measured vertical concentration profile of chloropicrin and 1,3-dichloropropene concentrations were the primary inputs used to calculate emission rates at each field. In addition, soil sampling was conducted at two depths for chloropicrin and 1,3-dichloropropene for concentration analysis.

AGRO 304

Science and technology of odor measurement

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Odors remain at the top of air pollution complaints to regulators and government bodies around the US and internationally. Ambient air holds a mixture of chemicals from everyday activities of industrial and commercial enterprises. A person's olfactory sense, the sense of smell, gives a person the ability to detect the presence of some chemicals in the ambient air. Not all chemicals are odorants, but when they are, a person might be able to detect their presence. Therefore, an odor perceived by a person's olfactory sense can be an early warning to them or might simple be a marker for the presence of air emmissions from some source. Either way, it is a person's sense of smell that can lead them to issue a complaint. When facility odors affect air quality and cause citizen complaints, an investigation of those odors might require that specific odorants be measured and that odorous air be measured using internationally standardized scientific methods. Point, area, and/or volume emmission sources can be sampled, and the samples sent to an odor laboratory for testing of

odor parameters following internationally recognized standards (e.g., ASTM and CEN), such as odor concentration, odor intensity, odor persistency, and odor characterization. Odor can also be measured and quantified directly in the ambient air, at the property line, and in the community, using field olfactometry practices. Furthermore, sensory testing can also be utilized to test chemical products and materials directly to consider their potential to emit odors or to compare chemical raw material or formulation alternatives.

AGRO 305

Sensory irritation from volatile chemicals

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At sufficient concentration, many chemicals stimulate somatosensory nerves. Mucus membranes like the eyes, mouth, and airways are sensitive primarily because they offer easier access to nerve endings than does dry skin. Resulting sensations range from clearly painful, like the sting and burn from pungent volatiles, to innocuous, like the cooling of menthol. Knowledge of underlying physiology has increased over the last couple of decades. For instance, the burning sensation from capsaicin, an important irritant in hot peppers, is mediated by a receptor protein that is also sensitive to physical heat. The cool sensation from menthol is mediated by a different receptor protein that is also sensitive to physical cooling. Work in humans has ranged from structure-activity studies aimed at predicting irritant potency based on molecular parameters to studies of how context and expectations influence responses to volatile irritants.

AGRO 306

Metam sodium shank compaction applications as a case study in mitigating airborne flux

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Regulatory initiatives at the state and federal level in the US have resulted in a reassessment of application methods for agricultural fumigants, with the objective of reducing airborne flux. This paper uses methyl isothiocyanate (MITC) emissions associated with applications of metam sodium as an example of how systematic steps to improve application methods, coupled with improved treatment zone preparation, can substantially reduce flux to the atmosphere without reducing rates or sacrificing efficacy. The paper compares airborne flux rates in the years 1990 through 2002 with more current flux rates based on four studies conducted during the period of 2008 through 2010 in California, Michigan, Wisconsin, and Washington State using current shank injection methods. This case study is offered as an example of how cooperative efforts involving registrants, applicators, and commercial farmers can effectively manage the evolving buffer zone requirements while still maintaining the treatment goals.

AGRO 307

Factors affecting the ability to detect and respond to environmental odors

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The sense of smell remains the least understood of our classic sensory systems. However, since the 1991 publication of experiments that identified an extensive olfactory gene family, for which the authors were awarded a Nobel Prize in Physiology or Medicine, we have learned that each person is likely unique in the ability to perceive odors because of the extensive variability in the genes that code for sensory receptor proteins. This genetic contribution is coupled with personal odor experiences, personality traits, and information about odors (or misinformation, e.g., "those toxic smells in the neighborhood") to further amplify individual awareness of and response to odors. Topics to be covered include: "smell blindness" or specific anosmia, gender differences, effects of age, extreme variability in hedonic responses to odor, and the potential impact of media coverage on community response to environmental odor.

AGRO 308

Modeling pesticide runoff from urban areas to assess impacts on threatened and endangered species in California

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Detections of pyrethroids and other insecticides in aquatic systems around urban areas in California have raised concerns about pesticide runoff from outdoor applications in urban and residential settings. A modeling system was developed to estimate the runoff of five widely-used pyrethroids across a 164,000 km^2 study area in California. County-level use data was spatially distributed across the study area using detailed land use data. Homeowner and professional applicator surveys were used to allocate pyrethroid applications to buildings, lawns, and other impermeable and permeable surfaces. Predicted urban mass loadings were relatively low and likely due to the large partition coefficient (K_d) of the pesticides used in the urban environment. Although, over 1,226,000 lbs of a.i. for four different chemicals were applied in the urban areas from 2000 – 2008, less than 1% was predicted to runoff in the urban environment and into surface water bodies. The assessment indicated that the greatest potential impacts on species of concern were predicted during the winter months.

AGRO 309

Evaluation of an approach for modeling the transport of residential pyrethroid applications

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Pyrethroid insecticides have both agricultural and residential uses and have recently been detected in urban waterways. Modeling pyrethroid environmental fate in a residential setting can help us to understand better the sources, transport pathways, and mitigation strategies for reducing environmental concentrations of pyrethroids. In this study, we compared concentrations of the pyrethroid bifenthrin predicted by the Storm Water Management Model (SWMM) with observed concentrations from a storm-drain outfall in southern California. The approach focused first on deriving pyrethroid wash-off characteristics from pervious and impervious surfaces based on plot-scale experiments. Research on the spatial and temporal patterns of bifenthrin applications in the study neighborhood was used in structuring the SWMM model to allow realistic application variability throughout the neighborhood. The results of the calibrated model simulations were used to determine SWMM's suitability for broader use in predictions of residential pyrethroid fate and transport and the effects of best management practices.

AGRO 310

Urban stressors for pesticide endangered species assessments: Should recent nutrient TMDLs and laws be considered?

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During 2000-2002, the US Environmental Protection Agency proposed new, stringent nutrient criteria under the Clean Water Act (CWA). Pursuant to §303(d) of the CWA, state agencies have designated more than 41,000 of their surface water bodies as “impaired.” Approximately 16,000 waters are impaired by nutrient-related pollution. Consequently, many TMDLs (total maximum daily loads) and state and local laws have recently been promulgated that target nutrients and the related parameters suspended sediments, dissolved oxygen, chlorophyll *a*, and temperature. Pesticide endangered anadromous fish assessments conducted by National Oceanic and Atmospheric Administration routinely list nutrients and temperature in urban and other environments as stressors that justify conservatism in their assessments. Full implementation of nutrient-based TMDLs would reduce the risk of eutrophication, which directly relates to dissolved oxygen concentrations. TMDL implementation can indirectly reduce urban runoff temperature increases as a result of vegetated BMPs. Thus these stressors can be reduced. A confounding factor is increased urbanization. Our initial focus on the Chesapeake Bay watershed and Florida is being expanded.

AGRO 311

Post-application irrigation reduces golfer exposure to the insecticide cyfluthrin

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A study to determine transferable residues and absorbed dose of cyfluthrin to golfers following application to turfgrass was conducted. Five applications were made to 100 m x 30 m bentgrass plots with (3X) and without (2X) post-application irrigation. Dislodgeable foliar residues were collected using the modified California Roller Technique. Volunteers simulated the play of golf for 4 hours starting 1 hour after application. Transferable cyfluthrin residues were measured on whole body dosimeters and with personal air samplers, while absorbed dose was estimated from urinary metabolites collected from volunteers wearing shorts and short sleeve shirts. Dislodgeable foliar residues were reduced by 93% (from 0.0197 to 0.0012 µg/cm^2) following post-application irrigation, significantly reducing the transferable residues collected on whole body dosimeters. Calculated Margins of Exposure (MOE) were > 200,000 for all applications based on the benchmark dose established by the US Environmental Protection Agency in the 2011 Pyrethroid Cumulative Risk Assessment.

AGRO 312

Design of an observational pest control operator worker exposure study

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To support products manufactured by Bayer CropScience (BCS) intended for indoor application to structures, an observational study consistent with the Protections for Subjects in Human Research Rule was designed to determine the potential exposure to Pest Control Operators (PCOs) involved in various work functions associated with crack and crevice treatments. This presentation will describe the need for the study, general experimental design, the processes used to identify and select the volunteers used in the study, and the analytical methodology developed for monitoring exposure.

AGRO 313

Epidemiology in public health risk assessments: A case study of 2,4-D

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In risk assessment, epidemiology studies are like a partial glass of water – some view it as half full, while others view it as half empty. Some consider an epidemiology study to be more important or to carry more weight than an animal study simply because it is occurring in real life and is in the target species. Others may view the epidemiology study sceptically because it is not as well controlled as an animal study. The epidemiological literature on the herbicide 2,4-dichorophenoxy acid (2,4-D) from the past decade will be reviewed. Biomonitoring exposure data for the general population, bystanders, and the occupationally-exposed will also be presented. These data demonstrate the rich and varied human information that is available for risk assessment on 2,4-D. The epidemiology results will be discussed in the context of the biomonitoring data and the consistency of study findings.

AGRO 314

Elicitation and metabolic engineering strategies to increase the levels of health-related polyphenols in root cultures

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Our group has used *Agrobacterium rhizogenes*-mediated transformation to develop hairy root cultures of peanut and American skullcap (*Scutellaria lateriflora*) as bioproduction systems for stilbenoids and flavonoids, respectively. These polyphenols have been associated with health benefits affecting cancer and neurodegenerative diseases. In order to increase their levels in plant systems, elicitation and metabolic engineering strategies were investigated. The combination of methyl jasmonate with cyclodextrin was the most effective elicitor treatment for both species. High levels of the bioactive, prenylated stilbenoids, arachidin-1 and arachidin-3, were induced in peanut. In skullcap, the non-elicited cultures produced the anticancer flavonoid wogonin. Interestingly, several putative phenolics were induced upon treatment with these elicitors. In addition, hairy roots of skullcap harboring a flavonoid-specific transcription factor (AtMYB12) were produced in efforts to increase the levels of wogonin. Hairy root cultures and these elicitation/metabolic engineering strategies provide a valuable tool for manipulating the levels of health-related compounds in plants.

AGRO 315

Metabolic engineering of lignan biosynthesis in *Forsythia*

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Sesamin, classified as a furofuran lignan, is water-insoluble lignan in sesame seeds and is biosynthesized through formation of two methylenedioxy bridges of a precursor lignan, pinoresinol, by a sesame cytochrome P450, CYP81Q1. Furthermore, sesamin was shown to lessen damages of the liver caused by ethanol and lipid oxidation as a new functional food. However, seed oil contains at most 0.4-0.6% (w/w) sesamin, indicating the need to develop a procedure for more efficient acquisition of sesamin. Recently, we have developed sesamin-biosynthesizing transgenic *Forsythia koreana* (Fk) cultured cells, CPi-Fk, which are stably transfected with sesame CYP81Q and an RNA interference sequence against an Fk endogenous lignan enzyme, pinoresinol/lariciresinol reductase. Moreover, CPi-Fk cells were found to increase the sesamin production under blue light. These results suggest that metabolic engineering of Fk leads to the establishment of a new platform for production of beneficial lignans.

AGRO 316

Production of pterostilbene in *Nicotiana* species and *Arabidopsis thaliana* via co-expression of peanut stilbene synthase and sorghum *O*-methyltransferase

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Pterostilbene, like its parent compound resveratrol, has a wide range of health promoting properties; however, pterostilbene is better than resveratrol in lowering lipid levels and in improving memory and cognition in aged rats. Pterostilbene has also been shown as a potent neuromodulator in aging and Alzheimer's disease, but not resveratrol. These interesting properties triggered engineering production of pterostilbene *in planta*. Pterostilbene-accumulating *Nicotiana tabacum* and *Arabidopsis thaliana* transformants were generated using a two-gene binary vector containing peanut stilbene synthase and sorghum *O*-methyltransferase, via *Agrobacterium tumefaciens* mediated transformation. GC-MS analysis showed accumulation of pterostilbene in 5 out of 15 tobacco lines and 8 out of 13 Arabidopsis lines. The tobacco transformants exhibited reduced floral pigmentation. Our studies demonstrated successful production of pterostilbene in transgenic plants; however, shunting of existing malonyl-CoA and coumaryl-CoA pools away from flavonoid synthesis must be taken into consideration.

AGRO 317

Quantification of allergenic lipid transfer proteins in maize kernels by liquid chromatography with ultraviolet and mass spectrometric detection

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Maize is not considered a major allergenic food; however, when food-induced allergenic and immunologic reactions have been associated with maize, lipid transfer proteins (LTPs) have been identified as the major allergens. An LC-UV/MS method was developed for LTP. The method allows for the differentiation between LTP and its variants. The present assay enables determination of LTP over a concentration range from 29 to 1030 µg/g in maize kernel samples. Assay recovery (% RE) was measured at 11 different concentrations ranging from 4 to 147 µg/mL and did not exceed 5.1%. The precision (% CV) was measured at 3 concentrations on each of 4 days and did not exceed 14.4%. The assay was successfully applied to determine and compare the levels of LTP in various commercial and transgenic maize lines. Further expansion of this method will be discussed for other major allergenic food crops such as soybean.

AGRO 318

Assessment of the natural variation of soybean protein expression through proteomics

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Genetic modifications to soybean have become inevitable to meet increasing demand. To ensure the safety of the crop for consumers, it is important to determine the natural variation in seed proteins, and any unintended changes that may occur resulting from genetic modification. Advances in proteomic technologies allowed for analysis of changes in protein profiles. We applied these technologies to determine the spectrum of proteins in soybean seed. We used two-dimensional polyacrylamide gel electrophoresis, matrix-assisted laser desorption/ionization time of flight mass spectrometry, and liquid chromatography-mass spectrometry to quantify and to identify different classes of soybean seed proteins. We observed significant variations of different classes of proteins between soybean varieties and differences in protein quantity and number of protein subunits among 27 soybean genotypes planted in three field experiments. This information is useful to determine whether the unintended expression of proteins found in transgenic soybean is within the range of natural variation.

AGRO 319

Comparison of aflatoxin and fumonisin levels in corn from Bt and conventional hybrids

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Few methods are available to control mycotoxin-producing fungi in pre-harvest crops. While published reports since 1999 have associated Bt expression in corn with reduced mycotoxin levels, subsequent field results have been inconsistent. We compared aflatoxin and fumonisin levels in corn from Bt and conventional hybrids. No consistent differences in mycotoxin levels were observed in 1998, 1999 and 2001 in Mississippi and Arkansas. In 2002, 2004, and 2005, fumonisin levels were lower in Bt hybrids than non-Bt hybrids at all plantings in both states. In 2006 and 2007, mycotoxin levels in Mississippi were less in harvested grain and debris from Bt than non-Bt corn. In 2010 and 2011, there was no significant difference in mycotoxin levels between Bt and non-Bt hybrids. More research is needed in order to identify the conditions under which Bt hybrids consistently yield corn with lower mycotoxin levels.

AGRO 320

Lactoferrin imparts resistance against fungal pathogens in transgenic plants

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Lactoferrin (LF) is a ubiquitous cationic iron-binding milk glycoprotein. LF is known to exert a broad-spectrum primary defense activity against bacteria, fungi, protozoa, and viruses in mammals. The Bovine LF (BLF) gene was introduced to tobacco (*Nicotiana tabacum* var Xanthi) and *Arabidopsis* (*A. thaliana*) plants via *Agrobacterium*. Detached leaves of transgenic tobacco plants exhibited high levels of resistance against a fungal pathogen *Rhizoctonia solani*. In addition, transgenic *Arabidopsis* seedlings were resistant to *R. solani* and did not show damping off symptoms. Previous studies have shown that LF also imparts resistance in plants against a bacterial pathogen *Ralstonia solanacearum*. This, together with the fact that LF is regarded as a safe food component, makes it a potentially highly-desirable candidate to introduce broad spectrum resistance against plant pathogens.

AGRO 321

Evaluating the economic benefits of the advanced biofuels targets under the RFS2

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This study evaluates the global economic effects of the renewable fuel standards under the USA Energy Independence and Security Act of 2007 (RFS2) focusing on the advanced biofuel targets. Three scenarios of the implementation of the RFS2 policy were simulated. Under the scenario that closely follows the current mandates, the global gross domestic product (GDP) increased by 0.21 percent in 2022. The GDP increased by 0.8 percent in the USA, whereas the effect on the rest of the world (ROW) was largely neutral at 0.02 percent. These positive economic effects are associated with the production of cellulosic ethanol from mature biochemical and thermochemical technologies and provide a basis for incentives to overcome cost and other barriers to the greater use of advanced biofuels in the USA. Future research is needed to compare the effects of cellulosic ethanol with those of other advanced biofuels among other refinements.

AGRO 322

Towards model-based identification of next generation biofuels: Aspects of product and process design

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Considering depleting fossil resources, biofuels offer great potential in ensuring future mobile propulsion. To this end, the Cluster of Excellence “Tailor-made Fuels from Biomass” at RWTH Aachen University investigates a holistic approach towards application-tailored biofuels by re-functionalizing biomass monomers. The multitude of possible organic fuel structures renders a solely experimental search strategy infeasible. Facing this challenge, a framework for model-based fuel identification has been elaborated. Complete coverage of the molecular space is achieved through a mathematically-rigorous generation of organic molecules. Model-based property screening relying on predictive structure-property-relationships is applied to reduce the quantity of molecules dramatically to a set of candidates predicted to exhibit optimal engine-relevant properties. Accounting for its major influence on synthesis efficiency, candidates are subsequently ranked regarding the similarity to available starting materials. Early stage process screening techniques are applied to the top-ranked candidates, determining key performance indicators of possible synthesis routes, and concluding the identification workflow.

AGRO 323

Efficient production of light olefins from biomass

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The U.S. has abundant biomass resources and with the right technology, has the potential to convert these renewable resources into valuable industrial products and bio-fuels. However, current thermo-chemical processes to convert renewable feed-stocks to chemicals such as pyrolysis and gasification or low temperature enzymatic processes are simply not cost-competitive with conventional fossil-fuel based processes. Exelus has developed a technology that applies novel reaction and reactor concepts with environmentally benign heterogeneous catalysts in a multi-step process that deconstructs and stabilizes biomass before conversion to light olefins – ethylene and propylene. The single biggest economic driver of this technology is a large reduction in production costs by efficient utilization of bio-mass raw material as well as lower capital costs than conventional steam crackers by eliminating the need to run the process at high reaction temperatures. The technology has been demonstrated using a variety of biomass including pure cellulose, switch grass and pine sawdust.

AGRO 324

Alternative processes for the bioconversion of waste into fuels and chemicals

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Wastewater treatment facilities are generally viewed only as a necessary component of industrial processes to comply with environmental regulations associated with protection of surface waters. However, the infrastructure of municipal and industrial wastewater treatment facilities, based on biotreatment, has the essential components necessary for a biorefinery (water nutrients, fermentation, biocatalyst production; cell concentration, recycling, and collection). Furthermore, many industrial wastewaters have organic compositions that can be transformed into valuable specialty chemicals. We will describe alternative configurations associated with specific wastewater treatment scenarios that could contribute to generation of sustainable feedstocks to produce fuels and chemicals, and thus, petroleum displacement and energy security. The proposed configurations also integrate the use of other sources of waste (municipal solid waste and agricultural residues) to enhance feedstock production rates. For example, results will be presented on the transformation of solid waste and liquid organic fractions into biogas, organic acids, and lipids for biodiesel production.

AGRO 325

Developing an industrial sugar-feedstock platform in the Mid-South for renewable chemicals and biobased products

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Sweet sorghum and sugar beets are targeted for agronomic production and processing in the Mid-South/Mississippi Delta as part of a regional strategy to establish an industrial sugar-feedstock (sucrose) platform for conversion to biofuels and renewable chemicals. A dual crop strategy can provide a year-round juice and syrup product in temperate regions. BioDimensions is developing an Advanced Rural Biorefinery (ARBR) based on sweet sorghum as the primary crop to establish supply chain logistics and demonstrate technologies suitable for the rural-scale biorefinery. Sugar beets are targeted as a flexible second off-season feedstock. Research at ASU is targeting biochemical processing of the beet pulp that will be generated from juice production to develop energy-efficient processing technologies and co-product streams to promote further economic viability. We will identify key benefits and challenges for the industrial sugar platform, present the current status of the ARBR, and summarize our laboratory studies for developing associated biochemical technologies.

AGRO 326

Giant panda intestinal microbes: Biofuels and conservation

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The use of giant panda (*Ailuropoda melanoleuca*) feces may hold the key to reducing the cost of biofuel production. The giant panda's fecal metagenome has elucidated multiple cellulolytic microorganisms that can be used in the conversion of lignocellulosic biomass-based biofuels. Preliminary evidence suggests that oleaginous microorganisms may also be present. Twelve species of cellulolytic microbes, including *Clostridium cellulovorans*, *Clostridium phytofermentans,* and *Pseudomonas fluorescens* were isolated using Ilumina sequencing. These microbes can be used to pretreat lignocellulosic biomass, a waste product of other agricultural processes, converting the biomass into simple sugars that can be used by oleaginous microbes to accumulate lipids. These lipids can then be converted into renewable diesel and biodiesel, thus creating a usable product from two waste materials and lowering costs associated with biofuel production. Further characterization of the microbes is currently underway to evaluate the activity of the enzyme systems and processes associated with these metabolic pathways.

AGRO 327

Fuel production from cellulose by subterranean termites

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Fuel production by wood-feeding termites was investigated by using cellulose as their food source. The bioconversion of cellulose to H_2 by the subterranean termites could reach as high as 3860 ± 290 µmol/g cellulose, suggesting that the termite gut system is unique and efficient in H_2 conversion from cellulose. Additionally, the effects of antibiotics on H_2 production and the gut symbionts in wood-feeding termites were investigated.

AGFD 7

Reversal of age-related motor deficits following stilbene dietary supplementation

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As the population over 65 increases, the incidence of age-related injuries will rise. Currently, there are few therapeutic regimens for age-related motor deficits. Resveratrol is a phytoalexin that has been shown to improve motor function in aged mice. To examine the effect of resveratrol or resveratrol analogs on motor function *in vivo,* mice (2, 10 and 22 months) were fed resveratrol or pinostilbene containing diet for 8 weeks. Motor function was examined using a challenge beam test and a cylinder test. To investigate the mechanisms that may underlie a reversal of motor deficits, dopamine (DA) and dopamine metabolite levels were examined in all groups and dopaminergic cells were treated with resveratrol or resveratrol analogs +/- DA. Additionally, dopaminergic cells were analyzed for ERK1/2 and ERK5 activation. Resveratrol and pinostilbene protected dopaminergic cells from DA-induced cell death. This research may lead to novel therapies for age-related motor deficits using natural compounds.

AGFD 8

Systemic and neuronal cross-talk: Effects of nature's products

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Plant foods, including fruits, vegetables, herbs and spices and certain oils have been consistently identified as key components of dietary patterns that reduce risk for the development of chronic diseases, including atherosclerotic cardiovascular disease, Alzheimer's disease, type II diabetes mellitus and some cancers. Recent epidemiological evidence has identified non-essential compounds, such as (poly)phenols that contribute favorably to the diet-disease relationship, presumably through their ability to modulate processes of oxidative stress/damage and inflammation. Anthocyanins and procyanidins are among those compounds showing systemic biological activity as well as neuronal activity. This presentation will discuss processes underlying disease, such as oxidative stress and inflammation and their relationship to chronic disease development, sources and inducers of oxidative stress and inflammation and impacts on neuronal signaling, and foods/food components and extracts that show biological activity systemically and centrally.

AGFD 9

Diverse cellular mechanisms underlying the neuroprotective effects of dietary polyphenols in ischemic injury in vitro

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Polyphenols, present in fruits and vegetables, possess anti-oxidant, insulin-potentiating, anti-inflammatory, and anti-apoptotic properties. Oxidative stress, inflammation, and apoptosis are key characteristics of cerebral ischemia, caused by an interruption of cerebral blood flow, and polyphenols exert neuroprotective effects in ischemic injury. Brain edema is an important consequence of ischemia and oxidative stress and inflammation are implicated in its pathogenesis. Astrocyte swelling is a major component of cytotoxic brain edema and, along with vasogenic edema, may contribute to increased intracranial pressure, brain herniation, and additional ischemic injuries. We investigated the protective effects of several polyphenols in attenuating cell swelling using C6 glial cultures. Polyphenol extracts from cinnamon, green tea, as well as purified type-A polyphenols from cinnamon, myricetin, and quercetin, attenuated cell swelling following oxygen-glucose deprivation (OGD), an *in vitro* model of ischemic injury. To study the mechanisms underlying the protective effects of such polyphenols we examined their effects on increased ROS production, nitric oxide (NO), mitochondrial dysfunction, and intracellular calcium $[Ca^{2+}]_i$, key factors that contribute to cell swelling, and on the reduction in glutamate uptake. All the above-mentioned polyphenols significantly reduced the OGD-induced increase in ROS. However, cinnamon and green tea augmented the OGD-induced increase in NO and concentrations of type-A polyphenols, that did not block ROS, significantly attenuated cell swelling, indicating that polypehnols may have multiple actions in reducing cell swelling. Blockade of the mitochondrial permeability transition (mPT) pore generally blocks cell swelling. OGD-induced dissipation of the inner mitochondrial membrane potential ($\Delta\psi_m$), a component of the mPT, was blocked by these polyphenols, but not by quercetin, even though quercetin blocked swelling. This indicated that the cellular mechanisms by which polyphenols reduce swelling are multi-factorial. OGD-induced $[Ca^{2+}]_i$ was significantly attenuated by myricetin, quercetin, and a type-A polyphenol from cinnamon. Further, blockade of $[Ca^{2+}]_i$, using calcium channel blockers (nifedipine, nimodipine, verapamil), BAPTA-AM, a calcium chelator, and dantrolene, an inhibitor of Ca^{2+}-release through RyR, significantly attenuated swelling indicating that one mechanism by which such polyphenols reduce swelling is through regulating $[Ca^{2+}]_i$, or a $[Ca^{2+}]_i$-mediated pathway. The type-A polyphenol component from cinnamon, as well as myricetin, but not quercetin, attenuated the decline in glutamate uptake after OGD, similar to cyclosporin A, a blocker of the mPT. These results indicate that polyphenols regulate $[Ca^{2+}]_i$, to exert their protective effects on cell swelling and some of the protective effects of polyphenols are mediated by mitochondria. In addition, given the differential effects of polyphenols on mitochondria, the neuroprotective effects of polyphenols may involve multiple intracellular signaling pathways that target diverse mechanisms.

AGFD 10

Use of cannabinoid receptors in the identification of biologically active secondary metabolites as immune-stimulants from foods

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Over the past 10 years, significant progress has been made in the field of the endocannabinoid system and in cannabinoid chemistry. Although much of this focus has been in the discipline of pharmacy, there are potential utilities of this system in the agrochemical and food industry. It is interesting to find there is a certain pleasure that comes from migrating across scientific disciplines. The feeling is much like seeing an old friend for the first time in many years. Perhaps another metaphor exists between pharmacy and agrochemicals with the common strand being chemistry. It is recognized that the receptor subtypes of the endocannabinoid system have broad utility. In particular the Cannabinoid Receptor Subtype 2 (CB2) has been suggested to play a role in influencing the immune system. This paper will describe the bioassay directed isolation and characterization of secondary metabolites from plants and food, which may stimulate the immune system.

AGFD 11

Exploring nature against depression, anxiety, and opioid withdrawal

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The ever-increasing demand for drugs that treat neurological conditions, coupled to the advancement of new techniques for the isolation and characterization of molecular targets as well as chemical entities, the exploration of natural products for neurological drug development is fast advancing. In collaboration with natural products chemists, research efforts in my laboratory have focused on establishing the potential of a variety of natural products to serve as drug leads for the treatment of various neurological disorders including anxiety, depression, as well as in the relief of opioid withdrawal symptoms. Phytocannabinoids isolated from high potency cannabis as well indole alkaloids isolated from marine sponges were evaluated for antidepressant-like actions in animal models of behavioral despair paradigms. The natural product pterostilbene showed significant anxiolytic activity that seems to correlate with down regulation of hippocampal ERK phosphorylation. Finally the potential for Kratom or mitragynine for pharmacological treatments of opioid withdrawal will be discussed.

AGFD 12

Anthocyanin effects in cognition and dementia: Probable mechanisms and future directions

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Anthocyanins are potent antioxidant and anti-inflammatory agents. Data suggests they have many biologically diverse roles. Anthocyanins are bioavailable after consumption of berries and reside in brain tissue longer than in plasma. This was unexpected, given normal assumptions of pharmacokinetics. The mechanisms by which anthocyanins contribute to neuroprotection remain poorly understood. As new data regarding their tissue concentrations comes to light, a better understanding is possible regarding the potential mechanism involved in preventing neurodegeneration and enhancing memory and cognition. Presently, limited data supports a causal relationship between the consumption of anthocyanins and behavioral outcomes. Supporting evidence will be presented with future directions proposed. Despite a decade of dramatic increase in understanding of the biology of flavonoids, they remain mistakenly portrayed as simply antioxidants. This is a significant barrier to advancing anthocyanins, and indeed flavonoids in general, to preclinical research.

AGFD 29

Effectiveness of the botanical drug candidate PBI-05204 derived from Nerium oleander in ex vivo and in vivo models of ischemic stroke

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Despite much study of the biochemical pathways triggered by ischemic stroke, molecular targets that have been targeted to date in clinical studies have failed to provide effective neuroprotection to injured neurons. Previously, we implemented a screen of known signaling pathways in a brain slice model for ischemic stroke, and found that several cardiac glycosides could provide direct neuroprotection to brain slices following ischemic injury induced by transient oxygen-glucose deprivation (OGD). Critically, we could show neuroprotective benefit of cardiac glycosides even when applied many hours after OGD, corresponding to the accessible time window for therapy in clinical stroke. The FDA-approved cardiac glycoside drug digoxin is a known substrate of P-glycoprotein, and thus therapeutic drug levels in CNS are not likely to be achievable. We show that the botanical drug candidate PBI-05204 provides dose-dependent neuroprotection in brain slice models of ischemic stroke. In addition we present evidence that such neuroprotection is mediated at least in part through its principal bioactive ingredient, the cardiac glycoside oleandrin. We further show that oleandrin can pass effectively across the blood-brain barrier, and present preliminary data for neuroprotection of CNS tissues in rodent models following systemic administration of PBI-05204. That PBI-05204 has already successfully completed a Phase I clinical trial in an oncology indication further suggests that this botanical drug candidate merits further evaluation for therapeutic use in ischemic stroke and related forms of CNS injury. This work supported in part by Phoenix Biotechnology, Inc.

AGFD 30

Attenuation of stress/age associated toxic protein accrual and tau-hyperphosphorylation in brain by berries and walnuts

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Phytochemicals protect the brain against stresses caused by oxidative free radicals and inflammation. The susceptibility of the brain to oxidative stress or inflammation increases with age, leading to degeneration and death of neurons with

pathologies of neurodegenerative diseases. We investigated whether feeding young rats blueberry- or strawberry-supplemented diets, followed by irradiation with high energy and charge particles, a model for accelerated aging, would protect brain cells from radiation-induced damage. Irradiation caused substantial hyperphosphorylation of tau proteins, a hallmark of Alzheimer's disease, in striatum and hippocampus, and caused substantial buildup of polyubiquitinated protein aggregates. Supplementing rat diets with blueberries and strawberries for 8 weeks, prior to irradiation, protected the brain against aggregation of PHF-tau proteins and attenuated polyubiquitinated aggregation via altering the levels of mTOR, Beclin1, and P62/SQSTM1. Aged animals fed with walnut-supplemented diets also elicited similar benefits in a normal aging brain, indicating benefits at the molecular level.

AGFD 31

Novel tetrameric galectin from a marine sponge potentiates mammalian glutamate receptor function

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Marine organisms are a rich source of molecules that alter mammalian neuroactivity. We carried out a bioactivity-guided screening using mouse behavior and highly sensitive *in vitro* electrophysiological assays. An aqueous extract from a *Cinachyrella* marine sponge potently modified the functional properties of mammalian ionotropic glutamate receptors. Further isolation, functional characterization, and structural resolution yielded a new tetrameric member of the sponge galactose-binding lectin, or galectin, family. The amino acid sequences of the CchGs confirmed that the proteins were distant orthologues of animal prototype galectins. The crystallographic structure of CchGs at 2.1 Å revealed that the lectin monomers associate non-covalently into a toroid-shaped tetramer that has not been observed in previously resolved galectin structures. Purified CchGs potentiated steady-state currents and slowed desensitization of mammalian glutamate receptors expressed in heterologous cells. This unexpected biological activity suggests that analysis of related mammalian galectin proteins will yield further glycobiological and neurophysiological insights.

AGFD 32

Novel neuroactive compounds from aqueous extract of marine sponges

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Aqueous extracts of marine organisms have provided us with interesting neuroactive molecules. We have reported novel kainate receptor ligands dysiherbaines from a Micronesian sponge and new purine derivatives with synaptic modulation activity from Palauan sponges. In the present paper, we outline isolation, structure and biological activity of these compounds. In addition, we present our recent progress in discovery of novel marine neuroactive compounds focusing on a novel peptide toxin Aculeins (ACUs) found form Okinawan sponge *Axynissa aculeata*. ACU A and B are isolated as toxic principals in the aqueous extract of the sponge. Aculeines are highly unique 44-amino acid peptide with three disulfide bonds. Amino acid terminals of ACUs were modified by long chain polyamines in an unprecedented manner.

AGFD 33

Neuroactive natural products from mollusks and their associated bacteria

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Cone snails are renowned for biological peptides, but we show that they also contain small molecules that act on neurons. Bacteria were cultivated from cone snails and other gastropods, and their extracts were screened using a phenotypic assay. These extracts yielded a variety of natural products, often exhibiting selective and potent activity against individual human receptors and ion channels. We are examining these compounds for their therapeutic potential. In addition, we show that some of these bacterial molecules contribute to the chemical arsenal of cone snails.

AGFD 34

Potential agents to enhance the expression of neurotrophins in the brain

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Neurotrophins are endogenous peptides responsible for development and repair of neurons in the brain. Depletion of neurotrophins could potentially lead to neurodegenerative disorders. Direct delivery of neurotrophins to the brain is not a practical solution. Therefore, there is an urgent need to discover safe therapeutic agents that can enhance the expression of neurotrophins in the brain. Carnosic acid has been reported to have the potential to enhance the expression of neurotrophins in the *in vitro* cell line models. Further, we investigated the brain bioavailability of carnosic acid in the brain by microdialysis sampling, following i.p and intranasal administration. The levels of Nerve generation factor (NGF) and Brain derived neurotrophic factor (BDNF) was found to be significantly higher in treated rats than in the control rats. Pharmacodynamic investigations were performed in depression induced rat model (BDNF depleted rats).

