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PICOGRAM V. 84

and Abstracts

AMERICAN CHEMICAL SOCIETY

246th National Meeting and Exposition

Chemistry In Motion

September 8-12, 2013

Indianapolis, Indiana, USA

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CROWNE PLAZA AT HISTORIC UNION STATION

POSTER SESSIONS

INDIANA CONVENTION CENTER

Mon: 1:30 - 5:30 PM in Halls F & G; Sci-Mix Mon: 8:00 – 10:00 PM, Halls F & G; Tues: 1:00 - 5:00 PM in Halls F & G
Cosponsored in ***ENVR*** Poster Session Wed: 6:00 - 8:00 PM in Halls F & G

Technical Program and AGRO Events List: pp. 67 - 89; **Abstracts:** begin on p. 90

SYMPOSIUM OR SESSION/SECTION	Room	Sun	Mon	Tue	Wed	Thu
Accurate Mass Analyses in Support of Agricultural Chemical Research & Develpmt	MILWAUKEE	A				
Advanced Bioanalytical Technologies for GM Detection	ILLINOIS STREET EAST	D				
Spray Application Technology	ILLINOIS STREET WEST	D				
ADME: The Motion of Veterinary Drugs and Xenobiotics	B&O	P				
Herbicide-Resistant Crops and Weeds: Current Status	MILWAUKEE	P				
21st Century Vision for Testing and Risk Assessment: Implications for Agrochemicals	B&O		A			
AGRO International Research Award	ILLINOIS STREET WEST		D			
Biopesticides: State of the Art and Future Opportunities	ILLINOIS STREET EAST		D	D	A	
Environmental Fate, Transport, and Modeling of Agriculturally-Related Chemicals	MILWAUKEE		D			
ENVR: Predicting Molecular Properties of Environmental Contaminants: Empirical and Theoretical Methods	PENN STATION A		D	A	E	
AGRO Education Award Poster Session	IND CONVCTR, F&G		P			
Pesticide Regulatory Science in the 21st Century Merging Research & Regulations	B&O		P			
ENVR: Air Monitoring	PENN STATION B		P		E	
High-Throughput Pesticide Residue Analysis	B&O			A		
Innovation in Chemistry of Agriculture Award	GRND CTRL STA A&B			A		
Journal of Agricultural and Food Chemistry Best Paper Awards	GRND CTRL STA A&B			A		
Sterling B. Hendricks Memorial Lectureship Award	GRND CTRL STA A&B			A		
Pollinators and Pesticides	ILLINOIS STREET WEST			D		
ENVR: Water: Global Problems, Local Solutions	VICTORIA STATION D			D		
Ecotoxicological Risk Assessment for Agricultural Use of Chlorpyrifos in the US	B&O			P		
Non-First Order Dissipation and Time-Dependent Sorption of Organic Chem in Soil	GRND CTRL STA A&B			P		
Protection of Agricultural Productivity, Public Health, and the Environment	IND CONVCTR, F&G			P		
AGFD: 2013 Kenneth A. Spencer Award: Symposium in Honor of Dr. Attila Pavlath	IND CONVCTR, 107			P		
ENVR: Status & Trends of Classical and Emerging Contaminants Across the World	PENN STATION A			P	E	
Pesticide Residues in Food and Feed: Scientific and Regulatory Global Needs	VICTORIA STATION A-C				D	A
Synthesis and Chemistry of Agrochemicals	ILLINOIS STREET WEST				D	
Terrestrial Field Dissipation Studies in Global Agrochemical Registration Programs	MILWAUKEE				D	
ENVR: Fate and Toxicology of Emerging Environmental Contaminants	VICTORIA STATION D				DE	A
Uptake, Translocation, and Distribution of Agrochemicals in Plants	ILLINOIS STREET EAST				P	
Air Quality at the Interface	MILWAUKEE					D
Assessing Potential Ecological and Human Health Effects from Fertilizer and Pesticide Use in Urban Environments	ILLINOIS STREET EAST					D
Regulatory Risk Assessment: New Paradigms for Human Health Exposure	ILLINOIS STREET WEST					D

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

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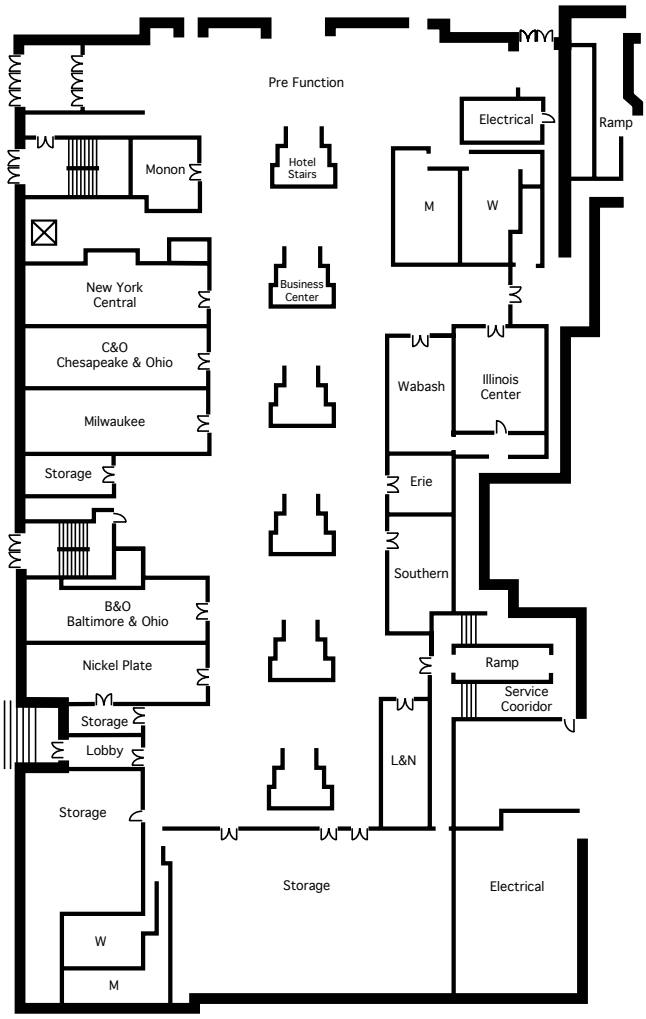
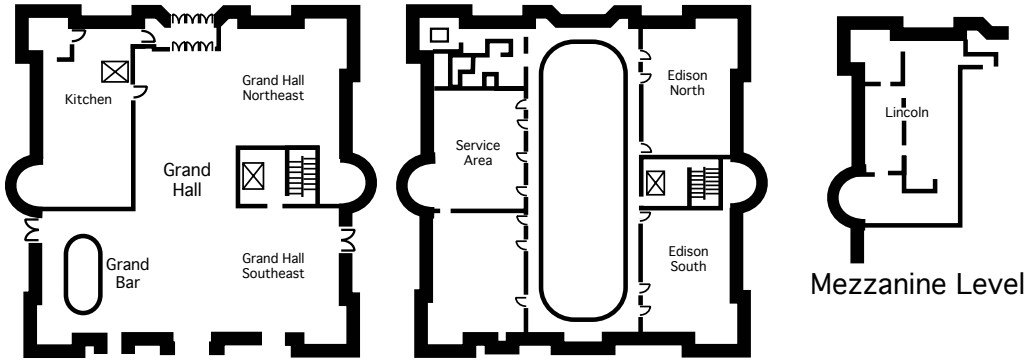
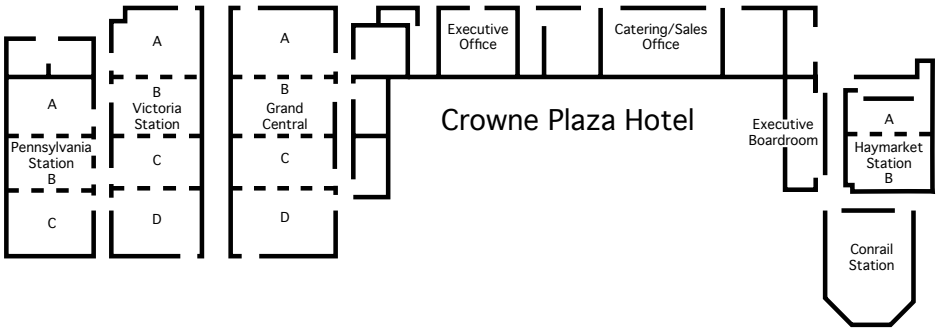


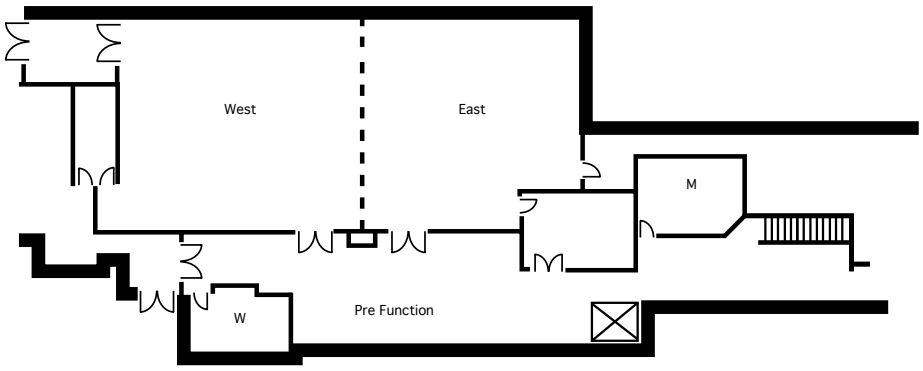
Conference Center

MEETING SPACE SPECIFICATIONS

CROWNE PLAZA HOTEL & CONFERENCE CENTER AT HISTORIC UNION STATION *(continued)*







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FROM THE CHAIR'S DESK

JOHN M. CLARK

The 246th National ACS meeting in Indianapolis is just a couple of months away, and planning for the combined ACS/AGRO-IUPAC/ICPC meeting is well underway for August 2014 in San Francisco. As in previous years, AGRO continues to reinvent itself by finding innovative ways to improve agricultural productivity and protect human health and the environment while maintaining a strong sense of community and support. Our current vision is to provide a supportive environment for professional growth through innovative programming, services, and opportunities for collaboration. To implement this vision, AGRO has focused on three areas central to our continued success as a valuable and growing professional society.

Fall Programming

246th ACS National Meeting – The AGRO technical program, put together by Steve Duke for the 246th ACS National Meeting in Indianapolis, *Chemistry in Motion*, is finalized and promises to be an exceptionally exciting and diverse program with 6 award presentations and symposia (AGRO Fellows, International and Innovation, Hendricks, JAFC Best Paper, Education, and New Investigator awards) and 21 technical symposia with 432 submitted abstracts. The implementation of a Programming Committee with Symposium Topic Champions and chaired by the Vice-Chair, the re-establishment of the Sunday Programming Meeting, and the continuation of the Blues and Brew wrap-up meeting appears to be paying off in robust and engaging programs.

IUPAC 2014 and 248th ACS National Meeting – From all accounts, the technical program being put together by Cathleen Hapeman and the Scientific Program Committee for the 248th ACS National Meeting, which will be held in conjunction with the 13th IUPAC International Congress of Pesticide Chemistry, in San Francisco in August 2014, is very likely to set a record in the number of symposia and in attendance. Details for the this meeting can be found on page 45. Volunteers are still needed for a number of committees for this meeting. Please contact either of the co-chairs, Ken Racke or Laura McConnell.

Additional AGRO Programming Accomplishments and Opportunities

Our Division has recently entered into two new and exciting programming opportunities by partnering with 1) the Foundation for the Study of Traditional Sciences and Arts (ECYART) in Peru and 2) the ACS Publication Division and the Journal of Agriculture and Food Chemistry (JAFC). In the first effort, Dr. Luis Ruzo in collaboration with John Johnston and Keith Solomon established ECYART as an educational-research entity in Peru and have now developed the first lecture series entitled, *Toxicology and Management of Pesticides*, at the Universidad Nacional Agraia La Molina in Lima, Peru to begin July 2013. In a similar development, Dr. James Seiber, Editor-in-Chief of JAFC, along with ACS Publications and the AGFD and AGRO Divisions has established a lectureship focusing on the *Research Article of the Year Award* for JAFC. The first two awards, one for the best paper in agrochemical research and one in the area of food chemistry, will be presented at the Indianapolis meeting. In addition to a monetary award, the awardees will present their work prior to the Innovation Award paper and the Sterling Hendricks Lectureship.

In addition to having a full technical program at the 246th ACS National Meeting, AGRO has recently co-programmed with the ENVR and SCHB Divisions by offering a 2-day symposium, "Arsenic Contamination of Food and Water," at the 245th National Meeting in New Orleans in April 2013. AGRO continues its effort to increase co-program and outreach activities in related conferences and is currently co-programming in the 50th North American Chemical Residue Workshop in St. Petersburg, Florida, (July 2013, contact Kevin Armbrust or Steve Lehotay) and in PacifiChem (the International Chemical Congress of Pacific Basin Societies) in Hawaii, December 15-20, 2015 (contact John Johnston). AGRO has also begun conversations with the Chemistry Advisory Group of the Society of Environmental Toxicology and Chemistry (SETAC) to improve the atmosphere and increase the potential for interactions for chemists with other disciplines within SETAC and between other chemistry organizations.

Finally, the Communication Committee and leaders, Laura McConnell and Julie Eble, have instituted the *AGRO Lunch and Learn Webinar Series*. Highlighting the best oral presentations given at recent ACS-AGRO National Meetings, six webinars have been presented. Recordings for all but one have been posted on the AGRO website and are freely available. Ideas and volunteer organizers for the 2013-2014 *AGRO Lunch and Learn Webinar Series* are being sought. This monthly series is sponsored by grants from the ACS and ABC Laboratories. Many thanks to all for this wonderful new addition to our programming efforts!

Governance

The health and prosperity of AGRO is completely dependent on members stepping forward and offering their services for the common good. Al Barefoot, the past chair and Chair of the Election Committee, has put together an excellent slate of candidates for new officers and executive committee membership to be decided in the on-going election. We will post the results on the website at the end of August. Good luck to all.

The financial health of AGRO is good overall, due to excellent support from our patrons, strong programming that maintains our revenue from ACS, special grants, and earnings from investments and financial reserves. Nevertheless, we still are spending more than we receive annually, a non-sustainable situation. To stem this revenue shortfall, we have recently created a "Sponsorship Champion" position that will work closely with the current Program Chair and is focused solely on raising money in the support of specific symposia in the technical program for each ACS/AGRO national meeting. Al Barefoot is currently the first Sponsorship Champion and is actively working with Steve Duke on the ACS/AGRO meeting in Indianapolis. To date, Al has generated in excess of $13,000 from 7-8 sponsors in support of symposium speakers. Nice job, Al.

Professor Toshio Narahashi (1927-2013)

Professor Narahashi of Northwestern University, passed away on April 21, 2013. He was widely regarded as one of the founding fathers of neurotoxicology, and his leadership will be missed.

AGRO Division Fellows

1971	Dr. Louis Lykken
	Dr. Tom H. (Bucky) Harris
	Dr. Herman Beckman (Posthumous)
1972	Mr. Wendell F. (Bud) Phillips
	Dr. Don G. Crosby
	Dr. Elvins Y. Spencer
1973	Mr. Roger C. Blinn
	Dr. Philip C. Kearney
	Dr. Julius J. Menn
1974	Dr. Morton Beroza
	Dr. James P. Minyard, Jr.
	Dr. Joe C. Street
1975	Dr. Hank F. Enos
	Dr. Maurice B. Green
	Dr. Charles H. Van Middelem
1976	Dr. Marguerite L. Leng
	Dr. Jack R. Plimmer
	Dr. Gerald G. Still
1977	Dr. Gustave K. (Bob) Kohn
1978	Dr. S. Kris Bandal
	Dr. Paul Hedin
1979	Dr. Rodney D. Moss
1980	Dr. G. Wayne Ivie
	Dr. John B. Siddall (Posthumous)
1981	Dr. Robert M. Hollingsworth
	Dr. Gino J. Marco
1983	Dr. John Harvey, Jr.
1985	Mr. Henry Dishburger
	Dr. Richard C. Honeycutt
1986	Dr. Gunter (Jack) Zweig
1987	Dr. Willa Garner
1988	Dr. Jan Chambers
	Dr. James Seiber
1990	Dr. Joseph Fenyes
1991	Dr. Nancy N. Ragsdale
1992	Dr. Don Baker
	Dr. Joel Coats
	Dr. Guy Paulson
1993	Dr. Larry Ballantine
1994	Dr. James Heitz
	Dr. Ralph Mumma
	Dr. Willis Wheeler
1996	Dr. John Bourke
1998	Dr. Hank Cutler
	Mr. Paul Giesler
2000	Dr. Barry Cross
2001	Dr. Robert Hoagland
2003	Dr. Judd O. Nelson
2005	Dr. Rodney Bennett
2006	Dr. Terry D. Spittler
2007	Dr. John M. Clark
	Dr. Ann T. Lemley
	Dr. R. Don Wauchope
2008	Dr. Allan S. Felsot
2011	Dr. Laura L. McConnell
2012	Dr. Jeffrey J. Jenkins
	Dr. John J. Johnston
2013	Dr. Stephen Duke
	Dr. Cathleen Hapeman
	Dr. Ken Racke
	Dr. Teresa Wehner

AWARDS COMMITTEE REPORT

Dr. René Feyereisen of INRA Centre de Recherche de Sophia Antipolis in France is the recipient of the 2013 International Award for Research in Agrochemicals. Dr. Feyereisen receives this award in recognition of his exceptional accomplishments in research into the regulation of insect development, leading to the discovery of biorational targets for insecticidal agrochemicals. A day-long symposium in his honor, organized by Dr. Jim Ottea, will be held Monday at the 246th ACS National Meeting in Indianapolis.

Dr. Keith Solomon of the University of Guelph, School of Environmental Sciences is the winner of the 2013 USDA-Agricultural Research Service Sterling Hendricks Lectureship Award. Dr. Solomon will present his lecture on Tuesday morning at the ACS National meeting in Indianapolis.

Dr. Jeanette Van Emon of the U.S. Environmental Protection Agency, Las Vegas, will receive the 2013 Award for Innovation in Chemistry of Agriculture, for her creative and extensive research into applications of immunochemistry technology for the detection and measurement of pesticides and other toxic chemicals in environmental samples and in foods. This award, sponsored by BASF, is given annually to an active researcher working in North America who has successfully demonstrated an innovation in the chemistry of agriculture, veterinary science, or public health. Dr. Van Emon will deliver her award lecture on Tuesday morning at the ACS National meeting in Indianapolis.

Dr. John H. Grabber USDA-ARS Dairy Forage Research Center in Madison, Wisconsin, is the recipient of the 2013 Journal of Agricultural and Food Chemistry Research Article of the Year Award Lectureship in the AGRO category. The Journal, in cooperation with the AGRO and AGFD divisions, sponsors two lectureships each year (one in the AGRO category and one in the AGFD category) for outstanding papers published in JAFC. Dr. Grabber's lecture, "Using biomimetic cell wall models to identify new plant lignin bioengineering targets for improving forage and utilization," will be presented at the ACS National meeting in Indianapolis on Tuesday morning. The awardee in the AGFD category, **Dr. Thomas Hoffman**, will be featured at the same symposium. His lecture is entitled, "Molecular determinants of the sweet-bitter Janus head of steviol glycosides and development of novel quantitation tools."

Drs. Stephen Duke and **Cathleen Hapeman** of USDA-ARS, **Dr. Ken Racke** of Dow AgroSciences, and **Dr. Teresa Wehner** of Merial Ltd. will receive the Division Fellow Award in recognition of their dedicated and enthusiastic service to the AGRO Division and to the science of agrochemicals.

Dr. Atilla E. Pavlath will be this year's recipient of the Kenneth A. Spencer Award. The Spencer Award is presented by the Kansas City Section of the American Chemical Society for outstanding achievement in food and agricultural chemistry.

Nominations for the 2015 International Award for Research in Agrochemicals and the 2014 AGRO Award for Innovation in Chemistry of Agriculture are currently being accepted. The nomination criteria for the 2015 International and 2014 Innovation Awards can be found on page 21 & 23, respectively. The Awards Committee is also accepting nominations for the Division Fellow Award. Criteria for the Fellow award and what to submit are shown below. The deadlines each year are March 31 for the Fellow Award and December 31 for the International and Innovation Awards.

Nominations for the 2014 Sterling Hendricks Lectureship Award are being solicited by USDA-ARS. The nomination criteria can be found on page 27. Nominations for the Kenneth A. Spencer Award are being solicited by the ACS Kansas City Section, and criteria can be found on page 29. Nomination criteria for the 2014 JAFC Research Paper of the Year can be found on page 31.

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

Respectfully submitted,
James N. Seiber, Chair
Awards Committee

CALL FOR NOMINATIONS
AGRO DIVISION FELLOW AWARD

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

Criteria shall be –

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

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

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

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ACS International Award for Research in Agrochemicals

René Feyereisen

AGRO Award for Innovation in Chemistry of Agriculture

Jeanette Van Emon

AGRO Fellow Awards

Stephen Duke, Cathleen Hapeman,

Ken Racke, and Teresa Wehner

USDA-ARS Sterling Hendricks Lecturer

Keith Solomon

2013 ACS Kansas City Section Spencer Award

Atilla E. Pavlath

AGRO New Investigator Award Finalists

AGRO Education Award Winners

Fun, Food, Drinks, Good Company, and Door Prizes

You MUST pre-register by August 31, 2013 for this event.
Please visit the AGRO homepage for registration link.

Tuesday, September 10, 5:30 - 8:00 PM

Location: Dow AgroSciences World Headquarters
9330 Zionsville Road, Indianapolis

Buses will be leave at 5 pm from the
Crowne Plaza Hotel at Union Station on Capitol Avenue Entrance

ALL AGRO DIVISION MEMBERS, SPEAKERS, AND
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ACS International Award for Research in Agrochemicals

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Insect P450 paradox: Too simple as targets, too complicated as detoxifiers?

Dr. René Feyereisen is the recipient of the 2013 ACS International Award for Research in Agrochemicals. Dr. Feyereisen was born and grew up in The Hague. He received his Ph.D. degree from Louis Pasteur University in Strasbourg, France in 1979. After postdoctoral fellowships at the Agricultural Research Council at the University of Sussex and in the Department of Zoology at the University of Toronto, he served on the faculty of the Departments of Entomology and Agricultural Chemistry at Oregon State University (1981-1991) as the insect toxicologist. He moved to the University of Arizona as Professor of Entomology (1991-2000) and then joined the National Institute of Agronomical Research (INRA) at the Sophia Antipolis Research Center in France, where he is currently Director of Research.

Dr. Feyereisen's early studies, initiated over 30 years ago, described the roles of cytochrome P450 enzymes in the biosynthesis of ecdysteroids and juvenile hormones (JH). His efforts began with the biochemical characterization of the enzymes, continued through the use of powerful inhibitors of JH biosynthesis and led to the molecular cloning and reconstitution of CYP15, the JH epoxidase. Feyereisen's lab has also made major contributions to our understanding of factors underlying the physiological regulation of juvenile hormone titers through the discovery of allatostatins as "brain-gut" peptides, neuromodulators of juvenile hormone synthesis. His studies of the metabolism of hormones regulating insect development and metamorphosis have greatly enhanced our fundamental knowledge of these systems, calling attention to these insect-specific target sites.

In addition, Dr. Feyereisen is perhaps best well known for his groundbreaking research on the role of cytochrome P450 enzymes in insecticide detoxification and resistance. In the late 1980s, his lab was among the first to apply molecular technologies toward the study of enzymes involved in insecticide metabolism and was the first to clone an insect P450 enzyme and the first to succeed in the heterologous expression and reconstitution of the various components of the insect microsomal cytochrome P450 complex, NADPH cytochrome P450 reductase, cytochrome b5 and various P450s. The reconstituted system of purified enzymes provided clean biochemical evidence for the wide substrate specificity of a major house fly P450, CYP6A1, which was shown to be responsible for metabolism of (and resistance to) many insecticides.

Dr. Feyereisen has continued to pioneer the application of molecular genetic technologies in research that is of key importance to agrochemical toxicologists, including DNA microarrays or detox chips. These efforts have yielded a more complete understanding of the regulatory mechanisms leading to the constitutive overexpression of insecticide-metabolizing enzymes in resistant arthropods. Feyereisen's work has increased our understanding of the evolution of the P450 gene family and these studies are especially relevant today, in an era when metabolic resistance has become a major impediment to the design and prolonged field use of pesticides.

In addition to his research, Dr. Feyereisen has written a number of influential reviews on JH biosynthesis, insecticide resistance, and on cytochrome P450 enzymes. He is currently co-editor of *Insect Biochemistry and Molecular Biology*, and has previously served on the editorial boards of *Pesticide Biochemistry and Physiology*, *Archives of Insect Biochemistry and Physiology* and on the Editorial Committee of *Annual Review of Entomology*. He co-chaired the 1997 Gordon Conference on Agricultural Science and served on the organizing committees of the IUPAC International Congresses of Pesticide Chemistry.

Please join us in a day-long symposium honoring Dr. Feyereisen on Monday, September 9, at 8:00 AM in Crowne Plaza at Historic Union Station, Illinois Street Ballroom West

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AGRO Award for Innovation in Chemistry of Agriculture

Sponsored by BASF Corporation

Immunochemistry in motion: Applications to agrochemicals

Dr. Jeanette M. Van Emon, an AGRO Councilor, is the recipient of the 2013 Award for Innovation in Chemistry of Agriculture. She is receiving this recognition for her creative and extensive research into applications of immunochemistry technology for the detection and measurement of pesticides and other toxic chemicals in environmental samples and in foods. The award will be presented at the Tuesday morning AGRO Awards Symposium, where she will also give a presentation.

Dr. Van Emon is a research chemist in the U.S. EPA National Exposure Research Lab in Las Vegas, Nevada. She became a member of the ACS during her graduate school days at UC Davis working in the labs of Bruce Hammock and Jim Seiber. Part of her graduate school research pioneered the use of immunoassays for measuring pesticides on clothing patches, air samples, and hand rinses taken during field monitoring and worker exposure studies. She credits ACS for providing her with many opportunities to interact with chemists and scientists across an array of fields from all over the globe. In 2012 she received the honor of ACS fellow for her work in applying some of the first immunoassays to environmental contaminants and for the development of the EPA Immunochemistry Summit meeting series. These meetings brought together government and academic researchers with chemical registrants for the first time to discuss the emerging area of environmental immunoassays. These meetings helped to foster the acceptance of immunoassay technology by building partnerships and facilitating information exchanges within and outside EPA. Some of these Summit meetings were held in conjunction with AGRO programming at national ACS meetings. She received the EPA Office of Research and Development Statesmanship Award, and she was twice awarded the EPA and American Chemical Society joint Science Achievement Award in Chemistry for her research and outreach to other agencies and organizations.

In addition to being an AGRO Councilor, she is a member of the Division Activities Committee and Innovative Project Grants Subcommittee. She is Chair of the ACS Western Regional Board and a member of the Editorial Advisory Board for the Journal of Agricultural and Food Chemistry. She is past Chair and Program Chair for the AGRO Division. She is a past editorial board member for Analytical Chemistry. She has been twice chairman for the Southern Nevada Local Section, co-organizer of the 2008 Western Regional Meeting, and is currently chair of the Section's Women Chemist Committee. She has organized several ACS symposia which have resulted in ACS symposium series books.

Dr. Van Emon will be presented this award prior to her paper in the symposium on Tuesday, September 10, at 10:15 AM in Crowne Plaza at Historic Union Station, Milwaukee

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

BASF The Chemical Company

AGRO Division Fellow Awards

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

Presented to Stephen O. Duke, Cathleen J. Hapeman, Kenneth D. Racke, and Teresa A. Wehner

Dr. Stephen O. Duke holds a BS in Biology (Henderson State U) and an MS in Botany (U Arkansas). After returning to the US from a stint in Vietnam as a Medical Service Corps officer, he earned his PhD (Duke U, 1975) in Botany. Shortly thereafter he joined the USDA-Agricultural Research Service (ARS) in Stoneville, Mississippi, where he became engrossed with the modes of action of herbicides and other phytotoxins and eventually become the Director of the Southern Weed Science Laboratory. In 1996, he become Research Leader of the USDA-ARS Natural Products Utilization Research Unit, which is embedded in the School of Pharmacy at University of Mississippi in Oxford.

Steve is probably best known for his research on the modes and mechanisms of action of herbicides. He has published almost 400 journal articles and book chapters, edited seven books, and co-authored one text book. These publications cover many aspects of agricultural chemical-related research, including discovery and modes of action of natural and synthetic herbicides and fungicides, mechanisms of resistance to herbicides, anti-malarial compounds, insect repellents, and biochemistry and physiology of herbicide-resistant crops. He has been a member of the many editorial boards including Plant Physiology, Weed Science, and Allelopathy Journal and is now Editor-in-Chief of Pest Management Science. He has received numerous awards including: Fellow of AAAS and the Weed Science Society of America, USDA-ARS Outstanding Senior Scientist Award, AGRO International Award for Research in Agrochemicals, Molisch Award of the International Allelopathy Society, and an honorary doctorate from University of the Basque Country (Spain).

As an AGRO active member since 1984, Steve has organized numerous AGRO symposia and edited four ACS Symposium Series books. He was a member of the AGRO Executive Board during 1996-98 and 2008-11, was elected 2012 Vice-Chair, and is currently the Program Chair. Steve looks forward to serving AGRO as Chair next year and to future involvement in AGRO symposia and publications. In his words, “Involvement in AGRO has been a major positive influence on my career. Good citizens of the scientific community attempt to repay such debts. I hope that I can play a helpful role in the careers of young scientists through my continued involvement in AGRO.”

Dr. Cathleen J. Hapeman earned her BS (Chemistry 1981) and PhD (Mechanistic Organic Photochemisty1986) at the University of Maryland, College Park and then promptly moved two miles down US Route 1 to USDA-ARS in Beltsville, Maryland. Her research has focused on both basic and applied aspects of pollutant fate, blending chemical proficiency and environmental process expertise with decades of experience in agricultural practices and acquired regulatory knowledge. She served as Research Leader for eight years where she learned very quickly that effectively communicating scientific achievements is as important as the discoveries themselves.

Cathleen has been involved with AGRO since she started her research career at ARS. She was the first recipient of the AGRO Young Scientist Research Award, making her keenly aware of how this support can boost a scientist in their early career. For several years she served as Coordinator of the New Investigator Award, which has recently been restructured to include an oral presentation competition. Cathleen has also organized many AGRO symposia and mentored others to organize and run symposia, frequently in collaboration with other Divisions. She has engaged non-research scientists, regulators, and policy makers to participate and to contribute their perspectives. As a member of the Communications Committee she has been involved in exploring non-traditional venues for providing AGRO members with useful information.

Although Cathleen has contributed in many ways to AGRO's success, perhaps her most substantial achievement to date has been as the editor of the *PICOGRAM* which has become a premier ACS Division publication. She reorganized the *PICOGRAM* format to meet membership needs and to provide a more informative document for the National ACS Meetings. Since 2006, she has worked closely with all the Division Program Chairs in preparing for upcoming meetings, including streamlining the proposals for Symposia (Call for Papers), editing abstracts, and modifying each *PICOGRAM* edition for each meeting.

A member of the Executive Committee since 2005, Cathleen currently serves as the 2013 AGRO Vice Chair. She is actively engaged in her upcoming role as AGRO 2014 Program Chair and Scientific Program Chair of the 13th IUPAC International Congress of Pesticide Chemistry. She looks forward to a year of intense activity working with co-organizers Laura McConnell and Ken Racke, the Scientific Program Committee Teams, and all the other committees and organizers.

AGRO Division Fellow Awards

Dr. Kenneth D. Racke is a global research leader with Dow AgroSciences in Indianapolis, Indiana. He received a BA in Biology from Trinity Christian College in 1981, a MS in Entomology from The University of Wisconsin in 1984, and a PhD in Entomology from Iowa State University in 1987. Ken has been with Dow since 1988 and has served in a variety of roles related to insecticide development and regulation. His interests include environmental chemistry, risk assessment, pesticide residues in food, and international trade standards.

Ken is a long-time member of and scientific program organizer for AGRO, and past symposia he has helped organize include sessions on enhanced biodegradation of soil pesticides, fate and significance of pesticides in urban environments, crop protection products for organic agriculture, pesticide residues in food and international trade, and pesticide regulation and endangered species protection. Ken has chaired the AGRO Young Scientist Recognition Committee and the International Activities Committee, and has served as a member of the Executive Committee and Long-Range Planning Committee. During 2011, he served as Chair of the AGRO Division, following his role of Chair-Elect for 2010 in organizing the AGRO program for the spring ACS meeting in San Francisco.

Ken has also been active for the past 20 years in promoting international crop protection chemistry activities through the International Union of Pure and Applied Chemistry (IUPAC). Through IUPAC, he has led the organization of international and regional pesticide chemistry workshops and projects which promote internationally harmonized approaches to evaluation and regulation of agrochemicals.

In serving as co-chair for organizing the 13th IUPAC International Congress of Pesticide Chemistry on behalf of AGRO for the Fall 2014 ACS meeting in San Francisco, Ken is bringing together his long-standing science and international interests and his commitment to both AGRO and IUPAC.

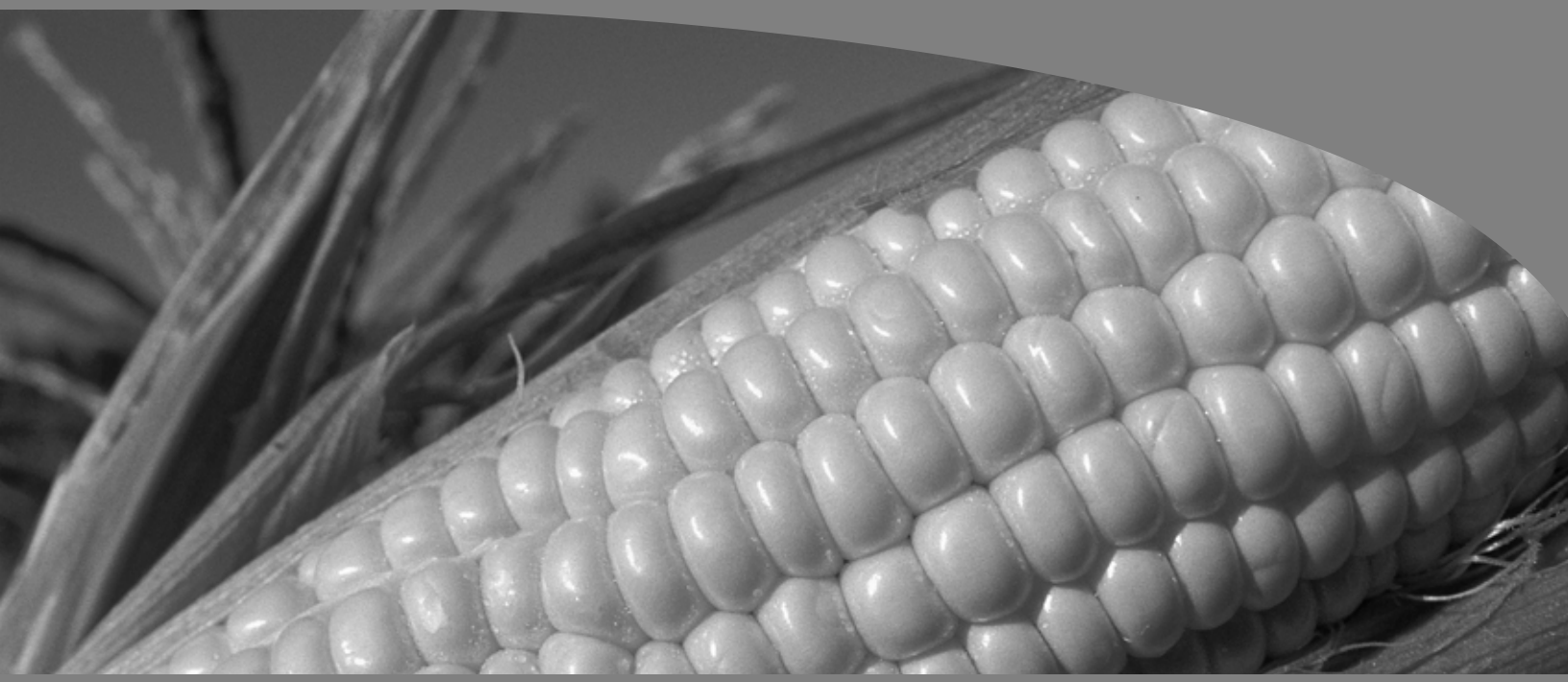
Dr. Teresa A. Wehner earned her BS in Chemistry from the University of California, Riverside in 1974. She worked briefly at Shell Oil Company in Houston, Texas and at the US Environmental Protection Agency in Washington, DC. She returned to graduate school at the University of California, Davis where she earned her PhD in 1982 under Dr. James Seiber studying pesticide residues in the air. During her studies, Teresa developed and implemented a multi-residue method using high pressure liquid chromatography fractionation and capillary gas chromatography for quantitation, the first of many residue methods that she would develop during her career.

Teresa was hired in 1982 by Merck Research Laboratories in Rahway, New Jersey. At Merck, she developed methods for determining the residues of various agricultural chemicals and veterinary drugs, including compounds from the anthelmintic or insecticide family of avermectins. She was fortunate to be teamed with many hard-working and imaginative scientists on projects that led to new products and commercial success. Through her teams, she was able to introduce some innovations to methods that would eventually be validated by regulatory agencies for surveillance or enforcement of residue limits in edible commodities. Following a normal industrial career progression, she received increasing responsibilities for managing people and projects and spent less time working in the laboratory.

In 1997, Merck formed a joint venture with Rhone-Poulenc (which eventually became Aventis, Sanofi-Aventis and then Sanofi) to create Merial, an animal health company, to which Teresa was assigned. Merial became solely owned by Sanofi in 2009. At Merial, Teresa has worked on veterinary pharmaceuticals in the Pharmacokinetics & Drug Metabolism department, part of Research & Development. She has been instrumental in teams obtaining or retaining approvals and marketing authorizations for more than 25 separate products, with registrations that span the globe, from Japan, Latin America, and Europe as well as the United States. These products maintain or improve the health of various species, ranging from cattle and sheep to horses, pigs, dogs and cats, as well as exotics such as deer, camel and bison.

Teresa has been a member of the American Chemical Society since 1975 and of the AGRO Division (and earlier iterations) since 1980 and served as a member of the Executive Committee for AGRO from 1999 to 2008. Teresa was instrumental in broadening the definition of the AGRO Division as chemistry for and from agriculture, emphasizing that agriculture includes more than crops. She has been privileged to collaborate one way or another with several previous AGRO Division Fellows, including Jeff Jenkins, John Johnston, and James Seiber. She co-organized symposia for the AGRO division programs at ACS meetings with other industry partners and state and federal scientists and policy makers. These symposia encompassed novel or emerging methods for determining residues or the environmental fate for agrochemicals. Teresa has elected to retire from Merial in August 2013 but will remain active in the AGRO Division.

Thank you Steve, Cathleen, Ken, and Teresa for all you have done for AGRO!



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2013 Sterling B. Hendricks Memorial Lectureship Award

Sponsored by USDA-Agricultural Research Service

Co-Sponsored by AGFD & AGRO Divisions

Arriving at the truth: Weight of evidence for assessing risks of agrochemicals.

Dr. Keith Solomon is Professor Emeritus and Associate Graduate Faculty in the School of Environmental Sciences at the University of Guelph. He is also Director of the Centre for Toxicology.

Professor Solomon teaches in areas of toxicology and pesticides at the University of Guelph and advises graduate students. He directs an active program of research into the fate and effects of pesticides and other substances in the environment, exposure of humans to pesticides and industrial chemicals, and risk assessment. He has, and continues to serve on several advisory committees on matters related to environmental toxicology and pesticides in Canada, the USA, and internationally. He is a member of the Society of Environmental Toxicology and Chemistry, the American Chemistry Society (Agrochemistry and Environmental Chemistry), and the American Association for the Advancement of Science. He is the recipient of the 1993 Society for Environmental Toxicology and Chemistry-ABC Laboratories award for Environmental Education, was elected as a Fellow of the Academy of Toxicological Sciences in December 1999, and is recipient of the 2002 American Chemical Society International Award for Research in Agrochemicals. In 2006, he was awarded the SETAC Europe Environmental Education Award and the Society for Environmental Toxicology and Chemistry Founders Award. He is co-author of the book, *Pesticides and the Environment*, which has been translated into Spanish and Portuguese and is used as a teaching text at the University of Guelph and in a number of universities around the world.

He graduated of Rhodes University with a B.S. (Honors) in Chemistry and Zoology and holds M.S. degrees from Rhodes University and the University of Illinois as well as a Ph.D. from Illinois. He has more than 40 years of experience in research and teaching in pesticide science and toxicology and has contributed to more than 400 scientific publications and reports in the fields of pesticides, environmental toxicology, and risk assessment. To date, he has advised or co-advised eight Post-Doctoral Fellows, 41 Masters Students, and 31 Doctoral Students and has given a large number of short courses on pesticides in Canada and around the world.

Dr. Solomon will deliver his lecture immediately following presentation of the Sterling Hendricks Award on Tuesday, September 10, at 11:20 AM, in the Crowne Plaza at Historic Union Station, Milwaukee

JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY

2013 Research Article of the Year Award Lectureship Awards

Sponsored by The Journal of Agricultural and Food Chemistry

Co-sponsored by AGFD & AGRO Divisions

Dr. John Grabber is a Research Agronomist with the USDA-Agricultural Research Service and has worked at the U.S. Dairy Forage Research Center in Madison, Wisconsin, since 1999. Previously, he was employed as a Postdoctoral Research Associate with the USDA and the Monsanto Company and as an Agronomist with the W.H. Miner Agricultural Research Institute. He received graduate degrees in Agronomy and Plant Sciences from the Pennsylvania State University and the University of Connecticut. A primary focus of Dr. Grabber's work has been to develop and utilize a biomimetic cell wall model for delineating how variations in lignin composition, structure, and cross-linking affect the susceptibility of cell walls to microbial fermentation, chemical pretreatment, and enzymatic saccharification. Recently, Grabber and colleagues have used the model to identify new lignin bioengineering targets for improving the conversion cellulosic biomass into biofuels and the utilization of fibrous feed by livestock. Other areas of collaborative research include improving methods for quantifying condensed tannins and assessing their effects on forage proteolysis and developing higher yielding alfalfa-based cropping systems for dairy farms. Results of these efforts have been disseminated in 65 peer-reviewed journal articles and 19 articles of other types.

The title of his lecture is, "Using biomimetic cell wall models to identify new plant lignin bioengineering targets for improving forage and biomass utilization."

Dr. Thomas Hofmann studied food chemistry at the University of Erlangen-Nürnberg and received his Ph.D. (1995) and habilitation (1998) at the Chemistry Department of the TU München (TUM). From 1999 to 2002, he was deputy director of the German Research Center for Food Chemistry of the Leibnitz Society. In 2002, he took over the Chair of Food Chemistry of the University of Münster, and since 2007 he holds the Chair of Food Chemistry and Molecular Sensory Science at TUM, is head of the BIOANALYTICS unit of the Center of Nutrition and Food Sciences of TUM, and is currently vice president for research and innovation of TUM. His scientific achievements in molecular sensory science is published in more than 220 papers and 25 patents, and he is honored by several awards such as the Kurt-Täufel Award of the Young Scientist, German Chemical Society (1999); Young Scientist Award of the Agricultural and Food Chemistry Division, American Chemical Society (1999); and the ACS Fellow Award of the Agricultural & Food Chemistry Division, American Chemical Society (2008).

The title of his lecture is, "Molecular determinants of the sweet-bitter Janus head of steviol glycosides and development of novel quantitation tools."

The Journal of Agricultural and Food Chemistry
Best Paper Awards Session
will be held on Tuesday, September 10, beginning at 8:25 AM
at the Crowne Plaza in Historic Union Station, Grand Central Station A&B

ENVIRONMENTAL MODELING
- Chemical Fate and Transport
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- Site-Specific Modeling and Calibration
- Hydrologic Modeling
- Monte Carlo and Traditional Statistical Analysis

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- Aquatic and Terrestrial Toxicology Assessment
- Study Monitoring and Testing Strategy
- Regulatory Strategy
- Registration Review Support

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- Vulnerability Analysis
- Spatial and Temporal Exposure Characterization
- Risk Mapping

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- Watershed and Ecological Monitoring
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Dr. Attila Pavlath was born in 1930 in Budapest and received all his education there. In Hungary he was an Assistant Professor at the Technical University of Budapest. He was the co-founder of fluorine chemistry research in Hungary. In 1956, after the Hungarian Revolution he escaped Hungary together with his family. After two years at the McGill University in Montreal, Canada he joined Stauffer Chemical Company in Richmond, California, to lead a research group on agriculture related problems. In 1967, at the invitation of the U.S. Department of Agriculture, he continued his research at the Western Regional Research Center, in Albany, California, where he headed various research to help U.S. agriculture. He officially retired in 2000, but continues as a Senior Emeritus Research Chemist.

In his 60+ years of teaching and conducting research, Dr. Pavlath pioneered research not just in fluorine chemistry, but also in areas of glow discharge, biomass, biodegradable films and various agricultural chemistry problems. He published more than 130 research papers, and he wrote 10 books and larger chapters. He also has 25 patents, some of which are commercialized. He has lectured throughout the world at various scientific meetings, universities, and research institutes. He received many awards; among them in, 1997 he was awarded the Pioneer of the Year by the American Institute of Chemists, and in 2004, he was elected to the Hungarian Academy of Science. He is the honorary lifetime President of the ACS Hungarian International Science Chapter.

In addition to his scientific accomplishments, he is equally well known for his various worldwide activities to help the chemical profession. One of them is the badly needed improvement of the public image of chemistry. He developed a worldwide program to educate the public about the benefits of chemical developments, which provide almost everything in our everyday life. He is also very well known in the American Chemical Society for his continuous activities to modernize the Society. In 1999, the members elected him as President, and he is still very active in these areas.

Please join us at an afternoon
AGFD *Symposium honoring Dr. Pavlath*
on Tuesday, September 10, at 1:00 - 4:00 PM
in the Indiana Convention Center, Room 107

Past Awardees of the Burdick & Jackson International Award

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

Past Awardees of the ACS International Award For Research in Agrochemicals

Co-Sponsored by BASF & DuPont Crop Protection

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

Sponsored by DuPont Crop Protection

2012 Dr. Thomas C. Sparks, Dow AgroSciences
2013 Dr. René Feyereisen, INRA, Nice, France

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

2015 Fall ACS National Meeting in Boston, Massachusetts

The ACS International Award for Research in Agrochemicals is given to a scientist who has made outstanding contributions to the field of agrochemicals at the international level. Their vision and sustained contributions will have opened new horizons for other investigators in their field and beyond.

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

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

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

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

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

Please email this information to:

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

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CALL FOR NOMINATIONS
AWARD FOR INNOVATION IN CHEMISTRY OF AGRICULTURE
Sponsored by BASF Corporation

2014 Fall ACS National Meeting in San Francisco, California

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

The Nomination email will include the following as attachments:

1. A **formal letter of nomination** that includes
   - Name, business address, phone and email address of the nominator
   - Name, birth date, business address, phone and email address of the nominee
   - A nomination statement (200-1000 words) giving reasons why the nominee should receive this award, stressing the chemical innovation and how it has enhanced agricultural or veterinary pest management and productivity.
2. The nominee's **current curriculum vitae**
3. One or two **letters of support**
4. Reference or e-mail link to 1 or 2 published **manuscripts that report on the work** which supports the award nomination

Deadline: Nominations should be received by the committee chair by ***December 31*** of each year.

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

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

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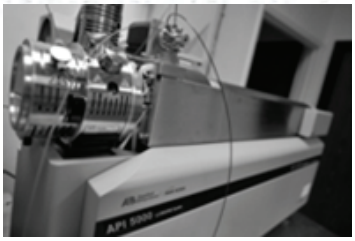


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Call for Nominations

IUPAC 2014 International Award for Advances in Harmonized Approaches to Crop Protection Chemistry

This award recognizes individuals in government, intergovernmental organizations, industry, and academia who have exercised personal leadership for **outstanding contributions to international harmonization for the regulation of crop protection chemistry**.

The award is administered by the IUPAC Advisory Committee on Crop Protection Chemistry, and is presented on a biennial basis during even-numbered years in conjunction with an IUPAC-sponsored conference or special symposium.

Awardees receive a $3,000 honorarium plus travel and per diem reimbursement to attend the award presentation ceremony. Corporate sponsorship for the award has been arranged with Dow AgroSciences.

Nominations will consist of:

- A **nomination letter** including the nominee's birthplace, date of birth, citizenship, business address, and a description (200-1000 words) of the reasons why the nominee should receive this award, stressing the individual's major accomplishments toward international harmonization for the regulation of crop protection chemistry.
- A **curriculum vitae** of the candidate that includes places and names of employment, professional affiliations, committee and working group assignments, and listing of relevant regulatory guidance documents, reports, and/or publications.
- One or more **letters of support**.

Nominations for the 2014 award are due **December 1, 2013**, and should be sent to:

Dr. John Unsworth, Chairman
IUPAC Advisory Committee on Crop Protection Chemistry
25 Vellacotts
Chelmsford, Essex CM1 7EA
UNITED KINGDOM
Phone: +44 1245 440 056
unsworjo@aol.com

PAST AWARDEES

2012 **Lois A. Rossi**, Office of Pesticide Programs, United States Environmental Protection Agency, Washington DC, USA

2010 **Denis J. Hamilton**, Animal and Plant Service, Queensland Department of Primary Industries, Brisbane, Australia

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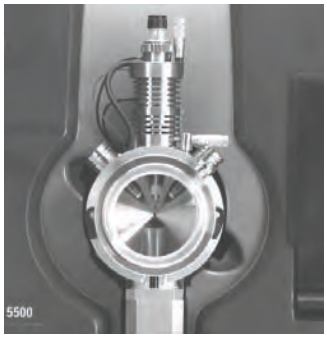

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2014 STERLING B. HENDRICKS MEMORIAL LECTURESHIP

Sponsored by USDA-Agricultural Research Service

Co-Sponsored by AGFD & AGRO Divisions

The USDA-Agricultural Research Service (ARS) is seeking nominations for the 2014 Sterling B. Hendricks Memorial Lectureship Award. This Lectureship was established in 1981 by ARS to honor the memory of Sterling B. Hendricks and to recognize scientists who have made outstanding contributions to the chemical science of agriculture. Dr. Hendricks contributed to many diverse scientific disciplines, including soil science, mineralogy, agronomy, plant physiology, geology, and chemistry. He is most frequently remembered for discovering phytochrome, the light-activated molecule that regulates many plant processes. The lecture should address a scientific topic, trend, or policy issue related to agriculture. Deadline is **December 1, 2013.**

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

Nominees will be outstanding senior scientists in industry, universities, consulting, or government positions. *Current ARS employees are not eligible.* The Award will be presented during an American Chemical Society National Meeting held in 2014 in San Francisco, California, prior to the Lecture. Giving the presentation is a requirement of the honor.

The **Nomination Package** includes:

- A letter explaining the nominee's contributions to chemistry and agriculture,
- A current *curriculum vitae*

Nomination packages may be sent electronically in pdf format (Adobe 8.0 or greater; no reformatting will be done) to:
Kim Kaplan, Lecture Coordinator, kim.kaplan@ars.usda.gov

Or, hard copy nominations packages may be submitted via courier to:
Kim Kaplan, Lecture Coordinator, ARS Information Office, Room 1-2253, Mail Stop #5128, 5601 Sunnyside Avenue, Beltsville, MD 20705, phone: 301-504-1637.

PAST STERLING B. HENDRICKS MEMORIAL LECTURESHIP AWARD WINNERS

1981	Norman E. Borlaug, Nobel Laureate, International Maize and Wheat Improvement Center, Mexico City
1982	Warren L. Butler, University of California, San Diego
1983	Melvin Calvin, Nobel Laureate, University of California, Berkeley
1984	Frederick Ausubel, Harvard Medical School and Massachusetts General Hospital, Boston, MA
1985	Alan Putnam, Michigan State University
1986	Ralph Hardy, Cornell University and BioTechnica International
1987	Mary-Dell Chilton, Ciba-Geigy Corporation, Research Triangle Park, NC
1988	Bruce N. Ames, University of California at Berkeley
1989	Sanford A. Miller, University of Texas Health Science Center at San Antonio
1990	Roy L. Whistle, Purdue University
1991	Peter S. Eagleson, Massachusetts Institute of Technology
1992	John E. Casida, University of California, Berkeley
1993	Philip H. Abelson, Deputy Editor, *Science*, and Scientific Advisor to AAAS
1994	Wendell L. Roelofs, Cornell University
1995	Winslow R. Briggs, Carnegie Institution of Washington
1996	Hugh D. Sisler, University of Maryland
1997	Ernest Hodgson, North Carolina State University
1998	Morton Beroza, USDA-ARS, Maryland (retired)
1999	Bruce D. Hammock, University of California, Davis
2000	William S. Bowers, University of Arizona
2001	Malcolm Thompson, USDA-ARS, Maryland (retired)
2002	Ervin E. Leiner, University of Minnesota
2003	Kriton Kleanthis Hatzios, Virginia Polytechnic Institute and State University
2004	Robert L. Buchanan, Food & Drug Administration
2005	Donald L. Sparks, University of Delaware
2006	Stanley B. Prusiner, Nobel Laureate, University of California, San Francisco
2007	Bruce E. Dale, Michigan State University
2008	Fergus M. Clydesdale, University of Massachusetts, Amherst
2009	Charles J. Arntzen, Arizona State University, Tempe
2010	Chris Somerville, Director of the Energy Biosciences Institute, Berkeley
2011	Deborah P. Delmer, University of California, Davis
2012	Eric Block, University at Albany, State University of New York
2013	Keith R. Solomon, University of Guelph

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Call for Nominations
2014 Kenneth A. Spencer Award
Sponsored by ACS Kansas City Section

The Kansas City Section of the American Chemical Society is soliciting nominations for the 2014 Kenneth A. Spencer Award. The award recognizes meritorious contributions to the field of agricultural and food chemistry. The Kansas City Section presents this award in the hope that it will give added stimulus in research, education, and industry to further progress in agricultural and food chemistry. The award has been awarded annually in Kansas City since 1955 and carries an honorarium of $6,000. At this meeting the recipient will deliver an address, preferably upon the subject of the work for which they have been recognized. Subsequently, that address will be published, if possible, in an appropriate journal. The Kansas City Section will reimburse the recipient and spouse for round-trip travel expenses to Kansas City for the presentation.

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

The nomination shall include a biographical sketch of the nominee containing minimum vital statistics, parents' names, education and professional experience; a list of published papers and patents; a specific identifying statement of the work on which the nomination is based; and an evaluation and appraisal of the nominee's accomplishments with special emphasis on the work to be recognized by the award.

Nominations are due before November 15, 2013. Forms and information can be found at http://cas.umkc.edu/chemistry/kcacs.

Contact HellmuthE@umkc.edu for questions and to submit nominations electronically.

Or, mail nomination to:

Spencer Award Committee
Kansas City Section of ACS Chemistry Department
University of Missouri-Kansas City
Spencer Chemistry Building, Room 210
5009 Rockhill Road, Kansas City, MO 64110 for FedEx, UPS
-or-
5100 Rockhill Road , Kansas City, MO 64110 for USPS

Past Kenneth A. Spencer Award Winners

1955	Ralph M Hixon, Iowa State University
1956	Conrad A Elvehjem, University of Wisconsin
1957	William C Rose, University of Wisconsin
1958	EV McCollum, Johns Hopkins University
1959	Karl Folkers, Merck, Sharpe & Dohme Res. Labs.
1960	CH Bailey, University of Minnesota
1961	HL Haller, USDA-Agricultural Research Service
1962	AK Balls, USDA-Agricultural Research Service
1963	CC King, Rockefeller Foundation
1964	Daniel Swern, Temple University
1965	Aaron M. Altschul, USDA-Agricultural Research Service
1966	Robert L. Metcalf University of California, Riverside
1967	Melville L. Wolfrom, The Ohio State University
1968	Herbert E. Carter, University of Illinois
1969	Edwin T. Mertz, Purdue University
1970	Lyle D. Goodhue, Phillips Petroleum Company
1971	William J. Darby, Vanderbilt University
1972	Emil M. Mrak, University of California, Davis
1973	Esmond E. Snell, University of California, Berkeley
1974	Roy L. Whistler, Purdue University
1975	Thomas H. Jukes, University of California, Berkeley
1976	E. Irvine Liener, University of Minnesota
1977	N. Edward Tolbert, Michigan State University
1978	John E. Casida, University of California, Berkley
1979	Charles W. Gehrke, University of Missouri-Columbia
1980	George K. Davis, University of Florida, Gainesville
1981	John Speziale, Monsanto Agricultural Products Co.
1982	Howard Bachrach, USDA-Agricultural Research Service
1983	Peter Albersheim, University of Colorado
1984	Richard H. Hageman, University of Illinois
1985	Bruce N. Ames, University of California, Berkeley
1986	John M. Brenner, Iowa State University
1987	Hector F. DeLuca, University of Wisconsin, Madison
1988	Boyd L. O'Dell, University of Missouri-Columbia
1989	Robert H. Burris, University of Wisconsin
1990	John E. Kinsella, University of California, Davis
1991	George Levitt, DuPont Experimental Station
1992	Clarence A. Ryan, Jr., Washington State University
1993	Bruce Hammock, University of California, Davis
1994	William S. Bowers, University of Arizona
1995	Robert T. Fraley, Ceregen, A Unit of Monsanto Co.
1996	James N. BeMiller, Purdue University
1997	William M. Doane, USDA-Agricultural Research Service
1998	Mendel Friedman USDA-Agricultural Research Service
1999	James A. Sikorski, Monsanto Co.
2000	Wendell L. Roelofs, Cornell University
2001	James Tumlinson USDA-Agricultural Research Service
2002	Daniel W. Armstrong, Iowa State University
2003	Eric Block, University at Albany, State Univ. New York
2004	Steven D. Aust, Utah State University
2005	Don R. Baker, Berkeley Discovery Inc.
2006	Russel Molyneux USDA-Agricultural Research Service
2007	David A. Schooley, University of Nevada, Reno
2008	Ron G. Buttery, USDA-Agricultural Research Service
2009	George P. Lahm, DuPont Crop Protection
2010	Clive A. Henrick, Trece, Inc.
2011	Michael W. Pariza, University of Wisconsin, Madison
2012	James N. Seiber, University of California, Davis

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As honey bee hive numbers decline, researchers are examining relationships between chemical, biological, managerial, and ecosystemic factors.

Concurrently, as the human population increases, pressure for higher agricultural production has prompted scrutiny of chemicals that may influence honey bees and other pollinators.

Regulators seek information to ascertain the benefits of a chemical's presence to deter the target organism(s), while mitigating the detrimental effects, if any, on beneficial non-target organisms.

Read about these regulatory developments in Smithers Viscient's Update on Pollinator Issues white paper.

Download the white paper and view additional resources and information at www.ThePollinator.net.

Smithers Viscient performs environmental and consumer safety contract research for the pharmaceutical, agrochemical, and chemical industries.
Smithers Viscient will attend the American Chemical Society National Meeting, September 8-12, 2013 in Indianapolis, IN, USA. Contact us to book an appointment.
Smithers Viscient locations:
Massachusetts, United States | North Carolina, United States | Harrogate, United Kingdom | Tokyo, Japan
Web: www.SmithersViscient.com | Email: info@smithersviscient.com

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JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY

CALL FOR NOMINATIONS

2014 RESEARCH ARTICLE OF THE YEAR AWARD LECTURESHIP

Co-sponsored by AGFD & AGRO Divisions

The Journal of Agricultural and Food Chemistry (JAFC) and the ACS Divisions of Agricultural and Food Chemistry (AGFD) and Agrochemicals (AGRO) are seeking nominations for the Research Article of the Year Award Lectureship. Two papers will receive awards – one in the subject area of agrochemicals (pesticides, biofuels and biobased products, and related), and one in agricultural and food chemistry (food, health, and related) for an outstanding article published in 2013 (either in an issue of JAFC or ASAP) that demonstrates creativity and impact on agricultural and food chemistry as a whole.

Each winner will receive an award plaque, $1000 USD, and travel expenses up to $1250 USD to attend the Fall 2014 ACS National Meeting in San Francisco, CA.

The winners will be announced in early 2014, and the award will be presented at the Fall 2014 ACS National Meeting held August 10-14, 2014, at a symposium featuring the awardees.

Nominations should include:

- Name, affiliation, and e-mail address of the nominator
- Nominee's article title and DOI (hyperlinked to the article if possible)
- Name, affiliation, and e-mail address of the corresponding author (no self-nominations)
- A statement of why the article is outstanding (< 500 words)
- Suggestion of a category AGFD or AGRO*
- The words "JAFC nomination" in the title of the email

*Nominees will be divided into two categories, one in the subject area of agrochemicals (pesticides, biofuels and biobased products, and related), and one in agricultural and food chemistry (food, health, and related). This will be subject to the discretion of the Editor-in-Chief.

Send your nominations by **February 14, 2014**, to: jafcaward@acs.org

PAST JOURNAL OF AGRICULTURE AND FOOD CHEMISTRY

RESEARCH ARTICLE OF THE YEAR AWARD LECTURESHIP AWARD WINNERS

2013:

John H. Grabber, Dino Ress, and John Ralph
Identifying New Lignin Bioengineering Targets: Impact of Epicatechin, Quercetin Glycoside, and Gallate Derivatives on the Lignification and Fermentation of Maize Cell Walls

Caroline Hellfritsch, Anne Brockhoff, Frauke Stähler, Wolfgang Meyerhof, and Thomas Hofmann
Human Psychometric and Taste Receptor Responses to Steviol Glycosides

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AGRO DIVISION
2013 NEW INVESTIGATOR AWARD FINALISTS
Sponsored by Dow AgroSciences

Chloé de Perre, Daniel Swale, Chitvan Khajuria

Please plan to attend presentations by our Three NIA Finalists

Dr. De Perre's talk will be at the Crowne Plaza at Historic Union Station, Milwaukee,
Drs. Swale and Khauiria will present at the Crowne Plaza at Historic Union Station, Illinois Street Ballroom East

MONDAY: Biopesticides: State of the Art and Future Opportunities

Environmental Fate, Transport, and Modeling of Agriculturally-Related Chemicals

9:50 – 75. Seed-coated clothianidin fate in corn and soybean fields using conservation tillage. **C. de Perre**, M. J. Lydy

Repellents and Attractants

2:40 – 92. Neurotoxicity and mode of action of *N,N*-diethyl-*meta*-toluamide (DEET) on the insect nervous system and mammalian neurons. **D. R. Swale**, B. Sun, J. R. Bloomquist

TUESDAY: Biopesticides: State of the Art and Future Opportunities

Products from Genetic Improvements

1:55 – 165. Functional analysis of four RNAi pathway genes in an economically important corn pest, western corn rootworm (*Diabrotica virgifera virgifera*). **C. Khajuria**, B. Siegfried, K. Narva

Dow AgroSciences

CALL FOR APPLICANTS
2014 Fall ACS National Meeting in San Francisco, California

The AGRO Division seeks nominations for the New Investigator Award to be awarded at the ACS meeting in San Francisco in August 2014. The purpose of the New Investigator Award is to recognize scientists who have obtained a doctoral degree and are actively conducting academic, industrial, consulting, or regulatory studies.

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

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

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

The Process:

- To be eligible for the award, the scientist must have obtained his or her doctorate no more than five years before the time of the Fall ACS National Meeting. Thus, for 2014, applications will be considered from ***scientists who have obtained their doctorates no earlier than the year 2009***
- A panel consisting of at least three AGRO members will chose up to three finalists based on their extended abstracts and letter(s) of recommendation
- ***Each finalist will receive up to $1000 for travel and meeting expenses***
- Each finalist will deliver an oral presentation (which will be judged by the panel) in one of the AGRO Program symposia. The winner, who will receive a plaque, will be chosen after all finalists have presented their papers

To Apply for the New Investigator Award:

1. Submit a **150-word abstract** to a symposium in the AGRO Division using ACS PACS abstract submission at *http://abstracts.acs.org/*
2. Submit an **extended abstract (maximum 2 pages) describing the candidate's research/studies**. Include the impact (or potential impact) of the results as it pertains to issues of concern to the AGRO
3. Submit least **one letter of recommendation** from a current supervisory scientist (e.g., post-doctoral mentor a business manager, departmental chair).
4. Deliver an oral presentation in AGRO at Division
5. For consideration of an award at the 2014 Fall ACS National Meeting, both the extended abstract and letter of recommendation must be received by the new coordinator of the New Investigator Award **no later than March 1, 2014**

All Graduate Students and Post-Docs

You Are Cordially Invited To Attend

AGRO Graduate Student Box Luncheon

Enjoy lunch on us and visit with professionals in academia, industry, and government to discuss career opportunities in the AGRO sector and your future involvement in AGRO

Monday, September 9 at 11:45 am – 1:15 pm
Crown Plaza -- Grand Central A

CONTACT: JULIE EBLE (Julie.Eble@criticalpathservices.com)
TROY ANDERSON (anderst@vt.edu)
RESERVATIONS ARE REQUIRED
Reservations made after by August 2 are on a space available basis.

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2013 AGRO EDUCATION AWARDS FOR STUDENT TRAVEL

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FIRST, SECOND, AND THIRD PLACE WINNERS WILL BE ANNOUNCED AT THE AGRO AWARDS & SOCIAL ON TUESDAY EVENING

Diana Aga and Marja Koivunen, *Organizers*

1:30 - 5:30 PM
Indiana Convention Center, Halls F&G

Sara Mueting. Multi-year field study of the fate and transport of three insecticides in an agricultural ecosystem. *Michael Lydy, Southern Illinois University Carbondale*, **AGRO 118**

Katia M Noguera-Oviedo. Assessing the removal of hormones and their potency as endocrine-disrupting chemicals in dairy wastes through an anaerobic digestion system. *Diana Aga, University of Buffalo*, **AGRO 119**

Amanda Parra. Determination of carbon nanotube uptake, translocation, and bioaccumulation in corn (*Zea mays L.*). *Jaclyn E Cañas-Carrell, Texas Tech University*, **AGRO 120**

Rolando S Mejorado. Evaluation of glufosinate and glyphosate translocation in young almond (*Prunus dulcis*) trees. *Bradley Hanson, University of California, Davis,* **AGRO 121**

Vurtice C Albright. Biological validation of enzyme-linked immunosorbent assays for detection of Cry proteins in the environment. *Joel Coats, Iowa State University*, **AGRO 122**

Katherine E Stain. Development and validation of a method to quantify Bt-Cry1Ab in water matrices. *Michael Lydy, Southern Illinois University Carbondale*, **AGRO 123**

Aaron D Gross. Deorphanization and pharmacological profile of a tyramine receptor from the southern cattle tick (*Rhipicephalus microplus*). *Joel Coats, Iowa State University*, **AGRO 124**

C Ian Johnston. Quantitative lipid analysis of gut microflora consortium in the Giant Panda. *Darrell Sparks, Mississippi State University*, **AGRO 125**

Joshua S Wallace. Assessment of conventional waste management and advanced waste treatment systems in removing veterinary antibiotics. *Diana Aga, University of Buffalo*, **AGRO 126**

Huizhen Li. Dynamic coupled fluxes of current-use pesticides in air-water/soil-sediment system in a city in southern China. *Jing You, Chinese Academy of Sciences, Guangzhou, China*, **AGRO 127**

Zhijiang Lu. Isomer-specific biodegradation of nonylphenol in river sediments. *Jay Gan, University of California, Riverside*, **AGRO 128**

Ngoc N Pham. Synergistic effects of verapamil on tacrine toxicity to vector mosquitoes. *Troy Anderson, Virginia Tech*, **AGRO 129**

Lacey Jenson. Voltage-sensitive potassium channels expressed by hormone treatment in mosquito cell lines. *Jeffrey Bloomquist, University of Florida, Gainesville*, **AGRO 130**

Nicholas R Larson. Evaluation of synthetic compounds as novel mosquitocides targeting potassium channels for control of *Aedes aegypti* and *Anopheles gambiae*. *Jeffrey Bloomquist, University of Florida, Gainesville*, **AGRO 131**

Juying Li. Influence of amendments on the degradation of pharmaceuticals in soil. *Jay Gan, University of California, Riverside*, **AGRO 132**

Congratulations to all our travel grant winners!

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CALL FOR APPLICANTS
2014 AGRO EDUCATION AWARDS
Sponsored by Bayer CropScience

UNDERGRADUATE & GRADUATE STUDENT RESEARCH

Support for Poster Presentations
At the 2014 Fall ACS National Meeting in San Francisco, California

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

Proposals are sought for the 2014 awards. Selected undergraduate and graduate students will be awarded up to $600 each to help defray costs of attendance to give poster presentations at the ACS 2014 Fall Meeting, which will be held August 10 – 14, 2014 in San Francisco, California. Posters will be displayed in a special poster session of the ACS AGRO Division. First, Second, and Third place winners will receive an additional cash award.

