PICOGRAM v. 75

and Abstracts

Chemistry for and from Agriculture

American Chemical Society

236th National Meeting and Exposition

August 17-21, 2008

Philadelphia, Pennsylvania, USA

AGRO DIVISION

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4th Pan Pacific Pesticide Conference
236th National ACS Meeting

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Thank you for your continued support!

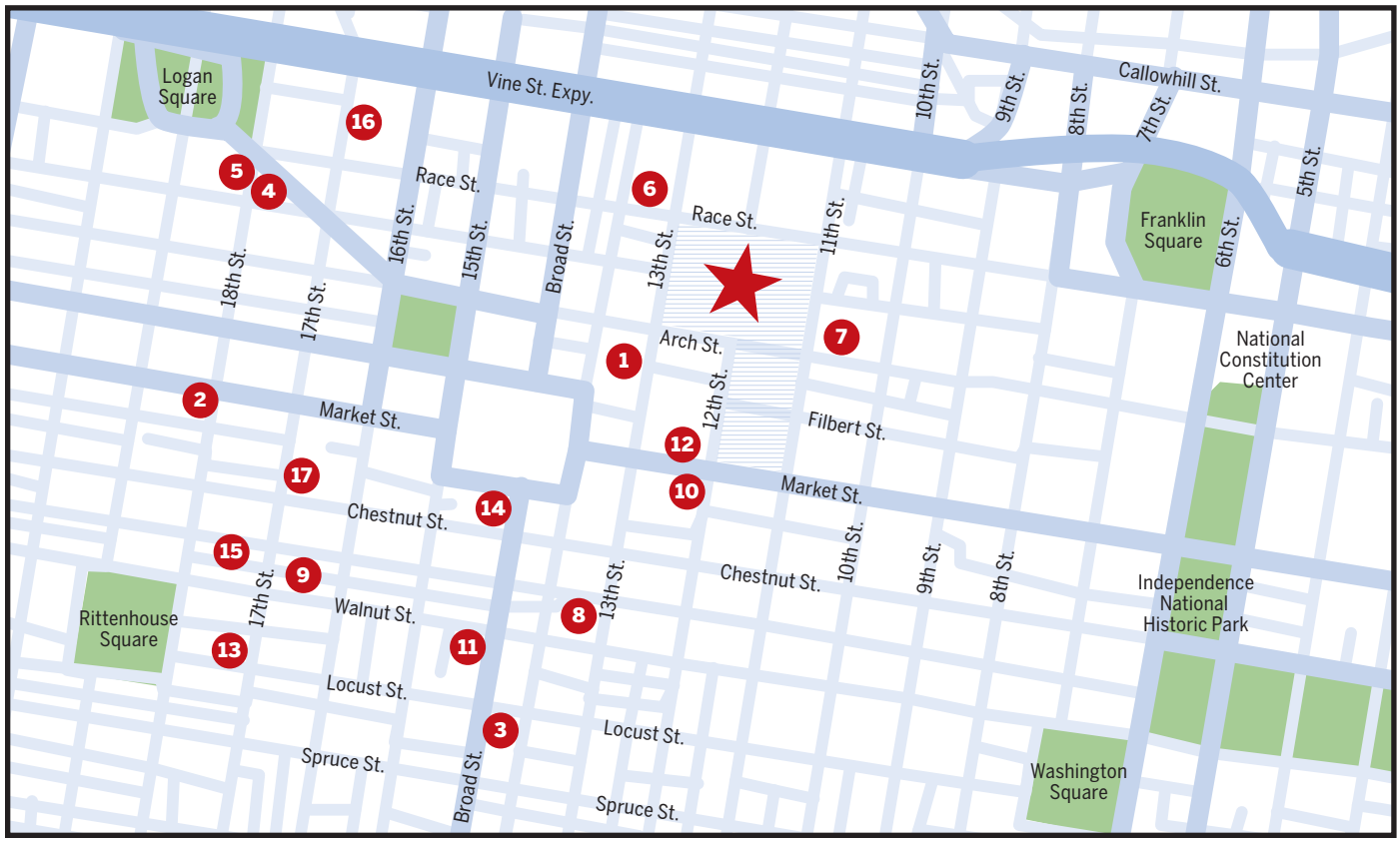
FALL 2008 AGRO MEETING SCHEDULE

Technical Program: page 53; Abstracts: page 70

Most SYMPOSIA & MEETINGS will be at the Crown Plaza City Center 2nd Floor Foyer, Liberty A/B/C, Independence A/B

SYMPOSIUM OR SESSION	ORGANIZER(S)	Sun	Mon	Tue	Wed	Thu
Agrochemical Residue and Metabolism Chemistry *Liberty C*	J. Johnston, D. Smith, T. Wehner	AM PM				
Synthesis & Chemistry *Liberty A*	T. Stevenson	AM PM				
Natural Products *Independence A/B*	C. Cantrell, S. Duke, P. Zubkoff	AM PM	AM PM			
AGRO Business Meeting - Open to all members *Declaration, Crown Plaza City Center*	J. Johnston	EVE				
AGRO Division Posters *Foyer*	K. Armbrust, J. Johnston		AM			
Evaluation of Agriculturally-Related Chemicals: Effects on Environmental, Animal & Human Health *Liberty A*	T. Anderson, E. Arthur, P. Rice, P. J. Rice		AM PM	AM PM		
Transitioning into Green Chemistry *Sheraton Philadelphia CC –Independence Blrm B*	Division of Chemical Education		AM PM			
Biological & Chemical Transformations of Animal Hormones & Veterinary Pharmaceuticals - *Liberty C*	D. Aga, P. J. Rice		PM			
Transitioning into Green Chemistry (Posters) *Sheraton Philadelphia CC –Independence Blrm B*	Division of Chemical Education		EVE			
Sci-Mix Poster Session *Pennsylvania Convention Center - Hall C*	K. Armbrust		EVE			
International Award for Research in Agrochemicals: Dr. David M. Soderlund - *Liberty C*	J. Bloomquist			AM PM		
Bioenergy Production: Challenges, Concerns, and Consequences - *Independence A/B*	C. Hapeman, J. Massey			AM PM		
Sterling Hendricks Memorial Lectureship: Dr. Fergus M. Clydesdale - *Liberty B*	J. Seiber, M. Tunick			Mid-day		
AGRO Social and Banquet *Liberty C*	J. Johnston			6-8p		
Agricultural Best Management Practices to Protect Chesapeake Bay Water & Air Quality - *Liberty C*	C. Hapeman, L. McConnell				AM PM	
Environmental Forensics *Independence A/B*	E. Arthur, G. Coimbatore, R. Cook, S. Mislankar				AM PM	
Reduced Risk Pesticides: Environmental Chemistry, Toxicology & Compatibility with IPM - *Liberty A*	A. Felsot, M. Brooks				AM PM	
Graduate Student Luncheon *Crowne Plaza, Location TBA*	L. McConnell, J. Johnston				noon	
Symposium Brainstorming, Brews & Blues *Independence A/B*	K. Armbrust				5-7p	
New Developments and Issues in Agrochemical Sciences - *Liberty C*	K. Armbrust					AM PM
Residential Pesticide Exposure Assessment Workshop *Independence A/B*	J. Driver, J. Evans, C. Lunchick, N. Tulve, D. Vogel, V. Zartarian					AM PM

Official Properties for the 236th ACS National Meeting in Philadelphia, PA



1 **Courtyard by Marriott Downtown**
21 North Juniper Street, Philadelphia, PA 19107
215-496-3200

2 **Crowne Plaza City Center**
1800 Market Street, Philadelphia, PA 19103
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3 **Doubletree**
237 South Broad Street, Philadelphia, PA 19107
215-893-1600

4 **Embassy Suites City Center**
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215-561-1776

5 **Four Seasons**
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6 **Hampton Inn Center City**
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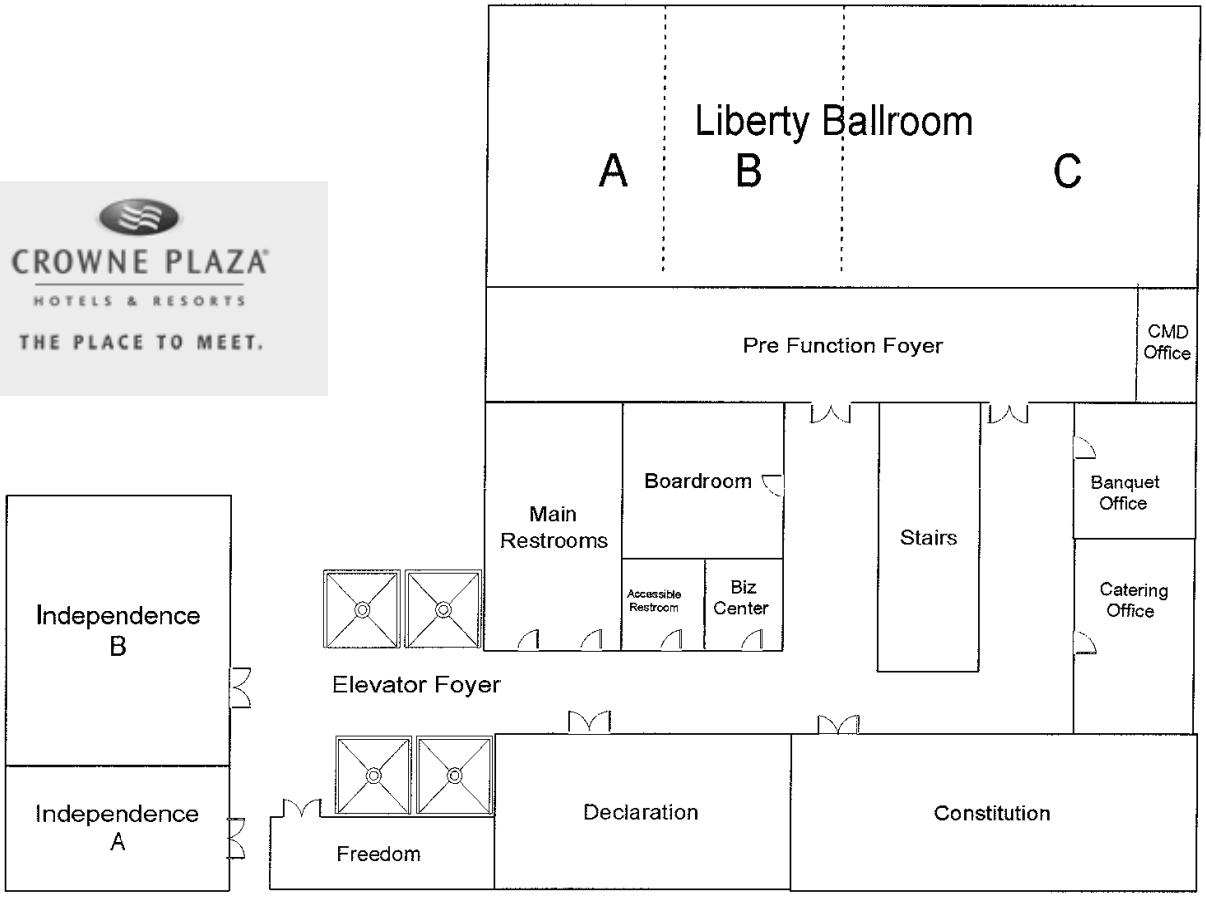

Crowne Plaza Hotel -Philadelphia Center City

2nd Floor Meeting Space

Editor's Notes

Color: The visual sensation dependent on the reflection or absorption of light from a given surface. The three characteristics of colors are hue, intensity, and value. (www.kn.att.com/wired/art2/guide/glossary.html)

Black & White versus Color

One of my professors from graduate school used to preach that things are either the same or they are different. Similar was just too squishy a word and we all chose to avoid it. We learned that experiments that yielded definitive results were easier to defend to colleagues, peer reviewers, and at the time, our dissertation committees. We learned that black & white was better, but then we came to understand that some comparisons and experiments do yield similar results; they are not cut & dry, black & white, or even the same or different.

We live in a world of color. Whether we perceive it or sense it or respond to it, color exists. As the color spectrum comes to AGRO, we turn to our more creative side with far-reaching possibilities. Colors are non-verbal communication; they can foster feelings of excitement, comfort, and even angst. But it's still chemistry! So be creative. Think in color. Reach outside the box. Expand your horizons. Explore the new ideas and venues in AGRO. We have a lot to offer.

Welcome to Philadelphia!
Cathleen J. Hapeman, PICOGRAM Editor
Communications Committee Chair

Special thanks to Laura, JJJ, Kevin, Peter, Chip, Sharon, John K., and others who have provided feedback and assistance in creating our new look and putting the PICOGRAM together. It wouldn't have happened without their help, insight, and appreciation of color.

Table of Contents

Hospitality Committee Report

Coffee Lounge – Boston

Fourteen companies have graciously donated a total of $1700 to support our Boston coffee lounge. Several firms provided literature to promote their services to meeting attendees. If you wish to join these companies in supporting our coffee lounge, please contact any of our committee members. Our coffee lounge offers a brief respite from our technical sessions as well provides an alternative forum for exchange of ideas. Those contributing to the coffee lounge in Boston are:

Compliance Services International
Environmental Turf & Services Inc.
Wildlife International, LTD
PTRL West Inc.
Waterborne Environmental, Inc.
Mandava Associates
North Coast Regional Science LLC
EN-CAS Analytical Laboratories
James F. Brady, Ph.D. LLC
Quality Associates Inc.
Critical Path Services
ADPEN Laboratories, Inc.
DAT Laboratory

AGRO Social – Boston

The AGRO Division Awards & Social was held at the Georgian Room of the Boston Park Plaza. Dr. Frederick Perlak was recognized as the recipient of the ACS International Award for Research in Agrochemicals. We also introduced the winners of the Young Scientists Pre- and Post-Doctoral Research Award Symposium to the revelers in attendance. Our inevitable prize drawing could not be stopped and drew smiles from surprised winners.

Patricia Rice, Joe Massey and Jim Brady have inherited the reins to the Hospitality Committee from Lillian Schwartz and Terry Spittler. We realize we have some awfully big shoes to fill but we are plunging ahead nevertheless.

SOCIAL CO-CHAIRS - Al Barefoot & Jeff Jenkins
HOSPITALITY COMMITTEE MEMBERS - James Brady, Julie Eble, Joe Massey & Patricia Rice

From the Chair's Desk

John J. Johnston

AGRO is GROWING STRONG!!!

For the first time in over a decade, our membership roster is growing!! AGRO's emphasis on delivering quality services to our members, expanding our scientific areas of interest and reaching out to other local, national, and international communities is proving to be a fruitful strategy.

AGRO Strategic Plan

Our Strategic Plan has energized AGRO membership. In line with our goal to provide increased value to our members, AGRO is developing workshops for professional enrichment to compliment the scientific symposia that we routinely offer at national meetings. Our goal to foster interactions among diverse communities led to AGRO's Environmental Impacts of Rodenticides Workshop at the Pan Pacific Conference. AGRO brought together a wide range of international scientists, regulators and applicators to identify improved approaches for using rodenticides to remove invasive rodents and permit subsequent restoration of rodent damaged ecosystems. AGRO growth in the international arena continues and is further detailed below. The strategic plan can be found on page 7.

National Meetings

For 2008 – 2009, AGRO will organize technical programming at one ACS national meeting per year. For 2008 and 2009, AGRO will be programming at the Fall National Meetings in Philadelphia and Washington, DC, respectively. Meeting selection for 2010 (Spring = San Francisco, Fall = Boston) is under discussion. If you have thoughts on the location of AGRO programming for 2010 (Boston and/or San Francisco), please email me. We will continue to supplement our programming at National ACS meetings with collaborative programming at a variety of national and international meetings.

Moving towards a Global Organization

It is clear that international collaborations offer increased opportunities for AGRO members. AGRO is planning collaborative meetings with:

1. **SETAC** (Society of Environmental Toxicology and Chemistry). AGRO will organize a symposium entitled "Modern Pesticides in Urban Environments: Risk Assessment and Management" symposium at the November 2008 SETAC North America Meeting in Tampa. Special thanks to Stewart Cohen and Pam Rice for leading this effort.

2. **GARP** (Brazilian Association of Professionals on Residues and Organic Pollutants), ABQ (Brazilian Chemical Association), and IUPAC (International Union of Pure and Applied Chemistry). We are planning to collaborate on a variety of symposia (e.g. Risk Assessment, Risk Management, Biotechnology) at the October 2009 International Workshop on Crop Protection Chemistry in Rio de Janeiro, Brazil. Given Brazil's vibrant agricultural industry, this should be an exciting meeting filled with a variety of opportunities for AGRO members. Laura McConnell is the AGRO lead on this project.

3. **FLAQ** (Latin American Federation of Chemical Associations). Kevin Armbrust, Cathleen Hapeman, and Joe Massey are co-organizing an Environmental Impacts of Bioenergy Symposium at the PRChem July 2008 symposium in Puerto Rico with Brad Miller, ACS-Office of International Activities.

4. **Fourth Pan Pacific Conference on Pesticide Science** (June, 2008) was a huge success with over 235 attendees! Kudos to AGRO organizers Al Barefoot and Joel Coats and to all those who served on the organizing and program committees.

From the Chair's Desk
(continued)

Providing Educational and Training Opportunities
In an effort to increase the value of AGRO membership and participation, we are adding workshops to our technical programming.

1. **Residential Pesticide Exposure Workshop** will be held in conjunction with AGRO programming at the upcoming National ACS meeting in Philadelphia.

2. At the **Pan Pacific Conference on Pesticide Science** (June 2008), we offered three unique educational opportunities for AGRO members
    - Environmental Risk Assessment Workshop
    - Rodenticide Chemistry and Environmental Impacts of Rodenticides Workshop
    - Stewardship of Neonicatinoids Workshop

3. AGRO is currently **soliciting ideas for future workshops** and training opportunities. Please forward your ideas to AGRO officers.

Improving Communication and Membership Services

1. **Communication Committee**
   The *Femtogram,* AGRO's electronic newsletter debuted this past year. As a supplement to our twice a year printed programs, the *PICOGRAM*, the *Femtogram* provides a means to keep AGRO membership abreast of important events, achievements, and opportunities throughout the year. Please forward all future *Femtogram* submissions to Tom Potter and *PICOGRAM* submissions to Cathleen Hapeman.

2. **AGRO Logo**
   We have a new logo for AGRO. The new logo was developed with input from a wide range of AGRO members and illustrates AGRO's expansive range of scientific interests. We believe the logo will attract a wide demographic of interdisciplinary scientists. The AGRO logo was unveiled at the Pan Pacific Conference and was well received. The new AGRO logo and supporting slogan can be found on the cover of this *PICOGRAM*.

3. **Electronic Voting**
   This year, we completed internet based voting for selection of new AGRO officers and committee members. The internet based voting process nearly doubled the percentage of AGRO membership that participated in the electoral process. And it was not as expensive as paper ballots! Kudos to Laura McConnell for spearheading this project.

4. **AGRO website**
   In line with our efforts to attract a broad membership base, the executive committee has agreed that AGRO needs to update our website. We hope to have the new site on-line by the Fall ACS meeting.

It has been a pleasure and an honor to serve as the 2007 – 2008 AGRO Chair. Thanks to everyone who helps to make AGRO a valuable, vibrant, and vivacious professional organization!

JJJ

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LFR

Three-year Strategic Plan for AGRO

Developed January 13, 2008

MISSION/OBJECTS
By-Law I. Name and Objects

Existing

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.

Recommended Replacement/Mission Statement

The AGRO Division promotes knowledge benefiting society
through advancements in agricultural, public health,
and environmental science and technologies.

VISION

The AGRO Division will increase its recognition as
a global leader in agriculture, public health, and environmental sciences
by engaging and energizing its membership to foster global interactions
that provide innovative solutions to challenges facing our world.

GOALS

Goal 1: Enhance the membership experience by providing accessible and innovative programs, educational products, mentoring and career services and opportunities for professional development and recognition.

Patricia Rice— patricia.rice@basf.com; 919-547-2668
Dan Stout— stout.dan@epa.gov; 919-541-5767

Goal 2: Foster constructive interactions among diverse communities to provide solutions to agricultural, public health, and environmental concerns.

Joe Massey— jmassey@pss.msstate.edu; 662-325-4725
John Johnston— john.j.johnston@usda.gov

Goal 3: Build the infrastructure for becoming a global center for solutions to problems of plant, animal, environmental, and public health protection, and advancing scientific and regulatory harmonization.

Chris Peterson— cjpeterson@fs.fed.us; 662-325-0199

Awards Committee Report

In 2008 and 2009, the International Award for Research in Agrochemicals will be co-sponsored by DuPont Crop Protection and BASF Corporation. **Dr. David M. Soderlund**, Cornell University, will receive the International Award at the Fall 2008 ACS National Meeting in Philadelphia, PA for his discoveries on the insect sodium channel and insecticides that disrupt its action. An award symposium has been organized by Dr. Jeffrey Bloomquist. **Dr. R. Don Wauchope**, retired USDA-ARS, will receive the International Award at the Fall 2009 ACS National Meeting in Washington, DC for his research on pesticide fate and in defining their chemical properties. His international contributions and dedication to AGRO have been extensive and extraordinary. A full-day award symposium is being organized.

Dr. Fergus M. Clydesdale, University of Massachusetts, will receive the 2008 Sterling B. Hendricks Memorial Lectureship Award for his work in food policy and regulation and for his research on the physiochemical changes in food that alter nutritional bioavailability, physiological effects, food quality, food acceptability, overall health, and quality of life.

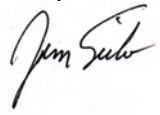
Dr. Ashli Brown will receive the AGRO New Investigator Award for her multifaceted research approach in renewable alternative fuels. She will present her paper in the Biofuels Production: Challenges, Concerns, and Consequences Symposium at the Fall 2008 ACS National Meeting in Philadelphia. This new award is sponsored by Dow AgroSciences. In addition, twenty-one students received the AGRO Education Awards which are sponsored by Bayer CropScience.

Dr. Allan S. Felsot, Professor and Extension Specialist, Entomology/Environmental Toxicology, Washington State University, will receive the Agrochemical Division Fellow Award at the Fall 2008 ACS meeting in Philadelphia. Dr. Felsot is recognized for his outstanding contributions to the endeavors of the Division and to the science of agrochemicals and his exceptional work over the years with students as the chair, organizer, and moderator of the young Scientists Research Recognition Award and Symposium.

Nominations for the 2010 International Award for Research in Agrochemicals are currently being solicited by the Awards Committee. The Awards Committee is also accepting new award nominations for the Division Fellow Award. The nomination forms and criteria for both awards can be found in the *PICOGRAM* on pages 21 and 23, respectively. Please consider nominating a deserving colleague. The deadlines each year are December 31 for the International Award and May 31 for the Fellow Award. Finally, USDA-ARS is seeking nominations for the 2009 Sterling B. Hendricks award. Deadline for nominations is November 5, 2008. Additional information can be found on page 25.

Congratulations to Drs. Brown, Clydesdale, Felsot, Soderlund, and Wauchope and to all our students!

Respectfully submitted,



James N. Seiber, Chair
Awards Committee

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- **Food Safety and Nutritional Safety.**

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You Are Cordially Invited To:

The AGRO Division Awards & Social

Meet with Friends Old and New
&
Celebrate AGRO's Award Winners

International Award for
Research in Agrochemicals
Dr. David M. Soderlund

AGRO New Investigator Award
Dr. Ashli Brown

AGRO Education Awards

Fun, Food, Good Company, Door Prizes, and a Cash Bar
6:00 – 8:00 pm Tuesday, August 19
Liberty C, Crowne Plaza City Center

ALL AGRO DIVISION MEMBERS, SPEAKERS AND THEIR GUESTS, SPOUSES/SOs,
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ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS

Presented by the AGRO Division of ACS
Co-Sponsored by BASF Corporation & DuPont Crop Protection

Dr. David M. Soderlund will receive the International Award for Research in Agrochemicals for his recognized work as a leading, international authority on the toxicology and mode of action of insecticides affecting ion channels, especially the pyrethroid insecticides. His research, which has spanned more than 30 years, has produced numerous important contributions to the science of insecticide toxicology. Dr. Soderlund has contributed to studies of the metabolism and mode of action of the precocenes and related insect anti-juvenile hormones, the actions of insecticides on the γ-aminobutyric acid (GABA) receptor/chloride channel complex, and the molecular biology of insect GABA receptors. However, he is best known for his research on the pyrethroids and other compounds affecting voltage-sensitive sodium channels.

Dr. Soderlund's early research on the *in vitro* metabolism of pyrethroids established structure-activity relationships for pyrethroid biotransformation and defined pyrethroid toxicokinetics in insects. In the mid-1980s, the focus of his research shifted to the elucidation of the mechanism of pyrethroid action on sodium channels. Studies with vertebrate brain preparations characterized the pyrethroid recognition site on brain sodium channels and its relationship to sites that bind other drugs and neurotoxins and also defined the action of two other chemical classes of insecticides, the *N*-alkylamides and pyrazoline-type compounds, on brain sodium channels.

Dr. Soderlund was among the first in the insecticide toxicology research community to incorporate the emerging tools and strategies of molecular neurobiology in research on insecticide action and resistance. His laboratory developed molecular probes to isolate sodium channel gene sequences orthologous to the para sodium channel gene of *Drosophila melanogaster*, which led to the molecular cloning of the house fly ortholog of para and the identification of sequence polymorphisms in susceptible and pyrethroid-resistant flies. The Soderlund group also achieved the functional heterologous expression of house fly sodium channels in the oocytes of the frog, *Xenopus laevis*, and employed this system to demonstrate that sodium channel sequence polymorphisms associated with pyrethroid resistance reduced the insecticide sensitivity of the channel. Dr. Soderlund's recent research has also exploited the heterologous functional expression of sodium channels to explore the actions of pyrethroid and pyrazoline-type insecticides on cloned rat and human sodium channel isoforms. These studies not only have identified differences in sensitivity between isoforms but also provide an experimental platform for the study of human sodium channels, an area of research with important regulatory implications.

Dr. Soderlund received a B.S. degree in Biology from Pacific Lutheran University in 1971 and a Ph.D. in Entomology from the University of California at Berkeley in 1976. After postdoctoral research at Rothamsted Experimental Station in the U.K., he joined the faculty of the Entomology Department at Cornell University's New York State Agricultural Experiment Station in Geneva, where he is currently Professor of Insecticide Toxicology and chair of the department. Dr. Soderlund is also Director of the Northeast Region IR-4 Program, part of a national cooperative program between the USDA and land grant universities to register crop protection tools for use on specialty crops.

An all-day symposium to honor Dr. Soderlund will be held on Tuesday, August 19.

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Solubility Studies
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Octanol/Water Partition Coefficient
Product Storage Stability
Corrosion Characteristics
Physical Chemical Properties
Release Rate of Biocides

Plant Sciences and Field Research

Project Management
Worker Exposure
Dislodgeable Residues
Import Tolerance
Efficacy - Field & Greenhouse
Confined Crop Rotation
Magnitude of Residue
Soil Dissipation

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Fish Bioconcentration
Marine & Fresh Water Organisms
Aquatic & Terrestrial Phytotoxicity
Sediment Toxicity Studies
Non-Target Insect Tests
Shellfish Residue Studies

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A Nutritional Odyssey: From Famine to Feast, Can Science & Policy Solve the Dilemma?

Dr. Fergus M. Clydesdale is one of the world's premier experts in food policy and regulation, a reputation based solidly on his outstanding research of physiochemical changes in food that alter nutritional bioavailability, physiological effects, food quality, food acceptability, overall health, and quality of life. He is one of the world's leading experts in food science communication. This combination of work in food science, nutrition, public health policy, and consumer acceptance gives Dr. Clydesdale a unique perspective in defining food policy.

Dr. Clydesdale is currently Distinguished Professor and Head of the Department of Food Science at the University of Massachusetts, Amherst, as well as Director of both its Strategic Research Alliance and Strategic Policy Alliance, also in the Department of Food Science. His work has led to many tasks including serving on numerous advisory committees concerning health, diet, and nutrition, such as those of the Federation of American Societies for Experimental Biology (FASEB), the U.S. Senate, International Life Sciences Institute-North America, Codex Alimentarius, and the Keystone Committee on National Policy on Diet and Health. He has also been a special consultant to the U.S. Food and Drug Administration (FDA).

In addition to having served as chair of the Food Forum of the Food and Nutrition Board of the National Academy of Sciences (NAS) three terms, Dr. Clydesdale served on the NAS Institute of Medicine Committee on the Use of Dietary Reference Intakes in Nutrition Labeling, the NAS Food Safety Oversight Commission, the Institute of Food Technologists (IFT) Expert Committee on Functional Foods (as chair), the 2005 Dietary Guidelines Advisory Committee, and the FDA Working Panel to evaluate Olestra (as chair) and the FDA Food Advisory Committee. He has also received the Council for Agricultural Science and Technology's Charles A. Black Award for scientific communication. He was inducted as an Honorary Member of L'Association Internationale Nicolas Appert, and was named a Lifetime National Associate of the National Academy of Sciences, honorary Fellow of the Australian Institute of Food Science and Technology, Fellow of the American College of Nutrition, and Fellow of the International Academy of Food Science and Technology. Dr. Clydesdale has published more than 375 scientific articles, coauthored or edited 20 books, and is the editor of Critical Reviews in Food Science and Nutrition.

Dr. Clydesdale will deliver his lecture immediately following presentation of the Sterling Hendricks Award on August 19 at 11:30 am in the Crowne Plaza City Center – Liberty B.

A reception will follow at 12:30 pm.

2008 AGRO Early Investigator

Presented by the AGRO Division of ACS
Sponsored by Dow AgroSciences

Dr. Ashli Brown is an Assistant Professor at Mississippi State University in the Department of Biochemistry and Molecular Biology. The rapidly depleting crude oil reserves and issues such as global climate change, environmental concerns, and energy security, have prompted her to focus her research on renewable alternatives such as green fuel, biodiesel, and bioethanol. She believes feedstocks which do not compete with food crops and the development of novel uses for the co-products (glycerol and distiller's grains) produced in these processes are required for these alternatives to become economically-feasible energy sources.

In collaboration with a team of researchers from the Renewable Fuels and Chemicals Laboratory at the David C. Swalm School of Chemical Engineering at Mississippi State University, Dr. Brown is using oleaginous yeast, which has been cultivated on medium containing glycerol alone and in combination with a variety of sugars as a potential lipid source. The oil produced by these microbes can be catalytically cracked to make bio-petroleum. She is identifying and characterizing the cellulase-hemicellulase complexes of the oleaginous yeast used in their microbial oil project in order to optimize the fermentation of biomass into biofuels. Dr. Brown and her colleague Dr. Jeffery Wilkinson (Biochemistry and Molecular Biology, Mississippi State University) with the help of Dr. Paul Williams (USDA-ARS, Corn Host Plant Resistance Unit) are characterizing critical factors in *Aspergillus* that control the degradation of aflatoxin in order to use aflatoxin contaminated corn as a substrate for ethanol production.

An additional challenge with biodiesel is its relatively short shelf life. Oil breakdown can occur through hydrolysis and oxidation of unsaturated fatty acid methyl esters resulting in an increased acid number and viscosity. Working in collaboration with the Mississippi State Chemical Laboratory (MSCL), she is currently developing a sensitive online, automated GC/MS method for monitoring oxidation.

Dr. Brown graduated with honors from the University of South Florida in December 2003, with a PhD in Chemistry. Her graduate research was focused in biochemistry where she characterized the enzyme arginine kinase from the American cockroach, a leading causative agent in allergenic asthma. The extensive kinetic inhibition studies conducted in this project are currently being evaluated for potential ways to control population growth. In 2006, Dr. Brown completed a postdoctoral fellowship with the USDA-ARS where she implemented a "push-pull" strategy to aid in the management of the multicolored Asian Lady Beetle. Critical to the success of this project was her design and development of a unique method to monitor swarming beetles using GC/MS in conjunction with ARC-GIS software. These educational experiences have led Dr. Brown to value multi-disciplinary approaches to agricultural challenges. It is her hope that her multifaceted research approach in renewable alternative fuels will increase the profitability and the bond between American agriculture and bio-refineries.

Dr. Brown will present her paper in the
Bioenergy Production: Challenges, Concerns, and Consequences Symposium
on Tuesday afternoon, August 19.

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Website: www.ptrl-europe.de

Internet Home Page: www.ptrlwest.com

Good science, no surprises.

Keynote Address

Bioenergy Production: Challenges, Concerns & Consequences

The Evolving Paradigm of Agriculture as a Supplier of Energy and Chemicals

Dr. Larry P. Walker is a native of Detroit, Michigan and a graduate of Michigan State University with a B.S. in physics. His interest in renewable resources and environmental research led him to complete M.S. and Ph.D. degrees at Michigan State University in agricultural engineering. During his 29 years at Cornell, he has been involved in a number of biomass to energy and chemical projects including an assessment of New York State biomass resources available for ethanol production, farm-scale methane production and co-generation, the application of nanotechnology characterizing and studying import biocatalysts for industrial biotechnology, and optimization of solid-state fermentation for the production of biocontrol products. His nanotechnology research is focused on using single molecule detection methods to study cellulase adsorption and hydrolysis mechanisms and the application of these methods to molecular ecology.

Dr. Walker is a professor of Biological and Environmental Engineering and is the Director of the Northeast Sun Grant Institute of Excellence. The Institute serves as a repository of information and data for the NE-SGI region biobased energy and products research, education and outreach activities. Dr. Walker is also the coordinator of a Cornell faculty cluster that is interested in the development of sustainable agriculture-based industries. He has served as a member of the National Biomass Research and Development Technical Advisory Committee, is currently a member of the Academic Steering Committee for the American Council for Renewable Energy, is Co-Chief Editor for the journal "Industrial Biotechnology," and is an ACS member.

Join us for Dr. Walker's inspiring presentation on this international issue on Tuesday morning, August 19.

In addition, several members of Dr. Walker's Laboratory will present posters at the AGRO Poster Session on Monday morning, August 18.

PAST AWARDEES OF THE BURDICK AND 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 WINNERS OF THE ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS

Co-Sponsored by BASF Corporation & DuPont Crop Protection

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

CALL FOR NOMINATIONS
ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS

Presented by the AGRO Division of ACS
Co-Sponsored by BASF Corporation & DuPont Crop Protection

I hereby nominate _____ as a candidate for this award.
(First) (Middle) (Last)

Complete the following for your candidate:

1. Birthplace Date of Birth Citizenship

2. Business Address:

3. **IMPORTANT** Please Attach:
   a. A **Curriculum Vitae** for your candidate which describes the individual's career data including: places and nature of employment, professional affiliations, honors received, and a list of publications and patents. Please provide 11 copies.
   b. A **description** (200 – 1000 words) of the reasons why your nominee should receive this award, stressing the individual's major accomplishments.
   c. Nominations often include one or two letters of support, but this is optional.

Submitted by: _____ Date: _____

Address: _____

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 at the spring meeting of ACS.

The nominating official(s) should be prepared to assist in organizing a symposium and dinner at the National ACS meeting in honor of the awardee.
Please, return this completed form to:

Dr. James Seiber
USDA-ARS, WRRC
800 Buchanan St.
Albany, CA 94710
510-559-5600 – phone
510-559-5963 – fax
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CALL FOR NOMINATIONS
AGRO Division Fellow Award

The Division has established the 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 AGRO Division of ACS and to the 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.

Dr. James Seiber
USDA-ARS, WRRC
800 Buchanan St.
Albany, CA 94710
510-559-5600 – phone
510-559-5963 – fax
James.seiber@ars.usda.gov

PAST WINNERS OF THE AGRO DIVISION FELLOW AWARD

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. Hollingworth
	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 Nelson
2005	Dr. Rodney Bennett
2006	Dr. Terry Spittler
2007	Dr. J. Marshall Clark
	Dr. Ann T. Lemley
	Dr. R. Donald Wauchope

PAST AWARDEES OF THE STERLING B. HENDRICKS MEMORIAL LECTURESHIP

Sponsored by USDA-ARS
and
Co-Sponsored by the AGRO & AGFD Divisions of ACS

1981 Norman E. Borlaug, Nobel Laureate and Director of International Maize and Wheat Improvement Center, Mexico City

1982 Warren L. Butler, Professor of Biology and Past Chairman, Biology Department, University of California at San Diego

1983 Melvin Calvin, Nobel Laureate and University Professor of Chemistry, University of California at Berkeley

1984 Frederick Ausubel, Professor of Genetics, Harvard Medical School and Massachusetts General Hospital

1985 Alan Putnam, Professor, Department of Horticulture and Pesticide Research Center, Michigan State University

1986 Ralph Hardy, President, Boyce Thompson Institute for Plant Sciences, Cornell University, and Deputy Chairman, BioTechnica International

1987 Mary-Dell Chilton, Director of Biotechnology Research for Ciba-Geigy Corporation, Research Triangle Park, North Carolina

1988 Bruce N. Ames, Chairman, Department of Biochemistry, University of California at Berkeley

1989 Sanford A. Miller, University of Texas Health Science Center at San Antonio

1990 Roy L. Whistler, Emeritus Professor of Purdue University

1991 Peter S. Eagleson, Professor of Civil Engineering, Massachusetts Institute of Technology

1992 John E. Casida, Professor of Chemistry and Toxicology, University of California at Berkeley

1993 Philip H. Abelson, Deputy Editor, *Science*, and Scientific Advisor to AAAS

1994 Wendell L. Roelofs, Liberty Hyde Bailey Professor of Insect Biochemistry, Cornell University

1995 Winslow R. Briggs, Director Emeritus, Department of Plant Biology, Carnegie Institution of Washington

1996 Hugh D. Sisler, Professor Emeritus, Department of Plant Biology, University of Maryland

1997 Ernest Hodgson, Head, Department of Toxicology, North Carolina State University

1998 Martin Beroza, Chief, Organic Chemicals Synthesis Laboratory, Agricultural Research Service

1999 Bruce D. Hammock, Professor, Department of Entomology, University of California at Davis

2000 William S. Bowers, Professor, Department of Entomology and Chemical Ecology at the University of Arizona

2001 Malcolm Thompson, Research Chemist, USDA-ARS, Beltsville, Maryland (retired)

2002 Ervin E. Leiner, Professor Emeritus, Biochemistry Department, University of Minnesota

2003 Dr. Kriton Kleanthis Hatzios, VA Agricultural Experiment Station

2004 Dr. Robert L. Buchanan, Food & Drug Administration

2005 Dr. Donald Sparks, University of Delaware

2006 Dr. Stanley B. Prusiner, Institute for Neurodegenerative Diseases, University of California, San Francisco

2007 Dr. Bruce E. Dale, Department of Chemical Engineering & Materials Science, Michigan State University

CALL FOR NOMINATIONS
2008 STERLING B. HENDRICKS MEMORIAL LECTURESHIP

The Agricultural Research Service (ARS), USDA's primary research agency, is seeking nominations for the

2009 Sterling B. Hendricks Memorial Lectureship

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. Nominees may be outstanding, senior scientists in industry, universities, or government positions. Current ARS employees are not eligible.

The Award will be presented during the American Chemical Society National Meeting held in Washington, DC on August 16-20, 2009 prior to the Lecture. (Giving the presentation is a requirement of the honor.) The Divisions of Agrochemicals and Agricultural & Food Chemistry 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.

To make a nomination, send
(1) a letter explaining the nominee's contributions to chemistry and agriculture, and
(2) a current curriculum vitae to:

Kim Kaplan, Lecture Coordinator
(301) 504-1637
at either
kaplan@ars.usda.gov
or
ARS Information Office
Room 1-2253, Mail Stop # 5128
5601 Sunnyside Ave
Beltsville, MD 20705

Electronic transmission is best; otherwise, use a carrier, such as FedEx.
The deadline for nominations is November 5, 2008 (COB, EST).

CALL FOR APPLICANTS
AGRO NEW INVESTIGATOR AWARD

Sponsored by Dow AgroSciences

The AGRO Division of ACS is sponsoring the New Investigator Award starting for the Fall meeting 2009 in Washington, DC. The purpose of the New Investigator Award is to recognize scientists who have obtained a doctoral degree and have been actively conducting academic, industrial, consulting, or regulatory studies.

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 meetings. Thus, for the first award, applications will be considered from scientists who have obtained their doctorates no earlier than September 2003.

Applications for the New Investigator Award will consist of the following elements:

1. Submission of a **maximum five page paper describing the area of research** or other work relevant to the broad mission of the Division of Agrochemicals. The paper may be structured as a research paper (i.e., contains the main elements of a typical journal article) or as a critical review of one's particular contributions to the scientific fields covered by the Division of Agrochemicals. The Division is especially interested in work on all aspects of agrochemicals. Agrochemicals 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.). Studies of veterinary pharmaceuticals and antibiotics are also included in the Division's mission. The Division is also interested in chemical products made from crops, including biofuels. The categorical areas of study related to agrochemicals are very broad and include environmental chemistry, toxicology, exposure assessment, risk characterization, risk management, and science policy. The Division especially encourages submissions related to public health protection as well as crop, livestock, aquaculture, and wildlife protection.

2. Submission of a **150 word abstract** for the submitted paper.

3. Submission of at least **one letter of recommendation** from a current supervisory scientist (e.g., a business manager, a departmental chair, etc.)

4. Both the paper and letter of recommendation should be **submitted** to Dr. Allan Felsot via email (afelsot@tricity.wsu.edu) **no later than February 20, 2009** for consideration of an award at the Fall meetings in Philadelphia.

The award winner will be expected to deliver an oral presentation in their area of interest in one of the Agrochemical Program sessions. The award winner will receive a $1000 honorarium, a commemorative plaque, one-year complementary membership in the Division of Agrochemicals, a meeting registration fee waiver, and reimbursement for travel expenses in association with the Philadelphia meeting.

AGRO EDUCATION AWARDS FOR GRADUATE STUDENT TRAVEL

Sponsored by Bayer CropScience

Twenty-one graduate students have been awarded AGRO Division travel grants to present their research posters at the ACS National Meeting in Philadelphia. First and second place winners will be announced at the AGRO Awards & Social on Tuesday evening. Abstracts can be found beginning on page 70.

A. Al-Taani, G. Miller. Thermal fixation of atmospheric nitrogen to nitrate on titanium dioxide and desert soil surfaces. *Department of Natural Resources and Environmental Science, University of Nevada.* AGRO 44

A. -M. Alves, S. B. Symington, J. M. Clark. Deltamethrin increases peak current and slows deactivation kinetics of the voltage-sensitive calcium channel ($Ca_V2.2$) from rat brain following PKC-dependent phosphorylation. *Molecular and Cellular Biology Program, University of Massachusetts.* AGRO 61

N. A. Andrade, L. L. McConnell, A. Torrents, M. Ramirez. Fate of PBDEs in biosolids and soil from commercial farms that receive biosolids application. *Department of Civil and Environmental Engineering, University of Maryland, College Park.* AGRO 49

M. M. Bigelow-Dyk, Z. Chen, Y. Li, H. Vega, R. I. Krieger. Determinants of human pesticide exposure following use of fipronil-containing pet products. *Department of Entomology, University of California-Riverside*. AGRO 56

Z. Chen, H. M. Vega, R. I. Krieger. Bis(chlorophenyl)acetic acid (DDA), a water-soluble biomarker of DDT metabolism in humans. *Department of Entomology, University of California-Riverside*. AGRO 57

A. B. Giasuddin, S. R. Kanel, J. Locklin, R. Chittaranjan. Removal of methyl parathion from water by nanoscale zero-valent iron. *Department of Biological and Agricultural Engineering, University of Georgia.* AGRO 52

A. D. Gross, J. R. Coats, M. J. Kimber, P. Ribeiro. Insecticidal activity of monoterpenoids at the octopamine receptor. *Department of Entomology, Iowa State University*. AGRO 59

R. E. Hunter, Jr., A. Riederer, P. B. Ryan. Method development for multiresidue pesticide extraction from food. *Department of Chemistry and Rollins School of Public Health, Emory University*. AGRO 53

L. J. Jenson, D. C. Klorig, S. L. Paulson, J. R. Bloomquist. Induction of neuronal phenotype in Sf21 insect cells. *Department of Entomology, Virginia Polytechnic Institute and State University*. AGRO 60

A. M. Jessick, K. L. Henderson, T. B. Moorman, J. R. Coats. Erythromycin: A look at a veterinary antibiotic's bioavailability in an aquatic microcosm. *Department of Entomology, Iowa State University*. AGRO 51

Y. Li, M. M. Bigelow-Dyk, Z. Chen, H. M. Vega, R. I. Krieger. Preformed organophosphorous insecticide biomarkers in fruits and vegetables: An in-depth study on California strawberries. *Department of Entomology, University of California-Riverside*. AGRO 55

J. N. Malin, P. L. Hayes, F. M. Geiger. Interactions of nitrate and cadmium ions at model environmental interfaces studied by second harmonic generation. *Department of Chemistry, Northwestern University.* AGRO 45

J. M. Mutunga, T. D. Anderson, P. R. Carlier, J. R. Bloomquist. Differential potency of bivalent anticholinesterases as a model for the molecular design of selective insecticides. *Department of Entomology, Virginia Polytechnic Institute and State University.* AGRO 62

D. A. G. Navarro, D. S. Aga, J. R. Coats, K. L. D. Henderson, T. Moorman, J. Bidwell. Determination of the effect of pH, ionic strength, and humic acids on the soil sorption coefficients (K_d) of tylosin and erythromycin antibiotics. *Department of Chemistry, University at Buffalo, The State University of New York, Buffalo.* AGRO 50

G. E. Paluch, J. R. Coats. Repellency of botanical sesquiterpenoids to arthropods. *Department of Entomology, Iowa State University*. AGRO 54

A. Podrygula, M. M. Bobylev. Accelerated Leuckart reaction in the synthesis of agrochemicals and pharmaceuticals. *Department of Chemistry, Minot State University.* AGRO 43

J. P. Strycharz, S. H. Lee, W. Sun, B. R. Pittendrigh, J. M. Clark. Polygenic resistance in the highly DDT-resistant 91-R strain of *Drosophila melanogaster* involves decreased penetration, increased metabolism, and rapid excretion. *Department of Veterinary and Animal Science, University of Massachusetts.* AGRO 58

F. Tong, J. R. Coats. Modulation of monoterpenoids on [^{3}H]-TBOB binding to house fly GABA receptor. *Department of Entomology, Iowa State University.* AGRO 63

M. E. Vasquez, R. S. Tjeerdema. Partitioning of etofenprox under simulated California rice growing conditions. *Department of Environmental Toxicology, University of California-Davis.* AGRO 47

Y. Yang, W. Hunter, J. Gan, S. Tao. Effects of black carbon on pyrethroid bioavailability in sediments. *College of Urban and Environmental Sciences, Peking University and Department of Environmental Sciences, University of California-Riverside.* AGRO 48

P. Ye, A. T. Lemley. Adsorption effect on the degradation of carbaryl, mecoprop, and paraquat by AFT in an Swy-2 montmorillonite clay slurry. *Graduate Field of Environmental Toxicology, Cornell University.* AGRO 46

Congratulations to all our winners!

All Graduate Students and PostDocs

You Are Cordially Invited To Attend

The Graduate Student Box Luncheon

Attendees will discuss:

- Potential outreach activities for graduate students and postdocs
- Student-led symposia in Washington DC and in 2010

Wednesday 12:00 – 1:00 pm
Crowne Plaza City Center – Room TBA

CONTACT ANY DIVISION OFFICER IF YOU WISH TO ATTEND
AS RESERVATIONS ARE REQUIRED

THE FOOD IS FREE!

CALL FOR APPLICANTS
AGRO Education Awards

UNDERGRADUATE AND GRADUATE STUDENT RESEARCH

SUPPORT FOR POSTER PRESENTATIONS AT THE 2009 FALL MEETING IN WASHINGTON, DC

The AGRO Division of ACS has established an endowment fund that will be used to promote an understanding of the role of chemistry in agriculture as embraced in the following areas related to chemistry for and from agriculture. Potential topics include synthesis, metabolism, regulatory, biotechnology, delivery, risk assessment, resistance, residues, mode of action, fate/behavior, biofuels, and bioenergy. To address this mission, awards will be made through the Division's Education Committee.

Proposals are sought for the 2009 awards. Undergraduate and graduate students will be awarded up to $600 each to help defray costs of attendance to give poster presentations at the ACS 2009 Fall Meeting, which will be held August 16 – 20, 2009 in Washington, DC. Posters will be displayed in a special poster session of the ACS Division of Agrochemicals. First, Second, and Third place winners will receive an additional cash award. The subject of the presentation should fall within the areas listed in the introductory sentence.

To apply, a graduate student should submit the following to be received no later than March 16, 2009 (tentative):

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 items 1 and 2 to the ACS OASYS abstract submission website.
Submit item 3 as a Word or pdf file to Dr. John Johnston at john.j.johnston@aphis.usda.gov.

Direct questions to:

Dr. John J. Johnston
USDA/APHIS/National Wildlife Research Center
4101 LaPorte Avenue
Fort Collins, CO 80521
(970) 266-6082

Abstracts will be reviewed by the Education Committee.
Submitters will be notified of their selection status in May 2009.

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Notes from the Program Chair

Kevin J. Armbrust

The 236th National Meeting in Philadelphia will feature a strong technical program with over 235 papers in three concurrent symposia on Sunday through Wednesday, and a special workshop addressing "Residential Pesticide Exposure Assessment" to be held on Thursday. Symposia included at this meeting will address reduced risk pesticides, agrochemical residue and metabolism chemistry, energy issues and agriculture, biochemical and chemical transformations of animal hormones and veterinary pharmaceuticals, evaluation of the impacts on human, environmental and animal health of agriculturally related chemicals, natural products including i-RNA technology, environmental forensics, and the synthesis of agrochemicals. A symposium exploring developments in agricultural best management practices to protect Chesapeake Bay water and air quality will also attract local interest. General oral and poster presentations are included in the "New Developments and Issues in Agrochemicals Sciences" symposia.

I encourage you to attend the awards-related programming activities during the week. The Sterling B. Hendricks Memorial Lecture by Dr. Fergus M. Clydesdale will be held on Tuesday with a lunchtime reception. Also on Tuesday, Dr. David M. Soderlund will be honored in a symposium as winner of the 2008 International Award for Research in Agrochemicals. Dr. Ashli Brown will receive the first AGRO Early Investigator's Award and present her paper in the "Bioenergy Production: Challenges, Concerns, and Consequences Symposium" on Tuesday afternoon. Twenty-one graduate and undergraduate students have received AGRO Education Awards to support their travel to the meeting, and they will be competing for best student poster awards during the AGRO poster session Monday morning.

AGRO has expanded programming to activities outside of ACS meetings. This year AGRO will sponsor a symposium entitled "Modern Pesticides in Urban Environments: Risk Assessment and Management" at the Society of Environmental Toxicology and Chemisty (SETAC) Annual Meeting in Tampa, Florida, November 16–19, 2008. This endeavor falls within our strategic plan goals for outreach to other societies and could ultimately enhance our membership. Several AGRO members are serving on the organizing committees of the 12th IUPAC International Congress of Pesticide Chemistry in Melbourne, Australia in 2010, and the 3rd International Workshop on Crop Protection Chemistry in Latin America in Rio de Janeiro, Brazil October 2009.

Next year we will be programming at the ACS Fall 2009 National Meeting in Washington, DC. I encourage young scientists to consider applying for the newly established New Investigator Award. This award is open to researchers in industry and government as well as academia who have received their doctoral degrees within the last five years. The winner will receive a $1000 honorarium in addition to their travel expenses to the meeting.

Our world and economies are rapidly changing and are becoming increasingly integrated. Solving problems related to issues of food, energy, and the environment will be critical to the future of our planet. AGRO will continue to address these issues in our programming. If you have ideas for future AGRO symposia or outside programming ideas, please contact any AGRO division officers or executive committee member. Have a great time in Philly and we look forward to seeing everyone in the District in 2009!!

AGRO Program Committee Report

The Program Committee is made up of the Division Officers, Executive Committee members, Standing members, Volunteer members, and a Long Range Program Coordinator to keep a continuous record of past and future programming. Some names may be listed twice as they are serving in more than one category. If you have an interest in serving as a volunteer member of this committee, or if you would like more information on participating in AGRO programming, please contact Laura McConnell, Joe Massey, or one of the division officers.

A list of standing topic areas was established which reflects better the broader areas of agricultural research being addressed by AGRO. These topics will be part of each AGRO program along with our normal awards, programming, and symposia to address ACS themes for each meeting and special topics of emerging or continuing interest.