AGFD 42

Bioactive potential of resveratrol oligomers of the *Carex* genus

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The *Carex* genus (family: Cyperaceae), consists of over 2000 species distributed worldwide. Although the genus has been shown to be a rich source of resveratrol based oligomers, the genus has received limited phytochemical

attention. We have initiated a study to determine the bioactive potential of the numerous *Carex* species growing in Pennsylvania, United States. Seed and leaf extracts for three *Carex* species have been shown to have a high content of antioxidant flavonoids. In addition, a resveratrol dimer (pallidol), two resveratrol trimers (*trans*-miyabenol C and alpha-viniferin), and three resveratrol tetramers (hopeaphenol, kobophenol A and kobophenol B) have been isolated. The compounds were evaluated for cytotoxicity against human colon tumor cell lines, and both alpha-viniferin and hopeaphenol exhibited strong antiproliferative effects against HCT-116 and Caco-2 cells lines, with IC_{50} values ranging from 2-32 microM. The presence of bioactive flavonoids and anticancer resveratrol oligomers in the *Carex* genus indicate the potential nutraceutical application of the genus.

AGFD 43

Anthocyanin content and percent polymeric color of commercial berry products

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Anthocyanin losses during storage of processed berries are accompanied by increased percent polymeric color values indicative of the formation of anthocyanin-flavan-3-ol polymers. In this study we evaluated the anthocyanin content and percent polymeric color of 21 commercial samples of various processed berry products. Anthocyanin content ranged from 11.2 mg/kg for strawberry jam to 6071.6 mg/kg for blackberry concentrate, while percent polymeric color values ranged from 13.2% for cranberry concentrate to 70% for blueberry and strawberry juice concentrates. Using MALDI-TOF-MS we detected the presence of anthocyanin-flavan-3-ol polymers in a sample of 100% cranberry juice stored at ambient temperature. A series of masses corresponding to peonidin 3-galactoside and cyanidin 3-galactoside linked to 1, 2, 3, and 4 flavan-3-ol units through an ethyl bridge were apparent. The observed masses indicated structural variation in the type of interflavan bonds (A and B-type), which increased in complexity with increasing polymerization of flavan-3-ol units.

AGFD 44

Whey protein hydrolysates inhibits hydrogen peroxide induced oxidative stress

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Whey protein hydrolysates (WPHs) contain various antioxidant peptides.In order to investigate the mechanism of WPHs' antioxidant activity in protecting against oxidative stress(OS),WPHs was prepared with pepsin and trypsin, PC12 cells model was bulit to observe the protective effect of WPHs against H_2O_2-induced changes of cell viability, Total Antioxidant Capacity(T-AOC) and apoptosis. The result indicates that WPHs attenuated cell viability loss by 18.60%,reduced apoptosis by 20%,and recovered T-AOC level. Intracellular ROS accumulation, calcium levels and mitochondrial membrane potential(MMP) were tested by flow cytometry, which indicates that WPHs suppressed the elevation of ROS and calcium, stabilized MMP by 16%. Anti-apoptosis/pro-apoptosis protein Bcl-2/Bax, PARP were investigated by Western blot, which indicates that WPHs could increase expression of Bcl-2 while inhibiting Bax and degradation of PARP. WPHs also block activation of Caspase-3 by 62%

In conclusion,WPHs could significantly protect PC12 cells against H_2O_2-induced oxidative stress, might be a good antioxidant addition agent.

AGFD 45

Curcumin inhibits metastasis of thyroid cancer cells

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Curcumin is a naturally occurring phenolic compound isolated as a yellow pigment from turmeric. In order to further advance our knowledge of the role curcumin plays in the metastasis of papillary thyroid cancer, we investigated its effect on K1 cell adhesion, spreading, invasion and migration. In vitro invasion assays was used to assess the changes in invasive behavior. Gelatin zymography and western blot were used to detect Matrix metalloproteinase activation and expression. After treated with different concentrations of curcumin, a series of motility related to matastasis of K1 was repressed in a dose-dependent manner, including adhesion, spread, invasion and migration. Up to now, we have also discovered the activation and expression of MMP-9 were depressed by curcumin. Therefore we demonstrate that MMPs are critical effectors of invasion in the papillary thyroid cancer cell line studied. Curcumin may be a effective tumoristatic agents for the treatment of aggressive thyroid carcinomas.

AGFD 46

Cytotoxic polymeric proanthocyanidins from Pourouma cecropiifolia fruit

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The anthocyanin-rich extract (ARE) of the Amazonian fruit *Pourouma cecropiifolia* showed moderate cytotoxicity toward different human cancer cell lines under MTT assay. Three fractions (F1-F3) were obtained by fractionation of ARE by gel filtration using Sephadex LH-20 and then analyzed by HPLC-PDA and LC-ESI/MS^n. F1 was composed of the monomeric anthocyanins delphinidin-3-*O*-*β*-glucopyranoside, cyanidin-3-*O*-*β*-glucopyranoside, and cyanidin-3-*O*-(6´´-malonyl)- *β*-glucopyranoside. F2 contained the isomeric flavonols quercetin 3-*O*-*α*-rhamnopyranosyl-(1→6)-*β*-galactopyranoside and quercetin 3-*O*-*α*-rhamnopyranosyl-(1→6)-*β*-glucopyranoside, the structures of which were confirmed by ^1H and ^{13}C NMR. F3 contained polymeric pigments, which were analyzed by tandem ESI/MS in an LCMS-IT-TOF equipment. The structures of two proanthocyanidin and two flavanol-anthocyanin condensed pigments were suggested based on their MS^n fragmentation patterns. The results of cell viability assays showed that only fraction F3 exhibited a cell growth-inhibitory effect similar to the one found for ARE. F3 significantly reduced the viability of HEp-2 larynx, MKN-45 gastric carcinoma, and MCF-7 breast cancer cells; in contrast, the pure compounds did not show promising citotoxicity toward cancer cells evaluated.

AGFD 47

Potential of coffee and coffee constituents for promoting body weight-maintenance in healthy subjects

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Epidemiological studies provide evidence that moderate coffee consumption is associated with a lower incidence of metabolic syndrome. Obesity is one of the major risk factors of metabolic syndrome which is becoming more common due to a rise in obesity rates among adults. Since it is possible to prevent or delay metabolic syndrome by maintaining a healthy body weight, there is growing interest in foods that may help to control energy intake and/or mimic energy expenditure by, e.g., inducing mechanisms of satiety or thermogenesis. Coffee, when consumed in moderate amounts of 3 – 4 cups per day, has been demonstrated to decrease the daily energy intake and to stimulate mechanisms of satiety in healthy volunteers, and to induce mechanisms of thermogenesis in cells in culture. Current research is focused on the identification of coffee components that act on these mechanisms, such as caffeine and chlorogenic acids.

AGFD 48

Anthocyanins as xenobiotic medicines

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Anthocyanins ward off plants predators and interfere with digestion and absorption of food in mammals, resulting in their classification as anti-nutrients. Yet millennia of evolution provided mammals with benefits. Anthocyanins are interesting among plant compounds as they are found to exert many metabolic effects in mammals. As xenobiotics, mammalian metabolism treats them as such; however, as observed since the time of Hippocrates, foreign chemicals can be potent medicines. Yet polyphenols, including anthocyanins, deliver contradictory research results in prevention of cardiovascular disease, cancer, diabetes and other health conditions. Most studies have been conducted at doses higher than reasonably attainable for most people. More studies in humans and more reliable data on the polyphenol content of foods are needed. Given the evidence we do have, how we do best approach the task of proving a benefit to consuming polyphenols, given funding time scales of modern medical research

AGFD 64

Comparison of antithrombotic activity and protective activities on alcohol gastric ulcer and immune system of different Fucoidan from Laminaria japonica

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In the present study, we compared the effects of four fucoidan fractions with different molecular weight and sulfated ester content from *Laminaria japonica* on antithrombotic activity and their protective activities of immune function and alcohol-induced gastric ulcer to find a safe fucoidan with good activity from a wildly-cultured brown seaweed Laminaria japonica in China. The results showed that oral admministraction of all fucoidan can effectively improve the immune system by increasing hemolysin content, ability of macrophages for celiac macrophage and delaying hypersensitivity level. After oral administration of low molecular weight fucoidan, the depth of alcohol-induced gastric mucosal injury was shallower and the bleeding was significantly reduced, better than middle molecular weight. Fucoidan can significantly improve the antioxidant enzymatic system and inhibited the oxidation of lipid in blood. In antithrombotic acitvity, molecular weight seems play a more important role in the antithrombotic and anticoagulant activity by venous injection of fucoidan. *In vivo* middle molecular weight fucoidan fractions exhibited better antithrombotic activity in electrical induced arterial thrombosis than low molecular weight fucoidan. Fucoidan fractions with different molecular weight acted on the antithrombotic action by different effect on coagulant system, platelet, TFPI, TXB2 and 6-keto-PGF1α activities.

AGFD 65

Effect of blueberry anthocyanidin extract on plasma cholesterol in hamsters fed a high cholesterol diet

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Interest in blueberry anthocyanidin extract (BAE) as a cholesterol-lowering nutraceutical is growing. The present study was to investigate the effect of BAE on blood cholesterol and gene expression of cholesterol-regulating enzymes in Golden Syrian hamsters maintained on a 0.1% cholesterol diet. Results showed dietary supplementation of 0.5% and 1.0% BAE decreased plasma total cholesterol (TC) in a dose-dependent manner. Supplementation of BAE was associated with a trend of increasing excretion of both neutral and acidic sterols. Real-time PCR analyses demonstrated BAE down-regulated the gene of NPC1L1, ACAT-2, MTP and ABCG, all of which are involved in cholesterol absorption. In addition, BAE was also be able to down-regulate the gene expression of hepatic HMG-CoA reductase. It was concluded that hypocholesterolemic activity of BAE was most likely mediated by inhibition of cholesterol absorption or synthesis via its inhibition on gene expression of intestinal NPC1L1, ACAT-2 MTP and ABCG, and hepatic HMG-CoA reductase.

AGFD 66

Dietary flavonoids: Red-ox ingredients or just simple "travellers" of plant foods?

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The extent to which antioxidant-rich plant foods are able to tune oxidative stress and the identification of the molecules involved is unclear. Flavonoids have been shown to display a strong *in vitro* antioxidant activity. However, the *in vitro* evidence might be somehow of limited impact due to the non-physiological concentrations utilized and to the low degree of absorption of flavonoids. Moreover, their extensive metabolism within the body, leading to molecules with different chemical structure and activity compared to the ones originally present in the food, have raised concerns about their antioxidant action in humans. The first systematic review of dietary intervention studies with plant foods and flavonoids on markers of antioxidant function and oxidative stress, will be presented. There is a strong need of increasing the existing knowledge on the efficacy of antioxidants *in vivo* to clarify if flavonoids are active red-ox ingredients or just ancillary “travellers” of plant foods.

AGFD 67

Plum fruit polyphenols differentially inhibit inflammation, and fat accumulation in cell models (adipocytes, macrophages, and HUVEC) associated to metabolic syndrome

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The effects of plum polyphenols against some components of the metabolic syndrome were studied using cell models including adipocytes to determine effects in differentiation, fat accumulation and inflammation representing events in fat tissue. In addition, we studied inflammation in macrophage cells and Human umbilical vein endothelial cells (HUVEC) associated to atherosclerosis events. Results indicated that plum polyphenols have multiple functions and could potentially work against the metabolic syndrome in different fronts simultaneously. A rich anthocyanin extract (RAE) inhibited adipogenesis or lipid accumulation by modulating key transcription factors, c/EBPα Pparγ and Pparα and reduced the inflammatory response in adipocytes or fat cells by modulating transcription factor NFkB and gene expressions of different pro-inflammatory cytokines. On the other hand, chlorogenic acid inhibited the inflammatory response in macrophages and HUVEC cells by modulating transcription factor NFkB and gene expressions of different pro-inflammatory cytokines and adhesion molecules associated to chronic inflammation and atherosclerosis.

AGFD 68

Effects of raspberry supplementation on measures of motor and cognitive function in aged rats

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Dietary supplementation with foods high in polyphenols has been shown to modulate decrements in performance in aged animals. A series of age-sensitive tasks assessing motor and cognitive skills was used to evaluate the effects of a raspberry diet. An extract was prepared from fresh ripe berries and incorporated at 2% into a standard well-balanced diet. Old rats were fed the supplemented or control diet for 11 weeks. The raspberry group scored significantly better on several motor tasks measuring strength, balance and agility. Performance on measures of learning and memory were unchanged. Results suggest that the bioactive components of raspberries may target age-related impairments in motor function thereby contributing to healthy aging. By affecting motor but not cognitive performance raspberry supplementation demonstrates a unique pattern of effects compared to other fruits and vegetables tested in our model. Future studies will address underlying differences in bioactive composition in relation to behavioral findings

AGFD 69

Colonic fermentation of dietary fibers is altered by background diet

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Dietary fiber must be considered as a major functional food in the diet. Fiber increases bulk in the GI tract, is fermented to short chain fatty acids and carries other food components through the GI tract to the colon where they are altered by the microbiota. Short chain fatty acids are considered highly desirable products of the fermentation by the microbiota. Changes in the diet alter the profile of the microbiota and consequently alter the nature of the fermentation of dietary fiber. When subjects are fed a diet rich in fermentable carbohydrates such as resistant starch, they produce high levels of short chain fatty acids (butyric and propionic) when alternative fibers are introduced. Conversely, when subjects are on low fiber diets they produce less butyric and propionic acids but higher levels of acetic acid. The effect appears to be driven by a shift in the dominant organisms in the microbiota.

AGFD 70

Stone fruit extracts revert insulin resistance and glucose insensitivity in cell models (muscle, hepatic, and pancreatic $_T$cells) associated to type 2 diabetes

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We report that stone fruit extracts (SFE) have multiple functions and could potentially work against insulin resistance and glucose insensitivity in different fronts simultaneously. All SFE reversed the glucose insensitivity in pancreatic-β-cells induced by palmitic acid. These extracts, by possible antioxidant (AOX) and AOX-independent mechanisms, increase insulin secretion. On the other hand, only plum extracts reversed the insulin resistance in hepatic cells induced by palmitic acid. Plum extracts reversed the effect by a mechanism that increased glucokinase activity. Similarly, nectarine and peach extracts reversed the insulin resistance in muscle cells induced by palmitic acid. Both extracts reversed the effect in muscle cells in a similar fashion as the drug metformin by an increase in glucokinase activity and a possible increase in glucose uptake. These results are very promising and indicate that SFE have potential health promoting properties against Type 2 Diabetes, which is an important event of the metabolic syndrome.

AGFD 85

Mechanism of inhibition of advanced glycation end products by bioactive compounds present in okra seed extracts: A comparison with the well known inhibitor aminoguanidine

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Advanced glycation end products (AGEs) have been associated with the micro-vascular complications in diabetes and other age-related neurodegenerative diseases. Recently we reported the bioactivity of okra seed extracts as potential inhibitors of advanced glycation end products (AGFD #95(2010),AGFD#157(2012). The studies involved examination of structurally defined flavonoids: quercetin-3-mono and di-glucosides, kaempferol-3-mono-glucoside, 3,5,7,3',4'- pentahydroxy flavonol-3-O-α-L-arabinofuranoside and rutinoside (Quercetin-3-O-rhamnosyl-glucoside). These compounds also showed potent antioxidant and antiproliferative activities. The present studies describe the mechanism of inhibition of advanced glycation end products by the bioactive compounds present in okra seed and their comparison with 2-aminoguanidine, a well known inhibitor of glycation. We incubated bovine serum albumin (BSA) and histone proteins with fructose, ribose, mannose and glucose with and without okra seed extract. After incubation the fluorescence of AGEs was measured with a fluorescence spectrophotometer (excitation 360 nm, emission 460 nm). After 7 days of incubation the fluorescence data exhibited an inhibition of glycation by the okra seed extract which was identical to the inhibition of glycation with 2-aminoguanidine in a dose dependent manner. We also noticed that okra vegetable mucilage, cinnamon and *Withania somnifera* (Ashwagandha) under these conditions did not exhibit any glycation inhibitory activity. Examination of inhibitory activity of okra seed extract with histone proteins did not exhibit a change in the intensity of fluorescence spectrum compared to BSA. We believe that glycosylation of BSA in the presence of okra seed extract leads to a change in the conformation of the protein probably due to an increased exposure of tryptophan residues. On the other hand, the non-enzymatic glycosylation of histones does not present a favorable glycosylation site and therefore no inhibition. Detail mechanistical implications of protein glycation inhibition with the 3-hydroxy substituted flavonoids present in okra seed extract and its comparison with 7-hydroxy substituted flavanoids will be also discussed.

AGFD 86

Portable nanoparticle-based sensor for the discovery of food antioxidants

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With the increased awareness of nutrition and the advocacy for healthier food choices, there is a need for a simple, easy-to-use test that can reliably measure the quality and content of food antioxidants. We report development of a portable nanoparticle-based sensor for the detection of antioxidants. The platform is based on immobilized nanoparticles that show a distinct color change in contact with antioxidants by means of redox and surface chemistry reactions. The sensor operates in a variety of environments and food products; it does not require specialized equipment or external reagents and can be used by unskilled personnel and the general population. This presentation will discuss fabrication and performance evaluation of this assay for the detection of common food antioxidants, and describe functionality of the assay in real samples, including tea, a variety of juices and food extracts. Validation of this sensor against commonly used USDA assays will be discussed.

AGFD 87

Alkylresorcinol as the major active components in wheat bran for colon cancer prevention

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Many studies have found that dietary cereal fibers protect against colon cancer, however, not all cereal fibers are equally effective. Wheat bran is the only cereal bran that shows consistent protection against colon cancer in laboratory animal models. We and others have reported that phytochemicals in wheat bran instead of fiber are the major active components for colon cancer prevention. However, the active components are still unknown. Using human colon cancer cells (HCT-116 and HT-29) as the guiding assay, we purified and identified fourteen 5-alk(en)ylresorcinols (ARs) from the active fraction of wheat bran. Among them, (10'*Z*,13'*Z*,16'*Z*)-5-(nonadeca-10',13',16'-trienyl)resorcinol is a novel compound and five ARs were purified as individual compounds for the first time. We evaluated the growth inhibition of these compounds on human colon cancer cells. Our results indicate that increasing the length of the side chain will diminish the inhibitory activity, and the existence of a double bond and a carbonyl group will strengthen such an activity. To further study the structure-activity relationship of ARs, we synthesized more than 20 ARs derivatives, the effects of the length of the alkyl side chain, the substitution pattern of the functional groups on alkyl side chain as well as the substitution pattern on the benzene ring will be discussed in this presentation.

AGFD 88

Activity-guided discovery of antioxidative and antidiarrheal components in bark extract of *Garcinia buchananii*

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The extracts and pure isolates from Garcinia plant species, genus *Garcinia*, familiy Guttiferae, exhibit multiple important biological activities such as antioxidant, anti-diarrheal, anti-inflammatory, analgesic, antimicrobial and anticancer. Stem and root bark extracts of *G. buchananii* are traditionally used to treat diarrhea, dysentery, abdominal pain, and a range of infectious diseases in Sub-Saharan Africa. In order to identify antioxidant and/or anti-diarrheal components in the bark extract of *G. buchananii*, activity-guided fractionation using in vitro-tests (H_2O_2 scavenging and ORAC assays for antioxidative activity) and guinea pig distal colon (anti-diarrheal activity) were performed and the most active principles were identified by means of UPLC-TOF-MS analysis, 1D- and 2D-NMR and circular dichroism (CD) spectroscopy. Finally, reconstitution experiments were done to evaluate additive and/or synergistic effects of the bioactive compounds identified. *Garcinia buchananii* is rich in important natural remedies.

AGFD 89

Cranberry fruit and leaves (*Vaccinium macrocarpon*) as a source of antimicrobial natural products

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Cranberry is known for urinary tract health benefits against *E. coli* bacteria. Fruit and leaves of North American cranberry (*Vaccinium macrocarpon*) were investigated for compounds possessing antimicrobial activities against a variety of bacteria and yeasts. Both leaves and fruit were found to be a rich source of A-type proanthocyanidin oligomers (PACs) and quercetin glycosides. MALDI-TOF MS analysis of cranberry leaf PACs showed a composition similar to that of fruit PACs, with oligomers of 2-12 degrees of polymerization. Several quercetin glycosides previously identified in fruit were plentiful in leaves, with quercetin-3-O-galactoside the major constituent. Cranberry leaf and fruit PACs inhibited biofilm formation by *S. aureus* with MBIC of 1.5-3.1 μg/mL; flavonol glycoside fractions also caused inhibition. Biofilm formation by oral bacterial communities and the growth of *Candida* species were selectively inhibited by both fruit and leaf PACs.

Thus, both cranberry leaves and fruit may be a useful source of antimicrobial compounds.

AGFD 90

Protective effect of steryl ferulate from bamboo shoot on experimental nonbacterial prostatitis in rats

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The protective effects of steryl ferulate from bamboo shoot (SFB) and its mechanisms on nonbacterial prostatitis (NBP) were investigated using experimental rat model and gene expression microarray. SFB could significantly inhibit absolute prostate weight, prostate index, total acid phosphatase, prostatic acid phosphatase and the expression levels of 238 genes, while SFB significantly increased density of lecithin corpuscles and the expression levels of 111 genes. Histologically, SFB treatment significantly suppressed the severity of the lesion in NBP rats. Gene ontology for functional analysis revealed that, biological processes (fibrinolysis, inflammatory response, etc.), cellular components (high-density lipoprotein particle, protein-lipid complex, etc.), molecular functions (enzyme inhibitor activity, peptidase inhibitor activity, etc.) were altered. Canonical pathway analysis indicated, metabolism of xenobiotics by cytochrome P450 and PPAR signaling pathway as the most important pathways. Thus, SFB may be useful for treatment of NBP by affecting the expression of genes in the related pathways.

AGFD 91

Effect of dietary tocopherol isomers on inflammatory response of adult- and infant-derived intestinal cell lines

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The effect of dietary tocopherol (Toc) isomers, including α-Toc, γ-Toc and δ-Toc, in modulating inflammatory response of intestinal cell lines derived from adult (Caco-2) and infant (FHs74Int) origin were determined. Toc isomers exhibited anti-inflammatory effect by reducing IL8 secretion from Caco-2 cells challenged with interferon gamma/phorbol mirystate acetate (IFNg/PMA). An opposing trend however was observed in the infant FHs74Int cells regardless of IFNg/PMA stimulation. At the same time, differential regulation of NfκB pathway signaling pro-inflammatory cytokines and Nrf-2 pathway signaling expression of antioxidant enzymes by Toc isomers in the two cell lines was observed. Δ-Toc was most effective in stimulating both NfκB and Nrf-2 pathways. In addition, the transcript level of two key enzymes involved in glutathione synthesis was down-regulated by δ-Toc in the infant FHs74Int cells, while no difference was observed in adult Caco-2 cells, suggesting potential differences in glutathione biosynthesis that may affect oxidative status thus IL8 expression.

AGFD 97

Fifty years of smelling sulfur: From Allium chemistry to olfactory detection of sulfur compounds

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The most distinctive characteristic of garlic, onion and other genus *Allium* plants is the formation of strong-smelling organosulfur compounds when they are cut. These sulfur compounds are thought to protect the plants from predators. After a brief overview of the history of genus *Allium* plants in civilization, I will describe our research elucidating the chemical processes that occur when alliums are cut, e.g., *Allium* chemistry, how the characteristic properties of *Allium* organosulfur compounds can be exploited in environmentally friendly bird repellents and pesticides, and how my fascination with strong-smelling organosulfur compounds led to a mouse model in which copper ions play a key role in the activation of olfactory receptors highly sensitive to organosulfur compounds.

AGFD 98

Where have all the polyphenols gone?

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One lingering question in the area of polyphenol research is the lack of mass balance. Three samples are measured; plasma, urine and feces. Plasma concentration of polyphenols or their metabolites is seldom as high as 10 µM and usually < 1 µM. The level in the urine is usually < 1 µM. Based on 2.5 L of total human plasma this calculates to be 0.3 mg for a molecular weight of 300 for the polyphenol/metabolite in 1 L of urine (24 hour) and 0.75 mg in plasma (1 uM). The fecal excretion is not well studied and thus unknown, but for black tea the combined excretion of catechins in all three routes is only 2% of dose. We investigated red blood cells (RBC) equilibrated with 12 polyphenols and their metabolites, and 8 polyphenols and their glycosides equilibrated with blood. Intracellular RBC levels (HPLC) for 10 µM polyphenol in the media were in the µM range for RBC when incubation was with RBC and less in blood where other proteins can bind polyphenols. From blood there was some methylation of the polyphenols. Thus RBC can metabolize polyphenols and can carry as much polyphenols or their metabolites as found in plasma. The physiological implications of this finding will be discussed.

AGFD 99

Health benefits of fruit polyphenols: Clinical evidence of fruit-derived polyphenol action in the postprandial state, and effects on blood pressure

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There is increasing evidence that the postprandial state is an important contributing factor in the development of chronic diseases. Modern day diets are characterized by high-calorie meals rich in processed, readily available carbohydrate and fat leading to exaggerated postprandial elevations in blood glucose and triglycerides, triggering a biochemical cascade resulting in oxidative stress, inflammation, dyslipidemia, insulin resistance and endothelial dysfunction. These postprandial changes repeated multiple times daily, and often with limited recovery, eventually lead to atherosclerotic risk factors and coronary artery disease. Polyphenolic compounds from various plant foods are the subject of increasing attention touted for their multiple

benefits promoting health and disease risk reduction. Polyphenolic compounds are most commonly known for their antioxidant properties; however, more recently they are recognized for their direct and indirect effects on cell signaling pathways imparting anti-inflammatory effects and improving metabolic- and endothelial- dysfunction. Certain fruits or their derived products have been investigated for their role in maintaining system balance during the described challenges of postprandial metabolism. Berry fruits, grapes, wine, and grape seed extract show particular promise in this area, although the science is young. Accordingly, only few studies have extended findings to examine the effects of supplementation on traditional coronary risk factors. The aim of this presentation will be to provide an overview of the clinical evidence of fruit-derived polyphenol action in the postprandial state, and effects of grape seed extract specifically on blood pressure regulation. Concluding remarks will include thoughts on research needs for advancing the clinical polyphenol evidence-based science and research considerations for the food industry to ensure delivery of health opportunities to consumers.

AGFD 100

Chardonnay grape seed flour reduces plasma lipids and increases expression of hepatic genes for cholesterol and fat synthesis in hamsters fed a high fat diet

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Chardonnay is a white wine grape variety with seed high in polyphenolics (over 10% by weight), a class of compounds with known bioactivity. Compared to male Syrian hamsters fed a high fat (HF) diet, animals fed a diet supplemented with flour made from chardonnay seeds (HFC) displayed a reduction in weight gain as well as lower blood lipid levels. These improved physiological changes correlate with the observed up-regulation of hepatic genes related to cholesterol and bile acid synthesis (CYP51, HMGR, SREBP2, CYP7A1) when compared to control. This suggests that the grape seed flour may reduce re-absorption of cholesterol and/or bile acid, therefore decreasing levels in the liver. Reduction in weight gain in the HFC group may be explained by hepatic gene up-regulation for fat oxidation (ACOX1) and down-regulation of fat synthesis (SCD1). The expression of adipose genes related to inflammation and adipocytokine production were also analyzed.

AGFD 101

Transplacental chemoprevention by dietary indole-3-carbinol (I3C) in a mouse model of T-cell lymphoblastic leukemia/lymphoma (T-ALL)

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In mice, transplacental exposure to the chemical carcinogen dibenzo[*def,p*]chrysene (DBC) causes development of T-ALL in young adult offspring leading to early mortality. Maternal consumption of the bioactive food chemical I3C, present in cruciferous vegetables, confers protection to offspring against DBC-initiated T-ALL. In this study, we investigated the timing of dietary I3C exposure prior to and during pregnancy and compared the efficacy of I3C to its major acid condensation product, 3,3'-diindolylmethane (DIM). I3C (500 ppm or 2000 ppm) fed during gestation and lactation provided significant ($P<0.01$) protection against DBC-initiated T-ALL in offspring (29% and 76% survival, respectively, compared to 14% for control animals). Pre-feeding dams prior to pregnancy with 2000 ppm I3C did not enhance this protection. However, dietary DIM (350 ppm) did not alter cancer outcome. These data suggest that I3C, or other acid condensation product, is likely responsible for the transplacental chemoprevention observed in this murine model of T-ALL.

AGFD 102

Chardonnay grape seed flour, not red grapes, reduce plasma cholesterol and body weight gain in hamsters on high fat diets

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The polyphenolic content of red wine is commonly associated with decreased risk of cardiovascular disease. However, some white grape seed varieties contain comparatively more polyphenolics than red seeds. Male Syrian hamsters were fed high fat diets containing 10% grape seed flours from chardonnay (CH), cabernet sauvignon (CS) and syrah (SY) grapes for three weeks. Low density lipoprotein (LDL) and very low density lipoprotein (VLDL) cholesterol respectively decreased by 66% and 72% with a diet containing CH, but not CS or SY, seed flour supplementation. Hamsters on the CH supplemented diet also had 31% reduced weight gain despite similar food intake to the CS and SY groups. Additionally, liver and epidydimal adipose weights were lower in the CH fed hamsters. The bioactivity of CH seed flour may be explained by its higher content of catechin and epicatechin compared to CS or SY.

AGFD 103

Nutritional and pharmaceutical applications of bioactive compounds of some edible berries and tropical fruits

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Extracts from Chilean and Polish berries and Thai tropical fruits decreased the proliferation of HT-29 and SW48 human colorectal cancer (CRC) cell lines. This effect was concentration dependent. The inhibition of cancer cell proliferation correlated with the levels of polyphenols, flavonoids and the antioxidant activities of investigated samples. DPPH kinetic measurements were used to compare, distinguish and discriminate the antiradical activity among berry extracts by multivariate analysis. The interaction between two flavonoids (catechin and quercetin), bovine serum albumin (BSA) and polyphenol extracts of berries and fruits was investigated by 3-D fluorescence and FTIR spectroscopy. The new kind of berries and fruits has a strong ability to decrease the intrinsic fluorescence of BSA and is comparable with quercetin. Supplementation of diets with berries and fruits positively affects plasma lipid profile, and antioxidant activity in rats fed cholesterol containing diets. The main histopathological changes were detected in the liver and aorta of rats fed a high-cholesterol diet without fruit supplementation. These changes were minor in rats with fruit supplementation. In conclusion, these findings suggest that the intake of berries and fruits, as a source of natural antioxidants, may reduce colon cancer risk. The consumption of berries and fruits as a supplementation to everyday human diet and for pharmaceutical applications is important for health effects.

AGFD 104

Total Western Diet (TWD) increases azoxymethane induced aberrant crypt foci (ACF) compared to the AIN93G diet

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The new TWD emulates average American intakes (at the NHANES 50th percentile) for micro- and macronutrients based on nutrient density. Mice were fed either TWD or AIN93G basal diets supplemented with or without 0.2% green tea extract in the drinking water. Green tea extract reduced bodyfat percentage in both the TWD and AIN93G groups ($P < 0.05$) and decreased fasting glucose levels in mice fed TWD ($P = 0.02$) but not AIN93G. Mice fed TWD without green tea had more ACF and a higher total crypt cell count compared to cohorts fed the AIN93G diet ($P < 0.001$). Interestingly, green tea extract decreased ACF and total crypt cells in the TWD group ($P < 0.001$) but not in mice fed AIN93G. These results suggest that the Western dietary pattern promotes carcinogenesis and that supplementation with chemopreventive bioactives, such as green tea, may be beneficial to populations consuming a poor diet.

AGFD 105

Synthesis of CLA isomers and their effect on milk fat production

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CLA in ruminant source foods originates as intermediates in the biohydrogenation of unsaturated fatty acids by rumen bacteria. There are over 20 CLA isomers in ruminant fat, most at trace levels. Under certain dietary conditions rumen fermentation shifts, increasing production of intermediates from minor biohydrogenation pathways, some of which are potent inhibitors of milk fat synthesis. *Trans*-10, *cis*-12 CLA has been most extensively studied and a 25% inhibition is observed at 0.02% of the diet in dairy cows. Effects are specific for milk fat; yields of milk and other milk components are unaffected. Mechanisms involve the SREBP transcription system and a coordinated reduction in mammary expression of genes for key lipogenic enzymes. Two additional CLA isomers have been found to inhibit milk fat synthesis, *trans*-9, *cis*-11 and *cis*-10, *trans*-12. Overall, CLA isomers produced in ruminant fermentation provide an example of nutrigenomics which offers exciting opportunities for agricultural application.

AGFD 106

CLA and its effect on dairy cow fertility with emphasis on low level inflammatory processes

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Low fertility and health are a major concern for dairy farms. In the last decades fertility decreased together with the increase of milk yield, but milk yield does not seem the main cause, since not always the most productive cows are the less fertile. Recently a strong negative relationship among inflammation in transition, milk yield and fertility has been observed. Surprisingly, cows with the highest milk yield showed a better energy balance and fertility, but the lower inflammatory status.

Despite the results from CLA-based experiments are still “in progress”, CLA supplementation in late pregnancy/early lactation of dairy cows exerts positive effects on reproduction, on inflammatory consequences (lower, likely for the inhibition of NFkB responsible of inflammatory gene expression) and on glucose/energy balance. This suggests to be reasonable a positive relationship between CLA feeding and better fertility through the reduction of inflammation effects and glucose/energy balance improvement.