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

To apply, a graduate student should submit the following to be received no later than
March 1, 2014 (PACS deadline):

1. An abstract formatted according to the directions given on the ACS website. Be sure to include name (of applicant), address, and e-mail address.

2. A two page extended abstract giving more detail of the research/presentation.

3. A short letter of nomination from the faculty advisor.

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

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

For more information, please contact the co-organizers:

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

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

Abstracts will be reviewed by the Education Committee.
Submitters will be notified of their selection status in May 2014.

Special thanks to our sponsor for their generous contribution!

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- Spray drift modeling with AgDRIFT/AGDISP
- Watershed-scale modeling (SWAT)
- Vegetative buffer modeling (VFSMOD)
- Groundwater modeling (RZWQM, LEACHP, PRZM-GW)
- Custom model development and modification

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- Endangered species assessments
- Watershed characterization
- Proximity analysis
- GIS tool development for environmental risk assessment
- Web-based mapping applications

Quality Assurance Unit (RQAP-GLP)
- GLP and NELAC audits and training

Field Studies
- Study design and directorship
- Drift reduction technology assessments
- Community drinking water monitoring
- Surface water monitoring
- Simulated rainfall runoff
- Prospective groundwater studies
- Regional groundwater monitoring

Risk Assessment
- Integrated partnership with Intrinsik Environmental Sciences to offer extensive capabilities in the areas of toxicology and risk assessment (see www.intrinsik.com)

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Michael Winchell / 802.229.1882
info@stone-env.com

Notes from the Program Chair

Stephen O. Duke

We have a full program for the 246th National ACS Meeting in Indianapolis of September 8-12, 2012, with 21 symposia, five award presentations, and two poster sessions (general and student), with a total of 334 abstracts for the entire program. There will be 38 half-day sessions with four concurrent sessions from Sunday afternoon through Thursday morning and three concurrent sessions on Sunday morning and Thursday afternoon. This will be a very busy and informative program, so come early and stay late, and don't forget to bring your *PICOGRAM* as a guide. There were so many oral sessions, that the General Session (*Protection of Agricultural Productivity, Public Health, and the Environment*) is scheduled as a poster session to held be at the Indiana Convention Center.

The most extensive symposium is ***Biopesticides:*** *State of the Art and Future Opportunities* that will run two and a half days. This symposium is partially supported by an ACS Innovation Grant. It will bring together top industry, university, and government officials and scientists to discuss the regulation, research, and future of this growing sector of pest management.

We will have several **emerging issue symposia**. AGFD and ANYL will cosponsor *Advanced Bioanalytical Technologies for GM Detection*, a crucial topic for transgenic crops. With the imminent introduction of transgenic crops resistant to auxinic herbicides (dicamba and 2,4-D), the symposium on *Spray Application Technology* is timely. Other timely symposia include: *Herbicide-Resistant Crops and Weeds – Current Status; Uptake, Translocation, and Distribution of Agrochemicals in Plants*; and *Pollinators and Pesticides.*

Some of the symposia fit the theme of the meeting: **Chemistry in Motion.** These include: *ADME - The Motion of Veterinary Drugs and Xenobiotics* (AGFD, ENVR cosponsors), *Environmental Fate, Transport, and Modeling of Agriculturally-related Chemicals* (ENVR cosponsor), and *Terrestrial Field Dissipation Studies in Global Agrochemical Registration Programs*.

Agrochemical regulation is the focus of three symposia: *Regulatory Risk Assessment: New Paradigms for Human Health Exposure*; *Pesticide Regulatory Science in the 21st Century: Merging Research and Regulations*; and *Pesticide Regulatory Science in the 21st Century: Merging Research and Regulations.* Several others consider **residue analysis**. Regulation is dealt with in part in *Pesticide Residues in Food and Feed: Scientific and Regulatory Global Needs. High-Throughput Pesticide Residue Analysis* will deal with analytical aspect of residue analysis.

Two symposia (*Accurate Mass Analyses in Support of Agricultural Chemical Research and Development* and *Synthesis and Chemistry of Agrochemicals*) relate to aspects of **agrochemical discovery**.

Toxicology of agrochemicals will be discussed in *21st Century Vision for Testing and Risk Assessment: Implications for Agrochemicals* as well as *Ecotoxicological Risk Assessment for Agricultural Use of Chlorpyrifos in the US.* Other aspects of **environmental chemistry** are covered by: *Air Quality at the Interface: Megacities and Agroecosystems* cosponsored by ENVR; *Assessing Potential Ecological and Human Health Effects from Fertilizer and Pesticide Use in Urban Environments*; and *Non-First Order Dissipation and Time-Dependent Sorption of Organic Chemicals in Soil: Measurement, Modeling, and Impact on Environmental Exposure Predictions.*

Also listed in the program are **five ENVR symposia cosponsored by AGRO**: *Fate and Toxicology of Emerging Environmental Contaminants*; *Predicting Molecular Properties of Environmental Contaminants: Empirical and Theoretical Methods*; *Air Monitoring*; *Status and Trends of Classical and Emerging Contaminants Across the World*; and *Water: Global Problems, Local Solutions.* In addition, AGFD and AGRO will cosponsor the Kansas City Section Spencer Award Symposium honoring Dr. **Attila Pavlath**.

I want to thank symposia organizers for their efforts to find external sources of funds to support their symposia. As you can see from the program, they were quite successful. I also gratefully thank the many companies and organizations that generously provided funds to support our program.

Marja Koivunen and Diana Aga have again organized our Education Awards and students' poster session. Steven Lehotay is in charge of the New Investigator Award in which three finalists will be judged by their oral presentations early in the week. The winner will be announced Wednesday afternoon. The **New Investigators Awards (NIA) finalists and the Student Poster Presenters** will be recognized with awards and grants for travel. Please plan on attending the poster session and the NIA presentations to encourage these budding scientists.

The achievements of **five of our most eminent colleagues** will be honored with award symposia. On Monday, we will honor Dr. **René Feyereisen** of INRA-CNRA, Sophia, Anipolis, France at the International Award for Research in Agrochemicals symposium that is sponsored by BASF. Four award presentations are planned for the same venue on Tuesday morning. First, will be presentations by the recipients (Prof. **Thomas Hoffman** of the University of Munich and Dr. **John Grabber** of USDA-ARS) of the newly instituted Best Paper Awards of the *Journal of Agricultural and Food Chemistry.* These will be followed by the BASF-sponsored AGRO Innovation in Chemistry of Agriculture Award lecture of Dr. **Jeannette Van Emon** of US EPA. Finally, Prof. **Keith Solomon** of the University of Guelph will give the Sterling B. Hendricks Memorial Lecture that is sponsored by USDA-ARS and co-hosted by AGRO and AGFD. Keith will speak on: *Arriving at the truth: Weight of evidence for assessing risks of agrochemicals*.

Finally, the venue for AGRO is the **Crowne Plaza at Historic Union Station**. The Indianapolis Union Station was **the first union station in the world**, opening Sept. 20, 1853. It is connected to the Crowne Plaza and the Indiana Convention Center via underground walkways. On Tuesday evening, there will be bus service to Dow AgroSciences, where Dow will host our **AGRO Awards Social** from 5:30 until 8:00 pm. Buses will depart at 5:00 pm at the Crown Plaza Hotel. **You must pre-register for this event by August 31**. See the link at the AGRO website.

We look forward to a productive and fun-filled experience with old and new friends and colleagues. ***See you in Indy!***

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Services include:

- **Environmental fate:**
  - Hydrolysis
  - Photolysis (aqueous and soil)
  - Metabolism in soils and sediments (aerobic and anaerobic)
  - Degradation in surface waters
  - Soil adsorption/desorption and column leaching
  - Soil volatility
- **Plant metabolism:**
  - Nature of the residue in crops
  - Confined rotational crops
- **Animal metabolism:**
  - Rodents: ADME
  - Livestock metabolism (goats and hens)
- **Livestock feeding studies:**
  - Cows and hens
- **Analytical Chemistry:**
  - Residues in soil, air and water
  - Residues in crops
  - Radio validation and ILVs
  - Operator exposure
  - 5-Batch analysis
- **Physicochemical characteristics**

Contact: Dr. David Dohn
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Dr. Luis Ruzo (Division General Manager)
lruzo@eaglabs.com

PTRL Europe

Services include:

- **Environmental fate:**
  - Hydrolysis
  - Photolysis (aqueous and soil)
  - Metabolism in soils and sediments
  - Soil adsorption/desorption
  - Soil volatility
  - Air sampling
- **Plant metabolism:**
  - Nature of the residue in crops
- **Analytical Chemistry:**
  - Matrices include: crops, animal, blood, urine, soil, water, air, operator exposure and others.
  - Development of new methods and modification/adaptation of old methods
  - Radio validations and ILVs
  - Operator exposure
  - 5-Batch analysis
  - Chemistry support of environmental effects studies
  - Blood cell isolation, RIA, FACS
- **Physicochemical characteristics**

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Dr. Luis Ruzo (Division General Manager)
lruzo@eaglabs.com

Wildlife International

Services include:

- **Environmental fate:**
  - Hydrolysis
  - Photolysis (aqueous and soil)
  - Metabolism in soils and sediments (aerobic and anaerobic)
  - Degradation in surface waters
  - Soil adsorption/desorption
- **Biodegradation**
- **Analytical Chemistry:**
  - Residue analysis
  - Method Development
  - ILVs
  - 5-Batch analysis
- **Physicochemical characteristics**
- **Ecotoxicology:**
  - Complete suite of fresh water and marine aquatic tests
  - Endocrine disruptor screening and testing with in-house histopathology
  - Bioaccumulation testing through aquatic and dietary exposure
  - Avian toxicology
  - Terrestrial and aquatic plant testing
  - Honey bee and earthworm testing

Contact: Annegaaike Leopold
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COMMENTS FROM THE VICE CHAIR

CATHLEEN J. HAPEMAN

The continued success of AGRO is highly dependent of long-term planning. Over this past year, Program Chair Steve Duke and the Programming Committee put together a strong program for Indy, but many of us were also working on preparations for the 13th Pesticide Congress which will be held at the ACS 248th National Meeting in San Francisco. See the following IUPAC 2014 section beginning on p. 45

It's time now to ***set in motion brainstorming ideas for Boston.*** Once again, we will call upon the Standing Program Champions to generate ideas but we still need more volunteers. Please let me know if you would like to participate in this important AGRO activity (cathleen.hapeman@ars.usda.gov). As always, we welcome all your comments and ideas. We invite everyone to attend the ***Brainstorming for Boston and Beyond*** meeting on Wednesday at 5 pm. We will be trying a slightly different approach this year...should be fun! And as we have done in the past, the drinks are free - provided you come with ideas!

You Are Cordially Invited To

AGRO Brainstorming for Boston & Beyond

Happy Hour

September 11, Wednesday 5 - 7 pm

Crowne Plaza, Grand Central A - C

- Share your ideas about AGRO programming
- Participate in brainstorming activities
- Learn more about organizing a symposium
- Tell us what topics are the most important to you
- Meet scientists with mutual interests

Free refreshments will be served

MEMBERS, SPEAKERS, GUESTS ARE ALL WELCOME

Topic Champions are strongly encouraged to attend!

AGRO Launches Lunch and Learn Webinar Series

In 2012, AGRO received funding from ACS Division Activities Committee for a proposal entitled, "Establish and Execute an Educational Webinar Program to Enhance the AGRO Membership Experience."

This project was launched using a live webcast of a symposium from the ACS National Meeting in Philadelphia entitled, "Perfecting the Communication of Chemical Risk" which included eight speakers. Outcomes from this symposium were recently highlighted in the *Journal of Agriculture and Food Chemistry* (2013, 61, 4676–4691).

Afterwards, the *ARGO Lunch and Learn Webinar Series* was developed by Julie Eble, Critical Path Services, and Laura McConnell, USDA-ARS. Five live webinars were presented from December 2012 to May 2013:

- Is Your Method Good Enough? Highlights from Philly 2012
- "What If" Approaches to Agrochemical Discovery - Highlights from Philly 2012
- Pesticides: The Global Need and Do Adjuvants Matter?
- The Future of Pyrethroids: Environmental Detection, Resistance, and Novel Spatial Repellents
- Pesticide Regulation and the Endangered Species Act: Recommendations for Improvement and Recent Developments -- Coordinated with the release of an ACS Symposium Series Book of the same title
- Designing Studies to Assess the Effects of Pesticides on Honey Bees

Recordings of all but one of these webinars are now freely available on-line at the AGRO website at:

http://www.agrodiv.org/2012-2013-agro-webinar-series/

Suggestions and volunteer organizers are needed to develop webinars for the 2013-2014 series. Webinars that highlight topics of international significance are desired as a means to promote the upcoming IUPAC International Congress of Pesticide Chemistry to be held in August 2014.

Contact Laura McConnell at laura.mcconnell@ars.usda.gov for more information.

AGRO Standing Programming and Champions

Long-term programming was identified as critical to the success of the AGRO Division. Currently AGRO programs technical symposia in 15 standing topics. Individual experts in each topic area have been identified from our membership to act as 'Champions' of that topic. These champions serve as liaisons to the current Vice Chair and Program Chair, providing ideas for new and timely symposia within their topic areas and identifying possible organizers. The champions long-term institutional memory of the Division's programming efforts because the officers rotate into and out of office. The Vice Chair is responsible for contacting them as necessary and organizing a conference call or two each year.

Additional Volunteers Needed for Boston 2015

Contact: Cathleen Hapeman, cathleen.hapeman@ars.usda.gov

Advances in Agrochemical Residue, Analytical and Metabolism Chemistry & Metabolomics
Kevin Armbrust, armbrust@msci.msstate.edu
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Michael Krolski, mike.krolski@bayer.com
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Teresa Wehner, teresa.wehner@merial.com

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Amrith Gunasekaram, amrith.gunasekara@cdph.ca.gov
Scott Yates, scott.yates@ars.usda.gov

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

Bioenergy, Bioproducts, and Biochars: Advances in Production and Use
Cathleen Hapeman, cathleen.hapeman@ars.usda.gov

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

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

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

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

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

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

Protection of Agricultural Productivity, Public Health and the Environment – General Session
Program Chair

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

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

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

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

Programming & Outreach Activities
2013 – 2015

Activity/Event	Leaders/ Champions	Status	Actions Required
2013/4 AGRO Lunch and Learn Webinar Series	Laura McConnell	• Program under development and will include IUPAC 2014 emerging topics	• Volunteers are NEEDED!! • Contact Laura McConnell
51st North American Chemical Residue Workshop July 2013 St Pete Beach, Florida	Kevin Armbrust Steve Lehotay	• Program to be developed winter 2013/4	• Submit abstracts for oral presentations by April 15.
248th ACS National Meeting 13th IUPAC Pesticide Congress San Francisco, California August 10-14, 2014	Laura McConnell Ken Racke Cathleen Hapeman Jay Gan	• Follow progress on website www.iupac2014.org • Symposia under review and finalized October 2013	• Committee Volunteers needed • Sign up for email updates • Submit abstracts when PACS opens in January
250th ACS National Meeting August 16-20, 2015 Boston, Massachusetts	2014 Vice Chair -- Elected July 2013	• Symposia planning at Brainstorming for Boston and Beyond, Wednesday, September 11, 2013	• Volunteers and champions NEEDED!! • Contact Cathleen Hapeman
Pacifichem 2015 December 15-20, 2015	John Johnston	• Symposium Proposals under Review	• Contact John Johnston

Future ACS National Meetings

247th ACS National Meeting & Exposition
Chemistry and Materials for Energy
March 16-20, 2014, Dallas, Texas

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

249th ACS National Meeting & Exposition
Chemical Resources: Extraction, Refining & Conservation
March 22-26, 2015, Denver, Colorado

250th ACS National Meeting & Exposition
A History of Innovation: From Discovery to Application
August 16-20, 2015, Boston, Massachusetts

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

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

254th ACS National Meeting & Exposition
August 20-24, 2017, Washington, DC

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

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

7 Easy Steps for Organizing a Symposium

Thinking about organizing a symposium for a future National Meeting?

It's really not that difficult. Here's how:

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

AGRO Support for Symposium Organizers

- Assistance with developing a symposium summary and Call for Papers
- Help with identifying co-organizers
- Funding to help with travel, non-member registrations ($500 each ½ session)

July 20-23, 2014

TradeWinds Island Grand

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Our workshop reflects the scope and international nature of
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pesticides, veterinary drugs, environmental contaminants, toxins,
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Expected Submission Deadlines:
Oral presentations: April 15; Poster presentations: June 1
Manuscripts related to the meeting maybe considered for publication
in a special section of *Journal of Agricultural and Food Chemistry*

www.nacrw.org

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

www.iupac2014.org

Join Us!

ON AUGUST 10-14, 2014

in San Francisco, California USA for the

13TH IUPAC CONGRESS OF PESTICIDE CHEMISTRY

CROP, ENVIRONMENT, AND PUBLIC HEALTH PROTECTION: TECHNOLOGIES FOR A CHANGING WORLD

Co-sponsored by IUPAC and ACS-AGRO

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

MAJOR TOPIC AREAS WILL INCLUDE:

- Emerging Issues and Challenges
- Mode of Action and Resistance Management
- Discovery and Synthesis
- Agricultural Biotechnology
- Environmental Fate and Metabolism
- Ecological and Human Exposure and Risk Assessment
- Residues in Food and Feed
- Formulation and Application Technologies
- Stewardship, Regulation, and Outreach

IUPAC 2014

SAN FRANCISCO

IUPAC INTERNATIONAL CONGRESS OF PESTICIDE CHEMISTRY

August 10-14, 2014, San Francisco, California

Organizer Co-Chairs:
Kenneth Racke, Dow Agrosciences, kracke@dow.com
Laura McConnell, USDA-ARS, laura.mcconnell@ars.usda.gov
Program Administrator:
Peney Patton, ppatton@iupac2014.org

ORGANIZING COMMITTEE

Responsible for overall planning and management of the Congress on behalf of the ACS AGRO Division and IUPAC. Directs the activities of committees, volunteers and staff for organization of the Congress. Maintains a high-level of coordination with both ACS and IUPAC. Ensures effective communication and implementation of the Congress vision. Recruits volunteers and establishes support positions and committees as needed to achieve Congress goals.

US Members:
Kevin Armbrust, Louisiana State University
Ellen Arthur, Bayer CropScience
Aldos Barefoot, DuPont
Rod Bennett, JRF America
Jeff Bloomquist, University of Florida-Gainesville
John Clark, University of Massachusetts
Stephen Duke, USDA-ARS
Jay Gan, University of California-Riverside
Cathleen Hapeman, USDA-ARS
Ann Lemley, Cornell University
John Johnston, USDA-FSIS
Sharon Papiernik, USDA-ARS
Pamela Rice, USDA-ARS
Patricia Rice, BASF
Jason Sandahl, USDA Foreign Agricultural Service
James Seiber, University of California-Davis
Jeanette VanEmon, EPA
Donald Wauchope, USDA Agricultural Research Service (ret.)
Scott Yates, USDA-ARS

International Members:
Rai Kookana, CSIRO, Australia
Xiongkui He, China
Yong-Hwa Kim, Korea Research Institute of Chemical Technology, South Korea
Jan Linders, RIVM, Netherlands
Keith Solomon, University of Guelph, Canada
Keiji Tanaka, Mitsui Chemicals Agro, Japan
John Unsworth, Consultant, UK

INTERNATIONAL ADVISORY COMMITTEE

Provides international advice/perspectives to the Organizing Committee for effective Congress planning based on past experience. Assists with communication of Congress plans and solicitation of inputs from international partner organizations. Promotes international participation in the scientific program of the Congress by liaising with scientific organizations, industry, and governments around the world. Supports efforts of the Scientific Program Committee to ensure an internationally diverse program of platform and poster presentations.

Chair:
Kenneth Racke, Dow AgroSciences, USA
Members:
Elizabeth Carazo, Univ. of Costa Rica, Costa Rica
Bernhard Johnen, CropLife International, Belgium
Hisashi Miyagawa, Kyoto University, Japan
Hideo Ohkawa, Kobe University, Japan
N.A. Shakil, IARI, India
Greg Simpson, CSIRO, Australia
John Unsworth, IUPAC, UK
Zhang Zhongning, Chinese Academy of Sciences, China

SPONSORSHIPS & FINANCE COMMITTEE

Responsible for development and implementation of a Congress budget of income and expenses. Establishes sponsorship guidelines and recruits sponsors. Provides financial guidance and advice to the Organizing Committee and other committees.

Chair:
Kenneth Racke, Dow AgroSciences, USA
Members:
Rodney Bennett, JRF America, USA
John Johnston, USDA-FSIS, USA
Del Koch, ABC Labs, USA
Scott Jackson, BASF, USA
Laura McConnell, USDA-ARS, USA
James Seiber, University of California-Davis, USA
Scott Yates, USDA-ARS, USA

COMMUNICATIONS & PUBLICITY COMMITTEE

Promotes interest and awareness of the Congress among potential attendees in the US and internationally. Develops promotional materials (brochures, flyers, ads, etc) and electronic communication for Congress including website postings, AGRO e-newsletters, a Facebook page, Youtube videos, blogs, and twitter. Coordinates dissemination of information with other ACS Divisions, scientific societies, industry associations, and affiliated organizations

Chair:
Ellen Arthur, Bayer CropScience, USA
Members:
Sarah Macedo, CropLife America, USA
Laura McConnell, USDA-ARS, USA
Kenneth Racke, Dow AgroSciences, USA
Pamela Rice, USDA-ARS, USA
Patricia Rice, BASF, USA

PUBLICATIONS COMMITTEE

Responsible for development and implementation of a post-Congress special publications plan of a series of books and special journal issues based on main scientific topic and/or symposia topic.

Chair:
Jay Gan, University of California-Riverside, USA
Members:
John Clark, University of Massachusetts, USA
Stephen Duke, USDA-ARS, USA
James Seiber, University of California-Davis, USA
Scott Yates, USDA-ARS, USA

Additional Volunteer Opportunities

LUNCHEON SEMINAR SERIES COORDINATORS

Chair:
Sharon Papiernik, USDA-ARS, USA
Members Needed
Responsibilities

- Coordinate with Organizing and Scientific Programming Committees in planning seminars.
- Coordinate food and beverage orders, room and A/V arrangements.
- Additional responsibilities under consideration.

LOCAL ARRANGEMENTS COMMITTEE

Responsibilities

- Organize social program events associated with the San Francisco IUPAC Congress.
- Plan the program for the Congress opening ceremony and reception on Sunday evening, including a memorable musical or performance-related component fitting for the San Francisco location.
- Plan the program for the Congress banquet on Wednesday evening, to include award presentations as well as a memorable performance related event.
- Plan the program for the Congress closing ceremony, including announcement of the 2018 Congress location and introduction of the organizers (with traditional hat exchange).
- Coordinate food and beverage orders, room and A/V arrangements for the opening ceremony, coffee breaks, banquet, closing ceremony in conjunction with the AGRO Social Committee and assigned ACS staff.

PANEL DISCUSSION COORDINATORS

Responsibilities

- Develop guidance for organization of panel discussions in conjunction with oral and/or poster symposia.
- Coordinate planning of panel discussions with the Scientific Program Committee, main topic team leaders, and symposia organizers.

NEWS MEDIA COORDINATORS

Responsibilities

- Explore new media options (web, webinar, email, blog, twitter, Youtube,…) and develop innovative approaches for disseminating events and outcomes of the Congress in cooperation with the Publications Committee and the Scientific Program Committee.
- Organize a press briefing event during the Congress to highlight hot issues and developments for invited news media.
- Serve as liaison for Congress news media efforts in cooperation with ACS headquarters.
- Develop summary articles concerning Congress activities for publication in the AGRO magazine *PICOGRAM*, the ACS publication *C&EN*, and the IUPAC news magazine *Chemistry International*.

IUPAC INTERNATIONAL CONGRESS OF PESTICIDE CHEMISTRY

August 10-14, 2014, San Francisco, California

SCIENTIFIC PROGRAM COMMITTEE

Chair: Cathleen Hapeman, USDA-ARS, cathleen.hapeman@ars.usda.gov
Associate Chair: Jay Gan, University of California-Riverside, jgan@ucr.edu
Poster Session Chair: John Johnston, USDA-FSIS, john.johnston@fsis.usda.gov

MEMBERS BY TOPIC AREA (*TEAM CHAIR*)

1. Emerging Issues and Challenges
Cheryl Cleveland, BASF, USA
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- Allan Felsot, Washington State University, USA
- Lei Guo, California Air Resources Board, USA
- David Gustafson, Monsanto, USA
- Ole Hertel, Aarhus University, Denmark
- Sharon Papiernik, USDA-ARS, USA
- James Seiber, University of California-Davis, USA
- Greg Simpson, CSIRO, Australia

2. Mode of Action and Resistance Management
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- Jeff Bloomquist, University of Florida, USA
- John Clark, University of Massachusetts, USA
- René Feyereisen, University of Nice, France
- Kazuhiko Matsuda, Kinki University, Japan
- Thomas Sparks, Dow AgroSciences, USA
- Klaus Stenzel, Bayer CropScience, Germany
- Arie Tsutomu, Tokyo University, Japan

3. Discovery and Synthesis
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- Joel Coats, Iowa State University, USA
- Peter Maienfisch, Syngenta, Switzerland
- Agnes Rimando, USDA-ARS, USA
- Xinling Yang, China Agricultural University, China

4. Agricultural Biotechnology
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- George Harrigan, Monsanto, USA
- Gijs Kleter, Wageningen University, The Netherlands
- Patricia Rice, BASF, USA
- Nick Storer, Dow AgroSciences,USA

5. Environmental Fate and Metabolism
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- Ettore Capri, Università Cattolica del Sacro Cuore, Italy
- Stuart Cohen, Environmental & Turf Services, Inc., USA
- Russell Jones, Bayer CropScience, USA
- Rai Kookana, CSIRO, Australia
- Weiping Liu, Zhejiang University, China
- Karina Miglioranza, University of Mar del Plata, Argentina
- Pamela Rice, USDA-ARS, USA

6. Exposure and Risk Assessment
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- Wenlin Chen, Syngenta, USA
- Qing Li, University of Hawaii, USA
- Curt Lunchick, Bayer CropScience, USA
- John Johnston, USDA-FSIS, USA
- Keith Solomon, University of Guelph, Canada
- Paul VandenBrink, Alterra, The Netherlands
- Joe Wisk, BASF, USA

7. Food Residues, Analytical Methods, and MRLs
Mike Krolski, Bayer CropScience, USA
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- Jerry Baron, Rutgers University/IR-4, USA
- Lori Berger, California Specialty Crops Council, USA
- Caroline Harris, Exponent, UK
- Dieter Jungblut, BASF, Germany
- Steve Lehotay, USDA, USA

8. Formulation and Application Technologies
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- Andreas Herbst, BBA, Germany
- Andrew Hewitt, Lincoln Ventures, Ltd, New Zealand
- Holger Tank, Dow AgroSciences, USA
- He Xiongkui, China Agricultural University, China

9. Stewardship, Regulation, and Outreach
Jeffrey Jenkins, Oregon State University, USA
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- Scott Jackson, BASF, USA
- Barbara Glenn, CropLife America, USA
- Kean Goh, California Department of Pesticide Regulation, USA
- Ivan Kennedy, University of Sydney, Australia

SCIENTIFIC PROGRAM TOPIC AREA DETAILS

1. Emerging Issues and Challenges

- Climate Change, Population Growth & Agriculture's Response
- Omics Technology in Agricultural Research
- Sustainability: A Greener Revolution?
- Pollinator Health through the Lens of Integrated Pest Management (IPM)

2. Mode of Action and Resistance Management

- Cutting edge approaches to mode of action discovery
- New mechanisms of action of fungicides, insecticides and herbicides
- Mechanisms of resistance: technologies/strategies to extend utility of existing and new pesticides

3. Discovery and Synthesis

- Design, isolation, synthesis, biology and/or structure-activity relationships
- New approaches and directions to crop health/yield enhancement, abiotic stress abatement, nematode control, biological control agents, natural products

4. Agricultural Biotechnology

- Molecular and RNAi-based technologies
- Challenges associated with biotechnology adoption globally
- Promote discussion and debate surrounding global regulations
- Evaluate biotechnology contributions to sustainable agriculture and food security

5. Environmental Fate and Metabolism

- Measuring/modeling of pesticide degradation, transport and bioavailability in soil, water, and air at nanoscale to macroscale from agricultural to urban environments
- Factors that influence fate and metabolism
- Effects of compounds/mixtures on environmental compartments and mitigation

6. Exposure and Risk Assessment

- Developments in hazard identification, exposure, dose-response, and risk characterization science for human exposures and environmental effects
- Estimating exposure through modeling and monitoring for drinking water and dietary assessments, worker exposure requirements, and ecological modeling
- Implementation of deterministic and probabilistic risk assessment methods

7. Food Residues, Analytical Methods, and MRLs

- Technical advances in analytical methodology
- Technology transfer between laboratories in different countries
- Global harmonization of regulations, maximum residue limits (MRLs), import tolerance value standardization

8. Formulation and Application Technologies

- Interaction between formulation physical properties and the application equipment such as spray nozzle or atomizer
- Latest innovations in agrochemical formulation and application
- Off-target losses affected by formulation properties and application variables

9. Stewardship, Regulation, and Outreach

- Bringing together those responsible for protecting the food supply and assuring consumer safety: food production, pest management science, pesticide regulation, registrants, public health officials, the medical community
- Examine data used for pesticide dietary risk from the farm gate to the table
- Consider how pesticide use practices are related to both international trade and national food safety and food security objectives

IUPAC INTERNATIONAL CONGRESS OF PESTICIDE CHEMISTRY

August 10-14, 2014, San Francisco, California

SPONSORSHIP OPPORTUNITIES

Every four years the international pesticide community comes together to share their latest research findings and to discuss emerging issues of global significance in agriculture. For the first time, an IUPAC Congress will be held in conjunction with the American Chemical Society (ACS) National Meeting and Exposition.

The AGRO Division of ACS, in collaboration with many state, national and international partner organizations, is developing an outstanding technical program that will attract scientists from around the world. Nine scientific topic areas have been selected.

Expected attendance is 1000 to 1500 delegates. Registration, housing, and social event planning will be supported by the ACS organization. San Francisco is a world-class destination and is typically the most popular of all ACS meeting locales. The Marriott Marquis Hotel will be the Congress venue, providing the feel of a standalone event. AGRO is seeking sponsors to support the technical program, social events, awards, and travel support for scientists from developing countries.

Congress Sponsor - $100,000
- Signage at Ceremonies and Plenary Lectures
- Acknowledged at Opening and Closing Ceremonies
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- Materials placed in Congress bag
- Full Page Ad in Program
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- Logo on Signage at Secretariat
- Largest Logo on Sponsorship Page of Program

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- Signage and display table at Welcome Reception and Acknowledged at Opening Ceremony
- 2 Comp Tickets to Congress Banquet
- 1 Comp Meeting Registration
- Materials placed in Congress bag
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- Logo on Sponsorship Page of Program

Major Scientific Topic Sponsor - $8,000 - $20,000*
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- Full Page ad in Program
- Logo on Meeting Website
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- Logo on Sponsorship Page of Program

Poster Award Sponsor - $10,000
- Listed as Poster Award Sponsor in Program
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- Materials placed in Congress bag
- Company Name Listed on Sponsor Page in Program

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Luncheon Seminar Sponsor - $5000 – $7,500
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Symposium or Webinar Sponsor - $2000 - $5000
- Signage at the Door
- Listed as sponsor in the Program
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- Company Name Listed on Sponsor Page in Program

IUPAC-AGRO Sponsor - $2500
- One page flyer in Congress Bag
- Distribute company/institution materials

* Lower level contributions as co-sponsorships available and to be reflected in shared credits in communication materials.

Advertisements
Program Booklet Advertisements are also available. Contact the organizers for more information.

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2013 AGRO Division Officers

John M. Clark
Division Chair

Stephen O. Duke
Program Chair

Cathleen J. Hapeman
Vice-Chair

Del A. Koch
Treasurer

Sharon K. Papiernik
Secretary

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1971	Wendell Phillips	1986	Henry J. Dishburger	2001	Jeffery Jenkins
1972	Philip C. Kearney	1987	James N. Seiber	2002	Terry D. Spittler
1973	Roger C. Blinn	1988	Paul A. Hedin	2003	Jeanette Van Emon
1974	Charles H. Van Middelem	1989	Gustave K. Kohn	2004	Rodney Bennett
1975	Henry F. Enos	1990	Willa Garner	2005	Allan Felsot
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1981	Marguerite L. Leng	1996	Barry Cross	2011	Kenneth D. Racke
1982	Gino J. Marco	1997	Willis Wheeler	2012	Aldos C. Barefoot
1983	G. Wayne Ivie	1998	Judd O. Nelson		

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(con't)

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Programming Committee - p.42

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

This just in.....

2013 Elections Results

Pamela Rice has been elected Vice-Chair to a 1-year term beginning September 12, 2013

Del Koch has been re-elected Treasurer to a 1-year term beginning January 1, 2014

Sharon Papiernik has been re-elected Secretary to a 1-year term beginning January 1, 2014

John Beck, Cheryl Cleveland, Ke Dong Marja Koivunen, and **Amy Ritter**
have been elected as the at-large members of the Executive Committee
to 3-year terms beginning January 1, 2014

Congratulations to our new 2014 Officers
and Executive Committee Members!

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AGRO Division Spring Conference Call Minutes

Tuesday, March 5, 2013

Attending:
Officers: John Clark, Chair, Steve Duke, Program Chair, Cathleen Hapeman, Vice Chair, Del Koch, Treasurer, Sharon Papiernik, Secretary
Others: Troy Anderson, Rod Bennett, Michael Barrett, Wenlin Chen, Joel Coats, Julie Eble, Scott Jackson, Jeff Jenkins, John Johnston, Mike Krolski, Steve Lehotay, Laura McConnell, Ken Racke, Pat Rice, Jim Seiber, Keith Solomon, Jeanette Van Emon, Diana Aga, Yelena Sapozhnikova

Secretary's Report – Sharon Papiernik

- 2012 Administrative report was prepared by Papiernik and submitted by Clark to ACS. Report, circulated to Executive Committee this week, is pending ACS approval.
- Papiernik noted that this year's report focused on volunteers and activities to engage members. The excellent cadre of AGRO volunteers and their work in providing webinars and other programming made a strong report.

2013 Nominating Committee –Al Barefoot

- Laura McConnell has replaced Cathleen Hapeman on the EC for the remainder of Cathleen's term.

Treasurer's Report – Del Koch

- 2012 Financial report was prepared by Koch and submitted by Clark to ACS. Report was sent to Executive Committee members this week. Report is pending approval from ACS. Koch noted that there was some debate on which sub-category should be used for some items. He explained that $25,000 in Donation income is from Luiz Ruzo for the Peru lectureship. Many of the funds for 2013 are designated, for example $25,000 for Peru lectureship; Innovative Project Grant funds are earmarked for those projects.
- So far in 2013:
    a. paid out about $3000 in expenses (officer training travel, graphics, etc. for IUPAC, webinars)
    b. $8300 in income from sponsorships and Picogram ads; also working on invoicing outstanding sponsorships from 2012.
    c. Del set up a checking account in Columbia, MO. Wells Fargo account will be kept open for at least a year to ensure that we don't lose any direct deposit funds.
    d. Thanks to Del and John for making the transition so smooth.

Finance Committee – Joel Coats

- 2013 Budget: budget expected to be within $8000 of breaking even
- 2014 Budget: no projections yet. Investments are doing well.

Awards Committee – Jim Seiber

- Fellow Awards: nominations are open until March 31
- International Award: will go to Ralf Nauen in 2014
- Innovation Award: will go to Jeanette Van Emon in 2013; presented at Indianapolis meeting
- JAFC Lectureship Awards: Being decided today for both AGRO and AGFD; to be presented in Indianapolis.
- Sterling Hendricks Award: Will go to Keith Solomon
- Kenneth Spencer Award: Selection has been made but not announced

Bylaws Committee – Rod Bennett

- Bylaws were published in the Picogram as required. Bennett received no comments; he asked if anyone on the call had heard any comments. Hearing none, the published version is deemed ready to go to ACS for review. He plans to submit the bylaws to ACS at the Spring 2013 meeting, with the hope of hearing back in time for the Fall (Indianapolis) meeting, and the possibility of finalizing revised bylaws in Spring 2014.

Early Career Scientist Committee

- Graduate Poster Awards – Diana Aga – Aga is soliciting applications for poster travel awards. These tend to be received the last week before they are due, and the deadline may be extended if needed. Current deadline is March 18 for abstract and letter of recommendation. Last year all applications were funded.
- New Investigator Award – Steven Lehotay – No applications have been received yet. The deadline is March 18. Verified that a selection committee is needed, because three awardees are to be selected, and there are typically more than three applicants. While the deadline can be extended until March 31, authors are still subject to the Mar. 18 abstract submission deadline. The abstract is used for assignment into the appropriate symposium.

Programming/Program Chairs

- ***Indianapolis – Steve Duke***
    a. Latest version was sent out to the Executive Committee this morning
    b. 22 oral symposia planned, which could translate into a maximum of 50 ½-day sessions: five full days of 5 concurrent sessions if all are held together.
    c. The RNAi (RNA interference) symposium will be cancelled.
    d. The general session will likely be all posters and invited speakers – for general topic oral submissions, an attempt will be made to place them into one of the specific symposia.

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e. Al Barefoot has been working on funding – they expect a total of $10,000 for Biopesticides, which would cover five ½-day sessions. Possibilities that other funding could support 10% of sessions (5 of 50) entirely by sponsorships. Assuming that AGRO would pay $500 per ½-day session for 40 sessions, this would total $20,000 for what should be a robust program.
f. E-mail programming reminders are being sent out. Attendees noted that the abstract deadline is very early this year. The question was posed whether a speaker slot can be reserved without an abstract – the answer is no, but Symposium Organizers can update abstract information until early April, and the Program Chairs can update abstracts until the end of April.
g. Jim Seiber mentioned the JAFC Best Paper Award session, in which the AGRO and AGFD speakers will present right before the Award ceremony.
h. Ken Racke announced that the AGRO Social will be held at Dow AgroSciences the evening of Tuesday, Sept. 10th. Dow will provide the food, but AGRO may be asked to help with transportation costs (about a 20 – 25 minute bus ride). In order to streamline the required visitor registration process, AGRO members and speakers can register on-line at http://events.signup4.com/ACSAgroSocial
i. Locations of programming have not been announced. Following past practice, Duke and co-programming groups (ENVR and AGFD) are preparing a joint letter to request that our venues be near each other. This request is usually accommodated by ACS.

- ***San Francisco (IUPAC) – Cathleen Hapeman***
  a. A lot of up-front work has been going on. Hapeman has met with nine team leads – still needs some of the team lead write-ups. She is taking names for plenary speakers, and has a sketch of the schedule in place.
  b. AGRO/IUPAC programming will be in the Marriott Marquis Hotel, right across from the Convention Center.
  c. There is a May 1 deadline for 2-page proposals. Hapeman hopes to have titles by May. Almost all speakers will be invited, with about 50% international. Along with the talks, panel discussions and highlighted poster sessions will be included.
  d. Hapeman will lead a brainstorming session for Boston 2015 at Indy's "Blues and Brews."

Co-sponsored Meetings

- ***50th North American Chemical Residue Workshop (NACRW) – Steve Lehotay***
  a. This year's meeting is the 50th annual meeting of what used to be known as the Florida Pesticide Residue Workshop, and will feature a special overview by George Fong (the historical force behind this meeting).
  b. Abstracts for oral presentations are due April 15th and for posters, June 1st.
  c. NACRW ties in with IUPAC by way of a $5,000 IUPAC Symposium Sponsorship. The NACRW website (www.nacrw.org) has the AGRO logo displayed.
  d. *JAFC* is publishing a group of papers submitted by presenters at last year's meeting.
- ***Pacifichem 2015 – John Johnston***
  o Round 1 of session proposals are due in April. Especially interested in rodenticides, international food safety, and others. Let Johnston know of any other session proposals.
- ***LAPRW –Bogota, Columbia 2013, Best Poster Awards –Steve Lehotay***
  a. In the past, AGRO funded $500 for 1st place and $250 each for 2nd and 3rd place, so AGRO commitment is $1000 [Correct minutes from Philadelphia meeting, which specified $100.]
  b. Short courses: FAO, IAEA, FAS, and others are looking into providing training.
  c. Lehotay is planning to go, sponsored by FAS. (Will sequestration affect that?) Lehotay will take IUPAC and AGRO materials, and AGRO will pay for the extra bag fee to transport.
- ***IUPAC 2014 (AGRO-ICPC) – Ken Racke, Laura McConnell***
  a. Racke sent a report to Executive Committee this week.
  b. Organizing committee will be meeting next week, March 12.
  c. Still looking for volunteers: local arrangements; program booklet development; poster session organizers; panel discussion organizers
  d. Networking with ENVR and AGFD – McConnell, Seiber, Johnston will pursue at New Orleans meeting. Van Emon and Bennett will present at Council meeting.
  e. Communications and Publicity committee has been busy (Ellen Arthur is chair). Considering Innovative Project Grant proposal to fund new media approach (You Tube, etc.) to engage early career members and encourage them to participate in AGRO/IUPAC.
  f. Programming Monday-Thursday. Several special events are planned for Sunday.
  g. Sponsors: IUPAC sponsorship guidelines were sent with AGRO sponsorship information. Racke is following up with ~100 potential sponsors.
  h. Looking for IUPAC 2014 ambassadors at meetings (ie, SOT, others)
  i. Looking into contract with administrative assistant to help with organization, communication

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- 5 Batch Analysis
- Phys-chem Studies
- Residue Trials - Analytics
- Field Trials
- Bio Analytical Studies
- Regulatory Services
- E-fate & Metabolism
- Ecotoxicology
  - Aquatic Studies
  - Terrestrial Studies

Councilor's Report – Jeanette van Emon, Rod Bennett

- Agenda for New Orleans is not established. One topic will be: What else should ACS do to help members thrive in the global chemical enterprise? If you have discussion items, forward them to Van Emon or Bennett.
- Kavli lecture series is expanding: In New Orleans, plenary lecture will be given by emerging leader.
- Councilors request that information on webinars be forwarded to them because Bennett is on a sub-committee on innovative programming, Van Emon will present to DAC.
- ACS is hosting additional officer and program chair training for the new program that will replace OASYS. Counselors are going to try to move deadlines forward.

Membership Committee - Dan Stout, John Johnston

- Executive Committee member questioned whether membership list is current; Membership Committee will verify.
- McConnell uploaded a fillable pdf membership form to the AGRO website. This can be e-mailed to ACS and should simplify application.
- Consider having a membership drive at the AGRO table, especially at IUPAC, maybe with some incentive. Membership Committee members are recruiting.

Action item: Organize membership drives at AGRO functions

Strategic Planning Committee – Laura McConnell

- McConnell sent a written update to the Executive Committee this week. AGRO has made excellent progress in meeting its goals. A conference call with Strategic Planning Committee is planned to articulate new goals.
- Webinars are going great, thanks to organizers, sponsors, and Innovative Project Grant funds. The 4th webinar, on pyrethroids, will be broadcast in March. Endangered Species Act is next (tied to Racke's ACS Symposium Series book). Suggestion to advertize webinars as training opportunities for professionals. Webinar page is 2nd most accessed page on AGRO web page.

Communications Committee – Cathleen Hapeman

- Website – Laura McConnell – Going well. Is updated very often.
- eNewsletter - Yelena Sapozhnikova – Going well.
- *PICOGRAM* – Cathleen Hapeman
  a. Hapeman reiterated her request for help with the *PICOGRAM*. Question was raised whether this volunteer position can be incentivized, because it is a large commitment. Answer: In some years, travel expenses were paid by AGRO for *PICOGRAM* editor to attend annual meeting.
  b. Hapeman has asked outside organizations for quotes to outsource *PICOGRAM* preparation.

Action item: have a proposal ready for possible action at the Indianapolis Combined Governance meeting.

- Public Relations – Jeff Jenkins – "old school" press releases are issued to outlets in conference city and hometowns of award winners. Executive Committee recognized need to update methods.

Social Committee – Pat Rice

- Thanks to Racke and Dow for setting up social in Indianapolis.
- Hospitality committee was merged with Social committee. Jenkins is chairing subgroup to set up the venue for the AGRO social and graduate student lunch. Jessica Malin volunteered to lead the program at the social program. Clark will invite Jenkins and Malin to co-chair the Social Committee.
- Suggestion that Development Committee send out one request for sponsorship for all AGRO functions.

Development Committee – Scott Jackson

- Continued to send out solicitations during December. Some new partners have been identified.

International Activities Committee – Ken Racke, Jay Gan

- Referenced co-sponsorship of international events discussed previously on the call. The International Activities Committee is focusing on IUPAC Congress. Goal is to leverage IUPAC to bolster AGRO's international presence.

Old Business from Philadelphia meeting:

- Managing AGRO Archives: Barefoot and Papiernik to implement.
- Operations Manual is posted on website. Consider revising Operations Manual to include recommendation that bylaws committee is responsible for maintenance and communication of the Operations Manual.
- Finance Committee to check into mechanism and cost of bonding AGRO Treasurer: Coats to investigate.
- Follow up on ILSI/HESI? One idea was to designate an AGRO member to work routinely with ILSI. Check with Barefoot; Keri Carstens may be interested

Old business since the Philadelphia meeting:

- Proposed lecture series at the Universidad Nacional Agraria La Molina, UNALM (the Agricultural University) in Lima, Peru. AGRO will collaborate with the Foundation for the Study of Traditional Sciences and Arts. Approved by e-mail vote November 2012.
- JAFC Research Paper of the Year Lectureship Agreement: AGRO to co-sponsor a half-day session. Approved by e-mail vote January 2013.

New Business

- Suggestion to create a Wikipedia page for AGRO. Some historical information about AGRO was put together by Nancy Ragsdale; this could serve as a starting point.

Action item: Establish a Wikipedia page for AGRO.

- Next conference call will be in mid-June.

Summary of new business requiring action:

- Organize a membership drive for the 2013 ACS Indianapolis and 2104 San Francisco national meetings (Laura McConnell and John Clark, co-initiators)
- Develop a Wikipedia page for AGRO (Nancy Ragsdale has a history of the Division that could be used as a start) (Laura McConnell, initiator)
- Develop a proposal for the incorporation of the Division, a process supported by ACS (Steve Duke, initiator)
- Develop a proposal to provide the *PICOGRAM* editor with profession and/or financial support to elevate some of their demands of this position (Cathleen Hapeman, initiator)

COUNCILOR REPORT

245th ACS NATIONAL MEETING
NEW ORLEANS, LA
APRIL 7-11, 2013

Hello Agro members! Both of your Agro Councilors attended the full Council meeting as well as several subcommittee meetings, business meetings and the Division Caucus! Many topics were discuss***ed throughout these meetings.*** We present a summary of topics of interest to the AGRO membership. If you would like any more details please feel free to contact either of us. Also, if you have any concerns you would like presented to ACS governance just let us know. Hope to see many of you in Indianapolis!

ACTIONS OF THE COUNCIL

Election Results
- The Committee on Nominations and Elections presented to the Council the following nominees for selection as candidates for President-Elect, 2014: G. Bryan Balazs, Charles E. Kolb, Jr., Carolyn Ribes, and Diane Grob Schmidt. By electronic ballot, the Council selected G. Bryan Balazs and Charles E. Kolb, Jr. as candidates for 2014 President-Elect.
- These two candidates, along with any candidates selected via petitions, will stand for the Fall National Election.

Society Finances
- Despite the sluggish economy, ACS generated favorable operating results in 2012. Total revenue was $490.7 million, which was $6.1 million or 1.3% greater than the approved budget, and 3.9% higher than 2011. The Net from Operations was $20.2 million, or $4.3 million favorable to budget. This was largely attributable to the favorable performance by ACS Publications and CAS, and represents the 9th consecutive year of positive operations.
- While operating performance was favorable, Unrestricted Net Assets declined $1.4 million to $100.6 million. The year ended with 80% compliance of ACS Board-established financial guidelines.

2014 Member Dues
- The Council voted to set the member dues for 2014 at the fully escalated rate of $154. This rate is established pursuant to an inflation-adjustment formula in the ACS Constitution and Bylaws.

Member Statistics
- Society membership at the end of 2012 was 163,322 which is 893 lower than the 2011 total despite recruiting 24,943 new members. The net loss occurred primarily in the Regular, full member category.
- There was continued growth in both the Student Member undergraduate and international categories, which helped mitigate the overall decline in membership.
- The Membership Affairs Committee approved five pilot market data tests to increase membership.

Attendance Report
- Approximate numbers for the ACS spring national meeting were: 15,596 registrants, including 8,105 regular attendees and 5,793 students.
- The meeting had 11,232 papers presented.

Divisional Activities Name Change Request
- The Divisional Activities Committee (DAC) received a request from the Division of Colloid and Surface Chemistry to change its name to the Division of Colloids, Surfaces and Nanomaterials.
- Six divisions have registered opposition to the proposed name, largely due to the use of the term 'nanomaterials'. DAC will ask Council to vote on the new name in Indianapolis, with a recommendation to approve. This is becoming a rather contentious issue for the Council.

Special Discussion Item
- A very interesting special discussion item was presented by ACS President Marinda Li Wu on "What else should ACS do to help members to thrive in the global chemistry enterprise?"
- ACS has established a strategic goal to "Empower an inclusive community of members with networks, opportunities, resources, and skills to thrive in the global economy." In support of this goal, President Wu commissioned a task force entitled, "Vision 2025: Helping ACS Members Thrive in the Global Chemistry Enterprise," to identify globalization opportunities and engage members in advocacy for improving the business and job climate.
- *Please let your AGRO Councilors know if you have anything you would like presented on this topic.*

ACTIONS OF THE BOARD OF DIRECTORS

The Board's Committees and Working Groups
- On the recommendation of the Committee on Professional & Member Relations, the Board voted to approve an alliance with the Latin American Federation of Chemical Associations (FLAQ) and to renew an alliance with the Chinese Chemical Society.
- The signing ceremony for FLAQ will take place at the Fall national meeting.

The Board's Open Session
- The Board held a lively, well-attended open session which featured a special forum focused on two questions:
  1. "What one thing would you like from ACS that you don't get now?"
  2. "What one thing do you get from another organization that you wish you got from ACS?"
- *Please give any input you would like brought to the Boards attention to an AGRO Councilor.*

FURTHERMORE:

- **m.wu@acs.org** – contact information for ACS President Marinda Wu
- **www.acs.org/leadscopeqa** - ACS vs. Leadscope questions and answers
- **www.acs.org/newmember** - information on "Why should I join the ACS?"
- **safety@acs.org** – for comments and suggestions about safety to the Committee on Chemical Safety
- **www.acs.org/ei** - information on the ACS Entrepreneurial Initiative
- **outreach@acs.org** – information on "Celebrating Chemistry" for 4th – 6th graders

Respectfully submitted,
Jeanette M. Van Emon,vanemon.jeanette@epa.gov
Rodney Bennett, rodney.bennett@jrfamerica.com

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***BYLAWS OF THE
DIVISION OF AGROCHEMICALS of the
AMERICAN CHEMICAL SOCIETY

*** *Proposed bylaws submitted August 2012.*
Effective TBD. 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 Society Affiliate of the SOCIETY may apply to the Secretary to become a Society Affiliate of the Division. Provided that Division dues established for Society Affiliates are paid, a Society 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 Society 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 one year 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.

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 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 The form of the ballot and procedures for balloting will be in compliance with the overall procedures of the Society. 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 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 and 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 Social 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 Communications Committee of at least three members. This Committee shall be responsible for coordination of the communication and publication activities of the Division, (including 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 Divison upon the usual authentication.

Bylaw VIII. Meetings

Section 1. There shall be a meeting of the Division at each a national meeting of the SOCIETY at least once per year, 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 one of the national meetings of the SOCIETY. The fall meeting of the SOCIETY will be designated as the annual meeting unless otherwise instructed by the Executive Committee. Division business requiring vote of the membership shall be conducted only at this meeting, except as provided elsewhere in these bylaws. 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.

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.

NOTES

American Chemical Society
AGRO Division
246th ACS National Meeting
September 8 - 12, 2013
Indianapolis, Indiana USA
S. Duke, *Program Chair* and J. Clark, *Division Chair*

PROGRAM

DIVISION BUSINESS AND PLANNING

AGRO Business Meeting
Sunday 5:00 – 10:00 PM
Crowne Plaza, Grand Hall Ballroom
All Members Welcome

IUPAC 2014 Scientific Committee Meeting
Sunday 11:30 - 1 PM
Crowne Plaza, Executive Board Room
Committee Members Only

IUPAC 2014 Organizing Committee Meeting
Monday 5:00 – 7:00 PM
Crowne Plaza, Victoria Station B
Committee Members Only

Brainstorming for Boston & Beyond – Long Range Program Planning & Social
Wednesday 5:00 – 7:00 PM
Crowne Plaza, Grand Central A-C
Beverages are FREE
All Members/Speakers welcomed; see page 41

SOCIAL EVENTS

Graduate Student Luncheon
Monday 11:45 – 1:15 PM
Crowne Plaza, Grand Central A
Reservations Required; see page 34

Sterling B. Hendricks Award Lecture Reception
Tuesday following the 11:30 AM lecture
Crowne Plaza, Grand Central Station A&B

AGRO Awards Social
Tuesday 5:00 – 8:00 PM
Dow AgroSciences World Headquarters
Buses depart at 5 pm promptly from
Crowne Plaza Hotel at Capitol Avenue Entrance
Members/Speakers/Guests welcome
Preregistration Required - August 31 Deadline
Go to www.agrodiv.org for link

SUNDAY MORNING

Advanced Bioanalytical Technologies for GM Detection Protein
Cosponsored by AGFD and ANYL
Financially supported by NanoString Technologies
A. M. Rimando, G. Shan, C. Zhong, *Organizers, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

8:00 Introductory Remarks.

8:05 – 1. Characterizing intractable targets using homogenous immunoassays. **R. Bosse**

8:30 – 2. Multiplexing protein analysis of transgenic plant samples using MSD technology. **A. Gao**

8:55 – 3. Immunoassay automation and its application in GM detection. **M. S. Yarnall**

9:20 – 4. Development and implementation of multiplexed LC-MS/MS strategies for the quantitation of plant-expressed proteins in genetically-modified crops. **T. J. Oman**, R. C. Hill, B. W. Schafer, J. R. Gilbert, G. Shan

9:45 – 5. Multiplexing protein quantitation of transgenic proteins in soybean tissues using tandem mass spectrometry (LC-MS/MS). **R. C. Hill**, T. J. Oman, G. Shan, J. Lawry, L. Wang, K. Smith, B. Wulfkuhle, A. Asberry, A. Cruse

10:10 Intermission.

10:25 – 6. Quantification of allergenic protein(s) in soybeans by 2D liquid chromatography with ultraviolet and mass spectrometric detection. **K. Kuppannan**, S. Julka, A. Karnoup, D. Dielman, B. Schafer, S. A. Young

10:50 – 7. Acceptance criteria for GLP validation of quantitative analytical methods for proteins by ELISA and LC/MS/MS. **L. M. Mallis**, J. E. Eble, C. Chen, G. Shan

11:15 – 8. Development of a sandwich ELISA for heat denatured Bt Cry1Ac protein. C. Zhen, **W. Baomin**

11:40 – 9. Bioanalytical technologies for GM detection in India. A. Seetha, S. Sivaramakrishnan, **J. K. Bhanushali**

Spray Application Technology
A. Hewitt, S. Jackson, *Organizers*
G. Kruger, *Organizer, Presiding*

Section B
Crowne Plaza, IIllinois Street Ballroom West

8:30 Introductory Remarks.

8:35 – 10. Wind tunnel testing of nozzles for reduction of drift. **J. P. Hanzas**, R. E. Wolf, B. N. Toth

8:55 – 11. Validation of the extrapolation of wind tunnel-generated spray droplet distributions to DRT classifications with field data. **P. L. Havens**, D. E. Hillger, A. J. Hewitt, G. R. Kruger, S. L. Wilson, J. J. Schleier

9:15 – 12. Comparison of multiple spray drift deposition data sets. **S. H. Jackson**

9:35 – 13. Ground spray drift modeling for pesticide application. **A. Hewitt**

9:55 – 14. RegDISP: A flexible tool for the prediction of pesticide spray drift deposition based on measured ground application data. **T. Estes**, B. Patterson, S. Jackson, M. Winchell

10:15 Intermission.

10:35 – 15. Drift-reduction for orchard applications: Practical adoption of low-drift nozzles while maintaining efficacy. **J. J. Schleier III**, S. Norman, D. Harris, E. Tescari, C. Vaj

10:55 – 16. Systematic literature review: Downwind spray drift from orchard air blast sprayers. **J. A. Bonds**, J. Z. Tang, S. Jackson, M. Ledson

11:15 – 17. Mechanisms, experiment, and theory of liquid sheet breakup and drop size from agricultural nozzles. A. Altieri,**S. A. Cryer**, L. Acharya, K. Qin

11:35 Discussion.

Accurate Mass Analyses in Support of Agricultural Chemical Research and Development
M. Saeed, *Organizer*
P. Reibach, *Organizer, Presiding*

Section C
Crowne Plaza, Milwaukee

10:00 Introductory Remarks.

10:05 – 18. Impact of high resolution accurate mass (HRAM) on metabolite identification for crop protection studies and regulatory submission. **M. Saeed**, P. Reibach

10:25 – 19. Use of accurate mass instrumentation for the differentiation of molecules with the same exact mass. **P. Reibach**, M. Fleischer, N. McHale, A. Grenier

10:45 – 20. Accurate mass for small molecule analysis. **J. Ferguson**

11:05 – 21. Metabolite identification using modern Q-TOF and Q-Orbitrap instrumentation. **J. L. Balcer**, J. R. Gilbert, Y. Adelfinskaya, A. Jackson, M. J. Hastings, L. Buchholz, B. M. Wendelburg

11:25 – 22. Applications of very high resolution UHPLC-MS data for metabolic fate studies of agrochemicals. **T. Stratton**, P. Bennett

11:45 Panel Discussion.

SUNDAY AFTERNOON

Advanced Bioanalytical Technologies for GM Detection Nucleic Acid

Cosponsored by AGFD and ANYL
Financially supported by NanoString Technologies
A. M. Rimando, G. Shan, C. Zhong, *Organizers, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

1:00 Introductory Remarks.

1:05 – 23. Status of GMO detection in Brazil. **R. M. Morello**

1:30 – 24. Current trends in DNA detection for biotech crops. **C. Channabasavaradhya**

1:55 – 25. Southern-by-sequencing: Molecular characterization of transgenic events. **M. Beatty**

2:20 – 26. New approaches in GMO detection as a solution for emerging problems. **J. Mano**, R. Takabatake, K. Kitta

2:45 – 27. Digital highly multiplexed gene-expression studies in plants: Mapping whole biological pathways in space and time using optical barcoding (nCounter Technology). **J. M. Beechem**

3:10 Intermission.

3:25 – 28. Use of QuantiGene® and QuantiGene® plex assays for direct RNA or gDNA copy number variation analysis direct from sample lysates: An introduction to the branched DNA technology from Affymetrix/Panomics Solutions. **M. M. Hughes**

3:50 – 29. Novel reference plasmid DNA for detection of genetically modified rice. **L. Li**, W. Jin, X. Zhang, Y. Wan

4:15 – 30. Inline, ultra high-throughput, Array Tape™ based end-point nucleic acid detection: Novel DNAble® v2.0 isothermal amplification system. **D. Shaffer**, S. Judice, L. Peters, B. Parker

4:40 – 31. Novel DNAble® v3.0 isothermal amplification platforms for GMO testing on-site at the grain silos and in the testing laboratory. **L. Peters**, S. Judice, J. Rudd, D. Shaffer, B. O. Parker

Spray Application Technology
G. Kruger, *Organizer*
A. Hewitt, S. Jackson, *Organizers, Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

1:30 Introductory Remarks.

1:35 – 32. Robust built-in spray drift reduction technology for pesticide formulations. **H. Shao**, M. Li, H. Tank, K. Qin, L. Liu, S. Wilson

1:55 – 33. Interfacial effects on the performance of emulsion-based antidrift spray solutions. **S. Wilson**, K. Qin, B. Downer

2:15 – 34. Agricultural spray tank mixing. **S. K. Ramalingam**, K. Qin, H. Jeon

2:35 – 35. Improvements in range and pasture formulations. **R. Acosta Amado**, L. Brinkworth, P. L. Burch, E. S. Flynn, N. T. Caceres

2:55 Intermission.

3:10 – 36. Effects of nozzles and drift reduction agents on droplet size distributions of dicamba and glyphosate mixtures. **T. B. Orr**, K. M. Remund, J. N. Travers, J. L. Honnegger, A. J. Hewitt

3:30 – 37. Field measurement of pesticides using passive, active, and laser sampling systems. **A. J. Hewitt**, R. Roten, C. Ferguson, C. Geoghegan, T. Corkins, E. Bachalo

3:50 Discussion.

Herbicide-Resistant Crops and Weeds: Current Status
J. Green, *Organizer*
T. Mueller, *Organizer, Presiding*

Section C
Crowne Plaza, Milwaukee

1:00 Introductory Remarks.

1:05 – 38. Glyphosate is not the herbicide it used to be: A North American perspective. **T. C. Mueller**

1:15 – 39. Surveys of herbicide resistances in Missouri waterhemp populations with a focus on correlations between field management practices and glyphosate resistance. **K. Bradley**, J. Schultz

1:40 – 40. Iowa survey of herbicide resistances in common waterhemp including glyphosate and other herbicide groups. **M. D. Owen**

2:05 – 41. Weed resistance in Arkansas: One crisis averted another begins? **B. Scott**

2:30 – 42. Glyphosate-resistant weeds: Lessons learned in Tennessee. **L. Steckel**

2:55 Intermission.

3:25 – 43. Complexity of weed management over the next five years. **B. Young**

3:50 – 44. Herbicide resistance by weeds: Its effects on and off the field. **H. Strek**, R. Beffa, T. Wilde

4:15 – 45. New tools for sustainable management of herbicide resistant weeds: The Enlist™ Weed Control System. **M. A. Peterson**, B. Braxton, R. M. Huckaba, D. M. Simpson

4:40 – 46. HPPD-inhibitor herbicide resistance in the USA: A Syngenta perspective. **L. Glasgow**, V. Shivrain, G. Vail, B. Manley, S. S. Kaundun, B. Miller

5:05 – 47. Strategies for sustainable weed management. **J. Kendig**, R. M. Cole, J. K. Soteres, J. N. Travers

ADME: The Motion of Veterinary Drugs and Xenobiotics
Cosponsored by AGFD and ENVR
T. Wehner, S. Lupton, *Organizers, Presiding*

Section D
Crowne Plaza, B&O (Baltimore & Ohio)

1:30 Introductory Remarks.

1:35 – 48. Role of ADME studies in veterinary drug development and registration. **T. A. Wehner**

1:55 – 49. Determination of hormone residues in rainbow trout muscle using liquid chromatography-tandem mass spectrometry. **P. Chu**, T. Johnson, W. Song, E. Evans

2:15 – 50. Pharmacokinetics and synovial fluid/plasma drug ratios of firocoxib and phenylbutazone in horses after repeated drug administration. **V. Kvaternick**, W. Cui, T. Nguyen, C. Zarabadipour, B. Fankhauser, H. Cheramie, C. E. Kawcak, C. McIlwraith, C. Lee

2:35 – 51. Validation of an LC-MS/MS regulatory method to determine and confirm three tetracyclines (oxytetracycline, chlortetracycline, and tetracycline) in bovine kidney, liver, and muscle. **L. Girard**, S. Smith, O. A. Chiesa, M. Lopez, S. Feng, P. Kijak, H. Li

2:55 Intermission.

3:15 – 52. Identification of a novel protein in rat bile that associates with POPs. **H. Hakk**

3:35 – 53. Determination of penicillin-G procaine in kidney, muscle, serum, and urine of heavy sows after intramuscular administration. **S. J. Lupton**, W. L. Shelver, D. J. Newman, S. Larsen, D. J. Smith

3:55 – 54. Quantitative method to measure five compounds simultaneously from cotton gloves. **L. D. Payne**, V. Kvaternick, V. Cooper

4:15 – 55. Physiologically-based pharmacokinetic model to estimate non-target exposure to rodenticides. **J. J. Johnston**

4:35 – 56. Pharmacokinetics of eprinomectin extended-release injectable for cattle. **T. A. Wehner**, V. J. Kvaternick, J. B. Fischer

4:55 Concluding Remarks.

MONDAY MORNING

Biopesticides: State of the Art and Future Opportunities
The Big Picture
Financially supported by American Chemical Society Innovation Grant and Ag Biotech Stewardship Technical Committee
A. D. Gross, J. Seiber, J. Coats, *Organizers*
S. Duke, *Organizer, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

8:00 Introductory Remarks.

8:05 – 57. Chemical ecology and biorational pesticide design. **J. A. Pickett**

8:50 – 58. USDA-Agricultural Research Service: Perspectives on biopesticides. **D. Strickland**

9:15 – 59. Microbially-derived pesticides: Challenges and opportunities. **B. C. Gerwick**

9:40 – 60. Bringing new biologicals to market. **M. Meadows-Smith**

10:05 Intermission.

10:25 – 61. Chemical ecoprospecting and biopesticides. **M. R. Berenbaum**

10:50 – 62. Market opportunities for biopesticides. **P. G. Marrone**, P. Himmel, A. Stewart

11:15 – 63. Botanical insecticides: A global perspective. **M. B. Isman**

11:40 Concluding Remarks.

International Award for Research in Agrochemicals

Symposium in Honor of Dr. René Feyereisen

Financially supported by
DuPont Crop Protection
J. Ottea, *Organizer, Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

8:00 Introductory Remarks.

8:15 – 64. Insect P450 paradox: Too simple as targets, too complicated as detoxifiers? **R. Feyereisen**

9:00 – 65. DDT, flies, and molecular biology. **R. H. ffrench-Constant**

9:30 – 66. How are recombinant cytochrome P450s and aryl hydrocarbon receptor (AhR) useful for biotransformation and biomonitoring of environmental chemicals? **H. Ohkawa**

10:00 Intermission.

10:15 – 67. P450s responsible for insecticide resistance in malaria vectors: Finding them, tracking them, stopping them? **H. Ranson**, M. Paine, C. Wondji, J. Vontas

10:45 – 68. Tale about an aphid and its insecticide-driven upgrade: *Myzus persicae* version 4.0. **R. Nauen**, C. Bass

11:15 – 69. Bed bugs evolved unique adaptive strategy to resist pyrethroid insecticides. **F. Zhu**

Environmental Fate, Transport, and Modeling of Agriculturally-Related Chemicals
Cosponsored by ENVR
S. Jackson, *Organizer*
T. Potter, N. Peranginangin, *Organizers, Presiding*

Section C
Crowne Plaza, Milwaukee

8:00 Introductory Remarks.

8:10 – 70. Atmospheric degradation of chlorpyrifos and chlorpyrifos-oxon. **A. Muñoz**, M. Ródenas, E. Borrás, M. Vázquez, T. Vera

8:30 – 71. Assessing risks from pesticide post-application volatilization. **R. Reiss**

8:50 – 72. Accumulation of pharmaceutical and personal care products (PPCPs) in vegetables under field conditions. **X. Wu**, J. L. Conkle, F. Ernst, J. Gan

9:10 – 73. Pesticide runoff risk during peanut production in the southern Atlantic Coastal Plain. **T. L. Potter**, D. D. Bosch, T. C. Strickland

9:30 – 74. Nutrient export in tile drainage: Comparing manure injection to fertigation. **S. K. Papiernik**, G. W. Feyereisen, C. D. Wente, J. M. Baker

9:50 – 75. ***New Investigator Finalist:*** Seed-coated clothianidin fate in corn and soybean fields using conservation tillage. **C. de Perre**, M. J. Lydy

10:10 Intermission.

10:30 – 76. Occurrence of neonicotinoid insecticides in water in two US regions. **M. L. Hladik**, D. L. Calhoun, K. L. Smalling, K. M. Kuivila, D. W. Kolpin

10:50 – 77. Estimating organic carbon sorption coefficients (K_{oc}) of nine pyrethroids based on feely dissolved chemical concentrations measured with solid phase microextraction (SPME). **T. Xu**, P. Hendley, K. Clark, B. Plastridge, S. Brown

11:10 – 78. Overview of a national aquatic risk assessment of pyrethroid use in agriculture. **J. M. Giddings**, M. Dobbs, P. Hendley, C. Holmes, A. Ritter

11:30 Questions.