If you have additional ideas for standing topics or programming that you would like to see included in AGRO, please contact one of the division officers or attend our AGRO future symposium Brainstorming, Blues & Brews Happy Hour on Wednesday, August 20 from 5:00 – 7:00 pm in the Crowne Plaza City Center, Independence A/B.

AGRO Program Committee			
Joseph Massey, 2006 – 2010 Long Range Program Coordinator		jmassey@pss.msstate.edu	
Division & Subdivision Officers			
John Johnston	Division Chair	John.J.Johnston@usda.gov	
Kevin Armbrust	Program Chair	armbrust@mscl.msstate.edu	
Ellen Arthur	Vice Chair	ellen.arthur@bayercropscience.com	
Bill Hall	Chair, FERT Subdivision	bill.hall@mosaicco.com	
Terry Spittler	Treasurer	tds2@cornell.edu	
Liliana Schwartz	Secretary	Liliana.Schwartz@usa.dupont.com	
Laura McConnell	Immediate Past Chair	laura.mcconnell@ars.usda.gov	
Barry Cross	Councilor	barry.cross@worldnet.att.net	
Standing Members			
Jim Seiber	Awards Committee Chair	jseiber@pw.usda.gov	
Allan Felsot	New Investigator Award Chair	afelsot@tricity.wsu.edu	
John Johnston	Education Award Committee Chair	John.J.Johnston@usda.gov	
John Clark	Special Conferences Chair	jclark@vasci.umass.edu	
Cathleen Hapeman	Communications Committee Chair	Cathleen.hapeman@ars.usda.gov	
Jason Sandahl	International Outreach Chair	Jason.Sandahl@usda.gov	
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Todd Anderson	todd.anderson@ttu.edu	Will Ridley	william.p.ridley@monsanto.com
Cathleen Hapeman	cathleen.hapeman@ars.usda.gov	Jay Gan	jgan@ucr.edu
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Scott Jackson	scott.jackson@basf.com	Scott Yates	syates@ussl.ars.usda.gov
Diana Aga	dianaaga@buffalo.edu		
Volunteer Members			
Steven A. Ripp	saripp@utk.edu		

Status of
Planned AGRO Programming & Outreach Activities
2009 – 2012

Activity/Event	Leader(s)	Status	Actions Required
SETAC North America 29th Annual Meeting, Tampa, FL, 16-20 November, 2008	Stuart Cohen, Pam Rice	• Full-day symposium on Modern pesticides in urban environments: Risk assessment and risk management has been included on the program	
238th ACS National Meeting August 16-20, 2009 Washington, DC	Ellen Arthur	• Call for Symposia & Papers TBA in PICOGRAM vols. 75 & 76	• Contact Ellen Arthur if you are interested in organizing a symposium
3rd International Workshop on Crop Protection Chemistry in Latin America, October 4-8, 2009, Rio de Janeiro	Irene Baptista de Alleluia, Ken Racke, Laura McConnell	• See announcement on page 36	• Contact organizers if you are interested in presenting a paper or poster
Activities beyond 2009			
239th ACS National Meeting March 21-25, 2010 San Francisco, CA And/Or 240th National Meeting August 22-26, 2010 Boston, MA	Ken Racke	• Call for Symposia & Papers TBA in PICOGRAM vols. 77 & 78	• Decide in 2010 if AGRO is returning to 2 national meetings per year
12th IUPAC International Congress of Pesticide Chemistry July 4-8, 2010 Melbourne, Australia	Greg Simpson, Ken Racke, Don Wauchope, Laura McConnell	• See announcement on page 41 for more information	• Contact organizers if you are interested in presenting a paper or poster
241st ACS National Meeting March 27-31, 2011 Anaheim, CA And/Or 242nd ACS National Meeting August 28-September 1, 2011 Denver, CO	2010 Vice Chair		
243rd ACS National Meeting & Exposition March 25-29, 2012, San Diego, CA And/Or 244th ACS National Meeting & Exposition September 9-13, 2012, New York, NY	2011 Vice Chair		

Future ACS National Meetings

237th ACS National Meeting & Exposition
March 22-26, 2009, Salt Lake City, UT

238th ACS National Meeting & Exposition
August 16-20, 2009, Washington, DC

239th ACS National Meeting & Exposition
March 21-25, 2010, San Francisco, CA

240th ACS National Meeting & Exposition
August 22-26, 2010, Boston, MA

241st ACS National Meeting & Exposition
March 27-31, 2011, Anaheim, CA

242nd ACS National Meeting & Exposition
August 28-September 1, 2011, Denver, CO

243rd ACS National Meeting & Exposition
March 25-29, 2012, San Diego, CA

244th ACS National Meeting & Exposition
September 9-13, 2012, New York, NY

245th ACS National Meeting & Exposition
April 7-11, 2013, New Orleans, LA

246th ACS National Meeting & Exposition
September 8-12, 2013, Indianapolis, IN

247th ACS National Meeting & Exposition
March 16-20, 2014, Washington, DC

248th ACS National Meeting & Exposition
August 24-28, 2014, San Francisco, CA

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

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

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

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

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

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

3rd International Workshop on Crop Protection Chemistry in Latin America: Environment, Safety and Regulation

4-8 October, 2009
Rio de Janeiro, Brazil

Co-Sponsoring Organiziations
GARP – Associação Nacional dos Especialistas em Resíduos, Contaminantes e Poluentes Orgânicos
IUPAC Division of Chemistry and the Environment
AGRO – American Chemical Society

Workshop Objectives

- Facilitate the exchange of information and ideas regarding harmonized approaches available for the scientific evaluation and regulation of crop protection chemistry
- Provide a forum for presentation of the latest research in the areas of agricultural biotechnology, environmental and human health protection, risk management and regulation of crop protection chemicals in Latin America

Technical Program
The workshop will include a plenary program with simultaneous translation from English to Portuguese and Spanish. All attendees are encouraged to present a poster of their work to be displayed throughout the workshop. Eight over-arching topics will be included:

- Risk management and Regulation
- Global Harmonization
- Quality and Constituents of Pesticides
- Biotechnology for Crops and Public Health
- Innovative Chemistry and Technology for Crop Protection
- Environmental Chemistry and Ecorisk Assessment
- Pesticides Residues in Food
- Education in Crop Protection

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AGRO 2009 ANNOUNCEMENTS CALL FOR SYMPOSIA & PAPERS

238th ACS National Meeting & Exposition
August 16-20, 2009
Washington, DC

AGRO is planning an exciting technical program in Washington, DC at the 2009 Fall National Meeting. Organizers are needed to plan symposia for standing program topics and to propose ideas for sessions addressing emerging topics in agricultural research. **Please contact the 2009 AGRO Program Chair, Dr. Ellen Arthur with your proposals at (913) 433-5328 or ellen.arthur@bayercropscience.com.**

Standing Program Topics

- Environmental Fate, Transport, Risk Assessment and Modeling of Agriculturally-Related Chemicals
- Technological Advances and Applications in Agricultural Science: Nanotechnology, Genetically Modified Organisms, and Biocontrol Agents
- Development of Value-Added Products from Agricultural Crops and Byproducts
- Bioenergy and Biofuels from Agriculture
- Natural Products, Pheromones, and Chemical Signaling in Agriculture
- Human and Animal Health Protection: Veterinary Pharmaceuticals, Antimicrobials, Worker Protection Products
- Advances in Agrochemical Residue and Metabolism Chemistry
- Urban Agriculture – Turf, Ornamentals, Household Products, and Water Re-Use
- Developments in Integrated Pest Management and Resistance Management
- Soil and Nutrient Management for Sustainable Agriculture
- Agrochemical Toxicology and Mode of Action
- Residue and Metabolism Chemistry
- Synthesis of Bioactive Compounds
- Exposure and Exposure Assessment Modeling

Award Symposia

ACS International Award for Research in Agrochemicals Symposium for R. Donald Wauchope

Sterling B. Hendricks Memorial Lectureship
Organizer: Jim Seiber, USDA-ARS, (510) 559-5600, james.seiber@ars.usda.gov

AGRO New Investigator Award
Organizer: Allan Felsot, Washington State University, 509-372-7365, afelsot@tricity.wsu.edu

AGRO Education Awards for Undergraduate and Graduate Student Travel: Research Poster Presentations
Organizer: John J. Johnston, USDA-NWRC, 970-266- 6082, john.j.johnston@aphis.usda.gov

AGRO 2009
CALL FOR SYMPOSIA & PAPERS
(continued)

Special Events

Research Poster Competition!

The top three AGRO posters will be awarded Amazon.com gift certificates. All posters not in the student competition are eligible; at least one author must be present.

EXCITING PRIZES!

Agricultural Research in Australia – Critical Issues Leading up to the 12th IUPAC International Congress on Pesticide Chemistry in Melbourne
Organizers: Laura McConnell, USDA-ARS, 301-504-6298, laura.mcconnell@ars.usda.gov, Ronald Hill, CSIRO, ron.hill@csiro.au, Ken Racke, Dow AgroSciences, kracke@dow.com

Symposia for Invited and Solicited Papers

Agrochemical Residue & Metabolism Chemistry
Organizers: Teresa A. Wehner, Merial Ltd; J. J. Johnston, USDA/APHIS/WS, 970-266-6082, john.j.johnston@aphis.usda.gov; David Smith, USDA-ARS, 701-239-1238, david.j.smith@ars.usda.gov

Application of Natural products in Organic Farming
Organizer: Kamal Chauhan, USDA-ARS, (301)504-5166, Kamal.Chauhan@ars.usda.gov

Chemical Use in Urban Environments
Organizers: Scott Jackson, BASF Corporation, (919) 547-2349, scott.jackson@basf.com, Paul Hendley, Syngenta, paul.hendley@syngenta.com

Ecological Exposure for Atrazine in Midwest Streams
Organizers: Paul Hendley, Syngenta, paul.hendley@syngenta.com

Lawrence A. Burns Memorial Symposium on Advances in Environmental Modeling of Pesticides
Organizers: Tharacad Ramanarayanan, Bayer CropScience, (913)433-5489, Tharacad.Ramanarayanan@bayercropscience.com, Ronald Parker, Office of Pesticide Programs, USEPA, (703) 305-5505, Parker.Ronald@epa.gov

New Developments and Issues in Agrochemical Sciences (Gen. Presentations/Posters)
Organizer: Ellen Arthur, Bayer CropScience, (913) 433-5328, ellen.arthur@bayercropscience.com

Non-dietary Human Exposure and Risk Assessment
Organizers: Mike Krolski, Bayer CropScience, (913) 433-5317; mike.krolski@bayercropscience.com, Curt Lunchick, Bayer CropScience , (919) 549-2986; curt.lunchick@bayercropscience.com

AGRO COMES TO SETAC!

Modern Pesticides in Urban Environments: Risk Assessment and Management

SETAC North America 29th National Meeting
Tampa, FL, November 16-20, 2008

Co-Organizers:
Stuart Cohen
Environmental & Turf Services, Inc.
ETSCohen@aol.com

Pamela Rice
USDA-ARS
Pamela.Rice@ars.usda.gov

PLANNING

You Are Cordially Invited To:

AGRO Brainstorming, Blues & Brews

Happy Hour

Wednesday, August 20, 5:00 – 7:00 pm
Crowne Plaza City Center, Independence A/B

- **Share your ideas about the future AGRO programming**
- **Learn more about organizing a symposium**
- **Let us know what topics are the most important to you**

Free refreshments will be served

ALL ARE WELCOME!

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12th IUPAC International Congress of Pesticide Chemistry

4-8 July 2010
Melbourne Exhibition and Convention Centre
Melbourne, Australia

Conference topics include:

- *Discovery of New Chemicals*— synthesis; natural products; molecular biology; mechanism-based discovery of crop protection chemicals; biology of pests, diseases, and weeds
- *Regulatory and Residue*— chemically induced crop traits; induced chemical defense in plants; globalization and harmonization
- *Crop Protection*— problems in emerging economies
- *Crop Biofactories*— emerging technologies
- *Formulation and Delivery*— chemical ecology; attracting beneficial insects for pest management; pesticide quality; application technology; public health pesticides
- *Environmental Fate and Safety Assessment*— modeling; environmental risk assessment; environmental persistence, degradation, and transport

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AGRO Congratulates New Officers and Executive Committee Members

Electronic Election

AGRO held its first electronic ballot election this year selecting a new Vice Chair, Councilors, and Executive Committee members to serve beginning in 2009. Secure electronic balloting over a three week period from May 26 – June 13, 2008 went very smoothly with approximately 19% of the membership casting ballots. Those without email addresses or with non-functional addresses received first-class post cards with a link and pass code to cast their ballot.

To all those who agreed to run for office, the division extends its gratitude for your willingness to serve.

Elected Officials for 2009

Vice Chair: Ken Racke
Secretary: Liliana Schwartz
Treasurer: Terry Spittler
Councilors: Jeanette Van Emon
Don Wauchoupe
Alternate Councilors:
Rodney Bennett
Barrington Cross
Executive Committee:
Steve Duke
Cathleen Hapeman
Keri Henderson
Ann Lemley
Chris Peterson

Submitted by **Laura McConnell**

2007 AGRO Treasurer's Report

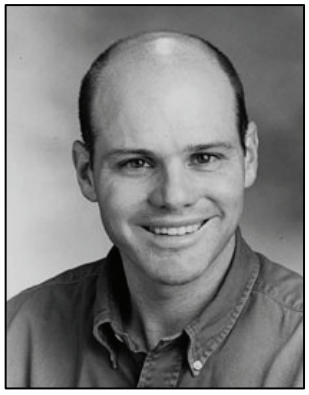
234th ACS National Meeting & Exposition
August 19, 2007
Boston, Massachusetts
Terry D. Spittler – Treasurer

DATE	**7/31/06**	**12/31/06**	**7/31/07**
CHECKING ACCOUNT	$47,999	$2,217	$41,397
INVESTMENTS			
Spectrum Income (T. Rowe Price)	195,073	204,706	170,005*
Prime Reserve (T. Rowe Price)	1,204	1,260	1,263
Educational Pool (JP Morgan)	421,439	439,716	464,977
ACS Investment Pool	23,173	25,406	26,880
TOTAL INVESTMENTS	**$640,891**	**$671,088**	**$663,125**
TOTAL ASSETS	**$688,890**	**$672,348**	**$704,522**

*$40,000 transferred Checking Account 3/07

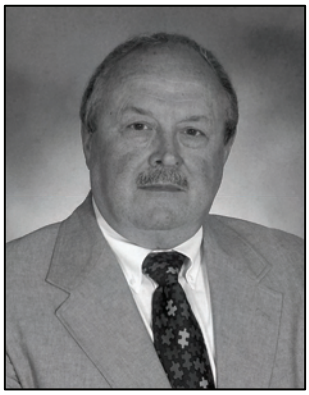
AGRO Division Officers

Dr. John J. Johnston
Division Chair



Dr. Kevin L. Armbrust
Program Chair

Dr. Ellen L. Arthur
Vice-Chair



Dr. Terry D. Spittler
Treasurer

Dr. Liliana Schwartz
Secretary

Officers and Committees of the AGRO Division

AGRO DIVISION OFFICERS			
Division Chair			
Dr. John J. Johnston	(970) 266-6082	FAX: (970) 266-6089	john.j.johnston@aphis.usda.gov
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Secretary			
Dr. Liliana Schwartz	(302) 999-4078	FAX: (302) 999-3720	liliana.schwartz@usa.dupont.com
Treasurer			
Dr. Terry D. Spittler	(315) 787-2283	FAX: (315) 787-2320	tds2@cornell.edu

EXECUTIVE COMMITTEE		
2006 – 2008	**2007 – 2009**	**2008 – 2010**
Dr. Todd Anderson	Mr. Tim Ballard	Dr. J. Marshall Clark
Dr. Cathleen Hapeman	Dr. Scott Jackson	Dr. Joe Massey
Dr. Patricia Rice	Dr. Diana Aga	Dr. Ken Racke
Dr. Luis Ruzo	Dr. Will Ridley	Dr. Pamela Rice
Dr. Jeanette Van Emon	Dr. Jay Gan	Dr. Scott Yates

COUNCILORS		
2005 – 2008	**2006 – 2009**	
Dr. Joel Coats	Dr. Barrington Cross	
Dr. Nancy Ragsdale, Alternate		

Division Committees

FERT Program Committee			
Mr. William Hall, **Chair**	(863) 428-7161		bill.hall@mosaicco.com
Nominating Committee			
Dr. Laura L. McConnell, **Chair**	(301) 504-6298	FAX: (301) 504-6298	laura.mcconnell@ars.usda.gov
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Dr. Allan Felsot	(509) 372-7365	FAX: (509) 372-7460	afelsot@tricity.wsu.edu
Awards Committee			
Dr. James Seiber, **Chair**	(510) 559-5600		jseiber@pw.usda.gov
Members			
Dr. John Casida	Dr. Robert Hollingworth		Dr. Willis Wheeler
Dr. Fritz Fuehr	Dr. Ralph Mumma		Dr. Izuru Yamamoto
Dr. Bruce Hammock	Dr. Nancy Ragsdale		
Dr. Ernest Hodgson	Dr. Jim Tumlinson		
Membership Committee			
Dr. Dan Stout, **Chair**	(919) 541-5767	FAX: (919) 541-0905	stout.dan@epa.gov
Dr. John J. Johnston	(970) 266-6082	FAX: (970) 266-6089	john.j.johnston@aphis.usda.gov
Communications Committee			
Dr. Cathleen Hapeman, **Chair**	(301) 504-6451	FAX: (301) 504-5048	cathleen.hapeman@ars.usda.gov
Members			
Mr. Tim Ballard – AG-LIST	Dr. Jay Gan – Abstracts Editor		Dr. Tom Potter – Femtogram Editor
Dr. Rodney Bennett – Books	Dr. Laura McConnell – Special Articles		Ms. Judy Ruppert – Website
Dr. Allan Felsot – Website	Dr. Sharon Papiernik – Awards		Dr. Terry Spittler – Publishing
Finance Committee			
Dr. Barry Cross, **Chair**			bcross@weidel.com
Dr. Terry Spittler, **Ex Officio**	(814) 272-1039	FAX: (814) 272-1019	tds2@cornell.edu
Members			
Dr. Don Baker	Dr. Ralph Mumma		
Dr. Willa Garner	Dr. Willis Wheeler		

Officers and Committees of the AGRO Division

(Continued)

Hospitality Committee			
Coffee Hour			
Dr. Jim Brady	(336) 643-1158	Cell: (336) 708-0097	jfbrady@bellsouth.net
Dr. Julie Eble	(302) 255-4700 x100		julie_eble@criticalpathservices.com
Dr. Joe Massey	(662) 325-4725	FAX: (662) 325-8742	jmassey@pss.msstate.edu
Dr. Patricia Rice	(919) 547-2668	FAX: (919) 547-2850	patricia.rice@basf.com
Social Hour			
Dr. Aldos Barefoot	(302) 451-5856	FAX: (302) 451-5941	aldos.c.barefoot@usa.dupont.com
Dr. Jeff Jenkins	(541) 737-5993	FAX: (541) 737-5001	jeffrey.jenkins@orst.edu

Special Committees

Bylaws Committee			
Dr. Don Baker, **Chair**			
Patron Relations Committee			
Dr. Scott Jackson, **Co-Chair**	(919) 547-2349	FAX: (919) 547-2407	scott.jackson@basf.com
Dr. Del Koch, **Co-Chair**	(573) 443-9003		kochd@abclabs.com
Future Special Conference Committee			
Dr. John M. Clark, **Chair**	(413) 545-1052		jclark@vasci.umass.edu
Dr. Robert Hollingworth			
Public Relations Committee			
Dr. Jeff Jenkins, **Chair**	(541) 737-5993	FAX: (541) 737-5001	jeffrey.jenkins@orst.edu
Members			
Dr. Ann Lemley	Dr. James Seiber		
Education Committee			
Dr. John Johnston, **Chair**	(970) 266-6082	FAX: (970) 266-6089	john.j.johnston@aphis.usda.gov
Dr. John Bourke, **Investment Coordinator**			
Dr. Allan S. Felsot, **New Investigator Award Coordinator**	(509) 372-7365	FAX: (509) 372-7460	afelsot@tricity.wsu.edu
Members			
Dr. David Barnekow	Dr. J. Harold Falls		Dr. Judd O. Nelson
Dr. John M. Clark	Dr. Vincent Hebert		Dr. Jack R. Plimmer
Dr. Joel Coats	Dr. Ann Lemley		Dr. Nancy Ragsdale
Dr. Barry Cross	Dr. Glenn Miller		Dr. William Ridley

PROGRAM COMMITTEE LISTING

See page 26

Past Chairs of the Pesticide Chemistry/AGRO Division

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

Minutes from the AGRO Division Business Meeting

Governance Meeting
Long-Range Planning Committee Meeting
Program Planning Committee Meeting

234th ACS National Meeting – Boston, MA
Sunday, August 19, 2007, 5:30 – 10:00 pm
Laura McConnell – Chair

I. Introduction – *Laura McConnell, Chair*

Laura started the meeting at 5:40 pm with the following AGRO initiative updates:

- Have Technical Program & Business Meeting only at the Fall ACS National Meeting each year.
- Add workshops (training and goal-driven at ACS and at separate meetings) to AGRO programming. Workshops are planned for Philadelphia and Pan Pacific Meetings.
- Recreate the program planning structure of the Division to provide continuity and sustained outstanding scientific programs. Program planning conference call prior to each National Meeting.
- Change the name of the Division to reflect more broadly its multidisciplinary focus. Re-branding AGRO to represent broader scientific area "Chemistry For and From Agriculture".
- Increase the Division's international participation, outreach and visibility through: participation in IUPAC workshops and conferences, representative at US Brazil Bioenergy Event, and sponsored scientist from Mali.
- Include regulatory agencies in program planning; e.g., cooperating with EPA to plan workshop in Philadelphia.
- Increase travel grants for young scientists/students, including the international ones.
- Involve students in program planning; e.g., graduate student luncheon initiated in Chicago to obtain feedback and provide information/services.
- Proposed AGRO Division involvement in the FAO/IAEA "infocris" pesticide information web site.
- Webcasted selected presentations from AGRO meetings; we are still searching for a volunteer.
- Planned Strategic Planning Meeting for AGRO in Washington, DC in January 2008.

II. Governance Meeting

A. 4th Pan Pacific Pesticide Conference June 1-5, 2008in Honolulu, HI - Al Barefoot, Nancy Todd, Joel Coats

- AGRO provides primary organizing effort
- Joint program committee with JSPS
- JSPS will provide registration and travel support to two speakers/session from Japan, students and several international speakers.
- Ten sessions are programmed, in which the Japanese side is well represented.
- A Japanese co-sponsor is needed.
- AGRO will provide funds for an equivalent number of speakers from US or other countries.
- New topics will be presented, such as Global Trade Issues, Invasive Species, Advances in Human Vector Control etc.
- Any excess funds will be revenue for AGRO.
- Any loss will be borne by AGRO.
- Estimated total expenses are $99,750.
- Estimated net revenues over expenses are $19,250.

Action: AGRO Division sponsors at least two students with Award Winner Poster represented at Pan Pacific Conference with a total expenditure of $4000. **Motion passed.**

B. Secretary's Report – Liliana Schwartz

- Presented the minutes of the last ACS meeting, in Chicago March 2007.
- Gave a short update on her recent activities; e.g., scheduled and arranged the Business Meeting.

C. Treasurer's Report – Terry Spittler

- Terry distributed a report indicating that we continue to enjoy good income from both our Division investment account and our Educational Endowment Fund.
- We are seeing a net erosion of the balances because of the significant expense of general programming and of our educational outreach to secure new members. The drop in the number of

dues paying members is, of course, also impacting our cash flow.
- While it has been discussed that overspending is not a sustainable practice, the consensus has been that we should invest in Division growth, even if it is not the best practice for the long term.

D. Councilor's Report – Joel Coats, Barry Cross

- At the spring meeting in Chicago two candidates, Thomas A. Lane and Howard M. Peters, were selected to stand for election as President Elect in the Fall National Election.
- Council voted to accept a petition on Multi - Year Due without discounts.
- The society ended 2006 with a $7.8 million budget with earnings of $12.2 million
- ACS closed 2006 with 160,491 members - the highest since 2002.
- Council voted to approve the Chemical Professional Code of Conduct as guidance for members in professional dealings, especially those involving conflicts of interest.
- We still did not pay the expenses for the Chicago meeting; the bill is going to be received in January 2008.
- Chicago meeting had a 50% approval/satisfaction rate by the ACS members in terms of hotel accommodations, Convention Center, logistics, losses in $600,000 – 700,000. As a result, ACS has decided to replace the next Chicago meeting scheduled in Fall 2011 with Denver.
- AGRO Division had a good representation in the oral presentation, but the posters presentations had 16.7% 'no shows', in which 50% of them are of students/scientists from China.
- Since the Division is interested in attracting diverse scientific activity, Laura McConnell suggested that the Division shouldn't reject papers, but in order to avoid these future situations, an improved communication between the AGRO Program Chair and the ACS staff is needed.
- Terry Spittler mentioned that the abstracts deadline is too early and therefore, it doesn't leave too much control over the abstracts' admission or cancellation.
- Any food cancellation beyond the admissible time will be penalized by the ACS.
- ACS Finance Meeting has decided to increase the registration fee by $10.

E. Membership Committee – no report

F. Guest Speaker – Brad Miller (ACS)

- Our guest has presented the 2006/2007 NSF Discovery Corps Fellowship Project on "Sustainable Energy and Chemical Sciences Collaboration in Biomass Conversion Research between the US and Brazil". A partnership of the Brazilian Chemical Society, EMBRAPA and the ACS Publications and ACS Technical Divisions, will develop an exchange/collaboration framework associated with crop-based and naturally occurring biomass, storage and transportation, and by-products/value-added co-products. Key project outputs include best science of biorenewable chemistry joint symposia, web/audio seminars, and coordinated site visits to research labs and production facilities in Brazil.
- The next steps of this initiative involve facilitating interactions between the Brazilian Research team with ACS Technical Divisions leadership (FUEL, PETR, BIOT, AGFD, CELL), identification of "Best of Bio-renewables" Technical Division content from ACS National Meeting in Chicago, and planning for joint symposia, web seminars, publication opportunities, and directory.

G. Communications Committee Report – Cathleen Hapeman (report given by Laura McConnell)

- The PICOGRAM for the Boston Meeting was sent "first class" since the time ran late. Third Class goes when it can, and there is no time limit on delivery.
- In spite of AGRO Division absence from the New Orleans Meeting in March 2008, the New Orleans PICOGRAM will be sent both as a hard copy and by e-mail.
- The website has been updated and we may re-do the AGRO website design in order to be closer to the ACS website.

H. E-mail Communication System – Tim Ballard

- Tim suggested that we need a person who will go through the membership list and will update all the e-mail addresses as it was done 2 years ago.

Action: In order to improve the communication with its members, the Division will hire a person who will update the members contact information. **Motion passed**.

I. Hospitality Committee – Patricia Rice, Joe Massey, and Jim Brady (report given by Terry Spittler)

- Fourteen companies have donated a total of $1700 to support our Boston coffee lounge. Several firms provided literature to promote their services to meeting attendees.
- The AGRO Division Awards & Social will be held at the Georgian Room of the Boston Park Plaza. We will introduce the winners of the Young Scientists Pre- and Post-Doctoral Research Award Symposium to the revelers in attendance.

J. Committee on Patron Relations

- **Scott Jackson** has volunteered for this position. **Laura McConnell** will be communicating with him.

K. Nominating Committee 2007 – Don Wauchope

- A draft with the ballot list will be prepared so that the elections for 2008 will be finalized on time (January 2008).

L. Public Relations Committee – Jeff Jenkins

- The Agrochemicals Division of the American Chemical Society (ACS) will present its International Award for Research in Agrochemicals to Dr. Frederick J. Perlak, Director for Cotton and Specialty Crop Technology and Distinguished Fellow, Monsanto Company. Dr.Perlak will be honored at the 234th ACS National Meeting in Boston, MA.
- The Agricultural Research Service (ARS), U.S. Department of Agriculture's primary research agency, the Agriculture and Food Chemistry Division, and Agrochemicals Division of the American Chemical Society (ACS) will award Dr. Bruce E. Dale with the 2007 Sterling B. Hendricks Memorial Lectureship. Dr. Dale will be honored at the 234th ACS National Meeting & Exposition in Boston, MA.

M. Education Committee - Allan Felsot, John Johnston

- 2007 Grad Student Travel Grant Recipients includes 16 students and 10 universities.
- 2008 Education Committee Symposia will include:
- Undergraduate and Graduate Student Travel Support for Student Research Poster Presentations sponsored by Bayer CropScience; the award will be opened to students conducting agricultural chemistry related research at North American Institutions of Learning.
- AGRO New Investigator Award sponsored by Dow AgroSciences, in which it will be opened to new investigators at research institutions, industries, and universities who have received their doctoral degrees within the last five years, prior to the application deadline.
- AGRO Graduate Student Luncheon, a real opportunity for AGRO to listen to the desires and needs of graduate students who are interested in agricultural chemistry, discussing also opportunities for students and finding jobs in science (government, industry, academics).

N. By-Laws Committee – Don Baker (no report)

- Recently, Don has experienced health problems and the participants at the meeting have shown concern. Several participants at the meeting will be contacting him.

O. Awards Committee – Jim Seiber

- **Dr. Frederick J. Perlak**, Monsanto Company, St. Louis, MO will receive the International Award for Research in Agrochemicals at the fall 2007 ACS Meeting in Boston, MA for his research contributions that led to the development of insect protected crops. This award will be sponsored by DuPont Crop Protection.
- **Dr. David Soderlund**, Cornell University and the New York State Agricultural Experiment Station, will receive the International Award for Research in Agrochemicals at the Fall, 2008 meeting of ACS, for his pioneering and continuing discoveries on the insect sodium channel and insecticides that disrupt its action. BASF Corporation and DuPont Crop Protection are the Award cosponsors. A symposium in Dr. Soderlund's honor will be organized by Dr. Jeffrey Bloomquist.
- **Dr. R. Donald Wauchope**, USDA-ARS (retired), has been nominated to receive the AGRO Division Fellow Award for dedicated and substantial contributions of time, talents, and service to the Division and to agrochemical science. The Strategic Planning meeting which Dr. Wauchope organized helped to instill new energy into the Division--a hallmark of Don's many contributions to the Division as Chair, officer, and many committee assignments. **Dr. Ann T. Lemley**, Cornell University, and **Dr. J. Marshall Clark**, University of Massachusetts, will also receive the AGRO Division Fellow Award.
- **Dr. Bruce Dale**, Professor of Chemical Engineering at Michigan State University, Associate Director of MSU's Office of Bio-based Technologies and leader of MSU's Biomass Conversion Laboratory, will receive the USDA-ARS Sterling B. Hendricks Memorial Lectureship award at the Fall, 2007, ACS meeting. Dr. Dale is being recognized for his research on biomass conversion and sustainability.
- Nominations for the 2009 International Award for Research in Agrochemicals are currently being solicited by the Awards Committee. Only one International Award will be presented in 2009. The Awards Committee is also accepting new award nominations for the Division Fellow Award. The nomination forms for both are found in the Picogram. Please consider nominating a deserving colleague. The deadlines each year are December 31 for the International Award and May 31 for the Fellow Award.

III. Long Range Planning Meeting – *Laura McConnell*

- The Strategic Planning Meeting is scheduled for January 11-13, 2008, Herndon, VA at Washington Dulles Marriott Suites.
- The meeting will be facilitated by ACS Staff, Dale Gaddy, at no cost for AGRO Division.
- The meeting will be attended by approximately 14 people, including officers and active representatives from different age groups and professional backgrounds.
- A draft plan will be developed by end of meeting.
- The plan will be circulated in Spring issue of PICOGRAM.

- The plan will be finalized by Fall Meeting in Philadelphia.

IV. Program Planning Meeting

A. ACS Western Regional Meeting, Las Vegas 2008 – Jeanette Van Emon

- Jeannette gave a short update on the September 24-27, 2008 Las Vegas meeting.
- This meeting examines some of the changes chemists are making in science and chemistry.
- More details can be found at: http://membership.acs.org/w/WRM2008

B. Boston, Fall 2007 – John Johnston

- According to the number of papers submitted for this meeting, AGRO is stronger than ever (around 380 papers compared to about 145 papers in 2002). In this way, AGRO is ready for Philly and Washington DC meetings too.
- AGRO is having 12 sessions at this meeting.
- An invitation was extended to new symposium organizers to attend the first AGRO Brainstorming, Blues & Brews for Wednesday, session on August 22, from 5:00 to 6:30 pm at Boston Convention Center, Room 259A was made.

C. Philadelphia, Fall 2008 - Kevin Armbrust

- 14 sessions, including an Urban Exposure Modeling Workshop, for the Philadelphia Meeting in Fall 2008 were presented.

D. AGRO Workshop Residential Pesticide Exposure Assessment – John Clark, Ken Racke

- This workshop is tentatively planned for two half-day sessions at the ACS Philadelphia Meeting, Fall 2008.
- The appropriate topics are being covered by EPA (OPP & ORD) and by non-dietary industry task forces/academic scientists. The workshop will have a common morning program with an update on revisions to the Residential SOPs, data requirements, and some general presentations on measurements, modeling and methods necessary for residential observational exposure studies.
- All breakout sessions will have demonstrations along with seminar-type presentations.
- The workshop will conclude with a roundtable discussion of "New Challenges" with government, industry, and academic participants.
- Draft list of potential topics for AGRO workshop were presented.
- Registration fee to this workshop has to be determined.

E. Washington, DC Fall 2009 – Kevin Armbrust

- The initial planning with topics in the main areas has been started.
- A replacement of Bill Hall - who just retired - on Soil and Nutrient Management for Sustainable Agriculture is needed.
- New topics, such as Agricultural Peptides and Proteins and Bio-farming have been proposed.

F. IUPAC Crop Protection Workshop, Beijing China, October 2007 – Ken Racke

- Info about this meeting can be found at: http://www.pesticidechemistry.com/index_en.htm

G. Info on Programming at or with SETAC – Laura McConnell

- SETAC is very interested in developing and implementing a joint symposium with the AGRO Division of the ACS. They agree that the urban risk assessment and risk management (including BMPs) topic is very relevant.
- Greg Schiefer, SETAC Executive Director suggests that the 2008 North America SETAC conference in Tampa would be most appropriate, but SETAC would be willing to consider other venues as well, e.g., an independent single theme conference in Washington, D.C. However, if the latter option is chosen, SETAC would not be able to provide any significant logistical support.

Laura adjourned the meeting at 10:00 pm.

Respectfully submitted,
Liliana Schwartz, Secretary

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
236th ACS National Meeting
August 17-21, 2008
Philadelphia, Pennsylvania
K.L. Armbrust and J. J. Johnston, *Program Chairs*

PROGRAM

DIVISION MEETING

AGRO Business Meeting
Sunday 5:30 – 10:00 pm
Crowne Plaza City Center, Declaration

SOCIAL EVENTS

AGRO Awards Social
Tuesday 6:00 – 8:00 pm
Crowne Plaza City Center, Liberty C
Members/Guests welcomed; see page 11

Sterling B. Hendricks Award Lecture Reception
Monday 11:30-1:30 pm
Crowne Plaza, Liberty B

Graduate Student Luncheon
Wednesdy 12:00 – 1:00 pm
Crowne Plaza, Room TBA
Invitation only; see page 29

Symposium Organizer Brainstorming, Blues & Brews
Wednesday 5:00 – 7:00 pm
Crowne Plaza, Independence A/B
All are welcome; see page 39

SUNDAY MORNING

Agrochemical Residue and Metabolism Chemistry
T. A. Wehner and J. J. Johnston, *Organizers*
D. J. Smith, *Organizer, Presiding*

Section A
Crowne Plaza City Center -- Liberty C

9:00 — Introductory Remarks.

9:05 —1. Modern GC-MS and LC-MS instrumentation techniques in the analysis of agrochemical residues. **K. Mastovska**

9:25 —2. SPE protocols for cleanup and UPLC-MS determination of acidic herbicides in fruit and vegetables after a rapid pretreatment procedure. **M. S. Young**, D. M. Diehl, J. C. Shia, K. M. Jenkins

9:45 —3. Structure elucidation of DNA adducts from pesticides via mass spectral analysis. **D. W. Boerth**, T. C. Andrade, E. Eder, P. Wanek

10:05 —4. Determination of 20,25-diazacholesterol residues in bird tissues. **D. A. Goldade**, C. A. Yoder, J. J. Johnston

10:25 — Intermission.

10:40 —5. Europium-sensitized luminescence determination of oxytetracycline residue in shrimp using an LED-based portable analyzer. **G. Chen**

11:00 —6. Determination of brodifacoum by ion exchange solid phase extraction followed by ion-pair high performance liquid chromatography in mussels and sparrow tissues. **T. M. Primus**, C. R. Wermager, J. J. Johnston, G. Howald, S. Buckelew

11:20 —7. Shikimate concentration determination in plant material. **T. C. Mueller**

11:40 —8. Utility of a rapid method for detecting herbicide residues. **P. J. Hannan**

Natural Products –
Allelochemicals and Natural Products for Pest Management
S. O. Duke, *Organizer*
C. L. Cantrell, *Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

9:20 — Introductory Remarks.

9:25 —9. Diffusive sampling of the rhizosphere using polydimethylsiloxane sorbents. **J. D. Weidenhamer**

9:45 —10. Preferential sorption of phenolic acids to soil and their allelochemical activity. **P. C. Bhowmik**

10:05 —11. *m*-Tyrosine, a root-exuded allelochemical produced by Chewing's fine fescue (*Festuca rubra* L. ssp. *commutata*). **L. A. Weston**, C. Bertin, F. C. Schroeder

10:25 — Intermission.

10:40 —12. Cyanamide in hairy vetch, tufted vetch, and black locust. **Y. Fujii**, T. Kamo, S. Hiradate, N. Hirai

11:00 —13. *p*-Hydroxyphenylpyruvate dioxygenase is a herbicide target site for natural β-triketones. **F. E. Dayan**, C. L. Cantrell, S. O. Duke, J. W. van Klink, N. B. Perry

11:20 —14. Phytotoxic eremophilanes from *Ligularia macrophylla*. **S. O. Duke**, C. L. Cantrell, F. E. Dayan, K. Grossmann, R. Niggeweg, N. Christiansen

11:40 —15. QSAR studies of allelochemicals. **F. A. Macias**, J. M. G. Molinillo, J. C. G. Galindo, R. M. Varela

Synthesis and Chemistry of Agrochemicals
T. M. Stevenson, *Presiding*

Section C
Crowne Plaza City Center -- Liberty A

8:45 — Introductory Remarks.

8:55 —16. Butenolides as seed germination stimulants. **M. Xu**, K. Sun, Y. Chen, T. Wagerle, M. Ruggiero

9:15 —17. Synthesis of new pyridine herbicides. **M. A. Hanagan**, Y. T. Henry

9:35 —18. HPPD inhibitor chemistry: A new generation of 1,3-diones. **R. Beaudegnies**

9:55 —19. Discovery of aminocyclopyrachlor (proposed common name) (DPX-MAT28): A new broad-spectrum auxinic herbicide. **B. L. Finkelstein**, G. R. Armel, S. A. Bolgunas, D. A. Clark, J. S. Claus, R. J. Crosswicks, C. M. Hirata, G. J. Hollingshaus, M. K. Koeppe, P. L. Rardon, V. A. Wittenbach, M. D. Woodward

10:25 — Intermission.

10:45 —20. Substituted 4-chloro-2-pentenamides: A unique class of protox inhibiting herbicides. **T. P. Selby**, G. R. Armel, K. A. Hughes, Y. Chen, M. Xu, T. M. Stevenson, B. Kamireddy, P. A. Mauvais

11:15 —21. Discovery and chemistry of flupicolide: A new agent for the control for oomycete diseases. **D. J. Mansfield**

11:45 —22. Substituted 1,2,4-triazin-6-ones and 4,5-dihydro-1,2,4-triazin-6-ones as agricultural fungicides. **K. G. Meyer**, S. S. Shaber, N. M. Niyaz, M. T. Sullenberger, B. J. Rieder, M. C. H. Yap, W. R. Erickson, F. D. Smith, C. Yao, T. Mathieson, Y. A. Adelfinskaya, S. Thornburgh

SUNDAY AFTERNOON

Agrochemical Residue and Metabolism Chemistry
J.J. Johnston and D. J. Smith, *Organizers*
T. A. Wehner, *Organizer, Presiding*

Section A
Crowne Plaza City Center -- Liberty C

1:30 — Introductory Remarks.

1:35 —23. Dos and don'ts for study directors of multisite studies. **P. J. Ourisson**, P. Swidersky

1:55 —24. Terminal residues in strawberry, tomato, and summer squash following soil applications of ^{14}C-furfural. **M. F. Kovacs Jr.**, W. E. Gledhill, M. E. Dix, N. R. Lentz, G. J. Burger, A. C. Katz

2:15 —25. Pesticide residues in pollen collected by foraging honey bees. **B. D. Eitzer**, K. A. Stoner

2:35 — Intermission.

2:55 —26. Leaching of thiacloprid in three different types of soil. **T. Jindal**

3:15 —27. Depletion of zilpaterol hydrochloride residues from the urine of orally-treated horses. **D. J. Smith**, C. J. Hammer, M. S. Mostrom, J. F. Thorson, W. L. Shelver

3:35 —28. Sorption of chlorpyrifos on agricultural soils. **M. K. Tiwari**, S. Guha

3:55 — Concluding Remarks.

Natural Products – Bioprospecting, Chemical Communication, and Quorum Sensing
P. Zubkoff, *Organizer, Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

1:30 — Introductory Remarks.

1:35 —29. How bacteria talk to each other. **B. L. Bassler**

1:55 —30. Use of microbial cell to cell communication and quorum sensing for controlling agricultural crop diseases. **M. A. Saleh**

2:15 —31. Chemical synthesis and biological characterization of structural analogs of the *Vibrio cholerae* autoinducer CAI-1. M. F. Semmelhack, **M. E. Pomianek**, C. M. Kraml, D. A. Higgins, B. L. Bassler

2:35 — Intermission.

2:50 —32. Red tides and harmful algal blooms (HABs): New technologies for detection of cells and toxins. **J. L. C. Wright**, D. M. Anderson

3:10 —33. Bioprospecting for novel fungicides in marine organisms. **D. E. Wedge**, N. Kasanah, M. T. Hamann

3:30 —34. Bioprospecting in extreme, deep-sea environments. **R. A. Lutz**

Synthesis and Chemistry of Agrochemicals
T. M. Stevenson, *Presiding*

Section C
Crowne Plaza City Center -- Liberty A

1:30 —35. Discovery and optimization of 1-alkoxy-4-amidinylphenyl analogs as fungicides. **C -P. Tseng**, M. C. Klapproth, W. K. Moberg, B. M. Reeves, S. I. Lewis, R. B. Sheth, W. Zhang

2:00 —36. Discovery and optimization of novel biphenyl ether fungicides. **J. F. Bereznak**, S. F. McCann, K. M. Patel

2:30 —37. Microcolin insecticides: Synthesis and structure-activity relationships. Z. L. Benko, C. V. DeAmicis, J. M. Gifford, J. R. Gilbert, V. Hegde, **J. E. Hunter**, P. Lewer, K. L. McLaren, N. Orr

2:50 —38. New heterocyclic analogs of Rynaxypyr™: Structure-activity studies in the anthranilic diamide class of chemistry. **G. P. Lahm**, T. P. Selby, T. M. Stevenson, B. L. Finkelstein, D. A. Clark, J. H. Freudenberger, W. Hong, M. Sethuraman, K. A. Hughes, C. M. Dubas-Cordery, B. K. Smith

3:20 — Intermission.

3:40 —39. Discovery of Cyazypyr™: A new cross-spectrum insecticide from the anthranilic diamide class of ryanodine receptor activators. **T. P. Selby**, G. P. Lahm, T. M. Stevenson, K. A. Hughes, I. B. Annan, D. Cordova, C. A. Bellin, E. A. Benner, K. D. Wing, J. D. Barry, M. J. Currie, T. F. Pahutski

4:10 —40. Pharmacophore design and parallel synthesis of phenylpiperidine/phenylpiperazine libraries as insect calcium channel inhibitors. **B. A. Lorsbach**, J. M. Ruiz, T. C. Sparks, J. D. Webster, M. T. Sullenberger, I. Morrison

4:30 —41. Syntheses and biologicial activities of insecticidal thieno[2,3-b]furans. **S. F. McCann**, Y. Hu, R. A. Coats, M. Hendrixson, W. Hong

4:50 —42. Synthesis and biological activity of cyclopropyl pyrazole insecticides. **W. von Deyn**, C. Koradin, D. G. Kuhn

AGRO POSTER SESSION

MONDAY MORNING
8:00 - 11:00

K. L. Armbrust and J. J. Johnston, *Organizers*

Section A
Crowne Plaza City Center -- Foyer

AGRO Education Awards For Undergraduate and Graduate Student Travel
Financially Supported by Bayer CropScience.

43. Accelerated Leuckart reaction in the synthesis of agrochemicals and pharmaceuticals. M. M. Bobylev, **A. Podrygula**

44. Thermal fixation of atmospheric nitrogen to nitrate on titanium dioxide and desert soil surfaces. **A. Al-Taani**, G. Miller

45. Interactions of nitrate and cadmium ions at model environmental interfaces studied by second harmonic generation. **J. N. Malin**, P. L. Hayes, F. M. Geiger

46. Adsorption effect on the degradation of carbaryl, mecoprop, and paraquat by AFT in an Swy-2 montmorillonite clay slurry. **P. Ye**, A. T. Lemley

47. Partitioning of etofenprox under simulated California rice growing conditions. **M. E. Vasquez**, R. S. Tjeerdema

48. Effects of black carbon on pyrethroid bioavailability in sediments. **Y. Yang**, W. Hunter, J. Gan, S. Tao

49. Fate of PBDEs in biosolids and soil from commercial farms that receive biosolids application. **N. A. Andrade**, L. L. McConnell, A. Torrents, M. Ramirez

50. Determination of the effect of pH, ionic strength, and humic acids on the soil sorption coefficients (K_d) of tylosin and erythromycin antibiotics. **D. A. G. Navarro**, D. S. Aga, J. R. Coats, K. L. D. Henderson, T. Moorman, J. Bidwell

51. Erythromycin: A look at a veterinary antibiotic's bioavailability in an aquatic microcosm. **A. M. Jessick**, K. L. Henderson, T. B. Moorman, J. R. Coats

52. Removal of methyl parathion from water by nanoscale zero-valent iron. **A. B. Giasuddin**, S. R. Kanel, J. Locklin, R. Chittaranjan

53. Method development for multiresidue pesticide extraction from food. **R. E. Hunter Jr.**, A. Riederer, P. B. Ryan

54. Repellency of botanical sesquiterpenoids to arthropods. **G. E. Paluch**, J. R. Coats

55. Preformed organophosphorous insecticide biomarkers in fruits and vegetables: An in-depth study on California strawberries. **Y. Li**, M. M. Bigelow-Dyk, Z. Chen, H. M. Vega, R. I. Krieger

56. Determinants of human pesticide exposure following use of fipronil-containing pet products. **M. M. Bigelow-Dyk**, Z. Chen, Y. Li, H. Vega, R. I. Krieger

57. Bis(chlorophenyl)acetic acid (DDA), a water-soluble biomarker of DDT metabolism in humans. **Z. Chen**, H. M. Vega, R. I. Krieger

58. Polygenic resistance in the highly DDT-resistant 91-R strain of *Drosophila melanogaster* involves decreased penetration, increased metabolism, and rapid excretion. **J. P. Strycharz**, S. H. Lee, W. Sun, B. R. Pittendrigh, J. M. Clark

59. Insecticidal activity of monoterpenoids at the octopamine receptor. **A. D. Gross**, J. R. Coats, M. J. Kimber, P. Ribeiro

60. Induction of neuronal phenotype in Sf21 insect cells. **L. J. Jenson**, D. C. Klorig, S. L. Paulson, J. R. Bloomquist

61. Deltamethrin increases peak current and slows deactivation kinetics of the voltage-sensitive calcium channel ($Ca_V2.2$) from rat brain following PKC-dependent phosphorylation. **A -M. Alves**, S. B. Symington, J. M. Clark

62. Differential potency of bivalent anticholinesterases as a model for the molecular design of selective insecticides. **J. M. Mutunga**, T. D. Anderson, P. R. Carlier, J. R. Bloomquist

63. Modulation of monoterpenoids on [3H]-TBOB binding to house fly GABA receptor. **F. Tong**, J. R. Coats

Congratulations to all our Student Winners!

AGRO POSTER SESSION

(continued)
MONDAY MORNING
8:00 - 11:00

Bioenergy Production: Challenges, Concerns, and Consequences

64. Fermentation stoichiometry of *Thermotoga neapolitana* and influence of temperature and oxygen on hydrogen production. **S. A. Munro**, S. H. Zinder, L. P. Walker

65. Microplate assay for characterization of plant cell wall degrading enzyme activity from crude fungal extracts. **M. K. Donnelly**, B. C. King, G. C. Bergstrom, D. M. Gibson, L. P. Walker

66. Supercritical CO_2 hydrolysis and explosion as pretreatment of guayule bagasse for fermentation feedstock. N. Srinivasan, N. M. Pinzon, **L -K. Ju**

67. Cellulosic ethanol production from *Saccharomyces cerevisiae* engineered for anaerobic conversion of pretreated lignocellulosic sugars to ethanol. **J. O. Rich**, K. Bischoff, S. R. Hughes

68. Properties of wood chars part 1: Elemental composition and acid functional groups. D. W. Rutherford, **C. E. Rostad**, J. A. Leenheer, R. L. Wershaw

69. Properties of wood chars part 2: Variation in surface area and porosity. D. W. Rutherford, **C. E. Rostad**, J. A. Leenheer, R. L. Wershaw

70. --Withdrawn

Analysis and Fate of Agrochemicals

71. Simulating hydrology at a Long Island turf study site using the model RZWQM98. **T. L. Estes**, C. T. Stone, J. Hanzas, J. L. Kunstman

72. Crop residue prediction in support of livestock feeding study dose selection. C. M. Kennedy, J. J. Anderson, N. Snyder, **M. T. Scott**

73. Raman microscopy of high P soil: In situ spatial compositional heterogeneity before and after Fe^{+3} amendment. E. E. Codling, L. Heighton, S. Mookherji, **W. F. Schmidt**

74. Analysis of residue samples: Effect of homogenization and sample size in extractions. **J. E. Eble**

75. Rapid UPLC-MS determination of tetracylines, sulfonamides, and penicillins in milk using mixed-mode SPE. **M. S. Young**, J. C. Shia, K. Tran, D. M. Diehl

76. An improved in vitro rearing system for the human head louse allows the determination of resistance to formulated pediculicides in a standardized format. **J. P. Strycharz**, K. S. Yoon, J. M. Clark

77. Determinants of human exposure to pet pest products: Fipronil. M. M. Bigelow-Dyk, **Y. Li**, Z. Chen, H. M. Vega, R. I. Krieger

78. Absorption and excretion of ^{14}C-labeled α-chloralose from Mallard ducks. **L. E. Hulslander**, D. L. Griffin, D. A. Goldade, J. J. Johnston

79. Biochemical and toxicological characterization of highly-selective anticholinesterases developed for malarial mosquito control. **T. D. Anderson**, J. Hartsel, M. Ma, J. M. Mutunga, A. Wysinska, B. T. Jackson, D. Wong, S. Paulson, P. R. Carlier, J. R. Bloomquist

80. Biochemical characterization of a putative insecticide target site in the acetylcholinesterase catalytic gorge of green peach aphid. **T. D. Anderson**, D. C. Hsu, P. R. Carlier, P. C -H. Lam, M. M. Totrov, J. R. Bloomquist

Synthesis and Chemistry of Agrochemicals

81. 2-Substituted 1-azabicyclo[2,2,2]octan-3-ones as novel insecticides. **W. Zhang**, A. X. Ding, C. Desmond, G. Seburyamo, K. A. Hughes, R. Kucharczyk, T. P. Selby, D. Cordova, M. Sacher

82. Synthetic atpenin analogs: Potent mitochondrial inhibitors of succinate-ubiquinone oxidoreductase (complex II). **K. A. Hughes**, T. P. Selby, J. J. Rauh, Y. J. Zheng, W. S. Hanna, P. A. Mauvais

83. Alkylsulfonyl benzophenone hydrazones as insecticides. **J. K. Long**, L. Jones, E. M. Keskeny, S. Lewis, T. M. Stevenson

84. Synthesis and herbicidal activity of *N*-isobutyl-*N*-substituted naphthalene methyl carboxylic acid amides. **T. Wagerle**, M. Xu, T. M. Stevenson, T. P. Selby, G. R. Armel, P. L. Rardon

85. Herbicidal 1,2,3-triazole carboxamides. **M. Xu**, T. M. Stevenson, M. Hendrixson, B. Kamireddy, X. Zhao, G. R. Armel, D. A. Baxter

86. Indoline insecticides. **T. M. Stevenson**, T. D. Neubert, C. M. Dubas-Cordery, R. Husted

87. Difluorobutenyl(thio)imidates as insecticides and nematicides. **T. M. Stevenson**, M. Xu, E. A. Marshall, T. Wagerle, C. M. Dubas-Cordery, W. Hong

88. Imidazopyridine based herbicides. **T. M. Stevenson**, C. M. Dubas-Cordery

89. Isonicotinamide herbicides. **T. M. Stevenson**, C. M. Dubas-Cordery

90. Pyrazolyl substituted pyridine herbicides. **T. M. Stevenson**, M. Xu, M. Hendrixson, C. M. Dubas-Cordery, M. J. Currie

91. Synthesis and fungicidal activity of 2-nicotinamidoalkylpyridines. **S. A. Bolgunas**, M. P. Walker, W. Moberg, D. Clark, J. Bisaha, D. W. Piotrowski, K. Patel, K -M. Sun, R. Shapiro, J. V. Hay, T. D. Neubert, S. Foor, T. P. Selby, T. M. Stevenson

92. Synthesis and insecticidal activity of novel 1,8-naphthalenedicarboxamides. **T. F. Pahutski Jr.**, K -M. Sun

93. Synthesis and optimization of bicyclic arylamidines as fungicides. **W. Zhang**, C. P. Tseng

94. Discovery of a new QoI fungicide, pyribencarb. **S. Fukumoto**, R. Tamai, M. Ozaki, M. Takagaki, S. Kataoka

95. Enantioenriched cyanohydrins: Versatile insecticide intermediates. **C. Moberg**, E. Wingstrand, F. Li, S. Lundgren, M. Penhoat

Natural Products for Pest Management

96. GreenMatch™ EX: A new broad-spectrum organic herbicide based on lemongrass oil. **C. Avila-Adame**, B. J. Campbell, L. E. Fernández, E. Tan, **M. E. Koivunen**, P. G. Marrone

97. Antifungal compounds from *Pimpinella* species active against plant pathogens. **N. Tabanca**, D. E. Wedge, N. Kirimer, K. H. C. Baser, E. Bedir

98. Antifungal activity of herbaceous essential oils protects wood from mold and decay fungi. **V. W. Yang**, C. A. Clausen

99. Tungstophosphoric acid and its compounds as agents against plant viruses. **S. Uskokovic-Markovic**, I. Holclajtner-Antunovic, D. Bajuk-Bogdanovic, J. Zakrzewska

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MONDAY MORNING

Natural Products –
Natural Products for Pest Management
S. O. Duke, *Organizer, Presiding*

Section B
Crowne Plaza City Center – Independence A/B

9:30 —100. Cyperin, a pathogenic fungi diphenyl ether phytotoxin, targets plant enoyl (acyl carrier protein). **F. E. Dayan**, D. Ferreira, Y -H. Wang, I. A. Khan, J. McInroy, Z. Pan

9:50 —101. New phytotoxins for biocontrol of *Cirsium arvense* and *Sonchus arvensis* (Asteraceae). **A. Evidente Sr.**

10:10 —102. Mevalocidin: A novel, phloem-mobile herbicide with potential as a bioherbicide. **P. R. Graupner**, B. C. Gerwick III, P. R. Schmitzer, S. C. Fields, W. K. Brewster, J. D. Webster, G. J. deBoer, T. A. Walsh, D. G. McCaskill, C. Pearce

10:30 — Intermission.