AGFD 107

Isomers of conjugated linoleic acid as important nutrients in the dairy cow

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Development of fore stomach fermentation in ruminants is associated with the formation of a wide range of positional and geometric isomers of conjugated linoleic acid (CLA) synthesized during ruminal biohydrogenation of dietary 18:2n-6 and 18:3n-3. More than 15 individual isomers of CLA have been detected in digesta at the omasum or duodenum with the amounts available for absorption being highly dependent on diet composition. Little is known about the metabolic fate and physiological activity of most CLA isomers in the host ruminant. However, ruminant tissues contain a wide range of CLA isomers indicating that these serve as substrates for essential functions including phospholipid synthesis. Virtually all of the evidence pertaining to the biological activity of CLA in cattle is based on post-ruminal infusions or feeding studies examining the effects of synthetic sources enriched in *cis*-9, *trans*-11 and *trans*-10, *cis*-12. Dietary supplements of rumen protected synthetic CLA (PR-CLA) decrease milk fat content in lactating cows, changes that are often accompanied by an increase in milk and milk protein yield and/or improved energy status. Effects of RP-CLA on lactational performance may, at least in part, to be mediated via the repartitioning of energy towards body tissues in the absence of changes in heat production or diet digestibility. Available data highlight a role of CLA in minimizing excessive mobilization of body tissues during periods of energy insufficiency in the dairy cow.

AGFD 108

CLA's role in biochemical processes

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Since its discovery as an anti-cancer component from ground beef, conjugated linoleic acid (CLA) has shown other biologically beneficial effects. One of the most interesting activities of CLA is its ability to reduce body fat, while improving lean and bone mass. CLA has tremendous effects on lipid metabolism and these effects of CLA contribute, either directly or indirectly, to its effects on muscle and bone metabolisms or vice versa. CLA fed animals showed increased activity levels and endurance capacity, which may link to its effects on increasing energy expenditure and fat utilization. In addition, CLA shifted bone marrow mesenchymal stem cell balance between bone marrow adiposity and bone cell formation in favor of bone mass, resulting in reducing marrow adipocytes and increasing osteoblasts. These suggest a great potential for CLA to be used to improve body composition along with current efforts to control obesity and osteoporosis.

AGFD 109

Dietary CLA reduces clinical signs of acute and chronic inflammatory disease

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Dietary CLAs are now recognized as naturally occurring anti-inflammatory fatty acids of animal origin. In acute inflammatory disorders, dietary CLA reduced endotoxin-induced cachexia and allergen-induced type 1-hypersensitivity. Reduced inflammatory mediator release in CLA fed animals was evident within the first 90 seconds of antigen stimulation. Dietary CLA was also effective in reducing disease associated chronic autoimmune inflammation. In a model of spontaneous autoimmune lupus, CLA extended survival 1.7 fold and reduced end stage body weight wasting by 25%. Severity of chronic autoimmune arthritis was reduced 30% up to 84 days after the onset of disease. The trans-10, cis 12-isomer of CLA appeared to have the greatest anti-inflammatory affect on collagen-induced arthritis, however, cis-9, trans-11-CLA was also shown to be effective in reducing disease progression. While CLA can decrease pro-inflammatory cytokines and eicosanoids in early stages of inflammation, dietary CLA continues to have anti-inflammatory effects long after plasma pro-inflammatory mediators have returned to baseline levels. New data shows that dietary CLA restored to normalcy a perturbed plasma metabolome associated with chronic inflammation. Our current hypothesis is that CLA may be a key upstream regulator of a feed forward loop that perpetuates inflammatory responses.

AGFD 110

CLA in obesity

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Among the multitude of physiological effects of CLA, the effect on body composition is one of the most controversial. Dozens of studies have assessed the effect of CLA on body composition in humans. They have varied in duration, design, subject selection criteria, and dose and isomer composition of CLA. Several studies have been underpowered or insufficiently designed (short duration or low dose) to detect an effect. Meta-analyses indicate CLA has a modest beneficial effect on fat loss and fat-free mass accretion in humans. Fat loss is dose dependent and nearly linear for about the first 6 months of treatment (0.09 ± 0.08 kg/wk, $P < 0.001$). Fat-free mass increases (0.3 kg ± 0.7 kg, $P = 0.05$), but is not time or dose dependent. In studies of natural weight gain (in growing children and adults over the holiday season), CLA also decreases body fatness. Additionally, studies using the same 36-item questionnaire found that CLA decreases adverse events. The body of evidence supports modest beneficial effects of CLA on body composition. These effects, coupled with decreased adverse events, have the potential to be clinically relevant.

AGFD 111

CLA in cardiovascular disease

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Conjugated linoleic acid is a mixture of positional and geometric isomers of octadecadienoic acid, the two major ones being cis9,trans11 and trans10,cis12 that occurs naturally in the diet. CLA is produced by biohydrogenation in ruminant animals and, as such, comes from dairy products and ruminant meats. There have been numerous *in vitro*, preclinical and clinical studies conducted which, although the findings are not always in agreement have demonstrated beneficial effects of CLA, as it relates to certain risk factors associated with cardiovascular disease (CVD). However, total and LDL cholesterol-lowering, the traditional markers for reductions in risk factors of early and more advanced stages of CVD by either nutritional and pharmaceutical interventions are not always associated with CLA administration, an observation we and many others have reported in preclinical studies in hamsters, rabbits and other animal species as well as clinical trials. Several studies report on CLA effects related to anti-inflammatory and anti-oxidative activity and the more recent associations with weight loss and/or increase in lean body mass. Although a recently published study showed that higher adipose tissue 9c,11t-CLA was associated with reduced risk of myocardial infarction, a clear mechanism remains to be elucidated. With the general recognized as safe (GRAS) status of CLA for use in foods, further studies of the mechanism(s) of action of CLA should be considered a high priority for investigation.

AGFD 112

Perspectives on CLA

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Conjugated linoleic acid (CLA) occurs naturally in the milk and body fat of ruminant animals. In 1986 it was shown that CLA inhibited chemically-induced epidermal neoplasia in mice, thus establishing that CLA possessed biological activity. Since then more than 2000 publications on CLA have appeared in the scientific literature, and it is now established that the two main biologically-active CLA isomers (c9t11 and t10c12 CLA), acting alone or in concert, are able to induce the known physiological effects of CLA. CLA presents many facets that are applicable to research on novel food ingredients, including the importance of pursuing promising if unexpected research leads, the discovery of multifunctional effects and the search for biochemical mechanisms to explain those effects, the importance of collaboration, the challenges and opportunities that arise from worldwide research interest, and the importance of perseverance in obtaining the data needed to assure safety, efficacy, and regulatory acceptance.

ENVR DIVISION

ENVR 1

Lab–on-a-chip devices for microbial monitoring and detection in water

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Lab-on-a-chip (LOC) devices can serve as ideal alternative detection systems to provide rapid, sensitive, specific, automated and portable features for on-site use. Using the most recent technological development in microlithography, micromachining and bonding techniques, small features (e.g., wells, channels, electrodes, and filters) can be created inside an enclosed silicon, glass or polymer substrate. These features eventually form a network interconnected to fluid reservoirs and reaction compartments, where samples and reagents are stored, and physical/chemical reactions are carried out. Incorporation of micropumps, microvalves and heating devices further enable sample/reagent dispensing, mixing and incubation, and biochemical reactions before analytes are detected through optical or electrochemical methods. Thus, sample preparation, biochemical reactions, and signal detection can be easily carried out to provide possible on-site solutions. LOC technology has the potential as key technology platforms for monitoring of biological contaminants in water. This presentation focuses on its potentialities in this new emerging field.

ENVR 2

Nitrogen-anchored granular activated carbon to remove perchlorate from groundwater

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A novel method for removing perchlorate has been developed, in which nitrogen containing compounds were anchored via chemical bonding to the graphene layer's edge sites within granular activated carbons (GACs). Two commercially available GACs tailored with four nitrogen-containing compounds with different chain lengths were evaluated for perchlorate removal capability by rapid small-scale column tests (RSSCT). While processing groundwater that was spiked with 30 ppb perchlorate, the bed volumes to 6ppb breakthrough increased from 1000 bed volumes up to 21,000 BVs for nitrogen-anchored bituminous (Ultracarb) carbon, whereas that increased from 300 BVs to 3000 BVs for nitrogen-anchored wood-based (Gran C) carbon. The mechanism occurred within these two carbons during the anchoring has been proposed via characterization of surface charge distributions, pore volume distributions and elemental analyses. Increased bed volumes to initial perchlorate breakthrough correlated to increased positive surface charges with R^2 higher than 0.93 on the N-anchored activated carbon.

ENVR 3

Novel tailoring activated carbons for enhanced removal of natural organic matter

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Adsorption of humic acid (HA) and fulvic acid (FA) by commerical activated carbon (F400) and novel tailoring activated carbons was studied. The adsorption ability of activated carbon is largely due to pore size distribution (PSD). To improve the adsorption kinetics and capacity of dissolved organic matter (DOM) (5-60Å), firstly two kinds of activated carbons with high mesoporosity and BET surface area were created from bituminous coal by KOH chemical activation. In addition, the presence of acidic functional groups and negative surface charge on activated carbon repel adsorption of HA and FA, which is also negatively charged. Thus four tailored activated carbons were further developed using outgassing and manganese impregnation to enhance surface chemistry. Tremendous higher rates of adsorption were found for the tailored activated carbons as compared to F400, indicating optimal PSD, yet the overall adsorption capacity was impacted by surface chemistry as was seen from the isotherm data.

ENVR 4

Synthesis and application of granular mesoporous carbon materials for removal of pharmaceuticals

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Granular mesoporous carbon (GMC) was synthesized by using new granulation method with various polymers such as carboxymethyl cellulose, polyvinyl alcohol, and microcrystalline cellulose as organic binders and then was impregnated with iron oxide nanoparticles (GMC-Fe). Use of the new granular method complemented previous studies by enhancing the physical properties such as surface area, pore volume, and pore size distribution. The granular mesoporous carbon materials (GMC and GMC-Fe) were characterized by BET, SEM, XRD, FT-IR, and element analysis and evaluated the adsorption capacity of pharmaceuticals, which are found ubiquitously up to $\mu g\ L^{-1}$ in environments and are considered as new emerging micropollutants. Adsorption kinetics, isotherms, and effect of water characteristics for removal of pharmaceuticals were investigated. The results suggest that the granular mesoporous carbon materials could be one of most versatile materials for removal of pharmaceuticals in water treatment.

ENVR 5

Development of novel cyclodextrin adsorbents for the removal of emerging contaminants from water

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Emerging contaminants (ECs) such as estrogen hormones, perfluoro-compounds (PFCs), bisphenol-A (BPA), and 1,4-dioxane have been detected in natural water at many places. The existing conventional wastewater treatment systems are not designed for the removal of these contaminants. This critical issue leads to the need for the development of advanced and effective technologies. β-cyclodextrin (β-CD) is a glucose-based molecule which has high affinity for different organic contaminants by the formation of host/guest inclusion complexes.

In this research, water soluble β-CD was reacted with certain crosslinking agents and copolymers to form water insoluble β-CD and to coat β-CD onto silica particles. The development of such novel inorganic-organic hybrid adsorbents provides high binding capacity with organic contaminants along with high mechanical strength. We have successfully developed β-cyclodextrin coated silica adsorbents for the removal of emerging contaminants.The adsorbents were synthesized under different experimental conditions. The developed adsorbent showed a good regeneration capacity in removing PFOA and estrogens over four successive cycles. The characterization of the adsorbents using FTIR, TGA, and TEM confirmed the coating of β-CD onto silica particles. The developed adsorbents were tested for the removal of ECs of interest (estrogens, PFCs, and BPA) under batch and column conditions from Milli-Q water. The adsorbent prepared by reacting β-CD with HMDI as crosslinking agent with the molar ratio of 1:8 showed best results in removing the target compounds. The adsorbent showed more than 95% removal of 17β-estradiol (in single component) and more than 90% of most of the estrogens (in multicomponent), more than 99% of PFOA, and a maximum of 90% removal in case of BPA. The removal of ECs of interest was dependent on the nature of both adsorbents and adsorbates. The nature of adsorbent such as type of crossliking agent, molar ratio between β-CD and crosslinking agents affect the removal of the contaminants. Similarly, the nature of adsorbates such as size, shape, and presence of functional groups affect the removal efficiency

ENVR 6

Removal of antibiotics from water using sewage sludge derived composite material

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A novel composite material was developed by the pyrolysis of a mixture of sewage sludge and waste oil sludge. The adsorption of a mixture of 11 antibiotics (amoxycillin, chloramphenicol, chlorotetracyclinie, enrofloxacin, ofloxacin, sulfadiazine, sulfamethazine, sulfamethoxazole, erythromycin, Penicillin-G, and oxytetracycline) and 2 anticonvulsants (carbamazepine and primidone) on the composite material was examined via batch experiments. Although the BET surface area of the waste derived composite material is only 10% of that of a model activated carbon, the total adsorption capacity of the composite material for antibiotics (~100 mg/g) is only slightly lower than that of the activated carbon (~360 mg/g). FTIR and thermal analyses suggest that physical adsorption, reactive adsorption (formation of salts) and specific polar interactions are the probable mechanisms of adsorption on the composite material. The effects of natural organic matter on the adsorption of the pharmaceuticals on the composite material were also investigated.

ENVR 7

Utilization of biowaste as a potential adsorbent for various pollutants in water

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Pollutants like heavy metal ions and organic compounds in waste water could affect human health, aquatic life and overall ecosystem adversely. Therefore, recently much emphasis has been given for the use of industrial waste material as economic adsorbents for removal of pollutants from waste water. In this study, tomato peel was used as the most efficient bio-material to remove toxic metal ions and organic pollutants from aqueous solution. Material was characterised using FT-IR and FESEM. Adsorbent dose, time dependent and pH dependent adsorptions were studied to establish optimum conditions. The maximum adsorption capacity was observed at different pH values for different pollutants. The equilibrium adsorption data were interpreted by using freundlich, langmuir and temkin isotherms. Results showed that Tomato peel, a waste material, have good potential as an adsorbent to remove various pollutants from water.

ENVR 8

Roles of black carbon on the fate of heavy metals and agrochemicals in soil

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Char(coal) and other black carbon materials can comprise up to 35% of total organic carbon in US agricultural soils, and are known to strongly and often irreversibly bind contaminants including heavy metals. Black carbon has received renewed interests in recent years as a solid co-product formed during thermochemical waste-to-energy conversion (slow/fast pyrolysis and gasification) of agricultural wastes such as plant residue, nutshell, and manure. Amendment of char product (biochar) in soil is a promising, cost-effective remediation strategy for contaminated soils and sediments, along with added benefits including carbon sequestration. This presentation will focus on biochar-induced changes in the fate of heavy metals and agrochemicals in both agricultural and contaminated soils, with a particular emphasis on the reversibility of contaminant sorption. The results suggest the importance of soil property (pH, CEC, TOC) and contamination scenarios in designing specific biochar for purported functions.

ENVR 9

Integrating field, lab, and modeling to assess the distribution of PCBs in a stream ecosystem

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The Sangamo Weston/Twelve Mile Creek/Lake Hartwell PCB Contamination Superfund Site in Pickens County, SC, resulted from effluent containing nearly 200,000 kg of three Aroclors (1016, 1242, and 1254) consisting of about 130 congeners in total. The large range of chlorination produces significant differences in the physiochemical properties that control the behavior of these compounds in natural systems upon their release. A multi-pronged approach to understand the distribution of the PCBs in the watershed will be discussed. Field work, laboratory studies, and modeling are integrated to describe the distribution of PCBs in different media (e.g., sediment, soils, groundwater, surface water, particulate organic matter, vegetation, and organisms) to provide a holistic view of the affected ecosystem. A synopsis of the results to date of intensive field campaigns including periphyton, decomposing leaves, organisms (e.g., fish, spiders, and insects), soil, sediment cores, distributed temperature sensing, and passive samplers will be provided.

ENVR 10

Organic chemical composition of $PM_{2.5}$ in vehicular exhaust: Gasoline and diesel light duty vehicles

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Fine particle emission from gasoline and diesel motor vehicles is a major source of particulate matter air pollution, especially in urban areas. In this study, organic speciation of fine particulate matter ($PM_{2.5}$, $d \leq 2.5$ µm) was carried out on 18 light-duty vehicles tested on a chassis dynamometer at the New York Department of Environmental Conservation (NYDEC) testing facility over different driving cycles.

A detailed chemical profile for organic compound mass emissions was constructed for the vehicle exhaust particulates collected from each vehicle and fuel type. More than 100 organic molecular marker compounds quantified by gas chromatograph/mass spectrometry (GC/MS). The major organic components identified were n-alkanes, PAH (polycyclic aromatic hydrocarbons), hopane, sterane, n-alkanoic acids and benzoic acids. The detailed chemical profiles corresponding to the fine organic PM will provide new apportionment and modeling tools to distinguish organic particulate pollution from gasoline and diesel powered vehicles.

ENVR 11

Moisture-filled porosity as a key parameter for accurate prediction of vapor intrusion rates

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Beginning in the 1990s, the issue of VOC vapor intrusion (i.e. the transport of VOC vapors from the subsurface into buildings through foundation cracks) began gaining regulatory attention. Since then, our understanding of vapor intrusion fate and transport has been largely advanced through the use of computational models. As part of this research, we solved a 3-D finite element model to evaluate the role of effective gas-phase diffusivity on vapor intrusion rates for a range of heterogeneous geologies. Our results show that the moisture-filled porosity (i.e. soil moisture) is an important variable due to its impact on the overall effective diffusivity. In fact, when considering a site with numerous contaminants, the soil moisture content itself appears to play a more important role than does the exact value of the pure-air chemical diffusivity for a given chemical (or suite of chemicals).

ENVR 12

Carbamazepine accumulation in soil and plants following land application of wastewater

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Carbamazepine (CBZ) has been one of the most detected and persistent pharmaceuticals in the environment. In this research, soil lysimeters of different arrangements – vegetated cover, no sunlight and with no plants, and open soil - at one meter height were installed inside a greenhouse to study the accumulation pattern of this compound in grass and soil. The columns were irrigated daily with synthetic wastewater consisting CBZ and drained monthly for one year. Afterwards, low rain and high rain seasons were simulated by manipulating the loading rates for a given time. Soil and water samples were analyzed using HPLC-UV and HPLC-MS. The results indicate that there is a significance difference ($p<0.05$) between the mean accumulated amount in the grass samples and in the soil samples and accumulated amounts in soil is varying by depth with the middle-depth samples showing higher values rather than top one-third and bottom one-third of the columns.

ENVR 13

Efficacy of in situ bioremediation of industrial wastes in Canada: Applications in PHC bioremediation and industrial soil fabrication

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The efficacy of bioremediation for the *in situ* treatment of industrial wastes and site remediation will be analyzed from a Canadian business perspective. This presentation will focus on bridging the gap between useful advancements in bioremediation and commercial application. The presentation will focus on business process, and case examples of PHC bioremediation fields and industrial soil fabrication with varying degrees of aeration, light exposure, and plant species.

ENVR 14

Ionic strength effects on the sorption of tylosin on clay minerals

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Tylosin, a widely used veterinary antibiotic and growth promoter in daily poultry and swine feed, is related to the prevalence of genes for the resistance of macrolide such as erythromycin, an important macrolide human antibiotic. As a result, there have been growing concerns on its possible adverse effects on natural ecosystems. As a weak base, the main mechanism for tylosin sorption in soil is cation exchange and the minerals play important roles. In this study, we investigated the sorption of tylosin by pure clay minerals in varies ionic strength and ions, as well as the interlayer interaction of tylosin on different type of montmorillonite. Sorption data were fitted with Langmuir-Freundlich-Hill sorption model to discuss the electrostatic and specific interaction for non-ideal adsorption. The sorption capacity of tylosin at different ionic strengths decreased with the order of 0.008 *M* > 0.051 *M* > 0.108 *M* > 0.508 *M*. For specific ionic strength, the sorption of tylosin decreased in the following order of ions: $K^+ > Na^+ > Ca^{2+} \geqq Mg^{2+}$. It should be noticed that the sorption displayed an opposite tendency for montmorillonite at low initial concentration of tylosin. It indicated that there might be existed the other interactive besides cation exchange in the sorption process. The sorption of tylosin on different montmorillonite decreased in the order of Ca-montmorillonite > Na-montmorillonite > K-montmorillonite. It seems that interlayer hydration could influence the sorption of tylosin.

ENVR 15

Equilibria of bisolute sorption on soil

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This study measured binary sorption equilibria for a soil using ten concentration levels for both phenanthrene and naphthalene. The results showed different competitive sorption equilibria between phenanthrene and naphthalene. Regardless of the loading sequence, naphthalene exhibited consistently lower sorption capacities and the ideal adsorbed solution theory (IAST) slightly underestimates naphthalene sorption equilibria. Conversely, sorption equilibria of phenanthrene depended upon the loading sequence of sorbates on the soil. Little competition from naphthalene on sorption equilibria of phenanthrene was observed when phenanthrene was loaded either simultaneously with or sequentially after naphthalene, but appreciable competition from naphthalene was observed when the soil had been pre-contaminated with phenanthrene. IAST slightly underestimates phenanthrene sorption equilibria observed in the latter system, but it cannot estimate phenanthrene sorption equilibria in the former two systems. The study demonstrates the effects of contamination history on sorption equilibria and provides insight information on the mechanisms of sorption by soils.

ENVR 16

Photocatalytic degradation of microcystin-YR using size-controlled monodisperse TiO_2 films

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Algal blooms occur very frequently because of change in climate and eutrophication of surface water. Recent research from Graham et al. reported the presence of toxin-producing cyanobacteria such as *Aphanizomenon*, *Cylindrospermopsis* and *Microcystis* in collected cyanobacterial bloom samples from 23 Midwestern lakes in America. All bloom samples contained microcystins (MCs), which are deleterious hepatotoxins. Although the toxicities of different congeners of MCs (MC-LR, MC-YR, MC-RR and MC-LA) have been studied, the degradation of MC-YR has been rarely studied. Therefore, the photocatalytic degradation of MC-YR in water is of great interest for water remediation. The particle size distribution, pore size distribution, surface area, and surface roughness of immobilized films are of great importance for the efficient use of titanium dioxide (TiO_2) films in photocatalytic applications. The adsorption of target compounds and the photochemical properties of the film (light absorbance, photonic efficiency, number of active sites) could be influenced by those properties. Therefore, understanding the role of structural properties of TiO_2 films on the degradation of MC-YR is important for the development of photocatalytic processes for water treatment. In this study, the effect of structural properties of TiO_2 films on the degradation of MC-YR was investigated. Size-controlled TiO_2 nanoparticles were immobilized on glass substrates using a dip-coating method and the prepared TiO_2 films were tested for the photocatalytic degradation of MC-YR under UV light irradiation. The concentration of MC-YR in water samples was analyzed using high performance liquid chromatograph (HPLC). Size-controlled monodisperse TiO_2 films were characterized with scanning electron microscopy (SEM), X-ray diffraction (XRD), atomic force microscopy, prosimetry analysis, and UV-Vis diffuse reflectance. Results on the effect of structural properties of TiO_2 films on photocatalytic degradation of MC-YR will be discussed.

ENVR 17

Visible light-sensitive Cu-grafted TiO_2 photocatalysts

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The metal ions (Cu, Fe, Cr and Ce) grafted TiO_2 has been demonstrated to enhance the photo-degradation efficiency under the visible light. In this study, the microwave-assisted impregnation method for preparation of Cu-grafted TiO_2 photocatalysts was reported. We adjusted the pH of the starting solution used for the grafting of Cu ions to control the amount of copper on the TiO_2. In addition, UV-Vis diffuse reflectance absorption spectra and ICP-OES were used to determine the band-gap and the weight ratio of as-synthesized Cu/TiO_2, respectively. From UV-Vis diffuse reflectance spectra results, the absorption intensity of TiO_2 starts to increase at 385 nm which is corresponding to the interband transition of P25 (3.2eV). In addition, another absorption region of Cu/TiO_2 around 700-800 nm which indicates the Cu d-d transition, is observed. It can be ascribed to the direct interfacial charge transfer from the valence band of TiO_2 to Cu. The ICP-OES result shows that the weight ratio of Cu/TiO_2 is in the range 0.005~0.008%. In addition, the photoactivity of the visible light-activated Cu/TiO_2 photocatalyst was examined by the photo-decomposition of sulfamethoxazole (SMX). The synthesized Cu/TiO_2 have the better photocatalytic activity toward SMX than that of Degussa P25, and the pseudo-first-order constant for SMX photodegradation by Cu/TiO_2 is 14 times higher than that of P25 under illumination of 465 nm visible light, clearly showing the excellent visible-light-driven ability of the Cu-grafted TiO_2.

ENVR 18

Oxidation of arsenite to arsenate on birnessite in the presence of light

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The photochemical oxidation of arsenite [As(III)] on birnessite was investigated as a function of pH. Irradiation of As(III), birnessite suspensions with visible light led to the oxidation of As(III) at a rate that was approximately two times faster than in the absence of light. At pH 5 the majority of the arsenate product, Mn(II) was released into solution. At pH 7.4 Mn(II) did not partition into the aqueous phase, instead adsorbed and went into the interlayers of the birnessite. In the absence of O_2 and presence of light, As(III) oxidation was similar to the As(III) oxidation by birnessite in dark. OH· and H_2O_2 produced in the presence of O_2, birnessite, and light, were responsible for this additional As(III) oxidation. TEM of the post-reaction birnessite

particles showed that the particles were smaller, edges are rounded compared to the pre-reaction birnessite particles, consistent with the dissolution of the particles during As(III) oxidation

ENVR 19

Application of potassium ferrite to remove contaminants: Role of nanomaterials

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This paper presents first the synthesis of potassium ferrite ($KFeO_2$) from the natural l waste ferrihydrite. The decomposing of $KFeO_2$ under humid condition formed monodisperse superparamagnetic maghemite (gamma-Fe_2O_3) nanoparticles. These nanoparticles will be shown be efficient as magnetic sorbents for copper and arsenic removal from water. Direct addition of $KFeO_2$ into water yielded in situ ferric hydroxide, which were efficient in removing copper. However, in situ phenomena of ferric hydroxide did not result in removal of arsenic. Causes of such differences will be briefly discussed.

ENVR 20

Nanoscale zerovalent iron (nZVI): Toggling between oxidative and reductive pathways for contaminant sequestration

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Nanoscale zerovalent iron (nZVI) is among the most extensively applied nanomaterials for groundwater and hazardous waste treatment. The nature of the nanoparticles, particularly its microstructure and surface chemistry, casts a profound influence on the particle reactivity and triggers different redox pathways for contaminant degradation and sequestration. In this work, the metallic-core-oxide-shell structure of nanoscale zerovalent iron (nZVI) was examined using a variety of characterization tools. The ambivalent redox behavior of nZVI is illustrated in two contaminant systems, namely, the sequestration of arsenic species and the degradation of chlorinated hydrocarbons. The findings presented here suggest that nZVI possesses more complex functionality than being a simple reductant. Careful control and engineering of the surface properties of nZVI may lead to optimal design of treatment systems and grant the nanoparticles with new applications.

ENVR 21

Dual redox functionality of nanoscale zerovalent iron: Fundamentals and applications in environment

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Zerovalent iron (nZVI) has been received great attention for more than a decade. It consisting of a core-shell structure has a particle size of 1-100 nm. nZVI is capable of treating a wide array contaminants including chlorinated organic compounds and heavy metals through chemical reduction and surface adsorption, respectively. The filed application of groundwater remediation using nZVI has been implemented in many countries including USA and Taiwan. Recently, the discovery of an oxidative ability of nZVI opens a new avenue for its application to target the oxidative contaminants. The dual redox functionality of nZVI offers insight into the fundamental chemistry and points out a new direction for advanced oxidation processes.

ENVR 22

Degradation of pentachlorophenol by well-suspended zerovalent iron nanoparticles

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Stabilized nanoscale zerovalent iron (NZVI) has been studied to treat pollutants recently. In order to prevent aggregation of nanoparticles, particle stabilization has been practiced by attaching a stabilizer onto the NZVI. However, the reactivity of NZVI was reduced due to surface coating. This study presents the treatment of pentachlorophenol (PCP) using NZVI with the assistance of ultrasonication. Removal efficiency of PCP was 56 % in 2 hours by ultrasound-dispersed NZVI while only 8 % and 11 % were found by sole sonication and NZVI process in 4 hours, respectively. With the assistance of ultrasonication, the removal rate of PCP with NZVI was accelerated due to the well dispersion of NZVI by ultrasonication, and enhanced the chloride release. The reaction mechanism and kinetics under different environmental conditions were performed. The combination of ultrasonication to NZVI could be a direct system to investigate the degradation reaction of halogenated compounds with fine-sized NZVI.

ENVR 23

Rapid detection of waterborne parasites in complex matrixes using piezoelectric-excited millimeter-sized cantilever (PEMC) sensors

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Rapid assays for *Cryptosporidium parvum* and *Giardia lamblia* in water using piezoelectric-excited millimeter-sized cantilever (PEMC) sensors were investigated at 5 to 10,000 (oo)cysts/mL. The sensor was functionalized with the corresponding IgG antibodies. The resonant frequency of PEMC sensor decreased in proportion to (oo)cysts concentration. Successful detection of *C. parvum* in both PBS and in proteinous background was done at 5 oocysts. Following the detection step, a second IgM antibody binding specific to *Cryptosporidium* was used for confirming detection. Detection of *G. lamblia* was carried out in a similar manner. Detection of as few as 10 cysts is feasible in 30 min. The specificity of the sensor was challenged with non-target cells. Detection was confirmed with eSEM. Detection of *G. lamblia* cysts spiked Schuylkill River (Philadelphia, PA) water showed feasibility without pretreatment. One liter samples at 1 cyst/mL or 10 cysts/mL were successfully analyzed. The authors acknowledge EPA STAR Grant R833007.

ENVR 24

X-ray photoelectron spectroscopy investigation of soluble manganese removal by MnO_x(s)-coated media

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Soluble Mn contamination in drinking water systems is a well-known problem that can lead to severe water discoloration and consumer complaints. X-ray photoelectron spectroscopy (XPS) and solution chemistry analyses were performed to investigate soluble Mn(II) removal by MnO_x(s)-coated media under experimental conditions relevant to drinking water treatment plants in the absence and presence of chlorine. While Mn(II) removal in the absence of chlorine was mainly due to adsorption, the detection of Mn(III) by XPS analyses of MnO_x(s)-coated media suggests that surface Mn-catalyzed oxidation occurred. Mn(IV) was predominant in all the XPS analyses of the MnO_x(s)-coated media recovered from experiments performed in the presence of chlorine, suggesting that initial adsorption followed by subsequent rapid surface-catalyzed oxidation was the mechanism for Mn(II) removal. These results confirm that combining the application of chlorine with the catalytic action of MnO_x(s) oxides is effective for soluble Mn(II) removal from drinking water.

ENVR 25

Magnetically activated charcoal (MAC): Synthesis from natural products, characterization, and green application in arsenic remediation

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This research describes a simple strategy for the synthesis of magnetically separable activated carbons (MACs). The method involves the formation of highly dispersed magnetite and nickel ferrite nanoparticles throughout the porous structure of activated carbon. These materials were prepared by including metal salts in the conventional recipe for activated carbon manufacture using high cellulose content natural products such as coconut shells, sawdust, and seaweed. Decomposition of these salts during the pyrolysis step yields the desired magnetic composites. MACs were characterized using BET surface area and pore size analysis, FTIR, and XRD, followed by utilization in environmental remediation of Arsenic and other heavy metals from water using Atomic Absorption Spectroscopy.

ENVR 26

Urine source-separation and treatment: Novel applications of ion exchange materials

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Urine source-separation and treatment has the potential to radically transform wastewater management whereby water, nutrients, and energy are recovered and toxic contaminants are sequestered. Despite the potential of urine source-separation and treatment, it has not been widely implemented because of an absence of engineering strategies that are efficient in contaminant removal, practical to implement, and acceptable to society. Accordingly, the research objective of this work is to generate new knowledge of physicochemical processes in urine to achieve sustainable urine separation, treatment, and resource recovery. The central research hypothesis is that ion exchange materials are robust, selective, and scalable, and as such, can be used as a foundational strategy for urine treatment. This presentation will highlight recent work that seeks to identify novel applications of ion exchange materials and reactor configurations in urine treatment that achieve maximum water conservation and selective recovery of nutrients.

ENVR 27

Effects of iron amended, naturally aerated soil on dissolved phosphorus retention within surface-flow constructed stormwater wetlands

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Dissolved P is difficult to remove in surface-flow constructed stormwater wetlands (CSWs), because of its likelihood of desorption from sediments into the water column. Soil amendment strategies are considered possible options for encouraging dissolved P retention. Phosphorus has a strong affinity towards iron and aluminum, however, when anaerobic conditions exist, iron releases dissolved P. The goal of this research was to study the effects of soil amendment strategies on dissolved P retention within surface-flow CSW's and to determine whether aerobic conditions could be maintained using natural wetland vegetation. Three identical laboratory mesocosms consisted of four separate flow chambers with soil treatments as follows: wetland soil, iron amended soil, densely vegetated + wetland soil, densely vegetated + iron amended soil. Periodic soil and pore water samples were taken and analyzed. A factorial analysis of variance design was chosen.

ENVR 28

Hybrid hematite / multiwalled carbon nanotube (ɑ-Fe_2O_3 / MWCNT) nanostructures as sorbents for metal contaminants in water

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A major hurdle in the application of nanomaterials for water treatment involves loss of reactive surface area from particle aggregation. Here, we develop a novel class of hybrid nanostructures through the growth of hematite (ɑ-Fe_2O_3) nanoparticles, which are recognized sorbents for heavy metals, on multi-walled carbon nanotubes (MWCNTs). The hybrid nanostructures were synthesized via hydrolysis of ferric nitrate in the presence of carboxylated MWCNTs, and examined as sorbents for metal pollutants (e.g., Cu(II) and chromate (CrO_4^{2-})). Characterization of ɑ-Fe_2O_3/MWCNT nanostructures revealed that the amount and size of hematite nanoparticles immobilized on MWCNT surfaces were tunable during synthesis. Generally, uptake of Cu(II) and CrO_4^{2-} was greatest on ɑ-Fe_2O_3/MWCNT relative to adsorption on either MWCNTs or freely suspended ɑ-Fe_2O_3 nanoparticles. Additionally, pH-dependent trends of metal uptake on ɑ-Fe_2O_3/MWCNT nanostructures suggest that the immobilized ɑ-Fe_2O_3 nanoparticles exhibit unique and enhanced surface reactivity relative to their freely suspended nanoparticle analogues.