21st Century Vision for Testing and Risk Assessment: Implications for Agrochemicals
C. Rowlands, K. Solomon, C. B. Cleveland, *Organizers*
M. Embry, J. McLain, T. Pastoor, *Organizers, Presiding*

Section D
Crowne Plaza, B&O (Baltimore & Ohio)

8:30 Introductory Remarks.

8:35 – 79. US EPA Office of Pesticide Program's 21st century vision and strategy for communication. **J. L. McLain**, V. L. Dellarco

8:55 – 80. New technologies for exposure assessment. **J. Wambaugh**

9:15 – 81. Adverse outcome pathways for neurotoxicity: An example using pyrethroid insecticides. **T. J. Shafer**

9:35 – 82. Evolution of the Endocrine Disruptor Screening Program (EDSP) in the 21st century. **M. Manibusan**

9:55 – 83. Cumulative risk assessment for human health: Asking the right questions. **K. Solomon**, M. Wilks, A. Moretto, A. Boobis, R. Philips, T. Pastoor, M. Embry

10:15 Intermission.

10:30 – 84. In vitro screening data within Tox 21: How to use it? **J. P. Bailey**, J. Mehta

10:50 – 85. Incorporating new technologies into toxicity testing and chemical risk assessment: Moving from 21st century vision to a data-driven framework. R. S. Thomas, **B. Wetmore**

11:10 – 86. Approaches for establishing scientific confidence in 21st century methods for toxicity evaluations. **R. A. Becker**, G. Patlewicz, J. Rowlands

11:30 – 87. HESI's RISK21 roadmap: A transparent risk assessment methodology. **T. Pastoor**, M. Embry, A. Boobis

11:50 Concluding Remarks.

ENVR Division

Predicting Molecular Properties of Environmental Contaminants: Empirical and Theoretical Methods Partitioning
Cosponsored by AGRO and COMP‡
E. Weber, K. Fenner, *Organizers*
P. G. Tratnyek, D. Ditoro, *Organizers, Presiding*

Section B
Crowne Plaza, Penn Station A

8:30 Introductory Remarks.

8:35 – ENVR 62. Perspective on the evolution and future of partition coefficients. **D. Mackay**, A. Celsie, M. Parnis

9:05 – ENVR 63. How accurate are physical property estimation programs for organosilicon compounds? **R. S. Boethling**, W. Meylan

9:25 – ENVR 64. Assessing the reliability of QSAR predictions for structurally complex chemicals. **T. N. Brown**, A. Stenzel, K. Goss

9:45 – ENVR 65. Physicochemical properties of C_{60} related to its environmental fate and exposure. **C. T. Jafvert**, P. P. Kulkarni, C. Chen

10:05 Intermission.

10:25 – ENVR 66. Molecular simulation-based thermodynamic protocol for computing physicochemical properties of environmental contaminants. **S. I. Sandler**, A. Ahmed

10:55 – ENVR 67. Applications of polyparameter linear free energy relationships (PP-LFERs) for evaluating environmentally relevant partition coefficients of organic chemicals. **S. Endo**, K. Goss

11:15 – ENVR 68. Predicting chemical partitioning to environmental phases using molecular structure. **D. M. Di Toro**, O. Dmitrenko

11:35 – ENVR 69. General linear free energy relationship models for predicting vapor pressure and boiling point of organic and organosilicon compounds. **G. E. Kozerski**

MONDAY AFTERNOON

Biopesticides: State of the Art and Future Opportunities
Repellents and Attractants
Financially supported by American Chemical Society Innovation Grant and Ag Biotech Stewardship Technical Committee
A. D. Gross, J. Seiber, S. Duke, *Organizers*
J. Coats, *Organizer, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

1:15 Introductory Remarks.

1:20 – 88. Semiochemicals to control orchard pests. **J. J. Beck**

1:40 – 89. Discovery of mosquito attractants and attraction-inhibitors. **U. R. Bernier**, M. Tsikolia, N. M. Agramonte

2:00 – 90. Discovery and development of repellents. **R. Roe**, R. D. Mitchell, A. Wallace, E. Hodgson, B. Bissinger, A. Carr, C. Apperson, C. Schal, D. Sonenshine, A. Dhammi, J. van Kretschmar, J. Zhu

2:20 – 91. SPLAT: A delivery technology for attractants and repellents. **A. Mafra-Neto**

2:40 – 92. ***New Investigator Finalist:*** Neurotoxicity and mode of action of *N,N*-diethyl-*meta*-toluamide (DEET) on the insect nervous system and mammalian neurons. **D. R. Swale**, B. Sun, J. R. Bloomquist

3:00 Concluding Remarks.

AGRO International Research Award: Symposium in Honor of Dr. René Feyereisen
Financially supported by DuPont Crop Protection
J. Ottea, *Organizer, Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

1:15 – 93. Enzymes, insecticides, and pests: Oh My! **T. C. Sparks**

1:45 – 94. Inhibitors targeting acetylcholinesterase with high selectivity for arthropod disease vectors. **J. R. Bloomquist**, J. Li, M. M. Totrov, P. R. Carlier

2:15 – 95. *Bacillus thuringiensis israelensis* toxins have multiple modes of action in *Aedes aegypti*. **S. S. Gill**, J. Chen, S. Lee, K. Aimanova

2:45 – 96. CYP genes in termites and their roles in termite biology. **M. E. Scharf**

3:15 Intermission.

3:30 – 97. G protein coupled receptors as targets for insecticide discovery. **D. A. Schooley**

4:00 – 98. Potential acaricidal targets in tick salivary glands. L. Simo, **Y. Park**

4:30 – 99. Using genomic tools to determine the mode of action of acaricides: The tale of chitin synthesis inhibitors in*Tetranychus urticae*. **T. Van Leeuwen**, R. M. Clark

5:00 Concluding Remarks.

Environmental Fate, Transport, and Modeling of Agriculturally-Related Chemicals
Cosponsored by ENVR
T. Potter, S. Jackson, N. Peranginangin, *Organizers, Presiding*

Section C
Crowne Plaza, Milwaukee

1:15 – 100. Higher-tier aquatic exposure estimation for agricultural pyrethroid-use patterns and associated model sensitivities. **D. A. Desmarteau**, A. M. Ritter, P. Hendley, S. Jackson, M. Dobbs, J. Giddings

1:35 – 101. PRZM-Hybrid modeling system utilizing an agronomic approach to define watershed-scale chemical applications.**P. Miller**, W. Northcott, C. Harbourt, M. Cheplick, P. Hendley, C. Truman

1:55 – 102. PRZM-Hybrid and VFSMOD modeling of chlorpyrifos transport in small agricultural watersheds in Minnesota, USA. **R. K. Gali**, **N. N. Poletika**, S. A. Cryer, S. S. Mishra

2:15 – 103. Predicting stream concentrations of selected pesticides using adjusted Watershed Regressions for Pesticides (WARP) models. **W. Stone**, R. Gilliom

2:35 – 104. Conceptual model for estimating exposure from the use of pesticides on rice. **A. Shelby**, K. White, M. Echeverria, D. Young, C. Peck, N. Thurman

2:55 – 105. Approach for predicting pesticide EECs in static water bodies based on spatially-explicit hydrography, landscape, and pesticide-use data. **M. Winchell**, N. Peranginangin, T. Estes, L. Padilla

3:15 Intermission.

3:35 – 106. GIS approach to identify vulnerable surface water monitoring sites to assess pesticide fate, transport, and exposure potential. **T. L. Negley**, T. Xu, D. K. Moore, D. G. Dyer, A. C. Newcombe

3:55 – 107. Comparison of three leaching models of different sophistication for estimating shallow groundwater concentrations. W. Chen, **T. Estes**

4:15 – 108. Validation and extension of a regional groundwater vulnerability assessment tool in Hawaii for agrochemicals at a national scale. S. Ki, **C. Ray**

4:35 Questions.

Pesticide Regulatory Science in the 21st Century Merging Research and Regulations
Financially supported by Council for the Advancement of Pyrethroid Human Risk Assessment
T. Osimitz, *Organizer*
M. Brooks, *Organizer, Presiding*

Section D
Crowne Plaza, B&O (Baltimore & Ohio)

1:15 – 109. Bridging the gap in quality assurance to academic settings for government regulatory science. **M. W. Brooks**

1:35 – 110. Use of a study protocol to assist in assuring appropriate documentation when conducting research in a non-GLP laboratory. **D. J. Minnema**

1:55 – 111. Non-GLP studies: Critical aspects required to help assure data integrity, accuracy, and study reconstruction. **R. J. Daniel**

2:15 – 112. Ensuring data quality for studies conducted in academic research laboratories. **J. V. Bruckner**, T. G. Osmitz

2:35 – 113. Development and use of a novel CAR direct activation assay to investigate species differences in mode of action with conazole-induced rodent liver tumors. **C. J. Omiecinski**, **R. C. Peffer**

2:55 – 114. Evaluation of an in vitro assay to characterize the effects of environmental contaminants on native ion channels in the spirit of good laboratory practices: Role of university labs. **S. B. Symington**, E. Murenzi, K. Yoon, J. Clark

3:15 Intermission.

3:35 – 115. Challenges and solutions for utilizing our research institutions' data to support regulatory decisions. **N. A. Assaf**

3:55 – 116. US EPA Office of Pesticide Program guidance for considering and using open literature toxicity studies to support human health risk assessment. **J. L. McLain**, B. May, V. L. Dellarco, J. Rowland

4:15 – 117. Twenty-first century toxicology and risk assessment: Going beyond guideline studies. **T. G. Osimitz**

4:35 Panel Discussion.

4:55 Concluding Remarks.

AGRO Education Award Poster Session

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

1:30 - 5:30 pm

Section E
Indiana Convention Center
Halls F&G

118. Multi-year field study of the fate and transport of three insecticides in an agricultural ecosystem. **S. Mueting**, K. Strain, M. Lydy

119. Assessing the removal of hormones and their potency as endocrine-disrupting chemicals in dairy wastes through an anaerobic digestion system. **K. M. Noguera-Oviedo**, S. A. Mackintosh, L. Su, J. S. Wallace, D. S. Aga

120. Determination of carbon nanotube uptake, translocation, and bioaccumulation in corn (*Zea mays L.*). **A. Parra**, B. Shrestha, F. Irin, M. J. Green, J. E. Cañas-Carrell

121. Evaluation of glufosinate and glyphosate translocation in young almond (*Prunus dulcis*) trees. **R. S. Mejorado**, M. L. Moretti, J. M. Abit, B. D. Hanson

122. Biological validation of enzyme-linked immunosorbent assays for detection of Cry proteins in the environment. **V. C. Albright**, R. L. Hellmich, J. R. Coats

123. Development and validation of a method to quantify Bt-Cry1Ab in water matrices. **K. E. Strain**, S. A. Mueting, M. J. Lydy

124. Deorphanization and pharmacological profile of a tyramine receptor from the southern cattle tick (*Rhipicephalus microplus*). **A. D. Gross**, M. J. Kimber, K. B. Temeyer, R. J. Miller, A. Y. Li, A. A. Pérez de León, J. R. Coats

125. Quantitative lipid analysis of gut microflora consortium in the Giant Panda. **C. Johnston**, C. Williams, D. Sparks, A. Kouba, S. Willard, A. Brown

126. Assessment of conventional waste management and advanced waste treatment systems in removing veterinary antibiotics. **J. S. Wallace**, K. Noguera-Oviedo, D. S. Aga

127. Dynamic coupled fluxes of current-use pesticides in air-water/soil-sediment system in a city in southern China. **H. Li**, Y. Wei, J. You

128. Isomer-specific biodegradation of nonylphenol in river sediments. **Z. Lu**, J. Gan

129. Synergistic effects of verapamil on tacrine toxicity to vector mosquitoes. **N. N. Pham**, T. D. Anderson

130. Voltage-sensitive potassium channels expressed by hormone treatment in mosquito cell lines. **L. Jenson**, B. Sun, J. Bloomquist

131. Evaluation of synthetic compounds as novel mosquitocides targeting potassium channels for control of *Aedes aegypti*and *Anopheles gambiae*. **N. R. Larson**, B. Sun, P. Carlier, M. Ma, J. R. Bloomquist

132. Influence of amendments on the degradation of pharmaceuticals in soil. **J. Li**, Q. Ye, J. Gan

ENVR Division

Air Monitoring
Cosponsored by AGRO, ANYL, and CHAS
J. Maclachlan, *Organizer, Presiding*

Section C
Crowne Plaza, Penn Station B

1:30 Introductory Remarks.

1:35 – ENVR 98. Comparison of Federal Equivalent Method (FEM) and Federal Reference Method (FRM) in evaluating $PM_{2.5}$ in Cincinnati, Ohio. **K. Li**, M. Lu

1:55 – ENVR 99. Characterization of particulate matter (PM) generated from commercial DC-8 jet burning petroleum-based JP-8 and synthetic FJ and HRJ fuels. **C. Huang**, R. L. Vander Wal

2:15 – ENVR 100. Impact of nanostructure on soot oxidation: Pressure and fuel comparisons. **C. K. Gaddam**, R. L. Vander Wal

2:35 – ENVR 101. Dynamics of airborne PCBs illuminated using a strategic deployment of active and passive samplers. **D. Hu**, T. Schulz, C. Persoon, K. Hornbuckle

2:55 – ENVR 102. Pyrolysis behavior of engineered carbon nanotube polymer composites. **C. J. Akinyi**

3:15 Intermission.

3:30 – ENVR 103. Modern high resolution gas chromatography: Air sampling approaches that exploit the high performance, small size, and low power requirements of person-portable GC-MS instrumentation now available. **P. A. Smith**

3:50 – ENVR 104. Personal PID chemical sensor coupled with a real-time location system to create a novel direct-reading exposure assessment method. **K. K. Brown**, K. R. Mead, P. B. Shaw, R. J. Kovein, R. T. Voorhees, A. R. Brandes

4:10 – ENVR 105. Tunable electronic noses for monitoring volatile small molecules. **K. Benkstein**, A. Vergara, C. Montgomery, S. Semancik

4:30 – ENVR 106. Assessing spatiotemporal commensurability for semi-volatile compounds in passive and active sampling through simulated passive air sampling rates and concentrations. S. N. Spak, N. T. Petrich, C. E. Shanahan, G. R. Carmichael, D. Hu, A. Martinez, Z. Rodenburg, **K. C. Hornbuckle**

4:50 Discussion.

5:20 Concluding Remarks.

ENVR Division

Predicting Molecular Properties of Environmental Contaminants: Empirical and Theoretical Methods Reactivity
Cosponsored by AGRO and COMP[‡]
D. Ditoro, K. Fenner, *Organizers*
P. G. Tratnyek, E. Weber, *Organizers, Presiding*

Section B
Crowne Plaza, Penn Station A

1:30 Introductory Remarks.

1:35 – ENVR 90. Reliable predictions of molecular properties for environmental studies. **D. A. Dixon**

2:05 – ENVR 91. Quantum mechanical modeling of PAH metabolic intermediates and their association with metals and minerals. **J. D. Kubicki**, H. D. Watts

2:25 – ENVR 92. Correlation analysis of oxidation kinetics for organic solutes: Meta-analysis of QSARs for the major aqueous oxidants. **P. G. Tratnyek**

2:45 – ENVR 93. QSAR for the suitability of activated carbon adsorption for EDC removal. **L. Morkowchuk**, A. Kennicutt, J. Kilduff, C. Breneman

3:05 Intermission.

3:25 – ENVR 94. Modeling remediation pathways available to environmental contaminants. **C. J. Cramer**

3:55 – ENVR 95. Quantifying the many possible hydrolysis reactions of nitroaromatic compounds using computational methods. **E. J. Bylaska**, K. Glaesmann, A. J. Salter-Blanc, P. G. Tratnyek

4:15 – ENVR 96. Effects of solvation methodology on hydrolysis and oxidation pathways of organophosphorus compounds: Implications for QSPR model development. **T. T. Sanan**, M. L. Magnuson, H. Mash

4:35 – ENVR 97. Quantum chemical vs. group contribution method based estimates of aqueous phase Gibbs free energy data for halophenols. **J. Dolfing**, I. Novak

MONDAY EVENING

8:00 - 10:00 Sci-Mix
S. Duke, *Organizer*

Section A
Indiana Convention Center, Halls F&G

118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132. See previous listings.
204, 205, 210, 212, 215, 217, 218. See subsequent listings.

TUESDAY MORNING

Biopesticides: State of the Art and Future Opportunities
Insecticides and Nematicides
Financially supported by American Chemical Society Innovation Grant and Ag Biotech Stewardship Technical Committee
J. Seiber, S. Duke, *Organizers*
A. D. Gross, J. Coats, *Organizers, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

7:55 Introductory Remarks.

8:00 – 133. Voltage-sensitive potassium channels as new target sites for biorational insecticide design. **J. R. Bloomquist**, M. M. Totrov, P. R. Carlier

8:20 – 134. Mosquito larvicidal lipopeptide produced by *Xenorhabdus*. **Q. Lan**, I. H. Kim, J. Ensign

8:40 – 135. Plant-derived products for control of ticks and biting flies affecting livestock. **A. Y. Li**, L. M. Costa-Júnior, L. M. Borges, A. A. Pérez de León

9:00 – 136. Natural product-based insecticidal structure activity relationship investigations. **C. L. Cantrell**, A. Ali, J. W. Pridgeon, J. U. Rehman, H. Nakano

9:20 – 137. Neuropeptides and receptors as targets for bioinsecticides. **R. J. Nachman**

9:40 – 138. G-Protein-Coupled Receptors (GPCRs): A target of plant terpenoids. **A. D. Gross**, M. J. Kimber, K. B. Temeyer, R. J. Miller, A. Y. Li, A. A. Pérez de León, J. R. Coats

10:00 Intermission.

10:15 – 139. Potent nematicidal activity of redox-active aromatic aldehydes against *Meloidogyne incognita*. **P. Caboni**, B. Liori, N. Ntalli

10:35 – 140. Phytochemically based strategies for nematode control. **D. J. Chitwood**

10:55 – 141. Natural and synthetic isothiocyanates for nematode control. **S. R. Yates**, D. Wang

11:15 – 142. Mode of action and anthelmintic activity of novel plant-based functional food additives. **B. W. Bissinger**, R. M. Kaplan, B. E. Storey, A. Akashe, D. J. Skrypec, S. M. Mitchell

11:35 – 143. Natural nematicides and analogs. **J. R. Coats**, A. Knips, D. Soo, R. Tsao, D. Park, G. Tylka

11:55 Concluding Remarks.

Pollinators and Pesticides
T. D. Anderson, R. Fell, *Organizers, Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

8:30 Introductory Remarks.

8:35 – 144. Honey bee colony health, bee decline, and pesticides. **R. Fell**

8:55 – 145. Pollinators, pesticides, and pathogens: Linking honey bee colony health to chemical exposures. **T. D. Anderson**

9:15 – 146. Agrochemical formulant toxicities for honey bees. **C. A. Mullin**, J. Chen, W. Zhu, M. T. Frazier, J. L. Frazier

9:35 – 147. Honey bee colony level responses to exposure of residues on flowers of the fungicide, propiconazole. **F. A. Drummond**

9:55 Intermission.

10:15 – 148. Comparative ecotoxicology of bee-pesticide interactions. **J. E. Cresswell**

10:35 – 149. Large-scale field study examining potential impacts on honey bees of exposure to clothianidin seed-treated canola. **G. Cutler**, C. D. Scott-Dupree, M. Sultan, A. D. McFarlane, L. Brewer

10:55 – 150. Honey bee field studies: Assessing hive health after four consecutive years of exposure to flowering crops grown from thiamethoxam-treated seed. **J. Overmeyer**, P. Campbell, M. Coulson, N. Ruddle, I. Tornier

11:15 – 151. Using data from semi-field enclosure studies for assessing the risk of pesticides to honey bees. **J. D. Wisk**

Journal of Agricultural and Food Chemistry Best Paper Awards

Cosponsored by AGFD
Financially supported by
Journal of Agriculture and Food Chemistry
J. Seiber, *Organizer, Presiding*

Section C
Crowne Plaza, Grand Central Station A&B

8:25 Introductory Remarks.

8:30 – 152. Molecular determinants of the sweet-bitter Janus head of steviol glycosides and development of novel quantitation tools. **T. Hofmann**

9:05 Discussion.

9:10 – 153. Using biomimetic cell wall models to identify new plant lignin bioengineering targets for improving forage and biomass utilization. **J. H. Grabber**

9:45 Discussion.

Innovation in Chemistry of Agriculture Award

Financially supported by BASF
J. Seiber*, Organizer, Presiding*

Section C
Crowne Plaza, Grand Central Station A&B

10:10 Introductory Remarks.

10:15 – 154. Immunochemistry in motion: Applications to agrochemicals. **J. M. Van Emon**

10:55 Discussion.

TUESDAY MIDDAY

Sterling B. Hendricks Memorial Lectureship Award

Cosponsored by AGFD
Financially supported by United States Department of Agriculture, Agricultural Research Service
K. Kaplan, M. H. Tunick*, Organizers*
S. Duke*, Organizer, Presiding*

Section C
Crowne Plaza, Grand Central Station A&B

11:20 Introductory Remarks.

11:30 – 155. Arriving at the truth: Weight of evidence for assessing risks of agrochemicals. **K. R. Solomon**

12:15 Concluding Remarks.

High-Throughput Pesticide Residue Analysis
Cosponsored by ANYL and ENVR
Financially supported by Monsanto
M. Saha, L. Riter, *Organizers, Presiding*

Section D
Crowne Plaza, B&O (Baltimore & Ohio)

8:30 – 156. Optimization of sample homogenization for pesticide residue analysis: Soil – an example for a difficult matrix. **H. Penning**, A. Altschuck

8:50 – 157. Validation of a modified QuEChERS version for high-throughput analysis of a wide range of pesticides in foods. M. Gonzalez-Curbelo, **S. J. Lehotay**, J. Hernandez-Borges

9:10 – 158. High throughput residue sample preparation. **C. E. Wujcik**, L. Riter

9:30 – 159. Development and implementation of high throughput techniques for use in residue and soil dissipation studies.**L. M. Mallis**, M. Pennell, S. Guess, C. Chen, S. Hill, J. E. Eble

9:50 – 160. Recent advances in flow injection mass spectrometry for high-throughput pesticide residue analysis in any complex matrix. **S. C. Nanita**, D. L. Bailey, E. A. Morgan

10:10 Intermission.

10:30 – 161. High throughput sample analysis using miniaturization and automation for residue analysis. **M. Saha**, R. Gooding, A. Finch, J. Jones

10:50 – 162. Increasing selectivity of LC/MS-MS analysis using differential mobility spectrometry. **P. C. Winkler**, L. S. Riter

11:10 – 163. High-throughput residue analysis for a water monitoring study using liquid-handling robotics and UHPLC/MS-MS. **S. R. Perez**, R. Perez, O. J. Almaraz, A. LaRosa

11:30 Discussion.

ENVR Division

Water: Global Problems, Local Solutions
Water Treatment
Cosponsored by AGRO, CEI, and IAC
Financially supported by Global Innovation Imperatives
A. M. Rimando, E. Contis, I. Urasa, *Organizers, Presiding*

Section A
Crowne Plaza, Victoria Station D

8:30 Introductory Remarks.

8:35 – ENVR 115. Water filters based on composite iron matrix: Fundamental studies and large scale deployment. **A. Hussam**

9:05 – ENVR 116. Sustainable and low cost approach for cleaning metal contaminated waters using pyrolized banana peel. **E. Sahle-Demessie**

9:35 – ENVR 117. Analysis of drinking water from the Blue Zone island of Ikaria Greece. **E. Tratras Contis**

10:05 Intermission.

10:20 – ENVR 118. Developing a bioreactor for water defluoridation: A university-community partnership. **I. T. Urasa**, T. B. Lash, W. J. Mavura, A. Kimaro

10:50 – ENVR 119. Removal of Pb by metal oxide nanoparticles. **M. Ossman**, M. Abdelfattah

11:20 – ENVR 120. Removal of Ni by activated carbon produced from Egyptian rice straw by chemical activation. **M. Abdelfattah**, M. Ossman

11:50 Concluding Remarks.

ENVR Division

Predicting Molecular Properties of Environmental Contaminants: Empirical and Theoretical Methods
Biodegradation, Toxicity, Risk
Cosponsored by AGRO and COMP‡
P. G. Tratnyek, D. Ditoro, *Organizers*
E. Weber, K. Fenner, *Organizers, Presiding*

Section B
Crowne Plaza, Penn Station A

8:30 Introductory Remarks.

8:35 – ENVR 121. External validation of regulatory QSBR models for predicting the biodegradability of xenobiotics. **J. Devillers**, P. Pandard, B. Richard

9:05 – ENVR 122. Application of cheminformatics tools for encoding the process science necessary for prediction of abiotic transformation pathways for organic chemicals in aquatic ecosystems. C. T. Stevens, **E. J. Weber**

9:25 – ENVR 123. On the role of vitamin B_{12} in the reductive dehalogenation of perfluorinated persistent organic pollutants: A DFT study. M. E. Duenas-Fadic, V. L. Ochoa-Herrera, M. A. Mendez, C. H. Zambrano, **F. J. Torres**

9:45 – ENVR 124. Complexation facilitated reduction of aromatic N-oxides by aqueous Fe^{III}–tiron complex: Reaction kinetics and mechanisms. **Y. Chen**, H. Zhang

10:05 Intermission.

10:25 – ENVR 125. Non-animal approaches for the predictive assessment of the aquatic toxicity of organic compounds. **G. Schüürmann**

10:55 – ENVR 126. Prediction of aquatic toxicity mode of action using linear discriminant and random forest models. **T. M. Martin**, C. M. Grulke, D. M. Young, C. L. Russom, N. Wang, C. R. Jackson, M. G. Barron

11:15 – ENVR 127. Predicting adverse health effects of transformation products formed from organic micropollutants during water treatment. **M. L. Card**, K. Fenner, B. I. Escher

11:35 – ENVR 128. Investigating the role of hydrophobicity in environmental transport prediction. **M. J. Wells**

11:55 Concluding Remarks.

TUESDAY AFTERNOON

Biopesticides: State of the Art and Future Opportunities
Products from Genetic Improvements
Financially supported by American Chemical Society Innovation Grant and Ag Biotech Stewardship Technical Committee
J. Seiber, J. Coats, S. Duke, *Organizers*
A. D. Gross, *Organizer, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

1:30 Introductory Remarks.

1:35 – 164. RNA interference in insect pest management: Assessing potential benefits and risks. **B. D. Siegfried**, X. Zhou, C. Khajuria, J. Jurzenski

1:55 – 165. ***New Investigator Finalist:*** Functional analysis of four RNAi pathway genes in an economically important corn pest, western corn rootworm (*Diabrotica virgifera virgifera*). **C. Khajuria**, B. Siegfried, K. Narva

2:15 – 166. Assessing the fate of RNA-based agricultural products in the environment. **J. Fischer**, S. Dubelman, B. Ayden, F. Zapata, J. Uffman, J. Warren, S. Levine, D. Carson

2:35 – 167. Toxins for transgenic resistance to hemipteran pests. N. P. Chougule, H. Li, S. Liu, L. B. Linz, K. E. Narva, T. Meade, **B. C. Bonning**

2:55 – 168. Mode of action of *Bacillus thuringiensis* toxins. **S. S. Gill**

3:15 Intermission.

3:30 – 169. Transcriptional responses to the ingestion of Cry1Ab protoxin and Cry1Ab corn leaves in the gut of Ostrinia nubilalis larvae. J. Yao, C. Khajuria, L. L. Buschman, **K. Zhu**

3:50 – 170. Using genomics and chemistry to screen for secondary metabolites in *Bacillus spp* biocontrol organisms. **C. Dunlap**, D. Schisler

4:10 – 171. Discovery of new insect resistance traits for control of insect pests in transgenic crops. **T. Meade**, K. E. Narva, N. Storer

4:30 – 172. Setting the stage for future transgenic insect control products. **M. E. Nelson**, G. Wu, J. Flexner

4:50 Concluding Remarks.

Pollinators and Pesticides
T. D. Anderson, *Organizer*
R. Fell, *Organizer, Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

2:00 – 173. Pesticide residues in bee hives: What levels are of concern? **D. L. Fischer**

2:20 – 174. Is planting corn killing bees? **K. Neal**

2:40 – 175. Analysis of pesticides in corn planter exhaust dust and dosimeters surrounding corn fields during planting. **B. Eitzer**, J. D. Holland, C. Krupke

3:00 Intermission.

3:15 – 176. Optimization of a method to quantify agrochemicals in bee tissues and wax. **M. J. Lydy**, D. Chen, Z. Chen, J. Trushenski, R. Kelley

3:35 – 177. Intersect of pesticides and pollinators: Challenges faced by state regulatory programs. **L. J. Fleeson**

3:55 – 178. Risk assessment framework for honey bees. **R. Baris**, K. Garber

4:15 – 179. Addressing new data requirements for chronic honey bee testing in the EU. **S. L. Levine**, J. Doering, S. Norman, P. Manson, P. Sutton, H. Thompson

4:35 Concluding Remarks.

Non-First Order Dissipation and Time-Dependent Sorption of Organic Chemicals in Soil Measurement, Modeling, and Impact on Environmental Exposure Predictions
Financially supported by Syngenta Crop Protection
W. Chen, S. Yates, S. Cryer, D. Young, *Organizers, Presiding*

Section C
Crowne Plaza, Grand Central Station A&B

1:00 Introductory Remarks.

1:05 – 180. Determining kinetic and nonequilibrium sorption behavior for chlopyrifos using a hybrid batch/column experiment. **S. A. Cryer**

1:25 – 181. Experiments and modelling to quantify irreversibility of pesticide sorption-desorption in soil. L. Suddaby, **S. Beulke**, W. van Beinum, R. Celis, W. Koskinen, S. Kuet, R. Oliver, C. Brown

1:45 – 182. Biphasic behavior of pesticide degradation in soils: Verification by pathway kinetic fits. **X. Huang**

2:05 – 183. Determining differential degradation of enantiomers in soil using data of no chiral separation. **W. Chen**, P. Francis

2:25 – 184. Statistical means for proper determination of kinetic half-lives. **S. H. Jackson**

2:45 – 185. Evaluations of regulatory kinetic analysis approaches. **J. Tang**, R. L. Jones, M. Huang, W. Chen, R. Allen, S. Hayes, R. Sur

3:05 Intermission.

3:20 – 186. Guidance on how aged sorption studies for pesticides should be conducted, analysed, and used in regulatory assessments. **S. Beulke**, W. van Beinum, A. Abu

3:40 – 187. Significance of time-dependent sorption on leaching potential: A comparison of measured field results and modeled estimates. **T. L. Negley**, K. Gehl, R. Allen, Z. Tang, D. G. Dyer, A. C. Newcombe

4:00 – 188. Effect of refined environmental fate properties on groundwater concentrations calculated with PRZM-GW. **R. Sur**, J. Tang, R. L. Jones, P. N. Coody

4:20 – 189. Influence of time-dependent sorption of flutriafol on predicted environmental concentrations. **Q. Ma**, R. Reiss, P. Whatling

4:40 – 190. APEX sensitivity to atrazine dissipation rate on surface runoff loss within a coastal zone in southeastern Puerto Rico. **C. O. Williams**, T. L. Potter, R. Lowrance, D. D. Bosch, T. Strickland, R. Williams

5:00 – 191. Soil dissipation kinetics: The use of a set of simple first order processes to describe a biphasic degradation pattern. **J. R. Purdy**, J. Cheplick

5:20 Concluding Remarks.

Ecotoxicological Risk Assessment for Agricultural Use of Chlorpyrifos in the US
Financially supported by Dow AgroSciences
K. Solomon, N. Poletika, J. Giesy, *Organizers, Presiding*

Section D
Crowne Plaza, B&O (Baltimore & Ohio)

1:00 Introductory Remarks.

1:05 – 192. Properties and uses of chlorpyrifos in the United States. **K. R. Solomon**, W. Williams, D. Mackay, J. Purdy, J. M. Giddings, J. P. Giesy

1:25 – 193. Towards a model of the environmental fate and long-range atmospheric transport of chlorpyrifos and its oxon.**D. Mackay**, J. P. Giesy, K. R. Solomon

1:45 – 194. Refined avian risk assessment for agricultural uses of granular chlorpyrifos in the United States. **D. R. Moore**, R. Teed, K. R. Solomon, J. P. Giesy

2:05 – 195. Refined avian risk assessment for agricultural uses of flowable chlorpyrifos in the United States. **D. R. Moore**, R. Teed, K. R. Solomon, J. P. Giesy

2:25 – 196. Exposures to aquatic organisms from the use of chlorpyrifos in North America. **W. Williams**, J. M. Giddings, J. Purdy, K. R. Solomon, J. P. Giesy

2:45 – 197. Risks to aquatic organisms from the use of chlorpyrifos in North America. **J. M. Giddings**, W. Williams, K. R. Solomon, J. P. Giesy

3:05 Intermission.

3:20 – 198. Ecological risk assessment for chlorpyrifos in terrestrial systems in North America: Conceptual model for pollinators. **J. R. Purdy**, G. Cutler, J. P. Giesy, K. R. Solomon

3:40 – 199. Risks of chlorpyrifos to pollinators: Risk assessment. **G. Cutler**, J. Purdy, J. P. Giesy, K. R. Solomon

4:00 – 200. Ecological risk assessment for chlorpyrifos in terrestrial and aquatic systems in North America: Overview and conclusions. **J. P. Giesy**, C. Cutler, J. Giddings, D. Mackay, D. Moore, W. Williams, J. Purdy, K. Solomon

4:20 – 201. Chlorpyrifos agricultural use and the Endangered Species Act: Do refinements in ecological risk assessment address uncertainty? **N. N. Poletika**, D. R. Moore, J. M. Giddings

4:40 – 202. Pesticides as POPs and PBTs: An assessment of chlorpyrifos. **K. Solomon**, N. Poletika, J. Anderson, J. Giesy

5:00 Discussion.

Protection of Agricultural Productivity, Public Health, and the Environment
S. Duke, *Organizer*

1:00 - 5:00 pm

Section E
Indiana Convention Center, Halls F&G

203. Investigations into the SAR of the aminosulfones. **A. M. Buysse**, M. J. Ricks, C. J. Klittich, J. Phillips, M. T. Iamauti, I. M. Morrison, B. Rieder, M. T. Sullenberger, W. C. Lo, T. J. Mathieson, M. B. Olson

204. Interaction of organic solvents with the epicuticular wax layer of wheat leaves. A. P. Parobek, **K. Myung**, J. A. Godbey, A. J. Bowling

205. Discovery and the structure activity relationship of a series of novel oxadiazole-based insecticides. **J. D. Webster**, B. A. Lorsbach, M. Olson, C. Geng

206. SAR Studies on 2-(2-arylidenehydrazinyl)-N-aryllpyrimidin-4-amine: A lepidopteran insecticide lead. **N. M. Niyaz**, T. K. Trullinger, T. Johnson, R. Hunter, A. V. Brown, K. Guenthenspberger

207. Discovery and optimization of isoxazolidines as novel insecticides. **W. Zhang**, W. Hong

208. Discovery and optimization of 4-aminomethylpiperidines as new class of insecticides. **W. Zhang**, K. A. Hughes

209. Triple mode of action herbicide tolerance utilizing the Enlist™ Weed Control System in soybeans. **G. Bradfisch**, C. Cui, B. Eby, B. Held, T. Hoffman, J. Mason, D. Pareddy, M. Peterson, S. Russell, V. Sekar, D. Simpson, A. Umthun, T. Wright, Z. Zhang

210. Toxicity of *Bacillus thuringiensis* to aquatic non-target organisms and its influence on toxicity of chloropyrifos. Y. Li,**J. You**

211. Comparison of aflatoxins analysis by test kit with liquid chromatography confirmation method. **H. Inerowicz**, K. Albert, Z. Bryant, V. S. Siegel

212. Multiresidue analysis of pesticides in brown rice and orange by liquid chromatography-tandem mass spectrometry. **Y. Jeon**, J. Hwang, J. Do, J. Oh, J. Hong, Y. Lee, J. Kim

213. Novel fluorinated strobilurin-pyrimidine acaricide: Design, synthesis, and acaricidal activity. **B. Chai**, C. Liu, J. Chang

214. Research directed towards the discovery of novel thymidylate synthase inhibitors as agricultural fungicides. W. K. Brewster, D. Camper, R. Gundla, G. D. Gustafson, **J. E. Hunter**, H. Joshi, W. J. Lo, B. A. Lorsbach, M. Loso, A. Mandaleswaran, R. Sanam, P. Arumugan, D. J. Pernich

215. Development and validation of a quantitative enzyme-linked immunosorbent assay (ELISA) for determining transgenic protein AAD-12 in soybean tissues. **G. Shan**, J. Smith-Drake, M. Sosa, P. Maldonado, B. Wulfkuhle, K. Smith

216. Development and validation of a sensitive and specific immunoassay for the detection of aryloxyalkanoate dioxygenase (AAD-1) protein in maize tissues. **E. H. Ma**, M. J. Sosa, B. E. Wulfkuhle, G. Shan

217. Application of AlphaLISA technology in testing genetically modified (GM) crops. **N. T. Theoharis**, F. M. Admana, S. Toledo, R. Belcher

218. Development and validation of a quantitative enzyme-linked immunosorbent assay for the detection of 2mEPSPS protein in soybean tissues. A. Cruse, G. Lin, E. Ma, **P. Maldonado**, V. Sekar, G. Shan, K. Smith, M. Sosa, B. Wulfkuhle

219. Systematic approach for validating enzyme-linked immunosorbent assay (ELISA) methods for protein quantification from soil. **A. Unger**, J. Anderson

220. Withdrawn.

221. Microbiome mining: Panda conservation and biofuels. **A. Brown**, C. Williams, I. Johnston, S. Willard, A. Kouba, G. Suen, D. Sparks

222. Metabolic engineering for improved microbial 2,3-butanediol production. **X. Ji**, **H. Huang**

223. Synthesis of enantiomerically-pure aryloxyphenoxypropioanate herbicides: Using biobased building blocks as starting material for agrochemicals. **B. J. Verkuijl**, M. Fleer

224. Large-scale particulate matter air sampling system for high density data measurments. **M. Buser**, A. Koller, D. Whitelock

225. Discovery of metazosulfuron: A new sulfonylurea herbicide for rice. **Y. Nakaya**, H. Kita, Y. Tamada, T. Yano, M. Saeki, K. Morimoto

2013 Kenneth A. Spencer Award

Symposium in Honor of Dr. Attila Pavlath
Sponsored by AGFD, Cosponsored by AGRO

E. Hellmuth, *Organizer, Presiding*

Section A
Indiana Convention Center, Rm. 107

ABSTRACTS ON PAGE 87

1:00 Introductory Remarks.

1:05 – **AGFD 95.** Food packaging and sustainability. **S. J. Risch**

1:25 – **AGFD 96.** Corn fiber gum and its synergistic effect on the viscosity of other polysaccharides. **M. P. Yadav**, F. Zhang, T. Luan, K. Ding, H. Zhang

1:45 – **AGFD 97.** Can bio-derived polymers compete? **M. Jaffe**

2:05 – **AGFD 98.** Edible films and coatings on processed fruits and vegetables. **A. E. Pavlath**

2:35 Intermission.

2:45 – **AGFD 99.** Inflammation of cardiovascular tissue by certain fatty acids and protection from the microbiome activity. **J. Finley**, A. Soto, J. Losso

3:05 – **AGFD 100.** Edible food coating derived barrier teat disinfectant for milk quality improvement. **T. C. Hemling**, **S. J. Leibowitz**

3:25 – **AGFD 101.** Further studies demonstrate PPARα activation and gene expression up-regulation by pterostilbene. **A. M. Rimando**, S. Khan, C. S. Mizuno, R. Guang, S. Mathews, H. Kim, W. Yokoyama

3:45 – **AGFD 102.** Dairy and functional foods research in the Agricultural Research Service. **M. M. Tunick**, P. M. Tomasula

ENVR Division

Water: Global Problems, Local Solutions
Source Water/Natural Water Assessment and Evaluation
Cosponsored by AGRO, CEI, and IAC
Financially supported by Global Innovation Imperatives
A. M. Rimando, E. Contis, I. Urasa, *Organizers, Presiding*

Section A
Crowne Plaza, Victoria Station D

1:30 Introductory Remarks.

1:35 – ENVR 146. Water availability and watershed management: Local solutions to global problems through USDA research. **M. R. Walbridge**

2:15 – ENVR 147. Determining contaminate sources to the Chesapeake Bay to discern the effectiveness of conservation practices. **C. J. Hapeman**, L. L. McConnell, G. W. McCarty, C. P. Rice, W. Hively, M. W. Lang, D. R. Whitall, A. M. Sadeghi, A. Torrents, A. Goel

2:45 – ENVR 148. Management of field edges in the agricultural landscape to mitigate farm chemical impacts. **M. A. Locke**, M. T. Moore, R. E. Lizotte, Jr.

3:15 Intermission.

3:30 – ENVR 149. Small infrastructure and development: Sustainable water and sanitation services for rural developing communities. **G. Louis**

4:00 – ENVR 150. Bringing relevant local and global water themes into the classroom. **J. C. Vites**

4:30 – ENVR 151. New global contamination generated from plastic. **K. Saido**, A. Okabe, **K. Koizumi**, M. Yamamoto, A. Nishino, H. Sato, Y. Togawa, S. Chung, K. Kogure

5:00 Concluding Remarks.

ENVR Division

Status and Trends of Classical and Emerging Contaminants Across the World
Cosponsored by AGRO and CEI
Financially supported by Global Innovation Imperatives
N. Savage, S. Ahuja, K. Hristovski, B. Loganathan, *Organizers, Presiding*

Section B
Crowne Plaza, Penn Station A

1:30 Introductory Remarks.

1:35 – ENVR 152. Spatial and temporal trends and possible sources of methoxylated polybrominated diphenoxybenzenes in herring gull eggs from the Laurentian Great Lakes of North America. **D. Chen**, R. Letcher

1:55 – ENVR 153. Environmental occurrences of nonylphenols. T. Romaine, **K. D. Hristovski**

2:15 – ENVR 154. Fate and risk of perfluorinated alkyl substances in environmental and food samples across the world (Spain, Brazil, Saudi Arabia, and Serbia). **D. Barcelo**, F. Perez, M. Farre, N. Al-Harbi, L. F. Silva

2:35 – ENVR 155. Classical and emerging metal contaminants in India: Associated problems and their solutions via green and sustainable pathway. **R. K. Sharma**, A. Puri

2:55 Intermission.

3:10 – ENVR 156. Water sustainability and reclamation: Bringing stakeholders together to solve problems. **S. Ahuja**

3:30 – ENVR 157. Affordable and clean drinking water using nanomaterials. **P. Thalappil**

3:50 – ENVR 158. Relative importance of *N*-nitrosodimethylamine compared to total *N*-nitrosamines in drinking waters. **N. Dai**, W. A. Mitch

4:10 – ENVR 159. Global contamination trends of persistent organic pollutants and their effect on wildlife and human health. **B. G. Loganathan**, K. S. Sajwan

4:30 Discussion.

4:35 Panel Discussion.

5:05 Concluding Remarks.

WEDNESDAY MORNING

Biopesticides: State of the Art and Future Opportunities
Economic, Regulatory, and Future Needs
Financially supported by American Chemical Society Innovation Grant and Ag Biotech Stewardship Technical Committee
A. D. Gross, J. Coats, S. Duke, *Organizers*
J. Seiber, *Organizer, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

8:30 Introductory Remarks.

8:35 – 226. IR-4 Project: A public sector program to facilitate the registration of biopesticides. **M. Braverman**, D. Kunkel, J. Baron

8:55 – 227. Biopesticides: State of the art and future opportunities. S. D. Goldblum, C. B. Warren, **R. P. Burlingame**

9:15 – 228. Growing need for bioherbicides. **S. O. Duke**

9:35 – 229. Registration of biopesticides. **K. A. Matthews**

9:55 – 230. Fascinating science, frustrating reality: Five barriers to broad utility of biopesticides. **D. Kittle**

10:15 Intermission.

10:45 – 231. Outlook for biopesticides in agriculture and public health. **J. N. Seiber**, J. R. Coats, A. Gross, S. O. Duke

11:45 Concluding Remarks.

Synthesis and Chemistry of Agrochemicals
T. Stevenson, V. Hegde, B. Lorsbach, D. Cudworth, *Organizers, Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

8:30 Introductory Remarks.

8:35 – 232. Discovery and optimization of cyclic carbonyl amidines as potent insecticides. **W. Zhang**, J. D. Barry, K. A. Hughes, S. F. McCann

8:55 – 233. Substituted cyclopropyl- and thiazolyl-1*H*-1,2,4-triazoles as insecticides and acaricides. M. L. Ash, T. J. Bruce,**D. P. Cudworth**, D. H. DeVries, L. P. Dintenfass, J. E. Dripps, J. M. Gifford, K. A. Guenthenspberger, V. B. Hegde, L. L. Karr, M. S. Kempe, T. P. Martin, D. C. McCormick, J. T. Pechacek, P. V. Ripa, J. R. Schoonover, F. E. Tisdell, M. C. Yap

9:15 – 234. Azetidinols and prolinols as insecticides. **W. von Deyn**, D. Breuninger, M. Puhl

9:35 – 235. SAR investigations into *N*-azinyl-*N*'-aryl ureas as insecticides. **T. K. Trullinger**, N. M. Niyaz, T. C. Johnson, R. Hunter, A. V. Brown, K. Bryan

9:55 – 236. Synthesis and insecticidal activity of new benzyl- and indanyl- oxazolines, thiazolines, and imidazolines. **A. C. O'Sullivan**, J. H. Schaetzer, C. Luethy, C. J. Mathews, C. Elliott, T. Pitterna, J. Pabba, O. Jacob, A. Buchholz, J. Blythe

10:15 Intermission.

10:35 – 237. SAR studies of the new sulfoximine sap-feeding insecticide, sulfoxaflor. **M. R. Loso**, Z. Yuanming, B. Nugent, J. J. Daeuble, G. T. Whiteker, T. C. Sparks, G. B. Watson, J. M. Babcock

10:55 – 238. Discovery of Sivanto™, a new butenolide insecticide. **R. Velten**, P. Jeschke, M. Haas, K. Kunz

11:15 – 239. Did we select lead chemistries for optimization based on MOA or activity? **E. Nagano**

11:35 – 240. Strategies and tactics for the synthesis of complex alkaloids. **R. Sarpong**

Terrestrial Field Dissipation Studies in Global Agrochemical Registration Programs
Financially supported by Waterborne Environmental Inc.
R. Gangaraju, M. Shamim, *Organizers*
R. Allen, *Organizer, Presiding*

Section C
Crowne Plaza, Milwaukee

8:30 Introductory Remarks.

8:35 – 241. OECD project on international harmonization of terrestrial field dissipation guidance and ecoregion crosswalk. **M. T. Shamim**, R. Gangaraju, M. Egsmose

9:00 – 242. Development and validation of a conceptual model of pesticide dissipation pathways under field conditions. **N. Peranginangin**, A. Sapiets, D. Simmons, C. Nichols

9:20 – 243. OECD guidance for pesticide field dissipation studies for obtaining DegT50 value. **C. M. Lythgo**, A. Massey, A. Boivin, M. Klein, M. Egsmose, J. Boesten

9:40 – 244. Experiences with planning and conduct of terrestrial field dissipation (TFD) studies in line with new EFSA guidance. **H. Bayer**, T. Richter

10:00 Intermission.

10:20 – 245. Interpretation of pesticide leaching in terrestrial dissipation studies using water content reflectometry. **R. Warren**

10:40 – 246. Inverse modeling for the derivation of degradation parameters in European and North American terrestrial field dissipation studies. **M. L. White**, G. P. Olchin, N. J. Snyder, A. C. Barefoot

11:00 – 247. Comparison of terrestrial field dissipation half-lives and trial sites between NAFTA and EU. **R. Sur**, D. Schaefer

11:20 Panel Discussion.

11:35 Concluding Remarks.

Pesticide Residues in Food and Feed: Scientific and Regulatory Global Needs
Financially supported by Golden Pacific Laboratories and Dow AgroSciences
H. Irrig, P. Brindle, C. Tiu, *Organizers, Presiding*

Section D
Crowne Plaza, Victoria Station A-C

8:00 Introductory Remarks.

8:05 – 248. Welcome to Indiana, where agriculture is an integral part of our state. **G. Sheets**

8:15 – 249. Regulatory Cooperation Council initiative on crop protection products. **M. Law**

8:40 – 250. Pilot project leading the way toward harmonized MRLs around the world. **L. Rossi**

9:05 – 251. Regulation (EC) 1107/2009: New residue data requirements coming into force January 2014. **K. Hohgardt**

9:30 – 252. Withdrawn.

9:55 Intermission.

10:10 – 253. US tolerance setting and alignment with Codex MRLs and other national authorities. **B. A. Madden**

10:35 – 254. What if CODEX expired? **C. Hunter**

11:00 – 255. Update on international cooperation and collaborations to address minor uses. **D. Kunkel**

11:25 – 256. Regulatory activities on sulfoxaflor, a novel product for insect control. **R. S. Brinkmeyer**

11:50 Panel Discussion.

ENVR Division

Fate and Toxicology of Emerging Environmental Contaminants
Cosponsored by AGRO
S. Uchimiya, B. Zhang, *Organizers*
X. Pan, *Organizer, Presiding*

Section A
Crowne Plaza, Victoria Station D

8:30 Introductory Remarks.

8:35 – ENVR 173. Biodegradational influence on poly and perfluoroalkyl substance (PFAS) release into landfill leachate. **M. Allred**, J. Lang, M. Barlaz, J. Field

8:55 – ENVR 174. Investigating crude oil-dispersant mixture-induced reproductive toxicity and its mechanism in *C. elegans*. **J. R. Polli**, Y. Zhang, X. Pan

9:15 – ENVR 175. Oil/dispersant induced the aberrant expression of miRNAs in *C. elegans*: Implications in reproductive toxicity. **Y. Zhang**, J. Polli, **X. Pan**

9:35 – ENVR 176. Determination of PCB 11 in human blood serum from populations in northwest Indiana and rural Iowa. **W. Koh**, P. S. Thorne, K. C. Hornbuckle

9:55 – ENVR 177. Chronic subtoxic exposure to chlorpyrifos increases risk of neurological disorders. **D. L. Dobbins**, F. A. Taki, X. Pan

10:15 Intermission.

10:35 – ENVR 178. Polycyclic hydrocarbons (benzo[a]pyrene and benzo[k]fluoranthene) in boiled, grilled, and roasted meat. **B. O. Opeolu**, O. S. Olatunji, O. S. Fatoki, B. J. Ximba

10:55 – ENVR 179. WITHDRAWN

11:15 – ENVR 180. Influence of nicotine on the expression of nAChRs and selected miRNAs in *Caenorhabditis elegans*. **J. R. Polli**, X. Pan

11:35 – ENVR 181. Mixture effects of triclosan and triclocarban on their aquatic chemistries. **K. Albanese**, R. Lanno, M. Chakraborty, C. Hadad, Y. Chin

WEDNESDAY AFTERNOON

Uptake, Translocation, and Distribution of Agrochemicals in Plants
Cosponsored by AGFD and ENVR
Financially supported by Dow AgroSciences
K. Myung, C. Kennedy, N. Satchivi, *Organizers, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

1:30 Introductory Remarks.

1:35 – 257. Withdrawn.

1:55 – 258. Co-penetration of actives and adjuvants and its significance for the matched pair liaison. **P. Baur**

2:15 – 259. Comparison of translocation properties of insecticides vs. herbicides that lead to efficacious control of pests as specifically illustrated by sulfoxaflor, a new insecticide, and halauxifen-methyl, a new herbicide. **G. J. de Boer**, N. Satchivi

2:35 – 260. Withdrawn.

2:55 – 261. Phloem translocation of xenobiotics in *Brachypodium distachyon*. **O. Castello**, G. DeBoer, A. Bowling

3:15 Intermission.

3:30 – 262. Withdrawn.

3:50 – 263. Activity of chlorantraniliprole and thiamethoxam seed treatments on rice water weevil as affected by distribution of insecticides in rice plants. **S. K. Lanka**, M. J. Stout, J. A. Ottea

4:10 – 264. Uptake, translocation, and accumulation of pharmaceutical and hormone contaminants in vegetables. **W. Zheng**, K. Wiles, N. Holm

4:30 – 265. Practical utility of dynamic plant uptake model assessed through application of probabilistic techniques. **K. M. Jernberg**, C. K. Kingston, N. J. Snyder

4:50 Concluding Remarks.

Synthesis and Chemistry of Agrochemicals
T. Stevenson, V. Hegde, B. Lorsbach, D. Cudworth, *Organizers, Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

1:00 Introductory Remarks.

1:05 – 266. Cyclin dependent kinases as starting points for fungicide discovery. Y. Chen, **P. L. Sharpe**

1:25 – 267. Substituted 2,2'-bipyridyls as agricultural fungicides. **K. G. Meyer**, M. T. Sullenberger, D. H. Young, F. D. Smith, C. Yao, G. E. Davis

1:45 – 268. Identification and optimization of pyrimidopyridines controlling speckled leaf blotch in wheat. **K. Lohmann**

2:05 – 269. Inhibitors of 4-hydroxphenylpyruvate dioxygenase (HPPD) in combination with a safener: New herbicide solutions for modern sustainable agriculture. **S. D. Lindell**

2:25 – 270. Accelerating discovery through risk-sharing collaborations. **B. A. Lorsbach**, V. Hegde, J. E. Hunter, W. T. Lambert, L. K. Lawler, D. J. Pernich, D. D. Young, N. Wang

2:45 – 271. Lead discovery and optimization through CRO collaborations. **G. P. Lahm**

3:05 Intermission.

3:25 – 272. Partnering for success with contract research organizations (CROs) to enhance discovery R&D productivity. **L. K. Lawler**, V. B. Hegde, B. A. Lorsbach, M. R. Loso, M. A. Pobanz

3:45 – 273. Thoughts on best practices and perspectives for working externally in a research environment. **R. Z. Brady**

4:05 Panel Discussion.

4:45 Concluding Remarks.

Terrestrial Field Dissipation Studies in Global Agrochemical Registration Programs
Financially supported by Waterborne Environmental Inc.
M. Shamim, R. Gangaraju, *Organizers*
R. Allen, *Organizer, Presiding*

Section C
Crowne Plaza, Milwaukee

1:30 Introductory Remarks.

1:35 – 274. OECD guidance for acceptance of foreign pesticide field dissipation studies and ecoregion concept. **R. Gangaraju**, M. Mitchell, M. Shamim, I. Nicholson, L. Montanarella, M. Egsmose

2:00 – 275. OECD guidance for acceptance of foreign pesticide field dissipation studies/ecoregion concept: Ecoregion Crosswalk model and demonstration. **D. J. Kroetsch**, R. Gangaraju, M. Shamim, M. Ballard

2:25 – 276. Novel approach to evaluate comparability of foreign soils used for environmental fate studies for agrochemicals with US agricultural soils. **J. Bang**, N. Peranginangin, A. Sapiets

2:45 – 277. What matters for predicting the similarity of TFD studies: Techniques, data, or pesticide characteristics? **T. Häring**, B. Erzgräber

3:05 Intermission.

3:25 – 278. Application of OECD ENASGIPS: User perspectives. **G. Hoogeweg**, S. Zelonis

3:45 – 279. Relevance of environmental fate and terrestrial field dissipation studies conducted in Europe and Canada to use environments in the United States. **S. Zelonis**, C. Mucha Hirata, G. Hoogeweg, N. J. Snyder

4:05 – 280. Use of the Europe-North American soil geographic information for pesticide studies tool (ENASGIPS version 2.0 tool). **M. Ruhman**, R. Gangaraju, M. T. Shamim

4:30 Panel Discussion.

4:45 Concluding Remarks.

Pesticide Residues in Food and Feed: Scientific and Regulatory Global Needs
MRLs and Trade
Financially supported by Golden Pacific Laboratories and Dow AgroSciences
H. Irrig, C. Tiu, *Organizers*
P. Brindle, *Presiding*

Section D
Crowne Plaza, Victoria Station A-C

1:30 Introductory Remarks.

1:35 – 281. OECD Residue Chemistry Expert Group (OECD RCEG): Progress report on recent efforts to prepare a comprehensive guidance document for rotational crops. **K. M. Jernberg**

2:00 – 282. Latest international developments in residue behaviour – proportionality approach. **K. Hohgardt**

2:25 – 283. Rates and residues: How proportional are they? **J. Stewart**

2:50 Panel Discussion.

3:10 Intermission.

3:25 – 284. Challenges of establishing and managing global pesticide magnitude-of-residue studies. **M. Braverman**

3:50 – 285. Residue analysis of plant protection products: Challenges and trends. **A. Reinold**

4:15 – 286. Matrix characterization: Challenges in obtaining and screening control sample materials suitable for use in pesticide residue analysis. **T. Moate**, R. Testman

4:40 Panel Discussion.

5:00 Concluding Remarks.

ENVR Division

Fate and Toxicology of Emerging Environmental Contaminants
Cosponsored by AGRO
S. Uchimiya, X. Pan, *Organizers*
B. Zhang, *Organizer, Presiding*

Section A
Crowne Plaza, Victoria Station D

1:30 Introductory Remarks.

1:35 – ENVR 210. Ecotoxicological effects of nanostructured titania to bacteria: Mechanistic insights of regulating factors. **T. Tong**, C. Binh, A. Shereef, J. Wu, J. J. Kelly, J. Gaillard, K. A. Gray

1:55 – ENVR 211. Impacts of the interaction of silver nanoparticles with microbial biofilm. **H. Jing**, B. Mezgebe, A. Hassan, E. Sahle-Demessie, G. Sorial, C. Bennett-Stamper

2:15 – ENVR 212. Transport behavior of nanoscale zerovalent iron stabilized with carboxymethylcellulose under simulated aquifer conditions. **L. L. Williams**, M. N. Goltz, **A. Agrawal**

2:35 – ENVR 213. ZnO nanoparticle induced phytotoxicity and differential anti-oxidative stress in green peas (*Pisum sativum* L.) cultivated in soil. **A. Mukherjee**, S. Bandyopadhyay, C. Rico, L. Zhao, J. Peralta-Videa, J. Gardea-Torresdey

2:55 Intermission.

3:10 – ENVR 214. Effect of cerium oxide nanoparticles on the metabolic activity of kidney bean plants and the first filial generation plants. **S. Majumdar**, J. Trujillo-Reyes, J. R. Peralta-Videa, J. L. Gardea-Torresdey

3:30 – ENVR 215. Toxicity assay comparing differing surface chemistries of nanoparticles on *Daphnia magna*. **J. Bozich**, S. Lohse, M. Torelli, C. Murphy, R. Hamers, R. Klaper

3:50 – ENVR 216. Toxicological effects of iron and copper nanoscale oxides and their bimetallic system in onion (*Allium cepa*). **J. Trujillo-Reyes**, S. Majumdar, J. R. Peralta-Videa, J. L. Gardea-Torresdey

4:10 – ENVR 217. Comparative eco-toxicities of nanoparticulate ZnO, bulk ZnO and ionic zinc ($ZnCl_2$) to the alfalfa-*Sinorhyzobium meliloti* system in soil matrix. **S. Bandyopadhyay**, A. Mukherjee, J. Peralta-Videa, G. Plascencia-Villa, C. Rico, M. José-Yacamán, J. Gardea-Torresdey

ENVR Division Poster Session

Air Monitoring
Cosponsored by AGRO, ANYL, and CHAS
J. Maclachlan, *Organizer*

Section A
Indiana Convention Center, Halls F&G

6:00 - 8:00

246. Chemical exposure monitor with indoor positioning (CEMWIP). **K. K. Brown**, P. B. Shaw, K. R. Mead, R. J. Kovein, R. T. Voorhees, A. R. Brandes

247. Nanostructure characterization of flat flame soot derived from petroleum-based, synthetic, and surrogate jet fuels.**C. Huang**, R. L. Vander Wal

248. Indoor and outdoor airborne PCBs in residential areas of East Chicago, IN and Columbus Junction, IA. T. Schulz, D. Hu, P. Thorne, J. DeWall, **K. Hornbuckle**

249. Atmospheric polychlorinated biphenyl congeners and synthetic musk fragrances in Chicago and Lake Michigan. **Z. L. Rodenburg**, D. Hu, Y. Ma, M. Venier, R. A. Hites, K. C. Hornbuckle

250. Improved quantitation of sulfur compounds in the atmosphere by hyphenated GC-FPD-PID. J. N. Driscoll, **J. L. Maclachlan**

251. Particulate PCBs and OH-PCBs in Chicago air. **A. Awad**, A. Martinez, R. Marek, W. Koh, K. Hornbuckle

Fate and Toxicology of Emerging Environmental Contaminants
Cosponsored by AGRO
B. Zhang, S. Uchimiya, X. Pan, *Organizers*

280. Reproductive toxicity and mechanism of ZnO nanoparticles in *C. elegans*. **B. O'Donnell**, J. R. Polli, X. Pan

281. Environmental fate of pharmaceuticals and hormones derived from water reuse. **W. Zheng**, Y. Zou, M. L. Machesky

282. Effects of Bisphenol A on growth and locomotion behaviors of *C. elegans*. **Z. D. Flood**, J. R. Polli, X. Pan

283. Trace analysis and imaging of heavy metal accumulation in rat tissues. **S. R. Wegst**, E. J. Mullin, D. Ding, R. J. Salvi, J. A. Roth, D. S. Aga

284. Predominant role of human CYP2B6 in the oxidative metabolism of BDE-47 and BDE-100 to potentially toxic metabolites. **M. S. Gross**, D. M. Butryn, B. P. McGarrigle, S. T. Singleton, A. L. Crane, J. R. Olson, D. S. Aga

285. Degradation potential of emerging contaminants by zerovalent zinc (Zn) and specific bimetallic reductants (Pd-Zn and Cu-Zn) in batch reactors. **C. S. Cushman**, **A. Agrawal**

286. Biodegradation of 4-*tert*-Octylphenol by bacteria: Kinetics and pathways. **K. Dong**, Y. Liu, J. Gan

287. Bench-scale degradation of emerging contaminants and recalcitrant organics by zerovalent magnesium and related bimetallic reductants. **B. Wang**, F. Yu, M. N. Goltz, **A. Agrawal**

288. Isomer specific reaction of HBCD with reduced sulfur species in aqueous solution. J. H. Wilson, **U. Jans**

289. Photochemical destruction of thyroid hormone. **X. Duan**, X. He, S. P. Mezyk, R. Marfil-Vega, M. A. Mills, D. D. Dionysiou

290. Interactions of functionalized nanomaterials on membrane gut of *Daphnia magna*. **G. A. Dominguez**, S. Lohse, M. Torelli, C. Murphy, R. Hamers, R. Klaper

Predicting Molecular Properties of Environmental Contaminants: Empirical and Theoretical Methods
Cosponsored by AGRO and COMP‡
D. Ditoro, E. Weber, K. Fenner, P. G. Tratnyek, *Organizers*

333. Predicting reduction rates of energetic nitroaromatic compounds. A. J. Salter-Blanc, **P. G. Tratnyek**, E. J. Bylaska

334. Gas-particle partitioning of polycyclic aromatic hydrocarbons: State of knowledge. **G. Lammel**, M. D. Mulder, L. Landlová, J. Klánová

335. Leaching potential of antibiotics estimated in soil and peat. **M. R. de Marchi**, P. Toledo Netto, C. Lourencetti

336. Identification of potential skin sensitizers based on non-animal chemoassay and in vitro bioassay information. A. Böhme, W. Zhang, **G. Schüürmann**

337. Effect of concentration and size of suspended sediment on nitrogen dynamics in freshwater ecosystem. **Q. Le**, C. Yoshimura, M. Fujii

Status and Trends of Classical and Emerging Contaminants Across the World
Cosponsored by AGRO and CEI
Financially supported by Global Innovation Imperatives
B. Loganathan, K. Hristovski, N. Savage, S. Ahuja, *Organizers*

338. Concentrations of perfluorinated chemicals and their precursors in wastewater matrices across United States. **K. Dasu**, M. A. Mills, K. Tadele, B. Crone

339. Tracing the temporal trends of inorganic elements and polychlorinated biphenyls using annual growth rings of pine trees from western Kentucky, USA. **B. Patibandla**, B. G. Loganathan

340. PCB congeners, chlorinated pesticides, and PBDEs in sediment and fish samples from riverine and brackish waters of Savannah, Georgia, USA. D. Benningfield, B. Cassidy, J. P. Richardson, **K. S. Sajwan**, B. G. Loganathan

THURSDAY MORNING

Assessing Potential Ecological and Human Health Effects from Fertilizer and Pesticide Use in Urban Environments
Financially supported by Pyrethroid Working Group
J. Gan, R. Jones, M. Shamim, *Organizers, Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

8:30 Introductory Remarks.

8:45 – 287. Factors influencing pesticide concentrations in dusts on residential outdoor impervious surfaces. **W. Jiang**, J. Gan

9:10 – 288. Factors affecting residential runoff transport of pyrethroids. **R. L. Jones**, P. C. Davidson, C. M. Harbourt, P. Hendley

9:35 – 289. Determining critical factors controlling off-site transport of pyrethroids in the urban environment. P. S. Miller, **P. C. Davidson**, C. M. Harbourt, X. Zhang, C. C. Boast, R. L. Jones, G. E. Goodwin, B. A. Sliz

10:00 Intermission.

10:20 – 290. Semimechanistic modeling of pesticide washoff from concrete surfaces. **Y. Luo**, F. Spurlock, S. Gill, K. S. Goh

10:45 – 291. Application of a modeling approach for predicting pyrethroid residues is urban water bodies for use in environmental risk assessments. **M. Winchell**, S. Jackson, G. Mitchell

11:10 – 292. Conducting ecological risk assessments for urban uses of pesticides. **M. T. Shamim**, J. Melendez, K. Sappington, M. Ruhman

Regulatory Risk Assessment: New Paradigms for Human Health Exposure
Considerations in Occupational, Residential Bystander Exposure Assessment
Financially supported by Dow AgroSciences
C. B. Cleveland, C. Lunchick, *Organizers, Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

8:30 Introductory Remarks.

8:35 – 293. Conducting an acute aggregate residential risk assessment. **C. Lunchick**, J. Driver

8:55 – 294. Risk assessment initiatives in Latin America. **X. Patino**

9:15 – 295. Development of a recombinant butyrylcholinesterase pulmonary bioshield to protect against OP inhalation exposure in macaques. **Y. J. Rosenberg**, B. Laube, L. Mao, X. Jiang, S. Hernandez-Abamto, R. Adams

9:35 – 296. Development of a generic seed treatment exposure database. **C. Lunchick**, D. Barnekow, L. Rosenheck, E. Kennedy

9:55 – 297. Acute nondietary exposure assessment. **J. Evans**

10:15 Intermission.

10:30 – 298. Considerations for estimating pesticide volatilization fluxes from various crops . **M. S. Majewski**, J. N. Seiber

10:50 – 299. Volatility and air dispersion modeling considerations for assessing bystander exposure and risk from semivolatiles applied to crops and orchards. **I. J. van Wesenbeeck**, S. A. Cryer, P. L. Havens, C. B. Cleveland

11:10 Panel Discussion.

11:30 Concluding Remarks.

Air Quality at the Interface
Megacities and Agroecosystems
Cosponsored by CEI‡ and ENVR‡
Financially supported by Society of Environmental Toxicology and Chemistry
G. P. Cobb, L. McConnell, P. Green, S. Madronich, *Organizers*
E. Ulrich, *Organizer, Presiding*

Section C
Crowne Plaza, Milwaukee

8:30 Introductory Remarks.

8:35 – 300. Understanding the origin of aerosols at the urban-regional interface. **S. Madronich**

9:05 – 301. Agricultural influences on air quality from California's San Joaquin Valley to the Chesapeake Bay area. **C. J. Howard**, J. Hu, M. J. Kleeman, P. G. Green, L. L. McConnell, C. J. Hapeman

9:25 – 302. Demonstration and evaluation of open-air tracer ratio flux measurements of methane and other trace gas emissions from pastured animals at low altitude, semi-tropical and higher altitude, semi-arid sites in Mexico. **C. E. Kolb**, S. C. Herndon, W. B. Knighton, C. Floerchinger, E. C. Fortner, J. R. Roscioli, T. Yacovitch, O. A. Castelán, J. K. Vera, E. Castillo, M. A. Zavala, L. T. Molina

9:45 – 303. Analysis and evaluation of measured trace gas emissions from farm animals in Mexico. **L. T. Molina**, M. A. Zavala, O. A. Castelán, J. K. Vera, E. Castillo, S. C. Herndon, W. Knighton, C. Floerchinger, E. C. Fortner, J. R. Roscioli, C. E. Kolb

10:05 Intermission.