10:50 —103. Antifeedant activity of rinsate constituents from camphorweed against lepidopteran larva. **M. Morimoto**

11:10 —104. Insecticides from plants against termites and mosquitoes. **K. M. Meepagala**, W. Osbrink, J. Pridgeon, J. Becnel, G. Sturtz, C. Burandt, A. Lax, S. O. Duke

11:30 —105. Discovery and development of natural products for insect pest management. **C. L. Cantrell**, N. Fokialakis, W. Osbrink, A. Lax, S. O. Duke

11:50 —106. Fungicides and insecticides from medicinal and aromatic plants. **D. E. Wedge**, N. Tabanca, B. J. Sampson

Evaluation of Agriculturally-Related Chemicals: Effects on Environmental, Animal, and Human Health –
Pesticides and Non-target Organisms
E. A. Arthur and P. Rice, *Organizers*
T. A. Anderson and P. J. Rice, *Organizers, Presiding*

Section C
Crowne Plaza City Center -- Liberty A

9:45 — Introductory Remarks.

9:50 —107. Value of herbicides in U.S. crop protection. **L. P. Gianessi**

10:10 —108. Fate and exposure pathways of Bt-endotoxins in terrestrial food webs. **J. A. Peterson**, J. D. Harwood

10:30 — Intermission.

10:45 —109. Pesticides and honey bee health: High levels of acaricides and crop protection chemicals in US beehives and its mitigation by gamma irradiation. **C. A. Mullin**, M. Frazier, J. L. Frazier, S. Ashcraft, R. Simonds

11:05 —110. Neonicotinoid insecticides: Assessing risk to bees. **A. E. Chalmers**, D. L. Fischer

11:25 —111. Phytotoxicity of four herbicides on *Ceratophyllum demersum*, *Vallisneria natans*, and *Elodea nuttallii*. **S -X. Gao**, H -Y. Pan, Q. Huang

Transitioning into Green Chemistry Academic
Sponsored by CHED, Cosponsored by ENVR, MEDI, ANYL, AGRO, FUEL, ORGN, CEI, CORP
J. D. Fair, Organizer, Presiding

Sheraton Philadelphia City Center -- Independence Ballroom B

8:30 — Introductory Remarks.

3:35– CHED 115. Microwave heating: A versatile tool for clean organic synthesis and biofuel production. **N. E. Leadbeater.**

9:10– CHED 116. Catalysis as a key technology and fundamental science for green chemistry. **W. Leitner**

9:45– CHED 117. Design, performance and mechanistic chemistry of Fe-TAML activators: Reducing and eliminating hazardous substances. **T. J. Collins**

10:20 — Intermission.

10:35– CHED 118. Green solvents: The good, the bad and the ugly. **J. F. Brennecke**

11:10– CHED 119. Green chemistry: Principles, practice, and economics. **M. M. Kirchhoff**

MONDAY AFTERNOON

Biological and Chemical Transformations of Animal Hormones and Veterinary Pharmaceuticals in Plants, Soil, and Wastewater Treatment Systems
Cosponsored by HEALTH
D. S. Aga and P. J. Rice, *Organizers, Presiding*

Section A
Crowne Plaza City Center -- Liberty C

1:25 — Introductory Remarks.

1:30 —112. Veterinary pharmaceuticals studied by nonlinear optics: Oxytetracycline and morantel interacting with model environmental interfaces. **P. L. Hayes**, A. L. Mifflin, C. T. Konek, J. M. Gibbs-Davis, M. J. Musorrafiti, K. A. Scheidt, F. M. Geiger

1:50 —113. Degradation of sulfonamides in aqueous solution by membrane anodic Fenton treatment. **K. Neafsey**, A. T. Lemley

2:10 —114. Reduction of chlortetracycline residues in manure from therapeutically-treated beef calves. O. A. Arikan, W. Mulbry, **C. P. Rice**

2:30 —115. Fate of sulfamethazine in surface water microcosms and bioaccumulation in sediment-dwelling invertebrates. **K. L. D. Henderson**, T. B. Moorman, J. R. Coats

2:50 — Intermission.

3:10 —116. Simultaneous analysis of estrogens and their conjugates in manure from dairy farms and poultry operations using LC/MS-MS. **J. Tso**, D. S. Aga

3:30 —117. Estrogen removal from dairy manure by pilot-scale reactors. **K. F. Knowlton**, Z. Zhao, J. A. Ogejo, N. G. Love

3:50 —118. Fate of estradiol and testosterone in anaerobic lagoon digestors. **H. Hakk**, G. L. Larsen, L. S. Sikora

4:10 —119. Degradation of zeranol by phytoremediation. **M. L. Card**

Natural Products – Genomics and RNAi in New Product Development
W. P. Ridley, *Organizer, Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

1:50 —120. Identification of key enzymes involved in the biosynthesis of the allelochemical sorgoleone. **S. R. Baerson**, A. M. Rimando, Z. Pan, F. E. Dayan, S. O. Duke

2:10 —121. Control of coleopteran insect pests through RNA interference. **J. A. Baum**

2:30 —122. Engineering broad-spectrum root-knot resistance in crops using RNAi silencing of a root-knot nematode parasitism gene. **R. S. Hussey**, G. Huang

2:50 — Intermission.

3:10 —123. Enhancing the value of cottonseed as a source of feed and food by RNAi-mediated, selective and substantial reduction in seed-gossypol. **K. S. Rathore**, G. Sunilkumar, L. M. Campbell, R. D. Stipanovic, L. S. Puckhaber

3:30 —124. High lysine corn generated by endosperm specific suppression of lysine catabolism using RNAi. **T. Malvar**, S. Huang, A. Frizzi, N. Houmard, L. Gilbertson, W. E. Brown, C. Bonin, A. Reyes, J. Mainville, W. Adams, M. Luethy, D. Brackenridge, C. Florida

3:50 —125. Intragenic options for specialty crop improvement: High health and quality without foreign DNA. **K. Swords**, J. Ye, C. Richael, H. Yan, C. Rommens

Evaluation of Agriculturally-Related Chemicals: Effects on Environmental, Animal, and Human Health
Environmental Fate and Modeling
T. A. Anderson and P. J. Rice, *Organizers*
E. A. Arthur and P. Rice, *Organizers, Presiding*

Section C
Crowne Plaza City Center -- Liberty A

1:45 — Introductory Remarks.

1:50 —126. Excel spreadsheet incorporating statistical tools for determining selection of regression models for analysis of E-fate datasets. **J. Aldworth**, S. H. Jackson, A. M. Wadley

2:10 —127. Mobility, longevity, and activity of fipronil at a rate labeled for the prevention of termite infestation in structures. **C. J. Peterson**

2:30 —128. Tillage-system impact on surface runoff and interflow transport of selected herbicides at the field scale. **T. L. Potter**, D. D. Bosch, T. C. Strickland

2:50 — Intermission.

3:05 —129. Management and modeling: Tools to improve water quality. **K. Kramer**, P. J. Rice, B. P. Horgan, J. Rittenhouse

3:25 —130. Pilot study to investigate options for catchment scale modeling of pesticides. **G. G. Hoogeweg**, C. M. Holmes, E. J. Pemberton

3:45 —131. Investigation of long-term trends in atrazine residues in raw waters supplying Midwest community water systems. **W. Chen**, B. Munoz

Transitioning into Green Chemistry Industrial
Sponsored by CHED, Cosponsored by ENVR, MEDI, ANYL, AGRO, FUEL, ORGN, CEI, CORP
J. D. Fair, Organizer, Presiding

Sheraton Philadelphia City Center -- Independence Ballroom B

1:30 — Introductory Remarks.

1:35– CHED 135. Successful academic-industry collaboration in green technologies through the federation model. **S. J. Downey**

2:10– CHED 136. Green chemistry through innovation at Merck: The synthesis of Januvia. **J. D. Armstrong III**

2:45– CHED 137. Lessons learned through measuring green chemistry performance of development routes at GSK. **D. Constable**, R. K. Henderson, C. Ruddick, C. Jimenez-Gonzalez, T. Roper, G. R. Geen

3:20 — Intermission.

3:35– CHED 138. Practice of sustainable chemistry at Dow: Historical and future perspectives**. V. A. Atiemo-Obeng**, A. A. Muellerweiss

4:10– CHED 139. Greening the pharmaceutical industry: Accomplishments and opportunities**. B. W. Cue, Jr.**

MONDAY EVENING

5:00 – 7:00
Transitioning into Green Chemistry Poster Session
Sponsored by CHED, Cosponsored by ENVR‡, MEDI, ANYL, AGRO, FUEL, ORGN, CEI, and CORP
J. D. Fair, Organizer

Sheraton Philadelphia CC
–Freedom Ballroom E/F

CHED 298. Green chemistry labs: An ongoing process at Siena College**. A. B. Todaro**, J. O'Donnell

CHED 299. Greening the organic chemistry laboratory at Widener University**. K. Gerhart**, L. D. Bastin

CHED 300. An approach to recycling scrap white athletic leather**. D. C. Shelly**, K. Kolomaznik, N. V. Phuoc

CHED 301. Progress in biodegradable poly-3-hydroxyalkanoate (PHA) polymer production: Cost reduction investigations. **D. J. Nicholson**, A. J. Stipanovic, C. T. Nomura, T. Bluhm

CHED 302. Screening biomass-derived fuel additives via emissions testing to evaluate the next generation of environmentally benign fuels**. N.-S. Chong**, S.Sirupa, B. M. Naah, R. W. Chong, B. G. Ooi

CHED 303. Studies of yeast strains for bioethanol production and the emission characteristics of biomass-derived fuel additives. **N. S. Chong**, K. R. Lankford, S. Sirupa, B. G. Ooi

CHED 304. Microwave heating for fast, easy biodiesel preparation. **L. M. Stencel**, T. M. Barnard, N. E. Leadbeater

CHED 305. Continuous-flow approaches to scale-up of microwave-promoted reactions. ***D. Gunn****, N. E. Leadbeater*

CHED 306. Palladium-catalyzed reactions with gaseous reagents: Carbonylation with carbon monoxide, Heck reaction with ethane. **C. M. Kormos**, N. E. Leadbeater

CHED 307. Beyond atom economy: A complete carbon-retentive process toward homoallylic amines. J. J. Chruma, **T. K. VanDervort**

CHED 308. Catalytic hydrogenation of aromatic compounds with carbon nanotube-supported metallic nanoparticles in supercritical fluid carbon dioxide. **H.-J. Chen**, H.-B. Pan, J.-F. Jen, K.-H. Chiu, C. M Wai

CHED 309. Magnetic beads-based bioelectrochemical immunoassay of polycyclic aromatic hydrocarbons and polychlorinated biphenyls. **Y.-Y. Lin**, Y. Lin, C. M. Wai

CHED 310. Green chemistry technique using algae fluorescence to monitor water quality. **Q. Wang**, H. H. Patterson, J. M. Peckenham

8:00 - 10:00
Sci-Mix
K. L. Armbrust, *Organizer*

Section A
Pennsylvania Convention Center -- Hall C

43-63. See previous listings.

International Award for Research in Agrochemicals Symposium in Honor of Dr. David M. Soderland

Financially supported by BASF Corp. and DuPont Crop Protection
J. R. Bloomquist, *Presiding*
TUESDAY MORNING

Section A
Crowne Plaza City Center -- Liberty C

First of two sessions

8:00 — Award Presentation.

8:20 —132. State-dependent actions of pyrethroid insecticides on voltage-gated sodium channels. **D. M. Soderlund**

9:05 —133. Identification of residues in the cockroach sodium channel critical for the binding and action of pyrethroid insecticides. Y. Du, J -E. Lee, Y. Nomura, **K. Dong**

9:35 —134. Role of the sixth segment of domain IV of the cockroach sodium channel in the action of sodium channel-blocker insecticides. **K. S. Silver**, S. Konanz, Y. Du, W. Song, J -E. Lee, V. L. Salgado, K. Dong

10:05 — Intermission.

10:20 —135. PKC-dependent phosphorylations modify the action of CS-syndrome pyrethroids on rat brain N-type ($Ca_v2.2$) voltage-sensitive calcium channel. **J. M. Clark**

10:50 —136. Molecular mechanisms and monitoring of permethrin resistance in human head lice. **S. H. Lee**, J. M. Clark, K. S. Yoon, D. H. Kwon

11:20 —137. Regulation of insect P450 expression: Genomic insights. **R. Feyereisen**, A. Brun-Barale, M. Giraudo, F. Hilliou, I. Jacovella, G. Le Goff

TUESDAY MORNING

Bioenergy Production: Challenges, Concerns, and Consequences
Cosponsored by ENVR
J. H. Massey, *Organizer*
C. J. Hapeman, *Organizer, Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

9:15 — Introductory Remarks.

9:20 —138. Keynote Address. The evolving of the paradigm of agriculture as a supplier of energy and chemicals. **L. P. Walker**

9:50 —139. Biomass production and processing economics: Implications for cost of reducing carbon emissions via biofuel. **J. A. Miranowski**

10:10 —140. A landscape vision for sustainable bioenergy feedstock production. **D. L. Karlen**, S. J. Birrell, D. A. Laird, R. M. Cruse

10:30 —141. Sustainable bioenergy production in the Chesapeake Bay agricultural landscape: Potential and peril. **W. D. Hively**

10:50 —142. Can biofuels be sustainable in an unsustainable agriculture? **D. De La Torre Ugarte**, C. M. Hellwinckel

Evaluation of Agriculturally-Related Chemicals: Effects on Environmental, Animal, and Human Health
Risk and Exposure Assessments
E. A. Arthur and P. J. Rice, *Organizers*
T. A. Anderson and P. Rice, *Organizers, Presiding*

Section C
Crowne Plaza City Center -- Liberty A

9:15 — Introductory Remarks.

9:20 —143. Use of structural analysis (QSAR) to predict fish bioconcentration factors for pesticides. **S. H. Jackson**, G. Thomas, C. E. Cowan-Ellsberry

9:40 —144. Assessing the importance of ionization state during environmental risk assessment of pharmaceuticals. T. W. Valenti Jr., **B. W. Brooks**

10:00 —145. Higher tier exposure modeling of veterinary pharmaceuticals: A UK case study. **C. M. Holmes**, K. L. Barrett, J. M. Cheplick

10:20 — Intermission.

10:40 —146. Experiences with NHDPlus and pesticide exposure assessment. **R. Vamshi**, P. Miller, C. M. Holmes

11:00 —147. New approaches to agrochemical monitoring studies: Update on the atrazine ecological exposure monitoring study. **P. Hendley**, S. M. Bartell, C. M. Harbourt, D. Volz

11:20 —148. Comparison of two water quality models for estimation of aquatic system bioaccumulation. **S. H. Jackson**

Sterling B. Hendricks Memorial Lectureship

Sponsored by USDA-Agricultural Research Service
Cosponsored by AGFD and AGRO
TUESDAY MIDDAY

M. H. Tunick, *Organizer*
J. N. Seiber, *Organizer, Presiding*

11:30 — Introductory Remarks.

11:45 — AGFD 101. Award Address: Fergus M. Clydesdale. A nutritional odyssey: From famine to feast, can science and policy solve the dilemma?

12:30 —Reception.

TUESDAY AFTERNOON

International Award for Research in Agrochemicals in Honor of Dr. David M. Soderlund
Financially supported by BASF Corp. and DuPont Crop Protection
J. R. Bloomquist, *Presiding*

Section A
Crowne Plaza City Center -- Liberty C

1:10 —149. A synergistic interaction between the two major mechanisms of permethrin resistance in mosquitoes, cytochrome P450 detoxification and *kdr*. **J. G. Scott**, M. C. Hardstone, C. Leichter

1:40 —150. Nicotinic acetylcholine receptors and resistance to neonicotinoids. **M. S. Williamson**

2:10 —151. Sulfonyl urea receptor in insect cuticular epidermis is likely the insecticidal target of benzoylurea type insecticides. **F. Matsumura**, G. Abo-Elghar

2:40 —152. Ligand-gated chloride channel gene family of *Drosophila*. **D. C. Knipple**, D. M. Soderlund

3:10 — Intermission.

3:25 —153. Glutamate-activated chloride channels: Unique fipronil targets present in insects but not in mammals. **T. Narahashi**, X. Zhao, T. Ikeda, V. L. Salgado, J. Z. Yeh

3:55 —154. Role of GABA and glutamate receptors in susceptibility and resistance to chloride channel blocker insecticides. **V. L. Salgado**, X. Zhao

4:25 —155. Anion channels/transporters as targets for new insecticides and nematicides. **J. R. Bloomquist**, D. R. Boina

Bioenergy Production: Challenges, Concerns, and Consequences
Cosponsored by ENVR
C. J. Hapeman, *Organizer*
J. H. Massey, *Organizer, Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

1:25 — Introductory Remarks.

1:30 —156. Enhancement and stabilization of biomass feedstock quality through utilization/recycling biological waste streams. **L. O. Pordesimo**, S. Capareda, S. Sokhansanj, S. Fernando

1:50 —157. Turning waste into energy: Biogas production on dairy farms. **M. C. Smith**, H. Ahn, J. White

2:10 —158. Estimating regional water use with changing cropping patterns. M. Stiles, **D. Pennington**

2:30 —159. Potential of biofuel production to complement Chesapeake Bay restoration efforts: Management strategies for grasses. **K. W. Staver**

2:50 —160. Renewable energy: Opportunities and breakthroughs for the future (AGRO New Investigator Award Winner). **A. E. Brown**, J. R. Wilkinson, W. P. Williams, T. J. Benson, D. L. Sparks, W. T. French, R. Hernandez, E. C. Rogers, W. E. Holmes

3:10 — Intermission.

3:25 —161. Sustainable bioenergy crop production. **F. M. Hons**, J. P. Wight, T. J. Gentry

3:45 —162. Sustainable corn-based bioenergy farming systems. **J. W. Singer**, D. A. Laird, C. A. Cambardella, D. L. Karlen, K. J. Moore, K. R. Lamkey, J. L. Hatfield

4:05 —163. Properties of wood chars for soil amendment and carbon sequestration. D. W. Rutherford, **C. E. Rostad**, J. A. Leenheer, R. L. Wershaw

4:25 —164. Considering the soil: Consequences of providing biomass for energy. **R. L. Graham**

4:45 — Panel Discussion.

Evaluation of Agriculturally-Related Chemicals: Effects on Environmental, Animal, and Human Health
Pesticide Risks and Benefits: Evaluations and Case Studies
T. A. Anderson and P. Rice, *Organizers*
E. A. Arthur and P. J. Rice, *Organizers, Presiding*

Section C
Crowne Plaza City Center -- Liberty A

2:05 — Introductory Remarks.

2:10 —165. Safety evaluation and regulation of crop protection chemicals in developing countries: A global human and environmental issue. **D. Wauchope**, J. F. Sandahl, L. Suguiyama

2:40 —166. Pecos River ecosystem restoration project: A case study. **C. E. Olivieri**

3:10 — Intermission.

3:30 —167. Contribution of environmental fate research to human health and the environment. **R. L. Jones**, E. L. Arthur

4:00 —168. Strengths and weaknesses of post-registration ranking systems for pesticides. S. H. Jackson, I. D. Kelly, A. C. Barefoot, K. Brugger, **P. Hendley**

WEDNESDAY MORNING

Agricultural Best Management Practices to Protect Chesapeake Bay Water and Air Quality
Chesapeake Bay Health and Pesticide Fate
Cosponsored by ENVR
C. J. Hapeman and L. L. McConnell, *Organizers*
G. Allen, *Organizer, Presiding*

Section A
Crowne Plaza City Center -- Liberty C

8:15 — Introductory Remarks.

8:20 —169. The role of agricultural research in the restoration of the Chesapeake Bay. **C. J. Hapeman**, L. L. McConnell

8:40 —170. Pesticides in groundwater and streams of the Chesapeake Bay watershed. **J. M. Denver**

9:00 —171. Pesticides in tidal regions of Chesapeake Bay. **L. L. McConnell**, C. P. Rice, C. J. Hapeman, K. Bialek, M. Fulton, A. K. Leight, G. Allen

9:20 —172. Assessing sediment quality in Chesapeake Bay. **M. J. Hameedi**, I. Hartwell

9:40 —173. Atmospheric delivery of herbicides to riparian buffer zones. **C. P. Rice**, K. Bialek-Kalinski, W. D. Hively

10:00 — Intermission.

10:15 —174. Modeling the effect of a riparian buffer strip on off-field entrapment of pesticides using REMM2008. **T. L. Estes**, R. Lowrance, R. G. Williams, R. D. Wauchope

10:35 —175. Modeling pesticide spray drift: Applications to the Chesapeake Bay watershed. **R. Williams**, C. M. Holmes

10:55 —176. Efficacy of trees to mitigate emissions from poultry houses. **G. W. Malone**, G. L. VanWicklen, S. L. Collier

11:15 —177. Can organic farming help protect Chesapeake Bay water and air quality? **M. A. Cavigelli**

Environmental Forensics
Cosponsored by ANYL and ENVR
E. A. Arthur, G. Coimbatore, and R. L. Cook, *Organizers*
S. Mislankar, *Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

8:50 — Introductory Remarks.

9:00 —178. Role of stable isotopes in environmental forensics. **R. P. Philp**, T. Kuder, J. Allen

9:20 —179. Following organic matter flow within the environment from a forensic viewpoint. **R. L. Cook**

9:40 —180. Perchlorate isotope forensics. **P. B. Hatzinger**, N. C. Sturchio, J. F. Bohlke, B. Gu, A. Jackson

10:00 — Intermission.

10:20 —181. Principles, techniques, and applications of environmental forensics in agroecology. **U. S. Tim**

10:40 —182. Identifying molecular changes in the chromophoric dissolved organic matter of oxidized waste streams. **W. T. Cooper**, D. Osborne

11:00 —183. Nanofluidics and mass-limited chemical analysis: Nanocapillary array membranes as switchable fluidic elements for coupled multidimensional analyses. **P. W. Bohn**

11:20 —184. Development of a new technique for the detection of heavy metals in aqueous media using modified nanomaterials. **A. K. Wanekaya**, J. Morton

Reduced Risk Pesticides: Environmental Chemistry, Toxicology and Compatibility with IPM
Cosponsored by HEALTH
A. Felsot and M. W. Brooks, *Organizers*

Section C
Crowne Plaza City Center -- Liberty A

8:20 — Introductory Remarks.

8:30 —185. Navigating the regulatory pathway for reduced risk pesticide registration. **M. W. Brooks**

9:00 —186. Spinosad to spinetoram: Evolution of the spinosyns. **J. E. Dripps**, C. V. DeAmicis, T. C. Sparks, G. D. Crouse

9:30 —187. Indoxacarb's fit in global IPM programs. **J. T. Andaloro**, H. E. Portillo, P. G. Marcon, A. Barefoot

10:00 — Intermission.

10:15 —188. Nonsteroidal ecdysone agonist insecticides: Mode of action, environmental fate, eco-toxicological profile, and fit in IPM programs. **L. E. Gomez**, T. S. Dhadialla, D. Paroonagian

10:45 —189. Rynaxypyr®: A new reduced risk insecticide for IPM programs. **P. G. Marcon**, J. T. Andaloro, A. Barefoot

11:15 —190. Ketoenols: Profile of a new class of low risk insecticides. **I. D. Kelly**, R. W. Heintzelman, J. W. Bell

WEDNESDAY AFTERNOON

Agricultural Best Management Practices to Protect Chesapeake Bay Water and Air Quality
Developing New Tools to Mitigate Nutrient Loads
Cosponsored by ENVR
G. Allen and C. J. Hapeman, *Organizers*
L. L. McConnell, *Organizer, Presiding*

Section A
Crowne Plaza City Center -- Liberty C

1:40 —191. Hydrologic and biogeochemical storm response in Choptank River basin headwaters. **A. I. Koskelo**, T. R. Fisher

2:00 —192. Buffer widths and removal efficiencies for TN, TP, and TSS. **S. Z. Cohen**, R. Baris, Q. Ma

2:20 —193. Sources and transport of suspended sediment in the Chesapeake Bay watershed. **S. W. Ator**, J. W. Brakebill

2:40 —194. Speaking in one voice: Developing a universal agricultural conservation language within the Chesapeake Bay watershed. **M. Dubin**

3:00 — Intermission.

3:20 —195. Developing nitrogen recommendations for corn with an on-the-go canopy reflectance sensor. **J. P. Schmidt**, A. E. Dellinger, D. B. Beegle

3:40 —196. Achieving nutrient reduction goals from Maryland cropland: What worked? What didn't? What will it take? **K. W. Staver**

4:00 —197. Innovative methods for measuring cover crop nutrient uptake on a landscape scale. **W. D. Hively**, M. W. Lang, A. Sadeghi, G. McCarty, L. L. McConnell

4:20 —198. Whole-farm simulation to determine effective conservation practices. **T. L. Veith**, C. A. Rotz

4:40 —199. Development of a GIS-based planning and land-use management tool for protecting water quality in Choptank River watershed. **M. S. Altinakar**, Z. He, G. W. McCarty, A. Sadeghi, D. Hively, J. Keppler, J. Rhoderick

Environmental Forensics
Cosponsored by ANYL and ENVR
E. A. Arthur, S. Mislankar, and R. L. Cook, *Organizers*
G. Coimbatore, *Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

1:40 —200. Immunosensors for the detection of low molecular weight contaminants. **D. A. Blake**, S. J. Melton, H. Yu, R. A. Foster, X. Zhu

2:00 —201. Multivalent glycoconjugates for *Escherichia coli* detection. **D. M. Hatch**, A. Weiss, R. R. Kale, S. Iyer

2:20 —202. Bioreporter genes for detection of specific compounds. **R. S. Burlage**

2:40 —203. Environmental forensics aspects of microbial contamination from concentrated animal feeding operations. **U. S. Tim**

3:00 — Intermission.

3:20 —204. Surface plasmon resonance based immuno-detection of environmental contaminants. **G. Coimbatore**, K. Ochoa, G. P. Cobb III

3:40 —205. Bis(chlorophenyl)acetic acid (DDA), a water-soluble biomarker of DDT metabolism in humans. **Z. Chen**, Y. Li, M. M. Bigelow-Dyk, H. M. Vega, R. I. Krieger

4:00 —206. Biological validation of dendrochemistry in environmental forensics. **K. T. Smith**, W. C. Shortle

4:20 — Concluding Remarks.

Reduced Risk Pesticides: Environmental Chemistry, Toxicology and Compatibility with IPM
Cosponsored by HEALTH
A. Felsot and M. W. Brooks, *Organizers*

Section C
Crowne Plaza City Center -- Liberty A

1:25 — Introductory Remarks.

1:30 —207. Fenamidone: A reduced risk fungicide. **S. Mislankar**, I. D. Kelly, R. W. Heintzelman

2:00 —208. Discovery and development of the reduced risk fungicide, mandipropamid. **A. Tally**, R. Rezaaiyan, F. Wilhite, D. Drost

2:30 —209. Paladin™ and Paladin EC™: A natural fumigant replacement for methyl bromide. **R. M. Bennett**

3:00 —210. Aminopyralid: A new reduced risk herbicide for invasive species control in range and pasture/IVM: Toxicology, ecotoxicology, and environmental fate profile. **J. J. Jachetta**, P. L. Havens, C. Tiu, S. C. Gehen, V. J. Kramer

3:30 —211. External, nonstandard studies: What impact do they have on glyphosate's public perception? **D. R. Farmer**, D. Goldstein, S. Mortensen

4:20 —212. Successes in the research, development, and adoption of reduced risk chemistry. **J. E. McFarland**, G. Watson, J. Abbott, P. Hertl, T. Pastoor

4:50 —213. Sustaining the new, reduced-risk-pesticide technology: Why IPM is more important than ever. **A. S. Felsot**

THURSDAY MORNING

New Developments and Issues in Agrochemical Sciences
K. L. Armbrust, *Organizer, Presiding*

Section A
Crowne Plaza City Center -- Liberty C

8:20 — Introductory Remarks.

8:30 —214. Common crop protection practices and the possibility of groundwater contamination in different types of soil through leaching of currently-used pesticides. **T. Jindal**

8:50 —215. Application volume and active ingredient concentration affect the initial soil penetration of aqueous termiticide formulations. **C. J. Peterson**

9:10 —216. Breaking down the substituent of the future: Environmental properties of pentafluorosulfanyl compounds. **D. A. Jackson**, S. A. Mabury

9:30 — Intermission.

9:45 —217. A new natural product pesticide for controlling fungal and bacterial plant pathogens. C. Avila-Adame, E. Tan, B. J. Campbell, H. Huang, L. E. Fernández, **M. E. Koivunen**, P. G. Marrone

10:05 —218. New biopesticides from plants and microbes. **M. E. Koivunen**, P. G. Marrone

10:25 —219. Esterase-based resistance in the tobacco adapted form of the green peach aphid, *Myzus persicae* (Sulzer), in the eastern US. **L. Srigiriraju**, P. J. Semtner, T. D. Anderson, I. V. Sharakhov, J. R. Bloomquist

10:45 —220. Study on preparation of pesticide microemulsion. **J. Wang Sr.**, **X. Yang Sr.**, G. Li Sr.

11:05 — Prize Drawing.

Residential Pesticide Exposure Assessment
J. Evans, D. Vogel, and V. Zartarian, *Organizers*
C. Lunchick and N. S. Tulve, *Organizers, Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

8:00 — Introductory Remarks.

8:20 —221. Overview of the evaluated observational children's pesticide exposure studies. **C. Lunchick**, D. E. Barnekow, J. H. Ross

9:00 —222. Relationships between environmental concentrations and measured urinary biomarker levels. **N. S. Tulve**, J. H. Ross, P. P. Egeghy, C. Lunchick, D. E. Barnekow, J. H. Driver

9:55 —223. Urinary pesticide metabolite concentrations in children following indoor pesticide applications. **J. H. Ross**, D. E. Barnekow, C. Lunchick

10:35 — Panel Discussion.

11:35 — Concluding Remarks.

THURSDAY AFTERNOON

New Developments and Issues in Agrochemical Sciences
Programming for Success
K. L. Armbrust, *Organizer, Presiding*

Section A
Crowne Plaza City Center -- Liberty C

12:00 — Introductory Remarks.

12:10 —224. Implementing AGRO's strategic plan. **J. J. Johnston**

12:30 —225. Standing topics for AGRO symposia. **K. L. Armbrust**

12:50 —226. Technical programming for DC and beyond. **E. A. Arthur**

1:10 —227. Making inroads in international venues. **L. L. McConnell**

1:30 —228. AGRO's communication to its membership. **C. J. Hapeman**

1:50 — Discussion.

2:20 — Concluding Remarks.

Residential Pesticide Exposure Assessment
J. Evans, D. Vogel, N. S. Tulve, and C. Lunchick, *Organizers*
J. H. Driver, *Presiding*
V. Zartarian, *Organizer, Presiding*

Section B
Crowne Plaza City Center -- Independence A/B

1:00 — Introductory Remarks.

1:10 —229. Presentation of standard operating procedures (SOPs): Equations and assumptions. **J. Evans**

1:30 —230. Presentation of equations, assumptions, and results for four post-application pesticide exposure models. **J. Evans**, V. Zartarian, J. Xue, B. Young, J. H. Driver, M. Pandian, N. S. Tulve

3:30 — Panel Discussion.

AGRO DIVISION

AGRO 1
Modern GC-MS and LC-MS instrumentation techniques in the analysis of agrochemical residues
Katerina Mastovska, *Eastern Regional Research Center, USDA-Agricultural Research Service, 600 East Mermaid Lane, Wyndmoor, PA 19038, Fax: 215-233-6642*

In recent years, gas chromatographic-mass spectrometric (GC-MS) and liquid chromatographic-mass spectrometric (LC-MS) instrumentation and techniques have scored dramatic developments, resulting in introduction of many useful tools for the analysis of agrochemical residues in various matrices. This presentation will discuss the application of state of the art GC-MS and LC-MS techniques in multi-class, multi-residue analysis of pesticides and veterinary drugs, emphasizing approaches that provide increased sample throughput and/or improved analyte detectability. With respect to GC-MS, the main focus will cover the use of time-of-flight MS for fast GC or for comprehensive, two-dimensional GCxGC. Whereas, for LC-MS, focus will be on the application of sub-2 µm particle LC columns in the LC-MS(-MS) analysis of pesticide and veterinary drug residues.

AGRO 2
SPE protocols for cleanup and UPLC-MS determination of acidic herbicides in fruit and vegetables after a rapid pretreatment procedure
Michael S. Young, *Diane M. Diehl, Jeremy C. Shia, and Kevin M. Jenkins, Waters Corporation, 34 Maple Street, Milford, MA 01757, Fax: 508-482-3100*

Recently, a rapid, solvent and salt-out partition, procedure has become popular for pre-treatment of fruits and vegetables prior to dispersion or pass-through SPE (solid phase extraction) cleanup. These procedures, known collectively as QuEChERS (quick, easy, cheap, effective, rugged, and safe) method, are designed to produce extracts for GC-MS and LC-MS analysis. The procedure has been demonstrated for many basic or neutral pesticides but the recommended SPE cleanup using PSA (primary/secondary amino bonded silica) is not appropriate for determination of acidic residues. This presentation will discuss options for SPE cleanup that are suitable for determination of acidic herbicides and other acidic analytes in samples processed using QuEChERS pre-treatment. Among the options discussed will be both dispersion or pass-through cleanup as well as retention and elution cleanup. Among the sorbents discussed will be various traditional sorbents such as PSA and silica as well as mixed-mode sorbents such as Oasis MAX. We will also demonstrate UPLC (ultra performance liquid chromatography) technology coupled with tandem mass-spectrometry for staightforward and rapid chromatographic analysis of these samples for acidic pesticides with no need for derivatization.

AGRO 3
Structure elucidation of DNA adducts from pesticides via mass spectral analysis
Donald W. Boerth[1], *dboerth@umassd.edu, Todd C. Andrade*[1], *U_T2Andrade@umassd.edu, Erwin Eder*[2], *and Paul Wanek*[2]. *(1) Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, North Dartmouth, MA 02747, Fax: 508-999-9167, (2) Institute of Toxicology, University of Würzburg, D-8700 Würzburg NA, Germany*

Formation of modified nucleotides in plant DNA from pesticide-treated crop plants has been previously detected in ^{32}P postlabeling studies carried out in our laboratories. These adducts result from direct binding with electrophilic sites on pesticide molecules or their metabolites but may also occur from electrophilic intermediates produced by oxidative stress or metabolic bioactivation of pesticides. Cyclic propanodeoxyguanosine derivatives of hexenal and 4-hydroxynonenal have already been identified and have been shown to be biomarkers of plant stress from lipid peroxidation. Additional potentially genotoxic adducts were also detected although structures were not determined. In this study, we have employed electrospray LC-MS and LC-MS-MS to elucidate putative structures of several adducts of deoxyguanosine formed from interaction with the pesticides, chlorothalonil, triclopyr, and dicamba.

AGRO 4
Determination of 20,25-diazacholesterol residues in bird tissues
D. A. Goldade, *Christi A. Yoder, and J. J. Johnston, National Wildlife Research Center, USDA/APHIS/WS, 4101 LaPorte Avenue, Fort Collins, CO 80521-2154, Fax: 970 266-6089*

Population explosions of pest bird species cause significant damage to crops and property in the US each year. Fertility control is a promising and often socially acceptable means of managing pest bird populations. One promising chemical for the control of bird populations is 20,25-diazacholesterol. This agent blocks steroid synthesis and prevents birds from forming viable eggs. As part of an effort to register this compound for use, an analysis of any potential secondary hazards from its use must be conducted. The method described was developed to analyze for 20,25-diazacholesterol residues in two of the test species: quail and crows. The method employs a polymeric cation exchange column to remove matrix components coupled with GC/MS detection.

AGRO 5
Europium-sensitized luminescence determination of oxytetracycline residue in shrimp using an LED-based portable analyzer
***Guoying Chen**, Eastern Regional Research Center, USDA-Agricultural Resarch Service, 600 E. Mermaid Lane, Wyndmoor, PA 19038, Fax: 215-233-6642*

Oxytetracycline (OTC) residue in shrimp is determined by europium-sensitized luminescence (ESL) using an LED-based portable analyzer. After extraction in pH 4.0 ethylenediaminetetraacetic acid-McIlvaine buffer, and deproteination in trichloroacetic acid, OTC is cleaned up using Oasis hydrophilic-lipophilic balance cartridges. Eu(III) is added to the eluate to form a Eu:OTC chelate at pH 8.5. When excited by a 385 nm LED, OTC transfers the absorbed energy efficiently to Eu(III). The 617 nm luminescence is detected by a gated photomultiplier tube and integrated over 25-1000 µs. The 25-µs delay rejects stray light from the light source as well as fluorescence and scattering from concomitant matrix components. This method achieves 80.0% recovery at 100 ng/g. The ESL signal is linear to OTC concentration over 3 orders of magnitude (10-10,000 ng/g). Limit of detection is 4.6 ng/g and relative standard deviation is 3.75%. The background, averaged over six shrimp samples of different origins, corresponds to 10.4 ng/g. This instrument-method combination provides high sensitivity for trace OTC-in-shrimp determination, high specificity to eliminate chromatography, and the possibility for field deployment.

AGRO 6
Determination of brodifacoum by ion exchange solid phase extraction followed by ion-pair high performance liquid chromatography in mussels and sparrow tissues
***Thomas M. Primus**[1], thomas.m.primus@aphis.usda.gov, Chad R. Wermager[1], chad.r.wermager@aphis.usda.gov, John J. Johnston[1], john.j.johnston@aphis.usda.gov, Gregg Howald[2], gregg.howald@islandconservation.org, and Stacey Buckelew[2], stacey.buckelew@islandconservation.org. (1) National Wildlife Research Center, USDA/APHIS/WS, 4101 LaPorte Ave., Ft. Collins, CO 80521, (2) Island Conservation Canada, Vancouver, BC V6B 2M9, Canada*

Invasive rats have contributed to the extinction of indigenous flora and fauna on islands. Pelleted brodifacoum baits inadvertently applied to surface water could potentially cause exposure to terrestrial, aquatic, and/or marine organisms. Additionally, grain based baits are potentially consumed by non-target birds and mammals. During field trials, non-target hazards were assessed by determining brodifacoum concentrations in surface water, intertidal mussels, and granivorous land birds to evaluate potential exposure. The method consisted of reversed-phase ion-pair liquid chromatography using fluorescence detection combined with a solid phase extraction clean-up. Mussel and sparrow tissues were extracted with acetonitrile and methanol. Extracts were dried, reconstituted with acidified methanol, and cleaned up by ion exchange solid phase extraction. Mean recoveries for common mussels and whole body sparrow tissue quality control samples were 105 ± 3.6% and 95.5 ± 14.9%, respectively. The mean MLOD (method level of detection) for brodifacoum in mussels and sparrows were 2.0, and 1.1 ng/g, respectively.

AGRO 7
Shikimate concentration determination in plant material
***Thomas C. Mueller**, Plant and Soil Sciences, University of Tennessee, 252 Ellington Plant Sciences, 2431 Joe Johnson Drive, Knoxville, TN 37996, Fax: 865-974-5365*

When glyphosate is applied to plants, the 5-enolpyruvylshikimate-3-phosphate synthase (EPSPS) is blocked and the chemical precursor shikimate accumulates. This report details the methods to quantify shikimate in plant material. Frozen plant tissue is finely ground in liquid nitrogen and extracted with 1 M HCl. A 5.0 mL aliquot is adjusted to a pH of 3.0 and diluted with 2.5 mL acetonitrile and filtered. UV detection at 215 nm is used for quantification. A Phenomenex Luna NH2 100A column (250 x 4.0 mm; 5 µm particle size) was used with an injection volume of 10 µL. The mobile phase was 85/15 (v:v) acetonitrile/deionized water + 1% phosphoric acid at a flow rate of 1.0 mL/min. Total run time was 30 min with a shikimate retention time of 8.9 min. The detection limit for shikimate is approximately 30 µg/g fresh weight in plant tissue.

AGRO 8
Utility of a rapid method for detecting herbicide residues
***Patrick J. Hannan**, NOWCC/SEE Grantee, U.S. Environmental Protection Agency, Retired, 5019 Centinel Dr, Bethesda, DC 20816, Fax: 703 305-6309*

The inability to detect residues of herbicides that have been applied at approximately one ounce per acre has led to unresolved litigations of spray drift incidents. However, a procedure based on the CO_2 uptake rate of algae has been shown to be an answer to the problem. In testing seven sulfonylureas and three triazines, sub-µg amounts were detected in less than 10 min. Even 0.005 µg of Londax was detected, though that amount required approximately 1.5 hr. Individual identities of the pesticides are not possible, but distinguishing between these two classes of herbicides presents no problem. In legal disputes such as those involving spray drift, identifying the class of herbicide applied would be very useful. Greatly increased sensitivity of the method is envisioned with plant seedlings as the test organisms. For example, the known sensitivity of lentils to sulfonylureas suggests that seedlings of these plants could show responses to a few thousandths of a µg in a matter of minutes.

AGRO 9
Diffusive sampling of the rhizosphere using polydimethylsiloxane sorbents
***Jeffrey D. Weidenhamer**, Department of Chemistry, Geology & Physics, Ashland University, Kettering Science Center, Ashland, OH 44805, Fax: 419-289-5283*

Polydimethylsiloxane (PDMS) sorbents are being applied to measure allelochemical fluxes from plant roots. In this study, 5 cm lengths of stainless steel wire coated with PDMS tubing were inserted into soil beneath marigold plants in the field. Probes were removed after 24 hours and analyzed by HPLC. Microgram quantities of both 5-(3-buten-1-ynyl)-2,2'-bithienyl (BBT) and α-terthienyl were detected on individual probes. The amount and relative proportion of each compound varied by plant and sampling date. Given the high potency of these thiophenes in bioassays, the concentrations found can readily be conceived to be biologically active. The distribution of marigold allelochemicals in the rhizosphere is spatially heterogeneous and dynamic over time. Other probe designs are being explored which can trap fluxes of allelochemicals in the rhizosphere for longer periods and provide integrated measurements of root exudation over time. These techniques appear to be broadly applicable to the analysis of lipophilic root exudates.

AGRO 10
Preferential sorption of phenolic acids to soil and their allelochemical activity
***Prasanta C. Bhowmik**, Department of Plant, Soil, and Insect Sciences, University of Massachusetts, Stockbridge Hall, Amherst, MA 01003-7245*

The soil environment largely determines the activity and fate of allelochemicals. The role of sorption to soil in modifying the availability of components in complex allelochemical mixtures is still not well understood and the research in this area has been limited. The phenomenon of allelopathy is often brought about by root exudates having complex chemical composition and containing various compounds with different degrees of varying toxicities. The preferential sorption to soil in altering the chemical composition of plant exudates was studied in a silt loam soil using representative mixtures of plant phenolics, namely hydroxybenzoic, vanillic, coumaric, and ferulic acids. Experiments were conducted using a batch-equilibration technique; data were fitted to a Freundlich isotherm. The concentration-dependent sorption coefficient (K_d) at 10 µg/mL was used to assess the sorption affinity of the phenolic acids across different systems. All of the phenolic acids exhibited strong site-specific sorption as evident from their non-linear isotherms. Removal of organic matter substantially decreased the sorption affinity of all phenolic acids, indicating its role in preferential sorption. Direct competition for sorption sites was observed even at low concentrations of phenolic acids. The K_d of hydroxybenzoic acid was decreased more than 90% in the presence of coumaric acid. About 95% of sorbed vanillic acid was displaced into the soil solution in the presence of ferulic acid. Hydroxybenzoic acid did not affect the sorption affinity of other phenolic acids significantly, whereas ferulic acid showed low displacement by other phenolic acids. The displacement pattern indicated directional sorption of phenolic acids with –OH and –COOH groups. Our results demonstrate that soil preferential sorption can alter the availability of plant root exudates and thus modify their phytotoxic activity.

AGRO 11
***m*-Tyrosine, a root-exuded allelochemical produced by Chewing's fine fescue (*Festuca rubra* L. ssp. *commutata*)**
***Leslie A. Weston**, leslieweston20@gmail.com, E H Graham Centre for Agriculture, Charles Sturt University, Wagga Wagga, Australia, Fax: 607-387-6410, Cecile Bertin, PharmAfrica, Research Director, Montreal Quebec, Canada, and Frank C. Schroeder, Cornell University, Boyce Thompson Institute, Ithaca, NY*

Fine fescue grasses displace neighboring plants by depositing large quantities of an aqueous phytotoxic root exudate in the soil rhizosphere. Via activity-guided fractionation, we have isolated and identified the non-protein amino acid *m*-tyrosine as the major active component. *m*-Tyrosine is significantly more phytotoxic than its structural isomers *o*- and *p*-tyrosine. We show that *m*-tyrosine exposure results in growth inhibition for a wide range of plant species at µM concentrations and propose that the release of this amino acid interferes with root development of competing plants. Microscopic study suggests that *m*-tyrosine is produced and released by epidermal cells in living fine fescue roots. Only certain cultivars of fine fescue such as Intrigue Chewing's fescue produce and release large quantities of *m*-tyrosine in root exudates. *m*-Tyrosine phytotoxicity is counteracted by certain protein amino acids, especially phenylalanine and *p*-tyrosine. The discovery of *m*-tyrosine, as well as a further understanding of its mode(s) of action, could lead to the development of biorational approaches to weed control.

AGRO 12
Cyanamide in hairy vetch, tufted vetch, and black locust
***Yoshiharu Fujii**[1], yfujii@affrc.go.jp, Tsunashi Kamo[1], Syuntaro Hiradate[1], hiradate@affrc.go.jp, and Nobuhiro Hirai[2], hirai@kais.kyoto-u.ac.jp. (1) Department of Biodiversity, National Institute for Agro-Environmental Sciences, 3-1-3 Kan-nondai, Tsukuba, Japan, Fax: 81-298-38-8338, (2) Department of Agriculture, Kyoto University, Kyoto, Japan*

Hairy vetch (*Vicia villosa*), tufted vetch (*Vicia cracca*) and black locust (*Robinia pseudo-acacia*) were found to be strongly allelopathic by bioassay. Cyanamide has isolated as a natural product from these plants and might be an allelochemical. Cyanamide has been synthesized as a nitrogen fertilizer, and is also effective against weeds, fungi, and pests. But the distribution of natural cyanamide appears to be limited. We have surveyed about 550 species, but we cannot find producing species other than these three species. Hairy vetch is a ground cover plant and is now being gradually distributed among Japanese farmers for weed control. Black locust is native to the United States, but now has been widely planted and naturalized in Japan and is considered an invasive species in some areas. Little vegetation is observed under this tree, and allelopathic activity might be explained by cyanamide. The biosynthetic pathway and mode of action of cyanamide are still unknown.

AGRO 13

_p_-Hydroxyphenylpyruvate dioxygenase is a herbicide target site for natural β-triketones

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p-Hydroxyphenylpyruvate dioxygenase (HPPD), a key enzyme in the biosynthesis of prenyl quinones, is the target site of β-triketone herbicides. Natural β-triketones and their analogues appear to bind to HPPD in a manner similar to sulcotrione. A Fe^{2+} interacts with the diketone of the inhibitors via an octahedral complex. A lipophilic region in the catalytic domain favors the binding of triketones with hydrophobic chains. However, compounds with very long chains have lower activity because they extend beyond the lipophilic domain within the catalytic site. The CoMFA (Comparative Molecular Field Analysis) model provided good prediction of the activity and the steric properties of the molecules had the greatest contribution to the model. Preliminary greenhouse data indicates that natural β-triketones do not have optimal structural features for in vivo herbicidal activity. However, surfactants may improve the herbicidal activity of β-triketone-rich essential oils sufficiently to be used as natural tools for weed management.

AGRO 14

Phytotoxic eremophilanes from *Ligularia macrophylla*

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Bioassay-guided fractionation of a methylene chloride extract of *Ligularia macrophylla* roots was performed to identify phytotoxic constituents. Four phytotoxic eremophilanes [furanoeremophilan-14β,6α-olide, 6β-angeloyloxy-10β-hydroxyfuranoeremophilane, eremophil-7(11)-ene-12,8α;14β,6α-diolide, and 3α-angeloyloxybakkenolide A] were isolated. These compounds strongly inhibited growth of the monocot *Agrostis stolonifera* (bentgrass) while demonstrating little activity against the dicot *Lactuca sativa* (lettuce) at 1 mM. In a dose-response screening of all compounds for growth inhibitory activity against *Lemna paucicostata* (duckweed), 6β-angeloyloxy-10β-hydroxyfuranoeremophilane was the most active with an I50 of ca. 3 μM. This compound also caused the greatest reduction of photosynthetic electron flow; however, its primary mode of action remains to be determined. A mode of action profile study suggested that this compound might inhibit mitosis or lipid synthesis, with a slight uncoupling of oxidative phosphorylation. An extensive metabolite profile after 48 hr of treatment did not fit any of thirty profiles caused by phytotoxins with known molecular target sites.