ENVR 29

Effects of surface functional groups on boron-doped diamond electrodes on organic compound oxidation and perchlorate formation

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Electrochemical oxidation using boron-doped diamond (BDD) electrodes is widely being studied as an alternative to other advanced oxidation processes (AOPs). However, recent work in our laboratories indicates that the oxidation of chloride-containing waters with BDD electrodes results in toxic perchlorate production, which is mediated by functional groups at the electrode surface. Thus, the objective of this work is to investigate the effect of electrode functional groups (e.g., C-H, C-OH, C-F) on both rates of organic compound oxidation and perchlorate formation. A series of batch and cyclic voltammetry experiments, coupled with XPS analysis were used to understand the relationship between reactivity and surface functional groups. Results indicate that perchlorate formation is limited on electrodes with a high density of C-OH groups. Additional studies focused on organic compound oxidation with a series of p-substituted phenols will be used to illustrate a relationship between electrode functional groups and organic compound oxidation rates.

ENVR 30

Activated carbon nanofiber anodes for microbial fuel cells

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Microbial fuel cells (MFCs) are an emerging technology capable of sustainable wastewater treatment. A significant impediment to their widespread adoption is a low power density. This can, in part, be addressed by the use of tailored anode materials. A suitable anode should have an open, porous structure with a large bioaccessible surface area for extensive biofilm formation and efficient nutrient transport. This investigation considers the use of activated carbon nanofiber nonwovens (ACNFN) as a novel anode for MFCs. ACNFN has an ultra-thin, porous structure with large bioaccessible surface area. ACNFN was fabricated by pyrolysis of electrospun polyacrylonitrile and subsequent steam activation. Preliminary tests in a single chamber MFC showed current densities of 2715 A/m^3 which is about 10% greater than the highest maximum obtained so far, with a conductivity of only one fifth that of the corresponding material. The performance of ACNFN was also compared to that of two commonly-used anodes.

ENVR 31

Estimating the polyethylene-water partition coefficients of organic chemicals using comprehensive 2D gas chromatography

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Hydrophobic organic chemicals often occur in the environment as complex mixtures, for which identification and quantification of each component is not feasible. For example, unresolved complex mixtures (UCMs) are commonly found at petroleum contaminated sites; and such hydrocarbons are known to cause narcosis toxicity in an additive fashion. An accurate evaluation of the risk associated with such sites must take into account the cumulative effects of all the chemicals in the UCM. To that end, we developed a method for inferring polyethylene-water partition coefficients using two-dimensional gas chromatography (GC × GC), thereby allowing simultaneous quantitation and characterization (but not identification!) of all UCM components with respect to their bioaccumulation potential. This implies that sampling sites of interest using a polyethylene passive sampler with GC × GC - flame ionization detector analysis will allow simultaneous determination of the freely dissolved concentrations of all organic compounds present in a contaminated sediment.

ENVR 32

Partitioning of polybrominated diphenyl ethers to dissolved organic matter

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Polybrominated diphenyl ethers (PBDEs) are a class of brominated flame-retardants that are ubiquitous in the environment and undergo long-range atmospheric transport to the Arctic. Large reported octanol-water partition coefficients (K_{OW}) of PBDEs (10^5 to $>10^9$ for decabromodiphenyl ether) enhance their susceptibility to dissolved organic matter (DOM) partitioning thereby altering both bioavailability and transformation. DOM partition coefficients (K_{DOC}) for BDE-47, 99, 153, and 209 were measured by solubility enhancement for DOM isolated from Toolik Lake, Imnavait Creek, and Oksrukuyik River in Alaska and Suwannee River and Pony Lake, (Antarctica). Log(K_{DOC}) for the Arctic DOM were similar regardless of source with a range of 4.88-5.08 for BDE-153 and 4.37-4.90 for BDE-99. Slightly higher partition coefficients were measured for Suwannee River DOM and are attributable to differences in DOM composition. Our study shows that DOM at levels present in Arctic surface waters can significantly bind and possibly alter the fate of PBDEs.

ENVR 33

Tidal effects on PAH concentration in the water column of an urban stream

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A study was conducted in an urban stream in Philadelphia to quantify tidal effects on the aqueous PAH concentration in the water column. Whole water samples were collected one foot below the water surface and one foot above the streambed at varying tides in one day. The PAH concentrations in both water and suspended solids were analyzed using a standard procedure. The concentration of 2-ring PAHs found in the water phase near the sediments at low tide was considerably higher than at any other location and time. High concentrations of 3-ring PAHs were found near the surface during high tide. The 4-and 5-ring PAH concentrations were highest during the falling and low tides near the sediments, but were relatively low and stable near the surface. The study indicates that the PAHs in the stream water fluctuate due to tide-induced varying hydrodynamics.

ENVR 34

Classifying landfill leachates using major ions

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Landfill leachates are complicated chemical mixtures, and it is difficult to differentiate and group sampling results in terms of overall chemistry. This methodology identifies leachates that share major ion chemistry, and distinguishes results that are different. A normalized version of Stiff diagrams creates subjective identification of general leachate classes, and principal component analysis makes a more objective understanding of similarities and distinctions. Applying the method to data from a New York landfill (652 samples collected over more than 20 years) found that 75% of the results fell into three general leachate groupings (classification efficiency rises to 90% if "early" results are not considered). The general leachate types conform to differences in wastes received in the different sections of the landfill, and to changes in landfilling practices. This modified Stiff diagram methodology has utility in assessing functionality of liner systems, and in determining causes of local groundwater impairments.

ENVR 35

Discarded plastics and priority pollutants: A multiple stressor in marine habitats

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Hazards associated with plastic materials have become an issue of concern among environmentalists, scientists, industry workers and policy makers. Plastic products have been questioned for their safety due to hazardous additives and monomers that make up the material itself. In the environment, discarded plastics have become a global environmental problem across several habitats. In the ocean, plastic pollution has been reported globally. In the marine environment, plastic waste sorbs priority pollutants such as persistent organic pollutants (POPs) and trace metals from surrounding waters. As a result, plastic itself may pose a threat to marine life, but may also be another medium for exposure to priority pollutants. Plastic material in combination with priority pollutants threatens organisms as a multiple stressor. To better understand the risks of discarded plastics in marine habitats we asked two questions: 1) what is the fate of POPs to different types of plastics in marine habitats, and 2) what are consequences of ingestion of plastic material and marine plastic debris in fish. Using field experiments replicated over space and time, we measured sorption of PCBs and PAHs to five types of mass-produced plastics (HDPE, LDPE, PP, PET and PVC) in San Diego Bay. Next, we selected low-density polyethylene (LDPE) plastic for dietary exposure experiments. Adult Japanese medaka (*Oryzias latipes)* were exposed to one of three treatments (control diet, diet spiked with 10% virgin LDPE and diet spiked with 10% ocean-exposed LDPE) for 1- or 2-month periods and tested for several toxic endpoints including: changes in gene expression, transfer of pollutants from plastic to fish tissue, and histopathology. We found that different types of plastics sorb different concentrations of PAHs and PCBs. Significant differences among plastic types ($p<0.001$) suggest that some plastics may be less hazardous as marine debris. In medaka, we found changes in gene expression from both virgin and plastic exposed to the marine environment. Results gathered to date regarding effects of polyethylene plastic material itself and in combination with priority pollutants to medaka will be presented.

ENVR 36

FSIS activities regarding dioxin

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FSIS will conduct its fourth dioxin survey in 2012-2013. The Agency will model the survey after the 2007-2008 survey. By using a survey of the same magnitude, duration, and statisical design, the Agency can determine trends in dioxin-like compounds (DLCs). The 2012-2013 study aims to monitor trends in the dioxin levels in animal fats and to detect and identify possible sources of dioxin into the food supply. FSIS will analyze 500 samples. FSIS and its federal partners and industry believe this effort will continue to ensure the safety of the nations's food supply, particulary meat products.

The National Academies of Science recently re-evaluated the EPA assessment of human exposure to dioxin in the food supply. On February 17, 2012, EPA issued the document entitled *Reanalysis of Key Issues Related to Dioxin Toxicity and Response to NAS Comments, Volume 1*. In the document, EPA derived a reference dose (RfD) 0f 7×10^{-10} mg/kg-day (0.7 PPT) for TCDD. Using the new RfD as a marker, FSIS analyzed exposure data for FSIS regulated products (e.g., beef, pork, chicken, and turkey). The ongoing dioxin surveys are vehicles for monitoring and assessing the meat and poultry exposure pathway. Exposure data included several variables, such as 1) lean vs. non lean meat/poultry; 2) highest vs. mean toxic equivalent (TEQ) values found in the most recent 2008 dioxin survey; 3) high calorie level vs. mean calorie level; and 4) usual U.S intake vs. recommended intake (dietary guidelines). FSIS determined that following recommended dietary guidelines, a typical American adult's exposure to dioxin from FSIS regulated products is below the new EPA established reference dose.

ENVR 37

Chemical dispersant synergy the Deepwater Horizon oil spill's toxicity on the growth, reproduction, and gene expression of Caenorhabditis elegans

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Caenorhabditis elegans are used as an animal model to test the impacts of crude oil and chemical dispersant. Our results show that both oil and dispersant were significantly inhibited the *C. elegans* reproduction. Oil exposure affected *C. elegans* growth and development at the early stage instead of later stage. However, the reproduction behavior of the L4-stage of *C. elegans* was more sensitive to oil exposure than that of the L1-stage of *C. elegans*. Oil dispersant synergistically interacted with oil to induce higher toxic in the aspects of worm growth and reproduction. Moreover L4 stage worms were more sensitive to dispersant and its interaction with oil. Transcriptional responses offer insights into the potential biological consequences. Results show that dispersant and the mixture of dispersant and oil induced the aberrant expression of 12 protein-coding genes. These genes are related to many biological processes, including egg-laying, oxidative stress, muscle movement and neuron functions.

ENVR 38

Effects of Marcellus Shale gas drilling wastewater discharge on trihalomethane formation

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This study examined the effects of untreated Marcellus Shale gas drilling wastewater on the formation of brominated trihalomethanes (THMs) in river water. Untreated Marcellus Shale gas drilling wastewater samples and Pennsylvania river water samples were tested for bromide and total dissolved solids (TDS). Composites consisting of river water and gas drilling water were treated with chlorine, incubated and tested for THMs. Results indicated an increase in brominated THMs and total THMs (TTHMs) with additions of gas drilling wastewater.

ENVR 39

Fluorescence detection of lead(II) ions through their induced catalytic activity of DNAzymes

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We have developed a fluorescence approach for the highly selective and sensitive detection of Pb^{2+} ions using AGRO100, a G-quadruplex DNAzyme. The sensing strategy is based on Pb^{2+} ions inducing increased DNAzyme activity of AGRO100 in the presence of hemin, which acts as a cofactor to catalyze H_2O_2-mediated oxidation of Amplex UltraRed (AUR). A test of eight aptamers of various sequences for the detection of Pb^{2+} ions revealed that AGRO100 performed the best in terms of sensitivity. The AGRO100-AUR probe exhibited high selectivity (>100-fold) toward Pb^{2+} ions over other tested metal ions. The fluorescence intensity (excitation/emission maxima, ca. 561/592 nm) of the AUR product was proportional to the concentration of Pb^{2+} ions over the range 0–1000 nM, with a linear correlation (R^2 = 0.98). For 5 mM Tris-acetate (pH 7.4) solutions in the presence and absence of 100 mM NaCl, the AGRO100-AUR probe provided limits of detection (signal-to-noise ratio = 3) for Pb^{2+} ions of 1.0 and 0.4 nM, respectively. We validated the practicality of using the AGRO100-AUR probe for the determination of the concentrations of Pb^{2+} ions in soil samples. This approach allows the determination of the concentrations of Pb^{2+} ions with simplicity, selectivity, and sensitivity.

ENVR 40

New double shell zero-valent iron nanoparticles with high potential of halogenated organic compounds removal

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Zero-valent iron nanoparticles (NZVI) are generally well known for their high efficiency of halogenated organic compounds decomposition. The efficiency of halogenated organic compounds removal can be based on NZVI reduction properties as well as on high sorption capacities of NZVI oxidation products. In this contribution, we will demonstrate a new kind of NZVI which has a double shell layer around zero-valent iron core. According to our recent results, the double shell protects the zero-valent iron core against air-oxidation and simultaneously allows a better trichlorethene decomposition in aqueous solutions. The finantial support by P108/11/P657 Grant awarded by GACR, the project of the Ministry of Industry and Business of the Czech Republic (project ID: FR-TI3/196), and the Operational Program Research and Development for Innovations - European Regional Development Fund (project CZ.1.05/2.1.00/03.0058 of the Ministry of Education, Youth and Sports of the Czech Republic) is gratefully acknowledged.

ENVR 41

Integrated decomposition of perfluorooctane sulfonate on nanoscale zerovalent iron

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Contamination of groundwater with perfluoroalkyl compounds (PFACs) widely used in fire retardants is a great concern. PFACs are stable and non-biodegradable which makes them persistent in the environment. We have attempted to develop effective in-situ remediation technologies for PFACs-contaminated groundwater. In order to remove PFACs more efficiently under various aquatic conditions, we have investigated integration of three proven treatment technologies (adsorption, oxidation, and reduction) into an innovative engineering system and to explore the associated reaction mechanisms and pathways in the complex system. The integrated treatment of PFACs will be implemented by introducing reactive activated carbon impregnated with various Fe nanoparticles (Fe oxides, zerovalent Fe (ZVI), and palladized Fe) in the presence of common oxidants. In this presentation, we will preliminarily discuss the heterogeneous decomposition of perfluorooctane sulfonate *via* reductive defluorination and/or advanced oxidation using nanoscale ZVI in the presence of hydrogen peroxide, peroxymonosulfate, and persulfate.

ENVR 42

Interactions of amines with activated carbons and potential catalyzed nitrosamine formation

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Activated carbon (AC) materials with micro- and nano-porous structures are commonly used in the solid phase extraction of nitrosamine contaminants in water, and for the removal of micropollutants in water treatment. Our research found that many commercial AC materials can catalyze transformation of secondary amines and certain tertiary amines to yield trace levels of carcinogenic *N*-nitrosamines under ambient aerobic conditions. The AC-catalyzed nitrosamine formation is highly influenced by the AC material properties and the amine precursor structures. Mechanistic investigation reveals that the reaction involves both atmospheric oxygen and nitrogen. AC's surface reactive sites react with molecular oxygen to form reactive oxygen species (ROS), which facilitate fixation of molecular nitrogen on the carbon surfaces to generate reactive nitrogen species (RNS) likely nitrous oxide and hydroxylamine that can react with adsorbed amines to form nitrosamines. AC's properties play a crucial role as more nitrosamine formation is associated with carbon surfaces with higher surface area, more surface defects, reduced surface properties, higher O_2 uptake capacity, and higher carbonyl group content. The chemical phenomena identified by this study are not only critical for minimization of nitrosamine formation in AC-based analytical procedures and water treatment, but may also be relevant for a wide range of processes involving synthetic and naturally-occurring activated carbons materials.

ENVR 43

Black carbon-mediated reduction of 2,4-dinitrotoluene: The role of electrical conductivity

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Currently, black carbon (BC)-mediated reduction of nitro compounds was increasingly investigated. However, the mechanism on the enhancement of reduction in the presence of BC was not clearly elucidated yet. In this study, we tried to prove our hypothesis that graphene moieties of BC can serve as adsorbent as well as electron conduit to promote the reduction of sorbed organic molecules. By using various types of BC material, including graphite, chemically-converted graphene (CCG), multi-walled carbon nanotube (MWCNT), and granular activated carbon (GAC), BC-mediated reduction was investigated with 2,4-dinitrotoluene (DNT), a model nitroaromatic compound. Results from batch experiments showed that CCG, MWCNT, and GAC could accelerate the reduction of DNT by dithiothreitol, a thiol reductant. Kinetic data analysis showed that the BC-mediated reduction of DNT is linearly proportional to electrical conductivity of BC, supporting that graphitic structure in BC may account for the role of an electron-transfer mediator.

ENVR 44

Comparative study for the adsorption of Cu(II) on functionalized nano graphene platelets and multiwall carbon nanotubes: Effect of size and morphology

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Nano graphene platelets (NGPs) are a new member of carbon nano-materials which can be seen as a flattened version of multiwall carbon nanotubes (CNTs), with few-layer thickness and two nano- or micro-dimensional sides. Basic manufacturing methods can use a graphite substrate to synthesize NGPs, with some exfoliating process to reduce the number of layers, and acid/purification process to add oxygen groups. The outstanding mechanical and chemical properties of the NGPs offer a potential of different applications in several technological fields, such as electronic industry, sensor, composites and in water treatment, with some advantages over CNTs. NGPs were characterized by TEM, SEM, XPS, FTIR, Zeta potential analyzer and BET surface area analysis. Adsorption capacity of copper on NGPs was studied by performing kinetics and isotherm experiments. However, the objective of this study is to compare the adsorption process variables, under the effect of the perimeter and the functionalized sites. Oxygen groups such as OH and COOH, tend to bond to the open ends of CNTs, and by similar mechanisms, bond mostly to the NGPs edges. The study involved estimation of the coefficients in a mathematical model, predicting the response and checking the adequacy of the model.

ENVR 45

Characterization of natural organic matter from Ohio River and investigation of their influence on stability and transport of engineered nanoparticles in water filtration system

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The presence natural organic matter (NOM) plays an important role in the transport and fate of nanoparticles (NPs) in the aquatic environments. NOMs can mobilize and facilitate the transport of NPs, which increase the potential hazard of NPs. However, the chemical structure and reactivity of NOM is highly heterogeneous according to the origin and extraction method. Many researches used commercial or artificially synthesized NOMs that have no relevance to water treatment. In this study water from the Ohio river was ultrafiltered and lyophilized to obtained concentrated form of NOM . The NOM sample was characterized in terms of NMR, LC-MS, electrophoresis mobility, TGA-GC-MS, DSC techniques for structural characterization. The influence of this NOM on the aggregation, transport and retention of nano Ceria, ZnO, Ag and TiO_2 was investigated. The interaction on NPs and biofilms that are present in biologically active filter that are commonly found in water treatment plants were studied.

ENVR 46

Mass loading effect of different lengths of polyethylene glycols on the enhancement of tetrachloroethylene dechlorination by zerovalent silicon

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The addition of polyethylene glycol (PEG) in zerovalent silicon (Si(0)) has proven to significantly enhance the dechlorination rate and efficiency of tetrachloroethylene (PCE) because of the inhibition of silicon oxide formation. A good relationship between the mass loadings of PEG-35000 and the k_{obs} for PCE dechlorination was also observed. PEG is a bi-functional polymer with various chain lengths and molecular weights and the effect of physicochemical property of PEG on the enhanced dechlorination of PEG is required and interesting to better understanding the inhibition mechanism for SiO_2 formation. In this study, different carbon lengths and amount of PEGs with MW of 2000-35000 were applied to the Si(0) system to examine the enhancement effect on PCE dechlorination and inhibition extent of SO_2 formation. Interestingly, the k_{obs} values for PCE dechlorination by Si(0) were similar when same concentration of various MW PEG was added. It was found when the same carbon mass loadings of each PEG were applied in Si(0) system. For example, the k_{obs} value was 0.19-0.24 h^{-1} when the loading amount of 4 various PEGs were 17.5 mg in 25 mL solution. The results in this study indicate that the loaded carbon mass of PEGs was the dominant parameter to enhance the reactivity of Si(0) system.

ENVR 47

First principles simulation of intermediate steps in nitrate reduction on metal catalysts

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Catalytic treatment is a potentially economical and low energy route to removing nitrogenous pollutants (nitrates, nitrites, and nitrosoamines) from drinking water. Pd and Pd alloy catalysts are catalytically active for hydrogenation of the nitrogenous compounds to harmless dinitrogen (N_2) and water (H_2O), but current formulations lack sufficient activity, selectivity, and durability for practical use. Here we report first-principles simulations of the adsorption chemistry and reaction of relevant intermediates (NO, N_2O, H, N, O, NOH, NH, NH_2, HNNO, H_2NNO) involved in nitrate reduction over model Pd surfaces. We show that Pd has a high affinity for NO, that this high affinity is important to reduction activity, that NO hydrogenation is the first step in the reduction chemistry and is facile in the presence of water, and that hydrogenation to NH3 competes with various NHx reaction with NO to form N-N bonds. The results are important for understanding observed catalysis and in designing superior materials.

ENVR 48

Structure sensitivity study of hydrogenation for waterborne contaminants using shape- and size-controlled Pd nanoparticles

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Catalytic reduction with Pd has emerged as a promising technology to remove a suite of contaminants from drinking water, such as oxyanions, disinfection byproducts, and halogenated pollutants. Here we systematically investigated the dependences of intrinsic catalytic activity and selectivity for nitrite, N-nitrosodimethylamine (NDMA), and diatrizoate reduction with Pd shape and size. Results show that turnover frequencies (TOFs) for nitrite, NDMA, and diatrizoate reduction are dependent on coordination number of surface Pd sites at low contaminant concentration, but TOFs for nitrite are constant at high contaminant concentration. Selectivity to ammonia for nitrite reduction decreases with increasing number of surface Pd sites for both low and high nitrite concentrations. However, selectivity for NDMA reduction is neither shape- nor size- specific, and ammonia and dimethylamine are the only products. Hence, our study suggests new insights that contaminant reduction activity and selectivity vary in respect with shape and size of Pd nanocatalysts, and that catalysts can be tailored for better performance for drinking water treatment.

ENVR 49

Treatment of perchlorate in waste ion-exchange regenerant brine with a Re-Pd catalyst

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Non-selective ion-exchange (IX) resins used to treat perchlorate (ClO_4^-) (often in combination with nitrate) must be regenerated using a brine solution, and this produces a concentrated waste stream. Treatment or disposal of ClO_4^- containing brine is a challenge for water treatment plants. Most current chemical and biological treatment systems for ClO_4^- reduction are negatively influenced by concentrated salt solutions. In this study, ClO_4^- reduction activity with a Re-Pd/C bimetallic catalyst was evaluated in synthetic and waste IX brine solutions (6% NaCl), using H_2 as the reductant at 25°C and 1 atm pressure. Catalytic activity in the synthetic brine was three times greater than the corresponding activity in DI water. However, catalytic activity in the waste IX brine was 65 times lower than in the synthetic brine. Both synthetic and real brines contained ClO_4^- at 100 mg/L. However, the real brine also contained nitrate (NO_3^-), at 2360 mg/L, which is also reduced by the catalyst. To explore the effects of nitrate on ClO_4^- reduction, nitrate was added to the synthetic brine, and the ClO_4^- reduction activity decreased by 20 times. The extent of this decrease is much greater than expected based on simple sequential reduction. Hence, NO_3^- appears to deactivate the catalyst surface for ClO_4^- reduction. Pretreatment of NO_3^- in the real brine using a In-Pd/Al_2O_3 catalyst, and subsequent treatment of ClO_4^- using the Re-Pd/C catalyst resulted in ClO_4^- reduction rate constants that matched the NaCl-only synthetic brine. A sequential treatment of NO_3^- and ClO_4^- is proposed as a promising strategy for waste recycling, and could reduce costs and environmental impacts associated with brine production and discharges.

ENVR 50

Zero-valent Fe/Al bimetal for water sustainability

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A zero-valent Fe/Al bimetal is synthesized by depositing zero-valent iron onto the surface of zero-valent aluminum. A dual functionality of Fe/Al bimetals for redox reactions has been discovered. The Fe/Al bimetal serving as an electron donor is capable of reductively degrading chlorinated organic compounds while it also possesses an oxidative ability to mineralize dye wastewater through the production of hydrogen peroxide. The oxidative ability was investigated using methanol as a probe. Methanol (initial concentration of 31.5 mg/L) was completely mineralized to carbon dioxide while formaldehyde was detected as an intermediate accounting for 7.1% of the total amount of methanol. Our study demonstrates the zero-valent Fe/Al metal is a reactive reagent for simultaneous treatments of a wide spectrum of contaminants including both reductive and oxidative compounds.

ENVR 51

Two approaches to achieve visible light upconversion for environmental application

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This talk summarizes our most recent advances in developing antimicrobial/biocidal materials that function through light frequency amplification process called upconversion (UC). The first approach is based on inorganic luminescent materials that can convert visible light into germicidal UVC and have been shown to inactivate microorganisms deposited on dry surface and deter biofilm formation under commercial fluorescent light exposure. Upconversion efficiencies of current phosphor systems are too low for practical antimicrobial/biocidal application, however, and methods of enhancing internal optical efficiency are required for further advancement. Lithium ion doping is a commonly employed, yet sparsely understood option for improving emission intensity in UC phosphors, including the visible-to-UV converting material $Y_2SiO_5:Pr^{3+}$. In this work, for the first time, we have identified and quantified the major mechanisms by which Li^+ enhances UC in a phosphor, using crystallographic and spectroscopic techniques in the form of X-ray diffraction, neutron diffraction, photoluminescence spectroscopy, and electron microscopy. Results show that 10 at.% doping with Li^+ improves UV emission 9-fold and is attributed to crystallite enlargement, induction of a phase change, and increasing inter-ion separation of the Pr^{3+} activator. The second UC approach is based on a completely different mechanism of sensitized triplet-triplet annihilation in an organic matrix. Moldable rubbery urethane materials generated from their corresponding polymeric precursors produce high efficiency regenerative green-to-blue upconverting solids when impregnated with benchmark palladium(II) octaethylporphyrin (PdOEP) sensitizers and 9,10-diphenylanthracene (DPA) acceptor/annihilator molecules. The cured soft materials promote sufficient diffusion at room temperature to support the sequential bimolecular reactions necessary for both triplet sensitization and triplet-triplet annihilation occurring between the precisely doped chromophores. UC quantum yields measured in linear incident light power dependence region exceeded 20%, over an order-of-magnitude greater than all previously investigated solids. These materials are intended as host materials enabling sub-bandgap sensitization of semiconductor photocatalysts such as TiO_2 to enhance visible light susceptibility in environmental decontamination application.

ENVR 52

Assessing long-term photocatalyst activity, inhibition, and deactivation by non-target water constituents when treating trace micropollutants

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Many studies report each year on new materials and catalysts that possess promising properties for water treatment applications (e.g., photocatalysts that are activated under a wider spectrum of light or degrade a target contaminant faster). Most catalyst development efforts have focused on improving material performance measured only in short-term batch experiments conducted in “clean” laboratory solutions devoid of non-target natural water constituents that are typically present in natural water matrices at concentrations (mg/L) many orders of magnitude higher than the target micropollutants (e.g., ng – µg/L). Comparatively little effort has been focused on improving long-term catalyst activity and stability when treating contaminants in these more complex matrices. Such efforts are needed to develop materials-based treatment technologies that are both economical and sustainable. Here, we report on the development of a laboratory continuous-flow photoreactor outfitted with fixed-film titanium dioxide (TiO_2) photocatalysts, and its application for assessing long-term (i.e., days to weeks) photocatalyst activity, inhibition, and deactivation when treating trace micropollutants in aquatic matrices (tertiary wastewater effluent, groundwater) containing diverse non-target constituents (e.g., natural organic matter, dissolved ions). Catalyst activity is tracked and post-mortem spectroscopic analysis of deactivated catalysts is used to identify deactivation mechanisms, information that can be used to develop more stable catalysts and strategies for slowing deactivation.

ENVR 53

Synthesis and optimization of photocatalytic TiO_2 nanofibers for treatment of impaired water supplies

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To achieve sustainable water resources, new treatment technologies are needed that can be applied to a broad range of undesirable constituents and water chemistries. In this work, we have synthesized photocatalytic TiO_2 nanofibers via electrospinning for use as a chemically reactive filtration technology. Through systematic tuning of material properties during electrospinning, TiO_2 nanofibers of controlled diameter, crystallinity and grain size were developed and their photocatalytic activity was tested toward a series of substituted phenols as a model pollutant class. Reactivity studies reveal that nanofiber photoreactivity ($\lambda > 305$ nm) is dependent upon nanofiber diameter and the relative amount of anatase and rutile TiO_2 phases. Notably, the most reactive nanofibers synthesized to date have outperformed commercially available TiO_2 photocatalysts commonly used in water treatment applications. Ongoing work aims to further establish links between nanofiber properties and reactivity, as well as their application in water treatment as nanofiber filter mats.

ENVR 54

Computational methods in the interpretation of reactivity of emerging contaminants by ozone-based technologies: Combined DFT QSAR approach

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Any chemical or biological contaminant introduced into clean water results in a lower water quality that may adversely affect human health or the environment. Emerging contaminants (ECs) generally refers to chemicals, biological agents and materials, that may pose a potential or real threat to human health or the environment, but which are not generally regulated at present or are expected to undergo changes in regulations. Ozone (O_3) is one of the strongest known oxidants with oxidation potential 2.07 V. It is widely performed for water and wastewater treatment. Mechanism of ozonation is similar to other disinfectants for water and wastewater treatment, which is based on the instability of O_3 in water [1]. The extra oxygen radical in an ozone molecule quickly binds to each component that comes in contact with ozone molecules [2]. The unique feature of ozone is its decomposition into hydroxyl radicals (•OH) which are the strongest oxidants in water. Ozone is a very selective oxidant, whereas hydroxyl radicals are non-selective and react fast with wide range of organic compound. Therefore, compounds persistent to molecular ozone are destructed by indirect reaction with the radical species that are formed when ozone decomposes in water. All the chemicals and reagents (high purity analytical or higher grade) were purchased from Sigma Aldrich. The setup comprises of ozone generator, bubble column, degassing unit, and destruct unit. The ozone generator (OZAT CFS-1 2G) was provided by Ozonia Ltd. The samples were taken at regular intervals and were prepared using solid phase extraction (SPE) (Oasis HLB carttriges, Waters) and analyzed using UPLC/MS/MS (Waters). The ozonation and chemically-assisted ozonation of several groups of ECs and endocrine disrupting compounds (EDCs) (bisphenol A, 1,4-dioxane) was investigated. The efficiency of the treatment varied from

one compound to another, which allowed making a conclusion about the applicability of these treatment methods to the certain group of compounds. The initial concentrations of all chemicals under study were initial concentrations of 100 µg/L. Pharmaceuticals were sufficiently removed (up to 100%) by direct ozone reaction during ozonation, whereas 1,4-dioxane degradation mostly occurred in hydroxyl radical reaction during peroxone treatment. All steroids were removed in approximately 1 min. No removal was achieved in ozone-based processes for the removal of *N*,*N*-Diethyl-*meta*-toluamide (DEET). The difference in reactivity can be attributed to the structures of ECs. Special study on the reactivity of seven estrogens and five progestins was accomplished by computational methods. However, the slight difference in reactivity between estrogens and progestins attributed to the presence of phenolic moiety in estrogens was found. The electronic structure of these compounds has been studied and several most important parameters were identified. As a result, qualitative structure activity relationship (QSAR) models for these two groups of steroids were developed. Emerging contaminants demonstrate different reactivity towards molecular ozone and hydroxyl radical. The selective treatability is attributed to the chemical nature of the compounds and can be interpreted via detailed structure analysis.

ENVR 55

Effect of organics on perchlorate byproduct formation during electrochemical oxidation of chloride-containing waters

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Waste streams from water treatment such as reverse osmosis and desalination contain high chloride concentrations. Electrochemical oxidation using boron-doped diamond (BDD) electrodes shows promise as a viable option for the treatment of these wastes streams but the formation of perchlorate, a human health risk, is an unwanted byproduct. Previous research in our laboratories has shown that perchlorate forms via the multi-step oxidation of chloride, where the rate-determining step is the oxidation of chlorate to perchlorate. Chlorate is first oxidized on the electrode surface via direct electron transfer, followed by the homogeneous reaction with hydroxyl radicals to form perchlorate. This presentation will focus on the effect that organic compounds have on perchlorate production. Several organic compounds with varying potential for participation in either direct electron transfer or hydroxyl radical scavenging reactions were studied, and results suggest that perchlorate formation is highly influenced by solution conditions.

ENVR 56

From waste to wealth using green chemistry

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Society is faced with the twin challenges of resource depletion and growing amounts of waste. The only sustainable solution is to stop viewing waste as something we wish to discard and see it as a resource. One of the key challenges to realise the enormous potential in these wastes is the difficulty of extracting valuable components such as metals and complex organic molecules. At present our technical ability to valorize waste is largely limited and based on "first generation" technologies such as anaerobic digestion which tend to have low efficiency and lose much of the valuable complexity of the wastes. New clean technologies that can help valorise wastes more efficiently include microwave processing and natural solvent extraction: these will be described and illustrated here along with the ultimate concept of zero waste biorefineries based on waste feedstocks.

ENVR 57

Valorisation of coffee grinds and unconsumed bakery waste from Starbucks Hong Kong for the sustainable production of chemical and materials

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The School of Energy and Environment at the City University of Hong Kong has recently started collaborating with coffee retailer giant 'Starbucks Hong Kong'. The partnership, which was facilitated by the NGO the Climate Group, will focus on the valorisation of spent coffee grounds and unconsumed bakeries via bio-processing. The collaboration is based on a support scheme and part of the “Care for our Planet” campaign: for every set of Care For Our Planet Cookies Charity Set sold, Starbucks will donate HK$8 to the School of Energy and Environment of City University of Hong Kong to support research on valorisation of food waste for sustainable production of chemicals and materials.

The aim of the research is to valorise the disposed coffee grounds and unconsumed bakeries to bio-plastics and detergents ingredients, facilitating the development of biomass use in Hong Kong and reduce the release of greenhouse gases and other air pollutants into the atmosphere.

The Hong Kong Starbucks project will focus on the use of acidic hydrolysis of non pre-treated spent coffee grounds and bakery waste, followed by fungal solid state fermentation for breaking down the carbohydrate into simple sugars for the subsequent succinic acid fermentation. One of the critical issues to be solved is to overcome the inhibitory compounds which affect the growth of *Actinobacillus succinogenes*, which is a facultative anaerobic bacterium used in the fermentative production of succinic acid.

ENVR 58

Integrated, catalytic strategy to enable production of cellulosic jet fuels

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γ-valerolactone (GVL) is a versatile bio-based chemical that can be prepared in good yields from cellulose (~70% of theoretical) through catalytic conversion via intermediate formation of levulinic (LA) and formic acids. As a platform, GVL offers many processing options to various fuels and chemicals. Of immediate interest is its role in facilitating production of cellulosic jet fuels.

Catalytic decarboxylation of GVL delivers butene monomers in nearly quantitative yields, and butenes can be coupled through acid-catalyzed oligomerization to form branched, higher molecular weight olefins. Here, we consider the kinetics and mechanism of GVL decarboxylation as well as varied product distributions achieved via oligomerization. Further, although GVL preparation (via LA hydrogenation) is straightforward, large scale accessibility is limited due to the cost of LA purification and mineral acid recovery. We therefore also consider recent developments which employ bimetallic catalysts to streamline LA purification (and thus GVL production) and further enable downstream technologies.