10:25 – 304. Field evaluation of EPA approved PM_{10} and $PM_{2.5}$ ambient FRM samplers for determining emission concentrations from agricultural sources. **M. Buser**, D. Whitelock

10:45 – 305. Field evaluation of EPA Method 201a (stack sampling methodology) for determining $PM_{2.5}$ and PM_{10} emission concentrations from an agricultural source. **M. Buser**, D. Whitelock

11:05 – 306. Oil and gas exploration impacts on air quality and their potential implications for agriculture. **E. P. Olaguer**

11:25 – 307. Air pollution in the metropolitan area of Buenos Aires: From emission inventories to air quality impacts. **D. R. Gomez**, V. Pereyra, M. Matranga, M. Diaz Resquin, M. Dos Santos, F. Fujiwara, L. Dawidowski, P. Smichowski, R. Abrutzky

Pesticide Residues in Food and Feed: Scientific and Regulatory Global Needs
Foreign Markets
Financially supported by Golden Pacific Laboratories and Dow AgroSciences
H. Irrig, *Organizer*
C. Tiu, *Presiding*

Section D
Crowne Plaza, B&O (Baltimore & Ohio)

7:30 Introductory Remarks.

7:35 – 308. Food commodity consumption data and new tools used by US EPA Office of Pesticide Programs. **J. L. Van Alstine**, D. J. Miller

8:00 – 309. What is the best use of available global data for regulatory assessments and harmonized Maximum Residue Limits (MRLs)? **C. B. Cleveland**, **C. Tiu**

8:25 – 310. Communicating the connection between MRLs and food safety. **A. Shulkin**

8:50 Panel Discussion.

9:10 Intermission.

9:25 – 311. MRLs as potential barriers to innovation, trade, and food security. **B. Innes**

9:50 – 312. US citrus industry perspective on MRLs and trade. **J. R. Cranney**

10:15 – 313. Import tolerance approval process in Japan. **A. Aoki**

10:40 – 314. Responses of export-oriented tree fruit producers to the challenges of meeting MRL requirements around the world. **M. Willett**

11:05 – 315. Challenges in establishing Maximum Residue Limits to support the export of raw agricultural commodities. **P. A. Brindle**

11:30 Panel Discussion.

11:50 Concluding Remarks.

ENVR Division

Fate and Toxicology of Emerging Environmental Contaminants
Cosponsored by AGRO
B. Zhang, X. Pan, *Organizers*
S. Uchimiya, *Organizer, Presiding*

Section A
Crowne Plaza, Victoria Station D

8:00 – ENVR 341. Fate of organophosphorus pesticides in water under environmental conditions. **M. G. Miller**, J. J. Kiddle, K. Clark, S. P. Mezyk

8:20 – ENVR 342. Chemical speciation of organotin compounds in seawater from Cape Town Harbour, South Africa: Seasonal variations and their toxicity effects. **O. S. Fatoki**, H. K. Okoro, F. A. Adekola, B. J. Ximba, R. G. Snyman

8:40 – ENVR 343. Fate of organic and inorganic contaminants in biochar amended soils. **S. M. Uchimiya**

9:00 – ENVR 344. Potential impact of biochar water-extractable substances on environmental sustainability. **C. R. Smith**, **J. W. Lee**

9:20 – ENVR 345. Assessing the role of natural organic matter in the photochemical degradation of lampricides. **M. B. McConville**, C. K. Remucal

9:40 – ENVR 346. Enhancement of carboxylic acids on the degradation of trichloroethylene with zerovalent iron. **C. Tso**, Y. Shih

10:00 Intermission.

10:15 – ENVR 347. Fate of aromatic nitrosamines in oxidative and reductive water remediation methods. **J. E. Toth**, B. Sjelin, J. J. Kiddle, S. P. Mezyk, K. A. Rickman

10:35 – ENVR 348. Degradation mechanisms during the removal of the emerging cyanobacterial toxin cylindrospermopsin by advanced oxidation. **X. He**, A. A. de la Cruz, D. D. Dionysiou

10:55 – ENVR 349. Photochemical reactions of ibuprofen, naproxen, and tylosin. **Y. He**, I. Hua

11:15 – ENVR 350. Photochemical fate of triclosan: Experimental and theoretical evidence for a radical pathway leading to dioxins and PCBs. **S. N. Eustis**, S. Kliegman, K. McNeill

11:35 Concluding Remarks.

THURSDAY AFTERNOON

Assessing Potential Ecological and Human Health Effects from Fertilizer and Pesticide Use in Urban Environments

Financially supported by Pyrethroid Working Group
R. Jones, *Organizer, Presiding*
J. Gan, M. Shamim, *Presiding*

Section A
Crowne Plaza, Illinois Street Ballroom East

1:30 – 316. Pyrethroid pesticides in municipal wastewater: A baseline survey of publicly-owned treatment works facilities in California. **J. C. Markle**, B. H. van Buuren, K. Moran, A. C. Barefoot

1:55 – 317. Analysis of pyrethroid insecticides in complex environmental samples using stable isotope labeled standards as surrogates. **K. Clark**, D. A. Koch, D. M. Tessier, J. C. Markle

2:20 – 318. Fate of pyrethroid pesticides through advanced wastewater treatment processes. **K. N. Ohlinger**

2:45 Intermission.

3:00 – 319. Potential influence of pyrethroids, metals, sediment characteristics, and water quality conditions on benthic communities in Cache Slough California in 2012. **L. Hall**, W. Killen, R. Anderson, R. Alden III

3:25 – 320. Pyrethroid monitoring of the Lower American River in California (USA). **C. M. Harbourt**, S. A. Clark, G. E. Goodwin, T. Albertson, M. Dobbs, K. Henry, G. Mitchell

Regulatory Risk Assessment: New Paradigms for Human Health Exposure Considerations for Dietary, Aggregate, Cumulative and FQPA

Financially supported by Dow AgroSciences
C. B. Cleveland, *Organizer, Presiding*
C. Lunchick, *Presiding*

Section B
Crowne Plaza, Illinois Street Ballroom West

1:00 Introductory Remarks.

1:05 – 321. Overview of updates to US EPA Office of Pesticide Programs dietary models and Residential SOPs. **J. L. Alstine**

1:25 – 322. Use of open literature toxicity and epidemiology studies in regulatory decision making. **S. C. Gehen**, **C. J. Burns**, **C. Thorp**

1:45 – 323. Impact of recent changes in pesticide exposure assessment procedures on dietary, residential, and aggregate exposure estimates. **J. Johnston**, A. Klemens, J. Van Alstine

2:05 – 324. What if there was no USDA Pesticide Data Program? Advantages and rigor of the US EPA tiered process for risk assessment. **C. B. Cleveland**, **C. R. Fleming**, J. Stewart, D. Haynes

2:25 – 325. Improving the estimation of drinking water exposure in dietary risk assessment. **M. F. Leggett**, N. N. Poletika

2:45 – 326. Pesticide dietary exposure and risk assessment: Incorporating monitoring data to address controversial issues.**C. K. Winter**

3:05 Intermission.

3:20 – 327. FQPA and health effects. **A. A. Li**, **B. M. Polakoff**

3:40 – 328. EU update on dietary risk assessment: An industry perspective. **M. B. Bross**

4:00 – 329. Cumulative risks: When do they add up? Using the Maximum Cumulative Ratio (MCR) to understand risks from concurrent exposures to multiple chemicals. **P. S. Price**

4:20 Discussion.

4:35 Concluding Remarks.

Air Quality at the Interface
Megacities and Agricultural Areas
Cosponsored by CEI‡ and ENVR‡
Financially supported by Society of Environmental Toxicology and Chemistry
G. P. Cobb, *Organizer, Presiding*

Section C
Crowne Plaza, Milwaukee

1:00 – 330. Can the oxidative stress responses in pine needles be used as reliable biomarkers to assess exposure to POPs?**K. S. Miglioranza**, M. Gonzalez, P. M. Ondarza, M. L. Menone, F. M. Mitton, G. Lukaszewicz, V. M. Shimabukuro, G. Fillmann

1:20 – 331. Design and performance of a study for the determination of trichlorofon transferrable residues from turf and residues in air. **M. E. Krolski**, C. Lunchick

1:40 – 332. Brominated flame retardants in the Great Lakes atmosphere. **A. Salamova**, R. A. Hites

2:00 – 333. Airborne steroids and growth promoters near concentrated animal feeding operations. **G. P. Cobb**, B. Blackwell, M. Buser, B. Johnson, M. Baker, P. N. Smith

2:20 – 334. Examining the fate and transport of α- and β-endosulfan in the atmosphere of South Florida. C. J. Hapeman, **L. L. McConnell**, T. L. Potter, J. A. Harman-Fetcho, C. P. Rice, B. A. Schaffer, R. Curry

2:40 Concluding Remarks.

2:50 Panel Discussion.

AGFD DIVISION

2013 Kenneth A. Spencer Award

Symposium in Honor of Dr. Attila Pavlath

AGFD 95

Food packaging and sustainability

Sara J Risch*, sjrisch@sbcglobal.net.Popz Europe Kft., Chicago, IL 60611, United States*

The food industry has been focused on sustainability. This is a very broad topic that ranges from water and energy issues to food production and distribution. Packaging has long been the target of environmentalists who want the absolute minimum amount of packaging used. Many people have been proponents of reducing, re-using and recycling packaging materials. While these are good ideas for some applications, they cannot be universally applied. In recent years, there has been an added emphasis on biodegradable and bio-based materials as replacements for traditional petroleum based plastics. New developments in food packaging will be reviewed. Challenges and potential compromises that might arise in the quest for sustainability in packaging materials will be discussed.

AGFD 96

Corn fiber gum and its synergistic effect on the viscosity of other polysaccharides

Madhav P. Yadav*[1], madhav.yadav@ars.usda.gov, Fei Zhang[2], Tu Luan[2], Kang Ding[2], Hongbin Zhang[5]. (1) SBCP, USDA-Agricultural Research Service ERRC, 600 E. Mermaid Lane, Wyndmoor (Philadelphia), PA 19038, United States (2) Shanghai Jiao Tong University, China (3) Shanghai Jiao Tong University, China (4) Shanghai Jiao Tong University, China (5) Shanghai Jiao Tong University, China*

Corn fiber gum (CFG) is an alkaline hydrogen peroxide extract of corn fiber, which is an abundant and low-valued by-product of corn kernel milling process. It has been known that CFG forms a low viscous solution and has a great ability to emulsify oil in oil-in water emulsions. Viscous synergism is well known for a mixture of polysaccharides with the viscosity of the mixture greater than the algebraic sum of its components' viscosity. In this study the effect of CFG on the aqueous solution of commercial polysaccharides including hyaluronan (HA, anionic polysaccharide), chitosan (CTS, cationic polysaccharide) and methylcellulose (MC, non-ionic polysaccharide) has been studied. It was found that the steady shear viscosity of CFG solutions at different concentrations was almost independent of the shear rate, and no obvious shear thinning phenomenon was observed even in very high shear rate range up to 1000 s^{-1}, revealing Newtonian-like fluid behaviour. Moreover, the steady shear viscosity of CFG solutions increased with an increase CFG concentration, but it was as low as about 0.3 Pa s even at a relatively high concentration (60 mg/ml), indicating low

viscous solution behaviour. Though CFG solution exhibited Newtonian fluid behaviour with a very low viscosity even at a high concentration, the mixtures of CFG and polysaccharide showed a pseudoplastic fluid behaviour. Furthermore, the viscosity of the mixture of each polysaccharide with CFG was much higher than the algebraic sum of its components' viscosity, showing a viscous synergism. The interesting viscous synergistic behavior of CFG towards these polysaccharides may be due their interaction by hydrogen bonding not ionic charges. Such combination of very good emulsifying properties, a low solution viscosity and a great synergistic effect on viscosity of many commercially available polysaccharides may generate a great commercial interest in CFG for formulating many products in food and non-food industries.

AGFD 97

Can bioderived polymers compete?

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A great deal of effort is being devoted to developing biological (sustainable) routes to monomers (propane diol, butane diol) and polymers identical to (PE, PET) or competitive with (PLA, PHA) petroleum-derived materials. While some success has been achieved, these materials struggle to be cost-competitive. Isosorbide is a sugar-derived diol that may offer competitive advantage to broad range of products including thermoplastics, thermosets, polymer additives and polymer modifiers. Recently, it has been reported that a cost-effective route to 2,5 Furan dicarboxylic acid has been achieved, renewing interest in a potentially enabling new monomer for polyesters and polyamides. In some cases the structural complexity of bio-derived chemistries may enable performance difficult to achieve with conventional chemistry; two examples of this are isosorbide modified PET with improved thermal stability and soy protein modified synthetic fibers with improved hand. Assigning a value to sustainability has been difficult but it appears sustainability and renewability are an advantage **if cost-competitiveness is achiev**

AGFD 98

Edible films and coatings on processed fruits and vegetables

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Why do we need edible films? While some product can be eaten in their original form, in most cases they need to be pared, cored, sliced, diced for immediate household use. If this is done in a factory before reaching the consumer, products start to dehydrate, deteriorate, loose appearance, flavor and nutritional values. Without special protection the product becomes immediately more perishable. The damage can occur within hours or days, even if this damage is not immediately visible. This can be prevented if after the processing the natural skin is replaced with an edible film. The right edible films can prevent moisture losses while selectively allowing the controlled exchange of important gases, such as oxygen, carbon dioxide and ethylene involved in respiration processes. The main components of our everyday foods, i.e., proteins, carbohydrates and fats, can fulfill requirements for edible films. The general rule is that fats reduce water transmission, polysaccharide films control oxygen and other gas transmission, and protein films provide mechanical stability. These materials can be added separately, or mixed provided they do not change flavor. The major deciding factor is whether the protecting films have the necessary physical chemical properties to maintain the transmission of the various gases and liquids at the same rate as the natural protection does. Each of these components has different properties, which are efficient in controlling one type of transmission while sometimes have detrimental effect on others. The lecture will describe their characteristics and discuss how they can be applied.

Pavlath, A.E. and Orts, W. Edible Films: Why, What and How? In Edible Films and Coatings for Food Applications, Eds. M.E. Embuscado and K.C. Huber, Springer, USA, N.Y. 2012? In Edible Films and Coatings for Food Applications, Eds. M.E. Embuscado and K.C. Huber, Springer, USA, N.Y

AGFD 99

Inflammation of cardiovascular tissue by certain fatty acids and protection from the microbiome activity

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It has been established that circulating fatty acids are risk factors for cardiovascular disease. The current study compared the effects of various fatty acids on inflammatory markers expressed in cardiovascular endothelial and smooth muscle cells. The inflammatory responses were influenced by chain length and degree of saturation of the free fatty acids. The study also investigates the influence of the anthocyanins and their degradation products by the microbiome on inflammatory responses of the cell cultures. The results indicate that although poorly absorbed the anthocyanins are protective against inflammation, but will not reverse existing inflammation. The microbiome degrades unabsorbed anthocyanins in the lower GI tract. The smaller degradation products as a result of the microbiome action on anthocyanins were demonstrated to be highly protective of the cardiovascular tissue from fatty acid induced inflammation. The results suggest that reduced exposure to certain fatty acids and incorporation of anthocyanins in the diet may help reduce risk of cardiovascular inflammation.

AGFD 100

Edible food coating derived barrier teat disinfectant for milk quality improvement

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Milk is an important source of dietary protein and fat. It is an important sustainable food source because the dairy cow converts non-human consumable food stuffs into valuable consumable protein. Quality milk must be low in bacterial count to maintain good protein levels and provide adequate shelf life. Bacteria in milk can come from a number of sources including shedding from infected mammary gland (mastitis). Mastitis is a bacterial infection with the dairy farm environment as a prominent source. Preventing mastitis is achieved by post milking teat disinfectants. The disinfectants can be formulated as barrier products, which provide a protective film to prevent bacteria from entering the teat gland. Edible coatings from Dr. Pavlath's USDA team were developed with DeLaval into barrier teat disinfectants. The successful coating material was based on similar requirements for these two seemingly divergent applications: acceptable for food contact, barrier to oxygen and bacteria, application as aqueous liquids.

AGFD 101

Further studies demonstrate PPARα activation and gene expression up-regulation by pterostilbene

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In an earlier study, we showed that pterostilbene is an agonist for the peroxisome proliferator activated receptor alpha isoform (PPARα). Activation of PPARα in rat hepatoma (H4IIEC3) cells by pterostilbene was compared with resveratrol and its methylether analogs, catechin, and epicathechin. The docking of these compounds into the PPARα ligand binding domain was also investigated. Of the stilbenes, pterostilbene demonstrated the highest PPARα activation. Pterostilbene also showed decreases in PPARα activation paralleling those of Wy-1463, a synthetic PPARα ligand, in the presence of chenodeoxycholic acid, a specific inhibitor of PPARα. Real-time gene expression analysis revealed pterostilbene significantly and dose-dependently (at 10, 20 and 50 µM) increased PPARα gene expression, and exhibited greater induction than fenofibrate at 100 and 200 µM. Docking experiments revealed that the stilbenes docked in a similar manner in the benzophenone pocket, and had H-bond interaction with amino acids considered essential for PPARα activation. The catechins did not dock in the active pocket. In animal studies, up-regulation of hepatic PPARα mRNA expression was observed in hamsters fed diet supplemented with 2% of an ethanol extract of blueberry fruit pomace (BBX). A significant negative correlation between liver LDL-cholesterol levels and PPARα expression was also observed. Catechin, epicatechin, pterostilbene and resveratrol were quantitated in the BBX by GC-MS analysis. Our studies provide further evidence that pterostilbene activates PPARα, and it may contribute to the hepatic LDL-cholesterol lowering and up-regulation of PPARα expression in hamsters fed BBX-supplemented diet.

AGFD 102

Dairy and functional foods research in the Agricultural Research Service

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The Dairy and Functional Foods Research Unit is the only group in the Agricultural Research Service that is dedicated to solving critical problems in milk utilization and fruit and vegetable byproducts from specialty crops. The many areas of investigation include development of specialty cheese, controlling cheese chemistry, bioactive peptide research, comparing milk from cows fed conventionally and on pasture, identifying milk components with possible nutritional advantages, utilization of milk protein for edible films, whey protein fractionation for nutritional products, and sustainable strategies for food processing. Another aspect of the program includes work on healthy carbohydrates, including bioactive oligosaccharides and active packaging films made from pectin and poly-lactic acid. Among the accomplishments resulting from this research are advances in the understanding of milk protein structure and cheese microstructure, reduced-lactose milk products, low-fat Mozzarella cheese for the National School Lunch Program, and rations for the Food for Peace program. The benefits provided by the Unit's work are felt by all Americans.

AGRO DIVISION

AGRO 1

Characterizing intractable targets using homogenous immunoassays

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AlphaScreen and AlphaLISA are fast and simple homogeneous immunoassay technologies allowing one to detect a wide range of analytes, either small (e.g., nucleotides) or very large (e.g., Titin = 4000 kDa), interacting with high (fM) or low (mM) affinities. The versatility of the Alpha technologies is due to a unique energy transfer process based on singlet oxygen diffusion occurring between nano-sized polystyrene beads over a distance ranging up to 200 nm, making possible the development of assays involving a wide diversity of binding partners engaging simple or complex interactions. AlphaScreen and AlphaLISA are used as enabling tools for developing applications with biological targets often intractable due their size, complexity, or scarcity. Various customer study cases will be presented and discussed with the audience.

AGRO 2

Multiplexing protein analysis of transgenic plant samples using MSD technology

***Ai-Guo Gao**, ai-guo.gao@monsanto.com. Biotech, Monsanto Company, Chesterfield, MO 63017, United States*

Quantitative protein analysis plays an important role in the agricultural biotech industry by supporting gene evaluation, event selection, safety studies, and product development. Although ELISAs are still the most commonly used assay for protein quantification, the rapid increase in the number of samples, complexity of proteins, and gene stacking have steered companies to explore new technologies to meet current and potential future needs and to increase efficiency. Meso Scale Discovery (MSD) is one of the technologies, which allows analyzing multiple targets in a single assay. Results from a multi-year sample analysis confirmed that MSD is a robust assay platform to process large numbers of gene stacked samples. In this presentation, technical details will be discussed with a focus on assay development and validation. Assay development centered on monoclonal antibody selection as capture reagents. Equivalence between results from the newly-developed multiplexed assays and the existing validated ELISAs was another important aspect in our studies. The linear range of the standard curves used on MSD is typically broader than ELISA. However, results from side-by-side comparisons illustrated that there is no significant difference between those two assay platforms. Variation between replicates is smaller on MSD. The overall rerun rate was significantly reduced on MSD. In summary, MSD based multiplexing protein assays have been successfully implemented at Monsanto. Details on assay development and validation will be provided in the presentation.

AGRO 3

Immunoassay automation and its application in GM detection

***Michele S Yarnall**, michele.yarnall@syngenta.com. Syngenta Biotechnology, Inc., Research Triangle Park, NC 27709, United States*

With the introduction of the first genetically engineered crop occurring less than 20 years ago, the incentive for automated technology in the agriculture detection field historically has not been as great as in the pharmaceutical or clinical diagnostic fields. However, the steadily increasing annual growth of genetically engineered crops and necessity for constant monitoring of these crops throughout every phase of the product life cycle (development, supply chain, and termination of product) have created a need for methods to screen large numbers of samples. Some practical and flexible ways to automate lab procedures specifically for the qualitative testing of plant extracts will be described. How different instruments can be used to automate each process and how to minimize cross-contamination, while keeping costs at reasonable levels, will be illustrated. Current available systems and alternative technologies that potentially will be useful for agriculture biotechnology in the future will be discussed.

AGRO 4

Development and implementation of multiplexed LC-MS/MS strategies for the quantitation of plant-expressed proteins in genetically-modified crops

***Trent J Oman**, oman@dow.com, Ryan C Hill, Barry W Schafer, Jeffrey R Gilbert, Guomin Shan. Dow AgroSciences, Indianapolis, IN 46268, United States*

Since the early commercialization of genetically modified (GM) crops in the mid-1990's, there has been a need in the field of agriculture to quantify transgenic proteins in plants. The quantitation of proteins in complex plant matrices requires robust analytical platforms with high sensitivity and specificity. The measurement of protein levels in GM crops has been achieved almost exclusively by immunoassays, such as enzyme-linked immunosorbent assays (ELISA); however, immunoassays rely upon the use of antibodies which are both highly specific and sensitive to the protein of interest, but may not be readily available in the early stages of the discovery process. In addition, many of the latest GM crops provide multiple modes of protection to the plant through the use of 'stacked traits' resulting in the simultaneous expression of several transgenic proteins. For product development, the expression level of each of protein must be measured. There has been recent interest in developing LC-MS/MS based methods to quantify several plant-expressed proteins in a single analysis. These 'signature peptide' analyses involve tracking protein expression levels by quantifying several highly specific digest fragments of the proteins of interest. This is typically accomplished using liquid chromatography coupled with selected reaction monitoring (SRM) tandem mass spectrometry. Several multiplexed LC-MS/MS platforms have been developed and utilized to quantify plant-expressed proteins in matrix with minimal sample manipulation. These methods have been evaluated 1) for analytical figures of merit including accuracy, precision, linearity, and limits of detection and quantitation, and 2) for other considerations including sample throughput, transferability, and ease of use. Subtle differences in protein expression levels among various tissue types and growth stages in several crops were

readily detected using the described LC-MS/MS technology. Parallel analysis of samples using ELISA demonstrated that LC-MS/MS can be used to complement or replace existing strategies to quantify multiple proteins in GM crops.

AGRO 5

Multiplexing protein quantitation of transgenic proteins in soybean tissues using tandem mass spectrometry (LC-MS/MS)

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Agricultural biotechnology relating to crop protection has evolved toward increasing numbers of transgenic proteins being co-expressed or "stacked" to achieve tolerance to multiple herbicides or multiple modes of action to insect resistance. Stacked proteins present a challenge to traditional technologies for quantifying transgenic protein expression such as Enzyme Linked Immunosorbent Assays (ELISA) to accommodate the volume of data generated per sample. A selective and sensitive multiplex method was developed and validated to quantify the double mutant 5-enolpyruvylshikimate-3-phosphate synthase (2mEPSPS), aryloxyalkanoate dioxygenase (AAD-12), and phosphinothricin acetyltransferase (PAT) proteins in soybean tissues using tandem mass spectrometry (LC-MS/MS). Signature peptides representing each protein were identified by an information-dependent acquisitions (IDA) followed by optimization in multiple reaction monitoring (MRM) for quantitation with a hybrid Q-TRAP mass spectrometer. The method was validated for its accuracy, precision, linearity, and limits of detection and quantitation in various soybean tissues as well as signature peptide stability. Whole protein calibration curves were compared to synthetic signature peptide calibration curves during the validation with heavy labeled synthetic peptides serving as internal standards. Finally, the validated LC-MS/MS method was compared to validated ELISA methods by examining protein expression across three generations of transgenic soybean root, grain, and leaf tissues. The stacked event that was analyzed in this abstract was co-developed by Dow AgroSciences and MS Tech.

AGRO 6

Quantification of allergenic protein(s) in soybeans by 2D liquid chromatography with ultraviolet and mass spectrometric detection

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Soybean (*Glycine max*) is considered a major allergenic food inducing allergenic and immunologic reactions in susceptible individuals. The soy allergens are considered complete food allergens in that they are capable of inducing specific IgE as well as eliciting symptoms ranging from mild rashes to anaphylaxis. Of the several soybean allergens, Gly m 4 has been identified to cause an allergic reaction; typically, the symptoms are localized affecting the skin, the gastrointestinal tract, or the respiratory tract. In this study, we have isolated, purified, and characterized an endogenous ~17 kDa Gly m 4 protein. The endogenous protein has 88.5% sequence homology with the theoretically-predicted Gly m 4 sequence. An assay was developed for quantification of endogenous Gly m 4 using two dimensional liquid chromatography with ultraviolet and mass spectrometric detection (2DLC-UV/MS). The linearity, accuracy, and precision of the assay was determined and found to be appropriate for the determination of Gly m 4 level in soybeans. The method was successfully applied to quantify Gly m 4 level in ten commercial soybean lines. Further expansion of this method will be discussed.

AGRO 7

Acceptance criteria for GLP validation of quantitative analytical methods for proteins by ELISA and LC/MS/MS

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To assess the safety of genetically modified organisms (GMO), the proteins expressed by those GMOs need to be quantified in a variety of matrices including plant tissues, grain, soil, water, etc. While the true impact of the protein levels can be determined by biological assays such as insect bioassay or enzyme assay, these tests are generally semi-quantitative and less sensitive; most researchers currently approach full quantitation with the use of either Enzyme Linked Immunosorbent Assay (ELISA) or LC/MS/MS method. However, no current government guidance exists for the minimum acceptance criteria for these two methods for genetically modified crops. In this talk, the authors present background on the differences between the two methodologies as well as suggested criteria for the two techniques. Example criteria are sensitivity, linearity, accuracy, precision, specificity, stability, etc. Acceptance parameters will be discussed for each criteria along with potential issues faced by the analytical chemist in validating these methods.

AGRO 8

Development of a sandwich ELISA for heat denatured Bt Cry1Ac protein

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A monoclonal antibody (designated as MAb 2B4C7E) which can recognize not only native but also heat-denatured Bt Cry1Ac protein was obtained. A sandwich ELISA was developed using the MAb 2B4C7E and rabbit polyclonal antibody to heat denatured protein. The detection limits for heat denatured and native Bt Cry1Ac protein was 30.5 and 0.5 ng/mL, respectively. The assay was able to detect heat-denatured Bt Cry1Ac protein extracted from boiled transgenic Bt corn which was undetectable with commercial Bt Cry1Ac ELISA Kit. The monoclonal antibody can also be used in Western Blotting of transgenic cotton and maize that contain Bt Cry1Ac gene.

AGRO 9

Bioanalytical technologies for GM detection in India

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The introduction of Genetically Modified Crops (GMO) has changed the traditional agriculture practices in the world. In India, the GM era started with the introduction of Bt cotton in 2002 which has grown from an area of 50,000 to about 12 million acres by 2012. The requirement for GMO testing comes from the seed industry as well as the regulatory authority of India who wants to watch closely and to regulate the movement of GMO according to the national guidelines. While the seed industry involved in selling GM

seeds wants to ensure the presence of modified trait in the GM seeds sold, regulatory agencies want to ensure that seeds sold to the farmers have only the approved events of GMOs. Of the several bioanalytical tools available for the detection of transgene in GMO, ELISA tests are the most popular in India. PCR testing is primarily done for zygocity verification. Rapid lateral flow immunostrips are rarely used because of cost constraints. Adventitious presence (AP) testing is normally not done in India. The current status and challenges for the application of these technologies in the light of GM detection in India will be discussed.

AGRO 10

Wind tunnel testing of nozzles for reduction of drift

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Wind tunnel testing at the University of Nebraska was conducted in October 2012 to compare 18 different ground spray nozzles for drift reduction of an insecticide. The nozzles ranged from the base-case flat fan to newer technology air induction nozzles. Labeled spray rate considerations of the insecticide for different crops required the testing of nozzles at different orifice sizes and pressures. After the initial tests were complete, additional testing was conducted on the best performing nozzles to determine if their lower production of driftable droplets was consistent irrespective of the amount of active ingredient in the spray mixture. Using the AgDisp model and the droplet spectrums for each nozzle, spray drift as a fraction of the total amount applied was reduced significantly by several of the nozzles types.

AGRO 11

Validation of the extrapolation of wind tunnel-generated spray droplet distributions to DRT classifications with field data

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Under the proposed US EPA Drift Reduction Technology (DRT) protocols, low speed wind tunnel testing can be used to define drift reduction potential for a given application technology. However, as the program is currently envisioned, emphasis has been placed upon equipment-based DRTs such as nozzles and shielded/shrouded spray booms. For chemistry-derived DRTs such as tank adjuvants, and, especially, formulation-based solutions, it is unclear how the drift reduction potential can be derived without significant field-scale testing. A test case will be described that suggests that wind tunnel-measures of the fraction of fine particles produced by a nozzle-formulation combination can be a successful surrogate for drift reduction and subsequently, a DRT rating. Results from a replicated operational-scale field study will be shown that strongly correlate with the fraction of driftable fines produced with the same nozzle-formulation combination. It will be proposed that the resulting correlations can then be used to extrapolate low-cost wind tunnel results to field-scale DRT ratings for chemistry-based drift reduction systems.

AGRO 12

Comparison of multiple spray drift deposition data sets

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With the advent of the US EPA registration review process and the launch of their Drift Reduction Protocol methodology, there has been renewed interest for evaluating differing deposition data and methods for predicting deposition. A summary of several deposition datasets as well as modeling prediction methods will be compared and contrasted. The focus of these comparisons will be the protection of non-target areas as well as keeping maximum product on target. Impacts that drift mitigation can have on crop protection labeling will also be discussed.

AGRO 13

Ground spray drift modeling for pesticide application

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Ground spray drift model validation is described for the AGDISP model using several data sets.

AGRO 14

RegDISP: A flexible tool for the prediction of pesticide spray drift deposition based on measured ground application data

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Current regulatory tools used for the prediction of pesticide spray drift from ground applications are limited by generalization of the underlying data used to make their deposition predictions. This has made these tools unable to represent specific conditions of nozzle type, boom height, and wind speed accurately. To address this, a new tool has been developed that allows the prediction of spray drift deposition based on specific conditions. This new tool, RegDISP, has been built around the AgDISP 8.26 interface and model. RegDISP contains an extensive collection of empirical drift deposition equations that have been derived from experimental data representing a wide range of pesticide application and environmental parameters. Users may choose to predict drift deposition from this collection of empirical equations, or enter a drift curve derived from their own experimental data. RegDISP provides access to the same Deposition Assessment and Stream Assessment tools found in AgDISP 8.26.

AGRO 15

Drift-reduction for orchard applications: Practical adoption of low-drift nozzles while maintaining efficacy

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Conventional orchard nozzles, such as the Albuz ATR, generate approximately 23% (by volume) of droplets < 100 µm in diameter. This fraction, referred to as the V_{100}, is

liable to drift from the target area. By contrast, air-inclusion nozzles have been developed for use in orchards and have a V_{100} of < 5%. A prime example is the Albuz TVI, which has a V_{100} of approximately 1%. In field experiments (UK, Netherlands, and Italy) using orchard air blast (axial flow) sprayers, this nozzle was shown to reduce drift by 90% compared with the Albuz ATR. The droplets produced by the TVI nozzle are classified as very coarse to extremely coarse, with inherent air bubbles producing an explosive effect aiding dispersion in the canopy. The question is whether such nozzles can be adopted in normal practice, while maintaining biological efficacy. Dow AgroSciences LLC has assessed biological efficacy of chlorpyrifos applications in orchards and vines using the Albuz TVI. The TVI nozzles demonstrated comparable efficacy to the ATR. A dedicated campaign in the United Kingdom, which is in its second season (www.saynotodrift.co.uk), has driven rapid adoption of TVI nozzles for chlorpyrifos sprays by fully engaging with growers and providing training on optimum sprayer set-up. These principles are also now being taken forward in a similar program in Italy.

AGRO 16

Systematic literature review: Downwind spray drift from orchard air blast sprayers

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Pesticide application in bush and tree crops requires an airblast to open and to penetrate the inner canopy. The airblast improves efficacy but can also lead to increased spray drift. Pesticide spray drift has been and continues to be of concern to the US EPA in its responsibility to ensure that pesticide use does not cause unreasonable adverse effects to human health and the environment. "Spray or dust drift is the physical movement of pesticide droplets or particles through the air at the time of pesticide application or soon thereafter from the target site to any non- or off-target site. Spray drift does not include movement of pesticides to non- or off-target sites caused by erosion, migration, volatility, or windblown soil particles that occurs after application or application of fumigants." Under 40 CFR part 158, US EPA requires data on drift to support the registration or re-registration of certain products. One of the data sources for the agency is a collection of studies conducted by a group of registrants, named the Spray Drift Task Force (SDTF). In addition to the collection of empirical data, the SDTF co-developed AgDRIFT with US EPA and USDA Forest Service. AgDRIFT is a model created to provide estimates of spray drift deposition under different pesticide application and meteorological conditions. The US EPA uses the conclusions from the SDTF data, AgDRIFT or other appropriate models, and open literature in its assessments of pesticides. This literature review aims to provide a better understanding of the level of precision and accuracy with respect to real-world exposures that can be obtained using the current tools for estimation.

AGRO 17

Mechanisms, experiment, and theory of liquid sheet breakup and drop size from agricultural nozzles

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Spraying of agricultural chemicals through spray nozzles is a standard delivery practice. Spray nozzles operate by discharging a liquid sheet or jet which subsequently breaks up into droplets. Droplets which are too small can become entrained in ambient air currents and carried off target, while droplets which are too large often reduce coverage and efficacy. Many agricultural chemicals are dissolved in an oil phase and subsequently formulated as an oil-in-water emulsion which is then sprayed. In this study, single phase (water) and two phase (oil-in-water) emulsion were investigated photographically, experimentally, and theoretically to isolate the relevant mechanisms of sheet disintegration and representative droplet size. Three distinct mechanisms of sheet breakup were observed, parameterized by different scaling of the Weber number. Mechanisms include wave growth, rim breakup, and hole growth. Wave and rim breakup were found to dominate in single phase sprays, while formation of holes within the liquid sheet and hole growth was dominant when an immiscible second phase was introduced. Existing models for wave growth and rim breakup leading to atomization, along with a novel model for hole expansion and subsequent sheet destruction compare favorably with droplet diameters obtained experimentally. A hypothetical case is presented when breakup due to hole growth competes with wave growth for a two phase oil-in-water formulation. Although the exact mechanism for hole creation is not definitely established, several possibilities are discussed and inferred from experimental observations. It appears that a second immiscible phase, if low- or non-wetting, creates the necessary precursor for hole formation within the liquid sheet leading to sheet breakup. If this mechanism is indeed correct, it should be possible to control the spray droplet size distribution from spray nozzles given the size and wettablity (hydrophobic nature) of solid or liquid immiscible particles/droplets within a two phase system.

AGRO 18

Impact of high resolution accurate mass (HRAM) on metabolite identification for crop protection studies and regulatory submission

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Today access to information is power and never more so than in the world of crop protection development. Having detailed knowledge of how the active ingredient is metabolized is crucial in the development process. Biotransformation data generated from metabolism studies defines the fate of a crop protection product in the environment and is required by governmental and environmental agencies as part of the registration process allowing their use. From an industrial perspective, efficient delivery of metabolism data can save time and precious resources and can maximize return-on-investment. High resolution accurate mass spectrometry (HRAM) plays an important role in this process, identifying metabolites and the site of metabolism. Recent advances in both mass spectrometry hardware and software have helped in this on-going challenge in simplifying metabolite identification, with ultra-high-resolution and sub ppm accurate mass to resolve

and identify metabolites from background matrix ions. This approach has become the technique of choice for metabolite identification because of its sensitivity and ability to analyse complex mixtures. But while signal sensitivity has improved over the past decade, detecting and identifying metabolites in the presence of complex matrices remains a challenge. This presentation covers the merit of modern HRAM by addressing the power of mass resolution, accurate mass measurements, elemental composition determinations, and the use of data-processing techniques. This includes mass defect filtering and isotopic pattern filtering to remove the vast majority of matrix-related background ions by using examples of actual data to show the impact to regulatory submission and efficient delivery of metabolism data.

AGRO 19

Use of accurate mass instrumentation for the differentiation of molecules with the same exact mass

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Many molecules in the Ag Chem arena can have the same exact mass and empirical formula but are structurally different. This can lead to false positives in screening assays, as well as difficulties during structure elucidation. For example, 2,4-dichlorophenoxyacetic acid, 2, 3-dichlorophenoxy acetic acid, methyl 3,5-dichloro-4-hydroxybenzoate, and 3,6-dichloro-2-methoxybenzoic acid (dicamba), all have the same exact monoisotopic mass (219.969406 Da) and empirical formula ($C_8H_6Cl_2O_3$) but all are structurally different. In many cases chromatographic separation can be used to differentiate structurally similar molecules. Fragmentation analysis is another way to differentiate these chemistries. Examples of how accurate mass spectrometry coupled with fragmentation analysis will be presented. Utilization of a SciEx 5600 Qtof and a SciEx 4000 Q-trap to confirm structures will be compared.

AGRO 20

Accurate mass for small molecule analysis

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The advantages of mass defect- and NL-triggered data collection for work in complicated (e.g., *in vivo*) matrices, quant/qual workflows in one experiment, and data correlation for comparison of sample sources will be presented. Data will include samples from rat plasma and from the environment. Confirmation and contraindication of Phase I and Phase II metabolites including glutathione adducts by accurate mass data will be illustrated. The use of fragmentation interpretation to identify where modifications of the test drug occurred will also be shown. Using the same data, sample correlation will be used to find unique metabolites, show metabolite appearance and disappearance, and differences in extent of metabolism. Data showing sample correlation by species, by sample treatment, and by time (PK data) will be presented. Absolute and relative quantification of metabolites will also be discussed. Accurate mass full scan along with fragmentation data will be presented to illustrate structural elucidation of metabolites and impurities. Data from two compounds separated by less than 40 mDa will be presented. Software using the accurate mass, isotope pattern, and fragmentation pattern of the molecules will also be used to help confirm the assignments. This software will also search for structures corresponding to the formula using the ChemSpider database. Accurate mass screening for known and unknowns will also be shown. Environmental samples will be screened for a battery of pesticides. The MS and MS/MS data automatically generated will be searched against an accurate mass library of fragmentation data. The data will be scored by three criteria: mass accuracy, match (and reverse match) to the library's MS/MS spectra, and by retention time match (if known) to known standards. The advantages of accurate mass MS and MS/MS in pharmaceutical, medical, and environmental applications will be shown using real-life sample data coming from a wide range of sources.

AGRO 21

Metabolite identification using modern Q-TOF and Q-Orbitrap instrumentation

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The development of new agricultural chemicals requires the identification of a variety of trace level unknowns. Some of the most challenging identification problems in compound development are encountered in the area of metabolite ID. These unknowns are generally present at ultra-trace (low pg) levels, precluding their identification with NMR. In these cases, their identification must be performed using LC/MS. In regulatory metabolite ID, radiolabeled metabolites are typically profiled using conventional LC to allow the injection of sufficient material for radiochemical detection. These metabolite samples may take weeks-months to form, and must be identified rapidly to avoid jeopardizing critical registration deadlines. To utilize these precious samples most efficiently, the post-column effluent is generally split between the MS and a radioactivity detector (RAM), and the effluent from the RAM cell is collected into a 96-well plate to allow the recovery of most of the LC-fractionated sample. In our work, metabolites were generated a combination of soil, plant cell culture, and whole plant systems. These samples were analyzed using LC separations on several LC/MS systems including: 1) a Thermo LTQ-FT Ultra (LIT-FTMS), 2) a Sciex 5600 (QqTOF), and 3) a Thermo Q Exactive (Q-Orbitrap). Radiolabeled metabolites were tracked using RAM detection, and ESI ionization was combined with accurate MS, and MS/MS data acquisition on each instrument. We will discuss the application of each of these techniques in the identification of trace level metabolites produced in whole plant, plant cell culture, and soil metabolism for several agricultural chemicals.

AGRO 22

Applications of very high resolution UHPLC-MS data for metabolic fate studies of agrochemicals

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The metabolic fate of chemicals released into the environment is an important aspect of development. Metabolism in target plants of food crops, as well as metabolism in soil or animals can all be considered. Here we demonstrate the use of high resolution accurate mass UHPLC-MS for determining the metabolic fate of four common herbicides in humans.The metabolic fate for 2,4-D, dicamba, thifensulfuron, and metolachlor was determined by incubation with human liver microsomes (0.5 mg/mL microsomal protein, 1 uM and 10 uM substrate concentration, 1 hour incubation duration). Samples were analyzed by UHPLC-MS on a high resolution accurate mass benchtop orbitrap mass spectrometer after separation on a C-18 column (Accucore Polar Premium 100x21 mm, 2.6 µm). Data was acquired using a polarity switching data dependant MS^2 method for full profiling. In addition, very high resolution acquisition using 140,000 resolving power (FWHM @ m/z 200) was also acquired. Metabolites of the herbicides studied were detected by analysis of the fragmentation of all detected peaks for similarity to the starting material. Briefly, fragment ion searching uses the

accurate mass of theoretical and observed fragmentation of the parent molecule to find related metabolites in the sample acquisition and begin to determine their structure. In addition, the application of common biotransformations increases the search capabilities by allowing for the metabolic modification of search fragments. The very high resolution data acquired in the 140,000 resolution run was used to confirm the formula and/or structure assignment of metabolites. For this data, the fine isotopic pattern in the isotopes was used to confirm the presence of specific elements proposed from the A0 isotope which further increased confidence that a detected component was a metabolite.

AGRO 23

Status of GMO detection in Brazil

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Currently in Brazil, there are 33 GMO events approved for commercial use: five of soybean, eighteen of corn, nine of cotton, and one of bean. The area in Brazil planted with transgenic seeds increased from 1.2 million hectares to about 37 million hectares in the last six years. An increase of 14% is estimated in the current crop this season. This is the first season in which the planted area with transgenic crops exceeds the area planted with conventional cultivars, representing 54.8% of 67.7 million hectares according to estimates. Due to this scenario of widespread adoption of GMO technology the Ministry of Agriculture, Livestock and Food Supply increased the number of inspections conducted from 300 in 2006 to an average of 1,400 inspections in the past two years. Currently 40% of the inspections are for control of research activities and 60% are for activities with GMOs for commercial use. The supervision of GMO's intended for commercial use is mainly perfromed to verify exclusion zones (where the farmers are not allowed to plant any transgenic cotton), the rules of coexistence between the GM and non-GM corn, and the detection of unauthorized events. Basically, the monitoring involving known events is carried out by the use of strip testing specific to the GMO protein. For research and quantification of GMOs in grains, food, and feed, there are two official laboratories and seven laboratories work according to ISO 17.025:2005, which mainly use the Real Time PCR. In the last two years, the samples for laboratories increased by 600%. In the first two months of 2013, the number of samples sent equaled the total number of samples sent in 2012, focusing on research with unauthorized GMOs and GMO allowed with restrictions. In 2013, it has been planned to start GMO analyses by digital PCR.

AGRO 24

Current trends in DNA detection for biotech crops

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With the increased trend in worldwide acceptance of genetically modified (GM) crops for cultivation and increased number of approved GM events available for commercialization, it has become increasingly important to have reliable GM detection methodologies for agricultural and food industries, government regulators, and international trade organizations. Widespread acceptance of GM crops in both developed and developing countries also increased the risk of unintended GMO contamination in food and feed samples. To enable efficient GM seed product development at industrial scale and to continue detecting all GM events in the final food and feed products, more robust and reliable bioanalytical GM detection technologies will become necessary. Current GM detection methodologies are focused on either DNA or protein detection of the target GM event(s). For most DNA-based detection, the polymerase chain reaction (PCR) is the preferred method, while most protein-based detection employs enzyme-linked immunosorbent assays (ELISA) with antibodies binding the novel transgenic protein. In addition to these widely-used detection methods, there are various novel technologies developed that include use of electrochemical signals versus use of traditional fluorescent probes, use of microarray, use of isothermal chemistries with or without DNA amplification (PCR) process, and sample screening achieved at nanoscale level. Evolution and recent trend in DNA detection technologies for biotech crops will be presented.

AGRO 25

Southern-by-sequencing: Molecular characterization of transgenic events

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Characterization of event quality is important when making advancement decisions in the transgenic pipeline. Assessment of copy number, integrity of the transgene cassette, and the absence of *Agrobacterium* backbone in a transgenic plant has traditionally been accomplished by Southern Blot analysis with multiple probes and enzyme digests. This method is time-consuming and expensive and can lead to ambiguous results. We have developed a new application, Southern-by-Sequencing (SbS), that utilizes the Illumina Sequencing technology to replace traditional Southern Blot analysis. SbS is accomplished by hybridizing whole genome libraries to biotinylated probes to enrich for transgene containing sequences. The enriched libraries are sequenced on the Illumina platform to a standard sequencing depth. Sequence data is analyzed via an analysis pipeline which identifies transgene copy number, fragments, rearrangements, and *Agrobacterium* backbone contamination.

AGRO 26

New approaches in GMO detection as a solution for emerging problems

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Along with the expansion of commercial use of GM crops, some problems in GMO detection have been emerging. We present new GMO detection methods as a solution to these issues. Due to the increasing number of commercially available GM events, testing with using a series of conventional PCR methods has become labor-intensive. To solve this problem, we developed a real-time PCR array method for comprehensive GMO detection. In this method, genomic DNA extracted from an agricultural product is analyzed using various qualitative real-time PCR assays on a 96-well PCR plate, targeting individual GM events, recombinant DNA segments, taxon-specific genes, and so on. Additionally, a comparative analysis with the data and publicly available information on GM crops approved in Japan allows us to assume the possibility of unapproved GMO commingling. We established the information handling process and then developed a Microsoft Excel spreadsheet application, Unapproved GMO Checker, which enables the easy assumption of unapproved GM crop commingling. Because of the increasing use of maize hybrids with GM stacked events, the commonly-used bulk sample methods for PCR quantification of GM maize in non-GM maize are prone to overestimate the GMO content, compared to the

actual weight/weight percentage of GM maize in the grain sample. As a solution for this, we designed and assessed a group testing strategy in which the GMO content is statistically evaluated based on qualitative analyses of multiple small pools of kernels. This approach enables the GMO content evaluation on a weight/weight basis, irrespective of the presence of stacked-event kernels. To enhance the method's user-friendliness in routine application, we devised an easy-to-use PCR-based qualitative analytical method comprising a sample preparation step in which maize kernels are ground in a lysis buffer and a subsequent PCR assay in which the lysate is directly used as a DNA template.

AGRO 27

Digital highly multiplexed gene-expression studies in plants: Mapping whole biological pathways in space and time using optical barcoding (nCounter Technology)

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Technologies developed by Seattle, WA-based NanoString Technologies that provide simple, automated, highly-multiplexed, digital profiling of single nucleic acid molecules will be described. The methodology is based on an optical digital molecular barcoding technology invented at the Institute for Systems Biology (ISB) under the direction of Dr. Leroy Hood (Nature Biotech 2008, 26:317-25). Up to 800 distinct nucleic-acid targets can be digitally counted in samples that range from single cells (10 pg input RNA) to complex plant tissue lysates (~ 100 ng total RNA). While digital gene expression has been extensively utilized in human studies, plant studies are rapidly expanding. Much of this growth is driven by the need in plant studies for highly precise and accurate gene expression that often must be followed in detail in both space and time. nCounter technology allows the examination of multiple plant biochemical pathways (800 targets, ~ 18 full pathways) with a precision of ≤ 20%. NanoString technology directly measures RNA-targets (no amplification) without the requirement of making cDNA or amplifying the cDNA, greatly simplifying the work-flow associated with gene-expression. Additionally, all of the reagents required to perform the study are pre-measured and pre-dispensed (all under GMP conditions) and utilized in a completely automated robotic process. Up to 12 samples (or 4 X 12 samples multiplexed) are measured per 1" x 3" cartridge, generating ~ 1 to 2 million nucleic acid reads per sample. Being completely digital, these gene-expression reads are directly comparable to and with Next-Gen-Sequencing (NGS) RNA-seq reads. In additional to counting RNA-targets, DNA-based target counting allows for copy-number-variations (CNVs), CHIP-String (analogous to CHIP-Seq), and gene-fusions (and RNA-fusion transcripts), to be measured in the same multiplexed manner. Unique features of recent plant-studies from peer-reviewed nCounter papers will be highlighted.

AGRO 28

Use of QuantiGene and QuantiGene plex assays for direct RNA or gDNA copy number variation analysis direct from sample lysates: An introduction to the branched DNA technology from Affymetrix / Panomics Solutions

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The Affymetrix branched DNA technology, known commercially as QuantiGene®, has been used for several years now in the plant biotechnology industry. Affymetrix has developed assays for direct RNA or gDNA copy number variation analysis using either purified RNA or DNA or sample lysates of plants, bacteria, yeast, whole blood, tissues, cells, and formalin-fixed, paraffin-embedded tissues. Papers using the single-plex technology have frequently been published since 1999. This linear assay, which allows for the detection of percent changes in gene expression, involves capturing the RNA directly onto an immobilized surface (plate) and then building a signal using a series of oligonucleotide hybridizations (400-fold signal amplification). This is all completed using numerous gene specific probe sets. First, capture extender (CE) probes hybridize to the Universal Capture probes chemically bound to the plate. Then, label extender (LE) probes hybridize to the RNA and become a platform for the bDNA amplifier. A third type of probe sets called blocking probes (BP) are used to help stabilize the RNA. In 2005, the first paper had been published using the QuantiGene® Plex 2.0 technology. This version of the assay is a Luminex® bead based assay which now allows for the true multiplex measurement of 3-80 different genes at one time in a single sample well. Affymetrix does a full QC to ensure there is no cross hybridization between targets. For an example of this technology published, please see Qi et al., *J Biol Chem*. 2012; 287:31482-93.

AGRO 29

Novel reference plasmid DNA for detection of genetically modified rice

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Rice is one of the most important food crops in the world. In rice, genetically modified (GM) technology has been used to confer herbicide tolerance and pathogen or insect resistance characteristics. Rice is a leading crop in China, and China is invested heavily into research on GM rice. By the end of 2012, at least 250 transgenic lines have been developed. Two varieties of Bt rice Shanyou 63 and TT51-1 approved for biosafety in 2009 are now undergoing extensive and rigorous field trials. With global expansion in the area of GM crops cultivated, the likelihood of contamination of non-transgenic varieties with GM products is increasing. To monitor the presence of GM rice ingredients in GM crops and foods, a reference plasmid of GM rice was constructed for qualitative and quantitative detection. Plasmid DNA (pBJGMM01) containing the elements and endogenous reference genes is used as real time quantitative PCR (qPCR) calibrant and positive PCR control. The pBJGMM01 plasmid was constructed based on pUC57 that includes the fragments of the cauliflower mosaic virus 35S promoter (CaMV 35S, 195 bp), the *Agrobacterium tumefaciens* nopaline synthase terminator (NOS, 180 bp), bar gene (430 bp), ubiquitin gene (314 bp) and Hyglomychl Phosphtobamfemse gene (hpt, 381bp) for elements gene detection; the fragments of sucrose phosphate synthase gene (sps, 287 bp) and phosphoenolpyruvate carboxylase gene (pepc, 271 bp) which enable positive control PCRs. The pBJGMM01 could be able to detect the GM rice lines of 97% according to statistics. The preparation, homogeneity, stability, and commutability of pBJGMM01 were assessed. To verify the correct copy number ratio in the plasmid, the sequencing data were generated from three independent laboratories and performed by digital PCR for batch characterization. The uncertainty was evaluated by the sources of homogeneity, stability, and batch characterization.

AGRO 30

Inline, ultra high-throughput, Array Tape™ based end-point nucleic acid detection: Novel DNAble v2.0 isothermal amplification system

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EnviroLogix' proprietary next generation DNAble v2.0 chemistry can rapidly and specifically amplify both RNA and DNA targets with single base resolution a billion-fold in 5-10 minutes at a single and constant temperature with results rivaling qPCR. Unlike PCR, DNAble can amplify a target sequence from a crude sample preparation. Assays can be adapted from single reaction point of care lateral flow test strips to fluorescent signal based assays that utilize our two, eight, and sixteen test DNAble portable systems. Standard real-time PCR instruments can run both 96 and 384 well tests for the next level of testing. Expansion of capability into ultra high-throughput applications requires unique instrumentation and chemistry solutions. Leveraging the DNAble chemistry, the Douglas Scientific Nexar system optimized for isothermal amplification and Array Tape™ has been successfully developed to include automating sample handling, master mix addition, array sealing, array incubation at a constant temperature, and fluorescence detection in a continuous reel-to-reel process flow to maximize throughput and reduce costs. This system can process over 122,880 samples per 8 hour day. Examples of validated HTP assays using the Nexar system will be presented and include GMO's from soy and maize.

AGRO 31

Novel DNAble v3.0 isothermal amplification platforms for GMO testing on-site at the grain silos and in the testing laboratory

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EnviroLogix' third generation of its proprietary DNAble assay technology can rapidly and specifically amplify both RNA and DNA targets with single base resolution a billion-fold in 5-10 minutes at a single and constant temperature with results matching the quality of qPCR. DNAble v3.0 can amplify a target sequence from an unpurified, crude sample produced simply by grinding a punch from a plant leaf in an extraction buffer and adding an aliquot to a DNAble reaction mix after heating the extract for 5 minutes. The same process can be performed with ground seed. We will show that the DNAble v3.0 assay platform is extremely flexible in regard to detection platforms, reaction volumes (1.6 – 50 mL) and applications. They can be adapted for Point-of-Care situations using end point detection on lateral flow test strips or end point fluorescent signal detection that utilize our eight and sixteen test DNAble portable systems. In addition, standard real-time PCR instruments can run both 96 and 384 well plate tests with quantitative detection in real (short) time for the next level of analysis. We will demonstrate results of DNAble assays that exhibit sensitivity down to 0.1% GMO in a background of 99.9% conventional seed. GMO assays will be discussed that show a positive target amplification result only when the amount of GMO in a conventional seed background is detected at 20% or more. Furthermore, we will demonstrate the conversion of pre-validated TaqMan qPCR assays directly into DNAble v3.0 molecular beacon assays, therefore eliminating the need for new candidate assay screening and validation for HTP GMO trait analysis in plant breeding programs.

AGRO 32

Robust built-in spray drift reduction technology for pesticide formulations

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Pesticide spray drift is the physical movement of a pesticide through the air, at the time of application or soon thereafter, to a site other than the intended target. Spray drift, can be an undesirable side-effect of pesticide application and remains a concern for possible environmental effects and property damage. Therefore, products and technologies that reduce and minimize spray drift or off target movement have become increasingly desirable, and sometimes essential in certain applications. This paper focuses on reduction of spray drift through formulation innovation. Spray nozzle selection and application parameters are critical to reduce the spray drift in pesticide application, yet the physical properties of the spray solution can have significant effects on the spray droplet size and distribution. Our research demonstrates that the potential for drift can be reduced by incorporating an oil-in-water emulsion in the spray solution. Two novel 2,4-D herbicide formulations with built-in low drift technology are described. Both 2,4-D herbicide formulations are aqueous-based salt concentrates that produce a spontaneous emulsion upon dilution in a spray solution. The spray drift reduction performance is demonstrated by substantially lowering the fraction of driftable fines (spray droplets ≤ 150 µm) in spray application. The effect of tank mix conditions (such as ammonium sulfate, drift reduction additive, and additional glyphosate salt product) on the performance of emulsion based spray solutions will be discussed.

AGRO 33

Interfacial effects on the performance of emulsion-based antidrift spray solutions

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Emulsion-based spray solutions have been shown to lower the fraction of fine particles produced in agricultural sprays which are prone to drift. Despite the demonstrated benefit of these systems for minimizing off-target spray movement, the actual mechanism by which emulsions suppress fine droplet formation is not well understood. In the present study, the interface of a series of methyl soyate emulsions was modified by incorporating a crosslinked polyurea capsule wall of varying thicknesses (0-50 nm) to impart rigidity at the droplet interface. Three different surfactant systems were used in the emulsion preparations to eliminate the possibility that the observations were limited to a specific system. The resulting emulsions were evaluated for their propensity for reduction in driftable fines produced during spraying. The measured driftable fines were seen to increase with crosslinked polymer wall thickness. The increase in fines with increasing interface rigidity implicates emulsion droplet deformability as a key factor in the spray sheet breakup mechanism, consistent with earlier proposals that shear induced droplet deformation is a necessary precursor for the early sheet breakup phenomenon to occur.

AGRO 34

Agricultural spray tank mixing

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During pesticide applications, constant mixing of the pesticide solution in the spray tank is critical for maintaining a homogenous solution to achieve uniform application. There are two major mixing mechanisms in commercial spray tanks, sparge tube mixing and jet nozzle mixing. Pumped jet mixers are established operations to blend miscible liquids in vertical cylindrical tanks. More than 50 years of studies and practice provide the proven guidelines for mixing operation in vessels with diameters ranging from 2 to 118 ft. A simple blend time correlation suffices for many jet mixing problems in vertical cylindrical tanks. However, the correlations have been shown to under-predict mixing times in horizontal cylindrical tanks by a factor of three or more. Mixing needs in unconventional tank geometries such as rails cars and agricultural spray tanks are frequently encountered by chemical industries. Agricultural spray tanks pose a unique challenge in that the shape of the tank is primarily designed to fit the back of a tractor and the pump system is coupled to the sprayers. Estimation of blend time and mixing efficiency in such tanks is of great importance in optimizing the mixing time for formulated products. To date, designing a jet mixing system with existing equipment such as tank and recirculation pump can be achieved only through CFD (computational fluid dynamics) analysis. In this study, Star CCM+7.02 is first used to validate the throughput of a ¼" HYPRO 3371 jet nozzle against experimental data. The blend characteristics of a spray tank mounted on a John Deere 4730 tractor with dual horizontal HYPRO jets are estimated computationally and the different mixing zones in the tank are identified for spray tank mixing design optimization.

AGRO 35

Improvements in range and pasture formulations

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Dow AgroSciences continues to lead the industry in bringing innovative solutions to the range and pastures weed control market. Dow AgroSciences is devoted to continuously improving the sustainability of its products through improved environmental profiles, new active ingredients and mixtures, and innovative formulations that exceed customer and regulatory expectations. The product design criteria to develop the next generation of range and pastures products devoted special priority to provide effective bio-efficacy with minimum toxicological and environmental impact while satisfying customer needs. Case study products are presented to exemplify how an innovative approach in crop protection formulations can assure consistently high standards in bio-efficacy while delivering added value attributes like better handling, reduced odor, and better label classification, as well as a significant reduction in potential emissions of volatile organic compounds (VOCs). Increased loading leads to an added advantage of a reduction in the amount of packaging material delivered to the market.

AGRO 36

Effects of nozzles and drift reduction agents on droplet size distributions of dicamba and glyphosate mixtures

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A series of wind tunnels studies were conducted to determine the effects of nozzle selection, nozzle, orifice size, spray pressure, and formulation composition on spray droplet distributions of dicamba/glyphosate mixes. The first study was conducted at the University of Queensland, Australia in 2012 and included 14 nozzles, three orifice sizes for each nozzle (03, 04, and 05), two spray pressures, and a total of four dicamba/glyphosate mixes, including two tank mixes (TM1, TM2) and two premixes (PM1, PM2). Spray pressures were adjusted to correspond to application volumes of 10 and 15 GPA. Droplet size distributions for all possible combinations of the four factors were measured using a laser in a wind tunnel. The data were statistically analyzed using a full factorial response surface model. The application parameters of nozzle selection and spray pressure had the largest effect on droplet size of the four primary factors evaluated in the model. Percent driftable fines (% volume < 150 µm) was primarily influenced by nozzle and pressure with nozzle selection being the most critical factor for reducing driftable fines. A follow-up study conducted at the University of Queensland in 2013 evaluated the effects of drift reduction agents (DRAs) on droplet size distributions of dicamba/glyphosate mixes using a subset of nozzles evaluated in the 2012 study. The effects of DRAs on droplet size distributions for dicamba/glyphosate mixtures for various nozzles will be presented.

AGRO 37

Field measurement of pesticides using passive, active, and laser sampling systems

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A field study was conducted in California to measure the emission of several active ingredient herbicides from a sprayed stubble field across a 6 hour period following initial spray application. Three different droplet size spectra were applied to separate fields. The passive samplers were petri dishes in both upward and inverted positions. The active samplers were air samplers with polyurethane foam sorbent sample tubes with a combined flowrate of 15 L air per minute. The laser system was a Phase Doppler Inteferometer sampling in two dimensions. The samplers were located in the center of the sprayed fields to sample airborne spray flux concurrently. Sampling media were collected and refreshed every few hours. An analytical laboratory measured the amount of each active ingredient sampled as a percentage of the application rate to the fields. The study results will be discussed with respect to the comparative performance of the sampling systems.

AGRO 38

Glyphosate is not the herbicide it used to be: A North American perspective

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Glyphosate is a special chemical, with the combination of low mammalian toxicity, favorable environmental profile, and broad spectrum control imparting a uniqueness to this herbicide. However, it was the development of glyphosate-tolerant crops that resulted in wide-scale adoption of glyphosate as a foundational herbicide over hundreds of millions of hectares in the Americas. For several years in the late 1990s, weed control was highly effective, economical, and simple. However, with this massive selection pressure, the evolution of weeds no longer controlled by glyphosate was inevitable, and this has occurred in numerous locations in several genera. The major agronomic examples of these weeds include *Conyza canadensis*, a winter annual that is problematic in no-tillage production systems, and *Amaranthus palmeri*, a tremendously competitive summer annual that is a growing problem in the southern United States. Incomplete control from glyphosate has also been reported on species from the *Sorghum*, *Ambrosia*, *Conyza*, and *Amaranthus* genus. This talk introduces the important topic of herbicide resistance in today's American agriculture. Issues discussed include comprehensive surveys of the occurence of herbicide resistance, how farmers are responding to this change, and future opportunities and responses to manage this problem.

AGRO 39

Surveys of herbicide resistances in Missouri waterhemp populations with a focus on correlations between field management practices and glyphosate resistance

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Herbicide-resistant weed populations have evolved rapidly in response to the selection pressures imposed upon them in current agricultural production systems. Specifically, in the Midwest the number of acres affected by glyphosate-resistant (GR) weeds has increased dramatically in recent years due to the rapid adoption of GR crops and the extensive use of glyphosate. One of the GR weed species that is currently infesting millions of corn and soybean acres in the Midwest is waterhemp (*Amaranthus rudis* Sauer). In Missouri, we have conducted a number of field surveys of waterhemp populations 1) to determine the frequency and distribution of glyphosate resistance in waterhemp, 2) to determine the percentage of waterhemp populations with multiple herbicide resistances, and 3) to determine if there are any field management factors that can serve as indicators of GR in future waterhemp populations. In a 2008-2009 field survey, glyphosate resistance was confirmed in 99 out of 144, or 69% of the total waterhemp populations sampled. These resistant populations occurred across 41 counties of Missouri. More recently, the incidence of multiple herbicide resistances to glyphosate, to 2,4-D, and to HPPD-, ALS-, and PPO-inhibiting herbicides is being determined in approximately 180 different Missouri waterhemp populations collected in 2012. Based on the data collected from each sampling site in the 2008-2009 survey, soybean fields confirmed with GR waterhemp were more likely to be free of other weed species, were more likely to occur where soybeans were continuously cropped, were more likely to occur where glyphosate was the only herbicide applied for several seasons consecutively, and were more likely to show obvious signs of surviving herbicide treatment.

AGRO 40

Iowa survey of herbicide resistances in common waterhemp including glyphosate and other herbicide groups

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Evolved herbicide resistance in common waterhemp (*Amaranthus tuberculatus*) has been a serious issue in Iowa agriculture when this weed first began to appear as a major production problem in soybeans in the 1980's. At that time, ALS inhibitor herbicides (Group 2) were applied to a majority of the corn and soybean acres across the Midwest and common waterhemp populations quickly evolved resistance. In the 1990's, concerns focused on the inevitability of evolved resistance to glyphosate (Group 9). The first glyphosate-resistant common waterhemp populations were identified coincidentally in Badger and Everly, Iowa in 1997. However, glyphosate resistance in common waterhemp was generally scattered in fields and had not become a major concern to agriculture. This changed as the adoption of glyphosate-based corn and soybean production systems became the dominate practice. It was clear that common waterhemp had become the major concern in Iowa soybean production and ultimately in corn production. The more recent identification of common waterhemp populations with evolved resistance to auxinic herbicides (Group 4) and the HPPD inhibitor herbicides (Group 27) as well as the historic resistance to the PSII inhibitor herbicides (Group 5) and PPO inhibitor herbicides (Group 14) leaves few herbicide options for the control of common waterhemp, particularly for postemergence strategies. In order to assess the extent of herbicide-resistant common waterhemp populations in Iowa, a project was initiated in 2011 with support from the Iowa Soybean Association. This project supplements a study conducted in 2008 where resistance to glyphosate was detected in 16% of approximately 220 Iowa common waterhemp populations collected arbitrarily.

AGRO 41

Weed resistance in Arkansas: One crisis averted another begins?

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Since 2002, six weeds (horseweed, common ragweed, giant ragweed, Palmer pigweed, Johnsongrass, and Italian ryegrass) have been confirmed to be resistant to glyphosate in Arkansas. Of these, horseweed and pigweed have by far had the greatest impact on farming practices. In addition to glyphosate resistance, pigweed populations also exist that are resistant to the ALS and dinitroanaline families of chemistry. Ryegrass populations exist that not only tolerate glyphosate but also ALS and certain ACCase chemistries, causing difficulties in not only spring burndown, but also wheat ryegrass control. Glyphosate resistant crops were grown on approximately 100 percent of the corn, cotton, and soybean acres in Arkansas by the year 2008. In 2010, it was estimated that most all cotton acres and at least 50% of the soybean acres had become infested with glyphosate resistant Palmer amaranth. Due to resistance management practices that were implemented statewide from 2009-2012, a true crisis in weed control has been averted in the state. Although pigweed is still both the most common and troublesome weed in both soybean and cotton, it is relatively under control. Many acres of cotton still require hand weeding for complete control, and farmers do still struggle in soybean with added input costs and time management. Pigweed control options and current management strategies will be discussed. In addition to pigweed in row crops, a

similar resistance situation is evolving in rice with barnyardgrass. This speaks to an overall greater concern with the lack of discovery of new herbicide modes of action and the bottlenecks that it creates for certain cropping systems, where only very specific herbicide recommendations will actually control weeds, which can inevitably lead to more resistance.

AGRO 42

Glyphosate-resistant weeds: Lessons learned in Tennessee

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There are six confirmed glyphosate-resistant (GR) weeds in Tennessee. Horseweed (marestail) and Palmer amaranth (pigweed) are now an issue on virtually every row crop acre in Tennessee. Horseweed was the first of these to show glyphosate resistance in 2001. Just four years later, Palmer amaranth was confirmed to be resistant to glyphosate and has in that short time become the biggest weed problem in the state. The effect GR horseweed had on the state of Tennessee was to increase producer costs and reduce conservation tillage acres. Management of this weed cost Tennessee producers an additional $20/acre and reduced conservation tillage acres 20% by 2004. These conservation tillage acres were mostly regained as soybean and cotton producers became comfortable with alternative burndown programs in recent years. Though GR horseweed was a problem, GR Palmer amaranth is proving to be the game changer with respect to weed control in Tennessee. Palmer amaranth is one of the most competitive plants in the world as it can grow 5 cm per day and in Tennessee has overwhelmed soybean fields to the point that they cannot be harvested effectively. Soybean producers have found that if they cannot control GR Palmer amaranth prior to it reaching a height of 7 cm, they cannot control it with any herbicide. As a result, in fields where a pre applied herbicide has failed, even with a good crop stand, the field is often tilled and replanted. With the unprecedented selection pressure now on glufosinate and PPO herbicides in controlling Palmer amaranth, the concern shifts to how long before resistance to these herbicides develops. The introduction of the new auxin tolerant traits in soybeans and cotton is slated for 2015. These new technologies should help alleviate some of this selection pressure on glufosinate and the PPO herbicides.