AGRO 15

QSAR studies of allelochemicals

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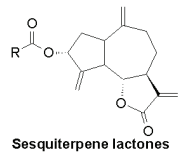
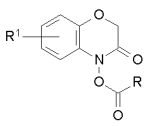
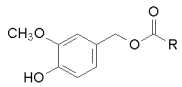
In the context of the new methodologies for bioactive compound design, quantitative structure-activity relationships studies (QSAR) constitute the key for a systematic analysis of structure and bioactivity properties. QSAR methodology was extensively employed for drug discovery, and its applications on new agrochemical design are starting to rise as the potential applicability of the physicochemical parameters employed in QSAR design of pharmaceuticals are discussed. The barriers that a crop protection agent must cross to reach its molecular target site may vary. Systemic transportation would be favored by a higher aqueous solubility, but some lipophilicity will be necessary to cross cell membranes and to reach the target site of action. Three different natural product skeletons have been modified in order to modulate their molecular properties and have been tested on cress, onion, lettuce, tomato, wheat, and the common weeds, rigid ryegrass and wild oat. The activity data were correlated with several molecular property descriptors.



Sesquiterpene lactones



Benzoxazinones



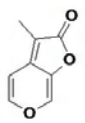
Capsinoids

AGRO 16

Butenolides as seed germination stimulants

Ming Xu, *Kingmo Sun, Yuzhong Chen, Ty Wagerle, and Marc Ruggiero, DuPont Crop Protection, Stine/Haskell Research Center, PO Box 30, Bidg 300, Newark, DE, 19714, USA, Newark, DE 19714*

The butenolide, 3-methyl-2*H*-furo[2,3-*c*]pyran-2-one (**1**), has recently been identified as a constituent of smoke. It has been shown to possess unique germination properties at extraordinarily low concentrations, as low as 10^{-9} M, and has therefore been postulated to play a role in field and forest restoration following fires. Here we report a new synthesis to the plant-derived butenolide 1 as well as the synthesis of analogs of formula **2**. Their biological germination activity will also be presented.



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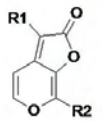
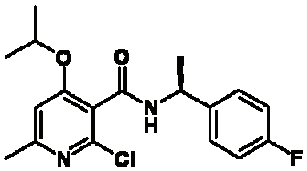


2

AGRO 17
Synthesis of new pyridine herbicides
Mary Ann Hanagan *and Yewande T. Henry, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

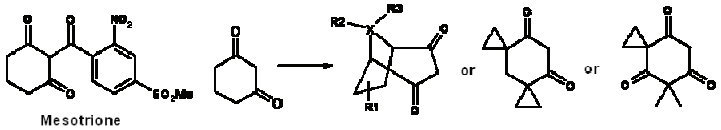
A series of novel 2,4-di- and 2,4,6-trisubstituted pyridines were prepared and their herbicidal activity evaluated. Compound **1** gave excellent control of grass and broad-leaf weeds both pre- and post-emergence in sugar cane at rates as low as 31 g/Ha. The structure activity relationship of the pyridines and their preparation is described. The mode of action of the herbicides is inhibition of protoporphyrinogen oxidase (protox), an enzyme target site in chlorophyll biosynthesis.



1

AGRO 18
HPPD inhibitor chemistry: A new generation of 1,3-diones
Renaud Beaudegnies*, Department of Chemistry, Syngenta Crop Protection, WST-820.1.35, Schaffhauserstrasse, Stein CH-4332, Switzerland, Fax: +41-61-3238529*

Triketone derivatives such as Mesotrione are potent herbicides which exert their action by the inhibition of hydroxyphenyl pyruvate deoxygenase (HPPD). In our quest to discover a new generation of HPPD inhibitors, some important issues remain to be addressed. In particular, higher intrinsic biological activity and crop selectivity along with optimal soil degradation need to be achieved. It has been demonstrated that substitution of the 1,3-dione scaffold can bring valuable solutions to these issues. In that context, we have investigated new generations of 1,3-dione moieties. The challenging syntheses of these building blocks will be presented.



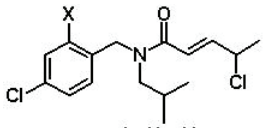
Mesotrione

AGRO 19
Discovery of aminocyclopyrachlor (proposed common name) (DPX-MAT28): A new broad-spectrum auxinic herbicide
Bruce L. Finkelstein*, Gregory R. Armel, Stephen A. Bolgunas, David A. Clark, Jon S. Claus, Richard J. Crosswicks, Cecilia M. Hirata, Gary J. Hollingshaus, Mary K. Koeppe, Patrick L. Rardon, Vernon A. Wittenbach, and Michael D. Woodward, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

Synthetic auxins have been in use for more than sixty years, yet they remain an important commercial class of herbicides widely used in both crop and non-crop situations. Today they have gained renewed significance as a tool in herbicide-resistance management strategies, especially for control of weed species resistant to glyphosate and to ALS (acetolactate synthase) inhibiting herbicides. This talk will focus on the discovery, chemistry, biology, and structure-activity relationships for a new family of highly-active, pyrimidine-based auxin mimics. Effort in this area has led to the commercial candidate aminocyclopyrachlor (DPX-MAT28) that provides outstanding broad-leaf weed control at low use rates. Aminocylopyrachlor is very effective on many hard to control weeds and is currently being developed by DuPont for use in turf, brush, and industrial weed control.

AGRO 20
Substituted 4-chloro-2-pentenamides: A unique class of protox inhibiting herbicides
Thomas P. Selby*, Gregory R. Armel, Kenneth A. Hughes, Yuzhong Chen, Ming Xu, Thomas M. Stevenson, Balreddy Kamireddy, and Patricia A. Mauvais, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714, Fax: 302-366-5738*

Patented by Kumiai in the early eighties, N-alkyl, N-benzyl substituted 4-chloro-2-pentenamides, e.g., **1**, were more recently reported to have herbicidal activity that is light-dependent. The 4-chloropentamide side-chain was determined to be critical for high activity. Causing rapid plant necrosis, compounds of this chemistry class were found to inhibit protoporphyrinogen IX (PPO, protox). There was particular interest in this herbicide class for barnyard grass (*Echinochloa oryzicola*) control in rice. In our subsequent investigation of this area, we found that novel 2-fluorobenzyl analogs were highly-active, postemergent herbicides that also showed rapid burn symptoms on plants. DPX-L8T33 provided excellent POST broadleaf weed control at rates as low as 8 g/Ha in greenhouse tests with some selectivity in maize and no significant re-crop injury. Interestingly, DPX-L8T33 showed much greater selectivity for the plant versus mammalian form of the PPO enzyme. Here, we wish to report on the background, synthesis and biology of novel fluorobenzyl derivatives of formula **2**. Differential activity of the two enantiomers of DPX-L8T33 will also be discussed.

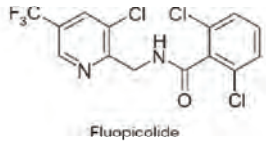


1 X = H
DPX-L8T33 X = F

2

AGRO 21
Discovery and chemistry of flupicolide: A new agent for the control for oomycete diseases
Darren J. Mansfield*, Fungicide Chemistry, Bayer CropScience, BCS AG-R-F-CFMON, Monheim, 6550, Germany*

Fluopicolide was discovered by AgrEvo UK Ltd in the late 1990's and developed by Aventis CropScience S.A. and then by Bayer CropScience AG. In this presentation, the discovery process leading to fluopicolide will be presented in detail. The key physical-chemical data for the compound will be described and the most important synthetic routes leading to the active ingredient will be discussed.



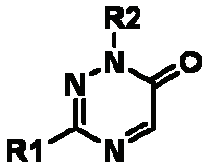
Fluopicolide

AGRO 22

Substituted 1,2,4-triazin-6-ones and 4,5-dihydro-1,2,4-triazin-6-ones as agricultural fungicides

Kevin G. Meyer[1], *kgmeyer@dow.com, Steven S. Shaber*[2], *Noormohamed M. Niyaz*[1], *Michael T. Sullenberger*[1], *Brent J. Rieder*[2], *Maurice C. H. Yap*[1], *William R. Erickson*[2], *Frisby D. Smith*[2], *Chenglin Yao*[1], *Todd Mathieson*[2], *Yelena A. Adelfinskaya*[1], *and Scott Thornburgh*[1]. *(1) Discovery Research, Dow AgroSciences, 9330 Zionsville Rd., Indianapolis, IN 46268, (2) N/A*

Substituted 1,2,4-triazin-6-ones(**1**) and 4,5-dihydro-1,2,4-triazin-6-ones (**2**) demonstrated high levels of control over a broad range of fungicidal pathogens of interest to agriculture. Details as to the synthesis, SAR and stability of these molecules will be reviewed.



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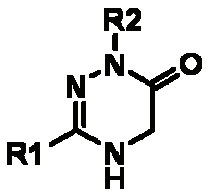

2

AGRO 23

Dos and don'ts for study directors of multisite studies

Philippe J. Ourisson *and Paul Swidersky, Quality Associates Incorporated, 8161 Maple Lawn Blvd., Fulton, MD 20759*

Study directors in multi-site studies have a much more complicated task of coordination than the study director of a single site study. This presentation will summarize the practical aspects of the US EPA GLPs (Good Laboratory Practices) for the typical multi-state, multi-participant, sometimes multi-lab, crop magnitude of the residue study. The presentation will use extensively the Consensus Documents prepared by the OECD (Organisation for Economic Cooperation and Development) on field studies (No.6), on study directors (No. 8), and on multi-site studies (No. 13).

AGRO 24

Terminal residues in strawberry, tomato, and summer squash following soil applications of ^{14}C-furfural

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Furfural is registered with USEPA as a nematicide on greenhouse ornamentals. To support food uses, ^{14}C-furfural metabolism was studied in strawberry, tomato, and summer squash mature fruits under greenhous-growing conditions to identify terminal residues following pre- and post-transplant soil applications of ^{14}C-furfural at proposed label rates. Terminal ^{14}C residues in mature fruit samples were identified using Waters IC-Pak Ion Exclusion and Phenomenex Rezex HPLC equipped with UV and radiochemical detection. Following multiple soil applications, neither ^{14}C-furfural nor its major soil metabolites 2-furoic acid and furfuryl alcohol were translocated into strawberry, tomato, or summer squash mature fruit. Citric, malic, and formic acids were identified as terminal residues in all three species. Predominant residues in fruit harvested 4 or 13 days after final application were: malic acid in strawberries and tomatoes (6.5 and 2.0 ppm, respectively) and formic acid at 26 days in squash (3.0 ppm). Citric and malic acids occur naturally in the 3 species tested, with formic acid also occurring naturally in strawberries.

AGRO 25

Pesticide residues in pollen collected by foraging honey bees

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Honey bees are an essential part of our agricultural system with a critical role in pollinating many fruit, vegetable, and nut crops. However, the number of honey bee colonies is currently in decline due to numerous threats, including parasitic mites, diseases caused by viruses and microsporidia, and the widespread use of pesticides. We are studying honey bee pesticide exposure by determining pesticide residues in pollen collected by foraging honey bees. Four hives representing urban, suburban, and rural locations are being monitored so that spatial and temporal differences in pesticide load can be determined. The pollen is extracted using a modified version of the QuEChERs procedure with an isotopically-labeled internal standard and analyzed with HPLC/MS/MS. The results show that honey bees are exposed to a wide variety of pesticides and that pesticide exposure varies with both hive location and time of year.

AGRO 26

Leaching of thiacloprid in three different types of soil

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Thiacloprid is currently recommended in Integrated Pest Management packages for pest control on various crops. Should thiacloprid gain access to ground water, it could adversely affect freshwater and marine species. Leaching of thiacloprid was studied in sandy soil (millet field), sandy loam (wheat field), and clay soils (cotton field). Leaching experiments were conducted in 30 cm soil columns and thiacloprid was analyzed in 5 cm soil fractions. After loading, 2.5 L of leachate was collected in fractions of 500 mL each. Major portions of thiacloprid residue were retained in the top 5 cm of sandy loam (96.8%), clay soil (98.2%), and sandy soil (93.3%). Thiacloprid leached to 10 cm (5.3%) in sandy soil. Leachate contained only 1.2% to 3.1% of thiacloprid residues in all the three soil types. It is unlikely that thiacloprid will leach into ground water when used in field conditions.

AGRO 27
Depletion of zilpaterol hydrochloride residues from the urine of orally-treated horses
David J. Smith[1], *david.j.smith@ars.usda.gov, C. J. Hammer*[2], *M. S. Mostrom*[3], *J. F. Thorson*[2], *and W. L. Shelver*[1], *Weilin.Shelver@ars.usda.gov. (1) Biosciences Research Laboratory, USDA-Agricultural Research Service, 1605 Albrecht Boulevard, Fargo, ND 58105, (2) Department of Animal & Range Sciences, North Dakota State University, Fargo, ND, (3) Department of Veterinary Diagnostic Services, North Dakota State University, Fargo, ND*

Zilpaterol HCl is a β-agonist feed additive that was approved for use to increase body weight gain and improve carcass composition in feedlot cattle. Because zilpaterol is a non-steroidal production enhancer, it has the potential to be used illicitly as a doping agent in species used for competitive racing. The purpose of this study was to determine the depuration of zilpaterol after oral administration to horses. Two mares and a gelding were provided an initial dose of 0.17 mg/kg body weight of zilpaterol in a corn-based feed supplement; a second dose of 0.022 to 0.043 mg/kg body weight was provided 24 hr after the initial dose. Urine was collected approximately 6 hr after dosing and at 24 hr intervals thereafter for 18 days. Mean urinary concentrations of zilpaterol, measured by indirect competitive ELISA after dilutions of 1:2 to 1:20,000, peaked at 1060 ± 550 ng/mL on day 2 of the study and remained detectable through day 18 of the study with mean concentrations of 1.3 ± 0.8 ng/mL (IC_{50}, 0.24 ng/mL in 50% control urine). These results suggest that a zilpaterol immunoassay may be useful for determining animals exposed to zilpaterol after prolonged depuration periods.

AGRO 28
Sorption of chlorpyrifos on agricultural soils
Manoj Kumar Tiwari *and Saumyen Guha, Department of Civil Engineering, IIT Kanpur, India, Kanpur 208016, India*

Batch experiments were conducted in duplicate to study the kinetics and equlibria of chlorpyrifos sorption onto agricultural soils. Kinetics of sorption were first order (rate constant 0.27 ± 0.06/hr; $r^2 > 0.95$). Sorption was nearly complete (>97%) within 6-9 hours. Agricultural soils containing 0, 8, and 20 mg/g of organic carbon were identified as zero (ZOS), low (LOS) and high organic soil (HOS), respectively. Sorption onto LOS ($r^2 = 0.96$) and HOS ($r^2 > 0.99$) followed a BET model with complete monolayer sorption amounts of 5.82 and 8.77 µg/g, respectively. The non-organic carbon sorption onto ZOS followed a Langmuir model ($r^2 > 0.95$) with maximum capacity of 0.92 µg/g. Deducting the maximum capacity of ZOS from the monolayer saturation amounts of LOS and HOS, and normalizing with the soil organic matter, we obtained partition coefficients of 3.58 and 3.82 log L/kg for LOS and HOS, respectively.

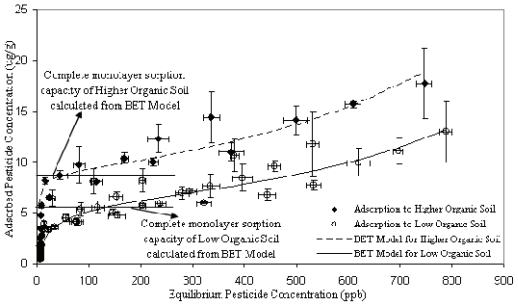

Figure 1: Adsorption Isotherm of Chlorpyrifos with Low Organic Soil (TOC = 8 mg/g) and Higher Organic Soil (TOC = 20 mg/g)

AGRO 29
How bacteria talk to each other
Bonnie L. Bassler*, Department of Molecular Biology, Princeton University, Lewis Thomas Laboratory, Washington Road, Princeton, NJ 08544*

Bacteria communicate with one another via production, detection, and response to secreted chemical signal molecules called autoinducers. This communication process is called quorum sensing and it allows bacteria to synchronize behavior on a populaton-wide scale. Bacterial behaviors controlled by quorum sensing are typically ones that are unproductive when undertaken by an individal bacterium acting alone but become effective when undertaken in unison by the group. For example, quorum sensing controls virulence, biofilm formation, bioluminescence, sporulation, and the exchange of DNA. Thus, quorum sensing is a mechanism that allows bateria to functiion as multi-cellular organisms. New research shows that bacteria integrate information from multiple autoinducers, some (acyl homoserine lactones and peptides) of which are used exclusively for intra-species communication while one auto inducer, generically called AI-2 (4,5-dihydroxy-2,3-pentanedione or DPD), is a universal signal and enables inter-species communication. DPD undergoes a series of spontaneous rearrangements. Structural studies of the active AI-2 ligands bound to cognate receptors from different bacterial species revealed that the receptors bind to chemically distinct AI-2 moieties derived from the common DPD precursor molecule. Interestingly, the active signal molecules inter-convert upon release from their respective receptors, revealing a surprisingly level of sophistication in the chemical lexicon used by bacteria for inter-species cell-cell communication. Current research is focused on the development of novel anti-bacterial therapies aimed at interfering with quorum sensing. Such therapies could be used to control bacterial pathogenicity. [A contribution of the Howard Hughes Medical Institute]

AGRO 30
Use of microbial cell to cell communication and quorum sensing for controlling agricultural crop diseases
Mahmoud A. Saleh*, Department of Chemistry, Texas Southern University, 3100 Cleburne Ave, Houston, TX 77004*

Many plant diseases are caused by microorganisms including bacteria and fungi. Biofilms, a common mode of microbial growth, are colonies of microbial cells encased in self-produced organized layers that are highly resistant to commonly-used pesticides. Biofilm formation is initiated by small, diffusible signaling molecules which are essential for quorum requirements. When a signal accumulates to a threshold concentration, the response regulator is activated within the the local population of cells, leading to biofilm formation. Acyl homoserine lactones, cyclic peptides, and the sesquiterpene farnesol are known to act as quorum sensing (inducer) molecules in gram-negative bacteria, gram-positive bacteria, and fungi, respectively. The utilization of quorum sensing molecules for controlling the microbial population and preventing biofilm formation is presented. This study also shows chemical structural requirements and a quantitative structural/activity relationship that enhances the selectivity and the potency of the target chemicals.

AGRO 31

Chemical synthesis and biological characterization of structural analogs of the *Vibrio cholerae* autoinducer CAI-1

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The bacterium *Vibrio cholerae*, the causative agent of the disease cholera, uses the cell-to-cell communication system of quorum sensing to regulate its life cycle and to control the expression of virulence factors. Quorum sensing is a process by which groups of bacteria control collective behaviors according to population density which is perceived through the secretion and detection of small organic molecules called autoinducers. The principal autoinducer of *V. cholerae* is CAI-1 (cholerae autoinducer-1) which is synthesized by CqsA (cholerae quorum sensing synthase) and detected by the transmembrane sensor-kinase CqsS (cholerae quorum sensing sensor). We have recently identified CAI-1 as 3-(*S*)-hydroxy-4-tridecanone. Chemically-synthesized CAI-1 initiates quorum sensing in *V. cholerae* and has a pronounced effect on the formation of the toxin-coregulated pilus crucial to virulence. To determine the effect of small structural changes on the ability of the autoinducer to communicate population density information and influence virulence factor production, we now implement straightforward synthetic strategies to access a variety of structural analogues of CAI-1. We evaluate the ability of CAI-1-like molecules that differ in characteristics such as stereochemistry, functional groups, acyl tail length, and steric bulk to activate the quorum sensing circuit of *V. cholerae*.

AGRO 32

Red tides and harmful algal blooms (HABs): New technologies for detection of cells and toxins

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Harmful algal bloom (HABs), commonly called "red tides", are phenomena caused by growth and proliferation of microscopic algae, some of which produce potent toxins. HABs are complex oceanographic phenomena that require multi-disciplinary study ranging from molecular and cell biology to large-scale field surveys, numerical modeling, and remote sensing from space. HABs take many forms and affect coastal countries. Impacts include poisonous shellfish, dead fish, and aerosolized toxin that can drive residents and tourists from beach areas, and ecosystem changes such as destruction of submerged aquatic vegetation or mortality of marine mammals and other organisms at all levels of the food web. Because human health and economic impacts of HABs are a significant challenge for those who are responsible for the management of coastal resources, there is strong incentive to develop capabilities for forecasting these events and mitigating their effects. Our understanding of the HAB phenomena is increasing dramatically, and with this knowledge comes technologies and management tools that can help reduce HAB incident and impact. This presentation summarizes the global HAB problem and some new technologies and approaches to monitoring, control, and management. These include molecular probe-based methods for cell detection, rapid and sensitive toxin assays, and large scale physical/biological models to analyze past blooms and forecast future ones. Field or operational application of some of these methods including some problems encountered are discussed with the prospects for incorporating these technologies into moored arrays for *in situ* detection of cells and toxins as part of the developing ocean observation system.

AGRO 33

Bioprospecting for novel fungicides in marine organisms

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Discovery of natural product fungicides is largely dependent upon the availability of high quality miniaturized antifungal bioassays. As part of a program to discover natural product-based fungicides, several sensitive assay systems have been developed for evaluation of naturally occurring antifungal agents. Bioautography was used to conduct basic bioassay-guided fraction, identify the number of antifungal compounds in an extract, eliminate nuisance compounds, and characterize antifungal activity against plant pathogenic *Colletotrichum* species. While bioautography techniques are successful in pre-screening large numbers of extracts or compounds this technique is especially important in evaluating lipophilic compounds and extracts. A second bioassay in a 96-well, micro-dilution broth format was used to evaluate pure compounds identified by bioautography. However, bioprospecting in marine organisms for new agrochemical compounds is complicated by the nature of the environment in which these organisms live. Marine natural products maybe complex, non-polar, lipophilic compounds that are not soluble in most aqueous-based, high-throughput, 96-well plate assay systems. We discuss several *in vitro* techniques and bioassays used to study the antifungal activity of kahalalide F, manzamine alkaloids, and the plakortides. The kahalalides are a family of natural depsipeptides isolated first from the Hawaiian herbivorous marine sacoglossan mollusk *Elysia rufescens* and later from its green algal diet of *Bryopsis pennata*. The manzamine alkaloids were isolated from *Acanthostrongylophora sp.* and the plakortides from the sponge *Plakortis halichondrioides*.

AGRO 34

Bioprospecting in extreme, deep-sea environments

***Richard A. Lutz**, Department of Marine and Coastal Sciences, Rutgers University, 71 Dudley Road, New Brunswick, NJ 08901-8521*

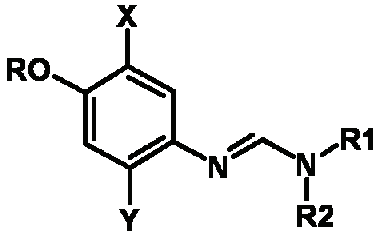
Deep-sea hydrothermal vents arguably represent some of the most extreme environments on the face of the planet and contain perhaps the most promising marine orgainisms for the production of unique bioactive compounds. These abyssal ecosystems are variously characterized by the presence of increased hydrostatic pressures, extreme temperatures (2° - 400°C), very low pH (as low as 2.6), and elevated levels of hydrogen sulfide (up to 100 mM), heavy metals (Co, Cd, Pb, Sr, Ba, etc.), radionuclides, and toxic polycyclic aromatic hydrocarbons. The spectrum of endemic organisms inhabiting these environments rely on normally toxic sulfides and hydrocarbons as their primary source of energy and nutrition. The capacity of these unusual organisms to utilize, detoxify, or degrade toxic compounds has led to the current intense interest on the part of numerous diverse corporations engaged in natural product discovery and bioremediation. Our ability to isolate and culture a wide variety of thermophilic microbes from these environments provides a potentially unlimited source of extracts for extensive screening for bioactive compounds. In addition, the development of recent techniques to culture tubeworms from deep-sea hydrothermal vents within the laboratory offers an exciting potential for further studies and analyses of these unique organisms that house symbiotic bacteria which, from our ongoing analyses, are of potentially significant commercial importance.

AGRO 35

Discovery and optimization of 1-alkoxy-4-amidinylphenyl analogs as fungicides

***Chi-Ping Tseng**, Michael C. Klapproth, William K. Moberg, Bonita M. Reeves, Stefanie I. Lewis, Ritesh B. Sheth, and Wenming Zhang, DuPont Crop Protection, Stine-Haskell Research Center, P.O. Box 30, Newark, DE 19714, Fax: 302-366-5738*

Plant diseases are ubiquitous and harmful to global agriculture. Safe and effective fungicides with novel modes of action are desirable since resistance has developed against many existing commercial fungicides. We have discovered novel 1-alkoxy-4-amidinylphenyl compounds are highly active as fungicides. This presentation will show our discovery and optimization of 1-alkoxy-4-amidinylphenyl analogs as fungicides.

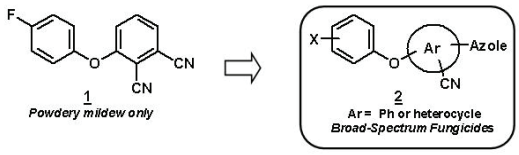


AGRO 36

Discovery and optimization of novel biphenyl ether fungicides

***James F. Bereznak**, Stephen F. McCann, and Kanu M. Patel, DuPont Crop Protection, Stine-Haskell Research Center, P.O. Box 30, Newark, DE 19714*

High-throughput screening efforts identified the biphenyl ether **1** as a viable starting point for fungicide optimization. An extensive synthesis program was initiated which eventually focused on the key azole structures **2** as broad-spectrum greenhouse fungicides. This talk will describe the synthetic aspects of this program, as well as the SAR evolution leading from **1** to **2**.

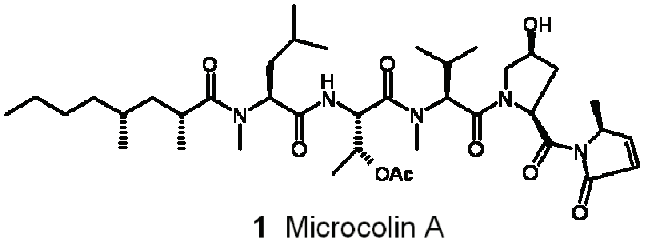


AGRO 37

Microcolin insecticides: Synthesis and structure-activity relationships

*Zoltan L. Benko[1], zlbenko@dow.com, Carl V. DeAmicis[1], cvdeamicis@dow.com, James M. Gifford[1], jmgifford@dow.com, Jeffrey R. Gilbert[1], jrgilbert@dow.com, Vidyadhar Hegde[1], vbhegde@dow.com, **James E. Hunter**[1], jehunter@dow.com, Paul Lewer[1], plewer@dow.com, Kevin L. McLaren[2], and Nailah Orr[1], norr@dow.com. (1) Discovery Research, Dow AgroSciences, 9330 Zionsville Road, Indianapolis, IN 46268, Fax: 317-337-3215, (2) N/A*

Microcolin A (**1**), an immunosuppressive tetrapeptide first isolated from the marine cyanobacterium *Lyngbya majuscula,* was subsequently reisolated by Dow AgroSciences' Natural Products group from blue-green alga extracts and discovered to be a broad spectrum insecticide. Leveraging synthetic protocols from two total syntheses of Microcolins reported in the literature, in addition to methods developed at Dow AgroSciences, a structure-activity relationship (SAR) investigation was conducted. The intent of the study was not only to define the SAR about Microcolin A, but also to distill down the natural product to a dramatically simplified, synthetically accessible insecticidal motif. This presentation will highlight those efforts with particular emphasis on modifications made to the fatty acid and proline lactam regions of **1**.



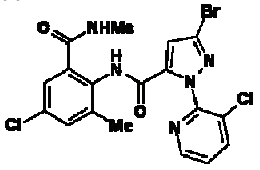
1 Microcolin A

AGRO 38

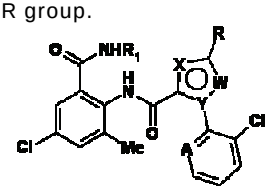
New heterocyclic analogs of Rynaxypyr™: Structure-activity studies in the anthranilic diamide class of chemistry

George P. Lahm, *Thomas P. Selby, Thomas M. Stevenson, Bruce L. Finkelstein, David A. Clark, John H. Freudenberger, Wonpyo Hong, Maya Sethuraman, Kenneth A. Hughes, Christina M. Dubas-Cordery, and Ben K. Smith, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

We recently described the discovery of the new anthranilic diamide insecticide Rynaxypyr™, that acts via activation of the ryanodine receptor (RyR). Ryanodine receptors regulate intracellular calcium levels and Rynaxypyr™ has been found to disrupt calcium regulation by blocking channels in a partially open state. The high selectivity for insect over mammalian receptors affords potent insecticidal activity coupled with high mammalian safety. Here, we report on the synthesis, biology, and structure-activity trends for a series of heterocyclic derivatives of formula **1** as well as new pyrazole substituents at the R group.



Rynaxypyr™



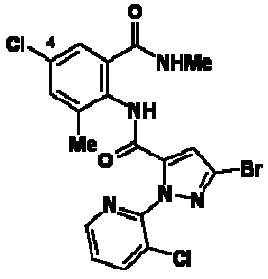
1

AGRO 39

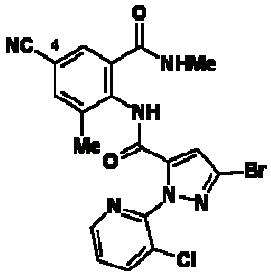
Discovery of Cyazypyr™: A new cross-spectrum insecticide from the anthranilic diamide class of ryanodine receptor activators

Thomas P. Selby[1], *thomas.p.selby@usa.dupont.com, George P. Lahm*[1], *Thomas M. Stevenson*[2], *Thomas.M.Stevenson@usa.dupont.com, Kenneth A. Hughes*[1], *I. Billy Annan*[1], *Daniel Cordova*[1], *Cheryl A. Bellin*[1], *Eric A. Benner*[1], *Keith D. Wing*[1], *James D. Barry*[1], *Martin J. Currie*[2], *and Thomas F. Pahutski*[1]. *(1) DuPont Crop Protection, Stine-Haskell Research Center, P.O. Box 30, Newark, DE 19714, Fax: 302-366-5738, (2) Stine-Haskell Research Center, DuPont Crop Protection, Newark, DE 19714*

Calcium channels are an attractive biological target for insect control due to the important role they play in multiple cell functions including muscle contraction. Anthranilic diamides substituted with a N-pyridylpyrazole were reported to be a new class of insecticides showing potent activity against a range of Lepidoptera by causing intracellular release of calcium mediated by the ryanodine receptor. Work in this area led to the discovery of Rynaxypyr™, an exciting new broad-spectrum product with outstanding insecticidal activity, especially against lepidopteran pests, at very low application rates. In our continued search for analogs with favorable systemic properties, we pursued substitution of the anthranilic diamide at various positions with a variety of polar groups such as cyano. Here, we report on the synthesis, biology and structure-activity trends for a series of lower log P derivatives of Rynaxypyr™ with a focus on cyano-substituted anthranilic diamides. This effort culminated in the discovery of Cyazypyr™, a second product candidate to emerge from this chemistry class showing excellent cross-spectrum activity against a wide range of insects including lepidopteran, hemipteran and coleopteran pests.



Rynaxypyr™ (DPX-E2Y45)



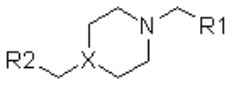
Cyazypyr™ (DPX-HGW86)

AGRO 40

Pharmacophore design and parallel synthesis of phenylpiperidine/phenylpiperazine libraries as insect calcium channel inhibitors

Beth A. Lorsbach[1], *balorsbach@dow.com, James M. Ruiz*[1], *jmruiz@dow.com, Thomas C. Sparks*[2], *tcsparks@dow.com, Jeffery D. Webster*[1], *jdwebster@dowagro.com, Michael T. Sullenberger*[1], *and Irene Morrison*[1]. *(1) Discovery Research, Dow AgroSciences, 9330 Zionsville Road, Indianapolis, IN 46268, Fax: 317-337-3215, (2) Dow AgroSciences, Indianapolis, IN 46268*

Disruption of calcium channels has been shown to cause lethal effects in insects. Known calcium inhibitors in the mammalian literature were leveraged to find chemical starting points as insecticides. Two such scaffolds, phenylpiperidines and phenylpiperazines, were selected and explored via a parallel synthesis approach to generate potential insect calcium channel blockers. Several *in vitro*/*in vivo* hits were identified from these early libraries. A pharmacophore model based on the screening results from the first two piperidine/piperazine libraries and literature pharmacophores was developed and used to design a third generation library. The synthesis and pharmacophore design of these libraries will be discussed in addition to the biological data.



X= C or N
R1 = alkyl, alkoxy, aryl, heteroaryl
R2 = alkyl, alkoxy, aryl, heteroaryl

AGRO 41

Syntheses and biologicial activities of insecticidal thieno[2,3-b]furans

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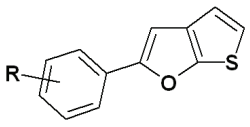
2-Aryl-thieno[2,3-b]furans, **1**, were found to be insecticidally-active. A number of synthetic approaches to **1** and general structures **1** were developed, including Suzuki arylations of a thieno-furan precursor and a *bis*-cyclization reaction based upon the Jacobi furan synthesis. These synthesis approaches will be described and the insecticidal activities of analogs **1** and **2** will be discussed.



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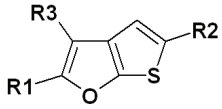

2

AGRO 42
Synthesis and biological activity of cyclopropyl pyrazole insecticides
Wolfgang von Deyn[1], *wolfgang.deyn@basf.com, Christopher Koradin*[1], *and David G. Kuhn*[2]*. (1) BASF, BASF SE, GVA/IO - B009, 67056 Ludwigshafen, Germany, (2) BASF, Research Triangle Park 27709*

A new class of pyrazole insecticides was discovered as a result of the continued efforts to improve the activity of amidrazone insecticides. Starting from the first hit, an improvement of spectrum and potency could be achieved by variation of the substituents on the 4- and 5- positions of the pyrazole ring. Further attempts to optimize the structure by modification of the phenyl moiety were not successful. The effects of substitution on the structure-activity-relationships will be presented.

AGRO 43
Accelerated Leuckart reaction in the synthesis of agrochemicals and pharmaceuticals
Mikhail M. Bobylev and ***Andrew Podrygula****, Department of Chemistry, Minot State University, 500 University Avenue West, Minot, ND 58707*

The Leuckart reaction is a unique one step method of reductive amination. It is a remarkably simple process that includes only two components: the carbonyl compound and formamide. The reaction is completed simply by heating the components at 160ºC to 185ºC for 6 to 25 hr. The long processing time seems to be the only shortcoming of the reaction. During their work with formamide fungicides, Bobylev *et al.* developed an accelerated procedure for the Leuckart reaction. The accelerated procedure transforms styryl ketones into respective phenylallyl formamides (formamide fungicides) in 15 min or less. In this work, the accelerated Leuckart reaction was successfully used for the synthesis of some known *N*-phenylalkylformamides of agrochemical and pharmaceutical interest. In some cases, the reaction was completed in 1 min or less making it the first instant Leuckart reaction ever. (The project is supported by NIH grant P20 RR016741 from the NCRR.)

AGRO 44
Thermal fixation of atmospheric nitrogen to nitrate on titanium dioxide and desert soil surfaces
Ahmed Al-Taani *and Glenn Miller, Department of Natural Resources and Environmental Science, University of Nevada, Mail stop 199, Reno, NV 89557*

A novel process for non-biological fixation of nitrogen to form nitrate has been identified in the presence of air or pure nitrogen gas, and is based on thermal treatment of titanium dioxide (TiO_2), anatase, and rutile. This finding was observed while preparing thin films of TiO_2 by thermal evaporation of an aqueous suspension in Petri dishes. An expanded series of experiments was carried out in a conventional oven in the absence of light; photocatalytic reactions are not involved. Nitrate was linearly produced over the temperature range of 50-200ºC after 2 hr. Under the conditions employed, the nitrate yield was a function of the TiO_2 area on the Petri dish, with the thinnest films producing over 40 mg/kg following a 2-hour thermal treatment at 200ºC. At temperatures >400ºC, nitrate formation was also observed, although the thermal degradation rate of nitrate tended to reduce the observed yields. Successive heat treatment and aqueous extraction of the same TiO_2 sample over 14 cycles resulted in effectively identical yields for each cycle, suggesting that this process is not a result of oxidation or release of nitrate that may have been contained in the TiO_2. The pH of the final extracted TiO_2 suspensions was lowered to approximately 3-5, consistent with the formation of nitric acid. Additions of stoichiometric amounts of sodium, potassium, or calcium hydroxide increased the amount of nitrate observed. The mechanistic pathway by which nitrate is formed is unknown, though it is presumably occurred via catalytic oxidation of elemental N_2 on heated TiO_2 surface. Formation of nitrate was also observed on certain arid-land soils heated to 70ºC for 15 hr, although the rate of production was generally lower. This observation suggests that thermal fixation/formation of nitrate on arid-land soils may contribute to elevated nitrate levels found in soils and groundwater in the western US.

AGRO 45
Interactions of nitrate and cadmium ions at model environmental interfaces studied by second harmonic generation
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The adsorption of nitrate and cadmium ions from aqueous solution onto a mineral oxide surface was studied using second harmonic generation (SHG). SHG is a surface specific, non-linear spectroscopy that allows interactions at a buried interface to be directly monitored in real-time and under flow conditions. Resonantly enhanced SHG was utilized to obtain adsorption isotherms for nitrate at the fused quartz/water interface. A binding constant and a free energy for this adsorption process were determined from the experimental data. The results indicate that nitrate anions are physisorbed to the fused quartz through H-bonding. The SHG chi-(3) technique was used to assess cadmium adsorption at the bare fused quartz/water interface, as well as an organic functionalized quartz/water interface. The free energies of adsorption on both surfaces revealed that cadmium cations are physisorbed via an outer shell mechanism. The results of the adsorption experiments were used in the K_d model to assess the mobility of nitrate and cadmium pollutants in soil systems similar to the model interfaces studied.

AGRO 46
Adsorption effect on the degradation of carbaryl, mecoprop, and paraquat by AFT in an Swy-2 montmorillonite clay slurry
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Adsorption and degradation of carbaryl, mecoprop and paraquat were studied in an Swy-2 Na^+-montmorillonite clay slurry. Adsorption isotherms for these three agrochemicals were obtained at given experimental conditions. The d spacing (d_{001}) of the clay layer before and after adsorption or degradation was measured by X-ray diffraction (XRD). Based on the change of d spacing, molecular disposition at the clay interlayer was inferred: both mecoprop and paraquat form a monolayer sitting flat and parallel to the clay siloxane surfaces. Results show that, due to different adsorption mechanisms, the adsorption effect on chemical degradation by anodic Fenton treatment (AFT) varies with pesticide: strong and tight adsorption of paraquat at the clay interlayer protects paraquat from being attacked by hydroxyl radicals; loosely adsorbed carbaryl or mecoprop is readily degraded. XRD analysis clearly indicates that AFT is capable of effectively degrading interlayer non-cationic organic chemicals that are not usually available for biodegradation.

AGRO 47
Partitioning of etofenprox under simulated California rice growing conditions
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A synthetic pyrethroid insecticide, etofenprox is of current interest to rice farmers in the Sacramento Valley due to its effectiveness against the rice water weevil. The objective of this study was to determine the equilibrium air-water partitioning (K_H) or Henry's constant for etofenprox and the soil-water distribution coefficient, K_d, and organic carbon normalized coefficient, K_{oc}, for etofenprox to two representative rice field soils in the Sacramento Valley. Experimental determination of Henry's constant revealed etofenprox partitioned onto the apparatus walls and did not significantly volatilize. Calculated values for Henry's constant were 1.8 x 10^{-5} Pa/mol m^3 at 5°C - 40°C based on estimated psolubility and vapor pressure at various temperatures. Both results agree that volatilization will not be a major dissipation pathway for etofenprox. The log K_{oc}, was experimentally determined to be 6.0 and 6.4 for the Princeton rice soil and the Richvale rice soil at 25ºC, respectively. The log K_{oc}, was 6.1 for the Princeton soil at 35ºC. Desorption of etofenprox from Princeton soil ranged from 1-3%(+/-1%) of adsorbed mass and 2-5%(+/-2%) in Richvale soil at 25ºC. High sorption coefficients and relatively insignificant desorption of etofenprox suggest its insolubility drives etofenprox to partition out of water and to sorb to soils with high affinity. Offsite movement is unlikely unless transported in a bound state.

AGRO 48
Effects of black carbon on pyrethroid bioavailability in sediments
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Pyrethroids are widely used insecticides. This research was conducted to understand the role of black carbon (BC) in governing the bioavailability of strongly hydrophobic pyrethroids in sediment. We evaluated pyrethroid uptake into polydimethylsiloxane (PDMS) fibers and 1-day bioaccumulation in *Chironomus tentans* as a function of BC amendment rates. There was a significant negative correlation between the content of pyrethroids in PDMS fibers and the BC level in sediment. When BC content was increased from 0 to 1 percent, pyrethroid uptake in the PDMS fibers decreased by 5.7-9.1 percent. The biota-sediment accumulation factor (BSAF) of *C. tentans* decreased from 2.8 to 1.7, as the BC content was increased from 0 to 1.5 percent. The concentrations of permethrin in different cellular fractions of *C. tentans* also correlated closely with BC amendment. This study suggests that BC affects the bioavailability of pyrethroids and may play an important role in sediment toxicity.

AGRO 49
Fate of PBDEs in biosolids and soil from commercial farms that receive biosolids application
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Polybrominated diphenyl ethers (PBDEs) are used as additives in consumer products for their fire-retardant properties. While PBDEs have been observed in various environmental media, little is known about their movement through the environment. This study examines the potential fate of selected PBDE congeners in soils treated with biosolids. Surface soil samples were collected from thirty fields at eleven commercial farms in the Mid-Atlantic region. Biosolids samples from the source WWTP were collected every two months over thirty months to evaluate PBDE concentrations. Preliminary data shows that concentrations of PBDEs (BDE-28, BDE-47, BDE-99, BDE-100, BDE-153, and BDE-154) in biosolids are in the range of 480 ppb - 1.3 ppm, with BDE-47 and BDE-99 being the major congeners. Concentrations on fields (BDE-28, BDE-47, BDE-99, BDE-100, BDE-153, BDE-154, BDE-183, and BDE-209) that have not received biosolids were 0.5 - 15 ppb, fields with a single application had levels of 17 - 71 ppb, and fields with multiple applications had a range of 10 - 210 ppb.

AGRO 50
Determination of the effect of pH, ionic strength, and humic acids on the soil sorption coefficients (K_d) of tylosin and erythromycin antibiotics
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Increased use of veterinary antibiotics such as the macrolides tylosin (TYL) and erythromycin (ERY) in concentrated animal feeding operations and use of manure as fertilizers raises concern with regard to their environmental impact. Sorption and desorption dictate mobility of these compounds once present in the environment. Sorption coefficients (K_d's) were evaluated for silty sand and clay sediments by batch equilibrium experiments analyzed via liquid chromatography with UV or MS detection (LC-MS) and liquid scintillation counting. The effect of pH, ionic strength and humic acid concentrations were investigated as well. Experimental values of K_d's ranged from 1.10x10^3 to 7.70x10^3 L/kg for TYL and 1.50x10^2 to 5.50x10^2 L/kg for ERY in both sediments. In all cases, sorption was seen to be greater for TYL compared to ERY which can be attributed to tylosin's more hydrophobic character relative to ERY. Sorption differences between TYL-A and TYL-B were also observed, but the differences are not statistically significant. K_d values were generally higher at low pH values, illustrating the influence of electrostatic

attraction in the sorption process. Additional electrolytes in solution appeared to have different effects on TYL and ERY sorption. Competition of different ions was evident in the sorption of ERY, which showed a 2.5-fold decrease in K_d with an 8-fold increase in ionic strength. Presence of humic acids in solution provided new surfaces where the compounds can sorb, resulting in considerably large K_d's for both TYL and ERY. Overall, the silty sand sediment had higher K_d compared to the clay type sediment.

AGRO 51
Erythromycin: A look at a veterinary antibiotic's bioavailability in an aquatic microcosm
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There is increased concern over the presence of veterinary antibiotics in the environment due to their widespread use in livestock feed for prevention of disease and growth promotion. Veterinary antibiotics in aquatic ecosystems are not well understood. In this study, the bioavailability of radiolabeled erythromycin was evaluated in an aquatic microcosm using C8-Empore™ extraction disks and comparing that data to uptake by the aquatic worm *Lumbriculus variegatus*. The Empore disks and aquatic worms were incubated in treatment water at various concentrations and time points. At the conclusion of the study, the disks and worms were extracted and uptake of ^{14}C-labelled-erythromycin was determined. Comparisons of relative uptake indicated a bioconcentration factor of 0.21 for *L. variegatus* compared to 15 for disks. The disk bioconcentration factor was 70 times the worm bioconcentration factor. This type of comparative data could be used for comparisons of compounds in aquatic environments if ratios of uptake are steady over a range of concentrations. Further research will focus on erythromycin's bioavailability and metabolism in sediment.

AGRO 52
Removal of methyl parathion from water by nanoscale zero-valent iron
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A highly efficient and versatile material, nanoscale zero-valent iron (NZVI) was synthesized in the laboratory. The NZVI was characterized using different microscopic and spectroscopic methods. From transmission electron microscopy and X-ray diffraction, its size, morphology, and chemical composition were confirmed. Our study shows that NZVI completely degrades methyl parathion (MP), one of the toxic contaminants used in agriculture, in a short period of time (30 min). Kinetic study of MP degradation by NZVI shows that 2 g/L of NZVI is sufficient to degrade 34 mg/L MP completely within 30 min at neutral pH. The results confirmed that NZVI has great potential to be used as a reactive material for *ex-situ* treatment for MP remediation from industrial/process wastewater or surface water as well as in deep groundwater for *in-situ* treatment.

AGRO 53
Method development for multiresidue pesticide extraction from food
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Pesticide residue extraction from food matrices was investigated using multi-residue extraction methods. Most multi-residue extraction methods are applicable to only one food (*e.g.*, wine or spinach), one type of food (*e.g.*, vegetables or fruits), and/or result in sub-optimal (< 70%) percent recoveries of the investigated pesticide residues. Consequently, we developed and implemented an accurate, high-throughput, multi-residue method for extracting organophosphates and pyrethroids from a range of composite food matrices, including non-dairy and dairy beverages, fruits, vegetables, grains, meats, beans/nuts/legumes, and fats. The modification of the sample extraction and solid-phase extraction (SPE) cartridge clean-up via primarily fine-tuning solvent polarity and the use of a SPE cartridge composed of a Supelclean™ ENVI-Carb-II layer and a polymerically bonded, ethylenediamine-n-propyl Supelclean™ PSA phase resulted in the effective clean-up of food matrices. Further, the combination of SPE layers allows the retention and subsequent elution of the target pesticide residues, diazinon, chlorpyrifos, malathion, permethrin, cypermethrin, cyfluthrin, and deltamethrin, which were quantified in different food matrices via gas chromatography with electron-capture detection (GC-ECD). Multi-residue pesticide extraction percent recoveries for an assortment of composite food matrices (*e.g.*, non-dairy and dairy beverages, fruits and vegetables, grains, meats, beans/nuts/legumes, and fats) were reproducible (n = 3) at ≥ 70% with an average standard deviation of 9.2 ± 6.3. The extraction protocol will continue to be evaluated to show further applicability to additional, relevant pesticide residues and dust and soil matrices in future work.

AGRO 54
Repellency of botanical sesquiterpenoids to arthropods
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In response to increased consumer awareness, toxicity concerns, and environmental impacts, there is a need for alternatives to traditional synthetic repellents for arthropod control. Some new repellents including picaridin and *p*-menthane-3,8-diol are recommended by the CDC as DEET alternatives, but the duration of protection provided is not as long-lasting as DEET. Preliminary work in our laboratory has shown that naturally occurring chemicals in plants such as the catnip (*Nepeta cataria*), Osage orange (*Maclura pomifera*), West Indian sandalwood (*Amyris balsamifera*), and Siam wood (*Fokenia hodginsii*) are capable of eliciting strong inhibitory effects against arthropods. Mixtures that include monoterpenes (provide good spatial repellency) and oxygenated sesquiterpenes (provide good contact repellency) result in good efficacy via both modes of action. Current research objectives are focused on the evaluation of newly isolated and purified plant-derived sesquiterpenoids in mosquito and tick bioassays and on the analyses of quantitative structure-activity relationships using physiochemical and electronic parameters.

AGRO 55

Preformed organophosphorous insecticide biomarkers in fruits and vegetables: An in-depth study on California strawberries

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The general population is exposed to organophosphorous (OPs) insecticides and their derivatives including dialkylphosphates (DAPs) mainly through diet. DAPs are important urine biomarkers to infer potential OP pesticide exposure. Malathion mono- and diacid are specific urine biomarkers also found in produce. Our previous research has shown that DAPs are present in fruits and vegetables. We have suggested that exposure to preformed biomarkers in produce can confound the interpretation of urine biomonitoring data. Source and time-metabolite concentration relationships in strawberry foliage and berries were studied at three times during three weeks after malathion application at a commercial strawberry farm in Santa Maria, CA. Malathion and derivatives including malaoxon, DAPs and malathion acids were measured. Malathion derivatives (total nanomoles) were higher in foliage than in berries at each interval. The foliage may be the limiting source of the berry residues long after disappearance of the parent insecticide residue, malathion.

AGRO 56

Determinants of human pesticide exposure following use of fipronil-containing pet products

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Applications of topical pet pest products inevitably result in human exposure. Characterization of the magnitude and duration of chemical transfer and exposure from these compounds is necessary for aggregate exposure assessment and mitigation. Currently, aggregate exposure assessments of topical pet products do not include characterization of indoor deposition of these pesticides, but instead rely on default assumptions. Fipronil, the active ingredient in Frontline®, is used for flea and tick control, roach and ant baits, as well as structural termite control. The potential for indoor exposure to fipronil and possible photoproducts is poorly understood and unstudied. Analysis of cotton gloves used as a dosimeter showed time-dependent levels of fipronil (66 µg/pair to 2.7 mg/pair) and derivatives. Other textile dosimeters, such as flooring and bedding, also show time dependent levels of fipronil and products (0.05 µg/cm^2 to 120 µg/cm^2). Future studies will investigate three potential urine biomarkers as indices of exposure.

AGRO 57

Bis(chlorophenyl)acetic acid (DDA), a water-soluble biomarker of DDT metabolism in humans

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DDT is sanctioned and used in some anti-mosquito campaigns in sub-Sahara Africa where malaria remains a serious health problem. DDT metabolism in humans yields DDA as a principle metabolite in urine. DDA elimination stops abruptly with DDT exposure. We developed a simple, rapid analytical method for DDA biomonitoring of human urine samples. We applied this method to the analysis of urine samples from Swaziland workers. The mean DDA elimination level was 59 ppb (range 5-400 ppb); the mean urine DDT level was 0.82 ppb (range 0.3–4.3 ppb). The mean mole ratio of DDA/DDT was ca. 90:1. These pilot studies show that urinary DDA excretion may be used to evaluate low level DDT exposure during anti-malaria campaigns. Since the analysis is sensitive, specific, and may be rapidly performed, the determination may be particularly useful for training and exposure assessment.

AGRO 58

Polygenic resistance in the highly DDT-resistant 91-R strain of *Drosophila melanogaster* involves decreased penetration, increased metabolism, and rapid excretion

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Resistance to dichlorodiphenyltrichloroethane (DDT) in the 91-R strain of *Drosophila melanogaster* is extremely high compared to the susceptible Can-S strain (>1000 times). Oxidative detoxification is involved in resistance but is not the only mechanism. Rates of penetration, metabolism, and excretion were determined radiometrically between resistant 91-R and susceptible Can-S strains. Contact penetration into 91-R was ~30% slower than Can-S and it had 50-78% more cuticular hydrocarbons likely resulting in penetration differences. DDT was metabolized ~30% more extensively by 91-R resulting in dicofol, DDE, an unknown metabolite, and polar conjugates being formed. 91-R also excreted ~5 times more radioactive DDT and metabolites, which is likely due to over-expression of *dMRP1* (CG-6214) (35% over-expression by qRT-PCR). Interestingly, verapamil reduced the LD_{50} value for 91-R flies topically dosed with DDT by 4.6-fold. Thus, DDT resistance in 91-R is polyfactorial and includes reduced penetration and increased detoxification and excretion.