ENVR 59

Catalytic hydrothermal processing for hydrocarbon production from waste lipid feedstocks using renewable hydrogenation agents

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Catalytic hydrothermal processing (C-HTP) is a promising technology for converting moisture-laden, high free fatty acid, waste lipid feedstocks directly into hydrocarbons. Water is used as the reaction medium, allowing for in situ hydrogen production via the water-gas-shift reaction. This study explores the conversion of highly unsaturated waste lipid feedstocks under C-HTP conditions (240-340°C, 7-21 MPa, 10-30% lipids) using mono and bi-metallic catalysts (Pt/AC, Re-Pt/AC) with renewable hydrogenation agents (glycerol, formic acid). Conversions were conducted with model and complex lipid feedstocks including oleic acid, corn oil, waste trap grease, and dried distiller's grain (DDG) oil. Conversion products and degree of saturation were monitored as the reaction progressed, and lipid and hydrocarbon constituents were identified and quantified by GC-MS and GC-FID. Favorable hydrocarbon yields demonstrate the potential of C-HTL for energy recovery from waste lipid feedstocks and highlight the promise of bimetallic catalysts and renewable hydrogenation agents for in situ hydrogen production.

ENVR 60

Integrated catalytic conversion of lignocellulosic biomass to chemicals and fuels

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Fractionation of lignocellulosic biomass increases process flexibility and allows for integrated processing of C5 and C6 sugars. Recent advances using acidic treatments to deconstruct biomass in combination with organic solvents to create biphasic systems have allowed for increased yields of platform chemicals such as furfural, hydroxymethylfurfural (HMF), and levulinic acid. Management of the mineral acids used in pretreatment steps remains a challenge, but proper organic solvent selection, such as sec-butylphenol, allows for complete recovery and recycle of mineral acid.

Using solvents with high partition coefficients for extraction of products in biphasic unit operations allows the concentrations of products to be increased and improves the efficiency of downstream processing options, such as distillation or further upgrading reactions. Overall, fractionation of lignocellulosic biomass allows for a flexible, integrated processing approach that we hope will advance biorefining operations, allowing commercial biomass processing to become a reality.

ENVR 61

Biomass gasification and gas conversion process for the recovery of useful gases

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There is currently a strong need for new and effective energy recovery from renewable resources, and in response, gasification and gas conversion technologies have been developed. In sequential processes, the benign catalytic production of CO and CH_4, from a syngas mixture of H_2, CO and CO_2, etc., is a key element, and the respective reactions take place at different temperature regions. In this study, a first-stage experiment was conducted using a gasification and reforming apparatus, operated at 750ºC, employing waste wood samples. In the second stage, the reverse water gas shift (RWGS) reaction at temperatures over 600ºC, and methanation at lower temperatures (350-400ºC), were investigated using a novel NiO/SBA-15 mesoporous catalyst. The results showed that the conversion efficiency in the methanation of CO_2 reached about 80%. Some challenging issues are involved in the RWGS reaction for CO_2 conversion; however, this new system would offer a sustainable form of chemical processing.

ENVR 62

Photocatalysis and biomass: An effective combination for the conversion of solar energy into chemical energy

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Biomass is the only current sustainable source of pharmaceuticals, plastics, and biofuels. The European Commission has set a goal that by 2020, 10% of the transportation fuels will be based on biofuels. It is expected that during the next 20 years renewable energy (solar, wind, geothermal and biofuels) will increase from 5 to 18% in the global scale. For this purpose, a number of processes have been developed. However, these processes require rigorous conditions, such as high temperature or high pressure and, therefore, are of high cost. Compared to them, photocatalysis could be a good approach since the process can be carried out under ambient conditions and driven by sunlight.[1] Thanks to the novel ultrasound-assisted methodology for nanomaterials synthesis (based on TiO_2), it was possible to synthesize photocatalytsts with special properties which applied under right reaction conditions were active and very selective (promising selectivity to glucaric and gluconic acids, 70% in total, Scheme 1A) in the photocatalyitc oxidation of 2.8×10^{-3} $molL^{-1}$ glucose solution at room temperature.[2] Interestingly, the incorporation of metals (e.g. Pt, Pd) into the structure of the previous synthesized TiO_2 and a post high-temperature-redox treatment of these hybrid materials, allows us to obtain a different and interesting photocatalysts for biohydrogen production from glucose solution (Scheme 1C).[3] The whole idea may be described as a photocatalytic selective conversion (either photoselective production of platform molecules or biomass photocatalytic reforming to biohydrogen, depending on the chosen catalysts preparation methodology and the reaction conditions) of organic wastewater at room temperature and represents an environmentally friendly and cost effective method for water purification with parallel production of energy and chemicals.

ENVR 63

SERS analysis of arsenic species in water

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Surface enhanced Raman scattering (SERS) is a promising technique for rapid, sensitive, and field analysis of arsenate and arsenite species. SERS analysis was performed by transferring 10 µL of water sample on an Ag nanofilm substrate or sensor and recording the SERS spectra under a Raman spectrometer for a few minutes. The characteristic SERS bands of As(V) and As(III) species were at 780 and 721 cm^{-1}, respectively. The effect of common cations and anions in natural water on the SERS analysis of arsenic was studied. Extended X-ray absorption fine structure (EXAFS) was used to investigate the bonding structures of adsorbed As(V) on the SERS substrate, as well as the mechanism of the Ca^{2+} effect on the SERS analysis of As(V). It was discovered that fluoride could be used to reduce the interference of Ca^{2+} and Mg^{2+} on the SERS analysis of As(V).

ENVR 64

Degradation of pentachlorophenol by surfactant stabilized Ni/Fe nanoparticles

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Nanoscale Ni/Fe particles stabilized with cetyl trimethylammonium bromide (CTAB) were used to evaluate the potential of dechlorination of the pentachlorophenol (PCP). The effects of Ni/Fe dosage, Ni loading, surfactant, temperature on the dechlorination of PCP were investigated. The increase of Ni/Fe dosage enhanced the removal of PCP. The removal rate of PCP increased with the loading percentage of Ni from 0.25 wt % to 0.5 wt %, but decreased with the loading percentage of Ni from 0.5 wt % to 2 wt %. CTAB remarkably enhanced the removal of PCP using Ni/Fe nanoparticles. The observed enhancement of PCP removal and reduction by Ni/Fe-CTAB attributed to the increased sorption of PCP onto iron surfaces and the increased local PCP concentration in the vicinity of iron surface, accelerating the reduction of PCP. The activation energy of the removal reaction of Ni/Fe-CTAB, 81.6 kJ/mole, indicated a surface-control mechanism.

ENVR 65

Identification of the amount of binding sites and dissociation constants of an ligand-receptor complex using AlGaN/GaN high electron mobility transistors

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Antibody-immobilized AlGaN/GaN high electron mobility transistors (HEMTs) were used for detecting peptides and revealing the amount of binding sites of an antibody for the peptide and dissociation constants. Two binding sites were found on this antibody for the peptide and the dissociation constants of the antibody-peptide complex were 2.723×10^{-11}M and 6.994×10^{-9}M for the two different binding sites, respectively. The estimated dissociation constants are consistent with the detection limit of the sensor showing the important role of the dissociation constants for the performance of the sensor. The results demonstrate that the AlGaN/GaN HEMTs not only can be used as a biosensor, but also can work as a good platform for the fundamental biological affinity study.

ENVR 66

DNAzyme based lead (II) ions biosensor development on a portable optic fiber sensing platform

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To reverse the negative effects of Pb^{2+}, an important first step is accurate, on-site and real-time detection and quantification of Pb^{2+} in the environment or in vivo. Herein, we report a novel biosensor for rapid, highly specific and sensitive detection of Pb2+ based on GR-5 DNAzyme. In the presence of Pb^{2+}, GR-5 DNAzyme cleaves its specific substrate DNA molecule, which further hybridizes with the complementary strands immobilized on the optic fiber sensor surface. Subsequent fluorescent signals of the hybridized fluorescent labeled fragment provides quantitative information on the concentrations of Pb^{2+} with a dynamic range from 2 to 40nM with a detection limit of 2.51nM(0.52 ngmL^{-1}). The proposed sensor also shows good selectivity against other mono and divalent metal ions. The sensor was regenerated with 0.5% SDS solution (pH1.9) over 100 times without significant deterioration of the sensor performance. This portable sensor system can be potentially applied for on-site real-time inexpensive and easy-to-use monitoring of Pb^{2+} in environmental samples such as effluents or water bodies.

ENVR 67

Multilayered microspheres as a signal amplification mode for sandwich immunoassays

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Devices used for the detection of infectious microorganisms include microfluidic systems, electrochemical microchips, colorimetric immunoassays, and many others. Most of the current techniques require expensive equipment and are labor intensive. In recent decades, studies have focused on improving sensitivity, enhancing the detection limit, and streamlining the processing time. Here, we design an amplified diagnostic detection method that is simple, rapid, and applicable in resource poor settings. An antibody coated platform is used to capture analytes from samples. Once the antibody-antigen sandwich complexes are formed, the self-assembly of modified micro- and sub-micrometer sized beads is triggered by the addition of cross-linking reagents. The microsphere aggregates can lead to detection of the sandwich complex using an optical microscope. This microsphere-based immunoassay may eliminate the requirement of expensive equipment and may be used for the detection of environmental pathogens in few simple steps.

ENVR 80

Comparison of silver- and copper-charged polypropylene feed spacers for biofouling control

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The productivity of membrane filtration is lowered by fouling, which is caused by accumulation of foreign substances on the surface and/or within pores. Biofouling is the growth of microorganisms on the membrane surface and on the feed spacer as present between the envelopes. The fouling of membranes has demanded and continues to demand considerable attention from industry and research communities. Many of these applications use membranes in a spiral wound configuration that contains a feed spacer. The goal of this project was to develop low-biofouling polypropylene (PP) spacers through the functionalization of PP by a spacer arm with metal chelating ligands charged with biocidal metal ions, investigate the use of this metal-charged polypropylene (PP) feed spacers that target biofouling control, and to use some traditional and one novel techniques to autopsy the membranes after filtration to gain a better understanding of the biofouling mechanism and how the modified spacers are affecting it.

ENVR 81

Antiadhesive and antibacterial coatings for biofouling control

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Operational problems caused by biofilm formation, i.e. biofouling, are a significant drawback for membrane technologies. This research evaluates super-hydrophilic & anti-bacterial coating films designed to prevent bacterial deposition and replication, thus, making biofouling less likely to occur. In a first screening, films with varying thickness, hydrophilicity and roughness were formulated to elucidate the effect of the film chemistry on reversible and irreversible bacterial adhesion. In general, less crosslinked PVA films prepared from lower molecular weight and less hydrolyzed PVA produced more hydrophilic and adhesion resistant films. Although highly dependent in bacterial type and water chemistry, dicarboxylic acid as PVA cross-linking agents showed the best adhesion resistance. In a second screening, antibacterial cation-exchanged zeolites were incorporated in the films. In general, no significant differences resulted from silver-zeolites incorporation. However, copper-zeolites resulted in higher bacterial inactivation rates, but also higher irreversible adhesions, most likely due to higher surface roughness and cell lysis.

ENVR 82

Understanding the relationship between osmotic membrane structure, chemistry, and performance

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Many technologies exploiting the process of osmosis have been introduced to augment the world's depleting fresh water sources – reverse osmosis (RO), pressure-retarded osmosis (PRO), and forward osmosis (FO). Integrally skinned cellulosic membranes perform minimally in FO/PRO applications, but lack appropriate mechanical and chemical stability. Conventional polyamide (PA)-polysulfone (PSf) composite membranes do not perform adequately in FO/PRO applications because of their hydrophobic, low porosity support materials. Traditionally, hydrophilic and high-porosity support membranes do not produce acceptable separation performance RO membranes, but recent evidence suggests they may work well for polyamide FO/PRO composite membranes. Herein, we introduce hand-casted PA-polyaniline (PANi) composite membranes as next generation FO/PRO membrane materials. Well-controlled experiments show that PANi support membranes interact fundamentally differently with the monomers used to form PA composite membranes, but monomer solution composition and concentration can be optimized to form high-performance composite FO/PRO membranes.

ENVR 83

Development of antifouling reactive electrochemical membranes for water treatment and water reuse

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The drastic reduction of permeate flux due to membrane fouling and the high cost of membrane replacement pose a significant problem in water separation applications. In this investigation, a novel reactive electrochemical membrane (REM) was developed utilizing a conductive tubular Ti_4O_7 electrode material to alleviate irreversible fouling. Crossflow filtration experiments were conducted to evaluate the separation performance as a function of solution conditions and the applied electrical charge. Results indicate that the permeate water quality is affected by a combination of electrochemical reactions, adsorption, and electrostatics at the REM surface. Results will be presented from a series of experiments conducted with model organic and inorganic species to illustrate the utility of the REM for water treatment. Development of a state-of-the-art characterization protocol is being developed to elucidate fouling mechanisms and determine the dependence of applied electrical charge on membrane-foulant interactions.

ENVR 84

Biomimetic membranes for water purification

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Water channel proteins, Aquaporins (AQPs), provide selective water transport across cell membranes at rates unparalleled in synthetic solute-rejecting membranes. Thus, cell membranes containing AQPs are excellent models for synthetic water purification membranes. In the last few years, interest and activity in the area of mimicking cell membranes with aquaporins has grown rapidly. This talk will review some of the research challenges and exciting new developments in the area of biomimetic membranes for water purification and then discuss our approach to these challenges. There are three major research challenges to the development of a water purification relevant membrane using AQPs. These include: incorporation of high numbers of functional AQPs in membranes, development of a application relevant flat form factor membrane incorporating AQPs, and most importantly, the stability, lifetime, and costs of such membranes. We will review the approaches used to address the first two issues and present our work on addressing these challenges. Stability studies as well as performance under realistic conditions are currently not being studied actively because of lack of membrane materials at a scale relevant to such work. We will also present our work on alternative aquaporins (currently work is mostly focused on the E. coli aquaporin, AqpZ) that may have a higher permeability and stability. Additionally, we will discuss our work with protein engineering eye lens aquaporins that form stable flat arrays in biological system but have low permeability to form high permeability mutants. These may have applicability to forming high permeability, protein-rich, flat membranes.

ENVR 85

Dendritic polymers, carbonaceous nanomaterials, and composite inorganic/organic nanoparticles as regenerable membrane coatings for trace contaminant removal and fouling control

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Two enhancements for membrane-based water purification can be achieved with regenerable coatings: (1) trace contaminant adsorption and (2) fouling control. Several materials have been evaluated for their ability to achieve these goals in ultrafiltration (UF) and reverse osmosis (RO) applications. Multi-walled carbon nanotubes (CNTs), nano-graphene platelets (NGPs), and superfine powdered activated carbon (S-PAC) were tested as adsorptive coatings on UF membranes. Silver and TiO_2 nanoparticles enmeshed in functionalized polymer shrouds were tested as regenerable coatings for fouling control on RO membranes. Dendritic polymers show capabilities as both adsorbents and regenerable coatings due to their internal hydrophobic structure for contaminant capture and their external functional groups for attachment and release from membrane surfaces. All the materials and filtration types are compared together here, leading to a broader understanding of the material properties required to produce regenerable coatings that improve both flux and contaminant removal in water treatment.

ENVR 86

Poly ethylene terephthalate electrospun nanofibrous membranes for water purification

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Electrospinning is a simple and versatile method for fabricating continuous fibers with diameters ranging from micrometers to several nanometers that is useful in water purification. Highly porous electrospun nanofibrous membranes currently gain considerable interests in water filtration applications. Poly(ethylene terephthalate) (PET) was selected as the polymer to synthesize the nanofibrous mats, due to its low cost to synthesis, high porosity and strength of membrane characteristics, and good electrospinning properties. The PET nanofibrous mats are obtained by electrospinning PET solutions in trifluoroacetic acid/dichloromethane. The goal of the present study is to further the understanding of relationships between the structural parameters of PET electrospun nanofibrous membranes (i.e., average fiber diameter, fiber diameter size distribution, membrane thickness and porosity) and microfiltration performance for water purification.

ENVR 87

Application of spray layer-by-layer assembled composite polyelectrolyte-clay thin films as selective layers in reverse osmosis membranes

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Development of novel, less-expensive, and highly-selective membranes for use in continuous reverse osmosis (RO) processes could reduce both the capital and operating costs for modern desalination operations. The flexibility of the spray layer-by-layer (spray-LbL) assembly process enables the deposition of composite polyelectrolyte/clay thin films on porous hydrophilic substrates to serve as a selective layer, and is particularly suited because large asymmetric films can be deposited orders of magnitude faster than with traditional dip-LbL. The composition and physical properties of spray-LbL assembled thin films can be fine-tuned by manipulating the film assembly conditions. Using mathematical modeling on data collected from dead-end and cross-flow permeation cells, permeability coefficients for water and salt through selective layers of varying film composition are calculated. Preliminary data have confirmed the viability of using composite polyelectrolyte-clay films to increase the selectivity of commercially available RO membranes.

ENVR 88

Benign synthesis of N-aryl sulfoximines and unnatural amino acids with dithiocarbamate side chain

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C-N cross coupling reactions play a vital role in the construction of many important organic intermediates and biologically active compounds. The ability of diaryliodonium salts in C-N cross coupling reactions pave the way for the rapid *N*-arylation of sulfoximines under eco-friendly conditions. The transformation was achieved by reacting sulfoximines with diaryliodonium salts in aqueous polyethylene glycol-400 using CuBr as catalyst under ultrasonic condition. Unnatural amino acids have high value in drug discovery and development. Herein, we present the first report of a new class of unnatural α-amino acids bearing a dithiocarbamate side chain. These unnatural α-amino acids containing the dithiocarbamate side chain were synthesized *via* a one-pot, regio- and stereo-selective ring opening of sulfamidates by dithiocarbamate anions (generated *in-situ*) in aerial atmosphere without any special precaution and in absence of any catalyst/additive.

ENVR 89

Green synthesis of glycerol carbonate: Biocatalytic alternative for glycerol industry

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Glycerol, by-product of biodiesel production is already considered a platform molecule for fine syntheses (*e.g.* classic esters and oligomers, telomers, epoxides, carbonate derivatives, etc) based on the exploitation of Green Chemistry.

We propose a green alternative for glycerol application to glycerol carbonate synthesis. Glycerol is lipase-converted to glycerol carbonate in solvent-free reaction system in which dimethyl carbonate has double role (*e.g.* coupling reagent and reaction medium). The biocatalytic system was tested for two different configurations, *e.g.* the lipase (*Aspergillus niger* lipase) biocatalyst freely dispersed in the reaction volume and lipase-enzyme supported on the magnetic nano-/micro-particles. The effects of the experimental parameters on the synthesis performance were investigated and evaluated (*e.g.* reagents concentration, biocatalyst concentration, immobilization approach, co-solvent content, incubation time and temperature). The development of the biocatalytic process under optimum experimental conditions allowed valuable glycerol transformation (74% and 60% glycerol conversion, and 84% and 80% glycerol carbonate selectivity for free and immobilized lipase, respectively).

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ENVR 90

Tuneable bifunctional water-compatible heterogeneous catalyst for the selective aqueous hydrogenation of phenols

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A water-tolerant bifunctional heterogeneous catalyst is able to effectively catalyse the selective hydrogenation of phenol to cyclohexanone in water at atmospheric pressure and room temperature with >99.9% selectivity to cyclohexanone at phenol conversions >99.9 %. The catalyst was found to be highly active and reusable, giving identical activities and selectivities after >5 uses. Moreover, this reported simple bifunctional catalyst is also able to hydrogenate a range of substituted phenols in high yields under the investigated aqueous conditions.

ENVR 91

Design of ionic liquids for green lignin extraction from woods

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Ionic liquids (ILs) have received strong attention as promising green solvent for lignocellulose pretreatment. We recently reported that amino acid type ionic liquids dissolved cellulose very well under mild conditions. Here, we report an efficient lignin extraction method based on the ionic liquid technology: several types of amino acid ILs dissolved lignin very well even at 60°C and green preparation of lignin from woods has thus been accomplished: 16 wt% of lignin was obtained from Japanese cedar chips using 1-(2-methoxyethyl)-1-methylpyrrolidinium lysine as extraction solvent.

ENVR 92

Fe/Al bimetal: A solid-phase hydrogen peroxide generator for effective mineralization of dye wastewater

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Textile wastewater includes a wide array of dyes and dyeing assistants causing the environmental challenge for textile industry. The Fenton reaction, a green chemical process, has been known as a homogeneous process for dye wastewater treatments. However, the overall cost and associated problems of secondary sludge generation limit its application. We present here a solid-phase hydrogen peroxide generator, zero-valent Fe/Al bimetal, for an effective mineralization of dye wastewater through the Fenton reaction. The Fe/Al bimetal consisting of zero-valent aluminum and iron can gradually and constantly release hydrogen peroxide at the concentration range of 20-50 mg/L. The slow release of hydrogen peroxide minimizes the sludge production and makes the Fe/Al bimetal a long-lasting green material for dye wastewater treatments. We have tested a large variety of dye wastewater containing acid, basic, reactive and disperse dyes in reaction with Fe/Al bimetal. The COD removal efficiency was in a range of 60-98%.

ENVR 93

Pd(II)-catalyzed cycloisomerization of alkynoic acids in water: New tandem cycloisomerization/click chemistry reactions

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The search for organic reactions proceeding with efficiency, selectivity and atom economy (*i.e.*, all atoms of the reactants end up in the final product), has emerged as a major goal in synthetic chemistry. Isomerization reactions are typical examples of atom economic processes as no by products are generated. In this sense, the catalytic cycloisomerization of γ-alkynoic acids (**1**) promoted by transition-metals represents a straightforward route to synthetically useful cyclic enol-lactones (**2**). It is important to note that, in most of the cases, this catalytic transformation has only been carried out in organic solvents or in biphasic mixtures with water.In this communication, we will present a simple and versatile iminophosphorane-Pd(II) complex **3** , as catalyst for the rapid, efficient and selective cycloisomerization of both terminal and internal γ-alkynoic acid (**1**) into their corresponding enol-lactones (**2**), which proceeds in water at room temperature and under air. In addition, the catalytic system could be also recycled in ten consecutive runs. Application of this methodology to the new tandem cycloisomerization/click chemistry reaction involving diynoic monoacids will be also discussed.

ENVR 94

UpScaling Microwave-assisted chemical reactions

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UpScale Microwave's tools and methods enable seamless scale-up from early-stage R&D to manufacturing without changing synthetic methods. Our proprietary microwave technology offers the opportunity to create materials at unparalleled scale in processes that are inherently cleaner, faster, and greener. We have recently expanded our reactor capability to include a bench-batch reactor (0.05 – 1 L reaction volume) and a continuous-flow reactor with a maximum flow rate of 2 L/min. These new reactors augment our existing floor-batch reactor (0.1 – 12 L reaction volume) giving a suite of microwave reactors capable of preparing materials from the laboratory bench top through to production. The scope of scaled-up microwave chemistries with our reactors includes platform chemicals such as biphenyls, pharmaceutical intermediates and building blocks, OLED intermediates, and fuels such as biodiesel. Our work in scaling microwave-assisted chemistry from bench to production highlights our ability to scale from 100's of grams to 100's of kilograms.

ENVR 95

Integrating water reuse systems in a self-sustaining outpost

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Supplying potable water to military personnel stationed in remote outposts represents one of the greatest challenges that often needs be addressed to achieve continuous military superiority in isolated and hostile environments. The aim of this project was to investigate the possibility of integrating water reuse systems for production of potable as part of a self-sustaining outpost design. The methodology incorporated an approach based on identifying potential water sources from other systems in the outpost, development of mass balance based model, assessing applicable water treatment technologies and energy requirements, and systems integration. Results demonstrate that combination of energy efficient systems incorporating microfiltration/reverse osmosis could be implemented to provide potable water for a platoon level unit for a period of 90 days without need of resupply.

ENVR 96

Modified polanyi-based model for mechanistic understanding of adsorption of phenolic compounds onto polymeric adsorbents

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A modified Polanyi-based Dubinin-Ashtakhov model was developed to obtain mechanistic insight into adsorption of phenolic compounds by two representative polymeric adsorbents, XAD-4 (polystyrene) and XAD-7 (polymethacrylate). The adsorption potential was re-defined by replacing the term (C_w/C_s) with the normalized equivalent concentration in *n*-hexadecane (C_{HD}), where C_w is the equilibrium concentration and C_s is the aqueous solubility of the solute. By fitting adsorption isotherms to the modified model using , a new normalizing factor (E_m) was obtained to quantify the contributions of specific interactions (i.e., H-bonding, dipolar/polarizability, etc.) to the overall adsorption energy. Significant linear correlation was established between "***A*** ", the hydrogen-bond acidity, and "E_m" for the target compounds. These results suggest that, in addition to hydrophobic interactions, hydrogen-bonding is predominantly responsible for the adsorption of phenols by XAD-4 and XAD-7. The newly developed model enables further development of predictive tools to estimate the removal of emerging contaminants by polymeric adsorbents.

ENVR 97

Nitrate assisted UV advanced oxidation in wastewater effluent

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Trace organic pollutants in wastewater effluents threaten the acceptance of water reuse for a number of applications. A large amount of research has been devoted to development of treatment technologies to degrade these compounds. Among them advanced oxidation stands out as one of the promising technologies. Typical ultraviolet based advanced oxidation processes require addition of chemicals such as hydrogen peroxide to generate hydroxyl radicals. Nitrate, a common constituent of wastewater treatment plant effluents, produces hydroxyl radicals when irradiated with low wavelength UV. This study evaluated the potential for using indigenous nitrate in effluents for generating enough hydroxyl radicals for considerable contaminant degradation at disinfection and advanced oxidation UV doses.

ENVR 98

Drying of wastewater sludge through a hydrophobic membrane: A novel approach to water protection and reclamation

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This research examined the drying kinetics of wastewater sludge across hydrophobic or "breathable" membranes. These membranes do not allow passage of liquid water, or of any contaminants within the water, but do allow transport of water vapor, driven by a difference in vapor pressure. The evaporated moisture can be condensed on the other side of the membrane to produce contaminant-free water. The process can also be conducted in contact with water or groundwater, with the vapor pressure gradient caused by a temperature difference. This work reports on systematic studies of operating condition variations: initial moisture content, temperature, thickness, and presence of the hydrophobic membrane itself. Experimental results are compared to available analytical models to predict sludge drying rate as a function of moisture content and other key factors. A model previously used only for fibrous materials is shown to be most applicable.

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ENVR 99

Water quality assessments using hydroxyl radical probes in gamma irradiations

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Most of the wastewater treatment facilities in the US treat through the secondary processing stage, as required by the Clean Water Act. While these facilities are required to report certain water parameters, the quality of discharged water varies substantially according to location, volume of water and type of treatment. Due to the growing list of organic pollutants now commonly detected in wastewaters, advanced oxidation technologies, which employ the hydroxyl radical oxidant, have garnered attention. In recent studies, caffeine molecules were shown to react 100% efficiently with hydroxyl radicals in pure water; the efficiency drops in treated wastewaters, but depends on the water make-up. Using caffeine as the probe molecule, secondary treated wastewaters from Southern California and Northwest Indiana were tested for its degradation, using radiation chemistry to generate hydroxyl radicals. The hydroxyl radical efficiencies showed significant differences between the two wastewaters, signifying the possibility of using this hydroxyl radical reaction probe for water quality assessment.

ENVR 100

Thermodynamic studies of wastewater treatment from rubber processing factory using snail shell

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Wastewater from rubber processing factory was characterised for their pollution potentials. Results of the raw wastewater show that the physicochemical parameters measured were all above regulatory limits for wastewater discharge in Nigeria. These high values for these parameters show that wastewater from rubber processing factory has high pollution potentials, and therefore need to be treated before discharge into the environment. Snail shell however proves effective in the treatment of this wastewater as it shows great improvement in the quality of the wastewater after treatment. Thermodynamic studies of the treatment show that the change in ΔG of the parameters in the treated wastewater has negative values except that of pH and dissolved oxygen. The positive values indicate that their treatment was not spontaneous. The values of the change in ΔS and ΔH were positive for most of the parameters in the wastewater while few were negative.

ENVR 101

Air-based membrane biofilm reactor (MBfR) for energy efficient wastewater treatment

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In the conventional activated sludge (CAS) process, around 40 – 60 percent of the energy is devoted to aeration. However, only 5 - 25 percent of oxygen supplied by blowers is transferred to the liquid phase. The Membrane Aerated Biofilm Reactor (MABR) is a novel technology that uses gas-supplying membranes to achieve essentially 100 percent gas transfer efficiency. The high transfer efficiency, along with the ability to match air supply with loading, can provide tremendous savings in energy. Cassettes of membranes can retrofit existing CAS processes in a modular fashion, with minimal disruption, or be used in new or decentralized treatment systems. The hybrid MABR process (suspended and biofilm) can remove BOD and total nitrogen (TN). The reactor used bundles of hollow-fiber membranes, and the reactor was well-mixed to minimize bulk BOD and avoid fouling. This presentation discusses recent bench and pilot-scale research on the MABR process, along with energy benefits.

ENVR 102

Water reclamation and reuse

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Although Earth is composed largely of water, freshwater comprises only 3% of the total water available to us. Of that, only 0.06% can be accessed easily. An estimated 1.2 billion people drink unclean water today. It is desirable to explore multiple opportunities to reclaim and reuse water that is not within drinking water standards in order to facilitate the maximum use of all water resources. So, it behooves us to classify water resources properly to allow better selection of procedures for reclamation. The commonly used classification system will be reviewed, and its advantages and limitations will be discussed. The lecture will discuss various contaminants that can be found in water, and focus on arsenic contamination from natural sources. It will also cover economical reclamation methods for reuse of water.

ENVR 110

Natural and nature-inspired materials for environmentally-friendly, green organic electronics

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Organic electronics has an extraordinary prospective for the development of electronic products that are non-toxic and environmentally friendly (bio)-degradable. An ideal alternative is given by the fabrication of such devices either from naturally occurring or from nature-inspired materials that have been proved to be degradable and/or biocompatible. Many naturally pigments are usually small hydrogen-bonded molecules as opposed to larger p-conjugated, synthetic materials like pentacene or oligothiophenes. The strong electronic coupling afforded by H-bonding yielded optical properties controlled by intermolecular interactions. Hydrogen-bonded, natural semiconductor materials have been recently investigated by our group in organic field effect transistors, and afforded performances on par with state-of-the-art synthetic organic materials. Among the materials we have exploited are naturally-occurring indigo and tyrian purple as well as a large family of synthetically produced indigoids, anthraquinones and acridones. We have demonstrated OFETs, OLEDs and integrated circuits featuring natural substrates, dielectric and semiconducting layers operating at state of the art performance. Nature inspires us to choose among a wide range of diverse materials for creating new electronic functionalities, coming closer to a vision of a green and sustainable electronics world.

ENVR 111

Environmental applications of iron oxide nanomagnets

Anna Cristina S. Samia, *anna.samia@case.edu.Department of Chemistry, Case Western Reserve University, Cleveland, OH 44106, United States*

This talk will provide a general overview of the different approaches that have been adopted to improve the performance of nanostructured magnetic iron oxide particles for environmental applications. The performance of iron oxide nanomagnets is improved by tailoring the properties of the magnetic nanostructures through engineering of morphology, composition, and surface functionality. These nanomagnets are expected to find applications in the microbial and heavy metal decontamination of water. The talk will cover aspects of nanomaterials synthesis and characterization methods, and will detail the mechanisms involved in the water decontamination applications.

ENVR 112

Biodegradable and biocompatible functional nanomaterials

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Modern electronics are based on rigid plastics, metals, semiconductors, and harsh production techniques that place a heavy burden on the environment. Our group focuses on the development of environmentally benign functional materials and processing techniques for flexible electronics, energy transducers, and stimuli-responsive surfaces. In this talk, we will discuss the development of environmentally benign materials based on alginate and chitosan, and cellulosic materials such as cotton, and inorganic semiconductors. Although inorganic semiconductors are intrinsically rigid and brittle, when the size, orientation, and shape are confined to the nanoscale, they can be combined with flexible biomaterial supports to elicit high functionality that may even surpass the performance of their traditionally produced counterparts. An electrospinning technique combined with room temperature hydrothermal growth was used to generate high surface-area-to-volume ratio materials. These materials house more functional groups for the specific application with minimum alteration on the bulk properties of the substrate.

ENVR 113

Green synthetic routes toward shape-controlled nanoscale materials

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Controlling the shape of metal nanoparticles is important for both fundamental science as well as industrial applications. Developing methods for synthesizing shape-controlled nanoscale particles in aqueous solvents is paramount for large scale production. The chemical and physical properties of anisotropic metal nanoparticles are unique relative to their isotropic counterparts. However, the synthesis of well defined anisotropic nanoparticles remains challenging. We report a facile, room temperature synthetic procedure for nanocrystalline anisotropic ruthenium, platinum and palladium particles. Vigilant control of the reactant concentrations and reaction conditions provided uniform anisotropic nanoparticles in high yield. Characterization of the nanoparticles was carried out using high resolution transmission electron microscopy (HRTEM), x-ray diffraction (XRD), small angle electron diffraction (SAED) and energy dispersive spectroscopy (EDS). The particles displayed unusual optical and catalytic properties relative to their bulk counterparts.

ENVR 114

Organic synthesis via magnetic attraction: Benign and sustainable protocols using magnetic nanocatalysts

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In homogeneous catalysis, the chemo-, regio- and enantioselectivity of the catalyst is better but the difficulty of catalyst separation from the final product creates economic and environmental barriers. Heterogeneous systems enable better separation but at the cost of reduction in the availability of active sites. The relative advantages of both these systems can now be retained using magnetic nano-catalysts via simple modification of iron ferrites. Because of the reduced size, in nm range, most of the catalyst surface is now available for the reaction. The added advantage is that the catalyst can be separated easily by using an external magnet and reused many times without loss in its activity. These developments including the influence of ligands in these reactions will be highlighted.