AGRO 43

Complexity of weed management over the next five years

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The era of glyphosate-resistant crops enabled, arguably, the most simplified and robust weed management system ever implemented by producers of major row crops. However, current trends over the next five years will necessitate the adoption of much more complex weed management tactics as no single technology or practice will translate into broad-scale effectiveness. More specifically, the complexity of weed management will potentially involve the pervasiveness of weeds with resistance to multiple herbicide groups, the selection of crop seed from several herbicide-resistant trait packages, the increased use of diverse herbicide chemistry, and an increased awareness to prevent off-target movement of herbicides. Glyphosate-resistant weed species currently infest millions of acres in the major crop production regions of the US, and the spread of resistance is anticipated to continue if altered management tactics are not implemented. The private industry sector anticipates the regulatory approval and commercialization of herbicide-resistant crop traits over the next five years, such as resistance to the herbicides 2,4-D, dicamba, isoxaflutole, and mesotrione with various combinations of these traits with resistance to glyphosate and glufosinate. Thus, weed management options will be driven, or limited, by the seed selected for planting well in advance of the weeds emerging in the fields. The integration of multiple herbicides with soil residual or foliar activity will require knowledge of herbicide site of action groups, soil factors, crop rotation restrictions, herbicide interactions, and optimal foliar application techniques that optimize herbicide efficacy while reducing the potential for off-target movement. Thus, the glyphosate-resistant crop technology that allowed for the most simplistic method for controlling weeds over the past 15 years will be followed by complex decisions on seed selection, herbicide combinations, application methods, and herbicide stewardship over the next five years.

AGRO 44

Herbicide resistance by weeds: Its effects on and off the field

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Resistance to herbicides has been a reality for several decades. In the past, products with new modes of action entered into the market and provided a ready fix for problems that arose. Beginning in the mid-to-late-1990s, crops containing genetically-engineered glyphosate resistance exploded onto the market and rapidly became the dominant and then the only weed control measure in the majority of American cotton, soybean, and corn crops. The number of alternative products used for weed control dropped significantly and resulted in a high level of selection pressure for resistance. With the advent of resistance to glyphosate in these crops, the effectiveness of this exceptional tool for weed control has been severely impacted. This development has, in some cases, rekindled the need for alternative weed control methods. For example, in Southern cotton fields, hand-hoeing is being implemented at considerable cost with the express purpose of reducing the contribution of single, escaping resistant weeds to the soil weed seed bank. Agriculture is at a crossroads with few new products in the pipeline and none with new modes of action foreseeable in the near future. Opportunities exist for new chemical weed control solutions, but they must pass ever higher hurdles for weed control and in their toxicological environmental profiles. Finding new solutions is not easy. We must preserve all the current tools while searching for new ones.

AGRO 45

New tools for sustainable management of herbicide resistant weeds: The Enlist™ Weed Control System

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Herbicides are essential to today's high-production agriculture, and in many areas, herbicide-tolerant (HT) crops broaden the utility of these products. Since the mid 1990s a dominant HT system has enabled widespread use of glyphosate across multiple crops. However, the continuous use of glyphosate without accompanying resistance management best practices has led to an increase in glyphosate-resistant weed species that threatens the future use of glyphosate and the benefits it has enabled. Dow AgroSciences is developing the Enlist™ Weed Control System which is based on a new family of herbicide tolerance traits, innovations in herbicide formulations, and novel approaches to technology stewardship. This system will add greater diversity to weed management programs

and help sustain the gains made with glyphosate-tolerant crops by enabling more flexible use of an innovative form of 2,4-D and other herbicides in maize, soybean, and cotton. Field studies have confirmed >90% control of a wide range of weed species (including many biotypes that are resistant to glyphosate) with a combination of a new 2,4-D plus glyphosate. Crops containing Enlist™ traits can withstand over twice the amount of 2,4-D plus glyphosate required for weed control with no significant impact on yield. New weed management technologies such as Enlist™ will require proper stewardship, including resistance management best practices, to ensure they remain viable over a long period of time. Effective resistance management programs must be based on scientific principles as well as compatibility with established production systems. Factors influencing the development of best management practices will be discussed. (™*Trademark of The Dow Chemical Company ("Dow") or an affiliated company of Dow. Regulatory approvals are pending for the Enlist™ herbicide solution and crops containing Enlist™ herbicide tolerance traits. The information presented here is not an offer for sale. Always read and follow label directions. ©2013 Dow AgroSciences LLC)*

AGRO 46

HPPD-inhibitor herbicide resistance in the USA: A Syngenta perspective

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Over the past 3 years, tall waterhemp (*Amaranthus tuberculatus* Moq. Sauer) resistance to 4-hydroxyphenyl-pyruvate dioxygenase (HPPD) inhibiting herbicides has been confirmed in Illinois, Iowa, and Nebraska seed corn production fields. Resistance to HPPD-inhibiting herbicides in Palmer amaranth (*A. palmeri* S. Wats.) has also been reported in Kansas. These populations are also resistant to other herbicides with different mechanisms of action (e.g., atrazine), and can therefore, be considered multiple-herbicide resistant populations. The existence of these HPPD-resistant populations illustrates the propensity of different species within this genus, to evolve resistance to HPPD-inhibitors, in addition to other mechanisms of action. The evolution of HPPD-inhibitor resistance in these seed corn production fields has been attributed to the limited diversity of cultural practices and of mechanisms of action of herbicides used, necessitated by the sensitivity of inbred lines to herbicides that are more widely available for use in field corn production. Nevertheless, this development is an early warning of potentially more widespread occurrences. In common with resistance in other herbicides, the risk of HPPD-resistance development is high if there is reliance on the exclusive use of HPPD-inhibiting herbicides for weed control, particularly in species with high genetic diversity and which are obligate out-crossers, such as *A. tuberculatus* or *A. palmeri*, in which resistance to other herbicide mechanisms of action has already evolved. Considerable resources have been employed in research to understand the mechanism of resistance and to assess the probability of evolution of further resistance to HPPD-inhibitors in waterhemp. In addition, research continues to explore the options for managing this issue from both proactive and solution-based approaches, in corn and soybean production systems. A diverse approach, which includes the use of multiple mechanisms of action and other methods of weed management, is critical to the sustainable use of HPPD-inhibiting herbicides.

AGRO 47

Strategies for sustainable weed management

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Weeds continue to evolve as agriculture places selection pressures on them. Weeds have shifted towards annual species in response to traditional tillage and towards shallow-emerging species with reduced tillage. From the 1960's to 1980s, species shifted when selective herbicides controlled some, but not other species. More recently, changes in growth habit (such as germination time) and herbicide resistance have occurred within species. To date, there are approximately 400 instances of resistance with species and herbicide modes of action groups (http://www.weedscience.com/Graphs/ChronologicalIncrease.aspx). With Monsanto's Roundup Ready systems, resistance in troublesome species such as *Amaranthus palmeri*, *Amaranthus rudus*, and *Conyza canadensis* has required proactive changes to weed control programs. With consultation from the academic community and other manufacturers, Monsanto launched the Roundup Ready PLUS platform which is based on Best Management weed control recommendations that include the use of residual herbicides and additional modes of action with glyphosate. The PLUS platform also provides growers with incentives to use residual and alternative MOA herbicides. Additionally, Monsanto and other companies are developing new trait-based herbicide systems that will allow new modes of action to be used in crops where they were not previously available to improve weed control further and to manage and prevent resistance. Currently, Monsanto is developing soybean and cotton with resistance to dicamba, a well established, broadleaf-controlling herbicide. Monsanto is also working to develop other herbicide traits and herbicides. The entire agricultural industry needs to remain vigilant, continue to develop weed control programs with diverse herbicide modes of action, and to recommend diverse cultural and herbicidal methods. However, growers are successfully adjusting their weed control programs with existing technology, controlling weeds, and maintaining crop yields.

AGRO 48

Role of ADME studies in veterinary drug development and registration

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ADME (absorption, distribution, metabolism, and excretion) studies play an important role in developing and registering veterinary drugs for use in animal health. Such studies assist in selecting formulations, determining the fate of the active ingredients, and supporting the safety or efficacy of the drugs. Regulatory agencies require information about ADME before a product can be approved for use. For food producing animals, human food safety also must be established. Antibiotics, antiparasitics, and analgesics provide examples of product classes that maintain or enhance the well-being of animals and for which ADME forms a key component in their development and registration.

AGRO 49

Determination of hormone residues in rainbow trout muscle using liquid chromatography-tandem mass spectrometry

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Hormones are used in food-producing animals to increase feed efficiency, to promote animal muscle development, and to improve meat quality. With the growing number of seafood products imported into the United States, analytical methods are needed to measure multiple hormone residues in seafood products. Our laboratory is developing an analytical method suitable for the simultaneous detection of sixteen conjugated hormonal drugs in rainbow trout muscle at 1 ppb. The sixteen hormones include testosterone, *cis*-testosterone, progesterone, 19β-nortestosterone, 17α-methyltestosterone, trenbolone, melengestrol acetate, megestrol, 17β-estradiol, 17α-estradiol, ethynyl estradiol, zeranol, estriol, dienestrol, diethylstilbestrol, and hexestrol. The method involves overnight incubation with glucuronidase to deconjugate the hormone glucuronides. After deconjugation, the analytes are extracted from fish muscle tissues followed by sample cleanup using a solvent partition and two solid-phase extractions. An atmospheric pressure chemical ionization (APCI) probe coupled with mass spectrometry analysis in a rapid polarity switching mode is used to quantitate both positively and negatively charged hormones. After method validation, we will use the method to assay muscle tissues derived from dosed rainbow trout. By comparing the hormone levels in dosed muscle tissues analyzed with and without enzymatic digestion, we attempt to address the question whether enzymatic digestion is needed for hormone analysis in rainbow trout muscle tissues.

AGRO 50

Pharmacokinetics and synovial fluid/plasma drug ratios of firocoxib and phenylbutazone in horses after repeated drug administration

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Synovial fluid drug concentrations are considered an important determinant of clinical response to NSAIDs used for joint pain and are likely to reflect blood/plasma concentrations because the synovial capsule is highly vascularized. To conform better with therapeutic conditions a study was conducted that evaluated synovial fluid and plasma drug concentrations after repeated drug administration rather than after a single dose. Results indicated that drug concentrations in synovial fluid increase with increasing plasma drug concentrations. For both drugs, average synovial fluid drug concentrations (Css,min) were >50% of the plasma drug concentrations (Css,min) at steady state. After 8 days of treatment, the average firocoxib plasma Css,min was 70.7 ± 22.9 ng/mL and the corresponding synovial fluid Css,min was 44.1 ± 20.0 ng/mL. The average phenylbutazone plasma Css,min was 772 ± 434 ng/mL and the synovial fluid Css,min was 380 ± 151 ng/mL. The depletion of drug from synovial fluid and plasma followed a similar exponential decay.

AGRO 51

Validation of an LC-MS/MS regulatory method to determine and confirm three tetracyclines (oxytetracycline, chlortetracycline, and tetracycline) in bovine kidney, liver, and muscle

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Oxytetracycline (OTC), tetracycline (TC), and chlortetracycline (CTC) are approved to treat bacterial infections in cattle. A tolerance has been established for the sum of the three tetracycline residues in bovine tissue as 12 ppm in kidney, 6 ppm in liver, and 2 ppm in muscle. The current regulatory method for these antibiotics is an obsolete microbiological assay which is non-specific, time consuming, and cannot provide information on the amount of drug present when multiple drugs are used to treat an animal. A faster, specific LC-MS/MS method for the determination and confirmation of the three tetracyclines in bovine tissues (kidney, liver, and muscle) has been validated according to relevant FDA guidelines. The new method involves performing liquid and solid phase extraction. Bovine tissue samples are chromatographically resolved with a Polar-RP Synergi column and analyzed by triple quadrupole tandem mass spectrometry. The new method was bridged to the existing microbiological method in kidney, the target tissue. Bridging involves testing samples from animals treated with the drugs to determine relationship between the analytical responses. This chemical method will replace the microbiological method for regulatory testing and has the potential to be expanded into a multiclass determinative and confirmatory method. In addition to the work that had demonstrated the applicability of the method to analyze each of the tetracyclines separately in both fortified and incurred samples, we produced incurred samples with the three simultaneously dosed tetracyclines to further validate the performance of this method.

AGRO 52

Identification of a novel protein in rat bile that associates with POPs

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Persistent organic pollutants (POPs) are of concern because they are toxic and possess an inherently low level of metabolism in most organisms. Due to their lipophilicity, POPs deposit into lipophilic stores within the body with very long half-lives. Elimination of POPs requires transport through the aqueous media of blood, bile, and/or urine. We have previously confirmed that proteins like serum albumin, α2u-microglobulin, and major urinary protein are carriers of POPs within blood and urine in mammalian systems. The goal of the present research was to isolate and to identify potential carriers of POPs in rat bile, which may facilitate the excretion of POPs into the feces. In quantitative protein binding studies conducted on rat bile collected following dosing with radiolabeled dioxin or brominated flame retardant congeners, an 84.8 kDa protein was identified that associated with the administered POPs. Tandem mass spectrometry of the bile protein tryptic fragments yielded sequence data that allowed the identification of this protein as the secretory component (SC) of polyimmunoglobulin receptor (PIGR). Equimolar doses of the POPs resulted in differential sorption to SC, suggesting a specificity of interaction. PIGR is an integral protein which mediates transport of dimeric IgA immunoglobulins across epithelial cells, and SC is its extracellular domain. Release of IgA into the epithelial lumen is accompanied by complexation with

the SC of PIGR, which is thought to protect the IgA from degradation. The results of our studies demonstrate that, consistent with our hypothesis, POPs do associate with biliary proteins, which may facilitate their elimination. However, based on the known function of PIGR, we additionally hypothesize that internalization of POPs via PIGR may represent a portal of entry into select organs, in particular mucosal tissues.

AGRO 53

Determination of penicillin-G procaine in kidney, muscle, serum, and urine of heavy sows after intramuscular administration

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The USDA Food Safety and Inspection Service (FSIS) recently adapted the use of the Charm Kidney Inhibition Swab (KIS) test for screening antibiotics on-site, along with a LC-MS/MS method for confirmation of KIS-positive samples. A study with 126 heavy sows (227 ± 31 kg) dosed intramuscularly with penicillin-G procaine at 5x the label dose (33,000 U/kg bw) for 3 consecutive days using 3 administration patterns was completed to determine if the 15-day withdrawal period recommended by Food Animal Residue Avoidance Databank (FARAD) is sufficient for swine. Urine and serum were tested to determine if they could be an alternative for ante mortem screening. Sows were slaughtered at 5, 10, 15, 20, 25, 32, or 39 withdrawal days and samples collected (muscle, kidney, urine, and serum). Tissues were first screened for penicillin-G residues using the KIS test, and subsequenstly penicillin-G residues were confirmed by LC-MS/MS following the FSIS method CLC-BLAC.03 and a modified method (M. Apley, unpublished report). Method limits of quantification are 6.1 ng/g, 2.4 ng/g, 4.1 ng/mL, and 5.0 ng/mL for kidney, muscle, urine and, serum, respectively. Method limits of detection are 1.8 ng/g, 0.7 ng/g, 1.1 ng/mL, and 1.5 ng/mL for kidney, muscle, urine, and serum, respectively. Skeletal muscle residues depleted most rapidly, whereas kidney and urine residues depleted slower. The residue data from the skeletal muscle supports the 15-day withdrawal period recommended by FARAD, however the kidney data suggests a longer withdrawal period is needed. Kidney is the more appropriate on-site tissue to screen for penicillin-G residues than muscle; urine is appropriate for pre-slaughter screening for penicillin-G residues. Collectively, the data suggest that a 15-day withdrawal period for penicillin-G treated sows could be followed provided that kidneys are excluded from human consumption.

AGRO 54

Quantitative method to measure five compounds simultaneously from cotton gloves

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BASi method SAP.1597 was developed to measure five veterinary compounds from cotton gloves simultaneously. It was successfully validated to regulatory standards. The method involves extraction of all five compounds from cotton gloves using acetonitrile. A 200 µL aliquot of the supernatant is diluted with water and injected onto a LC-MS/MS (electrospray interface in both negative and positive ion mode). The internal standard is added to the diluted sample which is injected onto a Varian® Pursuit® diphenyl (DP) analytical column maintained at 55°C with a Metaguard® Pursuit® DP precolumn and acetonitrile/ammonium acetate mobile phase. The standard range was 12.5-500 ng/mL. The extraction efficiency was > 95%, and the matrix effect was negligible (0-5%). Matrix and extract stability were established and covered the time period between sample collection and assay. Long term freezer stability in gloves was 130 days for all compounds except compound D (78 days). Extract freezer stability was 130 days for all compounds except compound D (90 days). The limit of quantitation was established as 12.5 ng/mL, which corresponds to 2.5 µg/glove, and no interference was noted from three lots of gloves tested for method selectivity.

AGRO 55

Physiologically-based pharmacokinetic model to estimate non-target exposure to rodenticides

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Rodents cause significant damage to agriculture and ecosystems. Rodents also carry vector diseases that can adversely impact public health. Anticoagulant rodenticides are widely used to reduce pest rodent populations and their associated negative impacts. Pest rodents that consume rodenticides may contain rodenticide residues. Non-target avian and mammalian species may be exposed to rodenticides via the consumption of rodenticide exposed target species. A physiologically-based pharmacokinetic (PBPK) model was developed and applied to estimate the magnitude of rodenticide residues in target species exposed to various baiting scenarios. This presentation will demonstrate the utility of PBPK models to identify baiting scenarios that minimize target species rodenticide residues and associated non-target hazards.

AGRO 56

Pharmacokinetics of eprinomectin extended-release injectable for cattle

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Eprinomectin extended-release injectable parasiticide (LongRange™) has been approved recently for use in the United States for the treatment and control of internal and external parasites of cattle on pasture with persistent effectiveness. Eprinomectin is a macrocyclic lactone in the avermectin family and is approved for use in a topical formulation. LongRange is a solution of eprinomectin (5% w/v) for subcutaneous injection at 1 mg/kg bw. LongRange has a unique plasma pharmacokinetic (PK) profile with two maxima that contribute to the product's persistent efficacy, providing control of parasites for up to 150 days after dosing. The PK is influenced by the formulation that contains poly(d,l-lactide-*co*-glycolic) acid (PLGA) which creates an in-situ forming gel that controls the release of eprinomectin and produces the extended plasma profile. *(LongRange™ is a trademark of Merial; registration pending in the United States of America.)*

AGRO 57

Chemical ecology and biorational pesticide design

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Biorational design of pesticides has been an elusive target, not because predicting intrinsic activity has eluded agrochemistry more than pharmacochemistry but because application is so distant from the target pest compared with application of human or veterinary medicines. Chemical ecology has given us a range of lead compounds that may not represent formally biorational design, but certainly biorational discovery in that natural phenomena, such as impairment of pest, pathogen or weed development, can be used in bioassay guided fractionation to provide the chemical structure involved. We have examples where valuable pesticides can then be designed and even where the natural product itself is utilised directly. However, many such leads are too weakly active and too broadly toxic for successful exploitation. Now that the provenance of such compounds in nature means that we can potentially use GM and other approaches for synthesis in plants, greater opportunities exist for exploitation, but we may for the long term consider more those compounds such as pheromones and other semiochemicals that act by sophisticated non-toxic regulatory mechanisms. This approach will be exemplified in detail from the laboratory to the farm.

AGRO 58

USDA-Agricultural Research Service: Perspectives on biopesticides

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The United States Department of Agriculture, Agricultural Research Sevice has a long history of research on the discovery and development of biopesticides, particularly in the area of biocontrol agents. Examples of some of these will be discussed, as well as our current research in this vital area of pest management.

AGRO 59

Microbially-derived pesticides: Challenges and opportunities

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Microbially-derived pesticides include living or killed microbes with enriched levels of pesticidal agents, such as, proteins or natural products, natural products purified from microbes, semi-synthetic modifications of microbial natural products, and fully synthetic pesticides inspired by microbial natural product starting points. Each of these approaches marks a different set of challenges and opportunities, including efficacy, production, formulation, and a likely path to registration. Among those microbial natural products produced by fermentation, only abamectin and spinosad are major products with sales in excess of $100 million annually, and similarly, only spinetoram and emamectin benzoate are major semi-synthetically, modified natural products of microbial origin. Challenges to discovery of microbial-derived pesticides such as these will be discussed.

AGRO 60

Bringing new biologicals to market

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This presentation will weave together three critical considerations in the development and commercialization of new biologic pest control products: the economics driving agricultural production, the regulatory environments in which biologics are measured, and the market drivers influencing farmers' agronomic decisions both today and into the future. As the Head of Biologics within Bayer CropScience and the former CEO of AgraQuest Inc., the presenter will present a unique view of the position biologics play in emerging offerings from leading multi-national agchem companies. Through this presentation, the presenter will demonstrate that biologics must meet performance, price, and production hurdles in order to justify R&D investment and grower acceptance. The presenter will show that sustainable agricultural relies on an integrated approach to biologics and conventional agchem technologies.

AGRO 61

Chemical ecoprospecting and biopesticides

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Despite the fact that plant-derived natural products have historically been the basis for multiple useful biopesticides, screening efforts over the last quarter-century have been far more likely to focus on identifying novel pharmaceuticals than on biopesticides. A hallmark of both enterprises, however, is their relatively low success rates, with associated low return on investment. Efforts to increase the success rate of screening for drugs have included conducting ethnopharmacognostical and zoopharmacognostical surveys and examining ancient classical texts for guideposts; more recently, ecological theory has been applied to guide screening and to predict general pharmacological activity. Ecological theory can be applied far more productively, though, to predict biopesticidal activity. Among theories predicting community-wide distribution patterns of bioactive chemicals, the majority (including the carbon/nutrient balance hypothesis and the growth-differentiation hypothesis) predict only allocation patterns of defense chemicals rather than modes of action or spectra of activity. Both optimal defense theory and apparency theory can be applied to predict with some success different types of bioactivity as well as different types of allocation patterns. Moreover, recent modifications of theories that incorporate new knowledge relating to multitrophic interactions and molecular mechanisms underlying plant responses have improved the prospects for predicting sources of new biopesticides.

AGRO 62

Market opportunities for biopesticides

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The biopesticide market is reported to be approximnately $1.7 billion annually out of a $45 billion total global pesticide market. Biopesticides are reported to be growing at 10-15% per year compared to chemical pesticide growth of 5-6%. When used in integrated pest management programs, biopesticides offer value to customers with higher yields and quality than chemical-only programs. Regulatory restrictions, residue/MRL issues on exported crops, pest resistance, and worker and environmental safety are added

benefits contributing to their increased adoption. These factors have fueled robust deal making where large agrichemical companies are licensing biopesticides for their portfolios and also acquiring entire companies. Trends and factors that will further increase biopesticide adoption will be discussed.

AGRO 63

Botanical insecticides: A global perspective

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According to the CAB Direct database of scientific publications, there has been an enormous growth in research on botanical insecticides over the past 30 years. In 1980, less than 3% of all journal papers on insecticides dealt with botanicals , whereas that proportion reached 20% in 2011. In particular, there has been explosive growth in studies on insecticidal properties of plant essential oils; over half of the 2,000 papers on essential oils as insecticides have been published since 2006. In contrast, commercialization of botanical insecticides has continued to proceed at a relative snail's pace, indicating a big disconnect between theory and practice. This is certainly the case in the jurisdictions with the most rigorous regulatory standards – the EU, USA, and Japan. Using California as an example, use data for botanical insecticides also suggests a very modest market presence. According to Cal DPR data from 2010, botanicals constituted only 5.6% of all biopesticides used and less than 0.05% of all pesticide use; however, some recently introduced products have seen modest success. On the other hand, there appears to be increasing commercialization of botanical insecticides in China, Latin America, and Africa, regions where socio-economic conditions have led to some of the worst examples of human poisonings and environmental contamination. Arguably, botanicals should be of greater value in developing countries where the useful plant species are often locally abundant, accessible, and inexpensive. In many tropical countries, semi-refined plant preparations are likely to be relatively safe for users and more cost-effective than imported conventional crop protection products. In G20 countries, botanical insecticides will probably remain niche products for use in public health, urban pest control, and organic food production, but with considerable market opportunities.

AGRO 64

Insect P450 paradox: Too simple as targets, too complicated as detoxifiers?

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The resistance problem continues to drive research in insect toxicology. Understanding insecticide metabolism and discovering new targets are two approaches taken in resistance management. The first is conservative; it can improve the selectivity and protect the efficacy of existing classes of insecticides. The second is progressive; it can provide new tools in the race with pests. Cytochromes P450 enzymes are increasingly important in the first approach, but remain absent from the second. This may seem paradoxical, because P450 enzymes have long been drug targets and a large number of fungicides target CYP51. Here, I will review the great diversity of P450 enzymes in insects and discuss possible directions towards insect P450 as targets and possible clues to their ubiquitous presence in resistance research.

AGRO 65

DDT, flies, and molecular biology

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I will take a historical perspective on the use of fruit flies in insecticide resistance work, focusing specifically on DDT resistance. I will begin by examining the work of Jim Crow and pass onto arguments about mono- versus poly-genic modes of inheritance. Resistance to DDT will be discussed both in terms of target site and metabolic resistance mediated via cytochrome P450s. The talk will conclude with recent work on the gene *Cyp6g1* and the number of resistance alleles it contains. The implications for fitness of resistance alleles and their succession in natural populations will be discussed.

AGRO 66

How are recombinant cytochrome P450s and aryl hydrocarbon receptor (AhR) useful for biotransformation and biomonitoring of environmental chemicals?

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Molecular mechanism of metabolism and biological actions of environmental chemicals are important for understanding biodegradability, bioaccumulation, and biological effects on ecosystems. In mammals, P450(CYP) monooxygenases participate in metabolism of foreign chemicals. These P450 genes were engineered in higher plants and examined for biotransformation of environmental chemicals. In mammals, AhR specifically combines with a dioxin-like ligand and induces certain P450 species including CYP1A1 and CYP1A2. AhR genes were engineered in higher plants and tested for monitoring dioxin-like compounds under environmental conditions. Usefulness of these recombinant P450s and AhRs for biotransformation and biomonitoring of environmental chemicals is discussed.

AGRO 67

P450s responsible for insecticide resistance in malaria vectors: Finding them, tracking them, stopping them?

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Insecticides play a key role in the control of mosquito borne diseases. The limited number of insecticide classes available for use in public health (currently four) and the growing levels of resistance to all of these chemicals in a range of mosquito species is a growing impediment to disease control. This problem is particularly acute in malaria control where the impressive gains achieved using insecticide treated bednets or indoor residual spraying with insecticides are in danger of being eroded by growing resistance in the Anopheles mosquito vectors. A variety of genetic screening tools have been used to identify the small subset of mosquito P450s that are over expressed in insecticide resistant populations. Recombinant proteins for each of these have been generated and screened against a panel of WHO approved insecticides. Antibodies have been used to identify the major tissues in which each of the major candidates are expressed and to confirm that these enzymes are expressed at elevated levels in insecticide resistant populations. Enzymes in the CYP6P, CYP6M and CYP6Z families have all been implicated in conferring insecticide resistance by this approach. Recently, a specific role for the

CYP4G enzymes in cuticular resistance has been proposed and is being further investigated. The next challenge is to develop molecular markers to track these resistance mechanisms in field populations to aid in resistance monitoring. Ultimately, it is hoped that knowledge on the P450s responsible for insecticide resistance and their mode of action will accelerate the development of new chemistries that are urgently needed for malaria control.

AGRO 68

Tale about an aphid and its insecticide-driven upgrade: *Myzus persicae* version 4.0

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The green peach aphid, *Myzus persicae* Sulzer (Homoptera: Aphididae), is a major sucking pest in numerous agricultural and horticultural settings worldwide. It damages crops by feeding, as a virus vector, and by honeydew excretions facilitating the growth of sooty mold, i.e., ascomycete fungi. To keep aphid pressure under economic damage thresholds, large scale insecticide treatments have a long tradition. Several chemical classes of synthetic insecticides addressing different biochemical modes of action have been introduced to control *M. persicae* over the past 70 years. These include organophosphates, carbamates, pyrethroids, and neonicotinoid insecticides. The insecticide pressure on *M. persicae* was and is still high in many cropping systems resulting in the selection of genotypes surviving such treatments as a consequence of toxicodynamic and pharmacokinetic adaptions. In this presentation, special attention is given to recently-discovered biochemical mechanisms of resistance to neonicotinoids, a chemical class of insecticides selectively binding to insect nicotinic acetylcholine receptors. Aphid ecology, a nicotinic acetylcholine receptor mutation, and an overexpressed cytochrome P450 monooxygenase are the principal characters in a special case of the evolution of insecticide resistance.

AGRO 69

Bed bugs evolved unique adaptive strategy to resist pyrethroid insecticides

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The extensive use of insecticides accelerated the accumulation of resistance related factors in survivors. Therefore, studies on the molecular basis of these factors are of theoretical and applied importance in understanding the evolution of insecticide resistance and devising constructive resistance management tactics. The physiological and biochemical mechanisms of insecticide resistance may evolve along several trajectories. Typically, a combination of diverse mechanisms provides significantly higher levels of resistance than one individual mechanism. Recent advances in genomics and post-genomic technologies have facilitated a genome-wide analysis of the insecticide resistance-associated genes in insects. Through bed bug, *Cimex lectularius*, transcriptome analysis, we identified 14 molecular markers related to pyrethroid resistance. Our study revealed that most of the resistance-associated genes belonging to diverse mechanisms are expressed in the epidermal layer of the integument, which prevents or slows down the toxin from reaching the target sites on nerve cells, where an additional layer of resistance (*kdr*, knockdown resistance) is common. This strategy evolved in bed bugs is based on their unique morphological, physiological, and behavioral characteristics and has not been discovered in any other insect species. RNA interference-aided knockdown of these genes showed the relative contribution of each mechanism towards overall resistance development. Understanding of the complexity of adaptive strategy employed by bed bugs will help us to design the most effective and sustainable bed bug control methods.

AGRO 70

Atmospheric degradation of chlorpyrifos and chlorpyrifos-oxon

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The photolysis and OH· initiated oxidation of chlorpyrifos (a widely-used insecticide) and its degradate product chlorpyrifos-oxon have been investigated at the large outdoor European Photoreactor (EUPHORE) in Valencia, Spain under atmospheric conditions. These facilities allow work under realistic atmospheric conditions, particularly as regards solar radiation intensity and wavelengths. The rate constant for reaction of chlorpyrifos and chlorpyrifos oxon with OH radicals have been measured using a conventional relative rate method. They give an atmospheric lifetime in relation to the reaction with OH· of approximately 2 h and 11 h for chlorpyrifos and chlorpyrifos-oxon, respectively. The main products detected from the degradation of chlorpyrifos in gas-phase are SO_2, chlorpyrifos oxon, and 3,5,6-trichloro-2-pyridinol. The mechanisms for their formation are proposed.

AGRO 71

Assessing risks from pesticide post-application volatilization

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Over the last decade, there has been increasing interest in the risks associated with pesticide volatilization after application. Specifically, efforts have been focused on estimating downwind concentrations and establishing buffer zones to protect bystanders from inhalation exposures. This process began, at the Federal level, with the assessment of fumigants and the use of an air dispersion-risk model called the Probabilistic Exposure and Risk model for FUMigants (PERFUM) to estimate buffer zones by the US Environmental Protection Agency (USEPA). Earlier efforts were made by the state of California. Fumigant registrants also conducted field flux studies to estimate emission rates as part of this process. The fumigants were a logical starting point as many of the fumigants are highly volatile and applied at relatively large rates. Current efforts are aimed at estimating risks for semi-volatile pesticides. USEPA has started this process with an assessment for chlorpyrifos and is expected to assess other semi-volatile pesticides in the future. This presentation will review the history of these pesticide volatilization risk assessments and provide a discussion of the likely implications for semi-volatile pesticides. The later discussion will focus on estimates of flux rates from the literature based on physicochemical properties and potential refinements to the air dispersion modeling methodologies.

AGRO 72

Accumulation of pharmaceutical and personal care products (PPCPs) in vegetables under field conditions

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Treated-wastewater irrigation and biosolid amendment in agriculture are increasingly practiced worldwide, and contamination of plants by pharmaceutical and personal care

products (PPCPs) from the treated wastewater and biosolids is an emerging concern. In this study, 8 common vegetable crops were grown in field plots and irrigated with tertiary-treated wastewater with or without PPCP spiking. The vegetables were analyzed for accumulation of PPCPs in the edible parts at harvest. The vegetables included carrots, bell pepper, tomato, cucumber, lettuce, spinach, celery, and cabbage, which were often consumed raw by humans. The results showed that a few PPCPs, especially carbamazepine, were taken up and accumulated in the edible parts. The study findings are valuable as they provide the first-of-its-kind information on the occurrence and potential risks of PPCPs in common vegetables under realistic conditions.

AGRO 73

Pesticide runoff risk during peanut production in the southern Atlantic Coastal Plain

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Peanuts are produced on approximately 200,000 ha in the Atlantic coastal region of Georgia. The humid subtropical climate promotes high yields; however, pest pressures are high. Crops are treated frequently with a variety of active ingredients for weed, insect, and disease control. In this presentation, we describe relative runoff risk of herbicides and fungicides from peanut produced under conventional and conservation tillage. Data were collected over ten years during a study when peanut and cotton were produced in an annual rotation. Total fungicide loss was up to 5% of applied and exceeded herbicide loss by more than 5-fold. This was due in part to the much higher frequency of fungicide application and the occurrence of runoff-producing storm events close to their time of application. Findings indicate that where fungicides are used intensively on crops like peanut, relative runoff risk may be high.

AGRO 74

Nutrient export in tile drainage: Comparing manure injection to fertigation

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Subsurface tile drainage of agricultural land is implicated as a major source of nutrients to the Mississippi River. To protect water quality, land application of manure should maximize crop nutrient use and minimize nutrient loss. Weather constraints and regulations restrict the period during which manure can be land-applied in the upper Midwest. We performed on-farm experiments at the large-field scale to test the concept of applying liquid dairy manure through center pivot irrigation during the growing season to silage corn. Our objectives were to compare subsurface drainage nutrient losses (nitrate and dissolved reactive phosphorus), corn silage yields for fall manure injection (standard practice), and fertigation with dairy slurry. Results showed that water flux and nutrient export had very high temporal variability, with most of the water flow occurring during the spring. Fertigation holds promise as a means to reduce nutrient export by subsurface tile drainage.

AGRO 75

Seed-coated clothianidin fate in corn and soybean fields using conservation tillage

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Neonicotinoids like clothianidin are systemic insecticides that are suspected to be toxic to non-target species, including honey bees. The objectives of this project were to evaluate tillage use and seed-coating rates on the fate and transport of clothianidin on large-scale fields in a corn/soybean rotation. As part of farming conservation practice, the site was split into three fields undergoing no-till and low-till practices. Clothianidin was introduced in the field only during corn planting through seed-coating treatments. Soil, run-off water, infiltration water, and ground water samples were collected over three seasons. Clothianidin was detected in almost all soil samples during the first two seasons, showing persistence of this compound in soil. Laboratory bioassays have also been conducted and the toxic levels will be compared to soil and water field concentrations to assess the environmental risk of this insecticide.

AGRO 76

Occurrence of neonicotinoid insecticides in water in two US regions

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Neonicotinoid insecticides are of concern in the environment, but little is known about their overall occurrence. Neonicotinoids are commonly used in both agricultural and urban settings, but most current research has focused on their fate near the point of application. These compounds are water soluble (log K_{ow} <1) and have aqueous half-lives on the order of months, so they have the potential for offsite transport. More information on their occurrence in water is needed to understand better the possible environmental effects of these insecticides. Water samples were collected from two different climatic, geographical, and land use regions in the United States (Georgia and Iowa) and analyzed for six neonicotinoids (acetamiprid, clothianidin, dinotefuran, imidacloprid, thiacloprid, and thiamethoxam). Two streams in Georgia, one draining a predominantly urban area and the other integrating a mixture of land uses (urban, forested, limited agriculture), were sampled bi-monthly for one year. Imidacloprid was detected in both streams and in all seasons except for late fall, with the urban stream having more frequent detections and higher concentrations. The Iowa locations consisted of select streams in agricultural areas (e.g., corn and soybeans) that were sampled in spring (May) and summer (July) during runoff conditions. The spring samples had detections of neonicotinoids associated with seed treatments (clothianidin, imidacloprid, thiamethoxam) while the summer samples also had detections of one associated with aerial applications (acetamiprid). The frequencies of detection and concentrations were generally higher in the spring compared to the summer samples. An additional set of samples was collected at a wastwater-impacted Iowa stream during winter low flow conditions (stream flow approximately 99% effluent at this time). Results document fairly conservative transport of chlothianidin and imidacloprid over an 8 km reach. Concentrations during such winter conditions indicate these compounds can persist long after initial application and are also present in wastewater.

AGRO 77

Estimating organic carbon sorption coefficients (K_{oc}) of nine pyrethroids based on feely dissolved chemical concentrations measured with solid phase microextraction (SPME)

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Pyrethroids are hydrophobic and bind strongly to soil/sediment and dissolved organic carbon. Thus, it is a challenging task to measure freely dissolved (C-free) and total pyrethroids (C-total) in sediment pore water for calculating the organic carbon sorption coefficients (K_{oc}) which is critical for ecotoxicological (ecotox) risk assessments for benthic organisms. Solid phase microextraction (SPME) and isotopic-D6-labeled standards were used to measure C-free and C-total in pore water simultaneously. C-free and C-total were measured and K_{oc}s were generated for nine pyrethroids (bifenthrin, cyfluthrin, lambda-cyhalothrin, cypermethrin, deltamethrin, esfenvalerate, fenpropathrin, permethrin, and tefluthrin) in three sediments (a fresh water sediment, a marine sediment, and OECD sediment) used for ecotox testing. As a comparison, C-total was also measured using a liquid-liquid extraction (LLE) from pore water and sediment. K_{oc} coefficients generated using LLE and SPME methods were compared between experiments using traditional K_{oc} study and simulated ecotox testing conditions; these differed markedly in sediment:water ratios. Because the K_{oc} coefficients generated using simulated ecotox test conditions using SPME reflect freely dissolved pyrethroid concentrations, these values are the most relevant ones to use in benthic organism focused ecotox risk assessments.

AGRO 78

Overview of a national aquatic risk assessment of pyrethroid use in agriculture

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Synthetic pyrethroids are used to control insect pests on many important crops including corn, soybeans, cotton, tree nuts, vegetables, and turf, among others. An ecological risk assessment is underway to quantify the risks of agricultural pyrethroid use to aquatic organisms and communities. Conservative screening-level risk estimates indicated concern for insects, crustaceans, and possibly fish for some agricultural uses. Refinement of exposure modeling to reflect mitigation practices specified on current pyrethroid labels (vegetative filter strips and spray drift buffers) and updated environmental fate parameters reduced the risk estimates but the potential for concerns remained for many uses. Several lines of higher-tier exposure analysis are being undertaken to address these concerns. Refined exposure analysis is proceeding along four paths: (1) probabilistic modeling to account for uncertainty and variability in critical exposure parameters; (2) simulation of processes affecting exposure in flowing water, especially sediment movement and chemical pulses; (3) a nationwide exposure modeling analysis of the vulnerability of stream reaches and catchments to pyrethroid input from runoff and drift; and (4) high-resolution landscape modeling of flowing and static water bodies in selected vulnerable watersheds. Assessment of aquatic effects includes analysis of single-species ecotoxicology data (Species Sensitivity Distributions), review of results from microcosm and mesocosm studies, population modeling for both fish and invertebrates, and bioassessments of stream communities. Findings of the risk assessment will be presented in several ways: deterministic Risk Quotients, probabilistic risk estimates, and qualitative evaluation of multiple lines of evidence. Uncertainties and limitations of the assessment will be discussed.

AGRO 79

US EPA Office of Pesticide Program's 21st century vision and strategy for communication

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US EPA Office of Pesticide Programs (OPP) is committed to protecting human health and the environment through the application of the latest scientific tools in assessing and managing pesticide risks. Traditional pesticide assessment approaches involve extensive studies that are often complex, expensive, use many animals, and are time consuming to conduct and to evaluate. OPP's vision (www.epa.gov/pesticides/science/testing-assessment.html) for advancing integrated approaches to testing and assessment (IATA) combines existing knowledge of hazard and exposure and predictive tools in a weight-of-evidence approach to predict better potential risks for specific exposure scenarios and focus testing on likely risks of concern. OPP's efforts in this area are coordinated with those across US EPA (e.g., OPPT, ORD), other federal agencies (e.g., FDA), the stakeholder community, and internationally through several venues (OECD, WHO, NAFTA, EFSA, etc). OPP established a workgroup under our Federal Advisory Committee the Pesticide Program Dialogue Committee on 21st Century Strategies (www.epa.gov/pesticides/ppdc/testing/index.html) which is made up of a diverse range of stakeholders (e.g., environmental and public health interest groups, worker protection groups, pesticide manufacturers and trade associations, state agencies, animal welfare groups, academics) to provide us with advice on communication and transition issues. In the future, pesticide assessment will employ increasingly sophisticated scientific tools and continue to protect human health and the environment. OPP's application of IATA is intended to minimize animal testing while evaluating more chemicals across a broader range of potential effects in a shorter time frame thereby enhancing the quality and efficiency of risk assessment and risk management decisions. An early and ongoing dialogue with stakeholders is critical to ensure this change will be successful. Stakeholders need to have an understanding of the new technologies and feel comfortable that society will benefit, i.e., trust that the approach is as good as or better than status quo.

AGRO 80

New technologies for exposure assessment

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Prioritization of chemicals requires reliable methods for screening on both hazard and exposure potential. High-throughput, typically *in vitro*, biological activity assays allow the ToxCast and Tox21 projects to investigate thousands of untested chemicals and compare the biological activity of chemicals with known *in vivo* toxicity to those with little or no *in vivo* data. Further, *in vitro* assays can characterize key aspects of pharmacokinetics and allow *in vitro-in vivo* extrapolation to predict the human uptake (mg/kg/day) that

might be sufficient to cause bioactivity *in vivo*. Without similar capability to make quantitative, albeit uncertain, forecasts of exposure, the putative risk due to an arbitrary chemical cannot be rapidly evaluated. Using physico-chemical properties and provisional chemical use categories, most of the ~10,000 Tox21 chemicals have been evaluated with respect to key routes of exposure. A mapping of chemicals to products and products to uses has categorized chemicals with respect to potential uses within the home. A Bayesian methodology was used to infer ranges of exposures consistent with biomarkers measured in urine samples and reported by the National Health and Nutrition Examination Survey (NHANES) in 2012. For each demographic group reported by NHANES we considered permutations of linear regression models, including as few as one and as many as all physico-chemical and use factors. Significantly associated factors provide heuristics for predicting exposures consistent with the NHANES data. For the Tox21 list, including hundreds of ToxCast pesticides, these simple heuristics alone were sufficient to make exposure predictions. These exposure predictions were then directly compared to the doses predicted to cause bioactivity for ~250 ToxCast chemicals. For chemicals with no other source of information, this approach allows prediction of a confidence interval within which the average human exposure due to near field sources is likely. (*This abstract does not necessarily reflect US EPA policy.*)

AGRO 81

Adverse outcome pathways for neurotoxicity: An example using pyrethroid insecticides

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The National Academy of Science report on *Toxicity Testing in the 21st Century* advocated the use of adverse outcome pathways (AOPs) as a critical aspect of predictive toxicity testing. AOPs catalog the evidence in the peer reviewed literature to describe the interaction of a chemical with a molecular target in the cell and the subsequent alterations in cellular, tissue, and organism function that describe toxicity following exposure to that chemical. For neurotoxicity, one of the best examples of an established AOP is for pyrethroid insecticides. These compounds bind to voltage-gated sodium channels in the membranes of neurons, prolonging the time that these channels remain open. Numerous studies have documented the relationship between prolonged sodium channel kinetics and altered membrane excitability due to excess entry of sodium. The changes in membrane excitability have been documented both *in vitro* as well as *in vivo* and contribute to the behavioral changes associated with pyrethroid neurotoxicity. This talk will outline the concept of AOPs and use pyrethroid neurotoxicity as an example of how to establish an AOP for a neurotoxicant. It will also use the AOP approach to discuss the role of other potential molecular targets in pyrethroid neurotoxicity to compare and to contrast the levels of evidence for different AOPs for pyrethroids. (*This abstract does not represent Agency policy.*)

AGRO 82

Evolution of the Endocrine Disruptor Screening Program (EDSP) in the 21st century

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Under the 1996 FFDCA and Safe Drinking Water Act, US EPA is required to screen all pesticide chemicals and those drinking water contaminants to which a substantial population is exposed for the potential to interact with the endocrine system. The combination of both pesticide and drinking water chemicals amounts to a universe of over 10,000 chemicals. The Agency must therefore prioritize which chemicals are listed for screening and testing in multiple biologically complex and resource intensive assays. In January 2013, the Agency brought a strategic prioritization scheme that combines physico-chemical properties, Structure Activity Relationship (SAR) and High ThroughPut (HTP) assays before the FIFRA Science Advisory Panel (SAP) for input on fit-for-purpose and regulatory application. The SAP provided key comments on the expansion of the SAR training set to cover a larger chemical universe and the approach to interpreting the HTP data to inform the SAR model. The SAP also provided recommendations on various aspects of the HTP data including transparency of how the data were generated, processed, and analyzed. These key recommendations will guide how the EDSP will evolve in the use of advanced robotics for rapid screening of the EDSP universe of chemicals.

AGRO 83

Cumulative risk assessment for human health: Asking the right questions

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When the current risk assessment–risk management paradigm as applied to humans was first elucidated in 1983, it did not explicitly include a problem formulation phase. The concept of problem formulation was first introduced in the context of ecotoxicological risk assessment (ERA) for the pragmatic reason to constrain and focus ERAs to the key questions. Subsequently, problem formulation has been introduced into human health risk assessment and is particularly pertinent in the context of cumulative risk assessment (CRA). In its broadest sense, CRA encompasses the combined risks from exposure via all relevant routes to all stressors, including biological, chemical, physical, and psychosocial. As part of the RISK21 program at HESI, we have proposed a framework for CRA that includes a problem formulation step. This framework is based on the tiered framework recommended for cumulative risk assessment of chemicals by WHO. Relative timing of exposures to multiple stressors is a major determinant of risks of adverse responses to cumulative exposures. In addition to contemporaneous, consecutive, or separate, exposures might also be important, depending on the kinetics of the chemicals, the duration of the response, any latency, and rate of recovery. Conceptual models for exposures in CRA need to include consideration and eventual quantification of non-chemical stressors such as physical environment, state of health and nutrition, and psychosocial status. At the highest tier, conceptual models for responses need to include measures of the interactions between stressors and the toxicodynamics and toxicokinetics that determine the cumulative response. This presentation will illustrate how conceptual models for exposures and responses can be developed, how data from new approaches to assessing responses can be used, and how testable risk hypotheses can be elaborated.

AGRO 84

In vitro screening data within Tox 21: How to use it?

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In 2007, the seminal National Academy of Sciences report, *Toxicity Testing in the 21st Century* (TT21C), was published. It strongly advocated for utilizing *in vitro* and omics tools to make predictions for *in vivo* outcomes and guide more-targeted animal testing. *In vitro* assays and *in silico* tools provide a natural fit into the early stage of a testing program and an opportunity to begin implementation of the concepts of TT21C. Most of these assays and tools capitalize on the rapid growth of knowledge in the modes of action (MoA) for *in vivo* toxicities, as well as the technological advances in modern molecular and cellular biology. Evaluation of discrete molecular endpoints, such as receptor binding, nuclear receptor transactivation, and gene expression modulation provide insight into potential *in vivo* toxicities and a basis for understanding adverse effects, the MoA, and the potential human relevance. For registrants, these targeted molecular assays can aid in identification of a chemical with the most desirable attributes without the use of resource-intensive early animal screening studies. *In vitro* screening data can then be used to prioritize more complex and definitive testing, which includes more complex *in vitro* assays and/or definitive animal studies. Integrated animal testing strategies reduce animal use even further and maximize information gathered from those animal studies. This tiered approach of *in vitro* screening information triggering more definitive decision-making assays provides a bridge between traditional *in vivo* testing and a complete *in vitro* strategy. Furthermore, it allows for confidence to be built in *in vitro screening* assay results and gathering of useful toxicological information for product evaluation while reducing initial early stage animal-based screening studies.

AGRO 85

Incorporating new technologies into toxicity testing and chemical risk assessment: Moving from 21st century vision to a data-driven framework

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A series of studies has been performed that together may provide a data-driven framework to address the large number of chemicals with limited toxicity information. The framework integrates new experimental technologies such as high-throughput *in vitro* screening and *in vivo* transcriptomics with computational modeling and bioinformatic analyses to identify both the relative selectivity at which chemicals interact with biological targets and the concentration at which these interactions perturb signaling pathways. The results are used to calculate a point-of-departure and are compared with human exposure estimates to yield a margin-of-exposure. The margin-of-exposure determines progression of the chemicals between tiers. Based on data collected, a significant percentage of chemicals could be eliminated from further testing using only *in vitro* assays or short-term *in vivo* transcriptomic studies in the early tiers. The framework provides a risk-based and animal-sparing approach to evaluate chemical safety, drawing broadly from previous experience but incorporating advances in technology to increase efficiency.

AGRO 86

Approaches for establishing scientific confidence in 21st century methods for toxicity evaluations

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Advances in high-throughput and high-content (HT/HC) methods such as those used in the fields of toxicogenomics, bioinformatics, and computational toxicology have the potential to improve both the efficiency and effectiveness of toxicity evaluations and risk assessments. However, prior to use, scientific confidence in these methods should be formally established. Traditional validation approaches that define relevance, reliability, sensitivity, and specificity, such as those in use by ICCVAM, may not be readily applicable. HT/HC methods are not exact replacements for *in vivo* testing, and although run individually, these assays are likely to be integrated together for decision making. Many of these assays rely on robotics, which may be unique in each laboratory setting. Building on the frameworks developed in the 2010 Institute of Medicine Report on Biomarkers and the OECD 2007 Report on (Q)SAR Validation, we present constructs that can be adapted to address the validation challenges of HT/HC methods. These constructs are both flexible and transparent, though require explicit specification of context and purpose of use such that scientific confidence (validation) can be defined to meet different regulatory applications. Transparency in the prediction model algorithms is a necessity to establish scientific confidence. Prediction models, filters, decision points, validation/performance data sets, and assay results should be publicly available and subjected to independent scientific peer review. We discuss some of the shortcomings of recently published models and recommend improvements, including how anchoring the assays and their prediction models to Adverse Outcome Pathways (AOPs) could facilitate the interpretation of results and support scientifically defensible fit-for-purpose applications.

AGRO 87

HESI's RISK21 roadmap: A transparent risk assessment methodology

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For decades, human health risk assessment has depended primarily on animal testing to predict adverse effects in humans, but that paradigm has come under question because of calls for more accurate information, less use of animals, and more efficient use of resources. Moreover, the disproportionate use of hazard information has overshadowed the important role of exposure science in determining the definition of reasonable measures for human safety. In addition, major risk assessments may lack transparency, thereby hindering a clear understanding of the conclusions and hamper communication of key safety messages. To help answer these challenges, the HESI-managed RISK21 project was initiated to develop a scientific, transparent, and efficient approach to the evolving world of human health risk assessment. RISK21 involved over 120 participants from 12 countries, 15 government institutions, 20 universities, 2 non-governmental organizations, and 12 corporations. RISK21 developed a tiered approach that is problem formulation-based, makes

maximum use of prior knowledge, and is led by exposure science to produce a highly transparent and flexible visualization of and approach to assessing human safety and risk. The general principles underlying the RISK21 approach as well as an overview of the RISK21 roadmap will be presented.

AGRO 88

Semiochemicals to control orchard pests

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Tree nuts – almonds, pistachios, and walnuts – are a significant agricultural commodity of California and supply a large portion of the world's consumption. The navel orangeworm (*Amyelois transitella*)is a major insect pest that inflicts significant monetary damage to California tree nuts. During their development, larvae of *A. transitella* feed upon the nut meat, which causes physical damage and ultimately lowers kernel quality. Moreover, infestation of *A. transitella* in tree nuts represents a serious food safety concern since the larvae have been purported to vector aflatoxigenic fungi into the food product. Aflatoxins are toxic metabolites produced by *Aspergillus flavus* and *Asp. parasiticus* – ubiquitous fungi in tree nut orchards. Semiochemicals play a large role in efforts to control or monitor *A. transitella* moths. For instance, a blend of almond host plant odors has recently been reported to attract both male and female navel orangeworm during field trapping studies. The origin of many of the components within this host plant blend appears to be from the almond host. However, new reports regarding the blend component, conophthorin, imply a fungal origin for this particular volatile. Discussed will be current applications for host plant semiochemicals to attract navel orangeworm as well as future opportunities.

AGRO 89

Discovery of mosquito attractants and attraction-inhibitors

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The United States Department of Agriculture (USDA) has developed repellents and insecticides for the U.S. military since 1942. A small component of this research program has aimed at the discovery of attractants that can be used to produce potent lures for haematophagous arthropods, with a primary focus on medically-important biting flies. Research on attractants in the late 1960s led to the discovery of *L*-lactic acid as one of the attractants for *Aedes aegypti* mosquitoes. In the mid and late 1990s, research involving multiple subjects led to the discovery of 277 compounds present on skin, and the results of this work produced lures that are highly effective at trapping *Ae. aegypti* in laboratory bioassays. As a result of these studies, it was discovered that some compounds on human skin inhibit the ability of mosquitoes to find hosts. These compounds are present on human skin at trace levels; however, when larger quantities of these attraction-inhibitors are presented with human odors to mosquitoes, they produce anosmia and hyposmia in test mosquitoes. This presentation will cover the USDA research to discover better mosquito attractants and novel means to deter mosquitoes from finding hosts.

AGRO 90

Discovery and development of repellents

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The synthetic compound, DEET, has been the gold standard for insect and tick repellents for over 50 years, and common thought was that it would be difficult to find something better than DEET. Since about one-third of the population in the US each year applies DEET to their skin or clothing at levels as high as 98% DEET, we should not be surprised of the public concern about its safety and demands for a green alternative. We have new data on the effect of DEET on total gene expression in primary human liver cells. A new, natural repellent, was discovered, BioUD, in a university laboratory. BioUD is more effective than DEET against mosquitoes and ticks, does not melt plastics like DEET, is non flammable, and is approved by the US EPA for use on children. The work on BioUD provides many lessons about technology discovery and commercialization in the University environment of "publish or perish". Tick attractants will be discussed with activities as high as 18,000 times that of carbon dioxide. The work on BioUD and tick attractants has led unexpectedly to a new herbicide, a new fumigant, and basic new information on how ticks taste and smell.

AGRO 91

SPLAT: A delivery technology for attractants and repellents

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ISCA Technologies specializes in the development of semiochemical-based products for pest management. Invariably semiochemicals tend to be volatile, labile compounds that require a specialized formulation to protect and to modulate their release over long periods of time. Despite decades of successful research, the bottlenecks to widespread adoption of semiochemical control techniques still remain. Current techniques 1) require high doses of semiochemicals per area to protect crops which may be cost-prohibitive, 2) require companion insecticide treatments, 3) require manual application, and 4) shown lack of consistency in control. SPLAT® is a biologically-inert matrix developed for pest management in agricultural, urban, and forest ecosystems to provide long-term release of insect pheromones, plant volatiles, insecticides, phagostimulants, and other compounds used for pest control. The amorphous and flowable properties of SPLAT allow it to be applied using a wide range of manual and mechanical methods such as electric and pneumatic grease guns, syringes, caulking guns, tractors, and even aerial applications. SPLAT formulations can be designed to provide species-specific control through mating disruption, repellency, attract and kill, and mass trapping techniques. We discuss three effective insect pest management systems that use SPLAT: 1) SPLAT EC, a mating disruption system that uses a mimic of the sex pheromone of the Carob Moth, a pest of dates, carob, pomegranates, almonds, and palms; 2) SPLATverb formulated with an anti-aggregation pheromone that protects individual trees and forest stands from mountain pine beetle attack; and 3) SPLAT MAT ME, formulated with an attractant combined with an insecticide and a phagostimulant that has resulted in an optimal bait-and-kill strategy for a number of Tephritid fruit flies.

AGRO 92

Neurotoxicity and mode of action of *N,N*-diethyl-*meta*-toluamide (DEET) on the insect nervous system and mammalian neurons

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Recent studies have suggested that DEET is an anticholinesterase and that this action may contribute to its repellent effects in insects and cause risk of toxicity in exposed humans. We have confirmed that DEET is lethal to mosquitoes (LD_{50} = 2-4 µg/insect), but observe that DEET is a poor anticholinesterase in mosquitoes (<10% inhibition at 10 mM). Neurophysiological recordings show DEET to possess neuroexcitatory effects to the housefly CNS at micromolar concentrations. Phentolamine, an established octopaminergic antagonist, blocked the CNS neuroexcitation of DEET and octopamine, but was ineffective against propoxur. These findings suggest DEET is targeting octopaminergic synapses and not acetylcholinesterase to induce neuroexcitation while indicating that anticholinesterase effects do not underlie toxicity or repellency. Additionally, DEET was found to block sodium and potassium currents of patch clamped rat neurons at micromolar concentrations, an action consistent with numbness of mucous membranes experienced in humans through contact exposure to DEET.

AGRO 93

Enzymes, insecticides, and pests: Oh My!

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Enzyme systems are widely involved in determining the action of insecticides on several levels including: a) differential toxicity between species, b) insecticide resistance, and c) as target sites for insecticides. Differential action of enzyme systems has provided the basis for differences in insecticide toxicity between target and non-target insect species. Likewise, resistance in pest insect species is frequently due to the enhanced or altered activity of enzyme systems towards selected, or in some cases a broad range, of toxicants. Finally, a number of enzyme systems have been targets for insecticides. Although inhibition of acetylcholinesterase has historically served as the basis for a large number of the insecticides developed, other new and under-utilized enzyme based targets are being exploited. The past, present, and future of each of these aspects will be considered.

AGRO 94

Inhibitors targeting acetylcholinesterase with high selectivity for arthropod disease vectors

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Chemical control has been effective in reducing malaria mortality, but insecticide-treated nets are losing efficacy due to emerging pyrethroid resistance. Thus, alternative insecticides are urgently needed. Anticholinesterase inhibitors selective for *An. gambiae* acetylcholinesterase could be useful additions to the malaria control arsenal if low mammalian toxicity and circumvention of existing resistance mechanisms was achieved. Over the past several years, we have explored the structural determinants of enzyme selectivity and potency of carbamates through side chain alteration and heterocycle ring replacement. Toxicity studies have evaluated *in vivo* mortality to *An. gambiae* mosquitoes of wild type G3 strain and the Akron strain possessing target site (G119S) and metabolic resistance mechanisms. All of these studies were augmented by *in silico* modeling of enzyme structure/ligand docking and toxicity versus physicochemical property relationships. Efforts to combine high *An. gambiae*/human selectivity with good contact toxicity towards WT and resistant mosquitoes will be presented.

AGRO 95

Bacillus thuringiensis israelensis* toxins have multiple modes of action in *Aedes aegypti

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Aedes aegypti is an important vector of human diseases, such as dengue fever and yellow fever. Its control has been attempted by eliminating breeding sites, using predators, and with chemical insecticides. However, such control is still difficult because of operational limitations and the development of insect resistance. Therefore, *Bacillus thuringiensis* has been used for decades instead of physical and chemical control methods. *B. thuringiensis israelensis* is highly active against *Ae aegypti*. The high insecticidal activity and the low toxicity to other organisms have resulted in the rapid use of *B. thuringiensis* as an alternative method for control of mosquito populations. This bacterial strain produces a variety of toxins which collectively show high toxicity to *Aedes aegypti*. Presently, it has been assumed that all the three Cry toxins in this strain act via a common mechanism, while the Cyt toxin acts via an alternative mechanism. We recently showed that the Cry toxins also act via different mechanisms. To assess the mechanism of action of the Cry toxins, we developed mosquito lines that express dsRNA for Aedes *Cad* and other receptor genes under control of a heat shock promoter. Our data shows that while the cadherin gene is important for Cry11A toxicity, Cry4Aa and 4Ba toxicity is mediated by other receptor(s).

AGRO 96

CYP genes in termites and their roles in termite biology

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Insect cytochrome P450s, encoded by CYP genes, play amazingly diverse roles in insect ecology, physiology, biochemistry, and toxicology. Termites are social insects with their own unique caste systems, behaviors, developmental physiology, chemical communication, chemical ecology, symbioses, and digestive processes. This talk with focus on recent advances in our understanding of termite P450-related biology with a special emphasis on the influences and contributions of Dr. Rene Feyereisen to this unique area of insect science.

AGRO 97

G protein coupled receptors as targets for insecticide discovery

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G protein coupled receptors (GPCRs) are a major target for drug discovery. Estimates in the literature are that somewhere between 30 and 60% of all drugs in use target these receptors. Of the human genome, about 4% of all proteins encoded are GPCRs. There are around 800 known human GPCRs, although many of these are olfactory receptors. All biogenic amine and most peptide hormone receptors are GPCRs. A huge number of drugs are agonist or antagonists of biogenic amines. Antagonists of corticotropin-releasing factor are under development for a variety of conditions; calcitonin is used for treating osteoporosis. This includes many of the best selling drugs, including histamine H_1 and H_2 receptors, α and β adrenergic receptor agonists and antagonists, etc. Fifty-six human GPCRs are drug targets. Yet to date, the only insect GPCR which is a target of a pesticide is the dopamine receptor, of which chlordimeform is the prototypical receptor agonist. Most vital life functions in insects are controlled by GPCRs presenting a huge number of possibilities for development of new selective insecticides. I will review the structure, function, and action of GPCRs.

AGRO 98

Potential acaricidal targets in tick salivary glands

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Ticks are obligatory ectoparasites causing global animal and human health problems. Tick salivary secretions are required for initiation and continuation of the feeding by injections of bioactive salivary components into the host and by osmoregulations upon ingestion of large quantity of blood. Nervous control of the salivary glands has been previously speculated. Dopamine has been described as a potent activator of salivary secretion. Our recent finding indicates presence of more complex mechanisms for control of the salivary glands. We identified at least two neuropeptides, myoinhibitory peptide and SIFamide, innervating the salivary glands in blacklegged ticks (*Ixodes scapularis* Say) which transmits the most important tick-born disease Lyme disease. We hypothesize that these neuropeptides control dopaminergic cells located on the base of acini in the salivary glands. Additionally, we find at least two different dopamine receptors with putative different functions in the salivary secretion. The fundamental knowledge obtained from this research is eventually expected to lead to the design of compounds and vaccines to prevent disease transmissions by ticks.

AGRO 99

Using genomic tools to determine the mode of action of acaricides: The tale of chitin synthesis inhibitors in *Tetranychus urticae*

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Acaricides are a diverse group of chemicals with excellent efficacy primarily on mite and tick species. The mode of action of acaricides is often less understood in comparison to insecticides. Spider mites are probably the most problematic mite pest species in plant production, as they are extremely polyphagous and have a tendency to develop resistance extremely fast. Recently, the genome of the two-spotted spider mite *Tetranychus urticae* was sequenced. Based on the availability of the small genome (90 Mb), we developed a population, multi-generational bulk segregant analysis (BSA) mapping method to uncover resistance mutations. When target-site resistance is the main resistance mechanism, this technique also potentially elucidates the molecular targets of acaricides. Etoxazole represents one of the several compound classes that act as potent chitin biosynthesis inhibitors and are of great agricultural importance for the control of arthropod populations. Using a BSA approach, we identified a non-synonymous variant in the major *T. urticae* chitin synthase enzyme that confers target-site resistance to etoxazole, suggesting a direct interaction between etoxazole and chitin synthase. Identification of the target-site of a chitin synthase inhibitor is important to exploit chemical structures fully. Intriguingly, the nature of the *CHS1* mutation underlying resistance is potentially informative as to why the exact mode of action of arthropod chitin biosynthesis inhibitors have remained elusive for decades: the target site mutation suggests that inhibition acts on a non-catalytic (but essential) function of *CHS1* complexes. Next to etoxazole, we have performed BSA analysis to uncover resistance mutations in strains resistant to a number of chemicals, and we will present the initial but exciting results.

AGRO 100

Higher-tier aquatic exposure estimation for agricultural pyrethroid-use patterns and associated model sensitivities

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This presentation will focus on potential aquatic ecological exposure from drift, erosion, and runoff from pyrethroid use on crops. USEPA Tier II modeling involves running the Pesticide Root Zone Model (PRZM) and Exposure Analysis Modeling System (EXAMS) models with standard crop scenarios to predict exposure concentrations in water, pore water, and sediment. Higher tier modeling (Tier II+) will be presented that reflects refined inputs including labeled mitigation practices such as drift buffers (calculated from AgDRIFT® model) and vegetative filter strips (modeled with VFSMOD). Additionally, higher tier results from modeling the standard pond waterbody with the AGRO model will be presented. The sensitivity of the models to parameters including K_{oc}, K_{ow}, soil organic carbon, drift droplet size, setback distances, and number of applications will be shown. A comparison of results from EXAMS versus AGRO models will be included. Ultimately, the results of these sensitivity analyses can be used to identify the key variables to include in probabilistic assessments of potential pyrethroid aquatic exposures in water bodies at the regional and crop-specific scales. This presentation provides further details on the refined exposure modeling.

AGRO 101

PRZM-Hybrid modeling system utilizing an agronomic approach to define watershed-scale chemical applications

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The PRZM-Hybrid system has been developed to predict residue values in chemographs from less-frequently-monitored time series by estimating when runoff events may have occurred in the watershed using local rainfall data and the Pesticide Root Zone Model (PRZM). The PRZM-Hybrid method simulates the environmental fate and transport of agrochemicals from field (~1 mi^2) and watershed (500 mi^2) scales. PRZM-Hybrid parameterizes the PRZM model using local rainfall/crop planting data and watershed-specific inputs to produce a daily time series of potential runoff event-based concentrations. In addition to standard PRZM parameterization, PRZM-Hybrid utilizes spatially-explicit high resolution NEXRAD radar rainfall data, additional meteorology data, field-scale soil properties from the US SSURGO database, and spatially-explicit land use data as input data to model daily watershed runoff. PRZM-Hybrid uses a combined Growing Degree Day (GDD) and soil "workability" approach for developing a window of probable crop planting and agricultural chemical application across fields in the watershed. Concentrations developed from this system represent watershed-scaled edge-of-field estimates and generally are similar to or over-predict measured concentrations. By using estimates of GIS-based watershed times of concentration and time to peak, watershed-scale concentrations simulated on a given day can be linked with monitored concentrations to predict concentrations between days with measured values. Also, using this refined version, model output for small watersheds can be used as stand-alone daily chemographs for comparative purposes, such as the estimation of potential year-to-year variability.

AGRO 102

PRZM-Hybrid and VFSMOD modeling of chlorpyrifos transport in small agricultural watersheds in Minnesota, USA

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Recent developments in field-scale mechanistic modeling of vegetated filter strips (VFS) at effectively removing soluble and sediment-borne pesticide residues enables greater accuracy in predicting the effectiveness of different BMP's. Simulations using the PRZM-Hybrid approach, previously applied to the herbicide atrazine employing high resolution local input data, were performed with various levels of assumed VFS implementation in small MN agricultural watersheds where the insecticide chlorpyrifos is used in agronomic crops. In this approach, a small watershed is represented as a combination of unique fields, where predicted field edge runoff of water, sediment, and chemical mass from all of the fields contribute instantaneously to the daily hydrology and chemographs for the watershed. PRZM3 edge-of-field predictions for water and sediment runoff was coupled with the VFSMOD model to address performance of VFS in reducing pesticide loadings from field edge and the impact this has at large within the watershed. Required data sets, model parameterization, and model assumptions are discussed. Predicted water concentrations from small watersheds in MN, discretized and simulated as a combination of unique fields, were compared to downstream monitoring data, with model performance evaluated against the actual conditions occurring in the watersheds in the 2012 cropping year. Predicted impacts of differing levels of adoption of VFS in reducing in-stream concentrations are summarized.

AGRO 103

Predicting stream concentrations of selected pesticides using adjusted Watershed Regressions for Pesticides (WARP) models

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Watershed Regressions for Pesticides for Multiple Pesticides (WARP-MP) models were developed to predict concentration statistics for pesticides in unmonitored streams. The WARP-MP models use the national atrazine WARP models in conjunction with a pesticide-specific adjustment factor that is based on the Surface Water Mobility Index and the vapor pressure of each modeled pesticide. The WARP-MP models perform well for pesticides with application timing and methods similar to those used with atrazine. For other pesticides, WARP-MP models tend to over predict concentration statistics for the model development and evaluation sites. WARP-MP models were applied to streams across the United States to illustrate their use in screening-level assessments to guide more intensive monitoring.