AGRO 59
Insecticidal activity of monoterpenoids at the octopamine receptor
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The concerns of environmental and health effects of currently used insecticides has led to increased research for alternative insecticides. Monoterpenoids constitute the largest portion of secondary metabolites in essential oils and provide sweet aromas which accounts for their wide usage in fragrance and perfume industries. Octopamine (OA) is a biogenic amine that is prominently found in invertebrates. OA has been compared to the mammalian adrenergic system with the activation of a “fight or flight” mechanism via G-protein coupled receptors (GPCR). The activation of these receptors leads to the production of cyclic AMP and calcium as second messengers. Competitive binding of monoterpenoids with the octopamine receptor will help us gain insight into the mechanism by which monoterpenoids exert their toxic effect. It has been shown that the toxic action of these agonists occurs mostly at higher concentrations. The higher agonistic concentrations cause the increased release of second messengers leading to tremors and eventually death. Therefore the release of second messengers upon activation of octopamine receptors produced by monoterpenoids and their role in toxicity will be monitored by expressing the *Periplaneta americana* octopamine receptor 1 (Pa oa 1) in the yeast *Saccharomyces cerevisiae*. The overall goal is to determine agonistic/antagonistic effects of natural products and conduct quantitative structure-activity relationships to design better insecticides for the future.

AGRO 60
Induction of neuronal phenotype in Sf21 insect cells
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The goal of this research is to produce insect neurons by transforming Sf21 insect ovarian cell lines. The procedure uses a culture of Sf21 cells and a mixture of transformation agents to induce differentiation. The cocktail consists of the molting hormone 20-hydroxyecdysone, which causes Sf21 cells to express neuronal morphology when added to the growth medium and the depolarizing agent, veratridine. Veratridine, a sodium channel activator, increased the number and/or survival of cells transformed into presumptive neurons by ecdysone, an effect that was blocked by 1 µM tetrodotoxin. A fraction of ecdysone-transformed cells (17%) showed elevated calcium-dependent fluorescence in response to a depolarizing pulse of K^+ ion, suggesting the presence of enhanced levels of voltage-sensitive calcium channels. Future studies will assess the presence of other neuronal marker proteins, test for the presence of any synaptic connections between the cells, and evaluate other differentiating agents, such as insulin and caffeine.

AGRO 61
Deltamethrin increases peak current and slows deactivation kinetics of the voltage-sensitive calcium channel ($Ca_V2.2$) from rat brain following PKC-dependent phosphorylation
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Pyrethroids are insecticides widely used since the 1970s. Derived from the natural insecticide pyrethrum, they are favored for their low mammalian toxicity, improved environmental stability and insecticidal potency. Insect voltage-sensitive sodium channels (VSSCs) are a known target but in vitro evidence indicates that voltage-sensitive calcium channels (VSCCs) are also targets. Site-directed mutagenesis of $Ca_V2.2$ (N-type), altering threonine 422 to glutamate (T422E), produces a mutant channel that acts as if permanently phosphorylated. 1R-deltamethrin increases peak current of T422E $Ca_V2.2$ compared to its antagonistic action on wild type $Ca_V2.2$ when expressed in Xenopus oocytes. Phosphorylation of wild type $Ca_V2.2$ is evoked by phorbol-12-myristate-13-acetate (PMA) by activating endogenous protein kinase C (PKC) in oocytes. 1R-deltamethrin now slows deactivation of the PKC phosphorylated channel, slowing channel closure, increasing Ca^{2+} influx and neurotransmitter release. 1R-deltamethrin treatment resulted in no effect on the deactivation kinetics of the unphosphorylated or T422E channels.

AGRO 62
Differential potency of bivalent anticholinesterases as a model for the molecular design of selective insecticides
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Acetylcholinesterase (AChE) is a target of conventional organophosphate and carbamate insecticides, which react with a conserved S200 residue in the active site, thereby causing toxicity to organisms. Due to the conserved nature of S200, conventional anticholinesterases are associated with cross-species toxicity. There is an urgent need to develop new selective chemicals with high insect toxicity and low mammalian toxicity with reduced propensity to elicit resistance. AChE has two ligand-binding sites, the peripheral aryl site (PAS) at the mouth and the catalytic active site (CAS) at the bottom of a deep narrow (20 Å) active site gorge. Tacrine dimers are bivalent inhibitors whose dual binding property on AChEs vary with tether length, and therefore serve as useful probes of AChE gorge geometry. We used tacrine dimers with linkers C2-C12 to systematically probe the *Drosophila melanogaster*, *Anopheles gambiae*, *Blattella germanica*, and human AChE gorge. We screened for both differential potency and dual binding ability of the bivalents in the AChEs. Tacrine dimers were found to be more potent to vertebrate and *Drosophila* AChEs, compared to that of other insects. The tether length dependence index (monomer IC_{50}/the most active dimer IC_{50}) was lowest in *Anopheles* and *Blattella* compared to

other organisms. AChE sequences were analyzed using Clustal-W to map candidate amino acid residues that are unique to insect AChE and hence possible targets for selectophore design. These structural data should prove useful for the molecular design of selective insecticides.

AGRO 63
Modulation of monoterpenoids on [3H]-TBOB binding to house fly GABA receptor
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Monoterpenoids and their derivatives showed good insecticidal activities in the previous studies, but the mechanisms of their action as natural pesticides are not known yet. In this research, modulation effects on [3H]-TBOB binding to house fly GABA (γ-aminobutyric acid) receptors of four monoterpenoids (pulegone, thymol, α-terpineol, and linalool) were studied in order to understand the mode of toxic action of monoterpenoids pesticides. In these four monoterpenoids, pulegone, thymol, and linalool potentiated the [3H]-TBOB binding to house fly GABA receptor with the maximum [3H]-TBOB binding= 270%, 475%, and 145% respectively. Another monoterpenoid, α-terpineol, showed neither enhanced nor inhibitory effect on [3H]-TBOB binding to housefly GABA receptor. The increasing [3H]-TBOB binding showed an interaction of house fly GABA receptor and those three monoterpenoids, but their binding sites are different from the [3H]-TBOB binding site (also known as the picrotoxin binding site).

AGRO 64
Fermentation Stoichiometry of *Thermotoga neapolitana* and Influence of Temperature and Oxygen on Hydrogen Production
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Batch experiments were conducted with *Thermotoga neapolitana* to determine the fermentation stoichiometry and influence of temperature on product yields and volumetric productivity rates at temperatures across the permissive range. The effect of O_2 on H_2 production was also tested. The carbon balance for 85°C was 2.5 mol H_2, 2 mol CO_2, 1.8 mol acetate, and 0.1 mol lactate produced per mol of glucose. The maximum rate and extent of H_2 production occurred at both 77°C and 85°C, but organic acid production was higher at 85°C. Yield coefficients and volumetric productivity rates indicated that 77°C is an appropriate temperature for H_2 production. H_2 production did not increase under aerobic conditions; providing additional evidence for the conclusion in the literature that *T. neapolitana* does not produce H_2 through microaerobic metabolism. The experimental results establish a reference point for future work to maximize H_2 productivity of *T. neapolitana*.

AGRO 65
Microplate Assay for Characterization of Plant Cell Wall Degrading Enzyme Activity from Crude Fungal Extracts
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Developing enzyme cocktails for cellulosic biomass hydrolysis complementary to current cellulase systems is a critical step towards economically viable biofuels production. Plant pathogenic fungi present a largely untapped resource for novel hydrolytic enzymes. Thus, a standardized method for rapid analysis of glycoside hydrolysis by fungal isolates was developed. Fungi were grown for 10 days on cellulose containing media and crude extracts were collected. Extract activity was measured on standard cellulose substrates and plant biomass, to better characterize cellulolytic ability. The standard DNS reducing sugar assay was previously adapted for small reaction volumes in 96-well plates. Color change was measured in a Synergy HT Microplate Reader. Significant interactions were identified among media composition, assay substrate and temperature, and variability within and among fungal species. Within a small initial sampling of phytopathogenic fungi, some species were identified with crude extract activities comparable to *T. reesei*, particularly when assayed at lower temperatures.

AGRO 66
Supercritical CO_2 hydrolysis and explosion as pretreatment of guayule bagasse for fermentation feedstock
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Guayule, a desert shrub, is planted for commercial production of hypoallergenic latex. Its resins also have unique applications. Latex and resins, however, make up only about 20% of biomass. Converting the waste bagasse to biorefinery feedstock for value-added products makes good economic sense. A supercritical CO_2-based process had been developed for extracting guayule resins and rubber. In this study, we demonstrated the feasibility of using a supercritical explosion-hydrolysis procedure, as part of the integrated process, to prepare/pretreat the bagasse for subsequent enzymatic and microbial conversion. Our approach used supercritical CO_2 and moisture for mild hydrolysis and, subsequently, explosion, created by sudden pressure release, to loosen and to expose the lignocellulosic structure for enzymatic hydrolysis. Optimizing the operating parameters such as temperature, pressure, moisture, and duration of hydrolysis can increase the sugar yield. Comparison studies showed that this method was more effective than other techniques such as acid hydrolysis and delignification.

AGRO 67

Cellulosic ethanol production from *Saccharomyces cerevisiae* engineered for anaerobic conversion of pretreated lignocellulosic sugars to ethanol

Joseph O. Rich, *Kenneth Bischoff, and Stephen R. Hughes, Bioproducts and Biocatalysis Research Unit, USDA-Agricultural Research Service, National Center for Agricultural Utilization Research, 1815 North University Street, Peoria, IL 61604*

Advanced high-throughput screening has resulted in the discovery of several yeast strains that are capable of anaerobically utilizing pentose, as well as hexose sugars. The growth and ethanol production of these developed strains will be described. The paradigm for using genetically engineered *Saccharomyces cerevisiae* strains in lignocellulosic ethanol production will also be discussed.

AGRO 68

Properties of wood chars part 1: Elemental composition and acid functional groups

David W. Rutherford[1], dwruther@usgs.gov, ***Colleen E. Rostad***[2]*, cerostad@usgs.gov, Jerry A. Leenheer[1], leenheer@usgs.gov, and Robert L. Wershaw[1], rwershaw@usgs.gov. (1) Water Resources Division, U.S. Geological Survey, Denver Federal Center, Building 95, MS 408, Box 25046, Lakewood, CO 80225, Fax: 303-236-3934, (2) Water Resources Discipline, U.S. Geological Survey, Box 25046 MS 408 (Bldg. 95), Denver Federal Center, Denver, CO 80225, Fax: 303-236-3934*

There is increasing interest in using pyrogenic carbon for carbon sequestration because it is more recalcitrant to degradation than unaltered organic matter. Chars produced as high surface area sorbents generally have been produced at high temperatures. For carbon sequestration, properties such as resistance to degradation or ability to improve soil fertility will need to be optimized and may require different charring conditions. A series of chars were produced from wood products using various times and temperatures to study the variation of composition and acid functional group content. Elemental analysis of char showed a preferential loss of oxygen compared to carbon during early charring when aliphatic carbon is being lost. In later stages of charring aromatic carbon is being preferentially lost. Charring conditions have substantial impact on the acid functional group content of chars. Low temperatures and long charring times produce chars with the highest acid functional group content.

AGRO 69

Properties of wood chars part 2: Variation in surface area and porosity

David W. Rutherford[1], dwruther@usgs.gov, ***Colleen E. Rostad***[2]*, cerostad@usgs.gov, Jerry A. Leenheer[1], leenheer@usgs.gov, and Robert L. Wershaw[1], rwershaw@usgs.gov. (1) Water Resources Division, U.S. Geological Survey, Denver Federal Center, Building 95, MS 408, Box 25046, Lakewood, CO 80225, Fax: 303-236-3934, (2) Water Resources Discipline, U.S. Geological Survey, Box 25046 MS 408 (Bldg. 95), Denver Federal Center, Denver, CO 80225, Fax: 303-236-3934*

Charring methods for production of sorbents have been optimized to create high surface area materials and usually employ high temperatures and activation. Properties of chars produced as soil amendments to enhance fertility and sequester carbon can be optimized at lower temperatures. To better understand the development of porosity in low temperature chars, wood, bark, cellulose and lignin samples were charred at temperatures ranging from 2500C to 5000C for times ranging from 1 hour to 168 hours. Structural changes were examined by changes in porosity as measured by nitrogen gas adsorption. 13C NMR spectrometry, mass loss, and elemental composition were combined to estimate the mass of aromatic and aliphatic carbon remaining in the char. Aliphatic components in the chars were either lost or converted to aromatic carbon early in the charring process. Porosity did not develop until loss of aromatic carbon occurred, indicating that micropores were developing within a fused-ring matrix.

AGRO 70

Competition for char phosphorous between microorganisms in the biodegradation of coexisting atrazine and dichlobenil in soil

Lei Xu and ***Daniel Sheng****, Zhejiang University of Technology, Hangzhou 310032, China*

A previous study demonstrated that nutrients from crop-residue-derived chars significantly enhance the biodegradation of single pesticides in soil. This work evaluated the role of char nutrients in the biodegradation of coexisting dichlobenil and atrazine by their respective degraders of DDN and ADP. Under growing conditions where the respective initial cell densities of DDN and ADP were $1x10^5$ and $3x10^4$ CFU/mL, the degradation of dichlobenil (10 mg/L) and atrazine (5 mg/L) as single pesticides in soil extract was slow. The degradation in extracts and slurries of char-amended solids increased with increasing char content over the tested range of up to 1% in soil, due to increased nutrient supply and thus enhanced stimulation on microbial activities. Supplementing the soil extract with P significantly enhanced the degradation of both pesticides, demonstrating that P was the limiting nutrient. When dichlobenil and atrazine coexisted, their degradation was reduced, due apparently to the competitive utilization of P by DDN and ADP. The nutritional competitions created a lag phase for ADP that was otherwise nonexistent. With a shorter lag phase, ADP grew earlier than DDN with the advantage of utilizing P first in insufficient supply to increase its population and metabolize atrazine. Reduced P concentration by ADP resulted in an inhibition on the growth of DDN and thus suppression on dichlobenil degradation. DDN being a poor competitor against ADP for P was verified by establishing the relationship between the initial degradation rate for both pesticides and P concentration.

AGRO 71

Simulating hydrology at a Long Island turf study site using the model RZWQM98

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A lysimeter field study was conducted on turf at a golf course in Long Island, New York during 2006 and 2007. A bromide tracer was applied during the conduct of this study to trace water movement through the soil profile at the study site. The USDA model, Root Zone Water Quality Model (RZWQM98), is used to simulate the hydrology at this study site. Predicted hydrologic results are compared to observed results from the study for both 2006 and 2007. Additionally, turf uptake of water at the study site will be examined for the two different weather conditions experienced at the study site during 2006 and 2007.

AGRO 72
Crop residue prediction in support of livestock feeding study dose selection
Coleen M. Kennedy[1], coleen.m.kennedy@usa.dupont.com, Jeffery J. Anderson[1], Nathan Snyder[2], and ***Martin T. Scott***[1], *Martin.T.Scott@usa.dupont. (1) Stine Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714-0030, Fax: 302-451-3570, (2) Waterborne Environmental Inc, Leesburg, VA 20175*

Crop protection product registrants are committed to conducting livestock feeding studies in support of product registration goals that meet all pertinent regulatory study design requirements including proper dose selection. Aggressive commercialization timelines often require setting doses before all residue data for calculation of a dietary burden are available. Using residue data in alfalfa obtained for other active ingredients, and through use of a residue prediction tool, regulatorily-acceptable doses will be set. Such an approach offers dose-setting capabilities based on a potentially larger database relative to those used for traditional dose-setting methods early in a product's development. At the same time, adherence to aggressive registration timelines is facilitated. The tool's methodology will be described as well as its application for this purpose.

AGRO 73
Raman microscopy of high P soil: In situ spatial compositional heterogeneity before and after Fe^{+3} amendment
Eton E. Codling[1], Lynne Heighton[2], Swati Mookherji[1], and ***Walter F. Schmidt***[1], *walter.schmidt@ars.usda.gov. (1) Beltsville Agricultural Research Center, USDA-Agricultural Research Service, 10300 Baltimore Avenue, Beltsville, MD 20705, (2) Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742-4454*

Recently, we reported that the interactions of phytate (the major organic form of P present in poultry litter) with soil components (mineral Cu^{+2} and Fe^{+3}) are highly pH dependent. Thus, processes used to isolate soil mineral complexes can dramatically alter the chemical interactions present one is trying to understand. Spatial homogeneity is present in solution. *In situ* analysis is essential in cases of spatial heterogeneity. Raman microscopy spectra of the high P Soil before and after Fe^{+3} amendment are presented and analyzed. Although soils can be highly heterogeneous, a very useful consequence of this is complex and diverse interactions and processes will be occurring simultaneously within the same sample. Without *in situ* examination, data from localized soil sites are signal averaged with data from the sites themselves are markedly dissimilar in composition. The site selective variability in components and interactions present in compositionally diverse soil sample can correspond to the molecular chemical processes present a wide array of soil type samples. Specificity in molecular processes at microscopically-discernable locations enables further studies to collect data from soil precisely at the microscopically-discernable sites that are most likely to contain the desired information independent of soil type.

AGRO 74
Analysis of residue samples: Effect of homogenization and sample size in extractions
Julia E. Eble*, Critical Path Services, LLC, 3521 Silverside Rd, Suite 1-I, Wilmington, DE 19810*

Crop samples from magnitude of residue studies are typically homogenized as the raw agricultural commodity in a food chopper with dry ice and subsequently extracted by a mechanical probe. Substantial savings in time and labor can be achieved by extracting samples in batches using beat beater technology rather than using mechanical probes. Such extractions in a batch mode are currently feasible but typically with sample sizes smaller than the norm for residue methods. The current work measures the impact of extraction sample weight on reproducibility as a function of homogeneity after chopping in a Hobart with dry ice. Sample sizes ranging from 100 mg to 10 grams will be tested to estimate a sampling constant and predict a minimum test sample size that would insure a coefficient of variation of ≤ 15%.

AGRO 75
Rapid UPLC-MS determination of tetracylines, sulfonamides, and penicillins in milk using mixed-mode SPE
Michael S. Young*, Jeremy C. Shia, KimVan Tran, and Diane M. Diehl, Waters Corporation, 34 Maple Street, Milford, MA 01757, Fax: 508-482-3100*

The current MRL (maximum residue limit) for the US and EU for the total of sulfonamide antibacterial residues is 100 ng/mL or 10 ng/mL for any single residue; MRLs for tetracyclines are similar. In this poster, we discuss mixed-mode SPE procedures suitable for multiresidue determination of sulfonamides and tetracyclines using tandem UPLC-MS. We will also discuss the suitability of the SPE protocols for UPLC-UV screening analysis. The analytes are first isolated from milk or tissue extracts using mixed-mode ion-exchange SPE (such as Oasis MAX). After cleanup, the extracts are analyzed by UPLC with MS-MS and UV detection. The results demonstrate simple and rapid methods with limits of quantitation (LOQ) well below 10 ng/mL for sulfonamides and tetracyclines. A modified protocol will be discussed for determination of penicillins at similar levels.

AGRO 76
An improved in vitro rearing system for the human head louse allows the determination of resistance to formulated pediculicides in a standardized format
Joseph P. Strycharz[1], *jstrycha@vasci.umass.edu, Kyong Sup Yoon[2], kyoon@vasci.umass.edu, and J. Marshall Clark[1], jclark@vasci.umass.edu. (1) Department of Veterinary and Animal Science, University of Massachusetts, Amherst, MA 01003, (2) Department of Veterinary and Animal Sciences, University of Massachusetts, Amherst, MA 01003*

Our *in vitro* rearing system allows the culturing of pediculicide-susceptible and -resistant strains of human head lice (*Pediculus humanus capitis*). To confirm resistance, treatments of 1% permethrin in acetone, Nix®, Rid® or Pronto Plus® to hair tufts were found highly efficacious (100% mortality) on susceptible lice but less efficacious (62–84% mortality) on resistant lice eight days post-treatment. Lice that survived the first treatment received an identical treatment eight days following the first treatment. Survivors (13–30%) developed to adults and females laid eggs that developed. Permethrin-resistant lice treated with an ivermectin formulation were completely controlled (100% mortality). Eggs exposed to ivermectin formulation-treated hair tufts hatched but none took a blood meal and all died within 24 hr. The delayed ovicidal action of ivermectin is likely due to paralysis of the sucking mouthparts.

AGRO 77
Determinants of human exposure to pet pest products: Fipronil
*Melinda M. Bigelow-Dyk, **Yanhong Li**, Zhenshan Chen, Helen M. Vega, and Robert I. Krieger, Department of Entomology, University of California-Riverside, Riverside, CA 92521*

Applications of topical pet pest products inevitably result in human exposure. Characterization of the magnitude and duration of chemical transfer and exposure from these compounds is necessary for aggregate exposure assessment and mitigation. Currently, aggregate exposure assessments of topical pet products do not include characterization of indoor deposition of these pesticides, but instead rely on default assumptions. Fipronil, the active ingredient in Frontline®, is used for flea and tick control, roach and ant baits, as well as structural termite control. The potential for indoor exposure to fipronil and possible photoproducts poorly understood and unstudied. Analysis of cotton gloves used as a dosimeter showed time-dependent levels of fipronil (66 µg/pair to 2.7 mg/pair) and derivatives. Other textile dosimeters, such as flooring and bedding, also show time dependent levels of fipronil and products (0.05 µg/cm^2 to 120 µg/cm^2). Future studies will investigate three potential urine biomarkers as indices of exposure.

AGRO 78
Absorption and excretion of ^{14}C-labeled α-chloralose from Mallard ducks
***Laura E. Hulslander**, Doreen L. Griffin, David A. Goldade, and John J. Johnston, Chemistry, USDA/APHIS/WS/National Wildlife Research Center, 4101 LaPorte Ave., Fort Collins, CO 80521*

α-Chloralose is an anesthetizing chemical used to aid in the capture of nuisance birds. It causes central nervous system depression which makes the affected birds easier to capture and minimizes injury to the birds during capture. To prevent possible human ingestion of α-chloralose, there is a 30-day moratorium on α-chloralose use with respect to hunting seasons; this moratorium limits the usefulness of this wildlife management technique. To generate pharmacokinetic data which could possibly lead to reducing the length of this moratorium, we conducted an experiment to identify the absorption and excretion of α-chloralose. Mallard ducks, *Anas platyrhynchos*, were given a single dose of ^{14}C-labelled α-chloralose. Results indicated that α-chloralose was slowly taken into the system and rapidly excreted. Only 10% of the administered dose was absorbed by the treated ducks. After 18 hr, tissue residue levels had dropped to near background levels.

AGRO 79
Biochemical and toxicological characterization of highly-selective anticholinesterases developed for malarial mosquito control
***Troy D. Anderson**[1], anderst@vt.edu, Joshua Hartsel[2], jhartsel@vt.edu, Ming Ma[2], mma@vt.edu, James M Mutunga[1], jmutunga@vt.edu, Ania Wysinska[1], Bryan T. Jackson[1], Dawn Wong[2], Sally Paulson[1], Paul R Carlier[2], pcarlier@vt.edu, and Jeffrey R Bloomquist[1]. (1) Department of Entomology, Virginia Polytechnic Institute and State University, 216A Price Hall, MC 0319, Blacksburg, VA 24061, (2) Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061*

The malarial mosquito, *Anopheles gambiae*, affects millions of people worldwide as a result of its disease-vectoring capacity. Acetylcholinesterase (AChE) is a proven target for high-efficacy, anticholinesterase insecticides; however, widespread resistance and poor selectivity towards humans limit their use to reduce the risk of the mosquito-borne infection. Our research focus is to develop highly-specific AChE inhibitors with high mosquito toxicity and low mammalian toxicity. We will demonstrate novel carbamate molecules with greater maximal potency (ca. > 1,000-fold) towards *An. gambiae* AChE compared to that of human AChE and examine the structural features of each anticholinesterase in relation to their differential sensitivities towards *An. gambiae* AChE. We confirm both contact and topical mosquito toxicity of these carbamates, with and without the use of synergists, and we will discuss the utilization of these mosquito-specific AChE inhibitors in malaria control programs.

AGRO 80
Biochemical characterization of a putative insecticide target site in the acetylcholinesterase catalytic gorge of green peach aphid
***Troy D. Anderson**[1], anderst@vt.edu, Danny C. Hsu[2], dhsu@vt.edu, Paul R. Carlier[2], pcarlier@vt.edu, Polo C-H. Lam[3], pololam@scripps.edu, Maxim M. Totrov[3], max@molsoft.com, and Jeffrey R. Bloomquist[1], jbquist@vt.edu. (1) Department of Entomology, Virginia Polytechnic Institute and State University, 216A Price Hall, MC 0319, Blacksburg, VA 24061, (2) Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, (3) MolSoft L.L.C, La Jolla, CA 92037*

The green peach aphid, *Myzus persicae*, elicits considerable economic damage on vegetable and ornamental crops. Acetylcholinesterase (AChE) is a proven target for hig-efficacy, organophosphate and carbamate insecticides; however, widespread resistance and poor selectivity towards humans limit their use in pest control programs. Sulfhydryl reagents inactivate AChE in aphids, but are ineffective against other insect and mammalian AChEs. Protein homology modeling of aphid AChE suggests a species-specific cysteine (Cys286) near the peripheral site of the AChE to which sulfhydryl reagents might interact. Cys286 is absent in mammalian AChE and, thus, may be exploited for selective anticholinesterase development. We will demonstrate a systematic screen of tacrine-linked AChE inhibitors to profile the catalytic gorge of *M. persicae* AChE and to examine the differential sensitivities of these compounds to Cys286. The implications of these structure-activity relationships to *M. persicae* AChE and other insect AChEs for insecticide design will be discussed.

AGRO 81
2-Substituted 1-azabicyclo[2,2,2]octan-3-ones as novel insecticides
***Wenming Zhang**, Amy X. Ding, Cheryl Desmond, Gilles Seburyamo, Kenneth A. Hughes, Roman Kucharczyk, Thomas P. Selby, Daniel Cordova, and Matthew Sacher, Stine-Haskell Research Center, Dupont Crop Protection, 1090 Elkton Road, Newark, DE 19711-3507, Fax: 302-366-5738*

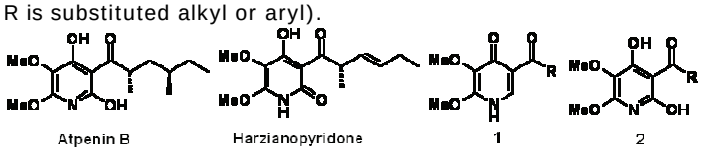
Nicotinic agonists are potentially useful insecticides and 2-substituted 1-azabicyclo[2,2,2]octan-3-ones have been shown as potent nicotinic agonists. We have discovered that 2-substituted 1-azabicyclo[2,2,2]octan-3-ones showed intriguing insecticidal activity. To optimize the insecticidal activity, we prepared different substitution derivatives altering the physical properties of those quinuclidines. This poster will outline the synthetic approaches we used to make the desired compounds as well as their biological activity.

AGRO 82

Synthetic atpenin analogs: Potent mitochondrial inhibitors of succinate-ubiquinone oxidoreductase (complex II)

Kenneth A. Hughes, *Thomas P. Selby, James J. Rauh, Ya Jun Zheng, Wayne S. Hanna, and Patricia A. Mauvais, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

Succinate-ubiquinone oxidoreductase (complex II) plays a critical role in the production of ATP by oxidative phosphorylation in the mitochondrial respiratory chain of animals, plants, fungi and bacteria. Specifically, complex II catalyzes the oxidation of succinate to fumarate thereby allowing for electron transfer to take place. Atpenins (isolated from *Penicillium sp.*) and harzianopyridone (a metabolite from *Trichoderma harzianum*) represent a unique class of penta-substituted pyridine-based natural products that are potent and specific inhibitors of mammalian mitochondrial complex II (no significant effect on complex I or III). Although antifungal activity has been reported for both atpenins and harzianopyridone, only modest *in vivo* activity was observed for harzianopyridone as a plant antifungal agent. In our continuing effort to discover new fungicides, we became interested in exploring synthetic atpenin analogs as potential plant protection agents that might interfere with ATP production in pathogens. Here, we wish to report on the synthesis, complex II inhibition (against mammalian and fungal forms of the enzyme) and antifungal activity of compounds of formulae **1** and **2** (where R is substituted alkyl or aryl).

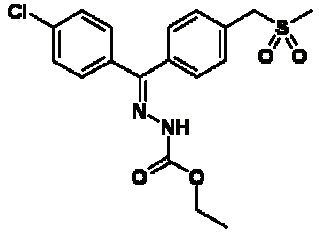


AGRO 83

Alkylsulfonyl benzophenone hydrazones as insecticides

Jeffrey K. Long, *Latasha Jones, Erno M. Keskeny, Stephanie Lewis, and Thomas M. Stevenson, Stine-Haskell Research Center, DuPont Crop Protection, P. O. Box 30, Newark, DE 19714*

Over the past 30 years, a variety of acyl hydrazones of benzophenones have been patented as insecticides, but no examples of this class have been commercialized. The majority of examples contain a sulfonate substituent that appears to be key for favorable biological activity. We examined the effects on insecticidal activity of replacing the sulfonate group with a variety of sulfur- and phosphorus-containing alkyl side chains, as well as changing aromatic ring substitution. Very good activity was demonstrated on a range of agricultural pests, including *Lepidoptera*, *Diabrotica*, and *Hemiptera*. The preparation and biological activity of these compounds will be presented.



AGRO 84

Synthesis and herbicidal activity of *N*-isobutyl-*N*-substituted naphthalene methyl carboxylic acid amides

Ty Wagerle, *Ming Xu, Thomas M. Stevenson, Thomas P. Selby, Gregory R. Armel, and Patrick L. Rardon, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

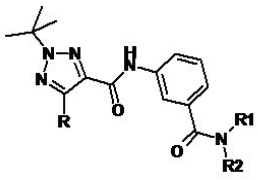
The successful strategy of using naphthalene as a surrogate for benzene in novel herbicide discovery is disclosed. A series of novel analogs with various substitutions around the naphthalene ring are synthesized as herbicides. The evaluation of their herbicidal activity will be presented in this poster.

AGRO 85

Herbicidal 1,2,3-triazole carboxamides

Ming Xu, *Thomas M. Stevenson, Maura Hendrixson, Balreddy Kamireddy, Xia Zhao, Gregory R Armel, and David A Baxter, Stine-Haskell Research Center, DuPont Crop Protection, Newark, DE 19714*

Some novel 1,2,3-triazole carboxamides were designed and synthesized as herbicides. In this poster, we will describe our synthesis of these interesting compounds as well as the results from herbicidal evaluations.

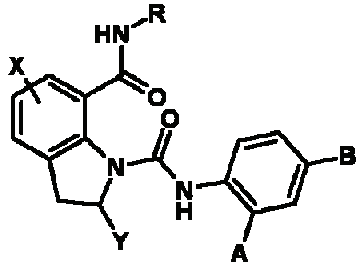


AGRO 86

Indoline insecticides

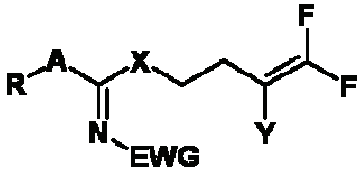
Thomas M. Stevenson, *Timothy D. Neubert, Christina M. Dubas-Cordery, and Rebecca Husted, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

Compounds which have common structural features of both the phthalic diamide insecticides and anthranilic diamide insecticides have been designed and synthesized. These compounds are based on the indoline nucleus and can be made from readily available starting materials. Optimally substituted compounds have excellent levels of activity on lepidopteran insects. This poster will focus on the design, synthesis, and biology of these potent insecticides.



AGRO 87
Difluorobutenyl(thio)imidates as insecticides and nematicides
Thomas M. Stevenson, *Ming Xu, Eric A. Marshall, Ty Wagerle, Christina M. Dubas-Cordery, and Wonpyo Hong, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

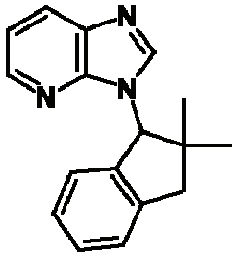
Many types of compounds containing the difluorobutenyl moiety have activity against both insects and nematodes. In this poster, we will describe a series of novel difluorobutenyl substituted imidates and thioimidates. These compounds were synthesized by a number of different methods which allowed us to prepare a variety of derivatives at various positions. The structure activity relationships and biological activity of these highly active insecticide/nematicides will also be discussed.



A = O, S
X = O, S
R = Alkyl
Y = H, F

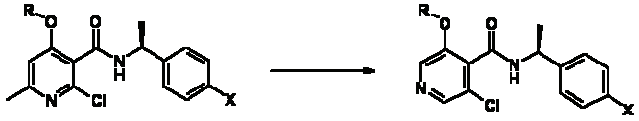
AGRO 88
Imidazopyridine based herbicides
Thomas M. Stevenson *and Christina M. Dubas-Cordery, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

Herbicidal inhibitors of Obtusifoliol biosynthesis discovered by Ciba Geigy in collaboration with Janssen Pharmaceuticals are known which are based on imidazole carboxylates. Noting the similarity of heterocyclic scaffold of the herbicidal imidazoles to the anti-hypertensive CosaarTM, we decided to make compounds based on synthetic strategies used in CosaarTM followup. Of particular interest was the work at DuPont and Merck on imidazopyridines as replacements for the imidazole carboxylate moiety. We made 5 different isomers of imidazopyridines substituted with groups which had previously imparted herbicidal activity to imidazole carboxylates. One of the isomers had significant activity on paddy weeds in flood testing. Synthesis and structure activity trends for these compounds will be presented in this poster.



AGRO 89
Isonicotinamide herbicides
Thomas M. Stevenson *and Christina M. Dubas-Cordery, Stine-Haskell Research Center, DuPont Crop Protection, P. O. Box 30, Newark, DE 19714, Fax: 302-366-5738*

A herbicidally-active byproduct isolated during an analoging program directed towards oomycete specific fungicides led to the discovery of a highly active class of herbicidal nicotinamides. In this poster, we will outline the synthesis and herbicidal activity of isonicotinic analogs of the lead structure. These compounds were accessible by completely different chemistry and also showed high activity as herbicides. The structure-activity relationships for the isomeric compounds was similar to that seen for the original class.

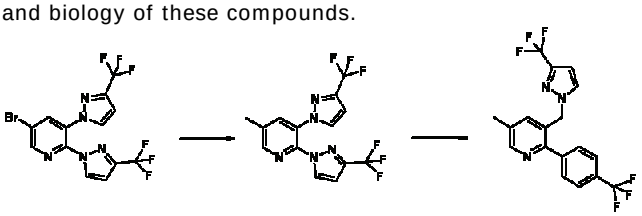


Nicotinamide Herbicides

Isonicotinamide Herbicides

AGRO 90
Pyrazolyl substituted pyridine herbicides
Thomas M. Stevenson, *Ming Xu, Maura Hendrixson, Christina M. Dubas-Cordery, and Martin J. Currie, Stine-Haskell Research Center, DuPont Crop Protection, P. O. Box 30, Newark, DE 19714, Fax: 302-366-5738*

During the optimization work that led to the discovery of the new insecticide Rynaxypr™ we discovered some interesting synthetic byproducts that were active herbicides which exhibited bleaching symptomology. Further study showed these compounds to act by inhibition of phytoene desaturase. By comparing the structures to known inhibitors of the enzyme we were able to design compounds which improved the activity and identified two different subclasses of active herbicides. This poster will outline the chemistry and biology of these compounds.



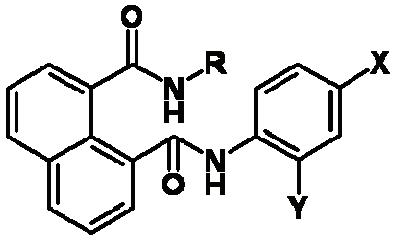
AGRO 91
Synthesis and fungicidal activity of 2-nicotinamidoalkylpyridines
Stephen A. Bolgunas, *Michael P. Walker, William Moberg, David Clark, John Bisaha, David W. Piotrowski, Kanu Patel, King-Mo Sun, Rafael Shapiro, James V. Hay, Timothy D. Neubert, Stephen Foor, Thomas P. Selby, and Thomas M. Stevenson, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

Certain nicotinamides of 2-(1-ethylamino)-3,5-dihalopyridines have been found to possess excellent levels of fungicidal activity on pathogens of grapes and potatoes. The synthesis and biology of these compounds will be presented.

AGRO 92
Synthesis and insecticidal activity of novel 1,8-naphthalenedicarboxamides
Thomas F. Pahutski Jr. *and King-Mo Sun, Stine-Haskell Research Center, DuPont Crop Protection, P.O. Box 30, Newark, DE 19714*

With the early discoveries of the diamide insecticides in 1999, we set out to find novel new ways of orienting the amide groups. Especially appealing to us was the concept of replacing the *o*-amide groups of the phthalic diamides with a naphthalene core containing amides at the 1- and 8-positions so as to occupy a similar region of space. Synthesis of these compounds led to the discovery of interesting levels of insecticidal activity which was characterized by a slightly different structure activity relationship than that seen for the

phthalic diamides. Similarly, we were able to apply the same concept to the anthranilic diamide insecticides.



AGRO 93
Synthesis and optimization of bicyclic arylamidines as fungicides
Wenming Zhang *and Chi Ping Tseng, Stine-Haskell Research Center, Dupont Crop Protection, 1090 Elkton Road, Newark, DE 19711-3507, Fax: 302-366-5738*

With increasing demand for food, feed, fuel, and materials through agriculture production, there is continuous requirement for novel pesticides. We have discovered a class of novel bicyclic arylamidines as fungicides. This poster will show our scouting efforts around arylamidines, discovering and optimizing bicyclic arylamidines with intriguing fungicidal activity.

AGRO 94
Discovery of a new QoI fungicide, pyribencarb
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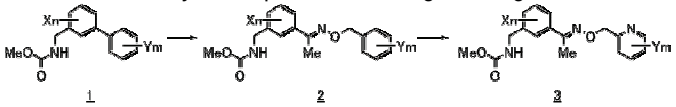
Pyribencarb is a new chemical class of QoI (quinone outside inhibitor) fungicides and provides a broad fungicidal spectrum, particularly effective against *Botrytis cinerea* and *Sclerotinia sclerotiorum*, with an excellent safety to a number of crops.The discovery of pyribencarb started with attempts to place chemical structures of existing strobilurin analogues and newly designed molecules on a two-dimensional hexagonal grid template and examine overlapped parts. First structural modifications based on the examination led to a potent series of *m*-biphenyl compounds **1**, with a -CH_2- linkage between the carbamate and benzene moieties. In further modifications, benzyloxyimino compounds **2** and 2-pyridylmethyloxyimino ones **3** showed excellent efficacy as well as penetrant activity. Finally, pyribencarb was selected as a promising compound to be developed as a new QoI fungicide. Pyribencarb has proven to inhibit the ubiquinol:cytochrome *c* oxidoreductase like other QoIs, but biologically demonstrates different and notable profiles including activities against QoI-resistant strains and safety to crops and non-targeted organisms.



AGRO 95
Enantioenriched cyanohydrins: Versatile insecticide intermediates
Christina Moberg*, Erica Wingstrand, Fei Li, Stina Lundgren, and Maël Penhoat, Department of Chemistry, KTH School of Chemical Science and Engineering, Stockholm SE 100 44, Sweden*

Several pyrethroid insecticides contain cyanoester functions. Many of these are today used in racemic form or, in case they contain more than a single stereocenter, even as a mixture of several stereoisomers, although it is known that both aquatic toxicity and biodegradation may differ for the two enantiomers. We have obtained enantioenriched *O*-acylated cyanohydrins by the addition of ketonitriles to prochiral aldehydes catalyzed by a chiral Lewis acid and an achiral Lewis base. By this procedure, (*S*)-*O*-acetyl 2-hydroxy-3-butenenitrile was prepared from acrolein and acetyl cyanide in 67% yield and 73% ee. This product can be used as an intermediate in the synthesis of glufosinate, (*S*)-2-amino-4-[hydroxy(methyl)phosphinoyl]butyric acid.

AGRO 96
GreenMatch™ EX: A new broad-spectrum organic herbicide based on lemongrass oil
Cruz Avila-Adame*, Brian J. Campbell, Lorena E. Fernández, Eunice Tan,* ***Marja E. Koivunen****, and Pam G. Marrone, Marrone Organic Innovations, Inc, 2121 Second Street, Suite B-107, Davis, CA 95618, Fax: 530-750-2808*

Essential oils containing terpene-like compounds have well-known pesticidal activities. GreenMatch™EX is a new non-selective, broad-spectrum burn-down herbicide. Due to its food-grade active and inert ingredients, it is exempt from EPA registration and also approved for use in organic farming. This natural product pesticide is based on lemongrass oil with good efficacy against both annual and perennial broadleaf and grass weeds. During its development, GreenMatch™EX was tested in California against a wide range of weed species to obtain efficacy and weed spectrum data. Studies with three dilution rates (7.5, 10, and 15%) and three spraying volumes (35, 60, and 100 gallons per acre) showed a significant correlation between concentration/water volume and percent weed control. The best control was achieved at 10 to 15% dilution rate (v/v) with 100 gallons of water per acre, which indicates that complete tissue coverage is required for highest efficacy. GreenMatch™EX performance was dependent upon the age of the weeds and the best control was obtained with young and actively growing plants. GreenMatch™EX at 15% was more effective than GreenMatch™O (*d*-limonene) and Matran™EC (clove oil) at the recommended commercial rates of 18% and 5%, respectively.

AGRO 97

Antifungal compounds from *Pimpinella* species active against plant pathogens

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The genus *Pimpinella* (Apiaceae) is represented by 27 taxa in the flora of Turkey and five of them are endemic. Essential oils from 19 Turkish *Pimpinella* taxa were analyzed by gas chromatography and gas chromatography-mass spectrometry techniques. Phytochemical investigation of *Pimpinella* oils resulted in the isolation of sixteen phenylpropanoids, 4 sesquiterpenes, and 2 azulene-type norsesquiterpenes. *Pimpinella* species are characterized by high contents of phenylpropanoid derivatives in their oils. The 2-hydroxy-5-methoxy-1-(*E*)-propenylbenzene skeleton of these compounds, known as pseudoisoeugenol, is unique to *Pimpinella*. Trinorsesquiterpenes (geijerenes and azulenes) were also found to be second characteristic constituents of most *Pimpinella* oils. Isolated compounds were also evaluated for their antifungal activities using direct-bioautography against plant pathogens: *Colletotrichum acutatum*, *C. fragariae*, and *C. gloeosporioides*. Subsequent evaluation of antifungal compounds in a 96-well micro-dilution broth assay showed that compounds 4-(3-methyloxiranyl)phenyl 2-methylbutyrate and epoxypseudoisoeugenol 2-methylbutyrate produced the most significant growth inhibition in *Phomopsis spp.*, *Colletotrichum spp.*, and *Botrytis cinerea*. Phenylpropanoids appeared to possess more antifungal activity against these important fungal plant pathogens than sesquiterpenes and trinorsesquiterpenes in *Pimpinella* oils.

AGRO 98

Antifungal activity of herbaceous essential oils protects wood from mold and decay fungi

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In recent years, concerns about structural damage and potential health risks due to mold and fungi growth on wood have increased dramatically in the United States. The combined damage from mold and decay fungi claims from homeowners, builders, and insurance companies exceeds several billion US dollars annually. Chemical fungicides that are commonly used to control the growth of mold or decay fungi on wood may not be appropriate for interior applications. Ideal fungicides must be nontoxic and hypoallergenic. There is a continuing need to develop new fungitoxic chemicals that are environmentally friendly. The objective of this study was to investigate the inhibitory effects of seven natural therapeutic essential oils on wood against growth of mold and decay fungi. Wood specimens dip-treated with thyme or geranium E. oil inhibited mold growth up to 22 weeks and wood specimens exposed to passive vapors of dill weed or rosemary oil also inhibited mold growth under laboratory conditions. Essential oils were also evaluated for their ability to inhibit weight loss by brown-rot and white-rot wood decay fungi on southern pine in standard laboratory decay tests. Results show no weight loss occurred in wood specimens. Gas chromatography (GC) analysis identified major components of the test oils that are believed to impart bioactivity. These findings demonstrate that bioactive essential oils could be used alone or as a co-biocide to protect wood against mold infestation and decay fungi.

AGRO 99

Tungstophosphoric acid and its compounds as agents against plant viruses

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Tobacco mosaic tobamovirus (TMV) is a very widespread and harmful plant virus. Even now in the 21st century, plant viruses are still fitopathogenic agents which cause huge economic losses. In our previous work, we confirmed the antiviral activity of tungstophosphoric acid (WPA) and its compounds, such as the magnesium salt and compounds with glycine and alanine, for antiviral activity on tobacco plants after foliar application on *Nicotiana tabacum*, var. Samsum infected with TMV, as host plant. Since the stability of Keggin anions depends on the medium pH, different spectroscopic methods (IR, UV-VIS and NMR) were applied in the present study to determine the dominant species of WPA compounds present in solutions of various pH. Special attention was paid to plant physiological conditions, so the fresh juice of tobacco plants was used in those experiments as well. As the result, the monovacant lacunary Keggin anion was found to be the bioactive form in the plant's juice. As an important step for further consideration of future application of WPA as an agent against plant viruses, its toxicity was tested in an experimental model on Wistar rats, after 7 weeks of oral administration of WPA in several dosages. According to our findings, it could be suggested that tungstophosphoric acid has protective effects on chemically-induced liver necrosis which could be explained by its antioxidant properties.

AGRO 100

Cyperin, a pathogenic fungi diphenyl ether phytotoxin, targets plant enoyl (acyl carrier protein)

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Cyperin is a natural diphenyl ether produced by several phytopathogens. Cyperin inhibits *Arabidopsis thaliana* enoyl (acyl carrier protein) reductase (ENR), which is also sensitive to triclosan. While cyperin was less potent than triclosan on ENR, both cause light-independent membrane degradation at their respective phytotoxic concentrations. A homology model of *A. thaliana* ENR was derived from the crystal structure of the protein from *Brassica napus*. Cyperin mimicked the binding of triclosan in the binding pocket of ENR. Both molecules were stabilized by the G-G stacking interaction between one of their phenyl rings and the nicotinamide ring of the NAD^+. Cyperin is a reversible inhibitor of ENR and is much less potent (I_{50} = 89.0 µM and K_i = 13.6 µM) than the slow tight-binding inhibitor triclosan ($I_{50,\ app}$ = 0.046 µM). Therefore, cyperin may contribute to the virulence of the pathogens by inhibiting ENR and destabilizing the membrane integrity of the cells surrounding the point of infection.

AGRO 101

New phytotoxins for biocontrol of *Cirsium arvense* and *Sonchus arvensis* (Asteraceae)

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Cirsium arvense (L.) Scop. and *Sonchus arvensis* L. (both from Asteraceae), commonly called Canada thistle and perennial sowthistle, are perennial weeds in different crops. Herbicides recommended for chemical control of the perennials are restricted to few active substances. Obviously, new compounds should be actually developed as herbicides against the composite weeds. Many phytopthogenic fungi produce phytotoxins responsible for disease development. Therefore, appropriate weed pathogens can be a source of such the useful metabolites. Several pathogens, *Stagonospora cirsii* Davis and *Ascochyta sonchi* (Sacc.) Grove (syn. *Phoma exigua* Desm. var. *exigua*) were found to be common for both host plants. *Septoria cirsii* Niessl. and *Phyllosticta cirsii* are specific foliar pathogen of *C. arvense*. The isolation chemical and biological characterization of the phytotoxins produced by the above cited fungal pathogens will be illustrated as well as their potential herbicide activity and the results as of structure activity relationships studies.

AGRO 102

Mevalocidin: A novel, phloem-mobile herbicide with potential as a bioherbicide

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Phloem mobility is a key attribute for robust herbicide performance under field conditions. In our herbicide natural product discovery program, we have biased the selection of extracts for isolation, structure determination and lead identification by focusing on actives exhibiting phloem mobility, an attribute that is primarily conferred by defined physicochemical properties. Accordingly, we have identified a wide range of small polar molecules such as the known nucleoside hydantocidin and larger macrolides such as the macrocidins. Recently we discovered a novel derivative of mevalonic acid, mevalocidin, from two soil fungi designated *Fusarium sp.* DA056446 and *Nodulisporium sp.* DA092917. Mevalocidin exhibited broad spectrum, post-emergent activity on grasses, broadleaves, and sedges. The effects on treated plants included chlorosis of new growth and necrosis of meristematic tissue. Further, mevalocidin exhibited a high degree of phloem mobility. The discovery was followed with a synthesis campaign and investigation of the biology, biochemistry, and plant metabolism of this novel active. Current efforts are focused on potential use of the mavalocidin-producing fungi and metabolites as bioherbicides.

AGRO 103

Antifeedant activity of rinsate constituents from camphorweed against lepidopteran larva

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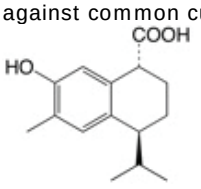
Camphorweed (*Heterotheca subaxillaris*) is a common annual or biennial Asteraceae weed that grows on sandy fields in the U.S.A. This species has a characteristic camphor-like smell and many glandular trichomes on the leaf surface. Additionally, the plant does not appear to be subject to damage from lepidopteran insects in the field. A dichloromethane rinsate was prepared from the aerial parts of this plant by dipping the plant into the solvent for ca. 5 seconds. The rinsate showed good insect antifeedant activity in a dose-dependent manner against 3rd instar common cutworms (*Spodoptera litura*). Constituents in this rinsate were isolated by Si-gel column chromatography and their structures identified based on their spectroscopic data. Three isolated calamenene-type sesquiterpenic acids, 2-hydroxy-, 2-acetoxy-, and 2-methoxy-calamenene-14-carboxylate showed insect antifeedant activity against common cutworms. Approximately 35% of the rinsate consisted of other major constituents. Of these, methylated flavonoids and borneol did not show significant antifeedant activity against common cutworms.



AGRO 104
Insecticides from plants against termites and mosquitoes
Kumudini M. Meepagala[1], *kmeepaga@olemiss.edu, Weste Osbrink*[2], *Julia Pridgeon*[3], *Julia.Pridgeon@ARS.USDA.GOV, James Becnel*[3], *James.Becnel@ars.usda.gov, George Sturtz*[4], *Charles Burandt*[5], *Alan Lax*[2], *alax@srrc.ars.usda.gov, and Stephen O. Duke*[1], *sduke@olemiss.edu. (1) Natural Products Utilization Research Unit, USDA-Agricultural Research Service, P.O. Box 8048, University, MS 38677, Fax: 662-915-1035, (2) Formosan Subterranean Termite Research Unit, USDA-Agricultural Research Service, New Orleans, LA 70179, (3) Center for Medical, Agricultural, and Veterinary Entomology, USDA-Agricultural Research Service, Gainesville FL 32608, (4) Aromagen, Albany, OR 97321, (5) University of Mississippi, University, MS 38677*

Plants produce secondary metabolites as part of natural defense mechanism against insects, fungi, bacteria, and other plants. Thus, this is one area to explore in order to search for environmentally benign insecticides. Several plant extracts were tested against Formosan subterranean termite, *Coptotermes formosanus*, and mosquitoes, *Aedes aegypti*. The active constituents were isolated by bioassay guided fractionation and the structures were elucidated by spectroscopic techniques. Based on these natural product leads more potent analogs were synthesized. Among the natural products that were tested, vulgarone B (isolated from *Artemisia douglasiana*), apiol (isolated from *Ligusticum hultenii*), and cinicin (isolated from *Centurea maculosa*) exhibited significantly higher mortalities compared to untreated controls in laboratory bioassays. Several synthetic and natural product amides have also shown high activities against both mosquitoes and termites. Some of these amides are piperidine derivatives. Isolation, synthesis, and biological activities of these compounds will be discussed.

AGRO 105
Discovery and development of natural products for insect pest management
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The desire for safer and more effective agrochemicals with reduced environmental and/or mammalian toxicity remains important. Essential to these efforts is identification of new lead candidates possessing high levels of desirable biological activities, reduced unwanted toxicities, new structural types and perhaps different modes of action, thereby providing protection from cross-resistance to currently used agrochemicals. Natural product-based pesticides offer advantages in that they can sometimes be specific to a target species and often have unique modes of action with little mammalian toxicity.
Many approaches can be utilized to identify and develop natural products or analogs thereof as candidates for insect pest management. Case examples will be presented and discussed for 1) utilizing botanical lore and traditional knowledge of pesticides, 2) random or selective screening of crude plant extracts, and 3) targeting, screening, and modification of certain classes of natural products with known insecticidal activities. Examples to be discussed will include the investigation and identification of insect-repelling constituents from American Beautyberry (Callicarpa americana), termiticides from Echinops sp., and substituted benzoquinones as termiticides.