ENVR 115

Synthesis and characterization of nanoscaled doped titanium dioxide with high nitrogen concentration for visible light catalysis

***Clemens Burda**, burda@case.edu.Department of Chemistry, Case Western Reserve University, Cleveland, OH 4106, United States*

Visible-light responsive nanoscaled nitrogen doped and co-doped titanium dioxide was synthesized using a sol-gel method. XPS spectra indicate that the nitrogen concentration is as high as 20%, even after sintering. The average size of the particles can be as small as 10 nm based on both the Scherrer calculation from the XRD results and measurements for particles in TEM images. There is no severe aggregation even for the particles calcined at higher temperatures although no protective surface ligand was used. Most particles show anatase XRD patterns with some amorphous phase. The photocatalytic performances were evaluated using photocatalytic decomposition of organic dyes. The latest progress on nanoscaled doped titania with high nitrogen content will be presented.

ENVR 116

Multi-electron transfer catalysts for conversion of biorenewables into commodity chemicals

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Well defined metallic and bimetallic nanomaterials have been developed to generate multiple electrons following photochemical irradiation. The development of new stabilizing ligands and reaction processes for nanoparticle stabilization has provided advantages toward obtaining well-defined nanoparticles with controlled morphology. Electrochemical, spectroscopic and x-ray techniques, as well as electron microscopy were used to characterize the nanoparticles. These nanoparticles have shown distinct reactivity in select hydrogenation reactions and have been effective in various chemical transformations, particularly, in the conversion of biorenewables to high value added chemicals. We demonstrate the efficiency of the metallic, bimetallic and metal oxide nanoparticles as effective catalysts for conversion of organic acids into commodity chemicals. The presentation will demonstrate that metallic, bimetallic and metal oxide nanoparticles offer the robustness for repeated use, and ability to withstand restructuring in aqueous environments.

ENVR 117

Facile hydrogenation of carbon-carbon double bonds using catalytic noble nanoparticles immobilized in microfluidic reactors

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Multiphase hydrogenation is critical in organic synthesis, but generally suffers from such challenges as mass transfer limitations, harsh reaction conditions and long reaction times. Noble metal colloidal nanoparticles (1-10 nm) have been shown to be efficient catalysts for hydrogenation due to their large surface-to-volume ratios, and can be used to eliminate or significantly reduce some of these challenges. Facile hydrogenation of carbon-carbon double bonds was achieved in a poly(dimethylsiloxane) (PDMS) microfluidic reactor with immobilized noble nanoparticles, using the conversion of 6-bromo-1-hexene to 6-bromo-1-hexane as a model reaction. The microreactor served as a platform to measure the intrinsic catalytic activity and turnover frequencies of palladium (Pd), platinum (Pt) and ruthenium (Ru) nanocatalysts. The turnover frequency (TOF, h^{-1}) of the nanocatalysts in the microfluidic reactor were hundreds of times larger than those measured in comparable experiments in Parr batch reactors.

ENVR 126

Abiotic transformations in the removal of estrogens during wastewater treatment: Effects of operating conditions

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Biological wastewater treatment of estrogens has been extensively studied in recent years. Lack of suitable analytical methodologies to identify the transformation products in complex environmental matrices led to the assumption that these compounds were mineralized and/or biotransformed to smaller molecules during wastewater treatment. This hypothesis led researchers to overlook the formation of other by-products resulting from chemical and/or catalytical redox reactions also occurring in the environment. Results will be presented from a comparison of two different wastewater treatment scenarios, conventional activated sludge and pre-denitrification conditions, in regard to estrogens removal. The difference in performance between the two treatments were found to be caused not only by the distinctive bacterial communities involved in the biodegradation, but also because of the minimization of the rate of the oxidative coupling of estrogens when the treatment involved anoxic stages

ENVR 127

Chemotaxis of pollutant-degrading bacteria to toluene droplets retained within the low permeable region in a heterogeneous porous microfluidic device

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Nonaqueous phase liquid (NAPL) contaminants are difficult to remove from groundwater due, in part, to the heterogeneous structure of soil. Chemotaxis toward the chemical pollutants, which bacteria degrade, provides a mechanism for bacteria to migrate to locations of high contamination, which may enhance the overall effectiveness of bioremediation. The chemotactic effect on bacterial abundance was studied within the low permeable NAPL-contaminated region in a microfluidic device with a structured pore network that mimics features of the natural contaminated groundwater system. Chemotactic bacteria migrated preferentially into the contaminated region, and accumulated near NAPL ganglia; the observations were also supported by computational simulations based on advection-dispersion type equations. Two key parameters in the mathematical model were the chemotactic sensitivity coefficient and the chemotactic receptor constant. Other microfluidic devices were designed to create well-controlled concentration gradients in order to obtain reliable values of these parameters. A ratchet structure is used to enhance the signal of bacterial concentration for optical detection.

ENVR 128

Bioregeneration of spent anion exchange resin produced in treatment of nitrate

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Anion exchange resin filtration is a commonly used technique for removal of nitrate in contaminated water. Although it is a rapid and simple technique compared dentrification process, nitrate is needed to release into brine solution to wait further treatment. A novel bioregeneration process has been developed for treatment of the spent resin through reduction of nitrate on the spent resin to nitrogen gas by denitrifying bacteria. This bioregeneration does not use brine solution. The effect of biomass to spent resin ratio, salinity and pH in the bioregeneration process was evaluated and optimized in this study. Bench-scale experimental results indicated that the spent resin produced in the filtration treatment of wastewater can be regenerated within several hours for reuse by contacting it with dentrifying bacteria. The dentrification is the rate limiting step in the bioregeneration process since release of nitrate from the spent resin is a rapid step.

ENVR 129

Anaerobic bioreactor system for treatment of groundwater contaminated with chlorinated volatile organic compounds

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An anaerobic, fixed film bioreactor system, inoculated with the WBC-2 dechlorinating consortium, is being evaluated at a bench scale (3 liters) and pilot scale (11,500 liters) for treatment of groundwater extracted from sites contaminated with mixtures of chlorinated volatile organic compounds (VOCs), including chlorinated ethanes and ethenes at two sites and chlorinated benzenes at another. Complete dechlorination of chlorinated ethanes and ethenes (inflow concentrations from 0.25 to 5.0 milligrams per liter) to concentrations below the permit requirements (0.1 milligrams per liter total VOCs) has been achieved with 15 to 20 hour retention times in the flow through system. Degradation rates and pathways have been quantified for individual chlorinated ethanes and ethenes with lactate, corn syrup, and hydrogen as electron donors. Initial testing with chlorinated benzenes is promising. Cost and carbon footprint analyses suggest that using a bioremediation system offers improved sustainability compared to a conventional treatment plant.

ENVR 130

Biological removal of chloroform by using biotrickling filter (BTF)

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Currently, the need for regulations to control and to limit the health risks from disinfection byproducts(DBPs) is becoming necessary and the concerns are elevated from possible cancer risks to other chronic health effects. Chloroform is a DBPs formed from chlorine disinfection process, a Trihalomethanes (THMs) group which have maximum allowable contaminant level of 0.08 ppm. It is the eleventh ranked hazardous and also the third highest among chlorinated organic substances. Removing chloroform by physical and chemical methods is expensive and may generate a secondary pollutant. But using Trickling bed biofilter as a biotechnological method can achieve a better removal. The dechlorination process is designed to achieve desirable elimination rate and sustained removal of chloroform. The primary objective of this project is to use an innovative technique for controlling the biological destruction of disinfection by-products, by operating the system anaerobically.

ENVR 131

Treatment of mixtures of hydrophobic and hydrophilic volatile organic compounds in trickling bed air biofilters

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A mixture of n-hexane, benzene, and methanol was investigated. Two Trickle-Bed-Air-Biofilters (TBABs) “A” and “B” were run under acidic conditions and received the following mixing ratios per volume of n-hexane:benzene:methanol 20:40:40% and 16.5:33:50.5%, respectively.

The experimental results have shown that for inlet n-hexane, benzene, and methanol loading rates of 8, 21, and 19 g $m^{-3}h^{-1}$ in TBAB “A” and 8, 21, and 29 g $m^{-3}h^{-1}$ in TBAB “B”, the overall VOCs removal efficiencies were 96 and 94% in TBABs “A” and “B”, respectively. Benzene and methanol removal efficiencies were more than 98% while for n-hexane degradation, the removal efficiency was dependent on the VOCs mixing ratio. 83% and 66% in removal efficiencies for n-hexane were obtained in TBABs “A” and “B”, respectively. The results achieved by TBAB “A” are higher than our previously published data for treating n-hexane in mixture with benzene. This implies that optimizing the mixing of multiple VOCs in TBAB could be a promising means for eliminating hydrophobic odors

ENVR 132

Remediation of metal-contaminated drinking water using electrospun alginate nanofibers

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We have electrospun nanofibers of the biopolymer alginate and have investigated their capacity to sequester toxic metals from water. Nanofibers are ideal for filtration applications because of their high surface-area-to-volume ratios.

Alginate interacts with a number of metals through a variety of mechanisms, including electrostatic and ionic interactions and coordination. The noted capacity of alginate to bind metals makes it a compelling candidate material for biological purification of metal-contaminated drinking water.

Nanofibers, with typical diameters of 500–600 nm, were electrospun and imaged using scanning electron microscopy. The nanofibers were initially crosslinked with Ca^{2+} and subsequently covalently crosslinked with epichlorohydrin, rendering them insoluble and suitable for repeated filtration applications.

Using colorimetric analysis, we have determined the nanofibers sequester significant amounts of Pb(II) ions from aqueous solutions. In ongoing studies, we are examining the binding of alginate nanofibers with additional heavy metal species of concern.

ENVR 133

Sustainable approach for simultaneous wastewater treatment and bio-energy production in mediator-less microbial fuel cell

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Among the new sources of clean energy, microbial fuel cells (MFCs) have gained lots of attractions in recent years. MFC is a device that directly converts the metabolic power of microorganisms into electricity using electrochemical technology. It is a promising green method to treat organic effluents and simultaneously produce electricity. In this study, electricity generation integrated with organic substrate biodegradation was investigated in a continuous two-chamber membrane-less and mediator-less microbial fuel cell. The performance of MFC was evaluated to treat domestic wastewater using alternatively actual aerobic sludge and anaerobic sludge. The average initial concentrations of COD and BOD in the actual wastewater were 350 and 200 mg/L, respectively. Results revealed that COD and BOD removal efficiencies were up to 80% and 72%, respectively using the anaerobic sludge. The effect of the inoculums type was evaluated under variable external resistance. Maximum power density of $21mV/m^2$ was observed with the anaerobic sludge.

ENVR 134

Feasibility of laccases for the removal of pharmaceutical compounds

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Pharmaceuticals are regarded as emerging environmental pollutants and their degradation implies an important challenge since conventional treatment plants can only attain partial elimination. Laccases have been reported to be a potential catalyst for the biodegradation of estrogens (such as estrone, 17β-estradiol and 17α-ethinylestradiol) by several investigations [1-2]. However, scarce references regarding the enzymatic removal of other type of pharmaceuticals are available. In the current work, we demonstrated the feasibility of two different laccases with different redox potential: from *Myceliophthora thermophila* (0.45 V) and *Trametes versicolor* (0.80 V), for the degradation of estrogens and anti-inflammatories (naproxen and diclofenac) with removal yields between 40 and 95%. Both enzymes were characterized to compare their pH and temperature optima, stabilities and kinetic parameters.

ENVR 135

Oxidation of bisphenol A and triclosan by laccase from *Trametes versicolor* and *Myceliophtora thermophila*

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Two types of laccase from *Trametes versicolor* and from *Myceliophtora thermophila* were used for the enzymatic oxidation of endocrine disrupting compounds: bisphenol A (BPA) and triclosan (TCS). BPA was almost completely removed after 30 min at pH 4 by *Trametes versicolor* laccase and HBT as a mediator and after 8 h at pH 7 in the absence of mediator with barely loss of enzymatic activity. TCS resulted more recalcitrant than BPA, and the use of laccase from *Myceliophtora thermophila* required the addition of the mediator. Nevertheless, laccase from *Trametes versicolor* at pH 4 achieved the removal of 95% of TCS after 24 h.

ENVR 161

Investigations into water quality indicators along southern Lake Michigan beaches

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The Laurentian Great Lakes are vastly important bodies of freshwater, which supply drinking water for over 40 million people. The ecosystems and the chemistry of the lakes have changed over the years due to natural and anthropogenic factors. This is especially prominent along the southern Lake Michigan basin, which is heavily industrialized and highly populated. During the warm weather months, beach health monitoring is of utmost importance along the southern beaches of Lake Michigan, and *E. coli* tests are performed regularly. Due to the drawbacks associated with these bacterial analyses, correlations between bacterial contamination and chemical markers continue to be investigated. During the 2011 summer, beach and tributary water samples were collected weekly. Filtered lake water was analyzed to determine anion concentrations and microbial levels. Larger water samples were filtered to collect phytoplankton, which were frozen and extracted to determine pigment content. Results of the data analyses will be presented.

ENVR 162

Determining indicator compounds representative of pharmaceuticals and personal health care products (PPHCPs) in water cycle

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The presence of pharmaceuticals and personal health care products (PPHCPs) in the aquatic environment has become a recent worldwide issue. The very large number of PPHCPs reported in the literature makes it difficult to interpret the potential environmental impacts and feasibility of their removal through treatment processes. Indicator compounds representative of PPHCPs detected in systems worldwide were determined based on five criteria, including usage, occurrence, resistance to treatment, persistence, and physicochemical properties that shed light on the potential degradability of a class of compounds. Additional constraints included feasibility of procuring and analyzing compounds. A list of fifteen indicator compounds belonging to 11 groups (antibiotics, analgesics, β-blockers, blood lipid regulators, antiepileptics, steroids, stimulant, fire retardants, metabolite, pesticides, and contrast agent) was obtained. These eleven groups of compounds presented the greatest resistance to treatment processes, were highly persistent in surface water, and were detected with significant frequency.

ENVR 163

Pilot plant study on indicator compounds representative of pharmaceuticals and personal health care products (PPHCPs) in the water cycle

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The presence of pharmaceuticals and personal health care products (PPHCPs) which include endocrine disrupting compounds (EDCs) in the aquatic environment is increasingly becoming a concern. Fifteen indicator compounds representing groups of PPHCPs were studied at United Water's Haworth pilot plant. Treatment processes studied including virgin granular activated carbon (GAC), pre- and intermediate ozonation with and without hydrogen peroxide (H_2O_2), ultraviolet/hydrogen peroxide (UV/H_2O_2), dissolved air flotation, chlorination, and dual-media filtration. Results revealed that the most effective processes involved UV/H_2O_2 with a dosage of 700 mJ/cm^2-15 mg/L and 500 mJ/cm^2-20 mg/L, virgin GAC, pre-ozonation with a dosage of 2 mg/L, and intermediate ozonation with H_2O_2 (2.5 mg/L-0.5 mg/L). Tri(2-chloroethyl) phosphate (TCEP) and cotinine were observed to be the most recalcitrant indicator compounds throughout this study. Furthermore, removal efficiency through ozone processes and GAC were found to be correlated to ozone rate constant (k_{O3}) and organic-carbon/water partition coefficient (K_{oc}), respectively.

ENVR 164

Degradation of iodinated carboxylic acid compounds in water

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The removal of toxic chemical contaminants from waters is an on-going struggle for water utilities. In particular, haloacetic acids are of serious concern due to their solubility, adverse health and ecological effects, and widespread use in industry. While some chlorinated and brominated haloactic acids are regulated, far less work has been performed on the iodoacetic acids. In this work, we have investigated the hydroxyl radical reactivity of a library of commercial and synthesized acetic, propanoic, butanoic and pentanoic iodoacids in support of potential advanced oxidation process water treatments. Reaction rate constants and degradation efficiencies have been determined utilizing a combination of electron pulse radiolysis and ion chromatography.

ENVR 165

Reactivity of the hydroxyl radical with International Humic Substances Society natural organic matter isolates

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The reactivity of Organic Matter (OM) with the hydroxyl radical ($HO^{\bullet}$) is important in both natural and engineered systems. In natural systems, $HO^{\bullet}$ is produced by the sunlight irradiation of OM, while in engineered systems OM acts as a scavenger of $HO^{\bullet}$ in Advanced Oxidation Processes (AOPs). Though much research has been done on the reaction between OM and $HO^{\bullet}$, there is still a lack of understanding as to which physiochemical properties of OM influence this reaction. In this work, we have measured the bimolecular reaction rate constants between OM and $HO^{\bullet}$ ($k_{OM\text{-}HO\bullet}$) for a suite of International Humic Substance Society purchased Natural Organic Matter isolates. These parameters are compared to the available ^{13}C NMR and measured average molecular weight data for these samples.

ENVR 166

Evaluation of the hydroxyl radical based degradation efficiency for antibiotics in water

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Efforts to minimize antibiotic levels in waste water effluents are essential to prevent the evolution of antibiotic-resistant bacteria. As standard water treatment methods do not quantitatively remove these contaminants Advanced Oxidation/Reduction Process (AO/RP) water treatment has been suggested as an appropriate final step. However, while the major AO/RP radical reactivity with antibiotics has been recently determined, the activity of the degradation products has not been extensively characterized. In this work we have established the efficiency of hydroxyl radical-based oxidation required to achieve complete removal of antibiotic activity in water. Different β-lactam and sulfonamide antibiotics were subjected to different levels of oxidation via steady state ^{60}Co irradiation, and product activity was investigated using *Escherichia coli* as a model system. EC_{50} values for these solutions were measured and correlated with the different antibiotics.

ENVR 167

Removal of antibiotics from water using the advanced oxidation/reduction process with sulfate radicals

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The deactivation of antibiotic activity in treated wastewaters is crucial because of the proliferation of antibiotic resistant bacteria. A potential method of removal is the advanced oxidation/reduction process (AO/RP) using oxidative radicals. While the reactions of the hydroxyl radicals have been established, another potential oxidant is the sulfate radical ($SO_4^{-\bullet}$). In this study, reaction rate constants and mechanisms for sulfate radical with two different classes of antibiotics were examined: tetracycline and sulfonamides. The average rate constant for the tetracycline class with $SO_4^{-\bullet}$ was determined to be (1.11 ± 0.88) x 10^9 $M^{-1}s^{-1}$. The average rate constant for the sulfonamide class with $SO_4^{-\bullet}$ was determined to be (3.98 ± 0.49) x 10^9 $M^{-1}s^{-1}$. A consistent reaction mechanism for each antibiotic class was inferred from the similarity of the measured rate constants.

ENVR 168

Emerging contaminants in water containing nitrogen-nitrogen single bonds: An examination of their degradation chemistry, reactivity, and products

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Over the past half century a number of compounds containing nitrogen-nitrogen single bonds have emerged as contaminants in water. Many of these compounds represent significant health hazards and are of serious concern. We have examined, in detail, the impact of advanced oxidation processes (AOP's) on these compounds and will present an in-depth perspective on their chemistry and interplay of these species in water during their degradation.

ENVR 169

Investigation of the dark reaction between hydrogen peroxide and chloramines

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The ultimate disinfection of water often utilizes chloramine rather than chlorine due to chloramine's longer residence time and less harmful byproduct formation. At relevant pH levels, it is likely that both monochloramine ($NH\text{-}_2Cl$) and dichloramine ($NHCl_2$) exist. However, for some recalcitrant chemical contaminant removal from waters, advanced oxidation process (AOP) treatments may also be required. At large-scale, many AOP treatments involve addition of hydrogen peroxide, and residual H_2O_2 may therefore react with added chloramine. There is currently no data on the kinetics or ultimate products of these reactions. In this work, the temperature-dependent rate constants for monochloramine and dichloramine's reaction with hydrogen peroxide were measured. Chloride is shown to be a quantitative product for the reaction of NH_2Cl. These results indicate that the reactions between peroxide and chloramines can possibly affect chloramine's residence time in the water distribution system, which could affect their disinfection ability.

ENVR 188

Nanomaterial contamination of agricultural crop species

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Zucchini was exposed hydroponically to bulk, ion, and nanoparticle Ag, Cu, Si, Au, fullerenes, and single/multi-walled nanotubes (S/MWCNT); biomass, transpiration, and NM accumulation were determined. Nanoparticle Ag, Si, and MWCNTs reduced biomass and transpiration by 30-91% compared to bulk materials; element accumulation was inversely related to particle size. Fullerenes, Au, and SWCNTs had no impact on growth. An evaluation of the toxicity of 12 nanoparticles to 12 agricultural crops under hydroponic and soil conditions is underway. Results show particle size-specific phytotoxicity, as well as concentration-dependent and species-specific response to NM exposure. Separately, the effect of fullerenes on *p,p'*-DDE accumulation by zucchini, tomato, pumpkin, and soybean was determined. Fullerenes promoted *p,p'*-DDE accumulation, suggesting enhanced uptake through a nanomaterial-pollutant complex. Our data demonstrates differential toxicity and accumulation of nanomaterials relative to bulk particles and ions. The implications of these findings for determining nanomaterial fate and transport in agricultural systems will be discussed.

ENVR 189

Synchrotron imaging of the uptake and speciation of ZnO and CeO_2 in soil cultivated soybean (Glycine max)

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The impact of metal nanoparticles (NPs) in biological systems is still not well understood. Little is known about the response of plants, the first trophic level, to NP exposure; consequently, their possible role on the fate and transport of NPs in ecosystems is unknown. In this study, soybean plants (*Glycine max*) were grown for 48 days in organic farm soil spiked with either ZnO or CeO_2 NPs. Micro X-Ray fluorescence (µXRF) maps were performed for different sections of the plant and X-Ray absorption near edge structure (XANES) spectroscopic analysis was performed on selected µXRF spots. Linear combination analysis showed no contribution from ZnO NPs in any of the plant XANES spectra suggesting different ligands for the Zn. XANES analysis revealed that the Ce in the plant remained as CeO_2 however little was translocated to the aerial part of the plant

ENVR 190

Phytotoxicity and biotransformation of Yb_2O_3 nanoparticles in cucumber plants

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With the increasing utilization of nanomaterials, there is a growing concern for the potential environmental and health effects of them. To assess the environmental risks of nanoparticles, better knowledge about their fate and toxicity in plants are required. In this work, we compared the phytotoxicity of nanoparticulate Yb_2O_3, bulk Yb_2O_3, and $YbCl_3 \cdot 6H_2O$ to cucumber plants. The distribution and biotransformation of the three materials in plant roots were investigated *in situ* by TEM, EDS, as well as synchrotron radiation based methods: STXM and NEXAFS. The decrease of biomass was evident at the lowest concentration (0.32 mg/L) when exposed to nano-Yb_2O_3. While at the highest concentration, the most severe inhibition was from the $YbCl_3$. The inhibition was dependent on the actual amount of toxic Yb uptake by the cucumber plants. In the intercellular regions of roots, Yb_2O_3 particles and $YbCl_3$ were all transformed to $YbPO_4$. However, only under the nano-Yb_2O_3 treatment, $YbPO_4$ deposits were found in the cytoplasm of root cells. We speculated that the dissolution of Yb_2O_3 particles induced by the organic acids exuded from roots played an important role in the phytotoxicity. While for nano-Yb_2O_3, the phytotoxicity might also be attributed to the Yb internalized into the cells.

ENVR 191

Impact of cerium oxide nanoparticles on Kidney beans (*Phaseolus vulgaris*)

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The uptake of nanoparticles (NPs) and their pertinent effects on terrestrial plants is not very clear till date. Among the edible plants, the red kidney beans (*Phaseolus vulgaris*) are of great ecological significance as they are consumed by a huge population as a source of protein. In this presentation we will discuss about the uptake of cerium oxide NPs (CeO_2 NPs) by bean plants and their impact on the physiological as well as biochemical parameters of the bean plants. Data on the stress imposed by the CeO_2 NPs on the antioxidant system and on the storage protein content of the bean plants will be presented. Microscopic studies will help us to localize the CeO_2 NPs within bean plant tissues on uptake and their fate thereafter.

ENVR 192

Comparative toxicity assessment of CeO_2 and ZnO nanoparticles towards nitrogen fixing gram negative species *Sinorhizobium meliloti*

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The use of engineered nanoparticles (ENPs) has risen due to the wide range of applications in the field of electronics, medicine, chemistry and biology. However, the impact of ENPs on biological systems is still not well understood. The aim of this research was to determine the effects of zinc oxide (ZnO) and cerium oxide (CeO_2) NPs towards the gram-negative nitrogen fixing bacterium *Sinorhizobium meliloti* (Rm 1021). Bactericidal effects of both the NPs were determined by Minimum Inhibitory Concentration (MIC), Disk Diffusion tests (diameter of inhibition zone i;e DIZ) and by dynamic growth measurements with Uv-Vis spectroscopy. Furthermore, Scanning transmission electron microscope (STEM) images helped to reveal the location of NPs on bacterial surface and suggested some structural changes along with the surface attachments. We reported the accumulation of CeO_2 and ZnO NPs into the periplasmic space of the bacteria. This was further investigated by the structural modification of extracted extracellular polysacharhides (EPS) present in bacterial cell envelope. The FT-IR spectra showed changes in protein and polysaccharide structure of bacterial cell surface upon application of NPs. We also reported the effect of CeO_2 NPs on *S. meliloti* is bacteriostatic whereas ZnO NPs act as bactericidal.

ENVR 193

TiO_2 NPs can be taken up by roots and translocated to leaves in cucumber (*Cucumis sativus*) plants

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Nanoparticles (NPs) are profusely used in consumer products, but little is known about their impact on food crops. In this research, the possible toxicity of TiO_2 NPs was studied in cucumber (*Cucumis sativus*) plants. Hydroponically grown cucumber seedlings were treated for 15 days with different concentrations of TiO_2 NPs. Seedlings growth and histological changes were determined. Micro x-ray fluorescence (µXRF) and micro x-ray absorption spectroscopy (µXAS), respectively, were used to track the presence and chemical speciation of Ti within tissues. Results showed that at 4000 mg TiO_2 NPs/L there was an increment in root and shoot elongation (average >300%) compared to control. Histological analyses showed that plant cells treated with TiO_2 at 4000 mg/L were three fold larger compared to control cells. µXRF analysis showed Ti in the vasculature of cucumber roots and leaves. µXANES spectra demonstrated that Ti was present as TiO_2 within the cucumber tissues.

ENVR 194

Uptake of fullerene (C60) induced catalase (CAT) activity in *Lumbriculus variegatus*

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With the rapid development of nanotechnology, nanomaterials have been mass produced and widely applied in recent decades. Fullerene (C60) with its unique physical properties in nano-size has been used in many products. The increased likelihood of direct fullerene release into the environment has raised interests in understanding its environmental fate and corresponding biological effects to living organisms. Few studies have emphasized fullerene uptake by benthic organisms and determination of resultant biochemical responses. In this study, the uptake of C60 and effects in *Lumbriculus variegatus* were tested over a 28-d time interval. The uptake of C60 in micro-sized agglomerates (µ-C60) was 192 ± 20 µg/kg dry weight sediment, while uptake for larger, bulk-sized, C60 was 23 ± 40 µg/kg dry weight. The size of C60 in sediment affects the C60 accumulation in *L. variegatus*. The corresponding catalase (CAT) activity has a significant increase on day 14 for *L. variegatus* exposed to µ-C60 ($p=0.034$) with the highest C60 body residue of 199 ± 80 µg/kg dry weight. No significant CAT activity changes were found by pyrene exposure with a 600 folds higher body residues compare to C60. This suggests that *L. variegatus* is more susceptible to C60 than pyrene at a relative low concentration. Relationship between C60 body residue and the increased CAT% was proposed in a power regression.

ENVR 195

Nanomaterials in food packaging and water: Addressing safety concerns

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Nanoparticle (NP) enhanced polymers have the potential to revolutionize food packaging and potable water pipe performance, though release of NPs from these materials has gone relatively unstudied. An extensive review of the food science, polymer science, environmental engineering, and medicine device literature was conducted to identify potential NP release pathways from nanocomposite materials into food and water. Results show little is known, and this lack of knowledge prevents responsible commercialization of safe and innovative nano-enhanced products, development of predictive health–risk models, and generation of science–based environmental, health, and safety focused regulation. Common limitations of past studies are that quantitative results were not described, NP detection methods were lacking, and metal ions were not differentiated from NPs. Science has not quantitatively determined if and under what conditions nanocomposites release NPs into food and water matrices. Future research needs are also identified.

ENVR 215

Nanosilver markets and global regulatory concerns

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Nanosilver metal has been an article of commerce for over fifty years. In the last ten, many new uses have been developed especially for medical and electronics use. Products containing nano silver metal are used as sprays and coatings to provide electrical and thermal conductivity. The highly efficient biocidal properties of all forms of silver against microorganisms have also been taken advantage of for medical, and for food packaging and processing uses. The proliferation of such uses has aroused concern among regulatory authorities in both North America and Europe about nanosilver particles in the environment. The silver industry trade organizations over the last three years have worked with the US Environmental Protection Agency to alleviate such concerns and to change policies regarding registration of products coming within regulatory agency jurisdiction. Similar efforts are now under way with European regulatory authorities for a similar purpose. It has also been recognized that if restrictive policies regarding silver were not challenged, these would also be applied to the other elements of the Periodic Table and their compounds. The presentation will focus on the issues involved and the roles of industrial, regulatory, and academic research institutions.

ENVR 216

Emerging trends in nanoparticle fate and transport

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Over the past three years the UC Center for Environmental Implications of Nanotechnology (UC CEIN) has been studying the toxicity and fate and transport of several important commercial nanoparticles, including metal and metal oxides, and carbon nanotubes. There are some

emerging patterns with regards to nanoparticle stability in natural media, rates of sedimentation, efficiency of attachment of the nanoparticles to sand and clays, dissolution patterns and photoactivity. Of critical importance is an understanding of the composition of the aqueous matrix in which the nanoparticles are suspended, particularly with regards to the concentration of organic materials, ionic strength, and the nature of the cations present. The nanoparticles are likely to remain suspended if there are more than a few mg/L of organic material, particularly at low ionic strength. Hard water *(i.e.,* with high [Ca2+] and/or other divalent cations) can quickly change the balance of the interactions among nanoparticles and between nanoparticles and the porous medium in which they are being transported. Coatings and organic capping agents on the surface of the nanoparticle can significantly increase the mobility of the nanoparticles in the environment. Understanding of the role of these various water constituents can be used to design either more effective injection of nanomaterials (*e.g*., nano-zerovalent iron) into the subsurface, or arrest their transport if they are unexpectedly mobile in groundwater.

ENVR 217

Environmental releases of engineered nanomaterial resulting from biosolids disposal to land and air

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The aim of this study is to assess the occurrence of engineered nanomaterials (ENMs) in land applied and incinerated biosolids and provide better understand their life cycle and environmental implications. High Resolution Scanning Transmission Electron Microscope (HR-STEM) equipped with energy dispersive X-ray microanalysis (EDS) and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) were used to identify and assess the occurrence and accumulation of titanium, zinc and silver based engineered nanomaterials at a biosolids application site near Austin, Texas.. The results confirmed presence of titanium based ENMs at depths reaching 1 m below the surface and with concentrations ranging between 2 and 5 mgTi/g dry soil. Although discrete silver and zinc ENMs could not be observed, the depth-concentration profiles of these elements suggested accumulation in the top 30 cm of soil. The transformation of the ENMs were characterized during lab-scale incineration of the full-scale biosolids and lab-scale produced biosolids embedded with commercial products containing ENMs, and interpretation is ongoing of the completed test results.

ENVR 218

Multimedia environmental distribution of nanomaterials

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Estimation of the exposure levels of engineered nanomaterials (eNMs) that may be released to the environment is crucial to assessing the potential environmental impact of eNMs. Accordingly, a generalized model was developed to evaluate the multimedia environmental distribution of nanomaterials. The modeling approach considers the multimedia environment as a collection of environmental compartments (e.g., air, water, sediment, soil, vegetation, biota), linked via fundamental intermedia transport processes (e.g., atmospheric dry and wet scavenging, soil wind resuspension, sedimentation and resuspension in water bodies). In order to enable rapid "what-if?" scenario analyses for the rapidly growing nanotechnology community, the model was developed via as cloud-computing application with a web-based graphical user interface (GUI). The user defines the modeling scenario by specifying relevant properties of the eNM, geography, meteorology, and source emission. The model then calculates the dynamic change of eNM concentrations in the various environmental compartments as well as their mass distribution within the ambient particulate phase (in air and water), and displays the result within the GUI in real-time. It is envisioned that the present multimedia analysis tool will assist regulators, industrial, and academic users in rapidly assessing the potential environmental implications of eNMs releases to the environment. Estimation of the exposure levels of engineered nanomaterials (eNMs) that may be released to the environment is crucial to assessing the potential environmental impact of eNMs. Accordingly, a generalized model was developed to evaluate the multimedia environmental distribution of nanomaterials. The modeling approach considers the multimedia environment as a collection of environmental compartments (e.g., air, water, sediment, soil, vegetation, biota), linked via fundamental intermedia transport processes (e.g., atmospheric dry and wet scavenging, soil wind resuspension, sedimentation and resuspension in water bodies). In order to enable rapid "what-if?" scenario analyses for the rapidly growing nanotechnology community, the model was developed via as cloud-computing application with a web-based graphical user interface (GUI). The user defines the modeling scenario by specifying relevant properties of the eNM, geography, meteorology, and source emission. The model then calculates the dynamic change of eNM concentrations in the various environmental compartments as well as their mass distribution within the ambient particulate phase (in air and water), and displays the result within the GUI in real-time. It is envisioned that the present multimedia analysis tool will assist regulators, industrial, and academic users in rapidly assessing the potential environmental implications of eNMs releases to the environment.

ENVR 219

Fate and occurrence of fullerenes in airborne particulate, combustion particles, contaminated soils and wastewater samples

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Fullerenes are carbon-based nanomaterials present in the environment due to several natural events and due to the human activity, including combustion processes, car-brakes, etc. During the recent years a new source of fullerenes to the environment can be expected through the increasing development of nanotechnology. Thus, a general consensus exists in considering fullerenes as a new family of emerging pollutants [1]. Nevertheless, analytical methods for these compounds are somehow scarce [2-4], and their extraction from some environmental samples is especially difficult. Traditional extraction techniques have been applied for this purpose with limited success and laser-desorption ionization sources have been extensively applied for their mass spectrometric analysis despite little quantitative information can be achieved and they entail risk of fullerene self-generation. There is a need of developing reliable, robust, accurate quantitative methods which allow assessment of the occurrence of fullerenes in environmental matrices, especially in soils and sediments. Different analytical procedures based on liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) will be presented for the analysis of eight fullerenes: C_{60}, C_{70}, C_{76}, C_{78} and C_{84} fullerene, C_{60} pyrrolidine tris-acid ethyl ester, [6,6]-Phenyl-C_{61} butyric acid butyl ester and [6,6]-Thienyl C_{61}butyric acid methyl ester in environmental samples, including: airborne particulate, soils, sediments, combustion particles and wastewaters. The fate of fullerenes in 22 wastewater samples from Catalonia (Spain) and combustion particles from Brazil will be reported. In addition, the results of 28 samples of airborne particulate collected from the Mediterranean Sea atmosphere [3], and 12 soils from urban and industrial districts of four different Saudi Arabia locations (Riyadh, Al-Diriyah, Yanbu' Al Bahr and Jubail) will be presented and discussed. Higher fullerene concentrations are generally associated with higher levels of Polycyclic Aromatic Hydrocarbons and legacy Persistent Organic Pollutants, such as PCBs. Fullerene sources are associated with the emission from urban and industrialized areas being a possible risk to the environment.