AGRO 104

Conceptual model for estimating exposure from the use of pesticides on rice

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Pesticide application to a rice paddy is a unique pesticide exposure scenario not fully addressed by previous regulatory aquatic exposure conceptual models. The goal of the conceptual model is to characterize concentrations of pesticide residue in the rice paddy and in water bodies receiving the released rice paddy water. In developing the conceptual model for use with EPA's Pesticides in Flooded Agriculture Model (PFAM), the following topics are considered: 1) agronomic practices associated with rice; 2) hydrology of rice growing regions; 3) locations of ecological receptors and human health drinking water intakes relative to locations of rice paddies; and 4) exposure durations of concern for ecological and human health assessment. Applications of the conceptual model beyond rice paddies are also considered (*e.g.*, cranberry bogs).

AGRO 105

Approach for predicting pesticide EECs in static water bodies based on spatially-explicit hydrography, landscape, and pesticide-use data

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The standard regulatory approach for estimating aquatic pesticide EECs in an ecological risk assessment is to use the PRZM/EXAMS model to simulate a ten-ha field draining into a one-ha pond. This approach assumes that 100% of the crop area draining into the pond is treated with the pesticide on a soil representative of the geographic region and crop.

In reality, the characteristics of pond drainage areas vary widely over the geographic extent of interest for a typical ecological risk assessment. To obtain a more robust estimation of aquatic exposure risk, an approach was developed to account for variability in soils, weather, percent cropped area, and pesticide use probability when estimating pesticide concentrations in vulnerable static water bodies. The approach uses spatially-explicit data and the PRZM/EXAMS model to identify a probability distribution of aquatic EECs reflective of conditions around actual ponds within the ecological setting of interest.

AGRO 106

GIS approach to identify vulnerable surface water monitoring sites to assess pesticide fate, transport, and exposure potential

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Focused monitoring studies, when designed correctly, can significantly increase the accuracy and confidence in pesticide exposure/risk assessments. The US Environmental Protection Agency (USEPA) estimates pesticide aquatic exposure potential by modeling a standard ecological pond scenario intended to represent upper bound exposure conditions. When necessary, monitoring data may be collected to assess the accuracy and conservatism of modeled estimates. To be useful in regulatory assessments, monitoring data should represent vulnerable environmental conditions by considering actual or potential pesticide use, surface water runoff potential, water body types and dimensions, contributing watershed area, and the fraction of the watershed treated. This paper demonstrates a Geographic Information System (GIS) approach that was used to identify candidate water bodies rapidly for inclusion in a monitoring study designed to assess the accuracy and conservatism of modeled surface water estimates.

AGRO 107

Comparison of three leaching models of different sophistication for estimating shallow groundwater concentrations

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Leaching of agricultural chemicals in soil depends on a number of factors, including field hydrological properties, local meteorology, chemical use, and environmental fate characteristics. Computer models for pesticide soil leaching assessment take into account these factors to a various extent. This presentation evaluates three models, SCI-GROW, PRZM3.12, and kinetic-PRZM, each of which represents a different level of sophistication for these factors. SCI-GROW is a Tier 1 regulatory model developed by the US Environmental Protection Agency (USEPA), which is based on a regression with shallow groundwater monitoring data. PRZM3.12 is a comprehensive field scale model which takes into account all major factors in an agricultural field. The model kinetic-PRZM was developed based on PRZM3.12 after incorporating sorption kinetics in the fate subroutine. A regional-scale soil data set is run by each of the models. Distributions of model outputs are compared to evaluate the sensitivity of the processes each model represents a group of statistical metrics. Propagation of variability in inputs and simplification of the environmental fate processes will be examined. Validity of using simple models for regional-scale leaching assessment will be discussed.

AGRO 108

Validation and extension of a regional groundwater vulnerability assessment tool in Hawaii for agrochemicals at a national scale

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We have previously reported the revision of a GIS-based pesticide leaching tool in Hawaii that can begin to assess regional groundwater vulnerability to new agrochemicals such as volatile organic compounds (VOCs). The updated tool includes two additional terms in the screening indices to account for volatilization loss from soils, illustrating the leaching potential of the VOCs using three (chemical, soil, and recharge) benchmark properties which are widely available. In the present study, we will discuss the validation of our statewide assessment tool with its extended use of national-scale vulnerability assessment. The statewide tool was examined with two different types of analytical (STANMOD) and numerical models (HYDRUS) in a given set of local conditions. Extensive soil and recharge databases for the conterminous United States, along with national-level fertilizer and pesticide sale data, were compiled to assess groundwater vulnerability on a national scale. Tentative findings from our ongoing research showed that the statewide tool provides an acceptable level of prediction accuracy with other models at high convective velocities (e.g., more recharge). However, the result of national-scale vulnerability assessed by the state level tool was quite different from that of a hybrid model used by the USGS (combining statistical model and GIS, often referred as WARP), due mainly to low recharge rates in the mid-part of the continental US. Therefore, this study highlights the importance of determining accurate annual groundwater recharge amounts for assessing groundwater pollution potential, especially for national-scale vulnerability assessment. At the end of this study, an alternative screening tool using the Meta Model that reduces the dimensionality of input data in the numerical model with neural networks is briefly discussed.

AGRO 109

Bridging the gap in quality assurance to academic settings for government regulatory science

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As the government requirements for data needed to conduct risk assessments on pesticides grow increasingly more complex, so does the need to guarantee sound reproducible science in areas exploring very unknown results. This poses a great dilemma as quality assurance principles require sometimes onerous documentation and constant recalibration and recalculations. While this ensures quality results, the cost and burden can be prohibitive to academic environments. At the same time regulatory bodies demand more and more cutting edge data. How can these two seemingly opposing forces be compromised and still produce accurate scientific data? This talk will focus on the changing face and pressures on the US EPA and their subsequent requests for data from registrants, data that require going outside the very controlled quality assurance environment of GLP labs. This talk will look at the evolution of the GLPs, the evolution of pesticide science, and how as 21st century regulatory consultants we bridge the gap between the two.

AGRO 110

Use of a study protocol to assist in assuring appropriate documentation when conducting research in a non-GLP laboratory

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This presentation will discuss the various means by which a protocol can assist in the conduct of a research study in an academic laboratory, specifically a research study that is designed to address potential regulatory issues, and as such may be submitted to a regulatory agency. A protocol is used to carefully detail the research objective and the experimental approach/design necessary to achieve that objective. In the process of preparing a study protocol, details of the planned research can be addressed to help insure that many of the major aspects of good laboratory practices (GLP) are fulfilled in a non-GLP laboratory setting. A GLP-consistent protocol can provide a detailed roadmap for conducting a study in a manner that will address issues relating the documentation of study-related activities. The protocol specific items to be discussed include: characterization of the test substance and other major reagents, description of the test system, experimental design, experimental endpoint (parameters to be assessed), description of procedures used to collect data, collection/storage/analysis of samples, statistical methods, maintenance of the study records/data, and description of how the study findings will be reported. Many of the details of laboratory procedures that are normally addressed by standard operating procedures (SOPs) in GLP-compliant laboratories can also be addressed using a study protocol; examples will be provided. Ultimately, documentation is the critical factor when performing studies in the spirit of GLP, and the protocol can be used to help assure that documentation of the critical aspects of a study is appropriately performed.

AGRO 111

Non-GLP studies: Critical aspects required to help assure data integrity, accuracy, and study reconstruction

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In some cases, it is impractical to implement a full GLP (US EPA Good Laboratory Practice Regulations, 40 CFR part 160) compliant infrastructure in a facility that conducts mainly non-GLP studies. This is typically the case when specialized equipment or processes are being utilized. Although such facilities can be at the top of their field in specialized procedures, they may have never been introduced to the concept of GLPs so would likely not have processes in place for documented training, written standard operating procedures, formal instrument calibration with documented maintenance, assuring study reconstruction, and/or quality assurance review of data generated and final report. This presentation will discuss the critical aspects required to help assure data integrity, accuracy, and study reconstruction when conducting non-GLP studies.

AGRO 112

Ensuring data quality for studies conducted in academic research laboratories

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The Interdisciplinary *Toxicology Program* at The University of Georgia is one of the primary collaborators with the Council for the Advancement of Pyrethroid Human Risk Assessment on a multi-year research effort. The overall objective of this project is to examine whether children are more sensitive to the neurological effects of pyrethroid insecticides. A number of different studies are being conducted at The University of Georgia to provide data for input into the physiologically-based pharmacokinetic models (PBPK) that are key to addressing this question. These parameterization studies include: measurement of plasma protein binding; determination of tissue:blood partition coefficients; measurement of *in vivo* pharmacokinetic parameters, and assessing whether pyrethroids are substrates for cellular transport systems. None of the university laboratories doing this work are true Good Laboratory Practice (GLP) certified facilities. Nonetheless, because the data are going to be used for regulatory decisions by the EPA, ensuring data quality and permitting the studies to be critically reviewed has required the Interdisciplinary *Toxicology Program* to embark on a broad effort to ensure that the studies are conducted in the spirit of GLP. A variety of different systems and approaches have been put into place to assure this happens. The challenges associated with this effort, as well as the approaches devised and benefits derived, will be presented.

AGRO 113

Development and use of a novel CAR direct activation assay to investigate species differences in mode of action with conazole-induced rodent liver tumors

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Sensitive and quantitative direct activation assays for human, rat, mouse, and dog forms of the constitutive androstane receptor (CAR) were developed in an academic-industry collaboration to address the link between CAR activation and high-dose liver tumors in rodents. The effectiveness of these novel CAR assays was demonstrated via activation with model substrates of each species' CAR and documented by publication in a peer-reviewed journal. The utilization of the assays to help elucidate the mode of action for mouse liver tumors with propiconazole, a registered conazole fungicide, will be described, along with study design elements and reporting approaches that provided an optimal product for submission and review by regulatory authorities. The CAR1 reference form of CAR exhibits high constitutive activity resulting in poor responsiveness in conventional reporter assays, because even in the absence of chemical activator, the background activity in control assays is near maximal. However, the CAR3 human splice variant lacks constitutive activity while retaining ligand interaction profiles characteristic of CAR1. Therefore, reporter assays that utilized the CAR3 variant were developed to provide sensitive and quantitative direct activation assays for human, rat, mouse, and dog CAR. In further studies, the CAR3 direct activation assay has also been utilized to help assess species differences for

propiconazole, a mouse liver tumorigen at excessive dose levels. Large increases above control levels in luciferase activities were observed with propiconazole treatment for mouse CAR (40-fold) and rat CAR (60-fold). In contrast, the maximal activation of human CAR (3-fold) with propiconazole treatment, which was only increased significantly at the highest concentration tested, revealed an inherent quantitative difference between rodent CAR and human CAR responsiveness. These results illustrate the utility of this novel CAR assay to understand species differences in chemical response and assist in regulatory evaluations of the human non-relevance of high-dose rodent liver tumors.

AGRO 114

Evaluation of an in vitro assay to characterize the effects of environmental contaminants on native ion channels in the spirit of good laboratory practices: Role of university labs

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Current approaches to toxicity testing are time consuming, expensive, and typically rely on investigations that evaluate observable changes to whole animals. New approaches capable of assessing environmental contaminants in a cost- and time-efficient manner are required to provide information necessary for sound evaluation of the health effects of adverse environmental agents by the US EPA and other government agencies. These agencies often require Good Laboratory Practices (GLPs) as a means to document the performance of a particular study so that the experiment can be successfully reconstructed from archived information at a future date. Many universities do not have a Quality Assurance Unit; regular review of performance standards and documentation, which is in compliance with GLPs, is limited. Instead, the peer review process serves as a mechanism to ensure the quality of the data and analysis. To this end, we evaluated neurolemma-injected *Xenopus* oocytes as a system to characterize the action of pyrethroids on voltage-sensitive sodium channels. Our results indicate that rat brain neurolemma-injected oocytes display several different native ion channels into their plasma membrane. Microtransplanted ion currents were sensitive to TTX, omega-conotoxin MVIIC, and chlorotoxin, indicating the presence multiple voltage-sensitive ion channels (voltage-sensitive sodium, calcium, and chloride channels) germane to the neuroexcitatory action of pyrethroids. This presentation will focus on the development of a high-throughput assay to characterize the effects of pyrethroids on different age rats in the spirit of GLP, including the documentation of test substances, calibration criteria for instrumentation and other methods employed to insure that the only variation observed is due to the biological preparation.

AGRO 115

Challenges and solutions for utilizing our research institutions' data to support regulatory decisions

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A survey of the current landscape of scientific research institutions from academia to contract laboratories reveals that the majority of the leading research institutions do not adopt the Good Laboratory Practice (GLP) Standards issued by the EPA in 40 CFR 160. This does not constitute an indictment of research conducted in these institutions, but it could mean that such research may not be accepted to support regulatory decisions by government agencies that adopted GLP requirements. However, in many cases the only relevant research and expertise required to advance our understanding of complex scientific issues with public health and safety implications comes from these institutions. In order to make it possible to use such valuable sources of knowledge and information to support regulatory decisions and to protect public health, an alternate set of standards is needed to provide assurances of data quality and integrity without adopting the GLP standard that has additional implications not compatible with the structure and mission of these institutions. This presentation will illustrate the problem and will explore possible solutions.

AGRO 116

US EPA Office of Pesticide Program guidance for considering and using open literature toxicity studies to support human health risk assessment

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In order to register a pesticide chemical (active and inert ingredients) in the US, industry is required to submit toxicology and/or exposure studies to US EPA. Office of Pesticide Programs (OPP). These submitted studies are most often conducted according to harmonized test guidelines (www.epa.gov/ocspp/pubs/frs/home/guidelin.htm). In addition, effects data from studies published in the open literature may also be considered in risk assessments. OPP has published guidance for considering and using open literature studies to support human health and ecological risk assessments (www.epa.gov/pesticides/science/literature-studies.html). The purpose of the open literature guidance is to assist in the conduct of open literature reviews and review of relevant publications for use in hazard and dose response assessment. It is intended to ensure transparency along with consistent consideration, use, and documentation of information. The document describes scientific considerations in reviewing open literature such as study design, relevance to adverse outcomes in humans, completeness of data reporting, statistical analysis, and public availability. According to the guidance, open literature studies are evaluated for their utility in risk assessment with respect to quantitative uses [e.g., establishing a No Observed Adverse Effect Level (NOAEL), Lowest Observed Adverse Effect Level (LOAEL), etc.]; or qualitative uses in weight of the evidence and risk characterization; or whether they are of insufficient quality and reliability.

AGRO 117

Twenty-first century toxicology and risk assessment: Going beyond guideline studies

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This presentation will highlight the types of studies that are increasingly becoming important for the assessment of the safety of chemicals. In contrast to the currently required studies (such as those in Section 158 for pesticides) that have been the subject of guidelines for carrying them out for a number of years, these new studies are often not fully validated, are subject to modification by the laboratories performing the studies, and are not presently carried out under strict Good Laboratory Practice (GLP) conditions. Nonetheless many of these studies are essential for making informed decisions about the safety of chemicals. In addition, given the National Academy of Sciences Toxicity Testing in the 21st Century report (Tox21), issued in 2007,

the traditional studies will become less important in the future as new testing methodologies emerge and are used for regulatory decisions. The Council for the Advancement Pyrethroid Human Risk Assessment (CAPHRA) has undertaken a multi-year research program designed to examine whether children are more sensitive to the neurotoxicity of pyrethroid insecticides than adults. Although many of these studies appear to be within the realm of academic research, they embrace the essence of the Tox21 approach, and the data derived has important applications for the safety assessment of chemicals currently in use. The program will lead to the development of a physiologically-based pharmacokinetic model to allow the prediction of brain levels of pyrethroids in humans. Because of this, CAPHRA has developed a careful, well-considered approach to ensuring data quality for studies conducted outside of traditional GLP facilities. Examples of the studies being conducted by CAPHRA, as well as other studies that are consistent with the Tox21 regimen will be discussed. An approach to ensuring data quality will be presented.

AGRO 118

Multi-year field study of the fate and transport of three insecticides in an agricultural ecosystem

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With the increasing prevalence of transgenic crops used in combination with insecticides, environmental fate is critical to understanding potential non-target species effects. Concentrations of Cry1Ab, a transgenic insecticidal Bt protein used in maize, tefluthrin, a pyrethroid insecticide, and two neonicotinoid insecticides used as seed coatings were measured in soil, runoff water, and soil pore water before, during, and after maize planting over three years. Runoff water samples frequently contained Bt-Cry1Ab and had the highest concentrations of any water samples. Tefluthrin was detected at the highest concentrations in soil samples and was not found to be transported by water. Neonicotinoid seed coating compounds were detected in water and soil samples with the highest concentrations found in soil pore water samples. While Cry1Ab proteins and neonicotinoids were not found in environmental matrices at ecologically relevant concentrations, tefluthrin was often detected at or above documented LC_{50} literature values during the growing season.

AGRO 119

Assessing the removal of hormones and their potency as endocrine-disrupting chemicals in dairy wastes through an anaerobic digestion system

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Manure generated by dairy farms contains excreted natural estrogens and their conjugates, as well as other hormones that have been used to increase milk production. Therefore, when manure is applied to fertilize croplands, these hormones may be spread in the environment and can potentially reach surface water by run-off, especially when a heavy rain event occurs immediately after land application. Livestock farms implement manure storage and treatment systems to decrease nutrient loading to the environment. Therefore, it is important to evaluate the extent at which estrogens are removed during storage or treatment of manure prior to land application. In this study, the concentrations of estrogens [estrone (E1), 17β–estradiol (E2), estriol (E3)] and their conjugated forms (glucuronides and sulfates) were evaluated in an advanced digestion facility (CH4 Biogas™). This facility includes a pasteurization step, followed by a 22-day anaerobic digestion process. All samples were analyzed by enzyme-linked immunosorbent assay (ELISA), yeast estrogen screen (YES) assay, and liquid chromatography- tandem mass spectrometry (LC/MS-MS). The results from YES assay showed a much higher E2-equivalent than the E2 concentrations observed in ELISA. This could mean that there are many other hormones present in the manure that have significant estrogenic activity. Increase in E1 concentration after digestion indicates deconjugation of glucuronides and sulfated conjugates. The sample matrix affected the analysis using both ELISA and LC/MS-MS, indicating that improved sample preparation is necessary.

AGRO 120

Determination of carbon nanotube uptake, translocation, and bioaccumulation in corn (*Zea mays L.*)

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Engineered carbon nanotubes (CNTs) have various applications in industries such as wastewater, environmental remediation, and agriculture. With their increasing usage, there is an increased likelihood that CNTs could enter the terrestrial environment where potential plant uptake and dietary exposure to humans may occur. This study was aimed to address uptake, translocation, and bioaccumulation of different types of CNTs in corn using a newly-invented microwave technique which can quantitatively determine CNT concentrations in biological samples. CNTs were characterized using thermogravimetric analysis and scanning electron microscopy (SEM). Corn was grown in 10, 100, and 1000 mg/kg multi-walled carbon nanotubes (MWNTs) in soil for 40 d. Corn was grown in 0, 10, and 100 mg/kg of unmodified, covalently modified, and surfactant stabilized single-walled carbon nanotubes (SWNTs) in soil for 40 d. MWNTs were taken up into roots at concentrations < 10 µg/g in plants exposed for 40 d. MWNTs were also translocated to above ground portions of the plant but at much lower concentrations (≤ 6 µg/g). Uptake and accumulation studies with SWNTs are ongoing. Roots, stems, and leaves were harvested, dried, grounded, and analyzed using a microwave technique to determine CNT concentrations. Further studies of CNT uptake, translocation, and accumulation in plants will lead to awareness of potential human exposure and risk assessment.

AGRO 121

Evaluation of glufosinate and glyphosate translocation in young almond (*Prunus dulcis*) trees

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Glufosinate is an important herbicide for weed control in California orchards. Although glufosinate is generally used as a contact herbicide, almond growers have expressed concern about injury to young almond trees suspected to be from translocation of the herbicide. The objective of this study was to evaluate uptake and translocation of glufosinate, in comparison to glyphosate, in young almond trees. ^{14}C-radiolabeled glufosinate or glyphosate was applied to leaf, green bark, or old bark (rootstock) of two-year-old almond nursery stock. Tissues were destructively harvested 1, 3, and 7 days after treatment. Absorption of glyphosate was greater than glufosinate regardless of application site. Most

of the herbicide applied to old bark remained in the treated area (52% of the glufosinate and 94% of the glyphosate). In contrast, when applied to leaf or green bark, only 17 to 19% of the glufosinate and 32 to 43% of the glyphosate remained in the treated area. For both herbicides, ^{14}C was recovered in roots, which suggests that there is long distance translocation of glufosinate that is comparable to glyphosate. However, more research is needed to determine whether the radioactivity recovered in almond roots was in the form of the parent compound or a metabolite. This work addresses almond grower concerns and increases our understanding of the mobility of glufosinate in woody specialty crops in California.

AGRO 122

Biological validation of enzyme-linked immunosorbent assays for detection of Cry proteins in the environment

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As the use of transgenic crops expressing genes for the production of insecticidal crystalline (Cry) proteins increases, concerns that these proteins may have adverse effects on non-target organisms also increase. Accurately detecting these proteins in various environmental matrices is essential for determining possible exposure of non-target organisms to these proteins. Enzyme-linked immunosorbent assays (ELISAs) have been widely used for detection of Cry proteins in the environment. However, their results are not typically validated biologically to ensure that only bioactive Cry proteins are being detected; therefore, accurate concentrations of the bioactive protein may not be properly represented in ELISA results. This could potentially lead to overly-conservative risk assessments and unnecessary regulation. Thus, in order to properly study Cry proteins in environmental matrices, standardized methods of detection that can be biologically validated are needed. This research project will improve methods of detection for Cry proteins in environmental matrices by developing a framework for biological validation of ELISA procedures. The first objective will be to develop a laboratory model system to degrade Cry1Ab. This will mimic degradation occurring in the environment and produce solutions of Cry1Ab fragments. In the second objective, aliquots of these solutions will be analyzed using ELISAs and bioassays. The results of the ELISAs and bioassays will be compared to determine anomalies in the data, i.e., if the fragments are detectable by ELISA but have no bioactivity and vice versa. Finally, specific guidelines for biological validation of ELISAs will be established.

AGRO 123

Development and validation of a method to quantify Bt-Cry1Ab in water matrices

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Genetically-modified crops expressing insecticidal crystalline (Cry) proteins derived from *Bacillus thuringiensis* (Bt) now dominate the agricultural landscape throughout much of the world. The wide-spread planting of Bt products has raised questions regarding the environmental fate of Bt toxins. Researchers have developed and validated methods to quantify Bt proteins in soil matrices using enzyme-linked immunosorbent assay (ELISA), but currently there is no published standardized method for the evaluation of Bt proteins in water. The objective of this research was to optimize the extraction of Bt-Cry1Ab from three water matrices collected from agricultural and forested sites in central and southern Illinois. The extraction methods were evaluated for matrix effects, extraction efficiencies, and precision using a series of ELISA experiments. The development of a standardized water extraction method bolsters the integrity of research involving the quantitation of Bt proteins in aquatic settings and provides a foundation for environmental risk assessments.

AGRO 124

Deorphanization and pharmacological profile of a tyramine receptor from the southern cattle tick (*Rhipicephalus microplus*)

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Tyramine is a biogenic monoamine commonly found in invertebrates and is the synthetic precursor to octopamine. Tyramine and octopamine exert various physiological/biochemical actions by interacting with G-Protein-Coupled Receptors (GPCRs). Octopamine receptors are well studied and have a defined pharmacological profile; tyramine receptors are not as well studied. Octopamine receptors are believed to be the target of formamidine insecticides. Previously, a putative octopamine receptor was isolated from amitraz-susceptible and amitraz-resistant southern cattle tick (*Rhipicephalus microplus*), but its ligand was never confirmed. The amitraz-resistant receptor displayed two nucleotide substitutions. Expression of these putative receptors in Chinese hamster ovary (CHO) cells resulted in a 41-fold higher functional response to tyramine versus octopamine. Furthermore, the pharmacological profile was similar to known tyraminergic compounds. Functional responses indicate that the putative octopamine receptor is actually a tyramine receptor.

AGRO 125

Quantitative lipid analysis of gut microflora consortium in the Giant Panda

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The giant panda, *Ailuropoda melanoleuca,* is a uniquely adapted member of the family Ursidae in that they are herbivorous with their main source of food being a variety of species of bamboo. Studies have shown that the giant panda lacks the innate capability to create cellulases that are necessary in the degradation of its woody sustenance. A previous metagenomics analysis has identified several cellulolytic organisms and oleaginous organisms. Fresh panda fecal samples were collected from two captive bears residing at the Memphis Zoo and kept under anaerobic conditions. These fecal samples where then used to inoculate an anaerobic media and allowed to grow under varying cellobiose concentrations. Sugar content determination was performed using an ELSD detector, while lipid production was quantified using gas chromatography by way of fatty acid methyl ester (FAME) analysis.

AGRO 126

Assessment of conventional waste management and advanced waste treatment systems in removing veterinary antibiotics

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The introduction of veterinary antibiotics to environmental systems is a salient concern due to the potential for the emergence and proliferation of resistant genes resulting from chronic exposure to low doses of excreted, unmetabolized antibiotics, leading to an eventual decrease in drug efficacy. Unmetabolized antibiotics are continuously introduced to croplands through repeated application of animal manure and undergo transport to surrounding surface waters, aquifers, and bodies of water. It is important to assess the effectiveness of various manure treatment and waste management practices in the elimination of antibiotics. Dairy animal waste management practices present a unique opportunity to minimize environmental exposure of these compounds through advanced treatment regimes. The removal efficiencies of four classes of environmentally-relevant veterinary antibiotics used in representative dairy farms in Western New York was examined using liquid chromatography tandem mass spectrometry (LC/MS-MS). Relative concentrations of tetracyclines, sulfonamides, macrolides, and penicillins in treatment influent and effluent were analyzed. Management systems examined included a mixed-waste anaerobic biogas reactor, conventional anaerobic digester, and traditional manure waste storage.

AGRO 127

Dynamic coupled fluxes of current-use pesticides in air-water/soil-sediment system in a city in southern China

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Dynamic coupled fluxes of organophosphate and pyrethroid pesticides were analyzed based on monitoring data to diagnose the key fate and transport processes in an air-water/soil-sediment system in Guangzhou, China. The total air-water fluxes including air-water exchange, dry particle deposition, wet particle deposition, and wet dissolved deposition exhibited deposition for chlorpyrifos, bifenthrin, and cypermethrin, while volatilization was observed for *lambda*-cyhalothrin and permethrin. The direction of water-sediment diffusion was from sediment porewater to overlying water for all the target pesticides. However, the net direction of pesticide transport was from overlying water to sediment, because suspended particle settling and sediment burial processes dominated the transport. Chlorpyrifos had similar total air-water and water-sediment fluxes, which suggested that atmospheric loading was one of the important sources for water and sediment budgets. Instead, the total air-water fluxes of pyrethroids were two to three orders of magnitude lower than total water-sediment fluxes, and suggesting that sediment-associated pyrethroids were not mainly from air deposition. The estimated soil runoff fluxes of pyrethroids were similar to the total water-sediment fluxes, which suggested that soil runoff might be one of the important sources for water and sediment budgets. Additionally, annual fluxes of current-use pesticides were calculated in Chebei Creek, the longest urban creek in Tianhe, Guangzhou. This is one of the limited studies assessing the dynamic fluxes of chlorpyrifos and pyrethroids in an air-water/soil-sediment system. The results gave a better description on the distribution and fate of pesticides among the environmental compartments and provided basic data for comprehensive risk assessment of current-use pesticides.

AGRO 128

Isomer-specific biodegradation of nonylphenol in river sediments

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Nonylphenol (NP) isomers are metabolites of non-ionic surfactant nonylphenol ethoxylates, are well known environmental estrogens, and are frequently detected in water and sediment. Recent studies showed that numerous NP isomers have different estrogenicity and biodegradability. In this study, for the first time, we investigated the biodegradability of 19 NP isomers in two river sediments under both aerobic and anaerobic conditions. Under aerobic conditions, NP isomers degraded efficiently. In one sediment, NP isomers underwent an initial rapid degradation period lasting 14-21 d after treatment; initial half-lives ranged from 0.86-13.2 d depending on the specific isomers. In another sediment, the NP isomers underwent an initial 7-14 d lag period, which was followed by a fast degradation phase with half-lives ranging from 15.1 to 20.0 d. Under anaerobic conditions, very slow or no degradation was detected. This study suggested the biodegradation of NP isomer in sediment was isomer and site specific.

AGRO 129

Synergistic effects of verapamil on tacrine toxicity to vector mosquitoes

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Mosquitoes affect human health worldwide as a result of their ability to vector multiple diseases. Widespread resistance is a serious public health challenge that limits the use of high efficacy insecticides to reduce the risk of mosquito-vectored diseases. P-glycoprotein is an efflux transporter that assists in maintaining the blood-brain barrier interface of mosquitoes and may serve as a first line of defense to insecticide exposures. Previous studies have demonstrated the blood-brain barrier of insects interferes with the target-site action of insecticides; however, the interaction of mosquito P-glycoprotein towards these chemistries is unclear. This research study is focused on the toxicological, biochemical, and molecular characterization of mosquito P-glycoprotein as a first step towards the identification of efflux transporter interactions and the validation of a potential resistance mechanism against insecticide exposures. Here, we will provide a: 1) toxicological analysis of tacrine and *bis*(7)-tacrine (acetylcholinesterase inhibitors) for mosquitoes alone and in combination with verapamil (P-glycoprotein inhibitor); 2) biochemical analysis of acetylcholinesterase for mosquitoes exposed to these chemistries; and 3) molecular analysis of P-glycoprotein in these mosquitoes. The long term goal of this research study is to provide a better understanding of chemomodulators that might be used to enhance the effectiveness of established and experimental insecticides that are substrates for mosquito P-glycoprotein.

AGRO 130

Voltage-sensitive potassium channels expressed by hormone treatment in mosquito cell lines

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The goal of this research was to evaluate the presence of insecticide target proteins from hormone-induced differentiated insect cell lines, which could lead to new, high-throughput screening methods and a way to mass produce insect proteins for basic research. This study used cultures of Sua1B cells with the application of 20-hydroxyecdysone (20-HE), an insect molting hormone, to initiate expression of insecticide target proteins and to evaluate insecticidal compound effects. Whole cell patch clamp techniques have shown the presence of K_{IR} inwardly rectifying and Kv_2 delayed-rectifier potassium channels expressed in as little as four hours after treatment with 20-HE. The expressed currents had current-voltage relationships diagnostic and were inhibited with an IC_{50}= 8 mM of tetraethylammonium (TEA), a well-established potassium channel blocker. The direct presence of ion channels and receptors in these cells will accelerate high-throughput screening for new insecticides and make screening more economical.

AGRO 131

Evaluation of synthetic compounds as novel mosquitocides targeting potassium channels for control of *Aedes aegypti* and *Anopheles gambiae*

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The successes of disease vector control have become increasingly threatened by the development of insecticide resistance. Therefore, continued disease control efforts require the development of insecticides with novel modes of action. Potassium channel-directed compounds have been screened in paralysis and lethality bioassays, as well as in electrophysiological assays, in the search for a selective and potent lead insecticide. In larval bioassays, many of the known potassium channel blockers have LC_{50} values >100 ppm. However, 4-aminopyridine, tetraethylammonium chloride, and 4-tert-octylcatechol have shown LC_{50} values that are <50 ppm. Electrophysiological assays, including muscle depolarization and muscle twitch force recordings show responses consistent with potassium channel block and with paralytic effects. Established and experimental blockers have also been tested on potassium channels of rat embryonic neurons, which generally show low sensitivity and suggest a favorable selectivity profile.

AGRO 132

Influence of amendments on the degradation of pharmaceuticals in soil

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Pharmaceutical and personal care products (PPCPs) are emerging contaminants in the environment. This study was carried out using ^{14}C-acetaminophen and ^{14}C-sulfamethoxazole to assess the influence of amendments on their degradation in soil. When incubated at room temperature, there was a gradual dissipation of both compounds. After 14 days, 18% of the applied acetaminophen was lost via mineralization from the unamended sandy clay loam soil. Enhanced $^{14}CO_2$ production was seen in soil with higher organic carbon content. Application of biosolids, compost, and activated carbon significantly decreased the transformation; mineralization decreased as the amendment ratio increased. For instance, only 2.4% of ^{14}C-acetaminophen was mineralized to $^{14}CO_2$ in the 10% biosolids amended soil, as compared to 18% in the soil without amendment. Addition of NH_4NO_3 temporarily inhibited mineralization, suggesting that organic amendments may serve as a more readily available N source than the pharmaceuticals resulting in the reduced transformation in amended soil.

AGRO 133

Voltage-sensitive potassium channels as new target sites for biorational insecticide design

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This presentation will discuss potassium ion channels from the perspective of biorational insecticide design. Potassium channels exist in a variety of molecular configurations, display a range of voltage-dependent properties, and are important for regulation of electrical excitability of nerve and muscle. Moreover, they are the targets of several classes of synthetic compounds and natural toxins, suggesting that they could be targeted for insecticide development. Examples exist of ligands that activate or block these channels to affect membrane potential or excitability. An effort to develop insecticidal chemistry from blockage of the calcium-activated potassium channel was recently disclosed. There is ongoing research into blockers of the Kir (inward rectifier) and Kv2 (delayed rectifier) potassium channels of mosquitoes. Interestingly, these two channels have opposite voltage-dependence, Kir channels activating at more negative potentials and Kv2 more positive potentials. Available results from initial studies targeting these channels will be discussed.

AGRO 134

Mosquito larvicidal lipopeptide produced by *Xenorhabdus*

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There is a critical need for improved agents to control mosquitoes due to the development of insecticide resistance. We have identified a mosquito larvicide produced by a strain of the *Xenorhabdus innexi* bacterium. The larvicide is a secreted low molecular weight peptidal molecule. The *Xenorhabdus* larvicidal lipopeptide toxin is highly toxic to larvae of the yellow fever and the malaria mosquito species. The *Xenorhabdus* mosquito larvicidal lipopeptide toxin has a different mode of action from *Bacillus* endotoxins. The specificity, the stability, and the mode of action of the *Xenorhabdus* larvicidal lipopeptide toxin make it potentially an effective alternative insecticide for integrated pest management for mosquitoes.

AGRO 135

Plant-derived products for control of ticks and biting flies affecting livestock

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Livestock production in many parts of the world, including the Americas, is severely affected by blood-feeding ectoparasites. The cattle tick *Rhipicephalus (Boophilus) microplus*, the horn fly *Haematobia irritans irritans*, and the stable fly *Stomoxys calcitrans* are economically important ectoparasites affecting beef and dairy cattle production systems. Their control has relied on synthetic chemical pesticides. However, the indiscriminate use of synthetic pesticides has led to the development of pesticide resistance. New chemical entities with novel modes of action are needed to manage problems associated with pesticide resistance. This review focuses on essential oils and other plant-derived natural products under evaluation against these target species. Essential oils extracted from several plant species have been tested for activity against different life stages of the cattle tick in different countries. The majority of this work has been done using *in vitro* assays, and few essential oil preparations have been tested on animals. The major chemical components of some essential oils have been identified, and the activity of individual compounds profiled against tick or biting fly species. Essential oils and related compounds demonstrated various levels of activity against livestock pests. Natural products tend to be evaluated as contact pesticides, and some of essential oils and related natural compounds were shown to be highly effective repellents against biting flies. Commercial formulations are under development in several countries for livestock pest control. The commercialization of plant-derived products for use in livestock pest control faces several challenges including an inferior efficacy profile under field conditions, relatively higher production costs, and supply issues to meet market demand. Little is known about the modes of action of plant-derived compounds shown to be toxic to livestock pests. It is expected that recent progress in toxicological and pharmacological studies will help elucidate the modes of action of these promising plant-derived natural products.

AGRO 136

Natural product-based insecticidal structure activity relationship investigations

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An *Aedes aegypti* larval toxicity bioassay was performed on compounds representing many classes of natural compounds including polyacetylenes, phytosterols, thiophenes, flavonoids, sesquiterpenoids, and triterpenoids. Among the compounds studied, two eudesmanolides, alantolactone and isoalantolactone, as well as many thiophenes showed larvicidal activities against *Ae. aegypti* and therefore were chosen for further structure-activity relationship investigations. Structural modifications were performed on both alantolactone and isoalantolactone in an effort to understand the functional groups necessary for maintaining and/or increasing its activity and to possibly lead to more effective insect control agents. Structure-activity evaluations of thiophenes found relationships between the number of thiophenes rings and acetoxy groups.

AGRO 137

Neuropeptides and receptors as targets for bioinsecticides

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Insect neuropeptides regulate critical processes and behaviors in insects, though they are unsuitable as tools for arthropod endocrinologists and/or as pest management agents due to poor biostability and/or bioavailability characteristics. Peptidomimetic and non-peptide analogs can overcome these limitations and either over-activate or block critical neuropeptide-regulated functions. Stereochemical and conformational aspects critical for the successful receptor interaction of several classes of insect neuropeptides were exploited to design/discover mimetic analogs with enhanced biostability and selectivity. These classes include the insect kinins, insectatatachykinins (or tachykinin-related peptides), and the pyrokinins. While natural, unmodified peptides of these three classes demonstrate little or no activity, biostable versions elicit potent antifeedant and/or insecticidal properties in insects such as aphids when delivered by an oral route. Some biostable analogs are inactive and do not elicit significant antifeedant or aphicidal effects. In some cases, the aphicidal effects can be blocked by neuropeptide antagonists, providing compelling evidence that the insecticidal activity is specific and mediated via a neuropeptide receptor. The mimetic analogs provide important leads for alternative aphicides. Diapause hormone (DH), an important sub-class of the pyrokinins, has been shown to terminate pupal diapause in heliothine species. Potent biostable analogs have been designed that can prevent the onset of pupal diapause via treatment of the preceding larval stage of a heliothine insect. Conversely, an antagonist, developed by a novel conformation-based strategy, can block the pupal diapause termination activity of DH. The observed activity of both agonists and antagonists is dependent on the presence of a DH core sequence. These mimetic DH analogs provide leads for the generation of agents capable of disrupting the protective state of diapause in economically important lepidopteran pests.

AGRO 138

G-Protein-Coupled Receptors (GPCRs): A target of plant terpenoids

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Plants have evolved beneficial and protection mechanisms including the production of essential oils. Essential oils are the odiferous component of plant extracts, which give plants a variety of unique properties. Essential oils are composed of various terpenoid compounds, particularly monoterpenoids and related aromatic compounds, along with sesquiterpenoids. A variety of terpenoids have been shown to have a toxic effect against insects. It is thought that this toxic action occurs through a neurological mechanism of

action. The presented research will focus on arthropod GPCRs which have been and continue to be an under-utilized target for pest control.

AGRO 139

Potent nematicidal activity of redox-active aromatic aldehydes against *Meloidogyne incognita*

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Sustainable agriculture providing with food quality and sufficiency is a major challenge for farmers, agro-industries, researchers, and governments. Synthetic nematicides have long had application in plant protection for the control of the root-knot nematodes (*Meloidogyne* spp.). Phytonematodes represent one of the most damaging pests causing more than $100 billion of crop losses in fruit and vegetable production annually. In the recent years, the environmental, food safety, and animal welfare issues pose the need for alternative nematode control measures. Plant secondary metabolites, involved in the complex chemical-mediated interactions between a plant and other organisms in its environment, can provide bioactive leading compounds to be studied further as innovative nematode control measures in Integrated Pest Management (IPM) programs. Here, we report the nematicidal activity of selected aromatic aldehydes against the root knot nematode *Meloidogyne incognita*. The most active aldehyde was phthalaldehyde with an EC_{50} value of 10.6 ± 5.9 mg/L followed by salicylaldehyde and cinnamic aldehyde with an EC_{50} of 10.8 ± 1.0 and 12.1 ± 5.3 mg/L, respectively. The reactivity of tested aldehydes against a synthetic peptide resembling the nematode cuticle was characterized by means of liquid chromatography mass spectrometry. We report that at the test concentration of 1 mM, the main adduct formation was observed for 3,4-dihydroxybenzaldehyde, 2-methoxybenzaldehyde, and 3,4-dimethoxybenzaldehyde. Considering that 2-methoxybenzaldehyde and 3,4-dimethoxybenzaldehyde were not active against *M. incognita* in *in vitro* experiments, we hypothesize a different mechanism of action rather than an effect on the external cuticle modification of nematodes. The results of this investigation reveal that aromatic redox-active aldehydes can be considered as potent nematicides, and further investigation is needed to clarify their mode of action.

AGRO 140

Phytochemically based strategies for nematode control

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One of the most important problems facing global agricultural productivity is the lack of chemically based control strategies for nematodes, a consequence of deregistration of numerous chemical nematicides because of environmental or health-associated problems. Because plant-based products or compounds are often safer than synthetic ones and consequently receive less regulation, researchers are utilizing several strategies for exploiting phytochemicals as nematode control agents. Specific experimental or practicable materials include the incorporation of nematode-antagonistic plant amendments to soil, the application of plant extracts or plant-based formulations, or the direct application of compounds discovered to be nematotoxic. Like any chemical nematicide, the ideal phytochemical or active analog would be inexpensive, effective only against agricultural pests and pathogens, and able to move in soils and persist in a manner that is agriculturally effective yet environmentally safe. Specific compounds and products will be emphasized.

AGRO 141

Natural and synthetic isothiocyanates for nematode control

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Methyl bromide (MeBr) had been widely used since the 1940s to control soil-borne pests prior to planting crops. Its success as a soil fumigant was largely due to its wide spectrum of control against plant pests and pathogens during many stages of life, the ability to rapidly penetrate soils, and the ease of application. However, in 1991, MeBr was identified as a stratospheric ozone-depleting compound, which has led to its phase-out in the United States. The MeBr phase-out has jeopardized production of high-valued crops, however, research is on-going to find suitable alternative chemicals and approaches to manage plant pests and pathogens. Alternative chemicals include a number of natural and synthetic pesticides, including isothiocyanates. Soil fumigation with alternative synthetic pesticides continues the conventional approach to prepare soil for planting. Biofumigation is an alternate agronomic practice that uses decomposing plant tissues (e.g., *Brassica*), or seed meal to produce volatile chemicals in soil. Isothiocyanates are the most common chemical produced from *Brassica* and are related to the active ingredient in commercial products, such as metam sodium and dazomet. Isothiocyanates have been shown to be toxic many soil-borne pests and pathogens. The purpose of this presentation is to provide an overview of some of the problems growers are facing in a post-MeBr world, provide information on the effectiveness of natural and synthetic isothiocyanates in controlling plant pests and pathogens, and to offer possible areas of future research that may assist in protecting the environment and lead to the continued use of this important class of chemicals.

AGRO 142

Mode of action and anthelmintic activity of novel plant-based functional food additives

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Ascaris lumbricoides is the most prevalent soil-transmitted helminth infection in humans, afflicting approximately 1.5 billion people and primarily burdening children in poor underdeveloped areas of the world. Synthetic anthelmintics are the current method of treatment; however, resistance could potentially develop. Challenges remain in providing inexpensive deworming treatments that do not require a complex and coordinated infrastructure; functional foods may help overcome this. A controlled study was performed in pigs infected with *Ascaris suum,* an important porcine pathogen closely resembling *A. lumbricoides*,to determine the efficacy of two microencapsulated essential oil blends, TTN1013 and TTN1014, as functional food compounds. Sixty-four Yorkshire-cross pigs aged 21–24 days were randomly assigned to one of four groups: TTN1013 at a dose rate of 0.5 or 1.0 mg/kg, TTN1014 at 1.0 mg/kg, or 1.0 mg/kg equivalent of empty capsules (placebo). Treatments were administered daily through week 10 inside cream-filled sandwich cookies. Pigs were inoculated with *A. suum* eggs 5 days/week for four weeks (20 eggs/kg/week) beginning three days post initial treatment. Pigs were necropsied during week 11. All worms were recovered, counted,

measured for length and volume and separated according to sex. Fecal egg counts (FEC) were conducted weekly starting at week 6. Data were analyzed using a Poisson regression model accounting for group-dependent over-dispersion. TTN1013 at 1.0 mg/kg yielded a significant reduction in total (77%) and female (76%) worm counts, FEC (69%), and worm volume (63%) compared to the placebo. A dose dependent effect for TTN1013 was observed for these parameters, but differences at 0.5 mg/kg were not significant. TTN1014 did not have a significant effect. All pigs remained clinically normal and showed no adverse reactions or signs of reduced intestinal health. Based on these results, TTN1013 at 1.0 mg/kg shows promise as a daily supplement to reduce *Ascaris* infection in pigs and possibly humans.

AGRO 143

Natural nematicides and analogs

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Plants produce numerous defensive chemicals, some of which are active against insect or disease pests. Glucosinolates, cyanohydrins, and monoterpenoids are three classes of botanicals with activity against insects and nematodes. Bioassays were conducted on nematode pests in the laboratory, focusing primarily on the soybean cyst nematode. Laboratory studies determined that several glucosinolate aglycones from rapeseed, crambe, and crucifers had activity against the soybean cyst nematode and stored-grain insect pests, as did several natural cyanohydrins (from cassava, flax, almonds, lima beans, etc.). Some natural nematicides had sufficient volatility to express bioactivity through the vapor phase only. Synthetic analogs of glucosinolate aglycones and cyanohydrins were also screened for their bioactivity.

AGRO 144

Honey bee colony health, bee decline, and pesticides

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Managed honey bee colony numbers have declined significantly in the US over the last 60 years with annual losses now averaging over 30%. The majority of colony losses occurs during the winter months and is thought to be due to a combination of multiple stressors affecting colony health. The introduction and rapid spread of parasitic mites (tracheal and *Varroa* mites) in the mid to late 1980s lead directly to increased winter losses, but the introduction of in-hive acaricides significantly reduced mite impacts. In late 2006, several commercial beekeepers reported unexpectedly high colony mortality that was associated with the sudden loss of the adult worker population. The condition was named colony collapse disorder (CCD) and was reported shortly thereafter as a major factor associated with colony decline across the country. No specific causes of CCD have been identified, but a number of possible causes have been suggested, including parasite loads, pathogens (viruses and *Nosema*), queen failure, nutritional stress, migratory stress, and pesticide contamination. Since 2007, investigations of colony losses and bee decline have focused on pesticides and pesticide residues in hives, particularly the neonicotinoids, imidacloprid and clothianidin. Pesticide contaminants and residues in comb have been shown to affect colony health through impacts on worker behavior, disease susceptibility, longevity, and queen and drone reproductive physiology. However, there is no evidence that specific insecticides like the neonicotinoids play a more significant role in colony decline.

AGRO 145

Pollinators, pesticides, and pathogens: Linking honey bee colony health to chemical exposures

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The honey bee is the most widely managed crop pollinator and provides our agricultural industry with the sustainability and economic viability needed to satisfy the food and fiber needs of our society. The excessive use of pesticides is implicated in the reduced number of managed bee colonies available for crop pollination services. However, there are several gaps in our knowledge with respect to pesticide exposures and the health status of managed bee colonies. Thus, it is necessary to gather information relevant to the areas where knowledge is lacking to enhance our ability to predict conditions that are either favorable or unfavorable for bee colony health. Here, we will summarize our research findings related to pesticide impact on the microbiota community structure and function of managed bee colonies and the resulting nutritional and immune deficiencies that threaten colony health. These data are being used to model the health profiles for managed bee colonies exposed to pesticides in order to provide a theoretical framework to explain bee colony health thresholds and failures. In turn, the information gathered in this study will be translated into utilizable management practices to reduce the loss of managed bee colonies for both the apicultural and agricultural industry.

AGRO 146

Agrochemical formulant toxicities for honey bees

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Adjuvant and pesticide co-formulants are largely assumed to be biologically inert and are subject to minimal scrutiny and toxicological testing by regulatory agencies. Recently, we have shown that honey bees are unusually sensitive to organosilicone spray adjuvants and the solvent *N*-methyl-2-pyrrolidone, common co-formulants used in agrochemicals and spray adjuvants. Effects include learning impairment for adult bees and chronic toxicity in larval feeding bioassays. Most formulations we tested were more toxic to bees than their respective active ingredients. Knowing relevant environmental levels of adjuvants and inerts would allow improved risk assessment of total chemical loads and exposures for bee pollinators and other non-target species. We anticipate that if 'inerts' are influencing pesticide levels and general hive stress, formulation recommendations can be optimized for use in bee foraging areas. Impacts of synergistic pesticidal blends on bees cannot be fully understood without identification and risk assessment of co-formulant residues and their agrochemical interactions.

AGRO 147

Honey bee colony level responses to exposure of residues on flowers of the fungicide, propiconazole

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Two field experiments (2011 and 2012) were conducted to assess honey bee colony level effects when foragers were exposed to flowers with residues of the fungicide, propiconazole, under typical pest management applications. In both years, isolated non-sprayed fields and isolated treated fields were selected to place 10-12 colonies in each field throughout bloom (period of 1 month). Every colony

was monitored every 2-4 weeks both during and after bloom. Colony worker population, brood population, queen presence and health, queen egg laying rate, larval survival, worker longevity, hypopharyngeal gland size, and disease and parasitic mite prevalence were measured. Flowers and pollen were also collected for residue (exposure) measurement. We found that honeybee health affects of the commonly-used fungicide, propiconazole, are not entirely consistent between years. Although we can conclude that negative effects were documented. We found that overall exposure of honeybee foragers to residues on flowers does not reduce colony strength of worker or capped brood populations. Queen laying and capped brood survival also does not appear to be affected by exposure to sub-lethal doses of this fungicide. We did find evidence in both years to suggest that workers reared as larvae during bloom result in young nurse bees whose longevity is reduced.

AGRO 148

Comparative ecotoxicology of bee-pesticide interactions

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Neonicotinoid insecticides are widely used in crop protection. They are systemic and appear at trace levels in the nectar and pollen of mass-flowering crops which bees consume. Recently, the results of several semi-field trials have appeared in high-profile journals, and these have increased the public's concern over the use of neonicotinoids across extensive areas of crops and their potential threat to honey bees, wild bees, and valuable pollination services for crops and wild plants. Here, I summarise my laboratory investigations into the comparative resilience of individual adult bees to dietary neonicotinoids. I show that honey bees are likely to make a poor sentinel for effects on wild bees in general because they have a substantive capacity for metabolic detoxification. I also compare the effects of different neonicotinoids on individual bumble bees to show that impacts vary among these chemicals. Finally, I explore the potential for laboratory observations to underpin models of demographic toxicity, i.e., population projections based on effects on birth/death rates. I argue that these models are valuable tools for exploring the relative resilience or fragility of bee populations. I use this review to show that bee-neonicotinoid interactions are complex and likely varied in outcome and that care must therefore be taken to accommodate this into the evolving frameworks for pesticide regulation and environmental protection.

AGRO 149

Large-scale field study examining potential impacts on honey bees of exposure to clothianidin seed-treated canola

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Numerous biotic and abiotic stressors have been suggested for the unusually high number of honey bee (*Apis mellifera*) colony losses experienced in many parts of North America and Europe the past decade. The neonicotinoid insecticides are widely used plant-systemic compounds. This class of insecticide contains the active ingredients imidacloprid and clothianidin and has perhaps been subject to more scrutiny and scorn than any other potential cause of honey bee colony declines. Many laboratory studies have shown that neonicotinoids may elicit various acute, chronic, lethal, or sublethal effects on honey bees. However, higher-tier studies where dietary exposure to pollen and nectar occurs from soil or seed treatment applications have failed to demonstrate significant colony level effects. Large-scale field studies are usually the most refined and realistic method of characterizing risks of agrochemicals to honey bees, but are rarely undertaken due to their complexity and high cost. In summer 2012, we initiated a large-scale field experiment in southern Ontario to determine whether or not exposure to clothianidin seed-treated canola has any adverse impacts on honey bees. Colonies were placed in the middle of clothianidin seed-treated or control canola fields during bloom, and thereafter they were moved to an apiary with no surrounding agricultural production. Colony weight gain, honey production, pest incidence, bee mortality, number of adults, and amount of brood were assessed in each colony throughout summer and autumn. Several of these endpoints and overall overwintering success will again be measured in spring 2013. Samples of honey, beeswax, pollen, and nectar were regularly collected and samples are being analyzed for clothianidin residues by GC/MS-MS.

AGRO 150

Honey bee field studies: Assessing hive health after four consecutive years of exposure to flowering crops grown from thiamethoxam-treated seed

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This study investigated the long-term potential risk to honey bee colonies under natural field conditions by assessing hive health over four years of consecutive exposure to corn and oilseed rape crops grown from thiamethoxam-treated seeds. To quantify exposure, pollen and nectar collected from honey bees after foraging on flowering corn (pollen only) and oilseed rape (pollen and nectar) were analyzed for residues of thiamethoxam and its primary metabolite CGA322704. Residues of thiamethoxam and CGA322704 in corn pollen collected from honey bees were low; ≤ 50% of the samples had quantifiable levels of thiamethoxam or CGA322704; maximum concentrations were 2 µg/kg for parent and the primary metabolite. For oilseed rape pollen and nectar, thiamethoxam was detected more frequently in nectar (83% of samples) compared to pollen (50% of samples), however maximum residues were also low, 1 µg/kg in pollen and 3 µg/kg in nectar. No quantifiable residues of CGA322704 were detected in oilseed rape pollen and nectar. Throughout the study, mortality, foraging behavior, colony strength, colony weight, brood development, and food storage levels were similar between treatment and control colonies. Detailed examination of brood development throughout the years demonstrated that colonies exposed to the treated crop overwintered successfully and had a comparable health status to the control colonies in the following spring. These data confirm low exposure with no resulting impact on honey bee health from potential residues in nectar and pollen following the use of thiamethoxam as a seed treatment on corn and oilseed rape.

AGRO 151

Using data from semi-field enclosure studies for assessing the risk of pesticides to honey bees

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North American pesticide regulatory agencies have recently developed a framework for assessing the risk of pesticides to

honey bees. The framework includes the use of data from higher-tier, whole colony studies to address uncertainties from first-tier, screening level assessments. This presentation will focus on the use of semi-field enclosure studies to refine risk assessments. Semi-field studies allow for the assessment of exposure to and effects on the whole colony under more realistic exposure conditions, and they bridge the gap between laboratory and full field studies. Specific study design elements to assess exposure to and effects on different life stages and casts of honey bees will be discussed. Examples of data obtained from such studies will be presented. Advantages of these types of studies over other study designs will be highlighted. Limitations on the data that can be obtained and how it can be interpreted will also be discussed.

AGRO 152

Molecular determinants of the sweet-bitter Janus head of steviol glycosides and development of novel quantitation tools

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Increasing consumer demand for natural low-calorie sweeteners, with no organoleptic drawbacks compared to sucrose, necessitates a new quality of knowledge on the organoleptic properties as well as the molecular determinants of the sweet and bitter taste of diterpenic glycosides of *Stevia rebaudiana*. Therefore, we correlated *in vivo* data obtained from human psychophysical experiments with *in vitro* data from cell-based taste receptor assays on the most common steviol glycosides. While sensory evaluation clearly demonstrated the structural features causing the sweet and bitter taste of these phytochemicals, comprehensive screening experiments with human bitter taste receptors indicated their sensitivity to hTAS2R4 and hTAS2R14. Interestingly, for some analytes, we observed a decline in their sweet intensity at supra-maximum concentrations. This effect did not arise from allosteric modulation of the hTAS1R2/R3 sweet taste receptor but for the first time indicate a cross-modal suppressing effect of the associated intrinsic bitter taste. Next to the analysis of the molecular determinants of taste, a stable isotope dilution analysis with LC-MS/MS detection was developed for the first time to navigate breeding of *Stevia rebaudiana* effectively and to improve post-harvest down-stream processing towards the production of sweet taste-optimized *Stevia* extracts.

AGRO 153

Using biomimetic cell wall models to identify new plant lignin bioengineering targets for improving forage and biomass utilization

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Bioengineering of lignin to contain atypical components derived from other metabolic pathways is increasingly being pursued to custom-design lignified cell walls that are inherently more digestible by livestock or more easily pretreated and saccharified for biofuel production. Because plants produce such a diverse array of phenolics that could serve as monolignol precursors for lignin formation, cell wall model studies are invaluable as a screening tool for identifying the most promising genetic engineering targets for forage and biomass crops. Our studies with such models demonstrated that copolymerization of normal monolignols with structurally related phenylpropanoid ester conjugates, such as coniferyl ferulate and rosmarinic acid, dramatically improved cell wall delignification by alkali and their subsequent saccharification by enzymes. Furthermore, copolymerization of normal monolignols with more divergent types of phenolics, such as epigallocatechin gallate (EGCG), yielded lignified cell walls that were intrinsically more fermentable by rumen microflora, as well as extensively saccharified following mild alkaline or acidic pretreatment than conventionally lignified cell walls. As with the aforementioned phenylpropanoid conjugates, oxidative coupling of EGCG with introduced monolignols easily cleaved ester linkages into lignin that facilitated delignification under mild pretreatment conditions. *Ortho*-OH groups on rosmarinic acid and EGCG also contributed to enhanced pretreatment/saccharification of cell walls and their intrinsic fermentability by blocking the formation of benzyl ether cross-links between lignin and structural carbohydrates. In addition to EGCG, several other flavonoid and gallate derivatives readily formed lignified cell walls that were more inherently fermentable or readily saccharified following mild pretreatment. Overall, less than 25% of the phenolics tested in our studies proved compatible with cell wall lignification or useful for modulating the adverse effects of lignin on cell wall utilization. These findings highlight the value of testing alternate monolignols in biomimetic cell wall models prior to attempting their bioengineering into lignin biosynthesis.

AGRO 154

Immunochemistry in motion: Applications to agrochemicals

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Dr. Rosalyn Yalow received the 1977 Nobel Prize in Physiology or Medicine for the development of an exquisitely-sensitive analytical technique to quantify minute amounts of biological substances. This antibody-based technique, radioimmunoassay (RIA), is still in use today and forms a foundation for all other immunoassay formats. Yalow and her colleague Solomon Berson used radioimmunoassay to measure insulin at concentration levels never before achieved, enabling new biomedical research approaches. The technique eventually transitioned to much smaller molecules of environmental interest, such as pesticides and other agrochemicals. The adaptation of using enzymes in place of radioactivity opened the technology to a myriad of applications such as field monitoring and in-home testing. Although highly capable, this new approach for environmental analysis was met with some resistance, similar to when RIA was first introduced, and had to be vetted via field testing and evaluation studies. The US EPA became interested in immunoassays in the 1980s and undertook methods development and evaluation studies, as well as outreach and educational activities through several avenues including the Immunochemistry Summit Meeting series. This presentation will chronicle the journey of immunoassay from biomedical to agrochemical applications. *(This is an abstract of a proposed presentation and does not necessarily reflect the US EPA policy. The actual presentation has not been peer reviewed by EPA. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.)*

AGRO 155

Arriving at the truth: Weight of evidence for assessing risks of agrochemicals

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Information and data on agrochemicals from studies published in the open literature are increasingly being used for assessment purposes by regulatory agencies in many jurisdictions, including North America and Europe. Because most of these studies are not conducted to the standards

required of GLP studies for regulatory agencies, there is a need to assess these studies for their quality and relevance to the regulatory endpoints being considered. Weight of Evidence (WoE) offers a consistent, objective, and transparent method for assessing these studies and including them in risk assessments. The need for WoE and a method for conducting these analyses will be presented with the herbicide atrazine as a case-example.

AGRO 156

Optimization of sample homogenization for pesticide residue analysis: Soil – an example for a difficult matrix

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The reliability of residue data strongly depends on the quality of sample homogenization prior to analysis. While in the last decade the sensitivity of instruments has strongly improved and was intensively discussed, information on the crucial step of sample homogenization is very limited in public literature. Yet, high quality of sample homogenization is needed, as for example, *Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration* (Sanco/10058/2005) requires a low degree of data scatter in order to obtain high significant degradation parameters. Therefore, we conducted a homogenization study for which we chose soil as the matrix. We modified a food processing machine so that it could with stand the strong exerted forces during homogenization. In the experimental design, we considered several influencing factors: (1) soil type (clay loam and sandy loam), (2) polarity of the pesticide (polar and non-polar), (3) type of sample (soil core and grab sample), and (4) sample size (600 g to 8 kg). Soil samples were spiked with 0.2 mg/kg pesticide, homogenized, and 5 g aliquots of each sample were analyzed. Factors influencing the homogenization quality could be distinguished by high replicate field sample analysis. Soil type and sample size influenced sample homogenization most, while other factors were of less importance. Homogenization was optimized by modification of scissor setup and processing duration. Our data show that such optimization of the homogenization technique is crucial and significantly improves representativeness of analytical results. However, even with the high effort taken, the variation of residue values after homogenization was always higher than the analytical error.

AGRO 157

Validation of a modified QuEChERS version for high-throughput analysis of a wide range of pesticides in foods

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In recent years, Nanita et al. of DuPont greatly increased sample throughput in pesticide residue analysis of foods and other matrices by using flow injection analysis in electrospray ionization – tandem mass spectrometry (FIA-ESI/MS-MS). They used the quick, easy, cheap, effective, rugged, and safe (QuEChERS) method for sample preparation, but had to modify the initial salting-out step because sodium chloride in the original version, or sodium acetate in the buffered version, did not volatilize, which posed problems in the analysis. Instead, they found that the more volatile salt, ammonium chloride, worked better in FIA-ESI/MS-MS, and still gave high recoveries for the pesticides of interest to DuPont. However, this modified QuEChERS version was not evaluated for a wider scope of diverse pesticides commonly monitored worldwide by gas and liquid chromatographic (GC and LC) methods. In this study, we validated the modified QuEChERS version using ammonium chloride for salting-out of 30 diverse representative pesticides using both GC/MS-MS and LC/MS-MS for analysis of fruits and vegetables.

AGRO 158

High throughput residue sample preparation

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The superior selectivity and sensitivity of modern LC/MS-MS instrumentation has enabled development of high throughput analytical methods for quantitation of pesticide residues in raw agricultural commodities (RACs). However, when the entire workflow from sample receipt to data reporting is taken into consideration, the throughput of the analytical instrumentation is often not the rate limiting step. A key factor affecting the net output of a residue workflow is sample preparation. This can be attributed to the common practice of preparing samples in larger extraction formats that restrict processing to small sets in a serial fashion. This presentation will focus on a series of process improvements that enabled high-throughput flow and processing in parallel. The main components that increased the net sample throughput will be addressed in the presentation, along with examples of how these elements were applied to both existing methods and development of novel methods for new chemistries.

AGRO 159

Development and implementation of high throughput techniques for use in residue and soil dissipation studies

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Market place demands have dictated that the number and size of field trial studies increase, thus the speed with which the samples are prepared for analysis is under constant scrutiny and must be evaluated. The use of LC in tandem with MS-MS continues to be a powerful tool in the quantitative analysis of small molecules as well as proteins. The much higher selectivity gained with this tool *vis-a-vis* LC/UV approaches has allowed method development, validation, and analysis times to be dramatically reduced. While the bottleneck of extracted sample analysis has been drastically reduced with these techniques, most residue studies still start with multi-gram samples, requiring large solvent volume extractions; these take a significant amount of time (and cost) to prepare. In our lab, we have been transitioning from 20 gram sample sizes, prepared using traditional extraction methods, down to 100 mg sample sizes prepared using geno-grinders and 96-well plate formats; the main issue is the homogeneity of the sample (and thus sub-sample) selected and extracted. Approaches to extract smaller sample sizes, while using more sophisticated instrumentation have allowed for improvements in precision, sensitivity, and speed of the analysis. Examples of these approaches will be presented.

AGRO 160

Recent advances in flow injection mass spectrometry for high-throughput pesticide residue analysis in any complex matrix

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Analytical chemistry research has continued at DuPont to improve flow injection tandem mass spectrometry (FI/MS-MS) for high-throughput quantitative analysis in complex matrices. The most recent work has resulted in lower limits of detection (LOD) and limits of quantitation (LOQ). An overview of FI/MS-MS applied to pesticide residue analysis will be presented. Emphasis will be given to the following recent results: (i) the development of a generic method for quantitation of pesticides in water, and (ii) extension of FI/MS-MS to novel agrochemicals and additional matrices. The new FI/MS-MS method for water analysis uses ammonium chloride salting-out extraction with the ratio of water/acetonitrile/salt adjusted to yield analyte preconcentration in the acetonitrile phase. This fast and simple sample preparation procedure was coupled to FI/MS-MS with a 30-second instrumental analysis acquisition time, resulting in LODs in water between 10 and 100 parts per trillion (ppt). A validation study was conducted in river, lake, ground, and drinking water for 13 pesticides, including anthranilic diamide insecticides, carbamate insecticides, sulfonylurea herbicides, as well as pyrimidine carboxylic acid, triazinone and phenylurea herbicides. The study demonstrated that for 10 out of 13 active ingredients, the water method meets the stringent 0.1 parts per billion (ppb) limit of quantitation (LOQ) specified by regulatory guidelines of the European Union. The LOQ for the 3 least responsive analytes (lowest ionization efficiency), i.e., chlorsulfuron, oxamyl, and methomyl, was 0.3 ppb. The ammonium chloride salting-out extraction FI/MS-MS method was also extended for residue analysis of oxathiapiprolin, a novel fungicide under development by DuPont. The method was successfully validated for this active ingredient with LOQs of 10 ppb, 1.0 ppb, and 0.1 ppb in food (potatoes and grapes), soil, and water, respectively. Other recent FI/MS-MS technology improvements will be discussed. An outlook of the technique will also be presented.

AGRO 161

High throughput sample analysis using miniaturization and automation for residue analysis

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It is a challenging task for industry, both from a time perspective and from technical constraints, to analyse thousands of samples to meet registration requirements. The tremendous demands for increasing sample throughput today are driven by regulatory trends around the globe. Consequently, short, rugged, and sensitive methods to quantitate multiple analytes are required for data generation. Towards these goals, BASF developed soil and crop methods using miniaturization and automation. These methods rely on cryogenic homogenization of bulk field samples in order to convert the sample to a fine powder for residue analytical methods. Smaller aliquots enabled the use of simpler and more automated extraction and clean-up procedures using 96-well plate, consequently increasing the sample analysis through-put. These types of miniaturized methods were developed with limits of quantitation as low as 0.01 ppm for numerous active ingredients and metabolites, in several plant matrices. Sample analyses utilizing miniaturization and automation (96-well plate) in conjunction with LC/MS-MS determination were achieved. The methodology and the results proving linearity, accuracy, and precision of the method will be presented and discussed in detail.

AGRO 162

Increasing selectivity of LC/MS-MS analysis using differential mobility spectrometry

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Over the last 20 years there have been significant improvements in both the sensitivity and specificity of LC/MS analytical methodology. Even with these improvements, however, there is still a need for improved specificity for especially challenging matrices such as those encountered in food and plant matrices. Differential Mobility Spectroscopy (DMS) is a technique that can be very useful for removing isobaric interferences that may arise from the matrix or for separating isomers by mobility instead of retention time. The principles of DMS will be presented and the optimization of important variables will be shown. Examples of the application of DMS to specific analytical challenges will be shown and the improvements in limits of detection and isomer quantitation will be discussed.

AGRO 163

High-throughput residue analysis for a water monitoring study using liquid-handling robotics and UHPLC/MS-MS

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It is common to investigate new or upcoming technologies to improve sample throughput in the analytical laboratory. Typically, laboratories will look to optimize instrument conditions or sample preparatory techniques. Our lab was tasked with a long-term water monitoring study, which required the analysis of several hundred water samples a week with expedited turnaround times. The analytical method utilized GC/MS and time-consuming sample preparation procedures. Several critical areas were identified for improvement from the original analytical procedure. These critical areas included a reduction in sample size, minimizing of time-consuming sample preparation procedures, improving repeatability of the procedure, and decreasing analytical run times. This presentation will describe the high-throughput residue analysis system which evolved at ADPEN Laboratories, Inc. The GC/MS procedure used initially, required large sample volumes, SPE clean-up, evaporation steps, and long run times. The improved procedure employs liquid sample handling robotics and a highly-sensitive UHPLC/MS-MS instrument and, along with an upgrade of the LIMS environment, increased sample throughput in our analytical laboratory. The high throughput procedure allowed the sample preparation of 80 samples in 3 hours versus 12-15 samples in an 8-hour work day. Additionally, instrument run times were drastically reduced from 17.8 minutes to 5 minutes.