AGRO 106
Fungicides and insecticides from medicinal and aromatic plants
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Essential oils isolated from medicinal and aromatic plants are a complex blend of secondary metabolites usually with low molecular weights. While many volatile oils are active against human pathogens and parasites, very few have been tested against crop pathogens and insect pests. Here, we summarize our most recent findings on the fungicidal and insecticidal activity of oils distilled from the tissues of several flowering plants: *Cupressus arizonica*, *Juniperus* spp., *Angelica* spp., *Arnica longifolia*, *Aster hesperius*, *Chrysothamnus nauseosus*, *Pimpinella* spp., *Haplopappus greenei*, and *Scaligeria tripartita*. TLC-based bioautography confirmed oxygenated monoterpenes and sesquiterpenes as the active antifungal agents in many of these oil extracts. The phenylpropanoid, epoxypseudoisoeugenol angelate (EPIA), in *Scaligeria tripartita* oil, inhibited *Colletotrichum fragariae* hyphal growth by 99.9% at 30 µM; an efficacy superior to the commercial fungicide, azoxystrobin. EPIA inhibited *Phomopsis obscurans* growth by 98.2 and 100% at 3 and 30 µM, respectively. Another phenylpropanoid, epoxypseudoisoeugenol tiglate, was less effective, yet reduced *C. fragariae* growth by 42.9%. *Pimpinella anisum* and *P. isaurica* oils rich in phenylpropanoids were tested for insecticidal activity and were moderately active against turnip aphids, *Lipaphis pseudobrassicae*. *Pimpinella isaurica* oil was more active than its three individual phenylpropanoid components: 4-(2-propenyl)phenylangelate, 4-(1-propenyl)phenyltiglate, and 4-methoxy-2-(1-propenyl)phenylangelate. A reconstituted mixture of these three phenylpropanoids in equal proportions was more active than the components by themselves. Of the 23 different plant oils tested, *Bifora radians* and those containing thymol and carvacrol (*Satureja*, *Origanum*, *Thymbra*, and *Origanum*) killed 90-100% of turnip aphids at concentrations as low as 0.3 to 1.0 mg/mL. Similar serial-time mortality bioassays targeting a major nursery and landscape pest, *Stephanitis pyrioides*, show terpenoid components in *Juniperus saltuaria* and *J. squamata* essential oils were more potent than the organophosphate insecticide malathion at the same dosage.

AGRO 107
Value of herbicides in U.S. crop protection
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Widespread herbicide use is a relatively recent development in U.S. agriculture in comparison with other pesticides. Insecticides and fungicides were routinely used in inorganic, naturally-derived chemical formulations on U.S. fruit and vegetable crops beginning in the early 1900's. Widespread use of herbicides to kill weeds did not begin until the

introduction of synthetic organic chemicals in the late 1940's. Currently, herbicides are routinely used on more than 90% of the area of most U.S. crops. The importance of herbicides to U.S. crop production can be understood through a historical perspective and examinations of the practices of organic growers. The historical record reveals that herbicides replaced or reduced the use of hand weeding and cultivation for weed control with an associated reduction in cost and increase in yield. The adoption of herbicides was spurred by a desire to reduce weed control costs as labor became scarce and more expensive in the years following World War II. Organic crop growers do not use herbicides to control weed populations. The problem of controlling weeds without herbicides has been cited numerous times as the single biggest obstacle to crop production that organic crop growers encounter.

AGRO 108
Fate and exposure pathways of Bt-endotoxins in terrestrial food webs
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Bt-transgenic crops are genetically engineered to express *Bacillus thuringiensis*, a bacterium with insecticidal proteins targeting certain agricultural pests. However, despite the reported specificity of Bt-endotoxins, there are concerns regarding the negative effects of exposure of these proteins to non-target food webs and tri-trophic movements through the food chain. Most Bt-crops express endotoxins throughout the plant, creating the potential for multiple pathways of exposure. These pathways include, but are not limited to: root exudates and plant biomass contaminating the soil, soil-dwelling detritivores, and their predators; ingestion of plant material or consumption of Bt-containing herbivores; and pollen feeding or consumption of pollen-dusted material. The complexity of terrestrial food webs and the cryptic feeding behavior of non-target arthropods can confound studying the fate and exposure pathways of Bt-endotoxins. However, molecular techniques have recently enabled the elucidation of trophic linkages in transgenic crops and quantified the uptake of Bt-endotoxins at multiple trophic levels.

AGRO 109
Pesticides and honey bee health: High levels of acaricides and crop protection chemicals in US beehives and its mitigation by gamma irradiation
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Recent bee disappearances threaten production of nuts, fruits, and vegetables. LC/MS-MS and GC/MS were used to analyze pollen, nectar, honey, brood, adult bees, wax, and royal jelly samples using a modified QuEChERS method. Unprecedented levels of the acaricides, fluvalinate (up to 204 ppm) and coumaphos, were found in all comb and foundation wax samples, while lower levels of 47 other pesticides and metabolites including: 8 pyrethroids, 5 organophosphates, 5 carbamates, 3 neonicotinoids, 3 chlorinated cyclodienes, 3 insect growth regulators, 2 organochlorines, 14 fungicides, and 6 herbicides prevailed in pollen and bees. Pollen averaged 5 with up to 17 pesticide detections per sample, including systemics. A 25 kGy dose from ^{60}Co reduced over 50% of wax acaricide residues. Mitigation of the toxic chemical burden from pollen and nectar foods and from the wax combs they inhabit may help preserve the pesticide-susceptible honey bee as a primary pollinator and sentinel species for environmental quality.

AGRO 110
Neonicotinoid insecticides: Assessing risk to bees
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Neonicotinoids are broad-spectrum insecticides with a generally favorable toxicological profile. Their efficacy against a wide range of pests combined with their low mammalian toxicity has led to rapid introduction into a variety of markets worldwide. Some neonicotinoids are intrinsically highly-toxic to bees and it has been hypothesized that use of neonicotinoids may be responsible for mysterious honey bee colony deaths (colony collapse disorder, or CCD) that have plagued US beekeepers in recent years. Here we review the available scientific data concerning toxicity and exposure of honey bees to neonicotinoid pesticides and present a risk assessment for registered agricultural uses of imidacloprid, the first neonicotinoid commercially developed and the one that beekeepers most frequently have suggested as a cause CCD.

AGRO 111
Phytotoxicity of four herbicides on *Ceratophyllum demersum*, *Vallisneria natans*, and *Elodea nuttallii*
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The physiological effects of widely used herbicides (butachlor, quinclorac, bensulfuron-methyl, atrazine) to 3 submerged macrophytes (*Ceratophyllum demersum*, *Vallisneria natans*, and *Elodea Nuttallii*) were tested under laboratory conditions. In addition to morphological responses, two physiological variables were examined: the relative growth rate and photosynthetic pigment content. All the herbicides tested herein affected the growth of the plants evidently; the morphological responses, such as chlorosis, curling of the leaves and fragmentation of plant, etc., were observed. Chl-a (chlorophyll-a) contents of all three species decreased as the herbicide concentration and the treatment duration increases. To evaluate the phytotoxicity of the herbicides, differences in Chl-a content of grasses receiving different treatment were analyzed by t-test and One-Way ANOVA. In all except only one treatment groups, Chl-a content decreased significantly. Results showed that submerged macrophytes may be used as sensitive plants in environmental monitoring or in the ecological risk assessment of herbicide contamination.

AGRO 112

Veterinary pharmaceuticals studied by nonlinear optics: Oxytetracycline and morantel interacting with model environmental interfaces

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The behavior of oxytetracycline (OTC) and morantel at model soil/water interfaces was investigated using the surface-specific spectroscopy technique second harmonic generation (SHG). SHG allows us to track the interaction of pharmaceuticals with aqueous/solid interfaces in real-time and to measure surface-specific binding parameters. A morantel adsorption isotherm follows the Langmuir model and results in a binding constant and a free energy of adsorption that indicates physisorption. The molecular orientation of adsorbed morantel was also determined. The strength of OTC adsorption was found to depend on the chemical identity of the organic moieties present at the functionalized quartz/water model interface, indicating that OTC adsorption is controlled by the chemical composition of soil natural organic matter. These SHG studies probe the fundamental interfacial properties that control the fate of agricultural pharmaceuticals in soils providing insight into chemical reactivity, mobility, and the corresponding threat posed to human health.

AGRO 113

Degradation of sulfonamides in aqueous solution by membrane anodic Fenton treatment

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Two agricultural antibiotics, sulfamethazine and sulfadiazine, used heavily in agriculture and found in manure lagoons and aquatic environments, were removed from an aqueous system by anodic Fenton treatment (AFT). This advanced oxidation technique has been shown to be effective in degrading various pesticides and other organics but has not been applied to antibiotics. The effects of the H_2O_2:Fe^{2+} ratio, the Fenton reagent delivery rate, and the initial concentration on the degradation of sulfamethazine by AFT were investigated. The optimal H_2O_2:Fe^{2+} ratio was determined to be 10:1 and the optimal Fenton reagent delivery rate was found to be between 39 µM/min and 54 µM/min. Under these conditions, sulfamethazine completely degraded at a range of concentrations commonly found in manure lagoons, contaminated rivers, and groundwater within 10 min. Using the same optimal conditions, the effect of pH on the degradation of sulfadiazine by AFT was analyzed. At 100 µM, sulfadiazine completely degraded within 6-8 min of treatment at a range of pH values that potentially could be found in the aquatic environment. Degradation products and pathways were proposed for both compounds and it was determined that the AFT degradation products of sulfamethazine and sulfadiazine are structurally unlikely to retain the same antibiotic properties as their parent compounds.

AGRO 114

Reduction of chlortetracycline residues in manure from therapeutically-treated beef calves

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Chlortetracycline (CTC) is one of only ten antibiotics licensed in the U.S. for use as growth promoters for livestock. The objective of this study was to determine the effect of composting on the fate of CTC residues found in manure from CTC-medicated beef calves. Five animals were medicated for 5 d with 22 mg/kg/d of CTC. Manure samples collected prior to and after medication were mixed with straw and woodchips; portions of these mixtures were treated in laboratory composters for 30 d. In addition, aliquots of the CTC-containing mixture were incubated at 25°C or sterilized followed by incubation at 25°C and 55°C (composting temperature). The presence of CTC did not appear to affect the composting process. Our results using sterile and non-sterile samples suggest that the decrease in concentrations of extractable CTC and its epimer at 25°C and 55°C is due to abiotic processes.

AGRO 115

Fate of sulfamethazine in surface water microcosms and bioaccumulation in sediment-dwelling invertebrates

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The antibiotic sulfamethazine can be transported from manured fields to surface water bodies. We investigated the degradation and fate of sulfamethazine in small pond water microcosms using ^{14}C-phenyl-sulfamethazine, and found a 2.7-d half-life in pond water and 4.2-d half-life when added to the water with a dilute manure solution that simulated runoff from manured land. Sulfamethazine concentrations in sediment accounted for 10 to 15% of the applied antibiotic within 14 d, and then declined thereafter. Sulfamethazine is transformed mainly into sediment-bound residue (40 to 60%) and smaller amounts of photoproducts. Biodegradation, as indicated by metabolite formation and $^{14}CO_2$ evolution, was less significant than photodegradation. Manure input increased sorption and bound residue formation. The bioavailability of sulfamethazine in pond water microcosms was evaluated using *Lumbriculus variegatus*. Bioconcentration factors (BCFs) were calculated following exposure to sulfamethazine in water or water-sediment systems. A significant inverse relationship between exposure concentration and BCF was observed, with log BCF of 2.17 at 0.05 mg/L during aquatic exposure. Log BCF following sediment exposure was 1.89.

AGRO 116
Simultaneous analysis of estrogens and their conjugates in manure from dairy farms and poultry operations using LC/MS-MS
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The detection of endocrine disrupting compounds in the environment is generating environmental and heath concerns. Among these endocrine disrupting compounds, estrogens are reported to be one of the most serious contributors because estrogencity can occur at ng/L concentrations. Since estrogens are excreted in their free and conjugated forms, a large interest has developed to determine whether the conjugated forms contribute significantly to the overall estrogencity of animal wastes. The conjugated estrogens are generally assumed to be inactive. However, these can be transformed back into the estrogenic parent compounds through enzymatic and hydrolytic reactions. Hence, an analytical method was developed to separate 14 analytes which include free estrogens and their conjugates in a single analysis. Separation and detection was achieved by high performance liquid chromatography with an electrospray tandem mass spectrometry (LC/MS-MS). Both natural and synthetic estrogens were evaluated along with their conjugated forms (sulfate, disulfate, glucuronide, diglucuronide, and sulfate-glucornide). This analytical method has been applied in the analysis of biosolids and manure from dairy farms and poultry operations.

AGRO 117
Estrogen removal from dairy manure by pilot-scale reactors
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17B-estradiol (E2) and total estrogenicity (E2-eq) removal from dairy manure was evaluated in six pilot scale reactors: two aerated reactors (60% and 100% aeration; AER60 and AER100), a nitrifying/denitrifying reactor (NDN), an enhanced biological phosphorus removal reactor (EBPR), an anaerobic digester (AD), and a nitrifying reactor (NIT) receiving AD effluent. In all reactors, the influent had greater mass of E2 and E2-eq than the effluent. In aerobic reactors, E2 and E2-eq removal efficiencies were expressed as % of influent mass and also as %/aerobic hour of influent mass (% and %/hour for AD). Reactors with influent anaerobic digestion pretreatment resulted in the same E2 and E2-eq removal in % and higher E2 and E2-eq removal in %/aerobic hour compared to those without. Estrogen removal efficiencies (% and %/aerobic hour) were similar in nitrifying and denitrifying reactors. Reactors with aeration supported greater estrogen removal than those without.

AGRO 118
Fate of estradiol and testosterone in anaerobic lagoon digestors
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Laboratory-scale lagoon digesters were constructed, and the fate of ^{14}C-labelled 17ß-estradiol (E2) and testosterone (T) were monitored for 42 d anaerobically under biological and sterile conditions. Hormone levels decreased in the liquid layer and increased in sludge with time. At 42 d, 27-40% of testosterone and 21-25% of estradiol remained in the liquid layer. E2 degraded to estrone (>90%) in 8 hr, but formation of estrone also occurred under sterile conditions after 14 d. For T, many metabolites formed; degradation was biological and non-biological. Daily gas production was monitored. For T, 3.5-10.7% was converted to methane, while for E2, 7.6-23.8% went to methane. CO_2 mineralization was 0.5-1.4% of the T dose, 0.3-0.5% of the E2 dose. Virtually no methane or CO_2 were generated under sterile conditions. Based on these laboratory studies, it would be expected that very little E2 or T would be released into the environment by land application of lagoon waste.

AGRO 119
Degradation of zeranol by phytoremediation
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The environmental fate of zeranol, an estrogenic-like growth promoter used in beef production, is not well understood. We are exploring the possibility of applying phytoremediation to remove zeranol from agricultural runoff and manure lagoons because it is potentially harmful to aquatic organisms. Specifically, we are evaluating its degradation by soybeans, poplars, and water hyacinths in hydroponic and soil experiments. We observed a rapid decrease in zeranol concentrations in hydroponic media exposed to hybrid poplars. Concurrent to its degradation an unknown has been identified by reverse phase high-pressure liquid chromatography. The unknown was not observed in control and blank replicates. The chromatographic peak for this metabolite surprisingly elutes after the parent compound, which suggests that it is more hydrophobic in nature. We are currently identifying this unknown metabolite using liquid chromatography-mass spectrometry and delineating the mechanisms responsible for zeranol loss, e.g., degradation or sorption to roots.

AGRO 120
Identification of key enzymes involved in the biosynthesis of the allelochemical sorgoleone
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Plant-derived natural products such as allelochemicals represent attractive alternatives to synthetic herbicides. The ability to engineer or manipulate their biosynthesis in crop plants could significantly reduce the reliance on synthetic herbicide input in future agricultural systems. The allelopathic benzoquinone sorgoleone, whose biosynthesis originates in root hair cells of all *Sorghum* species, acts as a potent, broad-spectrum inhibitor effective against many agronomically-important weeds and holds particular promise for development as a natural product-based herbicide. To clone genes involved in the biosynthesis of this compound, an EST (expressed sequence tag) data set derived from isolated *Sorghum* bicolor root hair cells was mined. Candidate sequences representing all of the required enzyme classes were identified including two alkylresorcinol synthase-type polyketide synthase (PKS) enzymes which have now been functionally characterized. The involvement of these PKSs in sorgoleone biosynthesis has been confirmed via RNA interference-based inhibition of the pathway in transgenic sorghum.

AGRO 121
Control of coleopteran insect pests through RNA interference
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Commercial plant biotechnology solutions for controlling lepidopteran and coleopteran insect pests on agricultural crops depend on the expression of insecticidal proteins derived from the entomopathogenic bacterium *Bacillus thuringiensis* (Bt). The deployment of insect control traits with a mode of action distinct from Bt proteins would be valuable for insect resistance management programs. Towards this end, we demonstrate that RNA interference (RNAi) can be triggered in a number of coleopteran species, most notably the western corn rootworm (WCR) *Diabrotica virgifera virgifera* LeConte, upon ingestion of dsRNAs (double-stranded RNA) supplied in an artificial diet. This results in target-specific gene suppression, larval stunting, and mortality. Furthermore, transgenic corn plants engineered to express WCR dsRNAs show a significant reduction in WCR feeding damage in a growth chamber assay, providing proof-of-concept that the RNAi pathway can be exploited to control insect pests via *in planta* expression of a dsRNA.

AGRO 122
Engineering broad-spectrum root-knot resistance in crops using RNAi silencing of a root-knot nematode parasitism gene
***Richard S. Hussey** and Guozhong Huang, Department of Plant Pathology, University of Georgia, Athens, GA 30606*

Secreted proteins coded by parasitism genes expressed in esophageal gland cells mediate infection and parasitism of plants by root-knot nematodes. An essential parasitism gene, designated as *16D10*, encodes a conserved root-knot nematode secretory peptide that stimulates root growth and functions as a ligand for a plant transcription factor. Plants were engineered to silence this parasitism gene in root-knot nematodes using RNA interference (RNAi). *In planta* expression of *16D10* dsRNA (double stranded RNA) in *Arabidopsis* resulted in resistance against the four common root-knot nematode species (*Meloidogyne* spp.). No known natural resistance gene elicits this wide and effective range of root-knot nematode resistance. Genetically modifying crop cultivars to express dsRNA that silence essential nematode parasitism genes represents a viable and flexible means to develop novel durable broad-spectrum root-knot nematode resistant crops. This strategy could also be used to develop root-knot nematode resistant crops for which natural resistance genes have not been found.

AGRO 123
Enhancing the value of cottonseed as a source of feed and food by RNAi-mediated, selective and substantial reduction in seed-gossypol
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In 2006, 44.2 million metric tons (MMT) of cottonseed was produced worldwide as a by-product of 24.8 MMT of cotton lint production (FAOSTAT). This amount of cottonseed, containing nearly 10 MMT of protein, can potentially provide the protein requirement for 500 million people/yr at a rate of 50 g protein/d. However, gossypol, a toxic terpenoid present in the glands, renders cottonseed unfit as feed for non-ruminant animals and as food for human beings. A major portion of this abundant agricultural resource is utilized simply as feed for ruminant animals either as whole seeds or as meal following oil extraction. Therefore, elimination of gossypol from cottonseed has been a long-standing goal of geneticists. We have successfully used RNAi to disrupt gossypol biosynthesis in the seed by interfering with the expression of the -cadinene synthase gene during embryo development. We demonstrate that it is possible to reduce significantly the levels of cottonseed-gossypol in a stable and heritable manner. Results from enzyme activity and molecular analyses on developing embryos were consistent with the observed phenotype in the mature cottonseeds. Most importantly, the levels of gossypol and related terpenoids that are derived from the same pathway were not diminished in the foliage and floral parts of these plants and thus remain available for defense against insects and diseases. Thus, a targeted genetic modification, applied to an under-utilized agricultural byproduct, provides a mechanism to open up a new source of nutrition for hundreds of millions of people.

AGRO 124
High lysine corn generated by endosperm specific suppression of lysine catabolism using RNAi
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Corn grain is limited in lysine content, therefore, synthetic lysine supplements are added to cornmeal-based, animal feed rations. The development of biotechnology, combined with the understanding of plant lysine metabolism, provides an alternative solution for increasing corn lysine content through genetic engineering. We report that by suppressing lysine catabolism, transgenic maize kernels accumulated a significant amount of lysine. This was achieved by RNA interference (RNAi) through the endosperm-specific expression of an inverted-repeat sequence targeting the maize bifunctional lysine catabolic enzyme lysine-ketoglutarate reductase/saccharopine dehydrogenase (LKR/SDH). We also report no systemic spreading of the short interfering RNA molecules (siRNA) or the presence of transitive RNAi, indicating that we can limit RNAi-mediated suppression to the endosperm tissue. The practical use of RNAi for plant genetic engineering will be discussed.

AGRO 125
Intragenic options for specialty crop improvement: High health and quality without foreign DNA
Kathy Swords*, Jingsong Ye, Craig Richael, Hua Yan, and Caius Rommens, Plant Sciences, J.R. Simplot Company, 5369 W. Irving Street, Boise, ID 83706*

Despite the broad acceptance of GM traits in the large acreage crops destined for feed, fiber, and highly processed products, genetic modification of specialty crops has been relatively stifled. Recognizing consumer sensitivity to modification of food crops, we developed new methods to improve quality by only modifying the plant's own genome. This Precise Breeding™ approach is readily coupled with insights gleaned from genomics and metabolomics research. Our focus on improvements beneficial to the consumer and production chain has yielded an intragenic potato with multi-gene trait silencing that delivers boosted quality, reduced cold-sweetening, improved flavor, and low acrylamide in the final fry product. Furthermore, by balancing potato gene over- and under-expression, we have dramatically boosted levels of the potato antioxidant, kaempferol, as a high-health consumer trait.

AGRO 126
Excel spreadsheet incorporating statistical tools for determining selection of regression models for analysis of E-fate datasets
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Many discussions on methods for fitting numerical solutions to experimental data sets have occurred over the past few years. Recently, a paper titled “Statistical tools for determining appropriate selection of regression models for analysis of environmental fate datasets” has been published. In that paper an approach was developed based on statistical fitting and diagnostics for determining appropriate kinetic models. In the paper, it was demonstrated that not only does the appropriate model have to be identified, but the appropriate transformation function also needs to be identified so that modeling can be done in the appropriate scale. Residual diagnostic procedures were proposed to identify the appropriate scale, and statistical testing procedures have been proposed to select the appropriate model within that scale. The focus of this presentation is implementation of the tools and methods in an easy to use, easily-distributable Excel tool that performs the fitting procedures and carries out the statistical diagnostics presented in the earlier paper.

AGRO 127
Mobility, longevity, and activity of fipronil at a rate labeled for the prevention of termite infestation in structures
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The mobility, longevity, and termiticidal activity of fipronil (Termidor SC™, BASF Corporation) at the termiticidal label rate for perimeter soil treatment were examined for 30 months in 45 x 10 cm (i.d.) PVC pipes. Vegetated and non-vegetated pipes were used, each receiving 200 mL water per week. Pipes were cut at 3-mo intervals into six 7.5-cm sections, the top two sections of which contained the treated soil. The soil was assayed for fipronil concentration, soil moisture, and insecticidal activity. Fipronil concentration in the treated soil decreased more rapidly in the top section than in the section immediately below, and decreased more rapidly for the first 18 months than afterward. Soil from the two treated depths remained toxic to termites in 3-d bioassays for the duration of the test. Toxicity of soil from untreated soil depths increased over time, indicating movement of fipronil into untreated soil depths, but toxicity generally decreased with increasing depth.

AGRO 128
Tillage-system impact on surface runoff and interflow transport of selected herbicides at the field scale
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Worldwide interest in conservation-tillage (CsT) of agricultural soils is increasing. Potential benefits include reductions in erosion and surface runoff of agrichemicals, increases in soil organic carbon content, and more efficient water use. However, net benefits on soil water availability and the potential for negative consequences due to leaching of agrichemicals remain poorly documented. For the past ten years our research group has focused on field-scale assessment of strip-tillage management in the Southern Atlantic Coastal Plain (USA) during rotational cotton and peanut production. Strip-tillage (ST) is a form of CsT which involves planting into strips tilled in cover crop surface mulch. ST is favored by farmers in the region. In this presentation, we describe measurements of surface runoff and interflow transport of cotton preemergence herbicides. Generally, CsT management contributed to reduced surface runoff but increased edge-of-field subsurface losses. Implications will be discussed in the context of the South Georgia landscape.

AGRO 129
Management and modeling: Tools to improve water quality
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Agricultural, urban, and suburban sources contribute to the contamination of surface waters, which has been observed by the detection of pesticides, excess nutrients, industrial pollutants, antibiotics, pharmaceuticals, and personal care products in both natural waters and treated wastewaters. The use of pesticides and fertilizers in highly-managed turf has raised questions concerning their impact on surrounding water resources and the contribution of managed turf systems to surface water contamination. Due to the time and expense involved in obtaining real-world measurements, computer simulation prediction modeling is a desired approach to estimating runoff volume as well as chemical composition and transport with runoff. In this study, measured experimental data was collected from creeping bentgrass plots managed as a golf course fairway under different management practices. Runoff from both simulated and natural precipitation events was collected and analyzed for pesticide and nutrient content. Hydrological transport models were tested to see how predictions of both runoff volume and runoff chemistry agreed with measured data. This discussion will focus on the importance of various input parameters to the performance of the models for the turf system under investigation and the influence of management practices to reduce chemical transport.

AGRO 130
Pilot study to investigate options for catchment scale modeling of pesticides
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A pilot study has been undertaken to investigate the accuracy of catchment-scale, modeled, pesticide predictions in the UK. Three catchments in the Anglian region of the UK have been studied: the Waveney, Yare, and Wensum. These catchments have been intensively monitored over the past year as part of the on-going England Catchment Sensitive Farming Delivery (ECSFDI); and as a consequence weekly monitored pesticide concentrations are available for the past year. Two catchment level models, the Soil and Water Assessment Tool (SWAT) and Pesticide Root Zone Model/Riverine Water Quality model (PRZM/RIVWQ) have been used to generate results. SWAT is a river basin scale model developed to quantify the impact of land management practices in large, complex watersheds. PRZM, is a field-scale model developed and used to estimate pesticide leaching and runoff. PRZM is linked with RIVWQ, a watershed-based model, to model impact of agro-chemical application and management practices on surface water. Results from these two models, will be compared with monitoring data and modeled predictions from a third pesticide model, CATCHIS.

AGRO 131
Investigation of long-term trends in atrazine residues in raw waters supplying Midwest community water systems
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Atrazine residues in drinking water supplies have been monitored for over 15 yrs and provide a rich dataset. Temporal trends were examined using atrazine residue data from raw surface waters supplying 103 Community Water Systems (CWS) primarily located in areas of high atrazine use and which also had 5 - 13 yrs of monitoring data measured between 1994 and 2006. Time-weighted annual mean (TWAM) and annual maximum 90 day rolling average (M90D) atrazine concentrations were calculated for each CWS-year and were analyzed using a mixed effect model. The dataset was stratified into subsets to evaluate potential trend changes between strata of different data magnitudes, monitoring durations, and time periods. There was little effect of monitoring duration on the monotonic decline trend, and few differences in trend parameters were seen between the 1994-1999 and 2000-2006 CWS monitoring periods. Results show significant and negative concentration-time trends for both variables (TWAM and M90D).

AGRO 132
State-dependent actions of pyrethroid insecticides on voltage-gated sodium channels
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Pyrethroids disrupt nerve function by altering the kinetic transitions between closed and open states of voltage-gated sodium channels that underlie the generation of nerve action potentials. Recent studies of pyrethroid action on cloned insect and mammalian sodium channel isoforms show that pyrethroids may preferentially bind to channels either in the closed or open state; the observed preference is determined by both the structure of the pyrethroid and the particular sodium channel isoform modified. This presentation will review the evidence for state-dependent modification by pyrethroids. It will also consider the implications of state-dependent effects for the development and testing of models of the pyrethroid binding site and the assessment of the cumulative risks of exposure to multiple pyrethroids.

AGRO 133
Identification of residues in the cockroach sodium channel critical for the binding and action of pyrethroid insecticides
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Pyrethroid insecticides are among the earliest neurotoxins that were found to act on voltage-gated sodium channels. They prolong the opening of sodium channels primarily by inhibiting deactivation, resulting in a slowly-decaying tail current associated with repolarization. Our previous studies showed that F1519 in the sixth segment of domain III (IIIS6) of the cockroach sodium channel is a key residue of the pyrethroid-binding site. To determine whether additional residues in IIIS6 are involved in the binding and action of pyrethroids, we made alanine substitutions of 21 residues flanking F1519 (10 upstream and 11 downstream of F1519) and examined the sensitivity of the mutant channels to deltamethrin (a pyrethroid insecticide). Our results reveal

that several additional residues in IIIS6 are critical for the binding and action of pyrethroids.

AGRO 134
Role of the sixth segment of domain IV of the cockroach sodium channel in the action of sodium channel-blocker insecticides
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Sodium channel-blocker insecticides (SCBIs), such as indoxacarb (DPX-JW062) and its bioactive metabolite, *N*-decarbomethoxyllated JW062 (DCJW), are a new class of insecticides with a mechanism of action different from those of other insecticides that target sodium channels. SCBIs block mammalian sodium channels in a manner similar to local anesthetics (LA) such as lidocaine. Several residues, particularly F1579 and Y1586, in the sixth transmembrane segment (S6) of domain IV (IV) of rat $Na_v1.4$ sodium channels are critical for the action of SCBIs and LAs and may form part of overlapping receptor sites. However, the binding sites for SCBIs and LAs in insect sodium channels remain undefined. We conducted systematic alanine scanning mutagenesis of 12 residues in IVS6 of the German cockroach sodium channel $BgNa_v1-1$, including F1817 and Y1824, which correspond to F1579 and Y1586 of rat $Na_v1.4$ sodium channels. We are currently examining the effects of SCBIs and lidocaine on the resultant mutant channels expressed in *Xenopus* oocytes.

AGRO 135
PKC-dependent phosphorylations modify the action of CS-syndrome pyrethroids on rat brain N-type ($Ca_v2.2$) voltage-sensitive calcium channel
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Isolated presynaptic nerve terminals (synaptosomes) were used to evaluate the action of a choreoathetosis-salivation (CS)-syndrome pyrethroid (deltamethrin) by measuring calcium influx and endogenous neurotransmitter (*L*-glutamate) release. Deltamethrin stimulated both calcium influx and *L*-glutamate release in a stereospecific and concentration dependent fashion, both of which were blocked by ω-conotoxin GIVA (Group IVA). These findings indicate that $Ca_v2.2$ is a target site for deltamethrin and this result is consistent with the observed *in vivo* release of neurotransmitter at the onset of the convulsive symptoms caused by CS-syndrome pyrethroids. Voltage clamp electrophysiological studies using $Ca_v2.2$ and its β-3-subunit coexpressed in *Xenopus* oocytes validated such an action. Deltamethrin increased the rate of activation, prolonged inactivation, and reduced peak current. Site-directed mutagenesis of threonine 422 to glutamic acid (T422E, one of five PKC-dependent phosphorylation sites) resulted in a channel that acted as if it were permanently phosphorylated (i.e., resulted in an increased probability of opening during depolarization and a reduced inhibition by the βγ subunit of heterotrimeric G-protein). Deltamethrin treatment of T422E enhanced peak current ~50% over ethanol-treated controls with an EC_{50} of 9.8×10^{-11} M. Deltamethrin also resulted in a significant slowing of channel deactivation when PKC-dependent phosphorylation was evoked by treatment with the phorbol ester PMA (phorbol 12-myristate 13-acetate). This effect was not seen with either wild type or T422E mutated channels. Thus, $Ca_v2.2$ is modified by deltamethrin but the resulting perturbations are dependent upon its PKC-dependent phosphorylation state.

AGRO 136
Molecular mechanisms and monitoring of permethrin resistance in human head lice
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Head lice resistance to permethrin is mainly conferred by the kdr trait, a voltage-sensitive sodium channel (VSSC) insensitivity factor. Three VSSC mutations (M815I, T917I, and L920F) have been identified. Functional analysis of the mutations using the house fly VSSC expressed in *Xenopus* oocytes revealed that the permethrin sensitivity is reduced by the M827I and L932F mutations when expressed alone but virtually abolished by the T929I mutation, either alone or in combination. Thus, the T929I mutation is primarily responsible for permethrin resistance in head lice. Comparison of the expression rates of channel variants indicates that the M827I mutation may play a role in rescuing the decreased expression of channels containing T929I. A step-wise resistance monitoring system has been established based on molecular resistance detection techniques. Quantitative sequencing (QS) has been developed to predict the VSSC mutation frequency in head lice at a population basis. The speed, simplicity, and accuracy of QS made it an ideal candidate for a routine primary resistance monitoring tool to screen a large number of wild louse populations as an alternative to conventional bioassay. As a secondary monitoring method, real-time PASA (rtPASA) has been devised for more precise determination of low resistance allele frequencies. To obtain more detailed information on resistance allele zygosity, as well as allele frequency, serial invasive signal amplification reaction (SISAR) has been developed as an individual genotyping method. Our approach of using three tiers of molecular resistance detection should facilitate large-scale routine resistance monitoring of permethrin resistance in head lice using field-collected samples.

AGRO 137
Regulation of insect P450 expression: Genomic insights
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Changes in the expression of P450 genes can have a profound influence on the level of insecticides reaching their target, as shown in many cases by the development of resistance. In well documented cases, increased production of one or a few P450 enzymes can lead to resistance. The coordinated expression of several P450 genes has been more difficult to study. The increasing availability of genomic tools and insights is now being put to use and we will present data on patterns of P450 expression in pyrethroid resistance, as well as on mechanisms of P450 gene regulation in noctuid pests.

AGRO 138
Keynote Address. The evolving of the paradigm of agriculture as a supplier of energy and chemicals
***Larry P. Walker**, Department of Agricultural and Biological Engineering, Cornell University, Ithaca, NY 14850*

Over one-hundred years ago, agriculture played an important role in providing energy, lubricants, dyes, surfactants and other industrial chemical. This role was significantly reduced with the evolution of the fossil fuels industry that has driven global human development for the bulk of the 20th century. However, this dominance is not likely to continue given the global challenges of tight petroleum supplies, climate change and global economic competition. These global challenges will creating opportunities for agriculture to return as an important resources base that will provide green energy and industrial chemicals for continue human development. These opportunities will be realized through exploiting many of the scientific and technological breakthroughs of the late 20th century, development of different business paradigm for securing energy and industrial materials, and through confronting some of the sustainability challenges associated with biofuels and bioproducts production.

AGRO 139
Biomass production and processing economics: Implications for cost of reducing carbon emissions via biofuel
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With the growing emphasis on sustainable energy and energy independence, cellulosic biomass has been advocated as a potential source for biofuel and a way to reduce greenhouse gas (GHG) emissions. We have developed an economic model to evaluate the feasibility of different cellulosic biomass feedstocks and to estimate the subsidy necessary to create a biomass market using four feedstocks: stover, switchgrass, miscanthus, and woody biomass. We first analyzed a cellulosic ethanol plant to determine the maximum amount that the biorefinery can pay, or the marginal willingness to pay (WTP) for the last dry ton of biomass delivered to the plant. Next, we estimated the minimum amount the biomass producer is willingness to accept (WTA) per dry ton of delivered biomass. The WTA is equal to the total cost to the supplier for delivering the last dry ton to the plant. For a biomass-based ethanol market to exist, the biorefinery's WTP must be at least as large as the supplier's WTA. Under current biomass processing and production technology and costs, the WTA is significantly greater than the WTP, so no market for biomass as an ethanol feedstock exists. Given the differential between the WTA and the WTP as well as the estimated carbon emissions reduction per ton of biomass feedstock or per gallon of ethanol, we estimated the subsidy cost per ton of carbon necessary to sustain a market or make the biomass-based ethanol industry viable.

AGRO 140
A landscape vision for sustainable bioenergy feedstock production
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Feedstock production for biofuel and other bioproducts is poised to rejuvenate rural economies but may lead to long-term degradation of soil resources or other adverse and unintended environmental consequences if the practices are not developed in a sustainable manner. This presentation will examine several of the initial assumptions regarding biomass production, discuss the multi-location research being conducted by the ARS Renewable Energy Assessment Project (REAP) team to develop sustainable crop residue harvest strategies, and present a vision for lignocellulosic feedstock production that simultaneously addresses water quality, carbon sequestration, wildlife habitat, aesthetics, recreation, community development, and other issues. Our vision is for a landscape management plan that utilizes a variety of plant species, conversion technologies, and co-product utilization in an integrated system rather than trying to satisfy our nation's energy appetite with current practices or single “one-size fits all” solutions.

AGRO 141
Sustainable bioenergy production in the Chesapeake Bay agricultural landscape: Potential and peril
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The current focus on corn-based ethanol production, while it has stimulated the farm economy through increased prices for grain crops, risks unsustainable side effects associated with increased pollution by nutrients, sediments, and pesticides, increased irrigation demands, and conversion of critical conservation areas into row crop production. The Chesapeake Bay Commission recently published a report estimating that increased corn acreage associated with biofuels will increase nitrogen loading to the Chesapeake Bay by five million pounds annually, unless conservation practices for corn land are substantially increased. In this circumstance, it is important to clearly evaluate the environmental effects of biofuels production, and to promote a diverse portfolio of environmentally and economically sustainable biofuel products. Positive sum practices under investigation include the use of winter small grains as ethanol feedstock, development of conservation crops such as switchgrass for cellulosic ethanol production, on-farm pyrolysis of chicken manure, bio-diesel production from waste chicken fat, and processing of wastewater byproducts.

AGRO 142
Can biofuels be sustainable in an unsustainable agriculture?
Daniel De La Torre Ugarte *and Chad M. Hellwinckel, Agricultural Policy Analysis Center, Department of Agricultural Economics, University of Tennessee, Knoxville, 325-A Morgan Hall, Knoxville, TN 37996-4519*

The expansion of biofuels has increased the utilization of grains, oilseed by-products, and sugar. Coincidentally, prices of agricultural commodities have substantially increased. Changes in land use driven by high prices are pressuring the expansion of agriculture into environmentally sensitive areas. Such expansion is leading some to question the sustainability of biofuels as a desirable source of energy. However, the increase utilization of agricultural commodities for biofuels can not completely explain the higher prices, indicating that there are other structural forces in agriculture, besides biofuels production, that need to be included in the debate. Land use, crop mix, crop production methods, and changes in food consumption patterns, must also be part of the biofuels debate. This presentation situates biofuels within the context of what is happening in agriculture and discusses avenues to enhance the sustainability of agriculture and biofuels.

AGRO 143
Use of structural analysis (QSAR) to predict fish bioconcentration factors for pesticides
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The focus of this research was to develop a model based solely on molecular descriptors capable of predicting fish bioconcentration factors (BCF). A fish BCF database was developed from high-quality, government-reviewed studies of pesticides that used the same laboratory protocol and the same fish species, *Lepomis macrochirus*. A commercially-available software program was used to create a quantitative structure activity relationship (QSAR) from the BCF values for 93 molecules. An additional 17 molecules were used to test the accuracy of QSAR model predictions for a variety of pesticide classes. The regression of the validation dataset of measured versus predicted log BCF values yielded a regression coefficient of 0.88. Based on results from this research, the ability to predict BCF by a QSAR regression model is improved using a fully structurally derived model based solely on structural data, like the number of atoms of a given type (e.g., $-CH_3$), or the local topology of each atom as derived from electron counts. Such descriptors provide insightful information on a molecule's potential BCF behavior in aquatic systems.

AGRO 144
Assessing the importance of ionization state during environmental risk assessment of pharmaceuticals
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Several pharmaceuticals that are likely to enter the environment are ionizable compounds. Although a multitude of variables will influence their ionization state in aqueous environments, the pH of the receiving system is perhaps the most pivotal. While abiotic factors predominantly determine baseline pH, biological components of ecosystems are also important to consider. Photosynthesis removes carbon dioxide, which may culminate in an increase in surface water pH during a photoperiod. Ionization state is integral to risk assessment as it influences the solubility as well as the bioavailability of contaminants. Unionized forms are less polar and have a greater propensity to cross cellular membranes, and hence are often regarded as posing a greater risk to biota. We shall present the results of toxicity tests completed over environmentally-relevant, surface-water pH gradients to assess whether adjustment factors may obviate uncertainty related to risk assessment.

AGRO 145
Higher tier exposure modeling of veterinary pharmaceuticals: A UK case study
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Veterinary medicines are present in treated animal manure which is land applied as a soil amendment. Therefore, there is a need to examine the potential for adverse environmental effects. The regulatory tool VetCalc provides environmental scenarios for use across the EU to address a range of agricultural and environmental conditions and incorporates models to simulate the fate of products in ground and surface water situations. VetCalc can also be linked to the FOCUS modeling framework used for pesticide risk assessment. FOCUS allows for factors such as long-term weather and refined application timing. However, FOCUS is also scenario based, with a set of pre-determined environmental situations that may not apply well to all locations. A UK case study for an antibiotic used in the treatment of poultry is presented in which each phase of the UK VMD regulatory process is illustrated. This includes running the standard VetCalc tool and linking VetCalc to FOCUS. Finally, GIS-based refined environmental parameters were then incorporated into the FOCUS/PRZM model to generate a scenario which best represents the environmental situation for the product.

AGRO 146
Experiences with NHDPlus and pesticide exposure assessment
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The National Hydrography Dataset (NHDPlus) was released in a 2006 workshop with the intent to communicate the structure and content of the newly enhanced data. These data, comprised of hydrologically-connected stream networks and corresponding drainage basins with associated attributes, provide a valuable foundation for many aspects of aquatic pesticide exposure assessments. Recently a second workshop in February 2008 was held, focusing on applications of the data and user experiences. This presentation summarizes our experiences using the NHDPlus data for a number of exposure related issues including; endangered species assessments, refined drinking water modeling scenarios, and appropriate watershed distribution and selection. Practicalities of using the data and tools over large geographic extents will also be discussed. Incorporation of cross-platform programming and automation was utilized to achieve the necessary efficiency in large volume data processing.

AGRO 147
New approaches to agrochemical monitoring studies: Update on the atrazine ecological exposure monitoring study
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In 2003, EPA requested a study to monitor small watershed streams to understand the magnitude and duration of potential atrazine exposures. This spatially extensive 40 site study generated over 80 site years of intensive atrazine monitoring data. In order to assess the impact of atrazine exposures on primary production, measured chemographs were evaluated using the Comprehensive Aquatic Systems Model parameterized for small Midwest streams (CASM_Atrazine). EPA used effects and exposure information from 32 microcosm/mesocosm studies to set a screening level of concern (LOC) using CASM_Atrazine. Data analyses show that 38 sites did not approach the LOC; however, two subwatersheds in north eastern Missouri characterized by continuous very shallow claypans on sloping cropped land experienced LOC exceedances. Detailed spatial analyses have shown that these watershed characteristics co-occur infrequently across the Midwest. Data generation continues at these two locations and in Nebraska where three monitored streams were frequently too dry to take samples.

AGRO 148
Comparison of two water quality models for estimation of aquatic system bioaccumulation
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Two modeling methods were evaluated to determine their appropriateness for predicting the potential of molecules to bioaccumulate in a multi-trophic level aquatic system. A new, dynamic, daily-time-step, water quality and food chain model was configured and run. Results from the new approach were compared to an established water quality model using the same food chain approach. Exposure was based on agricultural use of the compounds in a terrestrial system with subsequent unintentional introductions into an aquatic environment. Results from this evaluation indicate that the new water quality modeling approach was an improvement over the established model for differentiation of compounds that might be considered bioaccumulative. Additionally, results from this work indicate that static modeling approaches are inadequate for evaluation of compounds with episodic exposure profiles specifically those resulting from use in agricultural production systems.

AGRO 149
A synergistic interaction between the two major mechanisms of permethrin resistance in mosquitoes, cytochrome P450 detoxification and *kdr*
Jeffrey G. Scott, *Melissa C. Hardstone, and Cheryl Leichter, Entomology Department, Cornell University, Comstock Hall, Ithaca, NY 14853*

The evolution of insecticide resistance in mosquitoes is a growing and world-wide problem. The two major mechanisms that confer resistance to permethrin in *Culex* mosquitoes are target site insensitivity (i.e., *kdr*) and enhanced detoxification by cytochrome P450 monooxygenases. Interactions of resistance mechanisms are important to investigate as they dictate the level of resistance in the field and how they interact may be a determining factor in the speed at which resistance evolves. Using three strains of mosquitoes and crosses between these strains, we assessed the relative contribution of the two mechanisms to permethrin resistance, individually and when present together. We found that for all combinations tested, *Cx. p. quinquefasciatus* exhibited greater than additive interactions between P450 detoxification and *kdr*, whether the resistance alleles were homozygous or heterozygous. These results provide a basis for further analysis of the evolution and maintenance of insecticide resistance in mosquitoes.

AGRO 150
Nicotinic acetylcholine receptors and resistance to neonicotinoids.
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Nicotinic acetylcholine receptors (nAChRs) play an important role in excitatory synaptic transmission in both vertebrates and invertebrates and are the primary target site for the neonicotinoid insecticides. These compounds display a high selectivity towards insect nAChRs and are particularly active against a range of sucking pests (mainly *Hemiptera*) and certain beetles. Despite their intensive use over more than 15 years, they have generally proved to be relatively resilient to the development of resistance, although this may be changing as several cases of resistance have been reported recently including the first example of target site

resistance in brown planthoppers. This talk will discuss: 1) the current status of neonicotinoid resistance in Hemipteran pests; 2) the characterisation of nAChR subunit mutations that cause resistance in planthoppers; and 3) structure-based modelling studies of the insect nAChR to investigate some of the key residues that are likely to be involved in neonicotinoid selectivity and resistance.

AGRO 151
Sulfonyl urea receptor in insect cuticular epidermis is likely the insecticidal target of benzoylurea type insecticides
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To study the action mechanism of diflubenzuron (Dimilin®), we tested the hypothesis that the action site of diflubenzuron is a sulfonylurea receptor (SUR) operating in cuticular epidermis. When given to immature insects, glibenclamide, a typical SUR agonist, clearly caused toxicity, with a typical symptom of molting abnormality that is very similar to those induced by diflubenzuron. Its LD_{50} (0.47 µg/nymph) was approximately 2.8 times the value obtained for diflubenzuron (0.17 µg/nymph, topical) in German cockroach, *Blattella germanica* (L.). However, in terms of the inhibitory activities on chitin synthesis, in isolated integuments glibenclamide showed an identical potency to diflubenzuron in *B. germanica* nymphs. A competitive binding assay with [^{3}H]-glibenclamide and unlabeled diflubenzuron clearly established that the latter is capable of competitively displacing the former radioligand. These results support our conclusion that the sulfonylurea receptor (SUR) is likely the target of diflubenzuron in inhibition of chitin synthesis in these two insect species.

AGRO 152
Ligand-gated chloride channel gene family of *Drosophila*
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Heteromultimeric chloride channels gated by GABA (γ-aminobutyric acid), glutamate, and histamine are known to mediate synaptic inhibition and regulate cellular excitability in insects and other invertebrates. These receptors are functionally and pharmacologically similar to inhibitory GABA and glycine receptors of vertebrates. Insect GABA- and glutamate-gated chloride channels are also important targets for the action of insecticides. Four genes that encode subunits of ligand-gated chloride channels have been identified in *Drosophila melanogaster*. Each of these subunits appears to be a component of a distinct receptor, but the native subunit compositions of none of the receptors containing these subunits is known. Therefore, the existence of additional members of the ligand-gated chloride channel subunit gene family in *Drosophila* is predicted. Here, we identify seven novel members of this gene family in the *Drosophila* genome and compare the primary structures of their encoded proteins to previously described ligand-gated chloride channel subunits.

AGRO 153
Glutamate-activated chloride channels: Unique fipronil targets present in insects but not in mammals
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We have found that fipronil's selective toxicity is due to higher sensitivity of cockroach GABA (γ-aminobutyric acid) receptors than rat $GABA_A$ receptors and due, more importantly, to a high sensitivity of cockroach glutamate-activated chloride channels (GluCls) which are absent from mammals. The IC_{50}s of fipronil block were 30 nM in cockroach GABA receptors and 1600 nM in rat $GABA_A$ receptors. Moreover, cockroach neurons had GluCls with low IC_{50}s. Two types of glutamate-induced chloride current were recorded: desensitizing and non-desensitizing currents with fipronil's IC_{50}s of 800 nM and 10 nM, respectively. The non-desensitizing and desensitizing currents were selectively inhibited by trypsin and polyvinylpyrrolidone, respectively. In conclusion, the cockroach GABA receptors are more sensitive to fipronil than the rat GABAA receptors, and that the GluCls, which are absent from the rat, are highly sensitive to fipronil. Insect GluCls are an important target site responsible for a selective toxicity. (Supported by NIH grant NS14143.)

AGRO 154
Role of GABA and glutamate receptors in susceptibility and resistance to chloride channel blocker insecticides
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A point mutation in the GABA (γ-aminobutyric acid) receptor, chloride-channel pore conferring resistance to dieldrin and other polychlorocycloalkane (PCCA) insecticides is widespread and persistent in insect populations, so it is surprising that fipronil, which also binds at the PCCA site, remains effective in controlling dieldrin-resistant populations. Fipronil and its major sulfone metabolite also potently block GluCls (glutamate-activated chloride channels) which may play a role in the lack of serious fipronil resistance. In the present study, we examine the action of fipronil and its sulfone metabolite on native GABA receptors and GluCls of susceptible and dieldrin-resistant German cockroaches, to provide a better understanding of the effect of the *Rdl* mutation on the insecticide sensitivity of these three targets and its role in resistance. A survey of other chloride-channel-blocking insecticides shows that fipronil is unique in its multi-site action in insects. GluCls do not occur in vertebrates and are thought to contribute to fipronil's insect selectivity.

AGRO 155
Anion channels/transporters as targets for new insecticides and nematicides
Jeffrey R. Bloomquist *and Dhana Raj Boina, Department of Entomology, Virginia Polytechnic Institute and State University, 216 Price Hall, MC 0319, Blacksburg, VA 24061*

Four anion transporter (AT) blockers, DIDS (4, 4'-diisothiocyanatostilbene-2, 2'-disulfonic acid), 9-AC (anthracene-9-carboxylic acid), NPPB (5-nitro-2-(3-phenylpropylamino) benzoic acid), and IAA-94 (indanyloxy acetic acid) were evaluated for insect and nematode control. All the AT blockers showed slowly developing toxicity against second-stage larvae of *Meloidogyne incognita* and adults of *Caenorhabditis elegans*. Symptoms of AT blocker toxicity observed in *C. elegans* adults were increased pharyngeal muscle contractions and decreased locomotion. Exposure of *C. elegans* to double-stranded RNA (dsRNA) of *ceclc-1* and *ceclc-2* (genes coding for voltage-sensitive chloride channels) decreased their expression in F1 progeny. Reduction in expression of *ceclc-2* alone or together with *ceclc-1* significantly increased pharyngeal contractions and decreased locomotion, suggesting that AT blockers nematicidal activity primarily comes from inhibition of *ceclc-2* channels. AT blockers inhibited larval growth, increased the developmental time, and decreased survival of diet-exposed *Ostrinia nubilalis* (European corn borer). All the AT blockers decreased midgut alkalinity and inhibited chloride ion transport from midgut lumen into epithelia in fifth-instar larvae when fed for 3 h on treated diet. Positive correlations observed among growth, midgut alkalinity, and midgut Cl^- transport in AT blocker-fed larvae suggested that inhibition of chloride/bicarbonate exchangers decreased midgut alkalinity, affecting digestion and resulting in the observed lethal and sublethal effects.