ENVR 220

Effect of short-chain organic acids on the removal of pentachlorophenol with zerovalent iron in soil

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Pentachlorophenol (PCP) has been widely used as a pesticide and led to serious soil contamination. In this study, the effects of three short-chain organic acids (SCOAs) on adsorption of PCP in soil and the removal of PCP by zerovalent iron in the presence of SCOAs were investigated. In alkaline conditions, SCOAs inhibited the adsorption in the order: sodium citrate > sodium tartrate > sodium lactate because of providing more carboxylates. The sorption amount of PCP decreased in the presence of 1 mM to 100 mM of sodium citrate but increased as the concentration grows to 1000 mM. Furthermore, PCP could not be removed at pH 8.0, but SCOAs could promote the removal and sodium citrate enhanced largest among the selected acids. With their strong complexion, carboxylates could inhibit iron oxide or hydroxides on the surface of iron or refresh iron surface. These findings can facilitate the remediation of organic pollutants.

ENVR 221

Clay particles destabilize engineered nanoparticles in aqueous environments

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Given the ubiquity of natural clay minerals, the most likely interaction of nanoparticlesreleased into an aquatic environment will be with suspended minerals. Thus, thetransport of engineered nanoparticles in the subsurface and the water column willmost likely be altered by their interaction with these clay minerals. We studied theinteractions of two of the most produced nanoparticles, Ag and TiO2, and one of themost studied clay minerals, montmorillonite, to determine how heteroaggregationcan alter the stability of nanoparticle/clay mineral mixtures. Since at low pHmontmorillonite has a negatively charged basal plane and positively charged edges, itsinteractions with these nanoparticles at different pH lead to unusual behavior. There aresix different interactions for each clay-nanoparticle pair. At pH values below the pHPZCof montmorillonite edge site, montmorillonite reduced the stability of both negativelycharged Ag and positively charged TiO2 nanoparticles. Surprisingly this enhancedcoagulation only occurs within an intermediate ionic strength range. The spillover ofthe montmorillonite basal plane electric double layer to the montmorillonite edge mayscreen the electrostatic attraction between Ag and the montmorillonite edge at low ionicstrength, and a repulsion between TiO2 and montmorillonite face sites may restabilizethe mixture at low ionic strength. At pH 8, the presence of humic acid has no significanteffect on stabilizing TiO2/montmorillonite mixture; at pH 4, humic acid presenceleads to enhanced stability in TiO2/montmorillonite mixture due to the elimination ofelectrostatic attraction between TiO2 and montmorillonite basal plane.

ENVR 222

Stability of the coating in TiO_2-based sunscreens: Potential implications

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In sunscreen lotion (SSL) formulations, titanium dioxide ($nTiO_2$) nanoparticles are generally coated with an $Al(OH)_3$ layer to shield against the harmful effects of hydroxyl radicals ($^{\bullet}OH$), superoxide anion radicals ($O_2^{\bullet-}$), and other reactive oxygen species (ROS) (e.g. H_2O_2) generated when TiO_2 nanoparticles are exposed to UV radiation. Therefore, it is crucial to ensure their structural stability in the environment where the protective layer may be compromised and adverse health and environmental effects can occur. Results indicate that the presence of chlorine (swimming pool water) and ions in the simulated sea water increase zeta potential rendering rather unstable TiO_2 nanoparticles. Redistribution of a protective coating can be experimentally and statistically assessed using advanced analytic techniques such as scanning electron microscopy (SEM), high resolution transmission electron microscopy (HR-TEM) X-ray photoelectron spectroscopy (XPS), etc. Therefore, the outcome strongly suggests that water chemistry influences the characteristics of $Al(OH)_3$- coated TiO_2 in sunscreen environment.

ENVR 223

Influence of light on the formation of silver nanoparticles in aquatic environment

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There has been growing interest in silver nanoparticles (AgNPs) due to their antibacterial and antiviral properties. Increase in AgNPs in aquatic environment may cause risk to microbial communities and to ecosystems. In our research on AgNPs, the direct formation of AgNPs by the reduction of Ag^+ ion by humic acids (HAs) and fulvic acids (FAs) under different environmental conditions pH (6.0 - 9.0) and temperature (22 - 90 ^oC) was shown. Types of HAs and FAs (aquatic versus sedimentary) greatly influence the AgNPs formation. The present work focuses on the effect of light on AgNPs formation. The results of studies conducted on the formation of AgNPs under UV-light irradiation using HA and FA as reducing agents will be presented. Formation of AgNPs under natural daylight has also been conducted. Environmental implication of the results on the formation of AgNPs in the natural environment will be discussed.

ENVR 224

Impact of dry-wet cycles on the release of PAHs from wetland sediments in South Texas

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Wet-dry cycles are frequently occurring in wetland sediments in South Texas, and these cycles impact geochemistry of wetland sediments significantly. But how drying process affected the distribution of organic contaminants between water and sediment is less known. In this study, we showed that when dried sediments from south Texas wetlands were rewetted, certain polycyclic aromatic hydrocarbons (PAHs) including naphthalene, phenanthrene, fluoranthene and pyrene were preferentially released into solution (total amount from 10.85ng/L to 32.56ng/L) compared with wet sediments that have not been dried. The release of PAHs was mostly from the dominant finer fractions (<63µm), but when normalized to mass, PAHs were readily released from the 125-300 µm fraction. Source analysis showed that 125-300 µm fraction contained PAHs from incomplete combustion of petroleum-related products, which may lead to the readily release of PAHs to solution after a dry-wet cycle. Overall, this study provides valuable information how the water quality may change upon drought-flood cycles that often seen in South Texas.

ENVR 225

Examination of the diverse environmental impacts of long-term acid mine drainage on a Virginia stream ecosystem

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Although the local pyrite mines closed in the 1920s, acid mine drainage (AMD) continues to effect the water quality of Contrary Creek, in Louisa County, Virginia. This study looks at the extent of the chemical and toxicological impacts throughout the ecosystem by using interdisciplinary applications of chemistry. Correlation of chemical, environmental, and biological data can demonstrate the scope of adverse AMD effects. Soil samples along the creek and its tributaries were collected 5 m from the banks, with corresponding water and sediment samples. These samples were analyzed for pH, organic content, and metal concentrations. Each site was further surveyed for macroinvertebrate and plant species. These specimens were also collected, categorized, and digested for metal analysis. Chemical analysis on the streamwater, sediments, resident macroinvertebrates, and surrounding soils and vegetation reveal that, almost 100 years after the last mine closed, multiple contaminants persist throughout the ecosystem, significantly affecting biodiversity and environmental quality.

ENVR 226

Investigating of the levels, trends, and fate of pollutants in street dust in the Long Creek Watershed, South Portland ME

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Street dust is a known source of contaminants commonly associated with urbanized areas. Street dust typically contains metals, nutrients, polycyclic aromatic hydrocarbons and dioxins from vehicular exhaust, petroleum/combustion byproducts, asphalt, driveway sealants and from maintenance and landscaping activities. Contaminated street dust is transported via runoff from impervious surfaces into urban streams through stormwater disposal networks. In response to Residual Designation Authority under the Clean Water Act, public and private landowners in Long Creek, Maine's most studied urban watershed, have formed Long Creek Watershed Management District to implement the Watershed Management Plan. This unique partnership allows the District to evaluate water quality solutions based on site-specific data, and implement nontraditional methods on a watershed-wide basis (rather than by individual property) to improve water quality. This study evaluates contaminant trends within the Long Creek watershed to help the District implement best management practices to manage and reduce street dust contamination.

ENVR 227

Sorption of the chemical warfare agent VX to clay minerals

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Organophosphorus-based chemical warfare agents are unique military chemicals, which are extremely toxic, and could be found in soils of military installations and former production facilities. Little data exists on the fate and transport of these chemicals in soil environments. This poster will present data on the sorption of the chemical warfare agent VX to two different clay minerals: kaolinite and montmorillonite. Thermodynamic characteristics of sorption were obtained at temperatures ranging from 5 to 45 °C. Complementary sorption/desorption profiles and batch equilibrium sorption isotherms were also obtained. No VX sorption was observed with kaolinite, but VX sorption by montmorillonite was rapid. The predominant mechanism above the lower critical temperature (LCT) of VX was an exothermic physisorption process, consistent with an ion excahnge mechanism. Below the LCT, bimodal behavior was observed, with a second endothermic interaction occurring after the initial ion exachange. Additional details will be provided in the poster.

ENVR 228

Uncertainty analysis of vapor intrusion models using stochastic response surface method

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Different models have been developed over the past decade to predict the indoor air concentrations of chemicals originating from underground contaminant sources; however, the uncertainty of these models has not been studied systematically. The most widely applied model for predicting vapor intrusion potentials is the Johnson & Ettinger (J&E) Model. The purpose of this study is to assess the uncertainty of input parameters for the J&E model using probabilistic methods as opposed to computationally inefficient conventional tools such as Monte Carlo analysis. Specifically, this research incorporated Stochastic Response Surface Method (SRSM) to estimate the uncertainty within the J&E model. This method is based on chaos series expansion and a limited number of model simulations are required to determine the coefficients of chaos polynomial. Since the vapor intrusion models are dealing with random variables, the SRSM method could be employed to efficiently estimate the statistical characteristics of model outputs.

ENVR 229

Reactions of dehydropyrrolizidine alkaloids with valine and hemoglobin

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Metabolism of pyrrolizidine alkaloids (PAs) generates dehydro-PA(pyrrolic) metabolites which exert hepatoxicity and genotoxicity, including tumorigenicity. However, reaction of dehydro-PAs with cellular constituents, such as amino acids, proteins, nucleic acids, and DNA, has not been systematically studied. We report the reactions of dehydroriddelliine, dehydromonocrotaline, and dehydrohehiotrine, with valine and hemoglobin. The products were derivatized with phenylisothiocyanate, and upon HPLC purification, the resulting products were characterized by mass, UV-visible, and ^{1}H NMR spectral analysis. It was found that the reaction products were formed by linking the terminal amino group of valine and hemoglobin to the C7 and C9 positions of the necine base of dehydro-PAs. This represents the first full structure elucidation of protein conjugated pyrrolic adducts formed by linking the amino group of the amino acid to the necine base of dehydro-PAs (No official support or endorsement of this article by the U.S. FDA is intended or should be inferred.

ENVR 230

Debromination of HBCD-isomers by reduced sulfur species

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Hexabromocyclododecane (HBCD) is a brominated flame retardant widely used in polystyrene and textile products. Technical HBCD consist mainly of three diastereoisomers: α, β, and γ. HBCD is persistent and little is known about abiotic and biotic degradation reactions. Although the γ-HBCD is the dominant isomer in technical HBCD, the α-isomer is the isomer found at the highest concentration in biological samples. In this work we investigated the reaction of the individual HBCD-isomers with reduced sulfur species (bisulfide, polysulfide). The experiments indicate that the γ-isomer is reacting more than an order of magnitude faster with reduced sulfur species than the α-isomer. Therefore, abiotic reactions might shift the diastereoisomer distribution of HBCD in the environment.

ENVR 231

Contamination profiles of PCB congeners, chlorinated pesticides, and PBDEs in sediment and fish samples from riverine and brackish waters of Savannah, Georgia, USA

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Classical persistent organic pollutants and emerging new organic pollutants are of great concern due their negative effects on environment, wildlife and human health. Estuaries and coastal marine environments are considered the most sensitive areas to the accumulation of these pollutants. Objective of this study was to understand the contamination status of classical and emerging pollutants in the coastal waters off Savannah, Georgia. PCB congeners, chlorinated pesticides and PBDEs were analyzed in sediment and various fish species samples collected from riverine and brackish waters of Savannah, Georgia. Standard analytical procedures were followed to determine the concentrations of these contaminants. Results revealed that detectable levels of PCBs, pesticides and PBDEs were found in sediments and fish samples from this region. Certain PCBs and pesticides levels were below the FDA established limits for human consumption. The results also were compared with the earlier studies on these pollutants to discern temporal trends.

ENVR 232

Trace elements and PCB congener concentrations in annual growth rings of pine trees from western Kentucky

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Pollution trend monitoring studies are useful in understanding the historical contamination, present status and to predict future trends. Pine trees are used as biological indicators to assess environmental contamination by relating contaminant concentration in annual growth rings. The objective of the present study was to understand the trace elements including Cu, Mn, Cr, Pb, V, Ni, Zn, As, Ag, Cd, In, Sn and PCB congener concentrations in tree rings of pine trees from Western Kentucky. Pine tree core samples were collected from selected locations including industrial, national parks and undeveloped areas. Standard operating procedures were followed for tree core sampling and analysis using ICP-MS and GC-ECD. The results revealed that several elements and lower chlorinated PCB congeners were found in annual growth rings of pine trees. Tendency for increasing trends of Cr, Cu, Zn and slight declining trends for Pb and some PCB congeners were discernible.

ENVR 233

Effects of ozonation and UV radiation on the molecular and optical properties of natural water and wastewater effluent dissolved organic matter

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There is growing interest in finding alternatives to traditional chlorination for disinfecting drinking waters because of the formation of harmful chlorinated disinfection byproducts (DBPs). The combination of ozonation and UV radiation, considered an advanced oxidation process (AOP), has been used for the treatment and removal of harmful contaminates from both natural waters and effluent wastewaters. Dissolved organic matter (DOM) in both types of waters is of environmental concern for several reasons. It adds color, taste, and odor to aquatic systems, binds and enhances the transport of organic and inorganic contaminates, is a carbon source for microbial growth, and mediates photochemical processes. Here we report on studies of the effects of combined UV radiation and ozonation on the molecular weight distributions and optical properties of natural DOM and DOM in wastewater effluent (efDOM). Molecular weight distributions were determined by size exclusion chromatography (SEC) and time-of-flight mass spectrometry (TOF MS). Chromophoric and fluorophoric properties were characterized by ultraviolet-visible (UV-Vis) absorption spectroscopy and excitation emission matrix fluorescence spectroscopy (EEMS).

ENVR 234

Coking wastewater treatment plant as sources of polycyclic aromatic hydrocarbons to the atmosphere

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Polycyclic aromatic hydrocarbons (PAHs) were determined in air around a coking wastewater treatment plant (WWTP) using sorbent-impregnated polyurethane foam disk passive air samplers in 05.27-09.20 of 2010. Comprehensive gas chromatography-mass spectrometry analysis was performed to facilitate detailed chemical composition characterization of toxic PAHs. In total, 77 PAH compounds were positively identified in the atmosphere at the sites of primary clarifiers, aeration tanks and secondary clarifiers. The ∑PAH concentrations in the air were 2-18 times higher within the WWTP (957 to 11012 ng/m^3) compared to the references site (374 to 600 ng/m^3). 3 and 4-ring PAHs predominated in all these sites, and these compounds had the characteristics of coal combustion. The estimated lung cancer risks were between 0.4×10^{-3} and 3.7×10^{-3}, indicating the PAHs in the air near flotation-degreasing and aerobic tanks would have the potential lung cancer risk for the operating workers.

ENVR 235

Determination of haloacetic acids by 2D matrix elimination ion chromatography

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Treatment of drinking water with disinfectants is an important step in making water microbiologically safe for human consumption. Commonly used disinfectants react with naturally occurring organic and inorganic matter in source water to form disinfectant byproducts (DBP's). All drinking water in the United States is currently monitored for the presence of DBP's, which include Known carcinogens called haloacetic acids (HAA's). The US EPA has regulated five HAA's, which include monochloroacetic acid, dichloroacetic acid, trichloroacetic acid, monobromoacetic acid, and dibromoacetic acid. EPA Methods 552.1 and 552.2 are used to determine HAA's and require tedious derivatization and multiple extraction steps. This paper will demonstrate a two-dimensional matrix elimination ion chromatography method that diverts the matrix ions in the first dimension while analyzing the trace HAA's of interest in the second dimension using a high-capacity stationary phase. The method demonstrated good sensitivity, enabling the detection of all five regulated HAA's and four unregulated HAA's in the presence of typical drinking water matrix ions. The linearity, LODs, LOQs, an accuracy of the method to determine HAA's in drinking water samples will be reported.

ENVR 236

Preparation and characterization of polyamide-polyetheramide (PAPEA) copolymer membranes for reverse osmosis and nanofiltration

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The objective of this research was to prepare novel polyamide-polyetheramide (PAPEA) copolymers (See Figure 1) with improved chlorine stability for desalination of seawater by interfacial polymerization. The ratios of the amine terminated polyethylene glycol polymer (Jeffamine®) to different aromatic diamines such as p-phenylene diamine were dissolved in the aqueous phase and reacting with diacid chlorides in the organic phase. Poly(m-phenylene isophthalamide), an aromatic polyamide, was synthesized in the laboratory by high-speed stirring interfacial polycondensation of p-phenylene diamine and isophthaloyl chloride in water and tetrahydrofuran solvents, respectively. FTIR results confirm the polymer synthesis. The yield of the polymer obtained is ~90% of the theoretical value. Different RO membranes were synthesized from this aromatic polyamide (PA) under different casting conditions by varying the casting solution composition and casting thickness using N,Ndimethylacetamide (DMAC) as solvent. As a result, two different membranes were obtained containing PA concentration ranged from 2% to 5% with four different membrane casting thicknesses.

ENVR 237

Effects of environmental variables on coastal fecal indicator bacteria concentrations in Orange County, California

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The coastal zone is the significant environmental setting where ocean and land interface and it is economically important because of its high residential, commercial and recreational values. Meanwhile, in the United States, public coastal areas are increasingly off-limits due to elevated levels of fecal pollution and other contaminants. This study investigates the effects of rainfall, discharge, and wave heights on coastal fecal indicator bacteria (FIB) concentrations at several adjacent beaches in Orange County, California over three year period from October 2001 to September 2004. In order to identify the dominant temporal and spatial patterns along the coastal area, Empirical Orthogonal Function analysis was utilized for the three-year measurements of fecal indicator bacteria concentration data from 17 sampling stations. Through the statistical data analysis and the Empirical Orthogonal Function analysis, we found that the dominant factor effecting coastal fecal indicator bacteria concentration is precipitation event and consequent water discharge from Santa Ana River. The statistical analysis revealed the potential non-point fecal indicator bacteria sources around northern part of Huntington State Beach in addition to the alongshore transport by wave-driven surf zone current and offshore tidal currents.

ENVR 238

Overview of the remediation of cyanotoxins from water using physicochemical processes

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Cyanobacteria and cyanotoxins have been listed in the US Environmental Protection Agency's Contaminant Candidate Lists (CCL), with the more recent one (CCL 3) specifying for microcystin-LR, cylindrospermopsin, and anatoxin-a. In the presentation, Dr. Dionysiou will provide an overview of the cyanotoxin problems in the US and other countries, summarize some recent developments on the efforts of various stakeholders for the minimization of formation of such compounds in natural aquatic systems, and efforts towards their elimination from sources of drinking water supply; in situ in the aquatic systems or in unit operations of water treatment facilities. Details will also be provided on selected physicochemical processes that have demonstrated success on the removal of cyanotoxins from water as well as the mechanisms of removal.

ENVR 289

Towards a new organocatalyzed microwave-assisted isocyanate-free synthesis of [*n*]-oligourea: A new energy-saving, eco-friendly method generating oligourea using green chemistry approaches

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A new eco-friendly, energy saving method for the production of oligourea is reported using propylene carbonate and diamines with variable spacer length as a starting material *via* an organocatalyzed microwave-assisted, solvent-free synthesis. Furthermore, oligomers produced were analyzed by EA, ATR-FTIR, ^{1}H-, ^{13}C-NMR and thermal properties were analyzed using TGA, DSC. In addition to ^{1}H-NMR spectroscopy, molecular weight determination was further confirmed *via* HT-GPC using *m*-cresol. End groups can be tuned upon the right stoichiometry of the starting material. Several parameters were taken into consideration to be studied, organocatalyst, temperature, microwave power, time, catalyst loading and solvent. Amino alcohols under the conditions applied yielded bishydroxyalkylurea, making the method more chemoselctive towards aliphatic oligourea formation. Aromatic diamines were not successful at all to react with propylene carbonate.

ENVR 290

Performance of multilevel antimicrobials in clinical environment

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A multilevel antimicrobial coating based on contact-killing, release-killing and anti-adhesion strategy was developed based on encapsulated chlorine dioxide. The use of smart polymers enables the coating to response to touch and contamination by self-disinfection. Laboratory tests show the coating can render nonviable within 1 minute contact viruses (H1N1, RSV, EV-71), Gram-positive and Gram-negative bacteria. It is also effective against bacteria and fungal spores. The mechanism of inactivation is through oxidation of microbial outer coating and oxidative reactions with proteins and DNA.

The multilevel antimicrobial coating was field tested in hospital environment. Study were carried out at three Hong Kong public hospitals to evaluate safety, efficacy and compatibility of coating materials applied to medical items and hospital furnishings under real working conditions. The results indicate that the coating can render low viability of bacteria on surfaces for prolonged period of time. Thus, demonstrating the applicability of the coating in clinical situation.

ENVR 291

Efficiently Starbons based catalysts for biomass valorisation

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The production of energy, fuels, and chemicals from renewable biomass is currently an important issue for both academic and industrial communities. A great deal of effort has been put towards the valorisation of cellulose to value-added products by using efficient and environmentally friendly methods. Heterogeneous catalysts were used for such a purpose being involved in reductive splitting of cellulose to sorbitol and mannitol, degradation of cellulose to platform chemicals or saccharification of cellulose to glucose.Here, we report the development of novel functionalised Starbon®-based catalysts and their activities in three different applications: i) M (M = Ru, Ir, Ni)/Starbon for reductive splitting of cellulose, ii) Starbon-SO_3H for saccharification of cellulose, and ii) Starbon-CF_3SO_2 for the degradation of cellulose to levulinic acid. Tuning the chemical properties of the mesoporous carbonaceous materials from metallic to Lewis and/or Brønsted acids led to a large utilization of these catalysts.

ENVR 292

Waste valorisation practises: Changing problems into solutions

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Waste valorisation practises have attracted a great deal of attention over the past few years. In this work, we aim to provide a general overview of the different waste valorisation practises carried out in our laboratories to change the mentality of current society that sees waste as a problem rather than a resource, a solution

ENVR 300

Catalytic hydrodechlorination of dioxins over palladium nanoparticles in supercritical CO_2 swollen microcellular polymers

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Palladium nanoparticles embedded in monolithic microcellular high density polyethylene supports are synthesized as heterogeneous catalysts for remediation of 1,6-dichlorodibenzo-*p*-dioxin and 2,8-dichlorodibenzofuran in 200 atm of supercritical carbon dioxide containing 10 atm of hydrogen gas and at 50 ~ 90°C. Stepwise removal of chlorine atoms takes place first, followed by saturation of two benzene rings with slower reaction rates. The pseudo first order rate constant of initial hydrodechlorination for 2,8-di- chlorodibenzofuran is 4.3 times greater than that for 1,6-dichlorodibenzo-*p*-dioxin at 78°C. The catalysts are easily separated from products and can be recyclable and reusable without complicated recovery and cleaning procedures.

ENVR 301

Performance evaluation of CDI system based on electrode capacitance

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Water shortage is one of the most critical problems that endanger humankind. To solve this problem, there have been many efforts to secure fresh water by desalination. Capacitive deionization (CDI) technology could be an effective way of desalination. In spite of many researches for increasing the performance of the CDI, a few studies have reported the effect of important parameters such as electrode capacitance on CDI. Furthermore, most of the researches on CDI have been focused on the single-cell system only, though multi-cell system is required to secure a substantial amount of fresh water. This study evaluated the performance of single-cell (1 electrode pair) and multi-cell systems (40 electrode pair) in relation to electrode capacitance. The electrode capacitance was examined by using cyclic voltammetry and impedance spectroscopy. Afterwards, the obtained deionization performance of single-cell and multi-cell systems was correlated with the theoretical ion removal efficiency evaluated by electrode capacitance.

ENVR 302

Effect of pH on aqueous phase Hg(II) removal by nanoscale zero-valent iron

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We investigated the Hg(II) removal mechanism from the aqueous phase by nanoscale zero-valent iron (NZVI) under different pH conditions. At pH 3 after 1 min, 97% of the Hg(II) was removed from the solution phase: 74% of the removed Hg(II) remained in the solid phase and 23% of that was reduced to purgeable Hg(0). This result implies Hg(II) can be rapidly removed by not only the reduction but also the adsorption to the iron surface under acidic conditions resulting from the role of iron oxyhydroxide in a core-shell structure having high Hg(II) affinity. At pH 7 and 11, 16% and 23% of Hg(II) remained, respectively, in the aqueous phase due to the formation of stable Hg hydroxo complexes inhibiting Hg(II) sorption to the NZVI surface. This study suggests pH is the significant factor affecting Hg(II) removal using NZIV in aquatic environments.

ENVR 303

Modification of silica nanoparticles surface via "click" chemistry and their adjuvant effects

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Nanoparticles are increasingly used in commercial products, but the biological consequences from exposure to engineered nanomaterials are not well understood. Nanoparticle toxicity may result from their size, shape, surface chemistry, and tendency of aggregation. To determine such effects, we synthesized nanoparticles with specific sizes and surface chemistries. The surfaces of monodisperse silica nanoparticles were modified with alkynyl-substituted triethoxysilanes, which enable modification of particle surfaces via 'click' chemistry, the Cu-catalyzed azide-alkyne cycloaddition. Since the click reaction is the final step in the synthesis, the particles are identical except for the surface chemistry. We synthesized nanoparticles with carboxylic acids, amines, alcohols, and short methoxy-terminated polyethylene chains, and dynamic light scattering measurements in water confirmed that the nanoparticles had not aggregated. Nanoparticles with different surface chemistries showed enhanced Interferon (IFN)g and interleukin (IL)-2 production by CD8$^+$ T cells under OVA$_{257-264}$ stimulation at different levels.

ENVR 304

Degradation of cylindrospermopsin using brookite titanium dioxide under simulated solar light

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Titanium dioxide nanoparticles composed of mainly brookite phase (B-TiO$_2$) was synthesized using a temperature controlled oil bath method. The photocatalytic degradation of a hepatotoxic cyanotoxin, cylindrospermopsin (CYN), by B-

TiO_2 under simulated solar irradiation was studied. Experiments were carried out in a laboratory scale by using two15 W fluorescent lamps with the light intensity of 2.37 mW/cm^2. Almost complete removal of CYN with an initial concentration of 1 µM was achieved in 20 minutes when 0.1g/L photocatalyst was employed. When increasing the concentration of B-TiO_2 to 0.25g/L, a faster removal of CYN was observed. The effects of water quality parameters, such as pH, alkalinity and the presence of natural organic matter, were also studied. Natural water samples from St. Johns River, Florida and Lake Erie, Michigan have also been used to evaluate the utility of this technology on the degradation of CYN in natural waters. The formation of intermediates in the destruction process is also being studied and results will be presented.

ENVR 305

Stabilizing acetylcholinesterase on carbon electrodes to produce effective biosensors

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A biosensor for the detection of organophosphates (OPs) in water was produced by encapsulating acetylcholinesterase (AChE) enzyme in peptide nanotubes (PNTs) and attaching the encapsulated enzyme on a carbon screen printed electrode using Nafion. In this study, three versions of the sensor were used to detect the OP malathion. In one version, AChE was placed directly on the electrode. In the second, AChE was encapsulated in a PNT, and placed on the electrode. And in the third version, PNT encapsulated AChE was attached to the electrode using Nafion. The stability of the sensors was measured over 50 days of storage at 4°C. The sensors that were constructed without PNTs or Nafion were not stable. The biosensors constructed with PNTs, and with PNTs and Nafion, lost 17.3% and 14.2% of their activity, respectively, after 50 days. Detection of malathion on the order of nM was achieved.

ENVR 311

Adsorption of cationic and anionic dyes from aqueous solutions on KOH-activated multiwalled carbon nanotubes

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KOH dry-etching was explored to prepare activated multi-walled carbon nanotubes(MWCNTs) with higher specific surface area(534.6m^2/g) and pore volume(1.61cm^3/g), The activated MWCNTs (CNTs-KOH) were used for adsorption of representative dyes (anionic MO and cationic MB) in aqueous solutions, which can be efficiently removed with CNTs-KOH. CNTs-KOH can adsorb very large amount of both MO and MB via a specific interaction like electrostatic interaction and ion exchange between the dyes and the adsorbent. Experimental results indicated that the CNTs-KOH has good adsorption capacity (q_e) of MO (149 mg/g) and MB (399mg/g). The adsorption isotherms were fitted by the Freundlich model better than the Langmuir. Kinetic regression analysis results showed that the adsorption kinetics was more accurately represented by a pseudo second-order model, the overall adsorption process maybe jointly controlled by external mass transfer and intra-particle diffusion, and intra-particle diffusion was predominated over the external mass transfer. The findings indicate that KOH etching is a useful activation method to improve the adsorption affinity of dye contaminants on MWCNTs. Therefore, the CNTs-KOH is a promising adsorption nanomaterial for preconcentration and separation of organic pollutants from aqueous solutions for environmental remediation.

ENVR 312

Selective removal of Cu^{2+} and CrO_4^{2-} from natural waters by nanoporous sorbents modified by mono-/di-/tri- amino-organoalkoxysilanes

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Heavy metals in marine environment are a worldwide concern due to their adverse impact on marine organisms and human health. Sorption process remains the most economical means of removing heavy metals from seawater, but the high salt and organic content of seawater pose important challenges. Nanoporous sorbents were designed to selectively adsorb copper and chromium ions from natural waters in this study. Mono-/di- /tri- amino-organoalkoxysilanes were functionalized to MCM-41 for capture the copper ions; Fe^{3+} was then grafted to the above materials for selectively removing chromium anions. NH_2-MCM-41 is best one which can remove more than 99% copper with *Kd* of 10^6 from seawater with the other competing metal ions. It also demonstrated rapid Cu^{2+} sorption kinetics (minutes) and good sorption capacity (60mg Cu/g sorbents). Fe-NNN-MCM-41 is the best one for chromium removal with competing metal ions from natural waters with removal percentage >99% and Kd of 10^6.

ENVR 313

Removal of cesium ion by zeolite modified carbon electrode

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After Fukushima nuclear accidents, a fear of radioactive substances are spreading in the world. Their uncontrolled release may contaminate land, underground water, and ocean. If humans ingest a radioactive substance, it's accumulated in their body and believed to increase one's lifetime risk of developing certain types of cancer. Radioactive water from nuclear accident mainly contains cesium-137, and cesium-137 reacts with water producing a water soluble compound. To remove radioactive cesium in water, zeolite is considered one of the best absorbent materials to treat radioactive wastewater since zeolite can efficiently remove cesium by ion exchange. It also has high selectivity than other ions so it can be used for removing cesium ion in seawater. To increase the removal rate of cesium, we invented a zeolite mixed with carbon electrode and investigated the removal rate of cesium ion in comparison with applying voltage.

ENVR 314

Removal and recovery of phosphorous from contaminated waters using renewable resource-based magnetic nanocomposites

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Water pollution by phosphorous (P) has become one of the leading problems in water quality. Although several technologies exist to remove P from contaminated water, each has its own drawbacks. A novel microwave assisted synthesis of reduced iron oxide nanoparticles containing renewable resource based media for P removal from contaminated waters is discussed. The process is fast, easy, and economical. Nanoparticles were synthesized even without employing hydrogen or any inert gas. The prepared media were highly effective and efficient in removing P. A 100 % P removal efficiency was attained using a 1 mg / L standard P stock solution and a maximum adsorption capacity of 43.7 mg P/ g of composite was achieved using a 500 mg / L standard P stock solution. The present technique holds tremendous economic promise as the carbon source employed was a renewable resource material with a high regeneration capacity and a wide range of other metal/ carbon nanocomposites can also be synthesized. The present technology may also be used for arsenic removal from similarly contaminated waters.

ENVR 315

Removal of antibiotics from contaminated waters using natural zeolite

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Tetracycline (oxytetracycline, OTC and chlorotetracycline, CTC) and fluoroquinolone (ofloxacin, OFL and enrofloxacin, ENR) antibiotics have multiple pKa values and partial positive moieties at environmentally relevant pH. Natural zeolites have high cation exchange capacities and could be potentially used to remove these antibiotics from contaminated water. The sorption behavior of 4 antibiotics (OTC, CTC, OFL, and ENR) by natural zeolite at pH of 5, 7, and 9 was examined. The sorption capacities are 10, 6, 12, and 8 mg/g for OTC, CTC, OFL, and ENR, respectively, at pH 5. As the pH increased to 7, the sorption capacities decreased to 2, 4, 8, and 5 mg/L. At pH 9 only a minor amount of these antibiotics was sorbed. Zoelite could be used as the filtration bed in artificial recharge ponds where municipal wastewater is recharged to groundwater for the purpose of wastewater reclamation and reuse.

ENVR 316

Environmental safety of nanocomposites: Assessing degradation of nanocomposites under environmental condition

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Polymer nanocomposites are increasingly used in many industries, ranging from construction to medical applications. These polymer nanocomposites can have much better performance as compared to that of unmodified polymers due to unique combination of mechanical, thermal, dielectric and biodegradable properties. For example, structural and infrastructure applications of nanocomposites can be particularly promising due to the high strength to weight ratio of the materials, which would give them excellent fatigue resistance. However, the potential environmental and health hazards posed by the nanofillers are not completely understood. There is a lack of systematic studies of the release of the nanofillers from the composite matrix. This project looks into stability of CNT modified epoxy polymer composites subjected to UV and moisture degradation. These samples have been examined using SEM, FTIR spectroscopy and nanoindentation techniques. The implications of these results to environmental safety of nanocomposites are also discussed.