AGRO 164

RNA interference in insect pest management: Assessing potential benefits and risks

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Widely recognized as one of the premier functional genomics research tools, RNA interference (RNAi) has been used extensively in the post-genomics era to assign functions for genes annotated through small (expressed sequencing tags) or large (whole genome) scale sequencing efforts. Recently, the agricultural industry has recognized the potential to utilize RNAi as a mechanism to control the expression of target genes for pest control purposes resulting in a diversity of applications. Efficient delivery mechanisms, RNA stability, and RNA toxicity to the target organism remain as major technical challenges. However, a number of different approaches are being developed to overcome these challenges including transgenic crop plants that express RNAi traits (*in planta* RNAi). Although RNAi-based insect pest management technologies have yet to be commercialized, they are likely to become an important pest management tool that complements existing control practices including synthetic pesticides and *Bt* traits. This is especially important for target pest species, such as the western corn rootworm, where *Bt* traits are being challenged by resistance evolution. However, it is critical that the technology is used in a manner that is both sustainable and environmentally safe. The lack of a formalized/standardized ecological risk assessment (ERA) procedure remains as a major regulatory obstacle to integrate RNAi management approaches into sustainable pest management practices. An essential component of the ERA of RNAi plants involves *in vivo* RNAi toxicity testing under a defined worst-case scenario of exposure for both potential effects on non-target organisms and for resistance evolution. The studies described here are designed to answer questions directly pertaining to the risk of RNAi to non-target arthropods that are at greatest risk of exposure because of a shared environment and common molecular targets. In addition, studies to address the potential for resistance evolution are also described.

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Functional analysis of four RNAi pathway genes in an economically important corn pest, western corn rootworm (*Diabrotica virgifera virgifera*)

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RNA interference (RNAi) is being considered as an important tool to be used in insect pest management. Better understanding of the RNAi pathway will provide information to use this technology effectively for pest management and to inform decisions related to resistant management strategies for RNAi based traits. Four genes (*Dicer 2*, *Argonaute 2*, *Sid 1A* and *Sid 1C*) related to RNAi pathway were identified from transcriptome library generated from the gut of western corn rootworm (WCR). The expression of these genes was knocked down by injecting gene specific dsRNA into adult beetles, and then these adults were fed *vATPase A* dsRNA which has been demonstrated to cause mortality. The suppression of these genes apparently made the RNAi pathway less effective, thus reducing the mortality due to the second dsRNA treatment with *vATPase A* dsRNA. This research provides the basis for future studies aimed at improving RNAi technology as an insect resistance trait for WCR.

AGRO 166

Assessing the fate of RNA-based agricultural products in the environment

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Environmental fate data to characterize the extent of biodegradation of dsRNAs in environmental matrices is an essential element of a comprehensive environmental risk assessment of RNA-based agricultural products. The continued use of RNA-based gene suppression for agricultural products necessitates the development of novel analytical methods to determine the biodegradation potential of dsRNAs in the environment. Therefore, we have developed two complimentary techniques to assess the rate of degradation in soil of dsRNA from a biotechnology-derived *in planta* RNA-based insect-protected corn product. These techniques include a QuantiGene® assay to quantify the amount of dsRNA and an insect bioassay to measure functional toxicity. Results will be presented indicating that soil samples dosed with a dsRNA alone or with a dsRNA-corn tissue mixture demonstrate a loss of the parent dsRNA over time. Furthermore, results from insect bioassay indicate a corresponding time-dependent loss in biological activity. Results from complimentary methods support a lack of persistence of dsRNA in the soil environment and will be broadly useful for the exposure assessment needed to appropriately assess the environmental risk of RNA-based agricultural products.

AGRO 167

Toxins for transgenic resistance to hemipteran pests

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Transgenic crops expressing *Bacillus thuringiensis* (Bt) toxins have been widely adopted for management of lepidopteran and coleopteran pest species. In contrast, the sap sucking insects (Hemiptera) are not particularly susceptible to Bt toxins. We demonstrated that addition of a short peptide sequence selected for binding to the gut of the targeted pest species serves to increase toxicity against said pest. Insertion of a 12 amino acid pea aphid gut binding peptide by adding to or replacing amino acids in one of three loops of Cyt2Aa resulted in enhanced binding and toxicity against both the pea aphid, *Acyrthosiphon pisum* and the green peach aphid, *Myzus persicae*. This strategy may allow for transgenic plant-mediated suppression of other hemipteran pests, which include some of the most important pests of global agriculture.

AGRO 168

Mode of action of *Bacillus thuringiensis* toxins

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Numerous *Bacillus thuringiensis* strains are used for control of lepidopteran, dipteran, and coleopteran insects. In most strains insecticidal crystal proteins (Cry) are produced. In addition, these bacteria produce insecticidal proteins during the vegetative phase (Vips); and binary toxins that are structurally unrelated to Cry toxins also have been isolated. Further, all mosquitocidal strains produce cytolytic toxins (Cyt). These Cry, Cyt, Vip, and binary toxins are structurally, and appear to be evolutionarily, unrelated. Nevertheless,

these toxins all act on the insect midgut, where they lyse epithelial cells affecting cell function. The Cry and Cyt toxins act in multistage processes. Crystals are ingested by larvae and dissolve in the alkaline midgut environment. The inactive protoxins are cleaved by proteases yielding active toxin fragments, which bind specific membrane receptors on the midgut epithelium. This binding is a key factor in determining Cry toxin selectivity. For Cry toxins, these receptors are cadherin proteins or ABCC transporters, and with alkaline phosphatases and aminopeptidases also contributing to binding. Cadherins, ABCCs and alkaline phosphatases apparently bind domain II of the Cry1A toxins, while aminopeptidases bind a carbohydrate-binding pocket in domain III. This binding leads to the formation of an oligomeric toxin that migrates to and inserts into lipid rafts in the cell membrane, thereby leading to the formation of lytic pores. In contrast, Cyt toxin binding is dependent on unsaturated phospholipids. The bound toxins then aggregate through toxin–toxin interactions leading to formation of lytic pores. Pore formation in both toxins result in paralysis of the insect and eventual larval death. Mutations of cadherin, ABCC and aminopeptidase proteins in a number of insects have resulted in insect resistance. The talk will focus on mechanism(s) of toxin action, resistance mechanisms, and implications for such mechanisms in the field use of *Bacillus thuringiensis* toxins in insect control programs.

AGRO 169

Transcriptional responses to the ingestion of Cry1Ab protoxin and Cry1Ab corn leaves in the gut of Ostrinia nubilalis larvae

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We developed a DNA microarray representing 2,755 gut-specific transcripts from the European corn borer (ECB, *Ostrinia nubilalis*) larvae. Our microarray analysis putatively identified 174 genes whose expression changed by at least 2 folds after the early fourth-instar larvae of a Cry1Ab-susceptible strain were fed the artificial diet containing Cry1Ab protoxin. Among these, 17 up-regulated genes appeared to be involved in insect defense, signaling, and transport, and 43 down-regulated genes may be involved in binding and other biological processes. A total of 13 genes, putatively encoding 8 different serine proteases, 1 cadherin-like protein, 1 alkaline phosphatase, and 3 aminopeptidases, are potentially involved in Bt toxicity or/and resistance. We further compared the gut transcriptional responses to the ingestion of transgenic Cry1Ab corn (MON810-event) leaves in the early third-instar larvae between a laboratory-selected resistant (R) strain and a susceptible (S) strain. We putatively identified 398 genes from the S strain and 264 genes from the R strain with significantly increased or decreased expression (at least 2.0 folds) levels. When both the S and R larvae were fed transgenic corn leaves, the number of differentially expressed genes and the degree of their expression changes were generally greater in the S larvae than in the R larvae. Among these genes, 17 in the S larvae and 9 in the R larvae were potentially involved in Bt toxicity or/and resistance. Two aminopeptidase genes (contig 4776 and contig 1398) were down-regulated in the S larvae, but up-regulated in the R larvae as compared with the control larvae after they were fed transgenic corn leaves for 6 h. These studies represent the first large-scale surveys of Cry1Ab protoxin and transgenic Cry1Ab corn-induced transcriptional changes in the ECB larval gut and provide a platform for functional investigation of Bt-insect interactions.

AGRO 170

Using genomics and chemistry to screen for secondary metabolites in *Bacillus spp* biocontrol organisms

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The adoption of high-throughput DNA sequencing has greatly expanded our knowledge of the secondary metabolite potential of biocontrol organisms. By combining low cost sequencing and data mining software the ability to characterize the potential of new organisms is greatly enhanced. In the current study, we apply the approach to two *Bacillus* strains isolated to control Fusarium head blight in wheat. For *Bacillus amyloliquefaciens* AS 43.3, genomic data mining identified 9 gene clusters with the potential to produce bioactive secondary metabolites. The knowledge of the types of potential metabolites allowed us to develop extraction and mass spectroscopy approaches to confirm the metabolites are produced using traditional chemistry techniques. The results confirmed the presence of all 9 metabolites under liquid culture production. For *Bacillus subtilis* OH 131, genomic screening identified 5 gene clusters with the potential to produce secondary metabolites. Chemical techniques were able to confirm three of the metabolites, while the other two clusters are inactive due to a fatal point mutation in gene that makes a required precursor molecule for the synthetic clusters. Overall, the study highlights the growing interdisciplinary nature of studying the interactions of biocontrol organisms.

AGRO 171

Discovery of new insect resistance traits for control of insect pests in transgenic crops

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The first transgenic crop was deregulated in 1995 and the power of this technology to increase agricultural productivity is reflected in the fact that in 2012, transgenic crops were cultivated on 170 million hectares in 28 countries. First generation products containing transgenic insect resistance (IR) traits typically contained a single mechanism of action (MOA) targeting a specific pest complex, while the most recent products utilize pyramided MOAs. While there is an increased cost to the trait provider in pyramiding MOAs, a benefit is the opportunity to simplify grower production practices and increase product lifespan by incorporating the resistance-mitigating “refuge” seed (containing no IR traits) as a seed mixture with IR trait-containing seed. Pyramiding of traits, emergence of new pests, incorporation of IR traits into new crops, and the finite lifespan of commercialized IR traits, all drive the search for novel IR traits. Insecticidal protein genes from Gram-positive bacteria like *Bacillus thuringiensis* remain a significant focus of new IR trait discovery. Engineering these proteins to alter specific attributes has been used successfully to create novel IR traits. The advent of Next Generation Sequencing technologies and associated bioinformatics capabilities have enabled rapid sequencing of bacterial genomes and dramatically increased the rate of discovery of novel IR genes. These same technologies have enabled the creation of RNAi-based IR traits for some pests. Engineering plants to produce insecticidal or behavior-modifying small molecules also holds promise as a means to create novel IR traits. A challenge to sustaining innovation in the discovery and commercialization of novel IR traits remains creating value for growers and for the companies that invest in bringing these technologies to the marketplace.

AGRO 172

Setting the stage for future transgenic insect control products

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Transgenic insect control (IC) has important health and environmental benefits and provides a useful pest management option to growers. The success of transgenic crops has resulted in ever increasing adoption of this technology, but the possibility for resistance to IC traits remains. To be sustainable, future IC products will depend on the discovery of new modes of action to provide effective insect resistance management (IRM) features. This need drives considerable investment in research and development efforts aimed at identifying actives with novel modes of action. Appropriate characterization of these leads is necessary to understand how they can be best utilized in IRM strategies and includes the application of a variety of functional and biochemical approaches. Several of these approaches will be discussed.

AGRO 173

Pesticide residues in bee hives: What levels are of concern?

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Several recent published studies have performed chemical analysis of materials sampled from honey bee hives and suggested the frequency and levels of pesticides detected are high and likely cause for concern. However, these studies typically do not use risk analysis methods to confirm if in fact there is cause for concern. It would be helpful if a threshold Level of Concern (LOC) for concentrations in hive matrices were defined. Here I use published data and standard risk analyses approaches to define LOC values for commonly-detected pesticides in pollen, honey, and wax of honey bee hives. The LOC is defined as the threshold concentration that is likely to result in intake of a toxicologically significant dose for a worker honey bee. It is derived from endpoints measured in standard laboratory toxicity tests and conservative (near worst-case) assumptions for exposure levels. Ideally, a full data set consisting of acute and chronic test results with both adult and larval life stages of worker bees would be available. When data are lacking, conservative assumptions can be made to derive estimated toxicity values. Once LOCs have been defined, it becomes clear that pesticide residue levels reported in recent studies generally do not indicate there is cause for concern.

AGRO 174

Is planting corn killing bees?

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In the spring of 2012 the Office of Indiana State Chemist (OISC) investigated several incidents wherein beekeepers believed they were suffering losses to bee hives during planting season for corn. Dead and dying bees were gathered. Analysis in the OISC residue lab significant levels of clothianidin were found in the bees, pollen, and also in and around the hives. Clothianidin is the active ingredient in a seed treatment process for corn and it appears that the dust from the planting corn was exposing bees to this insecticide. Results of the investigations by OISC investigators will be presented.

AGRO 175

Analysis of pesticides in corn planter exhaust dust and dosimeters surrounding corn fields during planting

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During planting of corn fields, the outer coating of treated seed can be abraded and absorbed to materials, such as talc, that are added to the planter to keep the seed flowing. This creates a dust that can contain very high concentrations of pesticides and that, when exhausted from pneumatic planting equipment (or air planters), have the potential to contaminate the areas around the fields. If pollinators visit these surrounding areas, they may be exposed to these pesticides, sometimes at lethal rates. We have been studying this phenomenon by analyzing the pesticides deposited on dosimeters placed around fields during planting at a distance of 0 - 100 meters. Although the amount of pesticides found on a dosimeter slide varied greatly, as much as 87 ug/m^2 of an individual pesticide was observed during the 2012 tests. An additional set of fields will be monitored during the 2013 planting season, as well as planting with a newly developed seed lubricant. Methods of analysis and results for two years will be presented.

AGRO 176

Optimization of a method to quantify agrochemicals in bee tissues and wax

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An analytical method was developed to extract and to analyze simultaneously atrazine, chlorpyrifos, chlorothalonil, coumaphos, coralox, and τ-fluvalinate in bee tissues and wax. The optimized bee method used 3 g of bees and 30 mL of a 1:1 hexane:dichloromethane extraction solution. Cleanup was done using polystyrene-divinylbenzene cartridges capped with graphitized black carbon. The wax extraction method used 0.5 g wax and 10 mL of extraction solvent (same as for bees). Extracts were cleaned with a combination of Florisil solid phase extraction and gel permeation chromatography. Extracts were quantified using GC/MS-NCI for all of the target analytes, except atrazine, which was quantified using GC/MS-EI. Extraction efficiencies for the two matrices ranged from 70 to 120%, and minimum detection limits were well below reported toxicological benchmarks. In addition, total lipid extracts were conducted on the bees to separate the lipids into neutral and polar fractions and analyzed for fatty acid profile.

AGRO 177

Intersect of pesticides and pollinators: Challenges faced by state regulatory programs

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All pesticides must be either registered or exempted from registration by the US Environmental Protection Agency (EPA) before they can be sold or distributed in the US. As part of the registration process, EPA evaluates a pesticide to ensure that it will not have unreasonable adverse effects on humans, the environment, and non-target species. The legal

use of a pesticide is dictated by the instructions on the label that is developed as part of the federal registration process for all pesticide products and serves as an agreement between the EPA and the end user of the product. While the EPA registers pesticides, it is state pesticide regulatory programs that have primacy and ensure that pesticide use is consistent with the product label. State pesticide programs ensure compliance through routine inspections, pesticide use observations, and investigations of possible pesticide misuse. In situations where the use of a pesticide is in a manner inconsistent with the label, a state regulatory program will take appropriate enforcement action. But what about those situations in which the use of the pesticide is legal and yet there are adverse effects to non-target species, for example, pollinators? In this session, we will explore regulatory issues faced by state pesticide programs when the legal use of pesticides and the protection of pollinators are seemingly at odds and the current efforts to provide for both.

AGRO 178

Risk assessment framework for honey bees

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The US Environmental Protection Agency in collaboration with Health Canada's Pest Management Regulatory Agency and the California Department of Pesticide Regulation developed a tiered risk assessment framework for bees, relying heavily upon the honey bee (*Apis mellifera*) as a surrogate. This process was recently presented to a FIFRA Scientific Advisory Panel comprised of technical experts from academia and government. The framework identifies specific protection goals and assessment endpoints for which risk would be evaluated. At a screening level, risk is quantified based on dietary and contact routes of exposure for individual larval and adult bees, while higher tier assessments qualitatively evaluate potential risks to the entire colony. This presentation will provide a broad overview of the risk assessment process for bees by describing measures of exposure and effect and risk estimation. Emphasis will be placed on characterizing exposure of bees to pesticides using modeling and monitoring data.

AGRO 179

Addressing new data requirements for chronic honey bee testing in the EU

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To address new European Union (EU) data requirements for plant protection products, honey bee risk assessments are required where exposure of adults and larvae via direct contact or from residues in nectar and pollen cannot be excluded. Acute oral/contact toxicity studies are performed on adult bees and registrants may also be required to conduct Tier 1 larval chronic toxicity studies for which an OECD guidance is still under development or Tier 2 colony-level brood effects studies. For EU re-registration of glyphosate, potential exposure and effects on honey bee brood/colonies were assessed in separate studies. To quantify exposure, a greenhouse study involved a spray application of a glyphosate formulation to flowering *Phacelia tanacetifolia* during peak bee foraging. Glyphosate concentrations over time in forager-collected pollen and nectar were analysed. Mean glyphosate levels in nectar were >10X lower than in pollen and declined rapidly with DT_{50} values of 1-2 days. Pollen and nectar residue values were used as inputs to a bioenergetics-based exposure model to establish realistic worst case dose levels. To quantify effects on brood/colonies, a Tier 2 bee brood feeding study was performed using the Oomen test design. Colonies were tested at four dose levels including the control. Colonies were assessed 1 week prior and at weeks 1, 2, and 3 after dosing. Assessments tracked development of individual larvae and emergence, and the health of the colony as a whole with exposure confirmed by residue analysis of larvae collected from within the colony. No effects at any dose level were observed, consequently the No Observed Effect Level for brood development and adult survival was the highest dose tested, providing a sufficient margin of safety on the risk of glyphosate to honey bees. This conclusion is consistent with results of independently performed semi-field and field bee brood studies using a glyphosate-based formulation.

AGRO 180

Determining kinetic and nonequilibrium sorption behavior for chlopyrifos using a hybrid batch/column experiment

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Pesticide mobility in soil is strongly coupled to the chemical's sorption characteristics. A modified soil-column batch experiment was conducted to measure the transient nature of chlorpyrifos sorption and desorption from Cecil soil. This experimental system minimizes many shortcomings associated with obtaining sorption parameters by fitting soil column data to an advective−dispersive transport equation. Several chlorpyrifos formulations were investigated to determine how formulations affect soil sorption, and if this effect is adequately described using transient sorption/desorption algorithms. Both a second-order sorption with first-order desorption kinetic model and the two-site kinetic/equilibrium model were found to yield reasonable comparisons to experimental observations. Some reservations regarding the validity of the two-site model still need to be addressed since experiments using the same soil type under the same flow characteristics yield different values for an assumed fixed physical property of the two-site kinetic/equilibrium model (should remain constant under identical transport conditions). Although the two-site model can give excellent agreement between experiment and model predictions, this may just be a consequence of the additional free parameter that can be used to curve fit the solution to experimental data, with other simpler non-equilibrium sorption/desorption models offering similar comparison to experiment. Eliminating unnecessary free parameters helps distinguish any ambiguity between a general sorption−desorption model with a model that more closely describes the actual mechanisms involved in soil sorption. In general, the formulation temporarily decreases the sorptivity of chlorpyrifos and alters the time for equilibrium to be achieved.

AGRO 181

Experiments and modelling to quantify irreversibility of pesticide sorption-desorption in soil

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Characterization of irreversible pesticide sorption on soil has been confounded by procedural difficulties to differentiate between slow reversible and irreversible sorption. The isotope exchange technique developed by Celis and Koskinen (1999) eliminates experimental artefacts. It relies on establishing sorption equilibrium during an adsorption phase, then determining the proportion of sorbed pesticide that participates in exchange with a second isotope of the same pesticide. Celis and Koskinen's experiments indicated significant irreversibility (6-51%) in sorption in five pesticide-soil systems over 72 hours. We re-evaluated the experiments with a three-site sorption model that adds slow reversible binding on non-equilibrium sorption sites to instantaneously reversible and irreversible sites. The model matched the data closely, but only if irreversible sorption was absent. Non-attainment of sorption equilibrium could explain the observed asymmetry in binding of the two isotopes. Recent studies with chlorotoluron, prometryn, and hexaconazole in three soils showed that the isotope exchange technique is not powerful enough to differentiate between slowly reversible or irreversible sorption. Forced isotope exchange over protracted timescales (for chlorotoluron: 204 days, following 56 days adsorption and 14 days isotope exchange) and solvent extraction gave an indication of pesticide not participating in exchange between the soil and solution. Under abiotic conditions, irreversible binding was minimal, but desorption of the initially-sorbed pesticide occurred over exceptionally long time-scales. The presence of an active soil microbial community and formation of degradation products can play an important role in the binding of pesticides, and irreversible sorption is likely to occur to a greater extent under non-sterile conditions. This study provides a greater insight into the significance of irreversible binding for predicting pesticide fate. (*The authors wish to thank the EPSRC and Syngenta for financial support.*)

AGRO 182

Biphasic behavior of pesticide degradation in soils: Verification by pathway kinetic fits

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The biphasic behavior of pesticide degradation in soils is currently determined by fitting the data for the parent to a simple first-order (SFO) and a biphasic (DFOP, FOMC, and IORE) kinetic model. If SFO fit is rejected by visual and statistical assessment, degradation is considered biphasic. However, in some cases, SFO fit is acceptable, but a biphasic model provides a better fit, leading to very different degradation endpoints. The purpose of this study is to explore the feasibility of using a pathway kinetic fit approach to verify biphasic behavior of parent degradation. The basic premise is that the degradation behavior of parent must be kinetically consistent with formation of metabolites. Thus, a kinetic model for the parent can only be considered as a best-fit model, if it simulates both parent degradation and formation of metabolites in a pathway fit with all metabolites included. This approach can help discern a pseudo-biphasic behavior that does not correspondingly generate metabolites and avoid selecting over-conservative degradation endpoints for exposure modeling, although more datasets are needed to confirm its feasibility. The approach is illustrated with a real kinetic data set in this study.

AGRO 183

Determining differential degradation of enantiomers in soil using data of no chiral separation

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Non-first order can be caused by differential degradation of enantiomers of the same parent. Determining differential degradation in soil experimentally by chiral analysis can be challenging and costly. In this paper, we quantify isomer differential degradation by the degree of non-first order behavior and show that when differential degradation exists, initial enantiomer ratios influence the overall degradation pattern remarkably. This is also reflected in the DT_{50} and DT_{90} values, indicating experiments with different initial enantiomer ratios may help determine the existence of differential degradation and estimate the associated parameters without separate chiral measurements. Validity and limitations of the approach are discussed in case of complications of the non-first order pattern caused by other mechanistic processes such as sorption or microbial dynamics. Data sets from laboratory soil metabolism studies are used to evaluate the proposed approach. The analysis shows that a quick screening procedure can be developed for determining if full scale chiral experiments are necessary.

AGRO 184

Statistical means for proper determination of kinetic half-lives

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In the NAFTA regulatory community, a currently consistent methodology used to estimate dissipation times for environmental fate data has not applied. This work demonstrates through a case study that the inappropriate use of pseudo-first-order regression models can result in inaccurate estimates of degradation rates, and it proposes some statistical tools that can be used to identify an appropriate statistical model to fit a particular environmental fate dataset. Diagnostic procedures are proposed to identify the appropriate scale, and statistical testing procedures used to select an appropriate model within that scale. Results from this work demonstrate that, unless appropriate diagnostic and statistical procedures are used, inaccurate estimates of dissipation times may result.

AGRO 185

Evaluations of regulatory kinetic analysis approaches

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Environmental exposure assessment depends on environmental fate properties of an agrochemical, such as sorption and degradation behaviors. Therefore, kinetics evaluation of environmental fate studies is very critical to exposure and risk assessment. The FOCUS group in Europe

developed a kinetics guidance document in 2006, and the approach defined in this document is used on estimating degradation kinetics from environmental fate studies on agrochemicals for EU registration. For the similar purpose, a NAFTA kinetics guidance document was also developed in 2011 and is used by US EPA and PMRA of Canada for registration evaluations. An evaluation of the two kinetic approaches was performed using several datasets, and the derived kinetic endpoints were compared according to the model output and the FOCUS and NAFTA guidance. KinGUI, a kinetics evaluation tool, was used for kinetics characterization defined in the FOCUS guidance document. A NAFTA kinetics tool was used to implement the NAFTA kinetic approach. The datasets used in the evaluation follow simple first order degradation or bi-phasic degradation modeled by both kinetic tools. However, for the same datasets, the derived degradation half-life for exposure assessment can be very different, depending on the kinetics models that each approach uses to fit the datasets. The NAFTA approach tends to choose a fit with bi-phasic kinetics more than the simple first order, comparing to the FOCUS approach. When both approaches choose the bi-phasic model fitting, the resultant half-lives are similar.

AGRO 186

Guidance on how aged sorption studies for pesticides should be conducted, analysed, and used in regulatory assessments

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First-tier regulatory risk assessments for pesticides assume that pesticide sorption is instantaneous and fully reversible. In Europe, a change in sorption over time (aged sorption) is increasingly considered at the higher tier to revise predicted environmental concentrations in groundwater. To address a need in regulatory guidance in this area, the UK Chemicals Regulation Directorate (CRD) commissioned research that formed the basis of a guidance document. The guidance proposes (i) protocols on how to measure aged sorption, (ii) procedures to fit kinetic models to the experimental data, (iii) criteria to test the reliability of the model parameters, and (iv) procedures for use of the parameters in the groundwater exposure assessment. The draft guidance was presented to and discussed with European stakeholders at a workshop. The participants were positive about this initiative and agreed that the proposed principles should be applied to real datasets to gain more practical experience. Members companies of the European Crop Protection Association (ECPA) provided datasets and funding for testing of the guidance against 127 studies by an independent organisation (Battelle UK Ltd). The results were peer reviewed by Fera. Comments from the workshop and the results of the evaluation and peer review were incorporated into a revised guidance. This document is now under consideration for further development at EU level. The evaluation of aged sorption studies, estimation of model parameters, and their incorporation into regulatory assessments is detailed and complex. The current guidance applies to laboratory studies with directly dosed substances. Further UK Defra funded research is ongoing to investigate the estimation of aged sorption parameters for metabolites formed from dosed parent substances and for substances in field dissipation studies. The guidance document will be summarised and first results of the ongoing research will be presented.

AGRO 187

Significance of time-dependent sorption on leaching potential: A comparison of measured field results and modeled estimates

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Recently, the US Environmental Protection Agency (US EPA) and Canada's Pest Management Regulatory Agency (PMRA) released the Pesticide Root Zone Model for Groundwater (PRZM-GW) to estimate leaching behavior and potential groundwater concentrations following agricultural applications of crop-protection products. PRZM-GW assumes that soil sorption is linear and constant over time; however, some crop-protection products, such as clothianidin, often demonstrate soil sorption characteristics that are non-linear and increase over time, both being characteristics which can reduce mobility potential in soil. This paper demonstrates the importance of considering time-dependent sorption characteristics in leaching models to a complete understanding and evaluation of leaching behavior of a chemical by comparing the estimates from the US EPA PRZM-GW model and the European FOCUS PRZM model to measured residues from terrestrial field dissipation studies conducted across North America. Results are particularly significant for coarse-textured soils with substantial excess water inputs.

AGRO 188

Effect of refined environmental fate properties on groundwater concentrations calculated with PRZM-GW

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Non-linear and time-dependent sorption are common compound properties that allow for a realistic description of the transport and degradation of agrochemicals in the vadose zone of the soil. The groundwater model FOCUS PRZM 3.5.2 includes these soil processes following intensive evaluation and technical dialog among European stakeholders. This approach is used in the EU regulatory process and as such, laboratory data needed to describe the enhanced binding processes are often available. The PRZM-GW model considers only linear sorption. Non-linear and time-dependent sorption can be included in PRZM-GW with the US EPA environmental scenarios to demonstrate the effect on the predicted groundwater concentrations. In some cases, significant reductions can be obtained, and the predicted concentrations were in general agreement with SCI-GROW concentrations and the field study results from which SCI-GROW was developed. The results suggest that incorporation of Freundlich sorption isotherms and time-dependent sorption into the exposure assessments for plant protection products would result in more realistic estimates of groundwater concentrations when justified based on laboratory and/or field data. This approach is therefore suggested as an efficient means of improving drinking water exposure assessments for North America.

AGRO 189

Influence of time-dependent sorption of flutriafol on predicted environmental concentrations

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Sorption of flutriafol in the soil is time-dependent, with increasing apparent adsorption with time. This time-dependent sorption kinetics can lead to estimated environmental concentrations (EECs) that are significantly different from those predicted with equilibrium adsorption models. In this study, LEACHP, PRZM-GW, and RZWQM2 models were applied to six leaching-vulnerable locations representing different geographic conditions for predicting flutriafol concentrations in ground water. LEACHP and PRZM-GW models were parameterized assuming instantaneous equilibrium sorption, while RZWQM2 was parameterized with instantaneous equilibrium sorption as well as kinetics sorption. The predicted EECs in ground water by the three models were compared to evaluate the influence of sorption processes on EECs. These predictions were also compared with data collected from ground water monitoring studies. In addition, the potential impacts of the sorption processes on flutriafol risk assessment are also discussed.

AGRO 190

APEX sensitivity to atrazine dissipation rate on surface runoff loss within a coastal zone in southeastern Puerto Rico

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Simulation models are increasingly used to predict effects of conservation practices on transport of pesticides to water bodies. The Agricultural Policy/Environmental eXtender (APEX) model was used to predict the movement of the herbicide, atrazine, from treated fields to Jobos Bay National Estuarine Research Reserve located on Puerto Rico's southeast coast. The objective was to evaluate the sensitivity of APEX to atrazine half-life input values (DT_{50}, time to 50% dissipation) on atrazine in surface runoff. Hydrologic calibration and validation was performed. Atrazine DT_{50} values were measured in the treated field and adjoining riparian buffer soil and indicated accelerated degradation due to repeated atrazine application. Three scenarios were evaluated: 18-, 55-, and 146-day DT_{50}, representing measured field, measured riparian buffer, and the model default half-life values, respectively. APEX indicated use of the measured field soil atrazine degradation rate (18-day DT_{50}) resulted in 33% lower transport from the field. Findings demonstrated the utility of this model in evaluating atrazine fate and transport, emphasized that use of measured soil dissipation values can improve model accuracy, and that large storm events likely dominate herbicide transport to coastal waters in the region.

AGRO 191

Soil dissipation kinetics: The use of a set of simple first order processes to describe a biphasic degradation pattern

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The analytical results for a pesticide compound in a set of laboratory soil dissipation studies with a variety of different soil types from North America and Europe showed a range of behavior from linear simple first order to a pronounced biphasic pattern, with an initial phase of faster degradation followed by a period of much slower dissipation. Using a set of three simultaneous simple first order equations, representing reversible movement between two compartments in the soil, and irreversible degradation from one of the two compartments, it was possible to fit the data from all sites. The regression output was a set of three simultaneously optimized rate constants for each soil type, along with the goodness of fit statistics. The physical interpretation of this model was found to be unrelated to the movement of residues between bound residues and residues dissolved in soil pore water, but more associated with the movement of residues between a compartment that is bioavailable for the degradation processes and a compartment that is not bioavailable. The utility of the resulting rate constants for predictive modelling depends on the availability of measurable soil properties to predict the rate constants for the three equations from measured properties of the soil in the scenario being modelled. However, no relationship was found with typically available soil properties such as moisture content or organic matter content; the relationship with pH was found to be bimodal. The potential for measurement of bioaccessibility as a soil characteristic is discussed.

AGRO 192

Properties and uses of chlorpyrifos in the United States

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Physical properties and use data provide the basis for estimating exposures to chlorpyrifos (CPY) in the environment and assessing risks. The vapor pressure of CPY is small, solubility in water is less than 1 mg L^{-1}, and its log K_{ow} is 5. Chlorpyrifos has short to moderate persistence in the environment as a result of several dissipation pathways that might occur concurrently. Primary mechanisms of dissipation include volatilization, photolysis, abiotic hydrolysis, and microbial degradation. Volatilization dominates dissipation from foliage in the initial 12 h after application, but decreases as the formulation adsorbs to foliage or soil. Subsequent to application, CPY adsorbs more strongly to soil, penetrates more deeply into the soil matrix, and becomes less available for volatilization and other degradation processes become important. Degradation at application rates used historically for control of termites is much slower than that observed in agricultural uses where half-lives are shorter (1.2 to 120 d). The mean water-soil adsorption coefficient (K_{oc}) of CPY is 8,216 cc g^{-1}, negligible amounts of CPY enter plants via the roots, and it is not translocated in plants. Half-lives for hydrolysis in water are

inversely dependent on pH and range from 16 to 73 d. CPY is an inhibitor of acetylcholinesterase and is potentially toxic to most animals. Differences in susceptibility result from differences in rates of adsorption, distribution, metabolism, and excretion between species. CPY is an important tool in management of a large number of pests (mainly insects and mites) and is used on a wide range of crops in the US. Estimates of use in the US between 2008 and 2012 range from 3.2 to 4.1 M kg y^{-1}, about 50% less than that used prior to 2000. Application to corn and soybeans accounts for 46 to 50% of current annual use in the US.

AGRO 193

Towards a model of the environmental fate and long-range atmospheric transport of chlorpyrifos and its oxon

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The physico-chemical properties that influence the environmental fate and transport of chlorpyrifos (CPY) and CPY-oxon (CPYO) are briefly reviewed. These include vapor pressure, air-water and soil-water partition coefficients, half-lives in the atmosphere, water, and soils, and the kinetics of CPYO formation from CPY. The relatively high vapor pressure of CPY results in appreciable volatilization during and shortly after spraying, resulting in atmospheric concentrations at the site of application in the range 10 to 1000 ng/m^3. The plume disperses and degrades, notably to CPYO, thus causing long-range atmospheric transport (LRAT) in the days following application. CPY and CPYO are thus subject to deposition to terrestrial and aquatic systems in the hundreds of km downwind of sources as is confirmed by monitoring data, from the Central Valley and National Parks in California, the Mid-West and Eastern US, and Canada. A LRAT model suggests a characteristic travel distance for CPY of some 65 km, over which two-thirds of the CPY is degraded or deposited, but this distance is very sensitive to hydroxyl radical concentrations. A tentative mass balance model of dispersion, formation of CPYO, and deposition is outlined. It has the potential to simulate concentrations in air and other media such as precipitation yielding results that are broadly consistent with monitoring data. This model serves as a foundation for a more quantitative and site–specific quantification of the fate, transport and long-range transport, and potential effects of CPY and CPYO.

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Refined avian risk assessment for agricultural uses of granular chlorpyrifos in the United States

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Grit ingestion by birds is the most important route of exposure for granular pesticides. The Granular Pesticide Avian Risk Assessment Model (GranPARAM), a refined probabilistic exposure model, was used to estimate acute risk to a variety of focal bird species for a wide range of use patterns for granular chlorpyrifos. The model allowed the application scenario (e.g., crop and method and rate of application), bird species, and region of interest to be defined. The choice of region defined how much natural grit was available to birds using regional crop specific soil textures and soil pedon data. The scenario selected determined the number of pesticide granules potentially available as a source of grit to birds. The choice of species determined the amount of potential grit ingested and the proportion of time spent foraging in treated fields. The model simulated exposure of 20 randomly chosen birds on each of 1000 randomly selected fields from the region of interest. Each time a bird ingested a particle, the particle is either a pesticide granule or a piece of natural grit. Preference for selecting chlorpyrifos granules in comparison to natural grit was incorporated in the model. Dose was calculated from mass of pesticide per granule and compared to the dose-response curve for those focal species with toxicity data to determine if mortality occurred. For untested focal bird species, the dose was compared to each of three dose-response curves that represent species of high, median, and low sensitivity to chlorpyrifos. The results of modelling for granular chlorpyrifos across a broad range of use patterns indicated that birds are not at risk from this formulation. The results from avian field studies conducted with granular chlorpyrifos corroborated the predictions from GranPARAM.

AGRO 195

Refined avian risk assessment for agricultural uses of flowable chlorpyrifos in the United States

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The Liquid Pesticide Avian Risk Assessment Model (LiquidPARAM) was used to estimate risk for a wide variety of focal bird species and use patterns on the chlorpyrifos label. LiquidPARAM estimates the fate of each of 20 birds on each of 1000 treated fields. The model has a one hour time step, runs for 60 days, and estimates acute and chronic risk from single or up to three pesticide applications. The model included 29 bird species and accounted for their foraging behavior inside and outside treated fields as well as their specific diets. To estimate acute risk, the maximum hourly retained dose for each bird in each field was compared to the dose-response curve for those focal species with toxicity data and the fate of the bird calculated. For untested focal bird species, the dose was compared to each of three dose-response curves which represented species of high, median, and low sensitivity and were derived from a species sensitivity distribution (5^{th}, 50^{th}, and 95^{th} percentiles, respectively, combined with average slope for all tested species). For chronic risk, hourly doses were averaged over a duration selected to match the critical exposure period from chronic toxicity tests. The maximum running average was then compared to data on chronic effects. The results of modelling for chlorpyrifos across a broad range of use patterns indicate that sensitive bird species foraging extensively in fields treated at high application rates may experience some acute risk. The majority of bird species, however, are not at significant acute risk even for the use patterns with the high application rates. Chronic risk is not a significant concern for the flowable formulation of chlorpyrifos. The results from avian field studies conducted with flowable chlorpyrifos indicate that LiquidPARAM is likely over-predicting acute risk as little mortality was observed in those studies.

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Exposures to aquatic organisms from the use of chlorpyrifos in North America

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Environmental fate and transport models were used to supplement monitoring data to characterize potential concentrations of chlorpyrifos (CPY) in water and sediment for three watersheds in the United States: Orestimba Creek in the San Joaquin River basin in California, Dry Creek in the Flint River basin of southwest Georgia, and Cedar Creek in the Betsie-Platte River system in northwestern Michigan. The watersheds were selected by evaluating the relative runoff potential of CPY across the US under different use practices. Runoff of CPY was estimated using the European version of the Pesticide Root Zone Model (WinPRZM) based on its ability to simulate the dissipation of CPY via volatilization, microbial degradation, and transport in runoff, eroded soil, and from furrow/flood irrigation tail water. Loadings of CPY to water from spray drift were estimated with the AgDRIFT model. Concentrations in receiving streams were estimated using the Surface Water Assessment Tool (SWAT). Up to 30 years of CPY use were simulated to account for CPY runoff under a variety of weather conditions. The upper 90th centile 96-hour concentrations in water, determined from the annual maximum series, were estimated to be 1.32, 0.020, and 0.018 µg/L for the California, Georgia, and Michigan watersheds, respectively, based on the more persistent of two values used for CPY metabolism in soil (96.3-day half-life). Durations of concentrations exceeding 0.1 µg/L were generally less than 48 h. Monitoring from three relatively intensive sampling programs totaling 119,455 samples from 2002-2010 have reported median, 90th, and 99th percentile concentrations under 0.03, 0.3, and 0.9 µg/L, respectively.

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Risks to aquatic organisms from the use of chlorpyrifos in North America

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The risk of chlorpyrifos to aquatic organisms in North America was assessed. Exposure to organisms in the water column and sediments was estimated using refined transport models and available monitoring data. Ecological effects were evaluated using results of standard laboratory toxicity tests with single species as well as microcosm and mesocosm studies with complex aquatic communities. The upper 90th centile 96-hour concentrations (annual maxima) of chlorpyrifos in small streams in agricultural watersheds in Michigan and Georgia were estimated to be ≤0.02 µg/L. In a reasonable worst-case California watershed, the 90th centile 96-hour concentrations ranged from 1.32 to 1.54 µg/L. Measured concentrations of chlorpyrifos are smaller than the model estimates; the 99th centile for more than 10,000 records compiled by the US Geological Survey was 0.029 µg/L. Acute toxicity endpoints for 25 species of crustaceans range from 0.035 to 457 µg/L; for 19 species of aquatic insects from 0.05 to 27 µg/L; and for 24 species of fish from 0.53 to 806 µg/L. The No Observed Ecologically Adverse Effect Concentration in more than a dozen microcosm and mesocosm studies conducted in a variety of climatic zones is consistently 0.1 µg/L. These results indicate that chlorpyrifos concentrations in surface waters are rarely great enough to cause acute toxicity to even the most sensitive aquatic species.

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Ecological risk assessment for chlorpyrifos in terrestrial systems in North America: Conceptual model for pollinators

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Chlorpyrifos is widely used to control insect pests on a variety of crops. The potential for inadvertent exposure of pollinators such as honeybees to chlorpyrifos or its degradation product, chlorpyrifos oxon, after application involves the interaction of chemical, physical, biological, and behavioral factors that change with time. A conceptual model was constructed to define the network of routes of exposure in greater detail than has previously been done. This model reflects the scope of the pollinator risk assessment, guides its development, and illustrates the relationships among the potential exposure pathways. It also shows the distinction between primary exposure routes that affect foraging worker bees and secondary exposure of hive adults and immature life stages that receive food collected by foragers or produced by other hive bees. The conceptual model allows detailed consideration of the overall pattern of potential exposure, including the dynamics of exposure to various castes and life stages. It gives insight into the usefulness of honey bees as surrogates for non-*Apis* pollinators that may be exposed via portions of the network of pathways in the model. The conceptual model also aids in assessing the completeness of the risk assessment and identifying exposure pathways that require further investigation.

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Risks of chlorpyrifos to pollinators: Risk assessment

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The organophosphorus insecticide chlorpyrifos (CPY) is widely used in North America on a number of crops on which pollinators can forage. Bees, the most important pollinators of agricultural crops, were the focus of this risk assessment. The conceptual model identified a number of potential exposure pathways for pollinators, some more significant than others. CPY is toxic to honey bees by direct contact, but label precautions minimize the risk of CPY to pollinators through this pathway. The primary potential exposure for honey bees is dietary and contact exposure from flowers sprayed with CPY. Potential secondary exposure is mainly

through pollen and nectar brought to the hive by forager bees. Tier-1 estimates suggested that CPY poses a risk to honey bees through consumption of pollen and nectar. However, a Tier-2 assessment of concentrations reported in pollen and honey from monitoring work in North America indicated there is little risk of acute toxicity from CPY through consumption of these food sources. Models used to estimate CPY exposure through consumption of water from puddles or dew suggested that the risk is below the LOC for this pathway. Semi-field and field tests with honey bees, bumble bees, and alfalfa leafcutting bees indicate that exposure to foliage, pollen and/or nectar is hazardous to bees for up to 3 days after application of CPY within a crop. Pollinators exposed to foliage, pollen, or nectar after this period should be minimally affected. Reported bee kill incidents involving CPY are rare. Although there is a lack of exposure and toxicological data on non-*Apis* pollinators, we conclude that provided label directions and good agricultural practices are followed, the use of CPY in agriculture in North America does not present an unacceptable risk to honeybees.

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Ecological risk assessment for chlorpyrifos in terrestrial and aquatic systems in North America: Overview and conclusions

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Patterns of uses of the organophosphorus insecticide, chlorpyrifos (CPY) in North America have changed over the past decade. This along with emerging issues and new knowledge were considered in reassessing the risks of CPY to terrestrial and aquatic wildlife. Based on the physical-chemical properties of CPY, it would not be classified as a persistent or bioaccumulative chemical. Results of a model developed to predict long-range atmospheric transport were consistent with measured concentrations in areas remote from sites of application. Results of refined models used to predict concentrations in surface waters under a number of scenarios of use were consistent with measured values in surface waters. Both predicted and measured concentrations of CPY in surface waters were less than the threshold concentration predicted to cause adverse effects on aquatic organisms, except for a few situations in drainage ditches which receive irrigation return water directly from agricultural fields. Results of simulations of exposures of birds to CPY, which predicted *de minimus* risks to a range of species are consistent with the lack of incident reports under current label uses. Risk to honeybees is minimal. CPY poses *de minimus* risk to terrestrial and aquatic organisms near sites of application and the risk to aquatic organisms at locations more remote are even less. Concentrations of the oxon of CPY have been reported for rain and surface waters, but the oxon is very reactive and not accumulated into organisms and thus does not pose risks beyond those predicted for CPY. When used under conditions specified on the current US label, CPY is predicted to have *de minimus risks* to aquatic and terrestrial wildlife as well as honeybees in North America.

AGRO 201

Chlorpyrifos agricultural use and the Endangered Species Act: Do refinements in ecological risk assessment address uncertainty?

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Aquatic and terrestrial ecological risk assessments for chlorpyrifos require substantial refinement because wide-spectrum, highly-active insecticides do not pass early assessment tiers that are designed to be highly conservative. Generally, higher tier assessment iterations with more sophisticated problem formulations are intended to bring greater realism to the assessment and reduce uncertainty in the characterization of risk by considering additional data and multiple lines of evidence. The question of whether higher tier assessments, which often incorporate probabilistic statements of risk, can be used to help meet the protection goals of the US Endangered Species Act (ESA) is explored using examples from a recent chlorpyrifos ecological risk assessment for agricultural uses in the US. Topics discussed include scope of a national ESA assessment, data quality and relevance, probabilistic methods, ecological hierarchy theory, indirect effects, and extinction risk.

AGRO 202

Pesticides as POPs and PBTs: An assessment of chlorpyrifos

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In addition to the POPs (Stockholm) convention, regulations such as EC-1107/2009 in the European Union are placing focus on persistence (P), bioaccumulation (B), and toxicity (T) of pesticides. Clear and consistent guidance is lacking for categorization of POPs and PBTs. As a case-study, we assessed the organophosphorus insecticide, chlorpyrifos (CPY). When selecting these data, a quantitative weight of evidence (WoE) approach was used to evaluate relevance and strength (overall quality) of experimental data for P, B, and T. Since protection goals for POPs and PBTs are global or regional, mean values of relevant properties were compared to the triggers for categorization. A WoE assessment of data relevant to categorization of CPY as a POP or PBT was conducted. Based on the P in water, soils, and sediments, B in organisms, and its potential for long-range transport (LRT), CPY does not trigger the criteria for categorization as a POP under the Stockholm convention or EC-1107/2009. Like many pesticides, it is chronically toxic at concentrations less than the trigger value for T under EC1107/2009. This simple trigger needs to be placed in the context of the inherent properties of the molecule in the environment, duration of exposures, and small risks to non-target organisms in or close to the areas of use. Overall, CPY is judged to not trigger the PBT criteria of EC-1107/2009. A similar assessment of properties of the toxicologically-relevant metabolite, chlorpyrifos oxon (CPYO), shows that it does not trigger criteria for POP or PBT. However, the half-life in air is greater than the LRT trigger of 2 d. Because it has greater solubility in water and lesser K_{ow}, CPYO partitions into water where it degrades more rapidly. Overall

persistence is such that the potential for LRT is less, which is consistent with lack of detection of CPYO in remote regions.

AGRO 203

Investigations into the SAR of the aminosulfones

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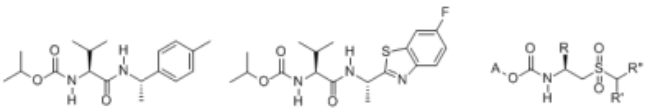
The aminosulfones, discovered at Dow AgroSciences, represent a proprietary class of chemistry used primarily for the control of *Plasmopara viticola* (PLASVI) in vines and *Phytophthora infestans*(PHYTIN) in potatoes and tomatoes. The key structural difference between the aminosulfones and related valinamide carbamate fungicides (e.g., iprovalicarb and benthiavalicarb) is the replacement of the amide moiety with a methylene sulfone. The fungicidal activity exhibited by the initial analogs prompted further investigation into the structure activity pattern (SAR) of this new class of chemistry. This paper will focus on the synthetic challenges and biological activity of this area.



AGRO 204

Interaction of organic solvents with the epicuticular wax layer of wheat leaves

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After foliar application, unabsorbed compounds remaining on the leaf surface can be removed by dipping or rinsing plant leaves in various dilutions of organic solvents in water. However, interactions between the solvent mixtures and the epicuticular wax layer have received little attention, and information on potential physical and chemical intactness to the plant surface by this method is limited. In this study, wheat leaves were dipped in organic solvents (methanol, ethanol, isopropanol, acetonitrile, and acetone) at different dilutions with water, and the major component of the leaf epicuticular wax layer, 1-octacosanol, was analyzed in the solutions to assess damage to the wax layer. Isopropanol and acetone removed more 1-octacosanol compared to methanol, ethanol, and acetonitrile; however, the extractable 1-octacosanol recovered in isopropanol and acetone was still less than 15% of that extracted in chloroform. Dipping leaves in dilutions of organic solvent as low as 60% by volume resulted in very low levels of 1-octacosanol, while no 1-octacosanol was detected in any mixtures containing less than 40% organic solvent. The differential extraction of 1-octacosanol in leaf samples by the solutions was found to be correlated with solubility of pure 1-octacosanol in the respective solutions. Furthermore, analysis of leaf surfaces by scanning electron microscopy showed structural intactness of the epicuticular wax layer, particularly when dipped in 20% or 40% organic solvent, which further supports our analytical data. Therefore, our results demonstrate that the epicuticular wax layer of wheat leaves is not altered physically or chemically by organic solvent solutions up to 40% by volume, and these findings provide new insights into the interaction of organic solvents with plant leaf surfaces.

AGRO 205

Discovery and the structure activity relationship of a series of novel oxadiazole-based insecticides

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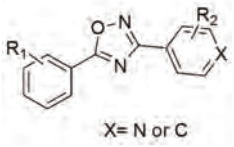
Bioactive scaffolds have been a source of new chemistry for lead generation in agrochemicals and pharmaceuticals. One such bioactive scaffold known in the literature is the substituted oxadiazole. Due to its potential for bioactivity and ease of synthesis, an effort was initiated to explore the oxadiazole scaffold. We opted to explore this scaffold *via* a parallel synthetic approach in an effort to generate novel molecules with relevant biological activity (Figure 1). Several *in vitro* and *in vivo* insecticidal hits, with activity against sweetpotato whitefly (BEMITA) and green peach aphid (MYZUPE) were identified from this initial library. A follow-up library led to molecules with increased efficacy and a broadened spectrum which included western flower thrips (FRANOC). A single pot microwave synthesis was utilized to efficently investigate the structure activity relationship (SAR) in an attempt to further increase activity and/or spectrum. The synthesis, design, and optimization of the hit generation library, as well as single analog synthesis and SAR of the active series, will be the focus of this poster.

Figure 1



AGRO 206

SAR Studies on 2-(2-arylidenehydrazinyl)-N-aryllpyrimidin-4-amine: A lepidopteran insecticide lead

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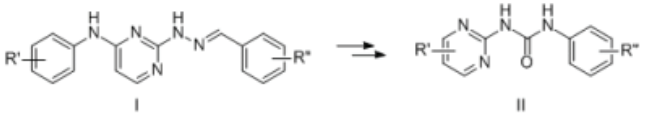
2-(2-Arylidenehydrazinyl)-*N*-aryllpyrimidin-4-amines (**I**) were found to exhibit broad spectrum control against commercially relevant lepidopteran pests. A SAR investigation about the aryl amine and 2-(2-arylidenehydrazinyl) motifs was undertaken. Details of this investigation, including the synthesis and biological characterization of hyrdrazones **I** , as well as the discovery of insecticidal ureas **II** will be described.



AGRO 207

Discovery and optimization of isoxazolidines as novel insecticides

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HTS (High Throughput Screen) composes a key source of generating agrichemical and medicinal chemistry Hits and

Leads. This paper will present one novel class of isoxazolidine as insecticides from HTS screen. The discovery and optimization of this class of chemistry will be presented.

AGRO 208

Discovery and optimization of 4-aminomethylpiperidines as new class of insecticides

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4-Aminomethylpiperidines are a new class of insecticides which were discovered through scouting projects in medicinal chemistry journals. This paper will present our efforts on the discovery and optimization of this area.

AGRO 209

Triple mode of action herbicide tolerance utilizing the Enlist™ Weed Control System in soybeans

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We report on a novel soybean trait that confers tolerance to glyphosate, 2,4-D, and glufosinate herbicides. Three herbicide tolerance genes, *2mEPSPS, aad-12* and *pat* were constructed into a single vector for constitutive expression. The stacked genes were introduced into the soybean line, Maverick via *Agrobacterium tumefaciens*-mediated transformation. The transgenic T0 plants were self-pollinated for several generations in contained and regulated field nurseries. Herbicide tolerance and molecular characterization were used for selection of events. The lead event was characterized, selected, and bred into elite soybean varieties. This event provided robust tolerance to single, sequential, and tank-mix applications of 2,4-D and glyphosate as well as to glufosinate. The trait will be identified as Enlist E3™ soybeans. Enlist E3™ soybeans will be used with a proprietary blend of glyphosate and a new 2,4-D choline. This product, Enlist Duo™, contains a number of innovations to reduce spray drift, post-spray volatilization, and odor and for improved handling characteristics. The combination of Enlist E3™ and Enlist Duo™ will provide soybean growers with more robust weed management options including the exceptional control of glyphosate-resistant and hard-to-control weeds. [™*Trademark of The Dow Chemical Company ("Dow") or an affiliated company of Dow. Components of the Enlist Weed Control System have been submitted for review and registration and have not yet received regulatory approvals in all countries. The information presented is not an offer for sale. Enlist Duo herbicide is not yet registered for sale or use as a component of the Enlist Weed Control System. Always read and follow label directions. ©2013 Dow AgroSciences LLC. Enlist E3 soybeans were co-developed by Dow AgroSciences and M.S. Technologies.*]

AGRO 210

Toxicity of *Bacillus thuringiensis* to aquatic non-target organisms and its influence on toxicity of chloropyrifos

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Since the commercialization of transgenic cotton, which expressed Cry toxins produced by *Bacillus thuringiensis* (Bt) in 1997, its cultivation has increased dramatically. Planting Bt cottons tremendously reduced the use of broad spectrum chemical pesticides, but the widespread cultivation of Bt crops has raised public concerns on their toxicity to non-target organisms. On the other hand, chemical pesticides were also noted to be applied in Bt cotton fields in some occasions. The current study investigated toxicity of Bt toxin to non-target aquatic organisms and its impact on toxicity of an organophosphate pesticide, chloropyrifos. Response surface methodology was used to optimize the extraction of Cry1Ac protein from solid matrices, and the optimum extraction conditions were at 21 ºC and 630 rpm for 2 h. The method showed high precision and sensitivity with the method detection limit of 0.8 ng/g dry weight and relative standard deviation of 7.3%. The dissipation of Cry1Ac protein in different matrices was investigated using a first-order kinetic equation, and DT_{50} values ranged from 0.8 to 3.2, 2.1 to 7.6 and 11.0 to 15.8 d in soil, sediment and water, respectively. Microbial degradation contributed the most to the dissipation of Cry1Ac protein, and high temperature accelerated the processes. While Bt proteins persisted for a longer time in aquatic systems than in soil, toxicity of Bt toxins to aquatic non-target organisms *Chironomus dilutus* and *Hyalella azteca* was limited. Last, joint toxicity of Cry1Ac protein and chloropyrifos was evaluated using mortality, movement, and acetylcholinesterase inhibition as toxic endpoints. Compared to the toxicity estimates using independent action and concentration addition models, an antagonistic interaction was noted when both pesticides were applied simultaneously in both sediment and water-only bioassays, while the organisms which were pre-fed with Bt proteins showed no change in susceptibility to chloropyrifos.

AGRO 211

Comparison of aflatoxins analysis by test kit with liquid chromatography confirmation method

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Aflatoxins are severely toxic fungal metabolites produced primarily by *Aspergillus flavus* and *Aspergillus parasiticus.* Their occurrence is stimulated by hot and humid field conditions; infection of a variety of crops may occur during either growth or post-harvest storage. In Indiana, drought conditions in the summer of 2012 provided an opportunity to investigate correlation of test results from screening and confirmatory testing methods. Accurate determination is required both to control the human health risk and to advance surveillance of the food supply. In a variety of corn and other animal feed ingredient samples, total aflatoxin content was measured using a rapid ELISA test kit and results were compared with those obtained using liquid chromatography with post-column photochemical derivatization (AOAC 2005.08). This paper will discuss possible reasons for some significant discrepancies in results between these two methods.

AGRO 212

Multiresidue analysis of pesticides in brown rice and orange by liquid chromatography-tandem mass spectrometry

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This study was carried out in order to establish a multiresidue analysis method applicable to the Positive List System (PLS) in Korea. A simple, sensitive, and selective method using liquid chromatography-tandem mass spectrometry (LC/MS/MS) has been developed to detect 88 pesticides in brown rice and orange. Samples were prepared using acetonitrile saturated with sodium chloride, followed by solid phase dispersive clean up. The quantification was done with matrix-matched calibration curves. The limits of quantification were in the range 0.0003-0.03 mg/kg and the limits of detection were between 0.0001 and 0.01 mg/kg. The recoveries at 0.02 and 0.1 mg/kg were within 70-120% (n=6) associated relative standard deviations < 25%. Based on these results, this multiresidue analysis method has been proven to be a highly efficient, robust, and accurate approach suitable for the monitoring of LC-amenable pesticides in accordance with PLS requirements. This method can surely be used as the official method for monitoring pesticides applicable to the PLS of imported agricultural products in Korea.

AGRO 213

Novel fluorinated strobilurin-pyrimidine acaricide: Design, synthesis, and acaricidal activity

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A new acaricide, pyriminostrobin, was discovered in our previous work. Based on the conception of introducing fluorine into pyriminostrobin to improve its bioactivity, a series of strobilurin-pyrimidine conjugates were synthesized and bioassayed. The compounds were characterized by ^{1}H-NMR, MS, and elemental analysis. Highly active compound **7e** was studied by X-ray diffraction. Preliminary bioassays demonstrated that compounds **7e** , **7f** , and **7i** exhibited notable control of *Tetranychus cinnabarinus* (Boisd.) at 1.25 mg L^{-1}. The relationship between structure and acaricidal activity was also reported. Two compounds of particular interest, **7e** and **7i** , exhibited potent acaricidal activity. The acaricidal potencies of these analogs are higher than fluacrypyrim in greenhouse applications, which are more efficacious than pyidaben and are comparable with pyriminostrobin and spirodiclofen in field trials. [Acknowledgments - The project was supported by the National Key Technology Support Program during the 12th Five-Year Plan Period (Grant No. 2011BAE06B00 and 2011BAE06B05) and the National Key Basic Research Program (973 Program) (Grant No. 2010CB126105 and 2012CB724501).]

AGRO 214

Research directed towards the discovery of novel thymidylate synthase inhibitors as agricultural fungicides

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Thymidylate synthase is a cytosolic enzyme that plays an essential role in DNA replication and repair in many organisms. X-ray crystal structures of thymidylate synthase from various organisms have been reported in the open literature as have non-endogenous ligands and biochemical assays for determining the potency of those ligands. Leveraging that information, computational models and a biochemical assay were developed directed toward discovering thymidylate synthase ligands which control agriculturally-relevant fungal pathogens. This paper will describe this research as well as the screening program and targeted synthetic efforts employed to identify novel fungicidal thymidylate synthase inhibitors.

AGRO 215

Development and validation of a quantitative enzyme-linked immunosorbent assay (ELISA) for determining transgenic protein AAD-12 in soybean tissues

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The aryloxyalkanoate dioxygenase (AAD-12) derived from *Delftia acidovorans* is expressed in soybean plants, where it provides tolerance to 2,4-dichlorophenoxyacetic acid. For the purpose of monitoring protein levels in plant, seed, and processed products, a specific, sensitive, and reliable quantitative detection method is needed. An Enzyme Linked-Immunosorbent Assay (ELISA) has been developed for the quantitative detection of AAD-12 recombinant protein in a sandwich format. In this format, a polyclonal antibody, specific for AAD-12, is immobilized on the microtiter plate, and an anti-AAD-12 monoclonal antibody is conjugated with an enzyme label. The resulting assay has a quantitative range of 0.5 -10 ng/mL with a limit of quantitation of 1.0 mg/g dry weight for AAD-12 protein for all soybean matrices. No cross reactivity was measured to other GM proteins tested. The method was validated for accuracy, extraction efficiency, precision, and ruggedness, which indicated that this AAD-12 ELISA is suitable for plant monitoring and seed testing. Application of this method for AAD-12 protein quantitation in field expression studies will be discussed.

AGRO 216

Development and validation of a sensitive and specific immunoassay for the detection of aryloxyalkanoate dioxygenase (AAD-1) protein in maize tissues

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A transgenic maize line has been genetically modified to express aryloxyalkanoate dioxygenase protein (AAD-1) providing tolerance to 2,4-dichlorophenoxyacetic acid (2,4-D) and aryloxyphenoxypropionate (fop) herbicides. An

Enzyme Linked-Immunosorbent Assay (ELISA) has been developed to specifically quantitiate the AAD-1 expression in maize tissues. The resulting assay uses two specific monoclonal antibodies in a sandwich ELISA format and was validated for its sensitivity, specificity, accuracy, precision and ruggedness. The validation results demonstrated that it is specific to AAD-1 with no cross-reactivity to other transgenic engineered proteins. The AAD-1 protein extracted from various maize tissues can be quantitated from a 1 – 32 ng/mL calibration curve with acceptable accuracy and precision. The validated LOD (limit of detection) and lower LOQ (limit of quantitation) were 0.20 and 0.40 ng/mg dry weight, respectively. The results demonstrate that the assay is specific, sensitive, and accurate for AAD-1 quantitation in maize tissues.

AGRO 217

Application of AlphaLISA technology in testing genetically modified (GM) crops

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Traditional technologies for testing genetically modified (GM) crops include Enzyme Linked Immunosorbent Assay (ELISA) and Lateral Flow Strip (LFS). These technologies are easily used in small scale GM testing. When GM testing on a larger scale is required, the limitations of these technologies, ELISA and LFS, become more apparent. These limitations include time, cost, and sensitivity. To meet the demands of greater throughput, the PerkinElmer amplified luminescent proximity homogenous assay (Alpha) technology was evaluated. The Alpha technology is a bead-based proximity assay that is easily adapted to use existing antibody (Ab) reagents developed for ELISA and LFS GM crop testing. The Alpha assay is homogenous with high sensitivity, can be adapted for high throughput, and is cost effective. These results indicate that the AlphaLISA technology is suitable for GM testing. This paper will introduce the detection of GM proteins, such as Cry1F and Cry34Ab1, in plant seed or tissues (e.g., corn) using AlphaLISA technology.

AGRO 218

Development and validation of a quantitative enzyme-linked immunosorbent assay for the detection of 2mEPSPS protein in soybean tissues

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A selective enzyme-linked immunosorbent assay (ELISA) was developed and validated to quantify double mutant 5-enolpyruvylshikimate-3-phosphate synthase (2mEPSPS) protein expression in soybean tissues. The 2mEPSPS protein is a modified maize EPSPS protein that when expressed in soybean, confers tolerance to glyphosate herbicides. The ELISA method developed to quantify this protein uses a sequential sandwich format in which soybean sample extracts are incubated in the wells of an immobilized anti-2mEPSPS polyclonal antibody coated plate. An enzyme-conjugated anti-2mEPSPS protein monoclonal antibody is sequentially added to the wells, which will bind to the immobilized polyclonal antibody-protein pair on the plate. The resulting assay has a quantitative range of 8 - 200 ng/mg dry tissue weight, with a lower limit of detection of 4 ng/mg dry tissue weight. The method showed no cross-reactivity to other herbicide tolerance transgenic proteins including CP4 EPSPS protein, and no false positive or false negative results were observed. Protein extraction efficiency was above 84% using a phosphate-buffered saline solution supplemented with Tween-20 and casein. Average protein recovery of fortified samples was above 76%. Method precision and ruggedness was assessed through inter-assay variability, which did not exceed 8% (%CV). Matrix effects were observed at lower sample dilution levels, requiring samples to be diluted at a 1:10 minimum dilution for accurate quantitation. All validation results confirmed that the 2mEPSPS ELISA method is suitable for its intended use. Application of the validated method in soybean tissue samples will also be discussed.

AGRO 219

Systematic approach for validating enzyme-linked immunosorbent assay (ELISA) methods for protein quantification from soil

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Validated methods for protein quantification by enzyme-linked immunosorbent assay (ELISA) are necessary for accurate reporting and analyses; however, developing methods for extracting and quantifying proteins from soil or other environmental matrices can present unique challenges. Oftentimes the buffer required to extract immunoreactive protein from soil can introduce potential interference by the soil matrix which can subsequently affect ELISA analysis. Central to ELISA validation are experiments designed to characterize interference due to the soil matrix or extraction buffer, as well as to optimize recovery of the protein from the soil matrix. Additional validation to determine accurate interpolation of the protein concentration at multiple dilutions and the use of well-characterized quality controls and acceptance criteria help ensure methods are robust and reliable. A systematic approach for conducting comprehensive ELISA validation experiments necessary to ensure accuracy and reproducibility of the method in environmental matrices will be presented.

AGRO 220

Absorption and penetration of glufosinate viewed in metabolism studies

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The resistance to glufosinate of two lines —genetically modified (GM) and unmodified (R and S, respectively)— of *Triticum aestivum* has been studied. In the GM line, the bar gene was introduced to increase the resistance to glufosinate. Experiments in a controlled growth chamber showed that line R presented a high resistance to glufosinate with an ED_{50} value of 478.59 g active ingredient per hectare (g ai ha^{-1}) versus 32.65 g ai ha^{-1} for line S. The activity of glutamine synthetase (GS) in leaf extracts from both lines was investigated. The I_{50} for line R was 694.10 µM glufosinate versus 55.46 µM for line S, with a resistance factor of 12.51. LC–TOF/MS analysis of glufosinate metabolism at 48 h after herbicide treatment (300 g ai ha^{-1}) revealed an 83.4% conversion of the herbicide (66.5% in N-acetyl-glufosinate metabolite), while in line S conversion of the herbicide was about 40% (0% to N-acetyl-glufosinate). Metabolism studies showed a higher and faster penetration of glufosinate in line S than in line R (6 times). These results suggest that metabolism of glufosinate by the bar gene is a key mechanism of resistance in line R that explains such high levels of herbicide tolerated by the plant, together with other mechanisms due to unmodified pathway, absorption and loss of glufosinate affinity for its target site. LC–TOF/MS analysis allowed an accurate analysis of both the absorption

and translocation of the herbicide without the use of radiolabelled compunds. Moreover, this method combined herbicide translocation data plus herbicide degradation to other metabolites, so herbicide metabolism in different parts of the plant could be studied.

AGRO 221

Microbiome mining: Panda conservation and biofuels

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Integrating next-generation metagenomic sequencing into giant panda conservation can provide insight into their gastrointestinal tract's (GIT) unique microbial system. GIT microflora can enhance giant panda conservation efforts through the greater understanding of microbes' involvement in digestion and their potential in producing second-generation lignocellulosic biofuels. Metagenomic analysis elucidated seventeen cellulolytic, six lignolytic, seven oleaginous, five nitrogen-fixing, and seven alcohol-producing microorganisms, and several organisms have been validated using species-specific PCR. These organisms play a major role in the giant pandas' ability to digest bamboo, but they can also be used as a pretreatment method in biofuel production. These organisms have been shown to degrade cellobiose (cellulose surrogate) and accumulate transesterifiable lipids under anaerobic conditions. Analyses indicate that cellobiose was consumed (HPLC/ELSD) and that transesterifiable lipids were accumulated (GC-FID) displaying giant panda microbes' ability to convert lignocellulosic biomass into lipids. The integration of new technologies and disciplines can substantially improve conservation efforts through advanced understanding of giant panda digestion and potential biofuel production.

AGRO 222

Metabolic engineering for improved microbial 2,3-butanediol production

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Many chemicals, which could only be produced by chemical processes in the past, could potentially be generated biologically from annually renewable resources. Microbial production of 2,3-butanediol (2,3-BD) is one of the examples. Its fermentative production process has attracted great interest due to the relatively higher product concentration that can be obtained, as well as its lower toxicity to microbial systems compared with other alcohols. However, some properties of the wild strains still hinder its large scale production. For example: 1) There are so many by-products in the fermentation broth that the conventional 2,3-BD fermentation process is not economically competitive because the formed by-products could inhibit 2,3- BD production, reduce 2,3-BD yield, and increase costs of product recovery and purification. 2) Different wild strains generally produce different 2,3-BD stereoisomers (meso-, (R,R)-, (S,S)-), but a mixture of two stereoisomers is generally formed, this would make it difficult to obtain the enantiomerically pure 2,3-BD stereoisomer which is vitally important for chiral synthesis. To resolve the abovementioned problems, the wild strain must be improved to be a robust and economical cell factory. In this presentation, we will discuss some case studies using metabolic engineering to improve the efficiency of the 2,3-BD producing strain. It involves both native 2,3-BD producers, i.e. homologous hosts, as well as microorganisms with acquired ability to form 2,3-BD via genetic manipulations, i.e. heterologous hosts. Aiming at reducing the by-products formation, a 2,3-BD hyper-producing *Klebsiella oxytoca* was successfully metabolically-engineered by altering the mixed acid-2,3-BD fermentation pathway. Using the modified proton-suicide method followed by gene insertional inactivation technology, a mutant strain with reduced by-product release was obtained. Aiming at producing the enantiomerically-pure (R,R)-2,3-BD, a synthetic metabolic pathway was constructed in *E. coli* by complementing the 2,3-BD biosynthetic pathway of *K. oxytoca* with (R,R)- specific 2,3-BD dehydrogenase from *Bacillus subtilis*.