AGRO 156
Enhancement and stabilization of biomass feedstock quality through utilization/recycling biological waste streams
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It can be argued that the success, sustainability, and security of a U.S. biofuels industry will not be based on only one or two biomass feedstocks available across the U.S. Rather, biomass production logistics (availability, supply, timeliness) and economics will in all likelihood demand that a core of biomass materials particular to given U.S. geographical regions will be feedstocks into bioconversion facilities for a year-round operation. With estimated annual supplies of 120, 377, and 446 million dry tons, respectively, forestry residues, agricultural crop residues, and dedicated energy crops will comprise this core. The variability in the feedstock properties can be minimized, their thermochemical value enhanced, and the consistency of the biofuel produced be assured by mixing with biological waste streams such as food processing residuals. This processing mindset opens a great opportunity to integrate all biomass including forestry, agricultural, and food processing residuals for bioenergy/biofuels production.

AGRO 157
Turning waste into energy: Biogas production on dairy farms
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Much of today's animal production is practiced in highly concentrated facilities known collectively as Confined Animal Feeding Operations (CAFOs). In some cases, dairy and swine, the manures are collected in a liquid form and are readily utilizable for the production of biogas through anaerobic digestion treatment of the waste. Many environmental benefits from anaerobic digestion beyond the production of biogas exist including odor reduction, reduction in COD (chemical oxygen demand), and conversion of organic nitrogen to more readily available inorganic forms. In states with strong net metering laws, large CAFOs are able to profit from generating electricity from the biogas they generate. To date, smaller operations have not been able to generate a positive economic benefit from anaerobic treatment of their waste stream. Work is needed to help small producers be more economically competitive through improvements in process design, process temperature, and possibly accepting/growing other feedstocks such as food wastes from local facilities or other biomass produced on the farm.

AGRO 158
Estimating regional water use with changing cropping patterns
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There are about 4 million acres of cropland in the Delta region of northwest Mississippi. Currently 3 million of those acres are irrigated with groundwater. The groundwater levels are declining in some areas due to withdrawals that exceed natural recharge. The number of acres of corn grown in the area is expanding. Corn uses more water than the cotton and soybeans than it replaces. A regional, water-demand model was developed combining USDA Agricultural Statistics land use classifications, the State's irrigated land polygons taken from the water use permitting data, and crop-water-use data collected by YMD (Yazoo Mississippi Delta) over the last 6 years. The model allows us to calculate regional water use under different future scenarios that include expanding the number if irrigated acres, the impacts of improved water conservation practices, and changing cropping patterns with related individual crop water needs.

AGRO 159
Potential of biofuel production to complement Chesapeake Bay restoration efforts: Management strategies for grasses
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Recent increases in fossil fuel prices and growing concerns regarding potential impacts of increasing atmospheric CO_2 concentrations have generated a surge of interest in renewable energy sources. The initial impact of this interest has been a rapid ramping up of grain ethanol production which has created a direct link between petroleum and commodity grain prices and a reversal of the long-term downward trend of inflation-adjusted prices of agricultural products. However the low net-energy return of current

grain-ethanol-production systems suggests that much more efficient biofuel systems will be needed to have a meaningful impact on fossil fuel consumption or CO_2 emissions. Ethanol production from cellulose appears to have potential for much higher net-energy returns, but this approach appears to have limited potential in the agricultural regions of the Chesapeake Bay watershed which already are net importers of grain. In the near term, warm season grasses appear to have potential for reducing subsurface nitrate losses while at the same time providing a fuel source for use in decentralized combustion systems.

AGRO 160
Renewable energy: Opportunities and breakthroughs for the future (AGRO New Investigator Award Winner)
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Depleting crude oil reserves and issues, such as global climate change, environmental concerns, and energy security, have intensified research in renewable alternatives (green fuel, biodiesel, and bioethanol). Feedstocks which do not compete with food crops and the development of novel uses for the co-products produced in these processes are needed for these alternatives to become economically-feasible energy sources. Results from oleaginous yeast cultivated on medium containing glycerol alone and in combination with several sugars suggests these microbes can be used as a potential lipid source. This oil can be catalytically cracked to make bio-petroleum. Additionally, we are investigating the enzymatic degradation of aflatoxin in order to use contaminated corn as a substrate for ethanol production. To address biodiesel oxidation, we developed a sensitive, inline, automated GC/MS method for monitoring oxidation. This multifaceted research approach will hopefully increase the profitability and the bond between agriculture and bio-refineries.

AGRO 161
Sustainable bioenergy crop production
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Biomass sorghums, other bioenergy crops, and crop stovers are potential biofuel feedstocks that may decrease dependence on fossil fuels and lower net carbon dioxide emissions associated with global climate change. However, a very negative outcome for society and the biofuel industry would be government and/or industry addressing near-term problems (over reliance on imported fossil fuels), while creating or aggravating longer-term problems (reduction in the productive capacity of soils). Concerns over stover and biomass removal initially focused on potential effects on water and wind erosion of soils. More recent concerns, however, are addressing quantities of stover that must be returned in order to sustain long-term soil quality and productivity. Results indicate that significantly more stover will have to be returned to maintain soil organic carbon and soil quality than for limiting erosion. The purpose of this review is to demonstrate what is known and to highlight what additional research is needed to make bioenergy crop production systems sustainable.

AGRO 162
Sustainable corn-based bioenergy farming systems
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Harvesting biomass from agricultural fields can decrease soil productivity if nutrients are not replaced and if biomass removal exceeds the C replacement value needed to maintain soil organic matter. Innovative farming systems that recycle nutrients and add C to soil may increase soil quality and thereby increase the quantity of biomass that can be sustainably removed. This presentation focuses on two potential components of such systems. Perennial groundcovers or living mulches growing concurrently with corn increase soil C inputs and provide other conservation functions. The use of biochar, a coproduct from fast pyrolysis of biomass, as a soil amendment will add a highly stable form of C to soils and is hypothesized to increase bioavailable soil water and enhance nutrient cycling. Preliminary results from and descriptions of research projects that are focused on developing sustainable farming systems for supplying bioenergy feedstock will be discussed.

AGRO 163
Properties of wood chars for soil amendment and carbon sequestration
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The US Geological Survey has had a long-term interest in pyrogenic organic materials as a part of the study of natural organic matter in soil, sediments, and water. Recently, interest has developed in using charcoal as an agricultural soil amendment because of its value to soil fertility and for carbon sequestration. Due to the difficulties of analyzing and separating pyrogenic materials from other forms of soil organic matter, chars were produced from wood and wood components under controlled conditions in the laboratory and the range of chemical and physical properties determined. Changes in composition were examined by Fourier Transform Infrared and Nuclear Magnetic Resonance spectrometry, mass loss, and elemental composition (carbon, hydrogen, and oxygen) of the char. Structural changes were examined by changes in porosity as measured by nitrogen gas adsorption. The Boehm titration method was used to measure the content of the acidic functional groups and lactones.

AGRO 164
Considering the soil: Consequences of providing biomass for energy
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There are many potential sources of biomass for bioenergy–grain and oil-seed crops, cellulosic agricultural wastes such as corn stover, thinnings from forests, and perennial energy crops such as switchgrass and poplar. The production and collection of these biomass resources is intimately intertwined with the soil and the need to maintain or to improve soil quality and fertility. Soil erosion, soil compaction, nutrient depletion, and carbon depletion are all considerations. In many instances but not all, the production and collection of biomass resources can be achieved without negatively-impacting soil quality. Achieving soil sustainability in the context of biomass collection requires a geospatially-explicit understanding of management options and outcomes.

AGRO 165
Safety evaluation and regulation of crop protection chemicals in developing countries: A global human and environmental issue
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Developing countries are global players in agriculture. For many food and fiber crops, they are becoming suppliers to the entire world, diversifying and enhancing diets with minor crops such as tropical fruits. How well are these countries regulating crop protection chemicals for worker safety, chemical residues in local and exported foods, human health and environmental monitoring? This not just an important local issue. Water and air do not recognize boundaries and chemical residues are typically a consequence of crop protection practices, leading to exported and local consumption of residues. As part of the Dominican Republic and Central American Free Trade Act or CAFTA-DR, US environmental and agricultural agencies are evaluating the regulation and food safety monitoring programs of Central American countries and the Dominican Republic. There is an emerging cadre of regulatory and environmental institutions and laboratories in the region, strengthened by regional cooperation and communication efforts and catalysed by visits of experts from their agricultural markets in Europe and the US. We will discuss trends, strengths, and weaknesses in food safety programs in the region, capacity-building in regulatory pesticide programs, and the relationship of these to global regulatory trends.

AGRO 166
Pecos River ecosystem restoration project: A case study
***Claudia E Olivieri**, Regulatory Affairs, BASF Corporation, 26 Davis Drive, Research Triangle Park, Durham, NC 27709, Fax: 919-547-2430*

Saltcedar (*Tamarix* spp.) was introduced into the United States to prevent soil erosion near rivers and lakes in the 1800's. However, saltcedar has displaced and threatened native plants species and changed wildlife diversity in the infested areas. Saltcedar absorbs large amounts of water and excretes saline solution increasing soil and water salinity considerably. In addition, saltcedar creates a dense canopy along the rivers making difficult for wildlife to have access to the river and increases fire and flood frequency. Saltcedar control is a complex task because saltcedar does not have natural enemies and spreads unchecked without human intervention. To solve this problem, the US Government Agencies agreed to use BASF herbicide ARSENAL® together with a-state-of-the-art application technology in a three year experimental project along the Pecos River. The Pecos River is part of an irrigation system that delivers water from a reservoir to nearby areas. For many years, the water available for irrigation has been a matter of contention between New Mexico and Texas, which adds another significant reason for saltcedar control to increase water availability. Results of experimental applications and monitoring programs have demonstrated a steady increase in the water flow of the Pecos River and its tributaries and a decrease in water salinity. Both factors have significantly benefited the farming communities around the area and eased the water conflict between states. The improvement in water quality and quantity has protected the Pecos fish from becoming endangered and increased native plant and animal wildlife diversity along the river.

AGRO 167
Contribution of environmental fate research to human health and the environment.
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The use of crop protection products, such as pesticides, provides benefits to the American public by reducing the cost and improving the quality of food. The production of affordable, high-quality food is certainly a positive contribution towards human health and minimizing production area is of overall benefit to the environment. However, these crop protection products sometimes have unwanted effects on terrestrial or aquatic non-target organisms or end up in drinking water in unacceptable concentrations. Research on the behavior of crop protection products and their metabolites in the environment can provide insight into making this risk-benefit decision. The authors will illustrate this with three cases based on their on experience. The first case was a candidate product where environmental fate research showed that the potential effects on the environment were too great to seek registration. The second case was a product where best management practices allowed continued use of the product except in all but the most vulnerable areas. The third case was a product in which environmental fate research showed it was safe to use throughout the U.S.

AGRO 168
Strengths and weaknesses of post-registration ranking systems for pesticides
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Pesticide registration under FIFRA (Federal Insecticide, Fungicide, and Rodenticide Act) requires that a high safety standard must be met. There must be no unreasonable adverse effects on the environment and reasonable certainty of no harm to humans when the practices and mitigation statements on the product label are followed. However, on the basis of local conditions, public perception, certification standards or participation in government funding programs, applicators, agricultural professionals or advisors may be required to justify product selection when several efficacious alternative products are available. Several evaluation indices have been designed with the intent of guiding pesticide users in selecting products with the lowest hazard to humans or the environment. These indices are problematic and contentious since, by virtue of the FIFRA evaluation and approval process, all registered products have acceptable risks relative to benefits. The strengths and weaknesses of these pesticide ranking schemes for registered agrochemicals will be discussed and common difficulties with these approaches reviewed. Alternatives will be suggested, such as landscape-based, best-agricultural- practices, for managing individual watersheds or fields largely independent of individual pesticide selection.

AGRO 169
The role of agricultural research in the restoration of the Chesapeake Bay
Cathleen J. Hapeman *and Laura L. McConnell, Beltsville Agricultural Research Center, USDA-Agricultural Research Service, 10300 Baltimore Avenue, Beltsville, MD 20705*

Nearly 25% of the land in the Chesapeake Bay watershed is used for agricultural production. According to the State of the Bay Report issued by the Chesapeake Bay Foundation, the health of the Bay is dangerously out of balance, falling one point in 2007 from 29 to 28 on a scale of 100. Clearly, better management strategies are required to reduce further the release of nutrients, pesticides, and sediments to the air and water and to improve ecosystem health. Agricultural scientists have an obligation to assist the farm community in producing commodities economically and efficiently but in a manner that reduces agriculture's environmental footprint. A better understanding of the processes from the molecular to field scale will lead to development of more effective management practices. Developing new measurement tools and improving predictive models and risk management tools will support policymakers and land use managers in identifying areas where mitigation is working and where new strategies and approaches are required. Scientists working with farmers, consumers, and local, state, and federal agencies can make the discoveries needed to preserve agricultural production and help restore the Chesapeake Bay.

AGRO 170
Pesticides in groundwater and streams of the Chesapeake Bay watershed
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Pesticides occur year-round at low levels (typically < 1 µg/L) in ground water and streams throughout the Chesapeake Bay watershed. Degradation products of pesticides are also found, often at concentrations higher than those of their corresponding parent compounds. The most-commonly detected pesticides are herbicides used on corn, soybeans, and small grains. Pesticide distribution reflects usage patterns, environmental conditions, and their chemical and physical properties. Pesticides usually occur at higher concentrations in ground water in areas underlain by permeable soils and aquifer material than in areas underlain by less permeable material. Increasing or decreasing use of pesticides can cause relatively rapid corresponding changes in overland runoff and streams; changes will be more slowly reflected in ground water and, therefore, in streams during base-flow periods. Therefore, lag times vary between management practices to reduce pesticides and corresponding changes in water quality.

AGRO 171
Pesticides in tidal regions of Chesapeake Bay
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In 2000, surface water samples were collected for pesticide analysis from 18 stations spanning the Chesapeake Bay. In a separate effort during July to September of 2004, 61 stations within several tidal regions were characterized with respect to 21 pesticides and 11 of their degradation products. In both studies, herbicides and their degradation products were the most frequently detected chemicals. The highest concentration for any analyte in these studies was for the ethane sulfonic acid of metolachlor (MESA) at 2900 ng/L in the Nanticoke River. In the agricultural tributaries, herbicide degradation product concentrations were more strongly correlated with salinity than the parent herbicides. In the two non-agricultural watersheds on the western shore, no gradient in herbicide concentrations was observed indicating the pesticide source to these areas was water from the Bay main stem.

AGRO 172
Assessing sediment quality in Chesapeake Bay
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This study described the spatial extent and severity of sediment contamination in Chesapeake Bay and its putative effects on benthic macrofauna. It was based on a probability-based sampling design and employed the Sediment Quality Triad approach, inferring weight of evidence from analyses of sediment chemistry, toxicity, and faunal distribution data. The triad results were presented as an index by developing a scoring system and estimating areas of triaxial plots in order to quantify and compare different sub-regions. Plotting of an index of sediment contamination and size of the triaxial plots showed a log-linear relationship that also discerned sets of stations where degradation was due to hypoxic conditions or associated with polluted harbors (Baltimore Harbor and Elizabeth River). Follow-up statistical analyses defined key environmental metrics and delineated groups of stations, but they did not account for high variability in benthic faunal distribution where salinity and sediment play a dominant role.

AGRO 173
Atmospheric delivery of herbicides to riparian buffer zones
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We have evaluated the ability of a riparian buffer to intercept herbicides from the air and deliver them directly by rainfall to a receiving stream in the buffer zone. The study was conducted over a four year period at a site within the Chesapeake Bay watershed. The rain collections included through-fall, stem-flow, and rain collected outside the buffer area. Herbicides are deposited on the leaves of trees and subsequently washed off during rain events. Late application of herbicides, accompanied by high temperature, high humidity, and dense foliage, resulted in a very small portion of herbicides in rain collected downwind of the forested area, i.e., less than 5% of that measured beneath the tree canopy. In contrast, these values were nearly 50% for metolachlor and around 30% for atrazine for the early spring application, when temperature and humidity were low and tree foliage less developed.

AGRO 174
Modeling the effect of a riparian buffer strip on off-field entrapment of pesticides using REMM2008
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A new version of the Riparian EcoSystem Management Model, REMM2008 is now available. This latest version contains an enhanced hydrology algorithm. Additionally, this new version contains an embedded pesticide module that can simulate pesticide movement within and out of a vegetative buffer strip adjacent to an agricultural field receiving pesticide application. Off-field movement of pesticides from agricultural fields can occur due to a combination of dissolved residues in runoff water, sorbed residues bound to eroded sediment, dissolved residues in off-field laterally moved water, and drift from pesticide application to an agricultural field. This paper will discuss details about the new pesticide module. Results from a riparian zone field study that was conducted by USDA will be compared to predictions from REMM2008 for hydrology. Vegetative buffer strip entrapment predictions for three pesticides will be discussed and compared to historical field study results.

AGRO 175
Modeling pesticide spray drift: Applications to the Chesapeake Bay watershed
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The potential for movement of pesticides to non-target aquatic areas via agricultural spray drift has been estimated using geospatial data on land cover and hydrology within a Geographic Information System. This produced a distribution of varying spray drift amounts across an agricultural landscape such as a watershed. Within the GIS, thousands of measurements were made between crop and water and were used to determine individual drift deposition rates based on the AgDRIFT model. The GIS also recorded information on the composition of the buffer, to see how this might influence spray drift. The Choptank River watershed in Maryland and Delaware provides an ideal landscape in which these approaches can be applied and ultimately combined with other pesticide and nutrient inputs to the aquatic system.

AGRO 176
Efficacy of trees to mitigate emissions from poultry houses
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Emissions of dust, ammonia, and odor from poultry facilities pose major challenges for the poultry industry. Cost-effective technologies to abate emissions from modern tunnel-ventilated poultry houses are limited. In 2002, a three-row planting of trees were installed opposite tunnel fans to evaluate vegetative environmental buffers (VEB) as a means of mitigating emissions from the poultry house. Efficacy of VEB to abate emissions has been evaluated over

the past five years during peak fan operation and emission potential. The relative change in concentration across this 6.7 meter wide VEB resulted in significant reductions in total dust (56%), ammonia (53%), and odor (18%). VEB appears to be a cost-effective means of partially abating emissions. As a proactive environmental and neighbor-relations initiative, the Delmarva poultry industry has hired a VEB coordinator to implement tree plantings on farms. This practice is being cost-shared in DE and MD with other states starting to implement similar programs.

AGRO 177
Can organic farming help protect Chesapeake Bay water and air quality?
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While organic farming practices do not in general contribute to pesticide contamination of the environment, other environmental impacts are not well studied. The USDA-ARS Farming Systems Project is a long-term cropping systems trial in Beltsville, MD designed to assess the sustainability of three organic and two conventional cropping systems. Initial results indicate that, among 3-year crop rotations, soil carbon to a depth of 1 m is 9 and 23% greater and N_2O flux is 64 and 27% lower in an organic (Org3) than in conventional no-till (NT) and chisel till (CT) systems, respectively. Predicted soil and nutrient erosion in Org3 is 33% lower than in CT but rates in NT are considerably lower than in Org3. Including a perennial forage crop into crop rotations and/or reducing tillage should improve the environmental sustainability of organic cropping systems in the Chesapeake Bay watershed. USDA-ARS research conducted in these areas will be discussed.

AGRO 178
Role of stable isotopes in environmental forensics
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As soon as organic compounds are spilled into the environment, changes will start to occur to them as a result of weathering process. Changes may result from water washing, evaporation, photo-oxidation, or biodegradation. An understanding of these processes is essential in understanding the origin and fate of these contaminants. In recent years, the use of gas chromatography-isotope ratio mass spectrometry (GCIRMS), has been applied to a number of environmental forensic problems. In this presentation, it is proposed to review how stable carbon and hydrogen isotopes can be used as a tool for correlating contaminants with their suspected sources and, where appropriate, used as a tool to monitor natural attenuation. Applications discussed will describe the fate of common contaminants, such as MTBE, PCE, and BTEX, in groundwater as well as less volatile compounds, such as PAHs and refined products. With the increasing popularity of natural attenuation as a remediation technique, monitoring the enrichment of heavier isotopes in the degraded residues is becoming a viable tool to determine when and if natural attenuation has commenced and the extent of the degradation.

AGRO 179
Following organic matter flow within the environment from a forensic viewpoint
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Tracking the flow of carbon (as well as nitrogen, phosphorous, and sulfur) in the environment is essential to our understanding of the dynamics of ecosystems over a range of scales, including continental watersheds. One of the major carbon carriers within the environment is natural organic matter (NOM) and its flow affects carbon cycling which, in turn, impacts a range of issues, such as climate change (global warming). NOM, being a highly complex and heterogeneous mixture, is very difficult to characterize. Recent advances in our understanding of NOM and in the development of analytical measurements and analysis methods have enabled us to distinguish between NOM from different sources. This presentation will focus on how these advances, in particular fluorescence-based techniques, can be used to track NOM within the environment from the forensic point of view.

AGRO 180
Perchlorate isotope forensics
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Perchlorate in soils and groundwater is derived both from natural sources and human activities including production and use for military purposes. Increased regulatory concern with this compound has generated appreciable interest in source identification. Comprehensive stable isotope analysis reveals that there are significant differences in the stable oxygen and chlorine isotope ratios among synthetic and natural perchlorates. Perchlorate in groundwater at several locations across the US with no known military installations reveals both synthetic and natural source contributions. Interestingly, stable isotope ratios of naturally-occurring perchlorate in groundwater at several locations in the western US do not match those of the well-known natural perchlorate from the Atacama Desert; these data may indicate either that natural perchlorate can form by different mechanisms or that it may be modified subsequently by biological, physical, or geochemical processes. Additional studies are ongoing to explain the genesis of isotopic variations in natural perchlorate.

AGRO 181
Principles, techniques, and applications of environmental forensics in agroecology
Udoyara Sunday Tim, *Department of Agricultural and Biosystems Engineering, Iowa StatevUniversity, Ames, IA 50011*

Environmental forensics, which uniquely integrates approaches and tools from disparate disciplines to analyze cases of environmental contamination, brings a new level of sophistication to ecological, agricultural, and life sciences. From the combination of investigative techniques from diverse fields (such as chemistry, isotopic analysis, toxicology, and epidemiology) to technologies ranging from aerial photography, statistical analysis, and mapping, to the principles of contaminant analysis and transport in the environment, and to mass spectrometry and other chemical fingerprinting methods, environmental forensics has enabled both the identification of how and when contamination took place and the quantification of the extent and potential impacts. In agroecology, the principles and techniques of environmental forensics have been applied to determine the source chemical and biological contaminants as well as pharmaceuticals and antibiotics. This paper provides a review of principles, methods, and applications of environmental forensics in agroecology. It details the application of tools, such as fate and transport models, and discusses the merits and pitfalls of existing investigative techniques.

AGRO 182
Identifying molecular changes in the chromophoric dissolved organic matter of oxidized waste streams
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Landfill leachates are complex, heterogeneous mixtures that containing levels of dissolved organic matter (DOM) that far exceed those in domestic wastewaters. On-site advanced oxidation followed by dispersed surface application has been suggested as a treatment option, but little is known about the oxidation potential of the high molecular weight chromorphoric component (CDOM) of leachate. We have used a combination of 3-dimensional excitation-emission matrix fluorescence spectroscopy (EEMS) and ultrahigh resolution Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) to characterize the changes in leachate DOM after oxidation by UV irradiation and ozonation. EEMS measurements indicate that about 93% of the fluorescent components of leachates can be removed after 2 hr of ozone or ozone/UV oxidation. High-field (9.4 Tesla) FT-ICR MS was able to resolve fully the individual compounds in the treated leachate DOM and to identify the fluorescesing components that were removed.

AGRO 183
Nanofluidics and mass-limited chemical analysis: Nanocapillary array membranes as switchable fluidic elements for coupled multidimensional analyses
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Motivated by problems as difficult as the detection of chemical and biological threat agents, a grand challenge problem for contemporary chemical analysis is the handling and characterization of mass-limited samples, i.e. samples consisting of a small absolute number of molecules. We are integrating nanometer-scale analytical unit operations into three-dimensional architectures to create integrated fluidic circuits - structures which handle fluids with the same digital control protocols used by integrated electronic circuits. Externally controllable interconnects, employing nanocapillary array membranes containing 1-10,000 nanometer-diameter channels, are used to produce hybrid three-dimensional fluidic architectures, in which controllable nanofluidic transfer is achieved by controlling applied bias, polarity and density of the immobile nanopore surface charge, and the impedance of the nanopore relative to the microfluidic channels. Such multi-level microfluidic structures are analogous to the massively three-dimensional architectures characteristic of VLSI (Very-large-scale integration) electronics and open the way for complex arrays of fluidic manipulations to be realized.

AGRO 184
Development of a new technique for the detection of heavy metals in aqueous media using modified nanomaterials
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Environmental forensics requires the continuous development of highly- sensitive and selective detection techniques for trace contaminants in the environment to enable accurate, rapid, and on-site testing. The information extracted from timely analysis is crucial in determining the source, fate, and transport of various anthropogenic species. In an attempt to achieve these goals, we describe a novel method for trace heavy metals detection using electrodes cast with modified nanomaterials. The use of the carbon nanotubes (CNTs) increases the sensitivity of the method because of their inherent catalytic activities. Further, due to their nanoscale dimensions, CNTs have high surface area to volume ratios that also lead to increased sensitivities. Modification of the CNTs by specific molecules and detection of heavy metals by electrochemical techniques demonstrate extremely sensitive quantification. The procedure was optimized with respect to the applied reduction potentials, pH, and concentration of the buffer solution used. The performance of this novel technique was evaluated and compared with established methods in the determination of trace heavy metal ions in some ground waters of southwest Missouri.

AGRO 185
Navigating the regulatory pathway for reduced risk pesticide registration
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Under FIFRA (Federal Insecticide, Fungicide, and Rodenticide Act) Section 3c(10), the US EPA is required to expedite the registration of pesticides which meet an overall determination of reducing risk. Risk can be fewer potential effects on human health, nontarget organisms, or water pollution or an increased integrated pest management strategy for the target crop. To make this determination, the EPA requires potential registrants to meet a stringent set of criteria. The reward is an expedited review of a new active ingredient. The focus of this presentation will be how the EPA makes this determination and what the potential benefits are for pesticides manufacturers. Types of data that are required and the possibility that a conventional chemical can meet the EPA's stringent benchmarks will be reviewed.

AGRO 186
Spinosad to spinetoram: Evolution of the spinosyns
***James E. Dripps**, Carl V. DeAmicis, Thomas C. Sparks, and Gary D. Crouse, Dow AgroSciences, 9330 Zionsville Road, Indianapolis, IN 46268*

The spinosyns are characterized by a unique macrolide structure and a novel, insect-selective mode of action. Spinosad consists of spinosyns A and D, the most active factors produced by a rare actinomycete, *Saccharopolyspora spinosa*. Spinosad was registered in 1997 under EPA's Reduced Risk Pesticide Initiative and won a Presidential Green Chemistry Award in 1999. Highly compatible with IPM programs, several spinosad formulations have been developed for foliar sprays to control major insect pests across a wide range of crops including one certified for organic production. Spinosad has proven to be very versatile, controlling stored grain insects, several urban and public health pests, and arthropod pests of livestock, poultry, and companion animals. It is also effective as a seed treatment and in baits controlling fruit flies and fire ants. Given the many positive attributes of spinosad, Dow AgroSciences sought to discover a significantly different and better spinosyn insecticide. Many approaches were explored, however, only synthetic modification yielded a candidate with the required efficacy, pest spectrum, and development cost. That candidate, spinetoram, was discovered using an artificial neural network-based QSAR analysis that identified ethyl substitution at the rhamnose 3'-position greatly improved activity. Eliminating the tetracyclic 5,6-double bond improved photostability. These modifications make spinetoram more potent, faster-acting, and longer-lasting than spinosad. Spinetoram controls a wider range of insect pests than spinosad in pome and stone fruits, citrus, tree nuts, and vegetables, yet maintains the favorable toxicological and environmental fate profiles of spinosad. Spinetoram was registered in 2007 under EPA's Reduced Risk Pesticide Initiative.

AGRO 187
Indoxacarb's fit in global IPM programs
***John T. Andaloro**, Hector E. Portillo, Paula G. Marcon, and Aldos Barefoot, Stine-Haskell Research Center, DuPont Crop Protection, 1090 Elkton Road, Newark, DE 19711*

Indoxacarb represents breakthrough insecticide chemistry with cross spectrum activity and classification by EPA as a reduced-risk product. Indoxacarb is from the new class of oxadiazine insecticides that have a novel mode of action and block the movement of sodium ions into nerve cell ion channels. Indoxacarb's selective toxicity on insect pests is due to its bioactivation to an active metabolite, while higher animals primarily degrade indoxacarb to inactive metabolites via alternate routes. The rapid metabolic degradation by mammals is a critical factor responsible for the high safety of indoxacarb to non-target organisms. Due to this new mode of action, indoxacarb is active on insects resistant to other insecticides. The primary route of entry into target insects is through ingestion, thus non-phytophagous insects, such as insect predators and parasitic wasps, are unaffected by contact with dried residue. Indoxacarb binds readily to organic matter, readily degrades in soil, and hence has low potential for transport to ground or surface water. The formulated product absorbs to the waxy layer of leaves, reducing potential for washoff, and provides excellent ultraviolet stability, resulting in good residual control of target pests. Indoxacarb has a positive temperature correlation providing consistent control under a wide range of conditions. Indoxacarb provides excellent plant protection in programs that use economic thresholds in combination with conserving natural enemies. Combined with its low impact on human health, low toxicity to non-target organisms, and environmental softness, indoxacarb remains one of the best choices for rotation in Integrated Pest Management and Insecticide Resistance Programs.

AGRO 188
Nonsteroidal ecdysone agonist insecticides: Mode of action, environmental fate, eco-toxicological profile, and fit in IPM programs
***Luis E. Gomez**, T. S. Dhadialla, and D Paroonagian, Dow AgroSciences, 9330 Zionsville Road, Indianapolis, IN 46268*

This paper will describe the mode of action of the non-steroidal ecdysone agonist insecticides, tebufenozide and methoxyfenozide, which are commercial insecticides sold under the trade names of MIMIC® , CONFIRM® and INTREPID®, and RUNNER®, PRODIGY®, and FALCON®, respectively. These insecticides have a novel and a very well understood mode of action. Both compounds interact with the ecdysone receptor at similar molecular sites as the natural insect molting hormone, ecdysterone, causing accelerated and lethal molting in larval stages. Both compounds, which are members of the diacylhydrazine class of chemistry, have been awarded a Green Chemistry Award by the US EPA. These compounds are mostly active only on lepidopteran larvae and have reduced risk, environmental fate, and toxicology profiles. In the field, both insecticides are presently being used for the control of a number of lepidopteran pests in row crops, vegetables, fruits, tree, nut and vine crops, as well as in forest areas. The novel mode of action, specificity of pest spectrum, low application rates, and reduced risk status make these compounds an ideal fit for integrated pest management and insect resistance management programs.

AGRO 189
Rynaxypyr®: A new reduced risk insecticide for IPM programs
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Rynaxypyr® is a new insecticide from the anthranilic diamide class of chemistry with exceptional activity on a broad spectrum of economically-important pest species. The novel mode of action of Rynaxypyr® is activation of insect ryanodine receptors. Activation stimulates release of stored calcium from the sarcoplasmic reticulum of muscle cells, causing impaired muscle regulation, paralysis, and ultimately insect death. Differential selectivity toward insect ryanodine receptors over mammalian receptors has been extensively demonstrated. Rynaxypyr® has remarkably low toxicity to mammals, fish, and birds and high insecticidal potency, setting a new standard for insecticides that led to a reduced risk decision by US EPA. The rapid cessation of feeding, strong residual activity, and excellent rainfast properties of Rynaxypyr® deliver nearly-immediate and long-lasting plant protection under a range of growing conditions at low use rates. The high larvicidal potency and long-lasting activity of Rynaxypyr® provide excellent crop protection, even when circumstances prevent optimal application timing, while its selectivity to non-target arthropods conserves natural parasitoids, predators, and pollinators. An extensive, resistance-risk-assessment, global study was conducted over a four-year period and indicates negligible risk of cross-resistance with existing insecticides, which suggests that Rynaxypyr® will be an excellent tool for growers in rotational programs within insecticide resistance management programs. The reduced risk status, novel mode of action, and unique selectivity against pollinators, and beneficial arthropods are key attributes of Rynaxypyr®, making it a suitable pest management tool with an excellent fit in integrated pest management programs.

AGRO 190
Ketoenols: Profile of a new class of low risk insecticides
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Modern insect control relies on a few modes of action (MOA) with only three modes accounting for approximately 70% of sales. Furthermore, the use of organophosphates, the major chemical class within this group, has been significantly restricted following US EPA's re-registration program under the Food Quality Protection Act. Additional modes of action are urgently required. Spiromesifen, a reduced risk insecticide/miticide, was introduced in 2005. It was the first of a new class of ketoenol chemistry, acting via inhibition of lipid synthesis. Further members of the class have followed; despite similar chemical structures, the individual ketoenols vary in their crop/pest activity as well as in their systemic properties. Together they bring a new MOA to a wide range of crops, providing a much needed resistance management tool that will extend the life of other chemical classes. Their favorable human and ecological risk profile and fit within IPM will be described.

AGRO 191
Hydrologic and biogeochemical storm response in Choptank River basin headwaters
***Antti I. Koskelo** and Thomas R. Fisher, Horn Point Laboratory, University of Maryland, 2020 Horns Pt. Rd., Cambridge, MD 21613*

During storm events, headwater streams transport large quantities of nutrients. During 2006-2007, we measured N and P during 10 storms at seven sub-basins (<26 km^2) of the Choptank River watershed. Farming and its associated fertilizer use is a major driver of nutrient export in this area. To mitigate the impacts, a variety of Best Management Practices have been applied, including nutrient management plans, winter cover crops, and riparian buffers. We found that nitrate and ammonium were depressed during storms, while phosphate and particulate P peaked. This suggests that P is transported during brief intervals (1 – 3 days) of overland runoff, whereas nitrate is transported by much slower groundwater pathways. Hydrologically, annual stormflow was about 45% of the total flow, a much higher estimate than previously thought. These findings support the idea of separate management strategies for N and P to account for transport differences and the high contribution of stormflow.

AGRO 192
Buffer widths and removal efficiencies for TN, TP, and TSS
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Upper parts of the Chesapeake Bay watershed are sensitive to TP (total phosphorus), and more saline areas are sensitive to TN (total nitrogen). TSS (total suspended sediments) is a contaminant which can also carry P and N. Most jurisdictions have either explicit or de facto regulations or guidelines for riparian buffers. Of the many buffer functions, this work focuses on contaminant removal in runoff and shallow subsurface. The literature was reviewed to determine the relationship between buffer width and pollutant removal efficiency. In addition, the relationship between buffer width and the onset of concentrated flow was examined. The relationship between removal efficiency (RE) and buffer width (W) is logarithmic, i.e., $RE(\%) = a(\ln W)+b$. R^2 values were 0.63, 0.57, and 0.42 for the TP, TN, and TSS relationships, respectively, for grass and grass/shrub buffers. All relationships were significant at $p = 0.01$, except TSS ($p=0.058$). This indicates that buffer width is a key factor but not the only factor. The second derivative of these plots can be used to estimate the 'point of diminishing returns', i.e., the approximate W at which a large increase in W results in only a relatively small increase in RE. These numbers were 18 m (60 ft), 20 m (65 ft), and 15 m (50 ft), for TP, TN, and TSS, respectively. We suggest that these distances are governed by the transition from overland/sheet flow to concentrated/channelized flow. Subsurface removal of TN seems to be minimally affected by buffer width.

AGRO 193
Sources and transport of suspended sediment in the Chesapeake Bay watershed
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The design of effective water-quality management practices in large watersheds requires an understanding of the sources and transport of important contaminants. A spatially-referenced, non-linear regression (SPARROW) model of suspended sediment has been calibrated for the Chesapeake Bay watershed. The model predicts mean annual suspended-sediment flux from specific upland and stream-corridor sources at more than 2,500 locations along Chesapeake tributaries. Effects of landscape and in-stream properties on sediment transport to and within stream channels are demonstrated. Agriculture is widespread and the largest overall source of fluvial sediment to Chesapeake Bay, although construction activities yield more sediment per unit area. Small stream channels above the Fall Line are also a significant source of sediment; net deposition occurs in the stream network in impoundments and along larger streams in the Coastal Plain. Natural conditions affecting the delivery of sediment from uplands to stream channels include soil permeability, erosion potential, and physiography.

AGRO 194
Speaking in one voice: Developing a universal agricultural conservation language within the Chesapeake Bay watershed
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The Chesapeake Bay Program (CBP) is a regional partnership facilitating the restoration activities of local, state and federal governments; non-profit organizations; watershed residents; and leading academic institutions throughout the watershed. A fundamental element of the CBP has been the measurement of progress by the partnership through the tracking of implemented conservation practices, also known as Best Management Practices (BMPs). Early in the program, the state partners chose not to utilize the existing USDA agricultural conservation language for reporting, but instead developed a language unique to the CBP, which still exists today. This use of a unique language has hindered the efforts of the CBP to fully engage USDA agencies in the restoration efforts and has subsequently prevented a thorough tracking of conservation implementation throughout the watershed. With the re-direction of staff resources by agencies and the partnership, including the completion of a new MOU in 2007, progress is now being achieved towards the development of a new universal agricultural conservation language.

AGRO 195
Developing nitrogen recommendations for corn with an on-the-go canopy reflectance sensor
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Our objective was to compare the potential for developing N recommendations for corn based on crop reflectance with those developed from more traditional approaches. Corn yield response to N was determined for N applied at the 8-leaf growth stage. Crop reflectance (590 nm and 880 nm) was determined prior to sidedress N applications. Relative Green Normalized Difference Vegetation Index (RGNDVI) was determined, as GNDVI(0) / GNDVI(280), based on reflectance from corn receiving 280 kg N ha-1 at planting. Traditionally used N recommendations deviated from the economic optimum N rate (EONR) by: i) -68 to 126 kg per ha N when determined by a soil testing lab; ii) -49 to 162 kg per ha N when based on the pre-sidedress N test; and iii) -139 to 115 kg per ha N when based on a chlorophyll measurements with a SPAD meter. EONR was strongly related to RGNDVI which offers the potential to improve N recommendations for corn.

AGRO 196
Achieving nutrient reduction goals from Maryland cropland: What worked? What didn't? What will it take?
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Agriculture has been the primary land use in the Coastal Plain region of the Chesapeake Bay watershed for several centuries and has been identified as a major source of nutrient inputs to the Bay. Despite more than two decades of effort to restore the Chesapeake Bay and repeated projections of significant reductions in nutrient losses, there is little apparent evidence of decreasing nutrient inputs to Eastern Shore tributaries. Much of the discontinuity between projected reductions in nutrient loadings and measurable changes in water quality has resulted from a lack of basic understanding of the processes that control nutrient transport rates in Coastal Plain watersheds. While early research efforts focused on identifying the causes of degraded water quality in the Bay, these efforts did little to identify effective strategies to restore the Bay. During the last two decades, terrestrial research efforts have gradually caught up to management activities and have identified what changes in agriculture will be necessary to reduce nutrient losses to target levels.

AGRO 197
Innovative methods for measuring cover crop nutrient uptake on a landscape scale
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Winter cover crops are recognized as an effective agricultural conservation practice for reducing nitrogen losses to groundwater and state cost-share programs have been established to promote cover crops on farms throughout the Chesapeake Bay watershed. Remote sensing provides a tool for real-time estimation of cover crop biomass and nutrient uptake on working farms throughout the landscape. This three-year study combined cost-share-program enrollment data with satellite imagery and on-farm sampling to evaluate cover-crop N uptake on fields within the Choptank River watershed on Maryland's Eastern Shore. Agronomic factors influencing cover crop performance included species (rye, barley, wheat) and varietal differences as well as planting date (September to November), planting method (drilled, broadcast, aerial), and previous crop (corn, soy). Combining remote sensing with farm program data can provide important insight into the success of various conservation practices, allowing programs to utilize more effectively scarce conservation resources while increasing water quality benefits.

AGRO 198
Whole-farm simulation to determine effective conservation practices
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Management decisions are made at the farm level, therfore, effective conservation practices must be both efficient in controlling air- and water-borne farm emissions and feasible with regard to farm production and profit. The Integrated Farm Systems Model (IFSM) provides a process-based simulation of farm production systems, enabling a comprehensive evaluation of the impacts of changing one or more production practices on net profit, ammonia and greenhouse gas emissions, and water-driven transport of nitrates, sediment, and phosphorous. IFSM is useful in evaluating relative benefits of practices, such as precision feed and forage management to reduce incoming nutrients and practices (e.g., manure separation, cover cropping, and forage or pasture management) to mitigate off-farm losses of excess nutrients. By using modeling to compare tradeoffs in controlling key pollutants with associated cost-effectiveness, management practices best suited to improving air and water quality of the Chesapeake Bay region can be determined.

AGRO 199
Development of a GIS-based planning and land-use management tool for protecting water quality in Choptank River watershed
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One of the major focus areas of the Choptank River Watershed Project, which has been underway since 2004, is to examine the effectiveness of various BMPs for protecting air and water quality at the watershed scale in the Choptank Watershed. A GIS-based, BMP planning and watershed management tool is being developed based on coupled-model watershed simulations using Annualized AGricultural Non-Point Source (AnnAGNPS) and CCHE1D models for unsteady flow, sediment transport, and water quality simulations in dendritic stream networks. The goal is to provide a practical and user-friendly tool that can be used by state conservation program managers for optimizing BMP implementation in the most cost-effective manner for the Choptank River Basin. Developed as an add-on extension to ArcGIS software by ESRI, the finished tool will allow a multi-criteria decision making approach which considers environmental, social, and economical aspects of watershed management in addition to purely technical and managerial aspects.

AGRO 200
Immunosensors for the detection of low molecular weight contaminants
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Prototype immunosensors based on the principal of kinetic exclusion method have been developed for the analysis of low molecular weight contaminants. This method produced assays that were 100- to 1000-fold more sensitive than indirect competitive ELISAs prepared using identical primary antibodies and analyte-conjugates. The lower limits of detection permitted sizeable dilutions of the environmental samples with a concomitant reduction in interference from the typical surface or ground water matrix. The 3 sensors under various stages of development in our laboratory include: 1) an in-line sensor that can process a sample autonomously and compare the results to an instrument-generated standard curve; 2) a battery-operated field-portable sensor that can analyze an operator-prepared sample in ~5 min; and 3) an underwater sensor designed to be installed on an autonomous underwater vehicle. These sensors have been used to develop assays for heavy metals and caffeine in environmental and food samples. (Supported by the DOE (DE-FG02-98ER62704), NOAA (NA06NOS4260226) and ONR (N00014-06-1-0307).)

AGRO 201
Multivalent glycoconjugates for *Escherichia coli* detection
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Cell surface carbohydrates decorate over 95% of all mammalian cells. Several toxins and pathogens use these molecules as unique recognition elements to bind and infect the cell. Using a versatile modular synthetic strategy, we have developed biotinylated bi- and tetra-antennary glycoconjugates to capture and to detect *Escherichia coli* and compared the binding affinity of these novel molecules to commercial polyclonal antibodies. Magnetic beads were coated with biotinylated glycoconjugate or antibody; these beads were used to capture, isolate, and quantify bacterial recovery using a luminescence assay. The glycoconjugate affinity reagents outperformed antibodies in sensitivity and in selectivity when compared under identical experimental conditions. Glycoconjugates could capture *E. coli* from stagnant water. The ability of a panel of glycoconjugates to capture a panel of pathogenic bacteria was also evaluated. To the best of our knowledge, this work represents the first comprehensive study comparing synthetic glycoconjugates and antibodies for the detection of *E. coli*. The glycoconjugate are also very stable and inexpensive.

AGRO 202
Bioreporter genes for detection of specific compounds
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The detection of specific chemical species in complex media, such as soil, sediment, and biological tissue, is often difficult. Specificity and sensitivity are both required and cost issues frequently arise when many samples must be analyzed. Processing of samples and waste problems frequently arise. We use a biological detector to determine the presence and approximate concentration of specific chemicals of interest. This biological detector is a bacterial species that has been genetically engineered to produce a visible signal when in contact with the chemical of interest. The visible signal is either fluorescence or bioluminescence (i.e., visible light) and is easily and sensitively detected using a variety of electronic instruments or even the naked eye. Although not as sensitive as other detection methods, the technique can be surprisingly specific for a class of compounds, or even for particular ionic species. The strains are inexpensive and reliable, and the applications are versatile. They are also used to describe gene expression from cell systems. The creation of a bioreporter strain is dependent on the exploitation of specific genes that respond to the chemical of interest. We have created bioreporter bacterial strains for organics (toluene, naphthalene), for heavy metals (mercury), and for explosives (TNT). These bioreporters have been used in a variety of settings, such as laboratory-based assays for the quantitation of organics, as a field kit for the identification of mercury in fish tissue and as a field release of bacteria for the detection of hidden explosives. Additional applications for analysis of plant stress and for Brownfield characterization are possible.

AGRO 203
Environmental forensics aspects of microbial contamination from concentrated animal feeding operations
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In the United States, tremendous progress has been made in restoring and maintaining the integrity and quality of soil and water resources. Today, the quality of rivers, streams, lakes, and estuaries has improved significantly with pollution control and conservation practices preventing billions of pounds of pollutants entering the nation's waters. However, despite this progress, concerns for air, water, and soil quality remain. Nearly 30% of the US waters assessed by the states in 2002 failed to meet designated uses, such as drinking, fishing, swimming, and other recreational uses. Anthropogenic pollution from sources such as agriculture, including concentrated animal feeding operations (CAFOs), and other sources continue to degrade environmental quality and pose threats to drinking water quality and human health. To manage the pollution problems from CAFOs and other anthropogenic stressors, numerous approaches, some of which fall under the general domain of environmental forensics, have been proposed. For example, environmental forensics techniques, such as fingerprinting, have been used to delineate and characterize the source(s) of microbial pollution of terrestrial and aquatic systems. This paper examines the use of environmental forensics techniques to differentiate and to characterize the source, fate, transport, and ecological effects of environmental contamination, focusing on microbial pathogen contamination from CAFOs. Through case studies, environmental forensic techniques are shown to offer a comprehensive toolbox that enables source differentiation and characterization as well as the tracking of contaminants, both chemical and biological. The implications of recent advances in ecological observatories and cyberinfrastructure on environmental forensic investigations are discussed.

AGRO 204
Surface plasmon resonance based immuno-detection of environmental contaminants
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Use of surface plasmon resonance for detection of low-level detection of contaminants in environment is well known. The past few years have seen a huge increase in trace detection methods of explosives. At the forefront are technologies that detect ppt levels of explosives, such as microcantilever based detection and surface-plasmon-resonance-based detection methods. Here we report our results on antibody based detection of explosives. We immobilized polyclonal antibodies on the surface of gold chip. The polyclonal antibodies were tested against explosives such as RDX, HMX, and TNX at ppb level concentrations. The results of their binding and relative sensitivities will be reported and discussed.

AGRO 205
Bis(chlorophenyl)acetic acid (DDA), a water-soluble biomarker of DDT metabolism in humans
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DDT is sanctioned and used in some antimalaria mosquito campaigns in sub-Sahara Africa. DDT metabolism in humans yields urine DDA as principle urinary metabolite, a potential occupational exposure biomarker. A simplified analytical method for DDA biomonitoring in human urine samples has been developed. Pentafluorobenzyl (PFB) bromide was used as derivatizing agent and diisopropylethylamine as catalyst to react for 1 h with dried hexane extracts of urine at room temperature. The DDA PFB-ester derivative was analyzed by GC-ECD. Limit of quantification is 2 ppb (confirmed by GC/MS in SIM mode). Urine samples from Swaziland workers were analyzed to evaluate the method. The results showed DDA (5 - 400 ppb) and a low DDT (0.3 – 4.3 ppb) elimination levels in urine of DDT applicators. The mean mole ratio of DDA/DDT is about 90:1. These pilot studies show that urinary DDA may be used to evaluate DDT exposure for risk assessment.

AGRO 206
Biological validation of dendrochemistry in environmental forensics
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Environmental forensics often seeks to establish the timing of changes in the chemical environment, such as the occurrence of a leak from a petroleum tank or a chemical spill. Dendrochemistry, the chemical analysis of precisely-dated tree rings, appears to provide a time-stamped sample to reconstruct events, such as chemical releases into the environment. High-resolution methods to analyze wood continue to improve in sensitivity and in precision. However, the valid contribution of dendrochemistry to environmental forensics requires an understanding of how tree biology affects chemical patterns in wood. These effects due to hydraulic conductivity, element exclusion and accumulation, wood anatomy, cellular respiration, and infection by microorganisms all follow basic chemical principles that need to be considered or at least acknowledged while providing forensic opinion.

AGRO 207
Fenamidone: A reduced risk fungicide
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Fenamidone is the first member of a new class of fungicide chemistry, the imidazolinones. While effective against a wide range of fungal pathogens, it has the unique property of being highly active against both late and early blight. It was introduced as a reduced risk chemical in 2002 and provided a needed alternative to older fungicides suffering use restrictions resulting from reevaluation under the Food Quality Protection Act. Fenamidone is produced in enantiomerically pure *S*-form which contributes to its low use-rate. Its chemistry, use in integrated pest management, and favorable human health and wild life profile will be presented.

AGRO 208
Discovery and development of the reduced risk fungicide, mandipropamid
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Syngenta Crop Protection, Inc. set a goal to develop a reduced risk chemical that would be efficacious on foliar oomycete pathogens. Syngenta synthesized 4468 compounds and screened for efficacy on leaf discs. Greenhouse tests were then conducted on 955 of the compounds and 72 of these were then field tested. Toxicology and environmental testing was initiated on the top 3 products and mandipropamid was selected for full development due to its excellent safety profile. Mandipropamid was classified by US EPA as a reduced risk chemical and was registered in 2008 for the control of downy mildew, blue mold, and late blight in many vegetable crops, grapes, and potatoes. Mandipropamid has superior efficacy compared to alternatives for control of late blight and is outstanding on several other downy mildew diseases. These diseases can be devastating and can cause up to 100% crop yield loss. Mandipropamid allows the opportunity to reduce application rates 10-30X compared to older alternatives. Mandipropamid has an excellent safety profile with regard to mammalian toxicity, ecotoxicity, and environmental fate characteristics. Mandipropamid degrades rapidly in the environment and is a low risk to non-target organisms and an excellent fit with IPM.

AGRO 209
Paladin™ and Paladin EC™: A natural fumigant replacement for methyl bromide
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Fumigants are an important class of compounds used for a variety of applications including: pre-harvest crop protection (soil fumigation); post-harvest crop protection (protection from pest damage to stored grains); removal of pests in harvested commodities (coffee, spices, etc.); and protection from structural pests (home/office and building materials). One of the most effective fumigants in the past has been methyl bromide. Unfortunately, methyl bromide has been determined to deplete ozone in the atmosphere. The Montreal Protocol on substances that deplete the ozone layer was a treaty originally signed in 1987. The treaty was modified and revised such that current stores of methyl bromide will be used until their depletion, estimated to be within the next few years. As a result of the phase out of methyl bromide, there is an urgent need to find a true replacement. Over the past several years, some combination of products have been investigated as replacements and some new products have been introduced into the market within the past year. From an efficacy and/or cost standpoint, no true methyl bromide replacement has been identified. The Arkema Group has two new formulations of dimethyldisulfide, Paladin™ and Paladin EC™, which have been demonstrated to be a true methyl bromide replacement. The current status of the new products will be discussed and how they are able to contribute to a more green approach to fumigation.

AGRO 210
Aminopyralid: A new reduced risk herbicide for invasive species control in range and pasture / IVM: Toxicology, ecotoxicology, and environmental fate profile
***John J. Jachetta**, Patrick L. Havens, Carmen Tiu, Sean C. Gehen, and Vincent J. Kramer, Dow AgroSciences, Indianapolis, IN 46268*

Aminopyralid is a new, systemic, low-rate, post-emergence herbicide in the pyridine carboxylic acid class for the selective control of noxious/invasive and agronomic broadleaf weeds in range and pasture, industrial vegetation management, and wheat. As its formulated product (Milestone®), aminopyralid exhibits low acute toxicity (Category III/IV). Overall, aminopyralid has a very favorable mammalian toxicity profile, with no evidence of teratogenicity, mutagenicity, carcinogenicity, or endocrine or adverse reproductive effects. Because of aminopyralid's low toxicity, risks to workers handling aminopyralid soluble liquid formulations are extremely low. Aminopyralid produces no significant soil or water metabolites except CO_2 and exhibits very low acute and chronic toxicity (practically nontoxic) to mammals, birds, fish, and aquatic invertebrates. Aminopyralid is slightly toxic to algae and aquatic vascular plants and is substantially below all of EPA's levels of concern for adverse effects to these organisms. The route of degradation in soils is aerobic biodegradation with a median field soil half-life at North American locations of 32 d and an average K_{oc} of 10.8 L/kg. Field experiments showed limited movement in the soil profile and aminopyralid demonstrates a low potential for groundwater concentration in EPA groundwater contamination models. In aquatic systems, the main route of aminopyralid degradation is photolysis with a half-life of 0.6 d. Aminopyralid does not have the physical/chemical properties similar to bioaccumulative compounds (Log K_{ow}<3). Aminopyralid was granted the Reduced Risk classification by the US EPA in October 2004 based on favorable toxicological, ecotoxicological, and environmental fate effects in combination with unique and improved features for invasive weed control.