ENVR 317

Applications for fluorescence and zeta potential measurements via nanoparticle tracking analysis

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When determining the limit of exposure for nanoparticles in the environment, the ability to measure nanoparticles in various media is critical in order to obtain accurate toxicology information. Sizing, 10 nm to 1 μm, and concentration measurements of particles in various media are obtained by nanoparticle tracking analysis (NTA) via particle-by-particle measurements. NTA is appropriate for screening environmental samples as the optimal concentration for detection is very low (108 particles/mL) and samples are commonly polydisperse. Recently, other parameters of detection, such as intensity, fluorescence and zeta potential, have been added to NTA, allowing for the identification of different nanoparticles within a single sample. Through combinations of these measurements, we will demonstrate with examples how NTA is a powerful, high resolution multi-parameter method with the capabilities to characterize and monitor particles in biological environments for toxicological studies and risk assessment.

ENVR 318

Competitive adsorption of toluene, ethylbenzene, and xylene isomers and heavy metal onto multiwalled carbon nanotubes in multisolute system

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A single-solute adsorption has reported in the literature, however, where multiple contaminants containing both heavy metals and organic contaminants may coexist in the environment. In this study, competitive adsorption of toluene, ethylbenzene and xylene isomers (TEX) and heavy metals on multi-walled carbon nanotubes (MWCNTs) was investigated. The results indicated that heavy metal ions Pb^{2+} evidently diminished the adsorption of TEX onto MWCNTs-3.2%O. Pb^{2+} decreased adsorption onto MWCNTs-3.2%O by 66.2, 50.2, 53.2, 54.6 and 52.8% for toluene, ethylbenzene, p-xylene, m- xylene and o- xylene by the expression as $(K_d^2 - K_d^1)/ K_d^1$, where K_d^2 and K_d^1 correspond to the distribution coefficients of TEX with and without heavy metals, respectively. The competition was much weaker in the effect of TEX onto Cu^{2+} and Pb^{2+} adsorption. TEX only deceased 15.8% of Cu^{2+} ions adsorption at initial concentration of 52.4mg/L by the same expression.

ENVR 319

Uptake and effects of multiwalled carbon nanotubes on germination and growth of various plant species

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Most of the studies related to carbon nanotube effects on plants have been conducted in a soil free environment, which is not necessarily environmentally relevant. A series of experiments were conducted on the uptake and effects of multi-walled carbon nanotubes (MWNTs) on germination and growth of various plant species (alfalfa, cotton, corn and sorghum) in soil. No significant effects were observed on germination, tap/primary root length, shoot length and shoot biomass in most of the species studied. Evaluation of lateral root density, lateral root length and number of lateral roots in corn and sorghum showed no significant differences from controls, except average sorghum lateral root length significantly decreased at 10 mgMWNTs kg^{-1} soil. Microwave analysis showed uptake and translocation of MWNTs within the stems of sorghum. The results of this study will be valuable in determining the risk posed by carbon nanotubes to plants and environment.

ENVR 320

Reduction of hydroxylated C_{60} (fullerenol) by Zn (0) in water: Reaction kinetics and product characterization

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Water soluble, hydroxylated fullerene (fullerenol) materials have recently gained increasing attention as environmentally relevant fullerenes as they have been identified as the primary product(s) during exposure of C_{60} (aggregated nC_{60}) to UV light in water. Further aqueous reactions however, have not been thoroughly studied. We examine the transformation mechanism(s) and reaction kinetics of fullerenol ($C_{60}(OH)_x(ONa)_y$) in a reducing aqueous environment, focused on a reduction reaction with Zn(0) through a series of batch reaction experiments spanning a range of environmental aqueous conditions (pH, Eh, etc.). Significant reduction of fullerenol was observed and the properties of the products were analyzed with ^{13}C-NMR, FTIR and UV-Vis. Interactions between resulting reduced fullerenol and two types of surfaces, polystyrene and silica, were studied through quartz crystal microbalance (QCM-D), indicating that hydrophobicity increased after reduction by Zn(0). The reaction rates under aerobic and anaerobic conditions were compared, indicating that the presence of oxygen has little effect.

ENVR 321 - Withdrawn

ENVR 322

Persistence of commercial nanoscale zero-valent iron (nZVI) and its by-products

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The use of nanoscale zero-valent iron (nZVI) for *in-situ* remediation of a wide scale of environmental pollutants has continued to gain momentum over the years. However, the long-term fate of the nZVI used for remediation is largely unknown. We aged three types of commercial nZVI in aqueous media under aerobic and anaerobic conditions and found that the bulk of the nZVI injected into polluted sites will end up in the sediment via aggregation-induced sedimentation of the nZVI and its insoluble oxides. Iron concentrations greater than 500 g/kg were detected in the sediment. This level of iron may potentially affect some organisms in that medium and also reduce the permeability of the aquifer, reducing transport through the aquifer. Solution chemistry and surface chemistry of the iron species showed that nZVI can remain reactive for more than one month and the reactivity of iron and its transformations are governed by environmental factors.

ENVR 323

Influence of morphology and phase on TiO2 photoactivity in natural waters

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The photoactivity of nanomaterials (NMs) in the environment is of particular concern considering the ability of metal oxide NMs to produce toxic reactive oxygen species. Titanium dioxide (TiO_2) has been heavily used and researched as a photocatalyst, although, little work has investigated the role of particle phase and morphology on photoactivity and even less is known about the environmental photoactivity. Using more than 10 different TiO_2 nanoparticles of different crystalline phase and morphology, we measured the photoactivity in deionized water, freshwater, groundwater and other natural waters. Under environmental conditions, our research has shown that anatase photoactivity is roughly one order of magnitude greater than rutile. We have also shown that amorphous particles are more reactive than dots, which are more reactive than spheres, which are more reactive than wires. Compared to DI conditions, photoactivity is generally reduced in all natural waters.

ENVR 324

Interaction between biofilms and nanoparticles

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The interaction of nanoparticles with bacterial biofilms has implications in evaluating the risk of nanoparticles in the natural environment including with aquatic animals. Investigation of the effect of nanoparticles on biofilms helps avoiding clinical infection, clogs or corrosion in an industrial or residential water distribution system. This study focuses on interaction and diffusion of nano ceria with biofilms from two types of microorganisms; *Pseudomonas Fluorescens* and *Mycobacterium Smegmatis*. Batch studies were conducted to understand adsorption and desorption kinetics and equilibrium of ceria. Live- Dead BacLight Bacterial Viability Kit and Confocal Laser Scanning Microscope were used to estimate the live and dead bacteria within the biofilm. Kinetics of adsorption and diffusion of nanoparticles with biofilm of different growth stage and viability were conducted. In addition, distribution of ceria penetration within the biofilm was observed by studying the distribution of dead and live cells within the biofilm thickness.

ENVR 325

High contrast two-photon fluorescence in vitro imaging using novel fluorescent polymeric nanoparticles

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Two-Photon-Fluorescence (TPF) has several advantages over the conventional confocal fluorescence microscopy, like better tissue penetration, reduced photo-damage and less photo-bleaching of the fluorescent molecule**.** Consequently, the design of novel materials with large two-photon absorption cross-sections continues to be of great interest. Numerous organic fluorophores with high TPF have been reported in literature, but their biological applications have been limited by their hydrophobicity and cellular toxicity. Here, we report the fabrication of fluorescent polymer nanoparticles (NPs) and their potential application as biomarker. These, NPs were fabricated using "mini-emulsion" technique. Strong TPF was observed from these polymeric NPs using femto-second laser pulses at 800 nm. Interestingly, these NPs were found to be non-toxic in a dose and time dependent manner in cell viability (MTT) studies. TPF microscopy imaging confirmed cellular uptake and two-photon activity of NPs in THP-1 cells. Diagnostic and theranostics applications of these novel NPs are been further explored.

ENVR 326

Toxicity of nZVI to freshwater and marine organisms

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Little is known about the impacts of using nano-scale zerovalent iron (nZVI) for groundwater remediation. This study investigated toxicity risks comparing two types of nZV and two iron chloride salts ($FeCl_2$ and $FeCl_3$. The focus was on sensitive organisms known to be indicators of toxicity, specifically marine and freshwater phytoplankton and a freshwater invertebrate. Toxicity studies indicate that nZVI can be toxic at concentrations greater than 0.5 mg/L total Fe. The response of different species of phytoplankton can be similar and show decreasing cell densities with increasing total Fe and less toxicity to $Fe2^+$ and $Fe3^+$. The response of the *D. magna* to nZVI suggests that nZVI istoxic even at 0.5 mg/L, with less toxicity to $Fe2^+$ and $Fe3^+$. For groundwater remediation it is important to consider the dilution down gradient and the significance of nZVI toxicity relative to toxicity of the pollutant in groundwater.

ENVR 341

Detection of carbon nanotubes in environmental and biological matrices using programmed thermal analysis

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Carbon nanotube (CNT) production is rapidly growing, and there is a need for robust analytical methods to quantify CNTs at environmentally relevant concentrations in complex organic matrices. Because physical and thermal properties vary among different types of CNTs, we studied 14 single- (SWCNTs) and multi-walled CNTs (MWCNTs). Our aim was to apply a classic analytical air pollution method for separating organic and elemental carbon (thermal optical transmittance/reflectance, TOT/R) to environmental and biological matrices and CNTs. An evaluation of the thermal properties of CNTs revealed two classes that could be differentiated using Raman spectroscopy: thermally "weak" and "strong." Using the programmed thermal analysis (PTA) method, we optimized thermal temperature programs and instituted a set of rules for defining the separation of organic and elemental carbon to quantify a broad range of CNTs. The combined Raman/PTA method was demonstrated using two environmentally relevant matrices (cyanobacteria and urban air).

ENVR 342

Surface analysis of carbon nanotubes and its application to understanding particle and nanocomposite properties in the environment

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As a result of deliberate functionalization strategies or incidental exposure to oxidizing conditions, hydrophilic oxygen-containing functional groups will often be present on the surface of carbon nanotubes (CNTs) in composites that incorporate CNTs and CNTs present in aquatic environments. I will show how quantitative information on CNT surface oxygen concentration determined by X-ray Photoelectron Spectroscopy, and oxygen-containing functional group distributions acquired from chemical derivatization has allowed structure-property relationships to be developed that quantify the effect of CNT surface chemistry on, (i) colloidal stability of CNT particles, (ii) CNT sorption properties with hydrophobic and divalent metal cations, (iii) CNT interactions with natural organic matter, (iv) photochemical stability of CNTs, (v) membrane properties and (vi) biofilm formation rates on CNT polymer composites. This information can be used to develop predictive models that describe the behavior of CNTs and provide the basis for more accurate risk assessment and cost benefit analysis.

ENVR 343

Development of a new detection method for carbon nanotube contamination in water

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Carbon nanotubes possess unique properties that have led to an increase in research in a wide variety of fields. This growing demand and use of carbon nanotubes poses a potential health risk and may have detrimental effects in the environment. There is a significant gap of information of the actual quantity of carbon nanotubes in the environment. However the detection methods that are specific to carbon nanotubes are very limited mainly due to the ubiquitous carbon chemistry of carbon nanotubes. In response to these deficiencies, a novel method that utilizes a structural differentiation of carbon nanotubes was developed for carbon nanotube detection in water. The specific affinity between single walled nanotubes (SWNT) and G/T alternating ssDNA was employed to capture SWNT in water.

A rapid, SWNT-specific separation was obtained by the use of magnetic field. Dual fluorescent labels that are attached to sandwich ssDNA probes were used for the precise quantification. A calibration curve ($r^2 = 0.90$) was successfully made using a range of SWNT concentration against the planar graphene that was used as a negative control. The findings of this research suggest that this method is of great sensitivity and specificity for carbon nanotube detection in aqueous environment.

ENVR 344

Measuring black carbon in geosorbents by elemental mapping

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Black carbon (BC), a ubiquitous, persistent, and sorptive carbonaceous component in the environment, is typically measured by bulk analyses. However, conventional BC methods often give widely varying results and provide little information on the distribution of BC at the particle scale. Hence, we explored the feasibility of quantifying BC using analytical electron microscopy (AEM) using a suite of standard BC and non-BC samples with and without the presence of sediment particles. Point analysis by energy dispersive X-ray analysis (EDX) showed that all BC samples have a characteristic O/C atomic ratio of ≤0.1 at the sub-micrometer scale. Areal analysis of the elemental images obtained by scanning transmission electron microscopy (STEM) yielded measurements of BC comparable with the conventional quantification methods. This study demonstrated the potential of using AEM to measure the abundance of nanomaterials in environmental matrices.

ENVR 345

Measuring particle interactions using total internal reflection microscopy

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Particles undergo interactions in the environment that occur on the *kT*-scale, where sensitive and quantitative measurements are needed to understand the detailed forces responsible for their behavior. Traditional scanning probe and light scattering techniques cannot accurately measure these forces, being either intrusive or insensitive respectively. In this work we use total internal reflection microscopy, a non-intrusive technique sensitive to nanometer changes in particle position, to track the three dimensional trajectories of various engineered particles in solution. Using this technique, we have quantitatively measured the force interactions of spherical silica particles and gold rods as they sample heights above silica surfaces. We also studied trends and changes in particle-surface forces when the solution chemistry (pH and ionic strength) of the system changes. Measurements of colloidal silica showed increased stability and deviation from DLVO theory, indicating the presence of a gel layer on silica surfaces that imparts additional stability through steric interactions.

ENVR 346

Donnan membrane technique: Separating nanoparticles from ions

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The dissolution products from engineered nanoparticles (NPs) are often toxic to aquatic organisms, yet accurately separating these two components is not a trivial endeavor. Physical and chemical processes such as sorption, thermodynamic equilibrium, and counter ion concentrations can hinder accurate dissolution product measurements. In this work, we demonstrate that the Donnan Membrane Technique (DMT) is a very suitable and robust technique for quantifying free ion concentrations in NP solutions. The DMT uses a cation exchange membrane that acts as a barrier to NP transport, thus promoting only ionic transport to the acceptor solution while maintaining chemical equilibrium in the donor solution. Using citrate-capped Ag NPs, we will compare the DMT with other size separation techniques, such as ultracentrifugation and membrane filtration.

ENVR 347

Environmentally relevant nanoparticle surfaces studied by vibrational sum frequency generation and second harmonic generation

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The application of vibrational sum frequency generation and second harmonic generation to study the surfaces of environmentally relevant nanoparticles is discussed in the context of Au, CdSe, and core-shell nanoparticles.

ENVR 348

Use of single particle – inductively coupled plasma – mass spectrometry for analysis of engineered nanoparticle stability in varied media

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Increasing use of engineered nanoparticles (NPs) in consumer products has led to concern that these materials will enter the environment. Once released, a variety of transformations such as dissolution and aggregation may alter the original material. Single particle – inductively coupled plasma – mass spectrometry (SP-ICP-MS) was used to determine size distributions over time for various sizes and shapes of NPs in varied environmentally relevant media. Silver nanowires were spiked into a simulated freshwater and a D. magna test media to monitor their size distributions. Samples were analyzed by SP-ICP-MS to observe transformations over toxicity test time periods. A decrease in the number of particles observed over time in both media suggests dissolution of nanowires. Tap water and wastewater were spiked with spherical Ag NPs, Ag^+, or a combination of the two at environmentally relevant concentrations. We determined under what conditions NPs may dissolve, aggregate, or form complexes, and if particles interact with free Ag^+ in solution. Water chemistry components, specifically chloride and sulfide, were investigated as to how they may transform Ag NPs or interact with dissolved Ag^+. Using SP-ICP-MS, changes in NP

size, through aggregation and complexation, were determined. Bioaccumulation tests were performed using the worm *Eisenia fetida* and both Au and Ag NPs. Worm tissue was extracted using a 25% tetrametylammonium hydroxide (TMAH) solution, allowing tissue to dissolve while leaving NPs intact. Differences in uptake of both Au and Ag NPs (size range 50 to 100 nm) were investigated with respect to particle size.

ENVR 349

Test protocols and results for the nanosilver containing pesticide AGS-20

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The US EPA granted a conditional pesticide registration for the nanosilver containing product HeiQ AGS-20. AGS-20 is a nanosilver containing composite with typical overall particle diameters of one micrometer (1 µm or 1,000 nm). AGS-20 will be incorporated into textiles to suppress the growth of bacteria, which cause textile odors, stains, and degradation. The final textile article cannot contain more than 0.01% silver by weight. As a condition of registration, EPA is requiring a number of studies including product characterization and stability testing to determine if nanosilver breaks away from AGS-20. If nanosilver is found to break away from AGS-20 or textiles treated with AGS-20, then additional testing will be triggered to determine the affect of AGS-20 derived nanosilver on humans and the environment. The scope and objective of each required study along with preliminary results will be discussed during this presentation.

ENVR 350

Tools and approaches for the assessment of nanomaterial induced oxidative DNA damage

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Hyphenated mass spectrometry (gas chromatography/mass spectrometry) techniques have been employed as one of the primary analytical tools for investigating the effects of ionizing radiation, chemical/biological carcinogens and oxygen derived free radicals on the induction and subsequent repair of oxidatively-induced DNA damage (DNA lesions) in living systems. Certain DNA lesions, such as 7,8-dihydro-8-oxoguanine (8-OH-Gua), are not only established mutagens, but have also been utilized as biomarkers of systemic oxidative stress. The National Institute of Standards and Technology (NIST) has established a comprehensive research program focused on identifying and characterizing the DNA damaging mechanisms of commercially relevant engineered engineered nanoparticles (NPs) using models of increasing biological complexity through the application of sensitive hyphenated mass spectrometry tools for the quantification of oxidatively-induced DNA damage. We present an overview of our recent findings from studies on metal (AuNP), metal oxide (CuO NP), and carbon-based (MWCNTs) nanomaterials.

ENVR 351

Lipid oxidation for measuring bioreactivity of iron nanomaterials

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Zero-valent iron nanomaterials participate in groundwater remediation, food fortification, and enter the environment through industrial dusts/products. Iron is known to participate in oxidative stress and lipid oxidation; these properties were investigated for assessing toxicological risks. In-vitro reaction of lipids in human saliva and biotissues (e.g., oleic, linoleic, linolenic acids) with iron species was monitored via the thiobarbituric acid substances (TBARs) method that is common for assessing oxidative stress. Results demonstrated that ferrous ion was the most reactive, zero-valent species had intermediate reactivity based on particle size, and ferric ion had low activity. The differences in reactivity among iron species have important implications. A positive is that lower lipid oxidation causes less damage to organisms. A negative is that because lipid oxidation causes the metallic flavor of iron, humans are less likely to detect an offensive iron flavor in groundwater or consumer products containing iron above recommended intakes.

ENVR 352

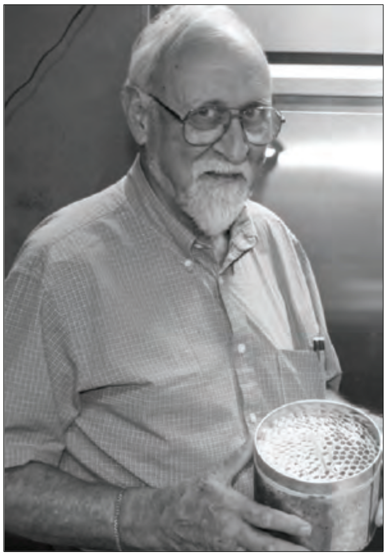
Nanomaterial Registry: Minimal information standards for well-characterized nanomaterials in environmental studies

Michele L Ostraat, *mostraat@rti.org, Karmann Mills, Damaris Murry, Kimberly Guzan.Center for Aerosol and Nanomaterials Engineering, RTI International, Research Triangle Park, NC 27709, United States*

Assessing the interactions and implications of nanomaterials with environmental systems is complex since interactions are not only a function of the system under consideration, but also of the nanomaterial characteristics and diverse analytical instruments, test methods, protocols, and assays used. Inconsistent and inconclusive reports of nanoparticle interactions with environmental systems continue to foster significant scientific debate concerning the suitability of analytical methods and the validity of research methods, findings, and conclusions in the characterization of nanomaterials. The Nanomaterial Registry seeks to systematically organize and evaluate existing research findings that demonstrate the impact of nanomaterials and their characteristics on environmental systems in a user-friendly, authoritative, web-based tool. To facilitate development of the Nanomaterial Registry, a minimal information standard for nanomaterials has be established, including detailed information on analytical instrumentation, process parameters, and experimental protocols. As an authoritative resource for diverse nanotechnology stakeholders, the Nanomaterial Registry incorporates data from existing resources

AUTHOR INDEX

HORACE G. CUTLER
NOVEMBER 21, 1932 – JUNE 1, 2011



Horace G. Cutler, Ph.D., a celebrated natural products chemist whose career spanned more than half a century, died June 1, 2011 in Watkinsville, GA at age 78, after suffering from cancer. He was born in London England on November 21, 1932 to Sir Horace Walter Cutler, O.B.E., K.C. and Betty Martin Cutler. He grew up in London during WW II and had many memories of the blitz. Dr. Cutler attended St John's Beaumont College Jesuit boarding school in Old Windsor, Trinity College, Dublin, Columbia University, New York and the University of Maryland, College Park. At the age of 20 he immigrated to Quebec City, Canada and then moved to New York City.

In 1954 he accepted a Union Carbide Fellowship with Boyce Thompson Institute for Plant Research in New York. During his Fellowship he realized his passion for natural products research while working with Lawrence "Larry" King on plant growth regulators. This passion drove him to embark on a 57 year career in natural products research. While working with Dr. King, he was involved with the development of the insecticidal agents possessing carbamates, which eventually lead to the discovery of carbaryl (Sevin®) by Union Carbide. In 1959 he accepted a position as a Plant Physiologist with Tate and Lyle, Ltd., Central Agricultural Research Station, Carapichaima, Trinidad, West Indies. While in Trinidad he was able to work with a team of researchers that investigated a wide-swath of plants for bioactive compounds. Among other developments, this work eventually led to the development by Tate and Lyle of the sweetener sucralose that and is currently sold in the US under the trade name Splenda®.

In 1963 he enrolled in the University of Maryland to earn a Master's of Science (1963-66) and Doctor of Philosophy (1966-67) degrees in botany with a focus on natural products chemistry. Upon graduating from the University of Maryland he was appointed Plant Physiologist with the United States Department of Agriculture – Agriculture Research Service in Tifton, GA to develop a modest natural products program within the USDA. It was during that time that he became interested in evaluating the secondary metabolites of plants, fungi, and aquatic organisms for their biological effects. In 1981 the USDA interests in the natural products program had grown to the point where his research group was relocated to the Richard B. Russell Center in Athens, GA. This afforded him the opportunity to become more engaged with his adjunct professorship at the University of Georgia and support graduate students of various departmental programs within the university system.

In the late 1980s he served on a USDA-ARS Special Committee to secure federal funding to build the Phase I of the National Center for Natural Products Research in Oxford, MS. His research group relocated to this site in 1995 when construction of the Center was completed. It was at that time that Hank retired from the USDA as a GS-15 Research Leader and volunteered his time at Mercer University College of Pharmacy and Health Sciences as a Senior Research Professor. This faculty appointment gave him the opportunity to educate pharmacy students and to direct graduate students working on PhD degrees in pharmacy research. He also held an adjunct professorship at the University of Mississippi School of Pharmacy.

During his 57 year career with the USDA and Mercer University, Dr. Cutler was recognized nationally and internationally for research on the isolation of biologically active natural products from fungi and plants. He published over 200 peer-reviewed papers, 33 book chapters, 13 books, over 150 national and international scientific presentations, and more than 50 US and international patents. He was a Fellow of the Agrochemical Division of the American Chemical Society, was awarded the Silver Medal for Research from the Japanese Society for the Chemical Regulation of Plants, the Plaque of Appreciation for Contributions to Science by the Korean Agricultural Chemical Society, and the Abbott Pharmaceutical Award. He served as President of the Plant Growth Regulator Society of America (PGRSA) and as its Chief Executive Officer. He was a member of the honor societies Sigma Xi, Rho Chi, Phi Lambda Sigma, and Phi Sigma as well as a member of the New York Academy of Sciences, the Georgia Academy of Sciences, and the American Chemical Society. In 1989 he was selected by the American Chemical Society as the state of Georgia Chemist of the Year. The USDA-ARS recognized him in 1990 by awarding him the Outstanding Award for Performance. He is survived by his wife of 56 years, Joanne Cutler, seven children; Frank Cutler, Paul Cutler, Chris Cutler, Kevin Cutler, Stephen Cutler, Elizabeth "Liz" Grow, and Holly Kendrick. He also leaves behind 12 grandchildren. We will all miss Hank's ready wit and wisdom.

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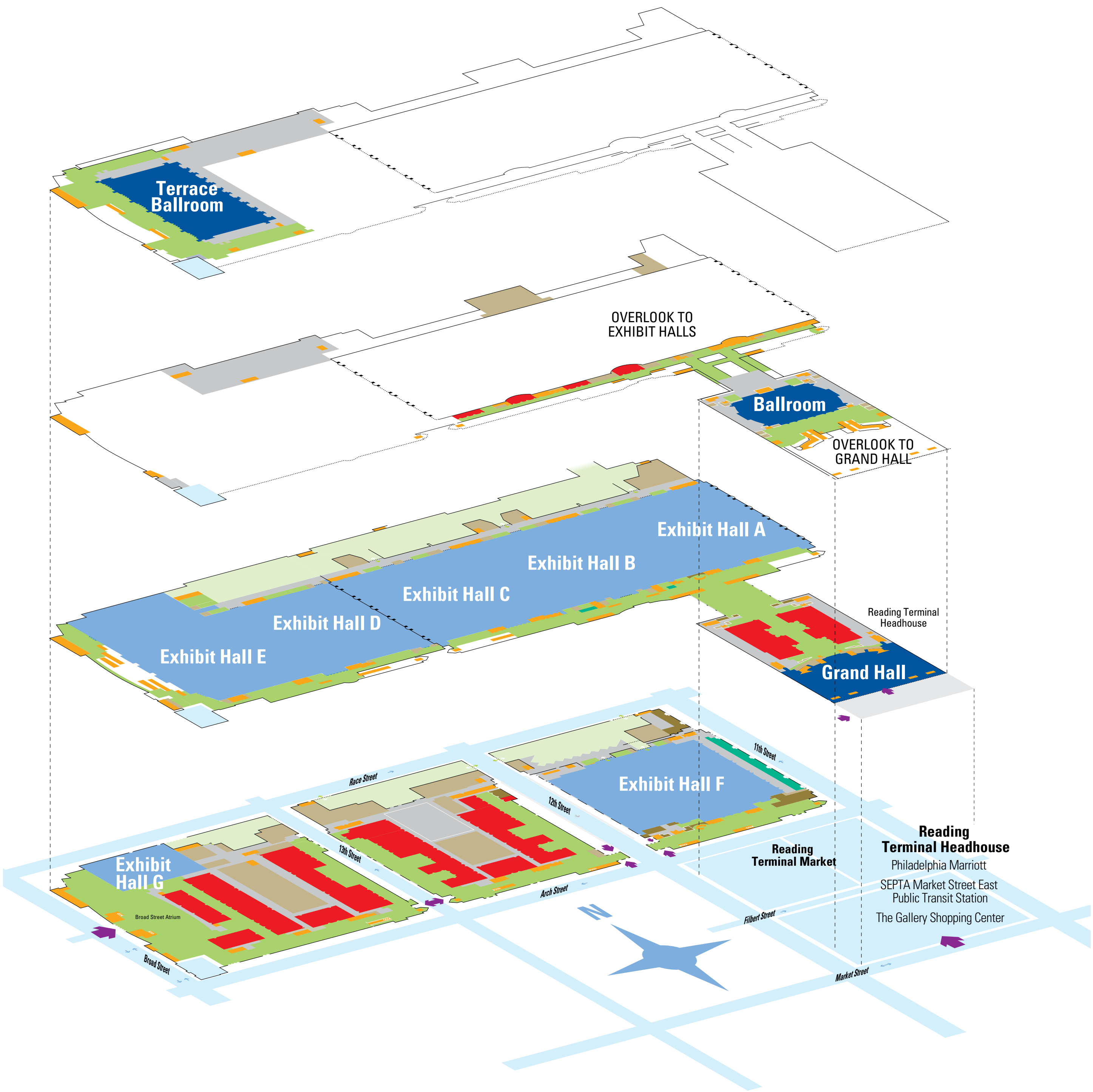

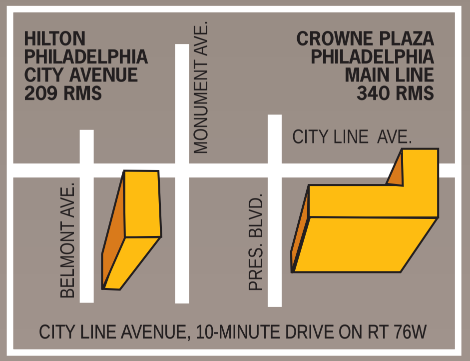

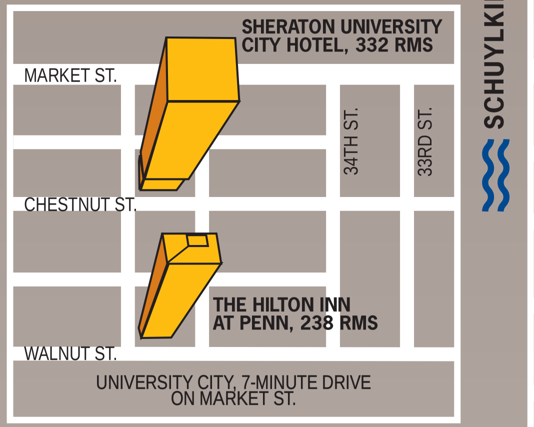

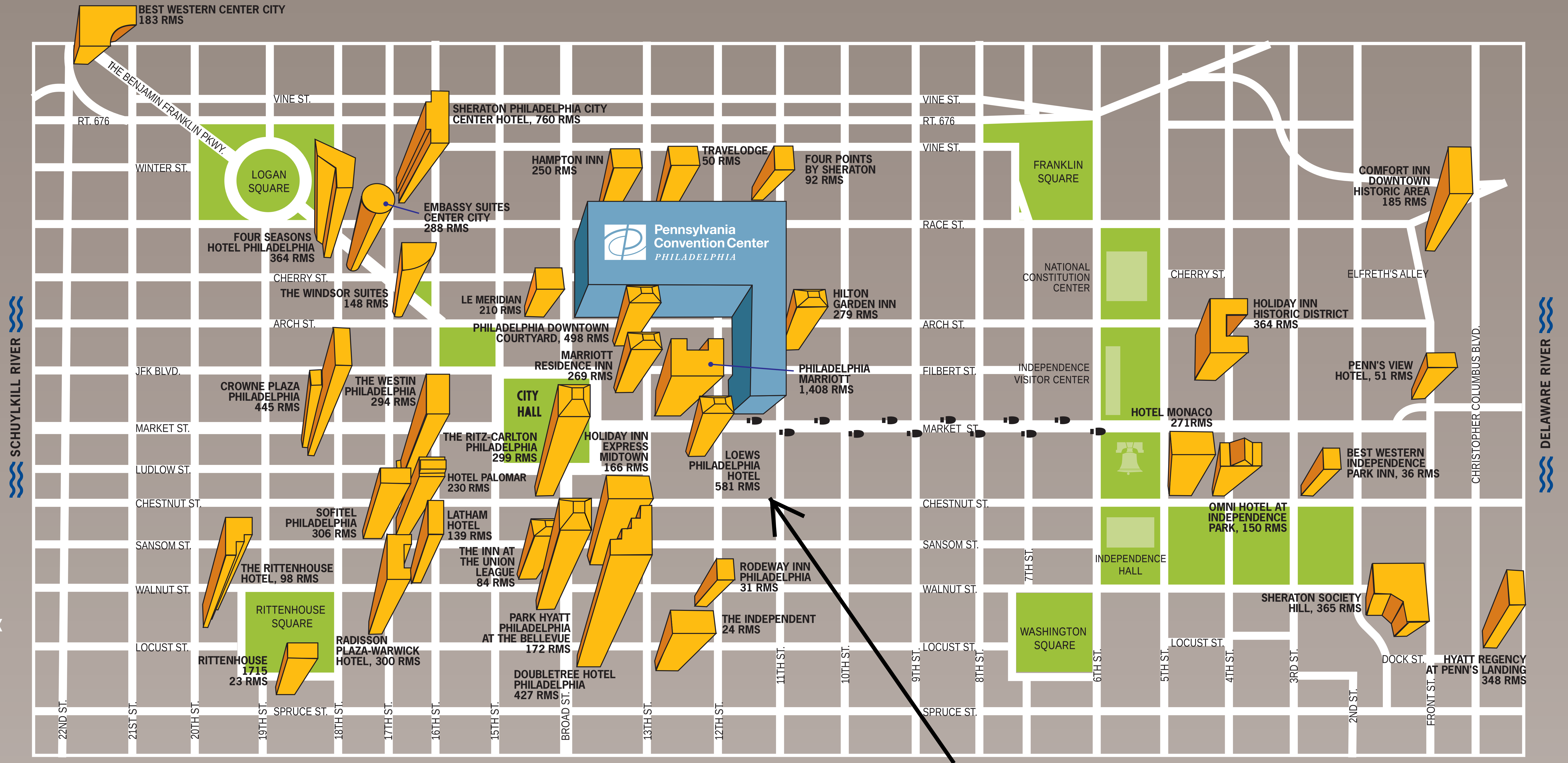

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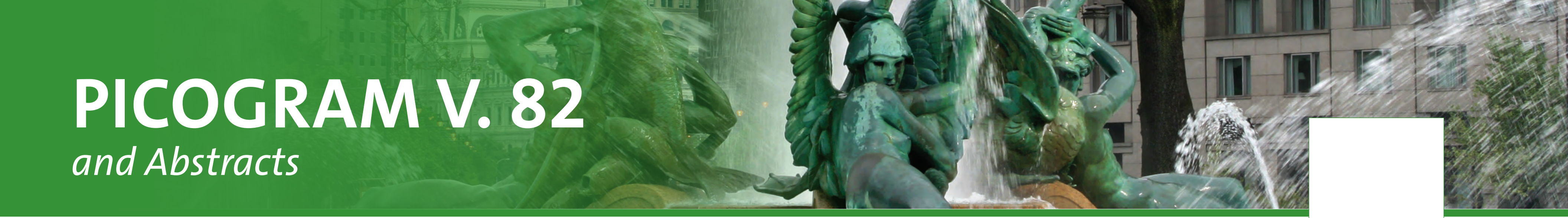

PICOGRAM V. 82

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