AGRO 211
External, nonstandard studies: What impact do they have on glyphosate's public perception?
***Donna R. Farmer**, Daniel Goldstein, and Spencer Mortensen, Regulatory Product Safety Center, Monsanto Company, 800 N. Lindbergh Blvd., Mail Zone 03, St. Louis, MO 63167*

Third-party studies have raised issues about glyphosate and other pesticides in the scientific literature. In almost all cases, these studies fall outside of current guidelines for accepted regulatory studies. Many have used test systems that are novel and have not been subjected to either replication or external scrutiny. The unvetted results of these studies have often moved quickly into the popular press with much fanfare - only to be widely, but quietly, dismissed by the scientific community. As a result, the public has been receiving a steady barrage of unrefuted pesticide safety concerns. Increasingly, the public questions whether any pesticides should be used, whether pesticides are contributing to public health problems and harming the environment. This can open a variety of other “what if” questions and lead to a loss of public trust in pesticide regulation. Issues raised regarding glyphosate and glyphosate formulations include endocrine disruption, cancer, reproductive problems, amphibian decline, altered water quality, and persistence. How does one address the concerns arising from these ad hoc, non-standard, studies? The answer lies in evaluating new findings against the depth and breadth of regulatory testing and experience. Glyphosate was introduced in 1974 by Monsanto and is used in agricultural, forestry, aquatic, industrial, turf, ornamental, and residential applications around the world. Glyphosate herbicides are sold in more than 100 countries. Numerous regulatory tests of glyphosate and glyphosate products, using rigorous protocols meeting international standards, as well as product post-marketing surveillance, have failed to reveal any untoward effects substantiating claims of adverse health and environmental outcomes. The public trust is maintained when governments make regulatory decisions upon sound scientific data, when pesticide manufacturers promote good science and good stewardship, and when media accept responsibility for balanced and accurate reporting.

AGRO 212
Successes in the research, development, and adoption of reduced risk chemistry
***Janis E. McFarland**, Greg Watson, John Abbott, Peter Hertl, and Tim Pastoor, Syngenta, Greensboro, NC 27419*

Syngenta Crop Protection, Inc. has developed and registered 6 new fungicides, 5 herbicides, and 5 insecticides that EPA classified as reduced risk chemistry or as organophosphate or methyl bromide replacements. The discovery and research on these 16 active ingredients focused on novel chemistry or new modes of action, development of methods with new catalysts or intermediates to target diastereomer and enantiomer syntheses, and improved formulation technologies. A 2005 survey of agricultural and seed treatment uses of 8 of these active ingredients in key crops showed that US grower adoption of the new products resulted in a use reduction of approximately 84 million pounds of older chemistry with a net reduction in pesticide use of 45 million pounds per year. Benefits of reduced risk/replacement chemistries for use in IPM include their excellent environmental and toxicological profiles and utility in resistance management. Syngenta's reduced risk technology has resulted in measurable reductions in volumes of pesticides transported and used, water quality improvements, reductions in organic carbon in production exhaust air and wastewater, and significant reductions in pesticide containers.

AGRO 213
Sustaining the new, reduced-risk-pesticide technology: Why IPM is more important than ever
***Allan S. Felsot**, Department of Entomology, Washington State University, 2710 University Drive, Richland, WA 99354, Fax: 509-372-7460*

The idea of green chemistry has overtaken the agricultural products industry, especially with regard to chemicals with insecticidal bioactivity. By comparison to the tumultuous history of using pesticides with broad spectrums of activity, the outlook for compatibility with chemical and biological control is better than ever. US EPA's reduced risk pesticide program has given somewhat of an advantage, as well as incentive, to those developers of products that meet the agency's perspective of low risk. From the viewpoint of a truly integrated pest management (IPM) program, as opposed to an integrated pesticide management program, the new chemistries have less possibility of adversely affecting natural enemies of insect pests. However, research shows that the new pesticides are not without hazard to natural enemies. Agricultural systems need to be studied and monitored on a case-by-case basis to make all population management tactics as compatible as possible. One risk of deploying the new compounds is perhaps a social one, wherein growers believing that the worst is over with the end of broad spectrum, high-toxicity products will revert to the easy spray-on-schedule methodology of yesterday. Such practices will ensure a quick evolution of pest resistance, as well as a disruption of the activities of natural enemies. The history of pesticide use teaches a lesson that none of the new technologies will be sustainable for future use unless the products are only used within the context of a well-defined and dynamic IPM program. Thus, IPM is needed more than ever as pest control is fine tuned to meet societal demands of abundant food produced with the least ecological disruptions possible.

AGRO 214
Common crop protection practices and the possibility of groundwater contamination in different types of soil through leaching of currently-used pesticides
***Tanu Jindal**, Science and Technology Innovation Foundation, Amity University, Block A, Amity University Campus, Expressway, Sector 125, Noida 201303, India, Fax: 91 120 26590520*

Imidacloprid, endosulfan, chlorpyrifos, and sulfosulfuron are currently commonly used in crop protection practices. Leaching studies were carried out at 100 ppm which is much higher than even double the recommended dose in sandy, loam, and clay texture soils. The major portion of all the studied pesticides was found in top 0 - 5 cm soil layer (86-99%). Pesticides could leach to 10 - 15 cm only in sandy soil. In leachate analysis, 0.2-6.3% of the studied pesticides could leach down in 3 different soil types. Leaching was highest in sandy soil followed by sandy loam and clay soils. The trend in leaching could be explained on the basis of organic matter and clay content. In natural field conditions leaching in soil as uninterrupted flow is rarely possible, therefore the actual magnitude of leaching will be much less. Possible groundwater contamination is unlikely due to leaching of imidacloprid, chlorpyriphos, endosulfan, and sulfosulfuron in theses three different soil types.

AGRO 215
Application volume and active ingredient concentration affect the initial soil penetration of aqueous termiticide formulations
***Chris J. Peterson**, Insects, Diseases and Invasive Plants Research Unit, USDA Forest Service, 201 Lincoln Green, Starkville, MS 39759, Fax: 662-325-6645*

The initial soil penetration of two termite insecticides, Premise 75® and Termidor SC®, containing imidacloprid and fipronil, respectively, were examined in five soils in the laboratory. Three application methods were tested: one treatment used the products at double the mixing rate but half the application volume (DR treatment), the second treatment used the two products at the label-recommended mixing rate and application volume (FR treatment), and a third treatment applied the products at half the mixing rate but double the application volume (HR treatment). In all cases, the DR treatment resulted in the highest active ingredient concentration in the top 1 cm, but the HR treatment resulted in the highest active ingredient concentration at depths below 2 cm. The DR treatment provides a thinner barrier of higher initial concentration while the HR treatment provides a thicker barrier of lower initial concentration.

AGRO 216
Breaking down the substituent of the future: Environmental properties of pentafluorosulfanyl compounds
***Derek A. Jackson** and Scott A. Mabury, Department of Chemistry, University of Toronto, 80 St. George St, Toronto, ON M5S 3H6, Canada*

The pentafluorosulfanyl (SF_5) functional group was investigated from an environmental perspective to ascertain its physical properties and photolytic fate. Five aromatic probe compounds were compared with their trifluoromethyl analogs. Water solubilities for SF_5 compounds ranged from 78 mg/L – 2.4 g/L. Octanol-water partitioning coefficients ranged from log K_{OW} = 2.9 to 3.6, all of which were approximately 0.5 - 0.6 log units more hydrophobic than their CF_3 analogs. The direct photolytic fate of SF_5

compounds was studied and the SF_5 group was found to completely degrade using actinic radiation with hourly half-lives. The reaction was followed by HPLC-UV, ^{19}F NMR and high resolution mass spectrometry. It was found that five equivalents of fluoride were released to form a benzenesulfonate as a final product of photodegradation. Finally, an SF_5 analog of fluometuron, a potentially new herbicide, was synthesized and likewise photolyzed. This study provides the first evidence that pentafluorosulfanyl can degrade under mild conditions.

AGRO 217
A new natural product pesticide for controlling fungal and bacterial plant pathogens
Cruz Avila-Adame, Eunice Tan, Brian J. Campbell, Huazhang Huang, Lorena E. Fernández, ***Marja E. Koivunen****, and Pam G. Marrone, Marrone Organic Innovations, Inc, 2121 Second Street, Suite B-107, Davis, CA 95618, Fax: 530-750-2808*

An aqueous formulation derived from an ethanolic extract of the plant giant knotweed, *Reynoutria sachalinensis*, is a biopesticide (MOI-106) that controls powdery mildews, downy mildews, and other important fungal plant pathogens, such as *Botrytis* sp. This natural product fungicide has prophylactic action and should be applied before the onset of the disease. The mode of action of MOI-106 has been described as a plant defense inducer, and two anthraquinones, emodin and physcion, are likely associated with this activity. Efficacy of MOI-106 controlling fungal diseases is dose-dependent as determined in a bioassay using cucumber plants infected with powdery mildew. In three experiments, two-week old cucumber plants were treated with MOI-106 at concentrations ranging from 0.008 to 1.0% (v/v). HPLC analysis indicated that MOI-106 contained 386 and 307 µg/L of emodin and physcion, respectively. Four hours after treatment, treated plants were inoculated with powdery mildew (*Sphaerotheca fuliginea*) conidia in water-suspension containing 21 to 64 x 104 conidia/mL. The ED_{50} values estimated 9 to 11 d after inoculation were 0.38 µg/mL for emodin and 0.31 µg/mL for physcion. In two other independent experiments, fractions containing either emodin or physcion alone demonstrated significant efficacy in controlling cucumber powdery mildew.

AGRO 218
New biopesticides from plants and microbes
Marja E. Koivunen *and Pam G. Marrone, Marrone Organic Innovations, Inc, 2121 Second Street, Suite B-107, Davis, CA 95618, Fax: 530-750-2808*

Chemical compounds in plant extracts have known activities against plant pathogens, insects, and weeds. In addition, microbes and microbial metabolites have been successfully used for natural product pesticides. Marrone Organic Innovations (MOI) is currently developing biopesticides from both plant and microbial sources. We have studied the herbicidal effects of lemongrass oil containing citral, a terpene aldehyde, in both greenhouse and field studies. Based on the results, lemongrass oil can be used as an effective burn-down, non-systemic herbicide controlling a wide spectrum of weeds. Plant extract-based compounds such as hinokitiol, physcion, and emodin are natural compounds that can be used to control common plant diseases. Hinokitiol (ß-thujaplicin) is a tropolone-analog that has long been used as a bacteriocide in Asia. MOI is developing this promising compound as a biopesticide against fungal diseases like grey mold (*Botrytis* sp.) and brown rot (*Monilinia* sp.). New active compounds in our product development include oxymatrine, a plant-extract-derived quinolizidine alkaloid with good insecticidal properties. On the microbial side, MOI screens for active compounds produced by bacteria, actinomycetes and fungi. The wide variety of whole-organism and enzyme-based assays for screening for herbicidal, fungicidal, insecticidal, and nematicidal activities will be discussed.

AGRO 219
Esterase-based resistance in the tobacco adapted form of the green peach aphid, *Myzus persicae* (Sulzer), in the eastern US
Lakshmipathi Srigiriraju*, Paul J. Semtner, Troy D. Anderson, Igor V. Sharakhov, and Jeffrey R. Bloomquist, Department of Entomology, Virginia Tech, 216 Price Hall, Blacksburg, VA 24061, Fax: 540-231-9131*

Organophosphates and carbamates remain as important alternatives to the neonicotinoids in resistance management programs for the tobacco-adapted form of the green peach aphid, *Myzus persicae* (Sulzer). General esterases, known to detoxify organophosphates and carbamates were assessed in the colonies collected from fields across nine different states over a four-year period (2004 to 2007). Esterase activity was quantified by microplate assay using 1-naphthyl acetate as substrate; toxicity of acephate (organophosphate) and methomyl (carbamate) were assessed with leaf-dip bioassays. The esterase genes, *E4* or *FE4*, that are responsible for increased production of esterases, were quantified using gene amplification methods. Esterase activities of many colonies were positively correlated with LC_{50} values for acephate and methomyl. A newly observed color morph with very high esterase levels had both *E4* and *FE4* genes amplified. Changes that occurred in esterase-based resistance in the tobacco aphids over the past two decades are discussed.

AGRO 220
Study on preparation of pesticide microemulsion
Jun Wang Sr., ***Xuzhao Yang Sr.****, and Gangsen Li Sr., School of Material Science and Chemical Engineering, Zhengzhou University of Light Industry, No.5 Dongfeng Raod, Zhengzhou 450002, China*

The butachlor microemulsion was investigated by the method of pseudo-ternary-component phase diagrams. The surfactants and the co-surfactants were selected to prepare the emulsifier by mixing of surfactants. The optimum emulsifier formula was as follows: the mass ratio of polyoxyethylene-(10)-nonylphenylether (TX-10) to calcium dodecylbenzene sulfonate (ABS-Ca) to butanol was 4:1:3. Phase diagrams of the TX-10/ABS-Ca/butanol/butachlor system will be presented. Microstructure was studied by conductivity measurement. The water-in-oil (W/O) region, oil-in-water (O/W) region, bicontinuous region, and liquid crystal region were determined. The stability of butachlor microemulsion was examined as well.

AGRO 221
Overview of the evaluated observational children's pesticide exposure studies
***Curt Lunchick**, curt.lunchick@bayercropscience.com, Product Safety Management, Bayer CropScience, 2 T.W. Alexander Drive, Research Triangle Park, NC 27709, D. E. Barnekow, debarnekow@dowagro.com, Environmental Chemistry, Dow AgroSciences, Indianapolis, IN 46268, and John H. Ross, jhross@surewest.net, infoscientific.com, Inc, Carmichael, CA 95608*

Multimedia data from three observational, exposure-measurement studies were used to evaluate the relationships between environmental and biological concentrations and to compare predictive-model outputs to measured biological concentrations following indoor insecticide applications. The first study was the Children's Total Exposure to Persistent Pesticides and Other Persistent Organic Pollutants (CTEPP) Study conducted by the US EPA. The CTEPP study was an aggregate exposure study of children aged 2 to 5 years and measured pesticide residues in air, dust, soil, hands, diet, water, and urine. The second study was a University of California-Riverside study that monitored the potential exposures of children aged 2 to 17 years to pyrethroid insecticides. The third study was an observational exposure measurement study conducted by the US EPA in nine homes. The study concurrently collected environmental samples of air, surface wipes, duplicate diets, sock dosimeters, and urine from children aged 4 to 6 years during a 24-hr period. This presentation will summarize these studies, highlight the data collected in each study and discuss the data inputs that were used for the other presentations in this session.

AGRO 222
Relationships between environmental concentrations and measured urinary biomarker levels
***Nicolle S. Tulve**[1], Tulve.Nicolle@epa.gov, John H. Ross[2], jhross@surewest.net, Peter P. Egeghy[1], egeghy.peter@epa.gov, Curt Lunchick[3], curt.lunchick@bayercropscience.com, David E. Barnekow[4], debarnekow@dow.com, and Jeffrey H. Driver[5], driverjh@comcast.net. (1) National Exposure Research Laboratory, US EPA, Research Triangle Park, NC 27711, Fax: 919-541-0905, (2) infoscientific.com, Inc, Carmichael, CA 95608, (3) Product Safety Management, Bayer CropScience, Research Triangle Park, NC 27709, (4) Environmental Chemistry, Dow AgroSciences, Indianapolis, IN 46268, (5) infoscientific.com, Inc, Manassas, VA 20111*

Observational exposure measurement studies may collect a plethora of information, including environmental (indoor and outdoor air, transferable residues, dust, soil), biological (urine, saliva), and personal (cotton garments, duplicate diet) samples, as well as activity patterns and questionnaire information. Data from selected studies were analyzed individually and then combined and analyzed collectively to evaluate the relationships between various environmental, personal, and biological concentrations for selected pesticides and their corresponding urinary metabolites. In this presentation, observations will be made on the relationships between the environmental concentrations and the measured urinary metabolite concentrations for the individual and combined analyses. Individual and combined data were evaluated using regression models. Preliminary data analyses indicated associations between analyte concentrations on socks data and measured urinary 3-phenoxybenzoic acid (3-PBA) concentrations (r^2 = 0.95) and the indoor air data and measured urinary 3-PBA concentrations (r^2 = 0.35) for a subset of the individually analyzed data (n = 9). Included in this presentation will be a discussion of the challenges often encountered when interpreting environmental and biological data, including variations in sample collection strategies, parent pesticide half-life, and the presence of pesticide metabolites in environmental media. We conclude by comparing our observations to the NHANES (National Health and Nutrition Examination Survey) and GerES (German Environmental Survey) population studies. (Disclaimer: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.)

AGRO 223
Urinary pesticide metabolite concentrations in children following indoor pesticide applications
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Urinary metabolite data from three observational biomonitoring studies were combined and analyzed to better understand children's potential exposures to pesticides following indoor applications to control insects. Each study collected urine ranging from days to weeks to determine metabolite concentrations at various times following pesticide applications. Fogger applications appeared to produce the greatest increase in urinary metabolite concentrations. In addition, the elevation of urinary metabolite concentrations following fogger use was not transient and appeared to persist in some cases for several weeks. Although intra-personal metabolite concentrations varied over time, trends were observed between family members in which the concentrations increased or decreased over time in a synchronized fashion. Consumer-applied hand-held indoor aerosol applications produced increases in urine metabolite concentrations that were highly variable and ranged from increases that were not discernable from pre-application concentrations to levels similar to fogger applications. In general, the crack and crevice applications produced slight and transient increases in urine metabolite concentrations compared to the individual's pre-application concentrations, but the concentrations were typically within the range of urine concentrations previously measured in the U.S. population. This presentation will further discuss these findings.

AGRO 224
Implementing AGRO's strategic plan
***J. J. Johnston**, National Wildlife Research Center, USDA/APHIS/WS, 4101 LaPorte Avenue, Fort Collins, CO 80521-2154, Fax: 970-225-1854*

In January, AGRO held a strategic planning meeting where the mission and vision statements were modified and specific goals were created. These goals formed the basis of a 3-year strategic plan. The overarching goals and details of their implementation will be discussed.

AGRO 225
Standing topics for AGRO symposia
Kevin L. Armbrust, *Office of the State Chemist - Mississippi, P.O. Box CR, Mississippi State, MS 39762, Fax: 662-325-7807*

As part of the overall plans for success in programming at one national meeting ACS per year, ACS-AGRO developed a list of standing topic areas that will form the basis of future programming at national meetings. It is intended that these topic areas will establish AGRO's presence and expertise within these scientific disciplines.

AGRO 226
Technical programming for DC and beyond
Ellen A. Arthur, *Metabolism Soil & Water, Bayer CropScience, 17745 South Metcalf Avenue, Stilwell, KS 66085, Fax: 913-433-5389*

Technical programming forms the heart and soul of a division. AGRO is no different. Specific plans for themes and talks for the 2009 meeting in Washington, DC will be discussed as well meetings for 2010.

AGRO 227
Making inroads in international venues
Laura L. McConnell, *Beltsville Agricultural Research Center, USDA-Agricultural Research Service, 10300 Baltimore Avenue, Beltsville, MD 20705*

Part of AGRO's new vision is to become globally recognized for its leadership within scientific disciplines and to provide program opportunities in other countires for its international membership. Consistent with this are current plans for collaborative meetings in Puerto Rico, Brazil, and Australia. These and other venues and opportunites will be discussed.

AGRO 228
AGRO's communication to its membership
Cathleen J. Hapeman, *Beltsville Agricultural Research Center, USDA-Agricultural Research Service, 10300 Baltimore Avenue, Beltsville, MD 20705*

Two important vehicles for communicating information to the membership are the PICOGRAM and the new newsletter, the Femtogram. AGRO also makes use of a LISTSERV and will unveil by 2009 a reformatted, more interactive website. New communication changes dictated by the changing needs of the division will be a presented.

AGRO 229
Presentation of standard operating procedures (SOPs): Equations and assumptions
Jeff Evans, *Office of Pesticide Programs, US EPA, 7509P, 1200 Pennsylvania, NW, Washington, DC 20460-0001, Fax: 703-305-5147*

EPA's Standard Operating Procedures (SOPs) for Residential Exposure Assessments are a compendium of algorithms developed to assess non-occupational human exposures to registered pesticide products. In this session, SOP algorithms and assumptions for post-application incidental ingestion, dermal, and inhalation residential exposure routes will be presented. These algorithms can be used in Tier 1 deterministic assessments or provide the framework for utilizing chemical specific residue and contact data used in higher tier assessments. They also form the basis of the exposure equations presented in alternative models such as the International Life Sciences Institute's (ILSI) Cumulative and Aggregate Risk Evaluation System (CARES) and Exponent's Dietary Exposure Evaluation Model (DEEM)/Calendex being presented in this workshop.

AGRO 230
Presentation of equations, assumptions, and results for four post-application pesticide exposure models
Jeff Evans[1], *evans.jeff@epa.gov, Valerie Zartarian*[2], *zartarian.valerie@epa.gov, Jianping Xue*[2], *xue.jianping@epa.gov, Bruce Young*[3], *bruce.young@bayercropscience.com, Jeffrey H. Driver*[4], *driverjh@comcast.net, Muhilan Pandian*[5], *muhilan@infoscientific.com, and Nicolle S. Tulve*[2], *Tulve.Nicolle@epa.gov. (1) Office of Pesticide Programs, US EPA, 7509P, 1200 Pennsylvania, NW, Washington, DC 20460-0001, Fax: 703-305-5147, (2) National Exposure Research Laboratory, US EPA, Boston, MA 02114, (3) Product Safety Management, Bayer CropScience, Research Triangle Park, NC 27709, (4) infoscientific.com, Inc, Manassas, VA 20111, (5) Infoscientific.com, Inc, Henderson, NV 89052*

Predictive algorithms and associated chemical- and scenario-specific input variables underlie residential exposure assessment methods. Alternative models (EPA/Office of Pesticide Programs' Residential Exposure Standard Operating Procedures (SOPs); EPA/Office of Research and Development's Stochastic Human Exposure and Dose Simulation (SHEDS) Model; International Life Sciences Institute's (ILSI) Cumulative and Aggregate Risk Evaluation System (CARES); and EPA/Office of Research and Development's Draft Protocol for Measuring Children's Non-Occupational Exposure to Pesticides by all Relevant Pathways) have been developed and used as the basis for deterministic, screening-level and higher-tier (probabilistic), quantitative, human-health risk analyses for pesticide-containing products that are proposed for use in and around homes. In this presentation, representatives from each of the four modeling groups will discuss the predictive equations, algorithms, and assumptions for incidental ingestion, dermal, and inhalation residential exposure pathways/routes. Outputs for selected ranges of model inputs (e.g., chemical application rates, environmental media concentrations, surface residue transferability to skin, relevant human activity information, and exposure factors) for an indoor residential exposure scenario will be presented for comparison. (Disclaimer: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.)

AUTHOR INDEX

AGFD DIVISION

AGFD 101
STERLING HENDRICKS MEMORIAL LECTURESHIP
A nutritional odyssey: From famine to feast, can science and policy solve the dilemma?
Fergus M. Clydesdale, *Department of Food Science, University of Massachusetts, Amherst, MA 01003*

Unquestionably, the tremendous increase in life expectancy in the developed world has resulted from a safer, more varied and healthier food supply. However, we have also experienced increases in age-related diseases and obesity. Lifestyle, including diet, may hold the key to reducing these seemingly intractable problems requiring both greater knowledge of food and its components at the molecular level along with appropriate legislation and knowledge to communicate benefits to the consumer. This will require the challenge of more cooperation between academic, industrial and government scientists and policy makers to meet the needs of society through both behavior change and changing the food supply.

CHED DIVISION

CHED 115
Microwave heating: A versatile tool for clean organic synthesis and biofuel production
Nicholas E. Leadbeater*, Department of Chemistry, University of Connecticut, 55 North Eagleville Road, University of Connecticut, Storrs, CT 06269-3060*

Microwave heating offers a versatile platform for preparative organic chemistry. It is possible to perform reactions in minutes instead of hours and, in many cases, obtain high yields of desired products. As the field develops, new avenues for microwave-promoted chemistry are developing. In this presentation we will show how we have incorporated the concepts of green chemistry into methodologies using microwave heating in our laboratory; taking advantage of the short reaction times and improved efficiencies. After a discussion of the use of water as a solvent for a number of carbon-carbon bond forming reactions, particular emphasis will be placed on approached to scale-up reactions using microwave heating. Applications to biofuel manufacture will be used as examples. The use of gaseous reagents in conjunction with microwave heating as well as development of in-situ reaction monitoring techniques will also be outlined.

CHED 116
Catalysis as a key technology and fundamental science for green chemistry
Walter Leitner*, Institute of Technical Chemistry and Macromolecular Chemistry, RWTH Aachen University, Worringerweg 1, D-52074 Aachen, Germany, Fax: +49-241-8022177*

Catalytic molecular transformations are of paramount importance to secure a sustainable chemical supply chain. They address the continuing need to utilize energy and ressources efficiently in waste-minimized chemical processes. The rapidly increasing interest in biomass derived feedstocks imposes also fundamentally new challenges on the develpoment of catalysts and catalytic processes. With this background, the present talk will highlight three areas of catalysis science:
- New catalysts and catalytically active materials
- Design of synthetic pathways and transformations
- New reaction engineering principles on basis of alternative reaction media

The direct relation of these fundmental scienitific challenges to the Green Chemistry principles will be discussed and illustrated with topical examples from current research.

CHED 117
Design, performance and mechanistic chemistry of Fe-TAML activators: Reducing and eliminating hazardous substances
Terrence J. Collins*, Department of Chemistry, Carnegie Mellon University, Institute for Green Science, 4400 Fifth Avenue, Pittsburgh, PA 15213, Fax: 412-268-1061*

Iron-TAML (Tetra-Amido-Macrocyclic-Ligand) activators are small molecule mimics of peroxidase enzymes. The key to their success has been a iterative design protocol carried out for 15 years to the prototype, and thereafter for further advancement, focused primarily on obtaining strongly electron-donating ligand systems where derivative complexes resist both hydrolytic and oxidative degradation. Ferric-TAML complexes with peroxides produce extremely reactive intermediates, probably several separately or jointly depending on the conditions, one of which is likely to be an iron(V)-oxo complex that has been trapped at low temperature. Fe-TAML catalysis is distinguished by low catalyst requirements (nM to low microM), efficacy under ambient conditions over a broad pH range (especially neutral to highly basic), rapidity, high efficiencies and turnover numbers, and flexibility for both selective and non-selective processes; the latter can be described as “fire-in-water”. Fe-TAML/hydrogen peroxide's use to purify water of numerous recalcitrant pollutants and hardy pathogens will be reviewed.

CHED 118
Green solvents: The good, the bad and the ugly
***Joan F. Brennecke**, Department of Chemical and Biomolecular Engineering, University of Notre Dame, 180 Fitzpatrick Hall, Notre Dame, IN 46556, Fax: 574-631-8366*

Solvents are a major source of atmospheric emissions, which contribute to poor air quality, climate change and decreased worker health and safety, by the chemical and related industries in the U.S. Efforts to replace traditional volatile organic solvents include solventless processes, use of water, lower volatility organic solvents, and supercritical carbon dioxide, as well as development and implementation of extremely low volatility ionic liquids. We will discuss the pros and cons of these alternatives, placing special emphasis on the rapidly developing field of ionic liquids. We will talk about their many potential uses, as well as the wide variety of toxicity one can achieve with various anions, cations and functional groups.

CHED 119
Green chemistry: Principles, practice, and economics
***Mary M. Kirchhoff**, American Chemical Society, 1155 Sixteenth Street, NW, Washington, DC 20036, Fax: 202-872-8068*

Green chemistry, the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances, is the most fundamental approach to pollution prevention. Green chemistry addresses the need to produce the goods and services that society depends on in a more environmentally benign manner. The focus of green chemistry is on pollution prevention, rather than treatment and disposal of hazardous waste after it has been generated. The implementation of green chemistry technologies has eliminated waste, improved safety, and saved industry money. This presentation will introduce the principles of green chemistry, provide academic and industrial examples of greener technologies, and highlight the economic benefits of adopting environmentally friendly processes.

CHED 135
Successful academic-industry collaboration in green technologies through the federation model
***Sandra Jayne Downey**, 621 Skytop Rd, Syracuse CoE Office for Industry Collaboration, 621 Skytop Rd, Syracuse, NY 13244, Fax: 315 443-8222*

The Syracuse CoE Office for Industry Collaboration (Syracuse CoE OIC), a not-for-profit 501(c)(3) corporation, has a vision to transform Central Upstate New York into a nationally and internationally known center for environmental and energy systems through close interaction with the Syracuse Center of Excellence, a federation of more than 200 firms and institutions focusing on Clean and Renewable Energy, Indoor Environmental Quality, and Water Resources for the built and urban environments.
This transformation is being accomplished by fostering collaborative projects between top academic institutions and industry, by providing a mechanism for funding research and technological innovation and by facilitating the identification, development, application demonstration, and commercialization of products and services.
Other key components of this successful collaborative model include the ability to financially assist companies in Central Upstate New York in order to host college level internships, in partnership with top academic institutions within the Syracuse CoE federation; creating a fundamental and necessary means of “knowledge transfer;” and increasing public understanding of key issues in the federation's three focus areas, through education, communications, and outreach programs. Finally, partnerships with local and state economic entities—along with other nationally known funding agencies—are essential for the entire model to succeed.
Successful execution of the collaborative federation model is evidenced by knowledge creation; the number of new products and services in the federation's focus areas developed and marketed; and the resulting wealth creation, and ultimately, job creation.

CHED 136
Green chemistry through innovation at Merck: The synthesis of Januvia
***Joseph D. Armstrong III**, Department of Process Research, Merck Research Laboratories, 126 East Lincoln Avenue, Rahway, NJ 07065*

Different approaches utilizing Green Chemistry to drive innovation at Merck will be presented. The specific case study for the syntheisis of Januvia will be detailed. An environmentally responsible new route for the manufacture of Januvia has been achieved through scientific innovation. Januvia is a new treatment for type II diabetes which is currently being evaluated in late-stage clinical trials. A first generation process, which used existing methodology to synthesize Januvia , was used to prepare over 100 kg of material and, with modifications, would have been a viable manufacturing process. However, in order to develop a highly efficient process for the preparation of Januvia, Merck researchers discovered a completely unprecedented transformation, the asymmetric catalytic hydrogenation of unprotected enamines. This new method provides a general solution to the synthesis of beta-amino acids; a class of molecules well known for their interesting biological properties. Merck scientists and engineers have applied this new method in a completely novel way, using it in the final step of synthesis, which maximizes the efficiency of the new route. This strategy is broadly applicable to other pharmaceutical targets and has been applied to the synthesis of several exploratory Merck drug candidates. Implementation of the new route on manufacturing scale has led to over an 80% reduction in the amount of waste produced and elimination of aqueous waste streams. The technology discovered, developed and implemented by Merck for the manufacture of Januvia is an excellent example of scientific innovation resulting in benefits to the environment.

CHED 137
Lessons learned through measuring green chemistry performance of development routes at GSK
***David Constable**[1], David.C.Constable@gsk.com, Richard K. Henderson[2], Richard.K.Henderson@GSK.com, Clare Ruddick[3], Concepcion Jimenez-Gonzalez[2], Conchita.J.Gonzalez@GSK.com, Tom Roper[3], and Graham R. Geen[3]. (1) Corporate Environment, Health & Safety, Glaxo Smith Kline, One Franklin Plaza, P.O. Box 7929, Philadelphia, PA 19101-7929, (2) Corporate Environment, Health & Safety, GlaxoSmithKline, Ware, Hertfordshire SG12 0DP, England, (3) Chemical Development, R&D, GlaxoSmithKline, Stevenage, Hertfordshire SG1 2NY, England*

One of the goals of GlaxoSmithKline's Sustainable Processing Team is to promote the design and development of more efficient chemistries and processes. By efficient we mean processes that use less mass and energy per kg of active drug substance, create less waste, use inherently less hazardous reaction conditions and chemicals, and in general move GSK towards more sustainable business practices.

In order to design more sustainable chemistries and synthetic routes, GSK systematically and continuously measures and monitors green chemistry performance throughout the development cycle. To do this, GSK has selected key green chemistry metrics and has designed tools to facilitate chemical, chemistry and process assessment. The tools include solvent and material selection guides, a Green Chemistry and technology guide, a chemical legislation guide, and others that have been previously reported. A set of agreed targets with benchmarks for each clinical development phase are provided and these are accompanied by guidance and interpretation that is communicated directly to the development scientists responsible for optimizing GSK chemistries and processes. Life cycle environmental impacts are also included as part of our continuing assessment of synthetic routes under development through our tool FLASC (Fast Life cycle Assessment of Synthetic Chemistry). The inclusion of life cycle metrics is especially important for supply chain management in light of the growing trend to outsource manufacturing within the pharmaceutical industry. This presentation intends to share GlaxoSmithKline's experiences with systematically measuring, comparing and evaluating synthetic chemistry routes using key 'green chemistry' metrics. It also explores the opportunities and challenges encountered in implementing green chemistry concepts within a research and development framework.

CHED 138
Practice of sustainable chemistry at Dow: Historical and future perspectives
Victor A. Atiemo-Obeng, *Victor.Atiemo-Obeng@dow.com, Core R&D - Engineering and Process Sciences, The Dow Chemical Company, 1776 Building, Midland, MI 48674-1000, Fax: 989-638-9674, and Adam A. Muellerweiss, AMuellerweiss@dow.com, Public Affairs - Sustainability, The Dow Chemical Company, Midland, MI 48674-1000*

Sustainability at The Dow Chemical Company received a lot of attention with the introduction in 2006 of the company's 2015 Sustainability Goals. The focus on sustainability at Dow however dates back much earlier. In this presentation specific examples encompassing both internal and external initiatives, programs and investments will be described and used to highlight Dow's long history in the practice of sustainability in the biggest chemical company in North America. How these efforts inform the current and future perspectives on Green or Sustainable Chemistry at Dow will discussed.

CHED 139
Greening the pharmaceutical industry: Accomplishments and opportunities
Berkeley W. Cue Jr., *Private Consultant, 12 Eska Drive, Ledyard, CT 06339*

The pharmaceutical industry has been at the forefront in adopting green chemistry and engineering as an important approach for the design of its active pharmaceutical ingredient (API) manufacturing processes, evidenced by winning the US EPA Presidential Green Chemistry challenge several times over its twelve year history. In 2005 several companies came together with the ACS Green Chemistry Institute to form a Pharmaceutical Roundtable, which, today, comprises eight member companies. These companies meet on a regular basis to discuss pre competitive and non competitive issues relating to green chemistry, and have made notable progress in achieving their common goals. These goals and accomplishments around greener chemical reactions, benchmarking environmental footprint reductions, legislative action, education and globalization will be discussed along with opportunities to expand membership, and take on some of the most challenging R&D problems facing this industry around environmental stewardship. The talk also will explore the challenging business environment in which the industry finds itself and its possible impact on these R&D efforts.

CHED 298
Green chemistry labs: An ongoing process at Siena College
Alicia B. Todaro, *todaro@siena.edu, Department of Chemistry and Biochemistry, Siena College, 515 Loudon Rd., Loudonville, NY 12211, and Jodi O'Donnell, jodonnell@siena.edu, Department of chemistry and biochemistry, Siena College, Loudonville, NY 12211*

Since 2006 the organic chemistry lab at Siena College has been transformed from using traditional experiments to a using greener chemistry experiments. This process, the principles used and some experiments will be presented in this poster. Plans for implementing green chemistry in the general chemistry lab and inorganic chemistry lab will also be presented.

CHED 299
Greening the organic chemistry laboratory at Widener University
Kaitlyn Gerhart, *kpgerhart@mail.widener.edu, Department of Chemistry, Widener University, One University Place, Chester, PA 19013-5792, and Loyd D. Bastin, bastin@pop1.science.widener.edu, Departments of Biochemistry and Chemistry, Widener University, Chester, PA 19013-5792*

In the past, the problem of waste disposal in the sophomore organic chemistry laboratory was combated by using microscale experiments. While the microscale approach reduces the amount of waste generated, it introduces several pedagogical problems. First, the microscale experiments require “special” glassware to deal with the small amounts of material used and produced in an experiment that are not always similar to comparable mini- and macroscale equipment. Second, the microscale experiments routinely result in little or no yields. This result is disheartening to students and leads to an unnecessary anxiety in the organic chemistry laboratory. Third, rescaling a reaction does not fully address the issue of hazardous waste disposal or the need for environmentally friendly methods. Therefore, in order to teach students about alternative solvents, reagents, and reactions, we redesigned the organic chemistry I laboratory. Here we describe our process of redesigning the organic chemistry I laboratory from a microscale into a green organic chemistry laboratory. Our approach involved an investigation of the current labs performed in the organic chemistry I and II laboratories to determine their pedagogical value. We also discussed the skills/knowledge that students should obtain from organic chemistry I and II laboratories with science faculty. From this information, we outlined the knowledge/skills that a student should gain in an organic chemistry laboratory and searched the current literature for “green” organic chemistry labs that met the developed course goals. We also developed a three step inquiry-based, green synthesis as a capstone experience for the organic chemistry I laboratory.

CHED 300

An approach to recycling scrap white athletic leather

Dennis C. Shelly, *kzdcs@ttu.edu, Dept. of Chemistry and Biochemistry, Texas Tech University, Box 41061, Lubbock, TX 79409-1061, Fax: 806-742-1289, Karel Kolomaznik, Faculty of Technology, Tomas Bata University, Zlin NA, Czech Republic, and Nguyen V. Phuoc, Environment Department, Univ. of Technology, Ho Chi Minh City NA*

The authors have partnered with the US-Asia Environmental Partnership (USAE P) and Nike, Corp. to develop scrap leather recycling technology for the athletic shoe industry. The focus of this technology is the panel stamping residuals and leather trimmings left over from athletic shoe manufacture in Viet Nam, particularly, and in Asia, generally. Employing alkaline hydrolysis and alkaline protease digestion techniques, a hybrid reaction scheme was developed for the industry in a “best practices” demonstration, recently. Trials were performed at both 600 g and 12 kg levels. We have shown how the scrap white leather can be converted to an aqueous protein (collagen) hydrolysate and a chromium/titanium bearing sludge in less than 12 reaction cycle. The protein hydrolysate has qualities amenable to an organic nitrogen fertilizer and the inorganic sludge can be used as a glaze for ceramics. Details of the biotechnology, as well as analysis for recovered products and the user interface (best practices demo) will be presented and discussed.

CHED 301

Progress in biodegradable poly-3-hydroxyalkanoate (PHA) polymer production: Cost reduction investigations

Daniel J. Nicholson[1], *beachbiofuel@msn.com, Arthur J. Stipanovic*[1], *astipano@esf.edu, Christopher T. Nomura*[1], *ctnomura@esf.edu, and Terry Bluhm*[2], *terry.bluhm@xerox.com. (1) Department of Chemistry, State University of New York- College of Environmental Science and Forestry, 1 Forestry Dr, Syracuse, NY 13210, (2) Xerox Corporation, Rochester, NY*

Microbiologically produced poly-3-hydroxyalkanoate (PHA) polymers are a well known biodegradable material with physical characteristics comparable to some commercially available plastics like polypropylene and polyethylene. PHA plastic production is ongoing, but has been constrained by high production costs. To decrease this cost, investigations at SUNY-ESF have focused on inexpensive substrates to replace glucose, which continues to rise in price. Poly-3-hydroxybutyrate-co-3-hydroxyvalerate copolymer (PHB-HV) has been produced from waste forest biomass hemicellulose/ xylose/ levulinic acid, to give good yields and desirable product characteristics. Waste glycerol from biodiesel production has also been used as a substrate to give medium chain length PHAs in significant yield with elastomeric characteristics. Another ESF research focus is decreasing PHA cost by augmenting the polymer matrix with low cost wood-derived hemicellulose “filler”. Blends of PHA have been created with a number of hemicellulose types and quantities, and analyzed for compatibility and strength characteristics. It is hoped that this approach will yield materials acceptable for commercial application at lower cost.

CHED 302

Screening biomass-derived fuel additives via emissions testing to evaluate the next generation of environmentally benign fuels

Ngee-Sing Chong, *Santhosh Sirupa, Basil Mugaga Naah, Reubyn William Chong, and Beng Guat Ooi, Department of Chemistry, Middle Tennessee State University, 1500 Greenland Drive, Murfreesboro, TN 37132*

The history of blending “clean-burning” additives in transportation fuels had been fraught with disappointing episodes of production bans for tetraethyl lead, manganese methylcyclopentadienyl carbonyl, and methyl tertiary butyl ether when it was discovered that such additives posed environmental and health hazards. Although many studies have been published for bioethanol and biodiesel with regard to the emissions of total hydrocarbons, carbon monoxide, nitrogen oxides, and particulate matter, the detailed results on hydrocarbon speciation, especially the partially oxidized polar organic compounds, are limited. Emission testing results based on canister and sorbent tube sampling followed by analysis with gas chromatography-mass spectrometry will be presented. The analytical data for polar organic compounds such as formaldehyde, acetaldehyde, and acrolein will be emphasized for emissions from a bus, a generator, and a lawnmover engine. The fuels investigated include bioethanol, biodiesel, recycled grease, a glycerol-based derivative, and biobutanol at various percentages of blending with gasoline and diesel.

CHED 303

Studies of yeast strains for bioethanol production and the emission characteristics of biomass-derived fuel additives

Ngee Sing Chong, *Kevin R. Lankford, Santhosh Sirupa, and Beng Guat Ooi, Department of Chemistry, Middle Tennessee State University, 1301 East main Street, Murfreesboro, TN 37132-0001, Fax: 615-898-5182*

Ethanol, a clean-burning fuel additive, and other higher alcohols with greater energy density and lower hygroscopicity, can be produced from sugars by microorganisms. In order to produce yeast strains that are tolerant to higher (>15%) ethanol levels, wine yeast strains are either grown in complete media containing 25-µg/mL ethidium bromide for several generations or grown in nitrogen base media containing 15 % ethanol. Some of the mutants selected were resistant to lycorine at concentration of 500µg/ mL, suggesting that these mutants were also rho0 or lack mitochondrial DNA. One mutant strain showed an increase in ethanol production compared to its parent strain. The emission characteristics of alcohols obtainable via microbial processing of biomass feedstock are studied by burning them as fuel additives in gasoline and diesel engines. The results of the comparative emission tests allow researchers to evaluate the relative merits of ethanol, isobutanol, 1-butanol, 2-methyl-1-butanol, and 3-methyl-1-butanol.

CHED 304

Microwave heating for fast, easy biodiesel preparation

Lauren M. Stencel[1], *lauren.stencel@huskymail.uconn.edu, T. Michael Barnard*[2], *mike.barnard@cem.com, and Nicholas E. Leadbeater*[1], *nicholas.leadbeater@uconn.edu. (1) Department of Chemistry, University of Connecticut, 55 North Eagleville Road, University of Connecticut, Storrs, CT 06269-3060, (2) Synthesis Division, CEM Corporation, Matthews, NC 28106*

Biodiesel is made through a transesterification reaction between vegetable oil and methanol using either an acid or base catalyst. The methyl ester products can then be used just as diesel fuel is in a car with only a few alterations to the engine. We have found that biodiesel can be prepared quickly and efficiently using a scientific microwave. The methodologies we have developed can be performed using either base or acid catalysts, used and new oil, as well as different alcohols. In our batch methodology we can processes up to 3 kg per run; the reaction time being only a few minutes with a 1:6 ratio of oil: alcohol and low catalyst loading. Our continuous flow approach involves using a 4 L reaction vessel, and processing at 7.2 L / min. Rudimentary energy balance calculations show the microwave method to be more energy efficient than conventional heating.

CHED 305

Continuous-flow approaches to scale-up of microwave-promoted reactions

David Gunn, *d.gunn@milestonesci.com, Milestone Inc, 25 Controls Drive, Shelton, CT 06484, and Nicholas E. Leadbeater, nicholas.leadbeater@uconn.edu, Department of Chemistry, University of Connecticut, Storrs, CT 06269-3060*

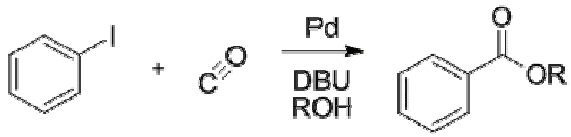
Within the organic chemistry community, it is now fairly well accepted that if a reaction requires heat then it can be performed faster using microwave as opposed to conventional heating. However, looking in the literature, the vast majority of reports are focused around small-scale synthesis. Significant attention is now being focused on scale-up of microwave promoted reactions. It is the aim of this poster to show how continuous-flow approaches have been developed for scale-up of a range of frequently-used organic transformations. As well as showing equipment that is currently available and which we have used in our laboratory, we will present up to the minute results from modifications we have made to make processing easier and allow us to increase throughput further.

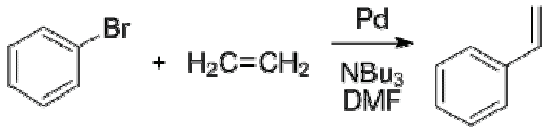
CHED 306

Palladium-catalyzed reactions with gaseous reagents: Carbonylation with carbon monoxide, Heck reaction with ethene

Chad M. Kormos *and Nicholas E. Leadbeater, Department of Chemistry, University of Connecticut, 55 North Eagleville Rd, University of Connecticut, Storrs, CT 06269-3060*

Gaseous reagents can offer a number of advantages over traditional synthetic equivalents, such as decreased waste and improved atom economy. Used in conjunction with a scientific microwave apparatus, gaseous reagents can be handled safely and dosed accurately. Microwaving heating can also be an energy-efficient route to elevated temperatures, decreasing reaction times. Within this paradigm, we have performed hydroxycarbonylation and alkoxycarbonylation reactions of aryl iodides in environmentally-benign water and alcohol solvents, respectively, and have optimized the protocols for low palladium catalyst loading. In addition, the carbon monoxide loading in the alkoxycarbonylation has been decreased to near-stoichiometric, eliminating the problems associated with carbon monoxide release following the reaction. More recently, the Heck reaction of ethene with aryl bromides has been optimized for selective conversion to a styrene intermediate, which can be subsequently transformed without purification in a one-pot two-step strategy to generate unsymmetrically-substituted stilbene derivatives via a second Heck reaction.



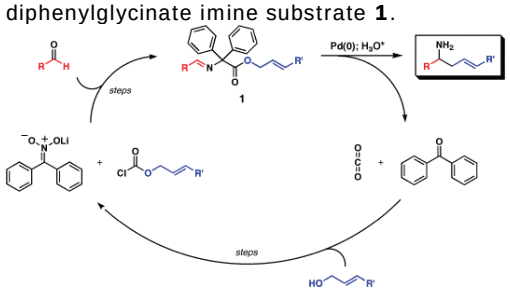


CHED 307

Beyond atom economy: A complete carbon-retentive process toward homoallylic amines

Jason J. Chruma and ***Tiffany K. VanDervort****, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, VA 22901, Fax: 434-924-3710*

Improving efficiency in organic synthetic processes has environmental and economic benefits. Of particular interest is the reduction of carbonaceous waste in the production of useful functionalized building blocks from petroleum derivatives and/or renewable resources. Inspired by the dialkylglycine decarboxylase/transaminase enzymatic cycle, we developed an efficient process for the conversion of aldehydes and allylic alcohols into homoallylic amines employing a benzophenone/diphenylglycine shuttle and a palladium-catalyzed decarboxylative allylation. The overall cycle proceeds with a zero net gain in carbon waste production, with most steps requiring ambient temperature and aqueous solvent mixtures. Furthermore, this cycle affords a nearly 20-fold cost reduction versus other routes previously developed in our group toward the required allyl diphenylglycinate imine substrate **1**.



CHED 308

Catalytic hydrogenation of aromatic compounds with carbon nanotube-supported metallic nanoparticles in supercritical fluid carbon dioxide

Hsing-Jung Chen[1], *hchen@uidaho.edu, Horng-Bin Pan*[2], *hbpan@uidaho.edu, Jen-Fon Jen*[1], *jfjen@dragon.nchu.edu.tw, Kong-Hwa Chiu*[3], *ckh@mail.nhlue.edu.tw, and Chien M Wai*[2], *cwai@uidaho.edu. (1) Department of Chemistry, National Chung-Hsing University, Taichung 402, Taiwan, (2) Department of Chemistry, University of Idaho, Moscow, ID 83844, (3) Department of Applied Science, National Hualien University of Education, Hualien 970, Taiwan*

Hydrogenation of benzene and biphenyl catalyzed by metallic (Pd, Pt, Rh) nanoparticles deposited on multi-walled carbon nanotube (MWCNT) in supercritical fluid carbon dioxide has been studied. In this study, a high pressure fiber-optic based reactor connected directly to a CCD array ultraviolet spectrometer was used for in-situ kinetic studies in supercritical fluid carbon dioxide. The experiment results are shown the carbon nanotube-supported metallic nanoparticles show better catalytic activities than the commercial carbon-based catalysts. The reaction order and rate constants are also presented. The significance of this green technique for converting toxic aromatic compounds such as benzene to eco-friendly cyclohexane will be discussed.

CHED 309

Magnetic beads-based bioelectrochemical immunoassay of polycyclic aromatic hydrocarbons and polychlorinated biphenyls

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Two simple, rapid, and sensitive bioelectrochemical immunoassay methods based on magnetic beads (MBs) have been developed to detect polycyclic aromatic hydrocarbons (PAHs) and polychlorinated biphenyls (PCBs). The principles of the two methods are the same but using two different substrates. It is based on a direct competitive enzyme-linked immunosorbent assay. A magnetic process platform was used to mix and shake the samples during the immunoreactions and to separate free and unbound reagents after the liquid-phase competitive immunoreaction. Several different parameters have been studied in detail and optimized. The detection limit of PAHs and PCBs are 50 pgmL-1 and 10 pgmL-1 which were obtained under optimum experimental conditions. The performance of these two methods were successfully evaluated with tap water spiked with PAHs and PCBs, indicating that this convenient and sensitive technique offers great promise for decentralized environmental applications with less organic solvent and power usage.

CHED 310

Green chemistry technique using algae fluorescence to monitor water quality

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This research has been carried out to determine the adverse effects of toxins on algae, and to provide methods to monitor and protect public water supplies. Changes in algae fluorescence can be used as an immediate indicator of quality changes in aquatic ecosystems. The introduction of toxins to water will damage the algae cells, and cause changes in the photosynthetic pigments in algae. The change of algal pigments can be detected by fluorescence techniques and monitoring different fluorescence intensities. The grab samples collected from Hermon Pond in Maine have been used to determine the toxic effect of copper sulfate to algal pigments. Experimental data indicate that the fluorescence intensity of the pond water algae significantly declined with the presence of copper sulfate (LC50=0.2ppm) at concentrations from 0.1 to 10ppm within 5mins incubation time. The kinetic tests for the copper sulfate introduced to grab samples shows that the respond of algae changes by copper sulfate is rapid (seconds). Our results indicate that the fluorescence of algae is very sensitive to the presence of different pollutants and this very quick response can be utilized to monitor water quality and protect water supplies.

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-Tim Ballard, tballard@en-cas.com
AG-LIST manager

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Please contact:

Dr David Dohn— d.dohn@ptrlwest.com
or
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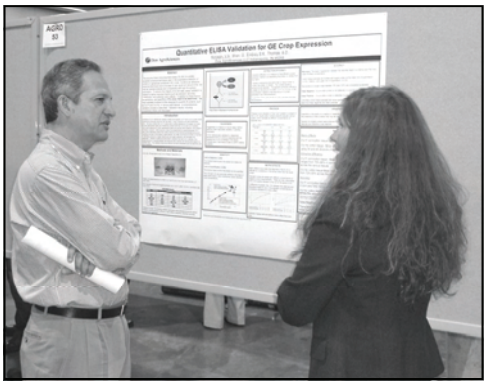

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