AGRO 223

Synthesis of enantiomerically-pure aryloxyphenoxypropioanate herbicides: Using biobased building blocks as starting material for agrochemicals

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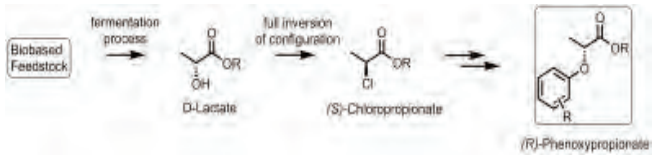
An important class of herbicides are the aryloxyphenoxypropionates. Studies have shown, that the *R* enantiomer is the active enantiomer in the inhibition of ACCase. The manufacturing process towards these compounds has proven tedious and is known to suffer from racemization. Here we present an alternative route, which uses D-Lactate as a key intermediate. D-Lactate consists of the unnatural enantiomer of lactic acid and is now a readily available compound that is produced from biobased feedstock with the use of a fermentation process. A detailed optimization study of the chlorination step has been conducted, which resulted in virtually complete inversion of configuration. This new and optimized route enables a more green and sustainable route towards higher quality herbicides.



AGRO 224

Large-scale particulate matter air sampling system for high density data measurments

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Increasing regulatory pressure on particulate matter emissions originating at agricultural operations and processing plants has created a needed for additional industry specific data. The required data generally includes point source or stack sampling and non-point source data. In this paper, the focus is non-point source data usually collected with ambient air samplers. For small sources or small scale sampling campaigns researchers generally use EPA approved ambient samplers, such as the TEOM. However for large scale sampling campaigns where twenty

or more sampling points are required, samplers like the TEOM become impractical due to their large size, high cost, low data storage capacity, and high power consumption. In the past, these drawbacks forced the researchers to work with very few sample points even when examining large processing plants that may cover several tens of acres. Consequently, the resolution of the resulting data sets was extremely limited, and verifying dispersion modeling results with this data is difficult if not impossible. In 2003, a project was initiated to develop a new air sampler that would mitigate the short comings of the currently available ambient air samplers. The completion of the design and development was eventually conducted at Oklahoma State University and the full system was deployed in 2008 with a total of 120 sampling points. Recent studies have incorporated the large scale comprehensive sampling setup and cover areas as large as 28 ha. This paper describes the design, development, and operation of this large-scale air sampling system.

AGRO 225

Discovery of metazosulfuron: A new sulfonylurea herbicide for rice

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Sulfonylurea (SU) herbicides have been in use for more than thirty years, and they still remain an important class of herbicides widely used in agriculture. In Japan, SU herbicides have been widely used in paddy fields; however, recently several paddy weed species showing resistance to SU herbicides are spreading nationwide. We have focused on discovering a new herbicide and investigated the herbicidal activity of pyrazolesulfonylurea derivatives on SU-resistant weeds. As a result, we found that some pyrazole-5-sulfonylureas showed high levels of herbicidal activity against SU-resistant weeds. Further evaluation of the pyrazolesulfonylurea chemistry led to the discovery of metazosulfuron. It is a new SU herbicide, which shows excellent herbicidal activity against annual and perennial weeds including SU-resistant biotypes in paddy fields. In this presentation, the structure-activity relationships of pyrazolesulfonylurea derivatives as well as the synthesis of metazosulfuron will be discussed.

AGRO 226

IR-4 Project: A public sector program to facilitate the registration of biopesticides

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The IR-4 Project was established 50 years ago to help to register pesticides in specialty crops or minor crops in addition to minor uses. IR-4 is a public sector organization, primarily funded by USDA-NIFA. Most biopesticides fill small but important segments of crop production, so like minor uses, it is difficult for small companies to justify investment in the registration process. Often researchers and small companies lack the expertise on how to prepare the information required by EPA. The biopesticide program was established in 1982 as part of IR-4 to assist in the federal registration of biopesticides with EPA. IR-4 is involved in assisting the registration of biochemical biopesticides such as plant extracts, pheromones, and minerals in addition to microbial and biotechnology products. This presentation will provide an overview of the IR-4 Biopesticide Program and recent registrations as well as current projects.

AGRO 227

Biopesticides: State of the art and future opportunities

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Terpenes are the most diverse class of biomolecules, with over 50,000 described compounds. Fifteen carbon sesquiterpenes are ubiquitous in nature and are known to be effective in a wide range of high value applications including flavors and fragrances, cosmetic products, food ingredients, pharmaceutical products, and insect control. There is rich literature on the use of sesquiterpenes for insect control. Work at the US Centers for Disease Control has demonstrated that nootkatone, the defining flavor and fragrance of grapefruit and also found in Alaskan yellow cedar, is a very effective tick acaricide and repellent. In those studies, it was further demonstrated that low concentrations of nootkatone have the ability to maintain effective acaricidal activity for up to six weeks. In addition to nootkatone, numerous other sesquiterpenes have been shown to control effectively insects such as mosquitoes, ants, fleas, and bedbugs. In spite of their proven efficacy, there has been little commercial development of sesquiterpenes as insect control agents due to their lack of availability at commercially viable prices. Allylix has developed proprietary technology for the production of terpenes using synthetic biology and metabolic engineering of *Saccharomyces cerevisiae* yeast. This technology provides the basis for sustainable production of sesquiterpenes and other terpenes from abundant inexpensive raw materials, allowing reliable cost-effective production of these compounds at consistent quality. The production process for nootkatone has been practiced at commercial scale, and nootkatone is currently sold in the marketplace. Allylix technology can also serve as a platform for discovery of new biopesticide products. Using straightforward chemical modification of various terpene scaffolds produced by fermentation, libraries can be generated and tested for insect control and other applications. These technologies provide mechanisms to discover and to produce terpene-based biopesticide products that can compete with conventional pesticides on both and efficacy and an economic basis.

AGRO 228

Growing need for bioherbicides

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Several factors have converged to make the need for bioherbicides perhaps more urgent than the need for other biopesticides. First, there is a critical need for new herbicide modes of action, as a new mode of action has not been introduced in more than 20 years, and new modes of action are needed to manage growing resistance to herbicides with old modes of action. Phytotoxic natural products that might be considered bioherbicides are a major source of novel modes of action. For example, many unused sites of action are known for microbial phytotoxins. Second, the biggest pest management need of organic farmers is new, effective tools for weed control. Thus, new bioherbicides that might be accepted by the organic farming community are a critical need for improving the economics and effectiveness of pest management in organic systems. Lastly, greener weed management with bioherbicides is highly desirable in order to reduce the environmental footprint of weed management in conventional crops. For example, the possibilities of RNAi as a bioherbicide in eliminating pesticide residues in the environment and in harvested crops, as well as eliminating non-target species effects are huge. There is tremendous

potential to solve all three of these needs with greater bioherbicide discovery and development efforts.

AGRO 229

Registration of biopesticides

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Federal law requires that all pesticides sold and distributed in interstate commerce in the United States be registered. The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) requires that the EPA determine that a pesticide, when used consistent with label directions, will not cause unreasonable adverse effects to human health or the environment. The US EPA, Office of Pesticide Programs, Biopesticides and Pollution Prevention Division is responsible for the registration and registration review of biopesticide products. Biopesticides include naturally occurring substances that control pests (biochemical pesticides), microorganisms that control pests (microbial pesticides), and transgenic plant pesticides, known as plant-incorporated protectants or PIPs. Biopesticides typically are distinguished from conventional chemical pesticides by increased specificity to target species, natural occurrence, low human toxicity, or low volume of use. This presentation will focus on the biopesticides regulatory scheme. Definitions and legal framework, key steps, and recent improvements will be reviewed.

AGRO 230

Fascinating science, frustrating reality: Five barriers to broad utility of biopesticides

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For more than a century, growers have understood the potential of biological control agents as effective tools for crop protection. The agriculture industry has yet to realize, however, many predictions about the pace of growth and adoption of biopesticides. Advances in science have increased the breadth of understanding about the potential of biopesticides while simultaneously deepening the realization of the challenge inherent in converting that potential into a robust solution. Learnings from the past decades of agricultural chemistry research have built a clearer understanding of the five key barriers to broad utility of biopesticides and the magnitude of improvements required.

AGRO 231

Outlook for biopesticides in agriculture and public health

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The authors will lead discussion on the status of biopesticide research, discovery, effectiveness, regulation, economics, and future outlook in the U.S. and internationally. The appropriateness of terms such as biopesticide, biorational pesticide, naturally-occurring, and 3rd generation pest control agents will be discussed, as well as, exploited targets and opportunities for biopesticides in integrated pest management.

AGRO 232

Discovery and optimization of cyclic carbonyl amidines as potent insecticides

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Neonicotinoids are a class of insecticides discovered in recent decades and have been adopted by farmers globally and applied broadly in the last couple decades. Given their supreme physical chemistry and biology profiles, there has been another surge of discovery activity on searching for new neonicotinoid insecticides. This presentation will disclose our efforts on this area. The discovery and optimization of a new class of neonicotinoids, i.e., cyclic carbonyl amidines, will be discussed.

AGRO 233

Substituted cyclopropyl- and thiazolyl-1*H*-1,2,4-triazoles as insecticides and acaricides

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Dow AgroSciences is a global crop protection company focused on the discovery of products that target fungi, weeds, and insects. A goal of the insecticidal research team is to develop new entities which provide broad-spectrum insect control of both chewing insects, such as *Lepidoptera* and *Coleoptera*, and some sap-feeding insects, such as whitefly, aphids, and mites. Classes of chemistry within substituted cyclopropyl- and thiazolyl-1*H*-1,2,4-triazoles were explored to address this goal. The efforts directed toward the synthesis and structure-activity relationship (SAR) of these compounds will be discussed.

AGRO 234

Azetidinols and prolinols as insecticides

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Neonicotinoid insecticides act as agonists of nicotinic acetylcholine receptors (nAChRs). Neurotransmitter receptors belonging to the same family have been targets for pharmaceutical drug discovery for a long time. Epibatidine, an alkaloid isolated from frog skin, binds to vertebrate α3/β4 and α4/β2 nicotinic receptors but also shows some insecticidal activity. However, the extremely-high mammalian toxicity would not allow the use in crop protection. Optimization of the analgesic activity of epibatidine led to the less toxic azetidinol derivative ABT 594. Due to their instability, the known azetidinol analogs are not suitable for agrochemical uses. We used the scaffold as a starting point for the discovery of new insecticides. Prolinols and azetidinols with improved metabolic stability, good activity against piercing sucking insects, and low mammalian toxicity will be presented.

AGRO 235

SAR investigations into *N*-azinyl-*N*'-aryl ureas as insecticides

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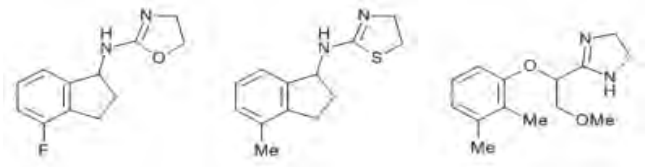
While investigating a series of dianilinotriazines, a new *N*-azinyl-*N*'-aryl urea scaffold was discovered which showed control of lepidopteran pests. Structure activity relationships (SAR) have been investigated to optimize the azinyl substitutions as well understand the optimal substitution patterns on the urea moiety. Chemistry developed to access these new molecules and their biological activity will be discussed.

AGRO 236

Synthesis and insecticidal activity of new benzyl- and indanyl- oxazolines, thiazolines, and imidazolines

Anthony C O'Sullivan[1], *anthony.osullivan@syngenta.com, Juergen H. Schaetzer*[1], *Christophe Luethy*[1], *Christopher J. Mathews*[2], *Clare Elliott*[2], *Thomas Pitterna*[1], *Jagadish Pabba*[3], *Olivier Jacob*[1], *Anke Buchholz*[1], *Judith Blythe*[2]. *(1) Syngenta Crop Protection, Crop Protection Research, Stein CH-4332, Switzerland (2) Crop Protection Research, Syngenta Crop Protection, Jealott's Hill International Research Centre, Berkshire RG42 6EY, United Kingdom (3) Santa Monica Works, Syngenta Biosciences Private Limited, Corlim Ilhas, Goa 403 110, India*

Compounds of the type shown below are examples of a new chemical class with potent activity against sucking insects, comparable to or greater than commercialised standards. Aspects of the discovery, synthesis, biology, and structure-activity relationships will be presented.



AGRO 237

SAR studies of the new sulfoximine sap-feeding insecticide, sulfoxaflor

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Sulfoxaflor is the first insecticidal product from the new sulfoximine class of insect control agents. A broad-spectrum insecticide exhibiting excellent efficacy against many sap-feeding insect pests, including aphids, whiteflies, hoppers, and *Lygus*, sulfoxaflor is comparable in activity with other classes of insecticides targeting sap-feeding insects, including the neonicotinoids. Importantly, sulfoxaflor exhibits little to no cross-resistance in insects that are resistant to the neonicotinoids and other insecticides. A comprehensive effort was undertaken to understand better the SAR of this unique chemotype including the synthesis of analogs designed to probe the conformational requirements for the putative recognition elements. The design, synthesis, and biological evaluation of these targeted molecules will be discussed.

AGRO 238

Discovery of Sivanto™, a new butenolide insecticide

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Sivanto™ is an innovative insecticide belonging to the new butenolide chemical class. The discovery of Sivanto™ was primarily inspired by the natural product stemofoline (isolated from the plant *Stemona japonica*). Its unique pharmacophore system represents a new bioactive scaffold selectively acting on the insect nicotinic acetylcholine receptor, one of the most important target sites for modern insecticides. The new butenolide-based chemistry provides a favorable pharmacokinetic and safety profile. Due to its physicochemical properties allowing versatile application methods, Sivanto™ offers excellent and fast efficacy against a broad spectrum of sucking pests in many agricultural and horticultural settings. Structure-activity relationship studies leading to the discovery of Sivanto™ and its biological profile will be presented.

AGRO 239

Did we select lead chemistries for optimization based on MOA or activity?

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Choosing lead chemical classes for optimization is always difficult to determine. In the early 1980s, we chose leads from patents, and a few successful optimizations were achieved at Sumitomo Chemical in IGR and herbicide areas. Better efficacy was good enough to develop a compound, even if the mode of action (MOA) was the same as a competitor's compound. Now we are concerned with resistance in any area of agrochemicals. The mode of action is thought to be a more important factor in choosing the lead. Examples of successes and failures in choosing the lead will be discussed.

AGRO 240

Strategies and tactics for the synthesis of complex alkaloids

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Strategies and tactics that accomplish the efficient syntheses of several alkaloids in an efficient manner will be discussed. Especially pertinent will be a discussion of metal-mediated methods for C-C bond formation and the synthesis of heterocyclic natural product like compounds.

AGRO 241

OECD project on international harmonization of terrestrial field dissipation guidance and ecoregion crosswalk

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An OECD project was initiated to develop harmonized guidance for conducting terrestrial field dissipation (TFD) studies and to develop an ecoregion crosswalk across North America and Europe. The TFD studies assess the transformation, transport, and fate of pesticides under representative actual use conditions. The major objective of this project is to facilitate the use of studies conducted at a specific site in North America or Europe across international borders based on the similarity of the ecoregion. The United States Environmental Protection Agency (US-EPA) has the lead for harmonization of the TFD guidance while the Pest Management Regulatory Agency (PMRA), Health Canada has the lead for developing the ecoregion crosswalk component. The European Food Safety Authority (EFSA) is the co-lead for both projects. This presentation will focus on the recommendations from the OECD TFD-ecoregion crosswalk workshop which was held March 2011 to solicit input from experts on issues related to harmonization of TFD guidance. It will also provide the status of the OECD project and the progress made in finalizing the draft guidance document. To harmonize the TFD guidance, the OECD Project Expert Group identified the following technical issues that needed resolution: conceptual model/modular approach based on laboratory studies; experimental layout, sampling, analysis, results; and use of pesticide TFD data in exposure and risk characterization by North American and European countries. The recommendations from the workshop were based on a consensus among the experts after in-depth discussions of these issues. It was concluded that the proposed OECD harmonized guidance should satisfy the need for both North American and European partners as well as provide the flexibility for the need of different endpoints between OECD countries. *Note: The content of this presentation does not necessarily represent the official views of the OECD or of the governments of its member countries and EFSA.*

AGRO 242

Development and validation of a conceptual model of pesticide dissipation pathways under field conditions

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This presentation describes a conceptual model for a pesticide that specifically addresses the question: Why does dissipation and mobility in the field differ from that observed under laboratory conditions? A conceptual model hypothesis was developed on the basis of established physical processes and experimental data and tested against a range of higher-tier laboratory studies to understand the mechanism by which photolysis acts as a major degradation route in the field. A re-parameterization of the USEPA regulatory model, Pesticide Root Zone Model (PRZM), was proposed to reflect a conceptual model describing the dissipation of the pesticide under actual-use conditions. The refined model predicted soil residues that were a significantly better match to the observed data from the field studies compared to those from unrefined modelling using standard regulatory modelling inputs. This suggests that the conceptual model is generally applicable and the use of the re-parameterized model for risk assessment is justifiable.

AGRO 243

OECD guidance for pesticide field dissipation studies for obtaining DegT50 value

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The objective of the DegT50 module is to provide field results, from which the degradation half-life (DegT50) in top soil at 20°C and at a moisture content corresponding to field capacity can be derived, following inverse modelling procedures (EFSA 2010; http://www.efsa.europa.eu/en/efsajournal/doc/1936.pdf). The geomean DegT50 is used as an input parameter in simulation models for environmental exposure to pesticides (leaching to groundwater, exposure of aquatic and soil organisms), within the EU. In the context of this DegT50 module, the definition of 'degradation' of FOCUS (2006; http://focus.jrc.ec.europa.eu/dk/) is used which considers soil bound residues as degradation products. For the exposure assessments, it is essential that the DegT50 reflects the degradation rate within the soil matrix, so excluding other loss processes such as photodegradation or volatilisation. This can be achieved either by designing the experiment so that the measured decline reflects almost exclusively the degradation within the soil matrix (e.g., by incorporating the dose immediately after application or covering the soil surface after application) or by spraying the substance onto the soil surface combined with an analysis of the data that ensures that other loss processes than degradation do not influence the DegT50 obtained (EFSA 2010). The inverse modelling procedure for estimating a DegT50 is based on the decline of the total mass per surface area that is present in the soil profile. So, the DegT50 module provides guidance for assessing this decline. [*Note: The content of this abstract does not necessarily represent the official views of the OECD or of the governments of its member countries and EFSA.*]

AGRO 244

Experiences with planning and conduct of terrestrial field dissipation (TFD) studies in line with new EFSA guidance

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Degradation parameters derived from field dissipation studies are important input parameters for environmental fate models. These parameters may only be used as input parameters for exposure models if surface processes like photodegradation and volatilization are excluded. Possibilities to exclude surface loss processes mentioned by EFSA[(1)] include incorporation of the substance into the soil by mechanical devices or washing the substance into the soil by irrigation or precipitation. Another possibility not explicitly mentioned by EFSA[(1)] is covering the soil surface with substrate (e.g., sand). This method is considered to represent an adequate alternative to incorporation and irrigation; first practical experiences with this study design, the use of sand as means to exclude surface processes, will be presented. *[(1)] EFSA Scientific Opinion, Guidance for evaluating laboratory and field dissipation studies to obtain*

DegT50 values of plant protection products in soil, EFSA Journal 2010; 8(12)1936

AGRO 245

Interpretation of pesticide leaching in terrestrial dissipation studies using water content reflectometry

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In many regulatory terrestrial dissipation studies, evaluation of the leaching mobility of the applied pesticide and its degradation products is an important goal. Leaching, or lack of leaching, can only be rationally interpreted if there is information on water movement through the sampled soil profile. Water content reflectometers (WCR) offer a reasonably convenient method for assessing soil water content with depth and time. Continuous soil water content measurements from WCR probes placed at different depths are captured in onsite data loggers for later analysis. The number, timing, and depth of water recharge events from the field surface through the monitored soil profile can be determined from the water content data and correlated with rain or irrigation events. While recent improvements in WCR technology have been made, e.g., to correct for temperature and salinity automatically, the most accurate results are obtained when soil specific calibration equations are used to relate WCR probe output period to volumetric water content. Use of WCR probes in regulatory terrestrial dissipation studies is discussed.

AGRO 246

Inverse modeling for the derivation of degradation parameters in European and North American terrestrial field dissipation studies

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Both USEPA field dissipation and EU FOCUS modeling guidance outline the use of inverse modeling as a means to understand dissipation pathways and derive degradation parameters for modeling endpoints from terrestrial field dissipation studies (TFD). As an alternate method to normalizing TFD studies, inverse modeling allows the model to take into account specific processes that may occur such as plant uptake, sorption, or photolysis, in addition to degradation. The modeling of two TFD studies are presented to illustrate the methodologies used to optimize input parameters against observed field data. The non-linear parameter estimation tool (PEST 9.0) was coupled with the USEPA PRZM model and separately the EU FOCUS PEARL model to estimate degradation parameters using site specific soils and weather data. Both models were able to predict observed pesticide residues accurately within the soil profile. Optimized parameters from inverse modeling can be used for further refinement of exposure assessments and provide added value for TFD studies.

AGRO 247

Comparison of terrestrial field dissipation half-lives and trial sites between NAFTA and EU

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Dissipation half-lives for about 20 active substances and metabolites derived from terrestrial field dissipation studies across North America and the European Union were compared following normalization to reference conditions for soil temperature and moisture using techniques approved for European regulatory exposure modeling. In the vast majority of cases there were no significant differences in dissipation rates. Potential reasons for the differences observed in a small number of cases will be discussed. Two approaches were applied to assess the representativity of the NAFTA field trial sites for the EU: (1) using a selection of soil properties and climatic data (as in the currently developed OECD “ecoregion crosswalk” tool), and (2) using mainly the soil types as integrative measure of ecological conditions. Based on the results of these investigations we propose to include soil type information into the “ecoregion crosswalk” tool. In addition, we recommend always to apply expert judgment to the outcome of semi-automated representativity analyses.

AGRO 248

Welcome to Indiana, where agriculture is an integral part of our state

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Welcome to the heart of agriculture. We are pleased to have you here in our state. The Indiana State Department of Agriculture has specific goal to advance agriculture. We are committed to establishing buffers and protecting wetlands, reducing sediment run-off, and increasing farmed riparian acreage. In addition to our many plans to better agricultural practices, we support many efforts to open trade of our crops in foreign markets.

AGRO 249

Regulatory Cooperation Council initiative on crop protection products

***Marion Law**, marion.law@hc-sc.gc.ca. Pest Management Regulatory Agency, Ottawa, Ontario K1A 0K9, Canada*

On February 4, 2011, the creation of the Canada-United States Regulatory Cooperation Council (RCC) was announced with its objective to increase regulatory transparency and coordination between the two countries. Regulation plays an important role in both countries. Effective regulations protect human health and the environment while supporting growth, investment, innovation, and market openness. Canada and the US each have well-developed, independent regulatory regimes and regulatory departments and agencies that support each of our domestic and legal policy requirements. While our regulatory systems are very similar in the objectives they seek to achieve, there is value in enhancing the mechanisms in place to foster cooperation to align these systems further. This presentation will provide an outline of the major action items underway as part of the U.S./Canada Crop Protection Initiative and the progress achieved 18 months into the plan. The goal of this initiative is to facilitate equal access to products and uses in both countries and to align maximum residue limits/tolerances where possible.

AGRO 250

Pilot project leading the way toward harmonized MRLs around the world

***Lois Rossi**, rossi.lois@epa.gov. Office of Pesticide Programs, US Environmental Protection Agency, Arlington, VA 22202, United States*

US EPA has been involved over the years with multiple initiatives supporting harmonization of regulations for pesticides registration and control. Feedback will be presented from a pilot project developed in cooperation with JMPR for parallel review with OECD-Joint Registration Review. Sulfoxaflor is new insecticide that has applied for registration for use on multiple crops in different countries,

based on a global registration package. Some details around the global joint-review and feedback from the pilot project developed with Codex process for setting MRLs will be presented.

AGRO 251

Regulation (EC) 1107/2009: New residue data requirements coming into force January 2014

***Karsten Hohgardt**, karsten.hohgardt@bvl.bund.de. Department 2, Plant Protection Products, Federal Office of Consumer Protection and Food Safety, Braunschweig, Germany*

About 10 years ago, European Commission requested experts to make proposals for updated data requirements for the approval of active substances and authorisation of plant protection products. Residue behaviour magnitude of residues in honey and the nature and magnitude of residues in fish will be asked for in future. Concerning the nature of residues in fish experts from industry, research, risk assessment, and risk management met a few times and discussed a study design which is available as a working document. Studies are only necessary for active substances that are fat soluble, i.e., substances with log Pow ≥ 3. Not common are housing conditions, stability of fortified feed, and calculation of dietary burden. These points are covered by the working document. A study design on magnitude of residues in fish and honey is not available up to now.

AGRO 252

Progress on MRL setting in China

***Xu Jun**, xujun1977927@163.com. The Institute of Plant Protection, Beijing, China*

This report is to introduce the progress on MRLs setting in China. (1) Background : Based on FSL, MOH, and MOA issued a joint declaration to confirm that the MOA will be in charge of the pesticide residue national standards, Jointly issued and published by MOA and MOH. (2) Outcome : In 2012, with the improvement of the integration of all MRLs, the new MRLs national standards in Food (GB2763-2012) were finalized. It covers 322 pesticides and 2293 MRLs. It will be put into force by March 1 2013. (3) Opportunities: the relevant government bodies attach more attention to pesticide residue control, which create favorable external environment for accelerating the pesticide residue standards development.

AGRO 253

US tolerance setting and alignment with Codex MRLs and other national authorities

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The Federal Food, Drug and Cosmetic Act (FFDCA) authorizes US Environmental Protection Agency (US EPA) to establish pesticide tolerances, the legal limit for a pesticide chemical residue in or on a food. US EPA seeks to harmonize US tolerances with international standards whenever possible. In accordance with the FFDCA, US EPA is required to consider the international maximum residue limits (MRLs) established by the Codex Alimentarius Commission (Codex). US EPA may establish a tolerance at a level that differs from a Codex MRL; however US EPA must have a valid reason for doing so. For US growers that export their commodities overseas, it may help facilitate trade to certain countries if the US EPA establishes a tolerance to align with a MRL of a national authority other than Codex. Harmonization of MRLs is a complex issue and there are many factors that must be considered in order to align US tolerances with Codex MRLs.

AGRO 254

What if CODEX expired?

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The use of CODEX to facilitate trade of treated commodities originally started out with promise to help growersand shippers. It has become the albatross that inhibits trade today for many countries with progressive pesticide registration regimes. In spite of repeated attempts to fix the problem, it remains locked in past approaches. CODEX has become time expired like a crate of week-old strawberries, and it too should be by-passed for a better system. Progressive pesticide regulatory authorities around the world can reach agreement on a better way to utilize their global evaluations, reach common MRL agreements, and facilitate their produce traders. Others could either join in, or continue to flog a dead horse. Here's how I see a better system working.

AGRO 255

Update on international cooperation and collaborations to address minor uses

***Daniel Kunkel**, kunkel@aesop.rutgers.edu. IR-4 Project, Princeton, NJ 08540, United States*

This paper will cover many of the areas of global collaborations that assist with international harmonization of pesticide uses as well as residue levels that may limit agricultural commodities in trade. Progress regarding the work plan developed during the second Global Minor Use Summit and the activities of the Global Minor Use Steering Committee will be presented. Activities of the OECD, especially with regard to the Expert Group on Minor Uses working group activities will be discussed. An update will be provided on the many actions taking place in Codex, including the Codex Electronic working group on Minor Uses and progress with Codex crop groups or extrapolation using representative commodities. Exploring prospects and examples for global residue data generation and gathering of existing data can serve as a means of providing robust data sets to regulators.

AGRO 256

Regulatory activities on sulfoxaflor, a novel product for insect control

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Sulfoxaflor, *N*-[methyloxido[1-[6-(trifluoromethyl)-3-pyridinyl]ethyl]-λ^4-sulfanylidene] cyanamide, is the first insecticidal product from the new sulfoximine class of insect control agents. Sulfoxaflor is a broad-spectrum insecticide exhibiting excellent efficacy against many sap-feeding insect pests, including aphids, whiteflies, hoppers, and *Lygus*. Sulfoxaflor acts via a unique mode of action and is classified by IRAC as 4C. No cross-resistance has been observed between sulfoxaflor and other insecticides. Some details around the global joint-review and other global regulatory activities of sulfoxaflor will be presented.

AGRO 257

Differences in herbicide uptake, translocation, and distribution as a source of herbicide resistance in weeds

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Herbicide resistance has been defined as the inherited ability of a weed population to withstand a herbicide at its use rate, brought about by a genetic change within the population due to selection by the herbicide. That resistance does not bode well for agriculture, which has grown extremely dependent on herbicides for cost-effective, labour-efficient, and soil-conserving weed management. All the mechanisms of herbicide resistance in weeds accounted for to date can be described *sensu lato* as the inability of the active ingredient to reach its original target site in a phytotoxic concentration. Indeed, plants are herbicide-resistant because the active ingredient fails to reach its target site as it is transformed into non-phytotoxic compounds on the way (herbicide metabolism), or it reaches a non-susceptible target (target site mutation). Surprisingly, herbicide resistance, due to the sheer absence of movement of the active ingredients towards their target sites, plays a minor role in the herbicide resistance universe. While herbicide metabolism or target mutations are due in most cases to small genomic mutations, restricting herbicide movements through and along the plant and plant tissues are complex physiological mechanisms usually involving polygenic traits. In addition, altered herbicide movement does not confer either a high degree of resistance (as in target site resistance) or cross-resistance (as in metabolism resistance). This paper provides a brief review of most of the described mechanisms of herbicide resistance in weeds dealing with the restriction of herbicide movement as a source of herbicide resistance, including foliar and root absorption, herbicide accumulation and sequestration in cells, and herbicide translocation. Mechanisms are discussed in depth, with scientific evidence related to herbicide-resistant weed biotypes supporting the different hypotheses.

AGRO 258

Co-penetration of actives and adjuvants and its significance for the matched pair liaison

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Most formulants and adjuvants are low molecular weight solutes, and they have the potential to be sorbed in the plant surface and deeper layers of the cuticle. This can have a huge impact on the sorption potential of actives and their mobility in the rate limiting barrier of the cuticle. Factors including volatility, photostability, plant compatibility, selectivity, salt compatibility, rainfastness, speed of action, weed control, residual efficacy, and the possible product combinations often depend primarily on the relative sorption and penetration and interaction of active and adjuvant. However, many factors affect the manifestation of these positive effects in practice like separation of active and adjuvant from the respective dispersion during evaporation, unmatched speed of penetration, or precipitation of active or adjuvant. Typically, adjuvants have several functions, and ignoring wetting effects here, they can act in the dry spray deposit as much as in the cuticle, for example they can solubilize actives in the former and mobilize them in the latter. For best results, a timely and rate fit is needed that is robust enough to withstand practical variability. Successful commercial formulations show a perfect match of active(s) penetration and adjuvant non-penetration. Three extreme examples will be shown for a model leaf cuticle system, and another extreme and striking example will be given that shows that plant structure can change the picture completely. The latter is a missed cause for the difficulty of proper product optimisation under field and particularly greenhouse conditions.

AGRO 259

Comparison of translocation properties of insecticides vs. herbicides that lead to efficacious control of pests as specifically illustrated by sulfoxaflor, a new insecticide, and halauxifen-methyl, a new herbicide

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An aspect of agrochemical effectiveness is its ability to translocate to the relevant sight of action for weeds or ingestion by insects. For modern synthetic insecticides, the most effective mode of translocation in plants is via xylem movement, allowing for even, uniform distribution throughout the foliage that is being attacked by sucking or chewing insect pests. In contrast, for modern synthetic herbicides, phloem mobility is far superior to xylem mobility as it allows for targeted concentration of the active material in the rapidly dividing tissue of the meristem. This presentation will illustrate general translocation properties of xylem-translocated commercial insecticides and phloem-translocated commercial herbicides and the specific attributes of two new agrochemicals from Dow AgroSciences. Sulfoxaflor, a xylem mobile insecticide for control of sucking insects, illustrates well the uniform distribution that leads to good control of aphids in the field. Halauxifen-methyl, a new cereal-selective herbicide, in contrast to sulfoxaflor, is translocated via the phloem where the active herbicide is concentrated to an effective dose in the meristematic tissue of the plant.

AGRO 260

Why are some weeds tolerant to glyphosate? The case of legominous weeds

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There are annual legumes with many valuable agronomic attributes as *Clitoria ternantea*, *Neonotonia wightii*,and *Mucuna pruriens*. As a ground cover, they reduce erosion, fix nitrogen, suppress weeds, reduce populations of some plant-parasitic nematodes, assimilate and sequester leftover nutrients, and increase crop yields. *C.ternantea*, *N. wightii*, and *M. pruriens* plants exhibit an innate, very high resistance (i.e., tolerance) to glyphosate similar to that of plants which have acquired resistance to this herbicide as a trait. We have been studying the mechanism of tolerance of these three legume species by analyzing the uptake of [^{14}C]-glyphosate by leaves and its translocation to meristematic tissues, the characterization of the leaf cuticle using scanning electron micrographs, and a putative metabolism capable of degrading the herbicide using 3D capillary electrophoresis. For all these experiments we used a glyphosate-susceptible *Amaranthus hybridus* biotype as susceptible population. ^{14}C-glyphosate absorption and translocation tests showed *A. hybridus* absorbed 30% more herbicide than the legumes 24 h after glyphosate foliar application. ^{14}C-glyphosate translocation, as measured by quantified autoradiography, revealed increased translocation of the herbicide to untreated leaves and roots in *A. hybridus* relative to the three legumes. The cuticular surface of *A. hybridus* exhibited very low wax coverage compared to the

epicuticular surface of *N. wightii*, *M. pruriens* and, especially, *C. ternatea*. Regarding glyphosate metabolism, only in *M. pruriens* were two concurrent pathways identified that were capable of degrading glyphosate to AMPA, Pi, glyoxylate, sarcosine, and formaldehyde. No significant degradation of glyphosate was detected in the other leguminous plants. These results indicate that the high glyphosate tolerance of *Clitoria ternatea*, *Mucuna pruriens*, and *Neonotonia wightii* is mainly a result of poor penetration and translocation of the herbicide to apical growing points in their plants. Enhanced glyphosate degradation was observed in *M. pruriens* as well.

AGRO 261

Phloem translocation of xenobiotics in *Brachypodium distachyon*

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Due to evolved resistance and environmental regulations, there is a particular need in the agricultural market for a new graminicide. An essential requirement of a novel graminicide is to have sufficient phloem mobility in the plant to reach meristematic tissues for the expression of activity leading to desired control of unwanted vegetative growth. A robust and reliable phloem bioassay utilizing monocot species is highly desirable for early stage experimental compounds. Vascular tissues and translocation patterns in *Brachypodium distachyon*, a new model organism for temperate grasses, was studied and compared to *Triticum aestivum*. *B. distachyon* has an advantage over *T. aestivum* due to its convenient biological and physical characteristics such as smaller size, plant height, and short generation time. Using confocal microscopy with fluorescent dyes and widefield microscopy with colorimetric dyes, we confirmed that *B. distachyon* has a xylem discontinuity functionally analogous to that found in *T. aestivum*. Based on the xylem discontinuity phenomena found in *B. distachyon*, ^{14}C radiolabeled studies using known xylem and phloem mobile pesticidal compounds showed that there was a significant difference in the amount of the xylem mobile compounds in the chaff and stem as compared to the phloem mobile compounds found in the grain. The findings described in this report suggest that *B. distachyon* can be used as a novel system for a rapid screening of phloem mobility in monocot species.

AGRO 262

Uptake of agrochemicals across seed coats

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The permeability of seed coats to solutes plays a major role in seed treatment with pesticides. An experimental setup was designed for investigating the mechanisms of seed coat permeation, which can be used to perform steady-state experiments with isolated seed coats of *Pisum sativum*. Permeances were measured for a set of organic model compounds with different physicochemical properties. The permeances measured correlated with the molecular sizes of the compounds and not with their lipophilicity. This shows that narrow aqueous pathways dominate the diffusion of solutes across pea seed coats. The aqueous permeation pathway is characterized by a small size selectivity and a small effect of temperature on permeation. The application of an osmotic water potential gradient across isolated seed coats leads to an increase in solute transfer proving that the aqueous pathways form a water-filled continuum across the seed coat allowing bulk flow of water. Thus, organic solutes can cross pea testae by (1) diffusion and (2) bulk water inflow which, however, is relevant only during imbibition. The uptake situation of treated seeds in the field is more complex than permeation in steady-state experiments. In a moist soil environment, the organic solutes in the formulation residue on the seed surface dissolve and can move either across the seed coat into the seed (by diffusion or bulk water inflow) or into the competing compartments of the adjacent soil. Under these conditions the active ingredient has to be dissolved in an aqueous medium prior to seed uptake and, thus, water solubility of the solute plays an important role. (Niemann et al., *Plant Cell Environ* 2013, http://dx.doi.org/10.1111/pce.12035)

AGRO 263

Activity of chlorantraniliprole and thiamethoxam seed treatments on rice water weevil as affected by distribution of insecticides in rice plants

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The differential activity of insecticides on life stages of rice water weevil, *Lissorhoptrus oryzophilus*, in rice plants treated as seeds with chlorantaniliprole (CAP) and thiamethoxam (TMX) were related to patterns of insecticide distribution (6-7 leaf stage). The differential activity on adults suggests poor inherent potency of CAP as an adulticide and/or its limited systemicity in foliage. The greatest activity of CAP on root feeding stages was consistent with the accumulation of CAP in roots, whereas the high adulticidal activity of TMX correlated with high above-ground concentrations of TMX. These results showed a potential for optimizing field use rates of CAP. A novel method was employed to determine dose dependence of adult mortality following exposure to foliage from TMX-treated plants (2-3 and 3-4 leaf stages). To estimate oral doses of insecticides, estimates of leaf biomass removed by adult weevils were used in conjunction with LC/MS-MS analysis of insecticide residues in leaves.

AGRO 264

Uptake, translocation, and accumulation of pharmaceutical and hormone contaminants in vegetables

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The widespread occurrence of pharmaceuticals and personal care products (PPCPs) and natural hormones in watersheds has been recognized as an emerging environmental issue. The potential uptake and internalization of these emerging contaminants in food plants that are irrigated with contaminated water is becoming a critical food safety issue. In the present study, uptake, translocation, and accumulation of seven PPCPs and three steroid hormones in lettuce and tomato plants grown under hydroponic conditions were investigated. An isotopic dilution method was developed for the analysis of trace PPCPs and hormones in vegetables using high-performance liquid chromatography-tandem mass spectrometry (HPLC/MS-MS), combined with solvent extraction and solid phase extraction (SPE) cleanup for sample preparation. All targeted PPCPs and hormones were detected in tomato roots, stems, and leaves, except for triclosan which was not found in the leaves of one cultivar of tomatoes. Concentrations ranged from 0.5 μg kg^{-1} up to 10 mg kg^{-1} when the plants were grown in hydroponic solutions containing each chemical at 50 μg L^{-1}. For most contaminants, root bioconcentation factors (BCF) were higher than the corresponding tomato stem and leaf BCFs, except for caffeine and carbamazepine

which had BCFs that were largest in the leaves. In addition, lettuce experiments showed that the uptake of each contaminant by plant roots was concentration-dependent. The accumulation of PPCPs and hormones in lettuce leaves increased with the increase of contaminant concentrations in hydroponic solutions. Using the BCFs and FDA acceptable daily intake levels for each compound, a critical threshold for each emerging contaminant in the irrigation water was calculated, which is very helpful in determining if agricultural irrigation with PPCP/hormone-containing water presents a food safety threat.

AGRO 265

Practical utility of dynamic plant uptake model assessed through application of probabilistic techniques

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Modeling of dynamic plant uptake of active substances affords potential advantage to the crop protection product business by aiding product development decisions related to use of varied product delivery options that ultimately impact assessment of human dietary safety of traded produce. Evaluation of the accuracy of predicting active substance uptake into the plant is needed relative to the accuracy required to derive business value. To this end, probabilistic modeling techniques are employed to account for the range of values for each relevant model input and the resultant range of values for predicted residue model outputs. Experimental data are gathered for a given active substance with insecticidal properties for the case of soil applications made to vegetable plants grown in a protected environment. These data are processed using the Percentage Exceedance approach as a means of validation of the dynamic plant uptake model.

AGRO 266

Cyclin dependent kinases as starting points for fungicide discovery

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Scouting around Syngenta's fungicidal cyclin dependent kinase area, led to the discovery that the reverse core retained activity. Several new cores were examined as fungicides and resulted in the new sub-class of symmetrical triazines.

AGRO 267

Substituted 2,2'-bipyridyls as agricultural fungicides

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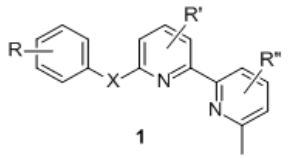
6-Substituted-2,2-bipyridyls are unprecedented in the agricultural literature. Mode of action studies suggested that the bipyridyls act by the same general mechanism as well-known fungicidal pyridylpyrimidines. Substituent effects were studied across the bipyridyl ring system through evaluation against a broad range of fungal pathogens of interest. The synthesis and biological efficacy of these molecules will be reviewed.



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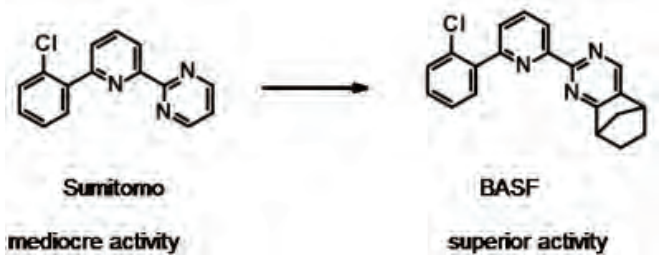
AGRO 268

Identification and optimization of pyrimidopyridines controlling speckled leaf blotch in wheat

Klaas Lohmann*, klaas.lohmann@basf.com. Global Research Agricultural Products, BASF SE, Ludwigshafen, Rheinland-Pfalz 67056, Germany*

Pyrimidopyridines have been described as fungicides in the late 1980s. Nevertheless, benchmark activity was not achieved. This presentation describes the further exploration of this class resulting in compounds with increased activity against *Septoria* leaf blotch.



AGRO 269

Inhibitors of 4-hydroxphenylpyruvate dioxygenase (HPPD) in combination with a safener: New herbicide solutions for modern sustainable agriculture

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Inhibitors of the enzyme 4-hydroxphenylpyruvate dioxygenase (HPPD) prevent the formation of carotenoid pigments in plants, thereby causing chlorophyll degradation and bleaching. Through combination with a suitable safener, the full potential of these herbicides for selective weed control can be realized in a variety of crops including cereals, maize, and rice. The safeners increase the rate at which crops are able to degrade metabolically the herbicides without affecting the level of weed control, even in resistant biotypes. This presentation will describe the discovery and development at Bayer CropScience of new HPPD-herbicide and safener combinations for use in sustainable arable crop protection.

AGRO 270

Accelerating discovery through risk-sharing collaborations

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Selectively leveraging the capabilities and expertise of contract research organizations (CROs) has become an integral part of many agrochemical and pharmaceutical companies' research strategies. Initially, CROs provided support in the form of research services, such as biological assay development, scale-up, combinatorial library production, clinical trials, and synthetic route optimization, which were outsourced on a contract basis. CROs range in size from large, international full-service organizations to small, specializing niche groups. Recently, some companies and CROs have joined forces by entering into true collaboration, in which the parties bring divergent expertise and share risk to achieve a common but aggressive goal. An overview of these risk-sharing collaborations will be the focus of this talk. Topics, such as when and why this type of collaboration may be favored over the more routine fee-for-service arrangement; attributes of a successful CRO partnership; and the strengths and weaknesses of large and niche CROs will be discussed, including case studies.

AGRO 271

Lead discovery and optimization through CRO collaborations

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A variety of chemistry programs aimed at new lead discovery and project optimization have been conducted in collaboration with the research group at GVK Biosciences. The focus of this talk will be on the practical aspects of this working relationship, the collaborative environment established, and the chemistry and biology investigated for several of these programs.

AGRO 272

Partnering for success with contract research organizations (CROs) to enhance discovery R&D productivity

Lori K Lawler*, lklawler@dow.com, Vidyadhar B Hegde, Beth A Lorsbach, Michael R Loso, Mark A Pobanz. Discovery Chemistry R&D, Dow AgroSciences, Indianapolis, IN 46268, United States*

Over the past two decades, outsourcing has become increasingly common in the pharmaceutical, biotechnology and agricultural industries with a transition in more recent years toward functional outsourcing where whole segments of an R&D organization are outsourced. Outsourcing of core functions including clinical trial management, manufacturing, and even entire therapeutic areas has been observed across industries. Dow AgroSciences has opted to leverage CROs within the Discovery organization involving both lead generation and lead optimization project teams in a highly integrated manner. This model creates supplemental resources for DAS scientists to utilize in the execution of ideas through direct collaboration with CRO project leaders and CRO chemists. The theory behind this strategy, logistics for execution, and metrics supporting the success of this program will be discussed.

AGRO 273

Thoughts on best practices and perspectives for working externally in a research environment

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Over the past decade, increasing emphasis has been placed on the externalization of chemistry. This has resulted in a dramatic increase in the number and size, particularly in Asia, of CROs. While the outsourcing of chemistry headcount provides opportunities for flexible and reduced FTE rates, the reality is variable from project to project and from organization to organization. To realize these benefits, sponsoring organizations need to understand fully why they are outsourcing, who they are outsourcing to, the strengths/weaknesses of each potential partner, and how the organizations will work together on sponsored programs. Organizations should pro-actively manage the incentives and engagement of their scientists to ensure they are aligned with the goals and drivers behind outsourcing. Selection of the right CRO is critical to success, and one should consider capabilities and price, but also emphasize culture and relationships. Organizations should also look to recent trends in the on-shoring of manufacturing which highlight the efficiencies of coupling research (from a discovery perspective = design and prioritization) and manufacturing (= synthesis) to select better the right partners and programs for working with external partners.

AGRO 274

OECD guidance for acceptance of foreign pesticide field dissipation studies and ecoregion concept

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Data on field dissipation/accumulation studies conducted at foreign sites are often submitted to the regulatory agencies worldwide under national and global joint reviews for the registration of pest control products. Region-specific soil characteristics (pH, organic carbon, and texture) and climatic conditions (precipitation and temperature) determine, to a large extent, the fate and behaviour of a chemical. A chemical is expected to behave similarly in ecoregions that are based on similar soils and climate. Studies conducted at foreign sites are generally considered if the study sites represent local use conditions. As no ecoregion analysis based on soils and climate together is currently available, ENASGIPS (Europe North America Soil Geographic Information for Pesticide Studies) is being developed under OECD to identify comparable ecoregions between Europe and North America. The purpose of ENASGIPS model is to compare and identify similar ecoregions and to assist in site selection. This model is based on ArcGIS and uses Harmonized World Soil Database for soils and MARS FOODSEC for climate to compare and identify similar ecoregions between Europe and North America. Thus, a field study conducted in Europe can be considered by the North American regulatory agencies and vice versa. Currently in the European Union, FOCUS guidance is used to facilitate use of overseas TFD studies for regulatory purposes. In addition, the model permits selection of field sites based on concerns identified by the conceptual model and acceptable to regulatory authorities in

both continents. It involves a series of selection of crops, soil and climatic parameters. Distribution of crops is based on Interpolated Census of agriculture to Soil Landscapes for Canada, US Agricultural Census (STATSGO) for USA and CAPRI EU15+EU12 for Europe. *Note: The content of this presentation does not necessarily represent the official views of the OECD and its member countries, the EU Commission, or EFSA.*

AGRO 275

OECD guidance for acceptance of foreign pesticide field dissipation studies/ecoregion concept: Ecoregion Crosswalk model and demonstration

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Data on field dissipation/accumulation studies conducted at foreign sites are often submitted to the regulatory agencies worldwide under national and global joint reviews for the registration of pest control products. Region specific soil characteristics (pH, organic carbon, and texture) and climatic conditions (precipitation and temperature) determine to a large extent the fate and behaviour of a chemical. A chemical is expected to behave similarly in ecoregions that are based on similar soils and climate. Studies conducted at foreign sites are generally considered if the study sites represent local use conditions. As no ecoregion analysis based on soils and climate together is currently available, ENASGIPS (Europe North America Soil Geographic Information for pesticide studies) a geospatial model is being developed under OECD to identify comparable ecoregions between Europe and North America. The purpose of the ENASGIPS model is to compare and identify similar ecoregions, assist site section process to identify worst case scenarios based on concerns identified in the conceptual model, and provide information on crops, soils, and climate in a particular region. This model was developed with ESRI ArcGIS v10.0 and uses WHSD (World Harmonized Soil Database) for soils data and MARS FOODSEC for climate data to compare and identify similar ecoregions between Europe and North America. In this way, a field study conducted in Europe is considered by the North American regulatory agencies and vice versa. In European Union, FOCUS guidance is used to facilitate use of overseas TFD studies for regulatory purposes. In addition, the model permits selection of field sites based on concerns identified by the conceptual model. It involves a series of selection of crops, soil, and climatic parameters. The model also provides generic information on soils, climate, and crops for any particular region.

AGRO 276

Novel approach to evaluate comparability of foreign soils used for environmental fate studies for agrochemicals with US agricultural soils

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Under the US Environmental Protection Agency's pesticide data requirements (40 CFR Part 158), selected environmental fate and transport studies (*e.g.,* leaching, adsorption/desorption, soil metabolism) are conducted in agricultural soils representative of those in intended pesticide use areas to determine the potential persistence and mobility of a pesticide in the environment. Foreign soils may be used in conducting these fate studies; however, it is required to demonstrate that the foreign soil have typical characteristics of agricultural soils at the intended pesticide-use sites. This study will present a quantitative approach using various geospatial data and techniques to evaluate foreign soils used for the regulatory studies. A comprehensive understanding of soil taxonomy, chemical and physical characteristics, and soil temperature and moisture regimes of the foreign soils together with those of agricultural soils in the proposed use areas in the US will allow an evaluation of their comparability and hence the suitability of foreign soils for use in regulatory environmental fate and transport studies.

AGRO 277

What matters for predicting the similarity of TFD studies: Techniques, data, or pesticide characteristics?

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Data characteristics and pesticides traits (e.g., pH dependency) are expected to influence the accuracy with which the transferability of terrestrial field dissipation studies to other geographical regions are predicted. In Europe, a new version of the EFSA GIS database has been published recently with considerable modification for several environmental parameters. Beside EFSA data, a huge amount of different GIS data on EU or country level have been used in the context of pesticide registration (e.g., MARS, CRU, worldclim). In this talk, we analyze different available GIS data from Europe in terms of comparability, map resolution, and transferability, and we assess the impact on prediction of similarity of TFD between North America and Europe. We see the need to establish a mutual quality- and version-control for GIS data and agreed methods in the context of pesticide registration.

AGRO 278

Application of OECD ENASGIPS: User perspectives

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One of the deliverables from the OECD Pesticide Dissipation Project is a GIS-based application to assess the similarity of ecoregions between Europe and North America. The objective of this tool is to find matching ecoregions which enable registrants to demonstrate that foreign test site conditions exist in either Europe or North America. This GIS application has the potential of being used in a variety of manners. In this presentation, we will explore how the tool and the underlying data can be used to find locations with conditions that match foreign test sites, how the tool compares with the current US EPA foreign soil guidelines, and the implications of registration of pesticides in Canada from an ecoregion perspective. In addition, we will address data-related issues, such as crop data, discuss the implications of using long-term versus short-term field data, and account for variability in climate and soil properties and the impact on site selection.

AGRO 279

Relevance of environmental fate and terrestrial field dissipation studies conducted in Europe and Canada to use environments in the United States

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USEPA, PMRA, EFSA, as well as EU Member State regulators are increasingly seeking to use all data that may be relevant to a registration review. In particular, registrants now have the ability to submit data from foreign environmental fate and TFD studies to their respective regulatory agency. We will describe the relevance of soils used in environmental fate and terrestrial field dissipation studies for a herbicide in Europe and Canada to soils found in potential use areas in the United States in response to Registration Review of the herbicide. The assessment used a beta version of the OECD ENASGIP tool and underlying database to identify areas in the United States with comparable environmental conditions to the European and Canadian test sites and soil source locations. This analysis was further expanded to include the use of higher resolution soils data from the USDA NRCS SSURGO database, which also includes data not available in the OECD database, e.g., soil taxonomy. The results demonstrate that terrestrial field studies conducted at sites in Europe and Canada or laboratory environmental fate studies using soils from Europe and Canada are relevant and applicable to soils in the United States, particularly those soils in USEPA regions with high reported usage.

AGRO 280

Use of the Europe-North American soil geographic information for pesticide studies tool (ENASGIPS version 2.0 tool)

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The ENASGIPS tool has been developed by Pest Management Regulatory Agency (PMRA), Health Canada and the US Environmental Protection Agency (USEPA) in collaboration with Agriculture and Agri-Food Canada and European Commission Joint Research Centre as part of the Organization for Economic Co-operation and Development (OECD) project on "Harmonization of International Terrestrial Field Dissipation and Ecoregion Crosswalk." The tool uses soil, climate, and crop databases to identify/quantify ecoregion similarities between the European and North American countries along with executing soil, climate, and crop queries for site selection based on concerns identified in the conceptual model. The presentation includes examples that demonstrate the ability of the tool to identify terrestrial field dissipation sites in North American and European countries. Results from these example runs will be used to explain the basis for decisions on site selection. Additionally, suggestions as to when and how the tool can be used will also be provided. *Note: The content of this presentation does not necessarily represent the official views of the USEPA or PMRA.*

AGRO 281

OECD Residue Chemistry Expert Group (OECD RCEG): Progress report on recent efforts to prepare a comprehensive guidance document for rotational crops

Kathryn M Jernberg, *kathryn.m.jernberg@dupont.com. Human Safety Assessment, DuPont Crop Protection, Newark, DE 19714-0030, United States*

There is movement in several OECD countries to add requirements for (1) rotational crop testing on permanent and semi-permanent crops (e.g., orchards, vines, strawberries), and (2) crop/rotational crop accumulation testing over multiple years, which may lead to different approaches of how residues in rotational crops are regulated. The absence of a harmonised approach to MRL setting for rotational crop commodities may create impediments to international trade. Common practices of how to handle inadvertent residues will support work sharing and joint reviews between OECD countries. This presentation will provide an update on OECD RCEG efforts to propose additional detailed guidance on the rotational crop residue studies conducted according to OECD TG 504 (Residues in Rotational Crops) with expanded flexibility in crop commodities to be tested. A tiered approach will be introduced which would ensure that consumers are not exposed to unacceptable residue levels and would support OECD countries in their efforts to harmonize MRLs for inadvertent residues in rotational crops.

AGRO 282

Latest international developments in residue behaviour – proportionality approach

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In 2010, JMPR considered the new concept of proportionality, and JMPR 2011 proposed MRLs based on this approach as CCPR requested to do so. In CCPR 2012, an electronic working group (EWG) was set up to develop principles and guidance for the use of the concept of proportionality to estimate maximum residue levels. An OECD Residue Chemistry Expert Group is still working on OECD Test Guidelines and OECD Guidance Documents. This group collected additional data to underpin the concept of proportionality. Results and statistics were intensively discussed in this group. On the basis of the overall results, the EWG came up with a proposal for CCPR Meeting 2013. Results of the discussion of the May 2013 meeting will be presented.

AGRO 283

Rates and residues: How proportional are they?

Jane Stewart, *jane.stewart@basf.com. Department of Consumer Safety, BASF, Research Triangle Park, NC 27709, United States*

Residue data recently collected from industry and government indicate that pesticide residues are proportional or nearly proportional to application rate for most crops and application types. The analysis of this data was used as a basis for recommendations and proposals for both OECD and CCPR for data extrapolation. Both statistical and pragmatic approaches were used to examine the data and to evaluate the relationship between residues and rate. This analysis will be described, along with a discussion of some of the factors which may lead to the statistical deviation from proportionality that was observed in some cases.

AGRO 284

Challenges of establishing and managing global pesticide magnitude-of-residue studies

***Michael Braverman**, braverman@aesop.rutgers.edu. IR-4 Project, Princeton, New Jersey 08540, United States*

The US Department of Agriculture, Foreign Agriculture Service and the Standards Trade Development fund are supporting the establishment of global hubs to generate pesticide residue data to support minor uses. This paper will discuss many of the challenges involved in these international collaborations to develop data for submission to regulatory agencies for registration on minor crops. The major types of challenges include technical, logistical, and legal-phytosanitary aspects. There are also cultural-linguistic and expressive-philosophical challenges when implementing Good Laboratory Practices and Standard Operating Procedures. Despite these challenges, successful GLP residue studies have been achieved through this capacity building process in developing countries. Strategies included unique and repeated forms of communication and standardization of trials to reduce potential errors. Pointed emphasis of educational resources and oversight were utilized to maximize success and assurance of data quality. The way in which these strategies reduced trial variability compared to experienced GLP researchers will be discussed.

AGRO 285

Residue analysis of plant protection products: Challenges and trends

***Anke Reinold**, anke.reinold@basf.com. BASF Corporation, Research Triangle Park, North Carolina 27709, United States*

Pesticides used today belong to a wide variety of chemical groups, and the spectrum of physic-chemical properties is further expanded by including their relevant metabolites and degradation products in the analysis. The determination of residues in food, feed, and environmental compartments is needed to support the registration and subsequent enforcement of maximum residue levels as well as for monitoring purposes. Consequently, adequate methods of these compounds are required that allow a selective and sensitive detection at trace levels. At the same time, a trend is developing towards multi-residue methods with high-throughput for efficient analysis. Instrumental advances have allowed for lower limits of quantification, for reduced time of analysis, and for increased separation of matrix and analytes. General issues of residue analysis like contamination and matrix effects and new challenges, such as the inclusion of small and polar/non-polar compounds and/or unusual matrices, will be addressed.

AGRO 286

Matrix characterization: Challenges in obtaining and screening control sample materials suitable for use in pesticide residue analysis

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Control matrix materials are necessary to support pesticide residue analytical research in generating method validation, field fortification, storage stability, and procedural recovery samples, among other uses. Obtaining matrix materials suitable for use in determining trace-level pesticide residues is a critical consideration for evaluation and control of analytical method performance. While it is desirable to have available control matrix materials which are representative of the crop group, homogenous, and free of analyte contamination, this is not always possible in the context of conducting field residue trials. In this presentation, alternatives for sourcing and evaluating matrices will be addressed. Strategies for dealing with inconsistencies in analyte recovery and interferences between specific matrix types within crop groups will be presented. Potential pitfalls and management of using field trial controls for analytical procedural recovery samples will also be discussed.

AGRO 287

Factors influencing pesticide concentrations in dusts on residential outdoor impervious surfaces

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Impervious surfaces are an important source of pesticides in residential runoff, and association with solid materials is the primary route of pyrethroid transport with runoff water. Although monitoring studies have showed temporal variations of pesticide runoff concentrations, their levels on residential outdoor surfaces are seldom measured directly, and the changes of their concentrations over time is unknown. We collected 360 dust samples in May, July, and September of 2011 from impervious surfaces around residential homes and used a linear mixed model to assess factors that may influence pesticide levels. Pesticides were detected in almost all samples, and in more than 75% of the dust samples, at least 5 pesticides were detected. Bifenthrin, permethrin, cypermethrin and cyfluthrin were found at highest levels, and bifenthrin also contributed >40% of total toxicity potential to aquatic invertebrates. Dust collected in July and September contained higher pesticide amounts than in May, and the curbside gutter samples showed higher contamination than sidewalk and street samples.

AGRO 288

Factors affecting residential runoff transport of pyrethroids

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Replicated runoff studies investigating the transport of pyrethroids applied to suburban residences were conducted at a full scale test facility in central California over 18 months. The first 12 months of results showed losses from historic practices mainly from applications made to impervious surfaces (such as driveways or walls adjacent to driveways) as a result of runoff generated by simulated or natural rainfall. Revised application procedures according to new product labeling specifying spot applications to impervious surfaces reduced runoff losses of pyrethroids by a factor of 40 compared to historic practices. The last 6 months of testing examined the effect of formulation on washoff from driveways or walls adjacent to driveways. Variability in runoff loses between product formulations under field scale conditions were considerably less than in small scale laboratory experiments. Also the ranking of runoff losses by product in laboratory experiments were not always the same as in the field experiments. This indicates that using laboratory studies to assess the effect of formulation on runoff losses under field conditions may not always be predictive of behavior under actual use conditions, thus field studies remain important for understanding washoff losses from residential pesticide treatments.

AGRO 289

Determining critical factors controlling off-site transport of pyrethroids in the urban environment

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Off-target pyrethroid transport from urban and suburban landscapes is not well understood, especially when compared to the off-target transport in agricultural production systems. Various combinations of pervious surfaces (lawns, flower beds, shrubbery) and impervious surfaces (concrete, asphalt, house siding) surfaces, lawn irrigation, and rainfall contribute to some of the variability. Different methods of product applications to those surfaces (general broadcast, target spraying, and applications to both horizontal and vertical surfaces) compound the complexity in these environments. In outdoor settings, additional variables control the washoff of pyrethroids, including the timing and number of applications, meteorological conditions (including rainfall, temperatures, and evapotranspiration), irrigation amounts and methods, product formulations, and mass remaining as a function of time. A full-scale experimental site was constructed in California and applications were conducted matching historic and newly-revised label recommendations for pyrethroids. Initial results indicate a time-based, three-phase process with washoff occurring, changing, and gradually slowing over time. Also, natural and simulated rainfall events accounted for the majority of mass loss from the study site when compared to mass loss under lawn irrigation and its associated urban drool. Additional results will be presented, including a multivariate analysis of pyrethroid washoff from various surfaces to determine critical factors influencing the process-based mass loss of pyrethroids under California suburban conditions.

AGRO 290

Semimechanistic modeling of pesticide washoff from concrete surfaces

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Pesticide uses over impervious surfaces like concrete significantly contribute to pesticide detection and aquatic toxicity in urban watersheds. California Department of Pesticide Regulation (CDPR) has been involved in multiple projects of lab/field experiments and surface water monitoring to evaluate urban pesticide use and their effects on the receiving water quality. In addition, regulations and mitigations have recently been proposed in California to restrict urban pesticide uses. A modeling approach is required for better characterization and prediction for off-site transport processes of urban pesticides. Presented here is a comprehensive study on pesticide washoff from concrete surfaces, including reviews of experiments and models, development of a new model, and its application. Analysis of experimental data indicated that pesticide washoff was generally associated with irreversible adsorption, dynamic dissipation rate constant, and dynamic effective diffusivity. The existing modeling approaches, mainly exponential function and power-law function, have limitations in explaining those processes. A mathematical and conceptual framework was developed to predict pesticide buildup and washoff processes on concrete surfaces, including the time-dependence of washoff potential after application and the dynamics in pesticide washoff during a runoff event. The model was applied to published data from controlled rainfall experiments. The model satisfactorily captured pesticide mass loads and their temporal variations for tested pesticides with a wide range of chemical properties (log K_{ow}= 0.6 - 6.9) and set times (1 - 238 days after application) under both single and repeated rainfall events (1 - 7 times). Results suggested that, with appropriate parameterization and modeling scenarios, the model can be used to predict washoff potentials of pesticide products from concrete surfaces and to support pesticide risk assessments in urban environmental settings.

AGRO 291

Application of a modeling approach for predicting pyrethroid residues is urban water bodies for use in environmental risk assessments

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Modeling pyrethroid environmental fate in an urban setting can help us to understand better the sources, transport pathways, and mitigation strategies for reducing their environmental concentrations. Recently, a modeling approach using the Storm Water Management Model (SWMM) has been developed and validated in a high density residential watershed in southern California. The approach incorporated pyrethroid wash-off characteristics from pervious and impervious surfaces, neighborhood characteristics, and pyrethroid application practices typical of the region. To extend this modeling approach to new geographic regions, a survey was conducted to gather regionally-specific, pyrethroid-use practices. These local use practices, along with local weather and neighborhood characteristics, have enabled the geographical extension of the California modeling approach to a diverse collection of locations. Application of the SWMM modeling approach to a broader population of residential neighborhood conditions has provided aquatic exposure estimates important for developing a comprehensive higher tier ecological risk assessment for pyrethroids at the national scale.

AGRO 292

Conducting ecological risk assessments for urban uses of pesticides

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Recent studies have reported pesticides in toxicologically-significant concentrations in surface water, sediments, stormwater, and POTW influent/effluent wastewater from residential uses at several locations across the United States. The US EPA faces many challenges in assessing the ecological risks from indoor and outdoor residential pesticide uses. Pesticides released to domestic wastewater from indoor residential uses are being assessed with the Exposure and Fate Assessment Screening Tool (E-FAST). Bench-scale treatability studies and POTW monitoring data will be used to refine exposure estimates of pesticides in wastewater, surface water, and biosolids resulting from indoor uses. It remains difficult to assess ecological impact from outdoor residential uses because existing urban models are inadequate to estimate exposure. Quantifying residential pesticide use at the national level remains an obstacle. Data are lacking on the timing, frequency, and location of residential pesticide application at a national scale. However, data are being collected on estimated run-off from impervious surfaces, housing density, application timing, method, and frequency for constructing representative residential exposure scenarios. In the absence of these data

and tools, the Agency has relied on urban monitoring data for conducting the ecological risk assessments. *(The content of this presentation does not necessarily represent the official views of the US EPA.)*

AGRO 293

Conducting an acute aggregate residential risk assessment

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Residential exposure and risk assessments and the underlying methodology have undergone significant evolution over the past few years. The US Environmental Protection Agency has evaluated significant amounts of exposure and use data relevant to the potential exposure of homeowners following residential pesticide applications. These data have been publically reviewed, presented to the FIFRA Science Advisory Panel, and published in the Agency's Residential Standard Operatoring Procedures. US EPA has made Excel spreadsheets available that permit deterministic exposure assessments. Distributional data provided in the SOPs were incorporated into the spreadsheets and probablistic assessments of the exposure following lawn and indoor applications were evaluated for two pyrethroid insecticides. The results of these stochastic assessments and a comparison to the deterministic assessments are presented along with an evaluation of the critical exposure variables for additional refinement of the exposure assessment. The potential of the stochastic assessments on conducting acute non-dietary risk assessments is also presented.

AGRO 294

Risk assessment initiatives in Latin America

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The first presentations and talks on pesticide risk assessment in Latin America date back to the 1990s, but not until 2001 was it introduced as a registration requirement for one country. In 2002 the Andean community published the regulation for registration of pesticides and settled the framework for performing environmental risk assessments. Since then, both authorities and industry have spent efforts to establish knowledge in the process and to achieve reasonable and sound practices for estimating the exposure both from the environmental and non-dietary human exposure. Within the last five years, initiatives to promote occupational risk assessment have arisen in various Latin American countries. Significant efforts are underway in the Andean region to address worker reentry. Peru has begun to use an operator exposure model to conduct operator risk assessments. In Brazil, there is an ongoing review of hazard and operator risk policy. Understanding the local conditions, agricultural practices, and variability has become a must to assess the exposure and the potential risk to workers in these countries.

AGRO 295

Development of a recombinant butyrylcholinesterase pulmonary bioshield to protect against OP inhalation exposure in macaques

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Native butyrylcholinesterase (BChE) is a potent, safe, and effective organophosphate (OP) and carbamate bioscavenger with very good *in vivo* stability but of limited availability. Alternative recombinant (r) forms of BChE require PEG-conjugation to achieve similar plasma stability following parenteral delivery (im, sc, iv). However, while BChE has broad antidotal properties, the large size of PEG-rMaBChE (>800,000 MW) and the 1:1 stoichiometry of BChE:OP, means large treatment doses will be required, and thus the route of systemic delivery, which determines the pharmacokinetics (PK) of clearance, becomes critical to efficacy and to safety. Because of the challenges using parenteral delivery of large molecules and because inhalation OP exposure serves as a major means of intoxication due to rapid accesses of the OP to the blood, we have delivered an aerosolized form of rBChE, which is too large to leave the lung and which can neutralize inhaled OP *in situ* and prevent its entry into the blood and inhibition of RBC-AChE and plasma BChE. The results to date, indicate that unmodified aer-rMaBChE and rHuBChE (~5-9 mg/kg) pretreatment given 1-40 hr prior to >1 LD50 of aer-paraoxon (Px) prevented inhibition of circulating cholinesterase in a dose-dependent manner. These studies are the first to show protection by rBChE against a pesticide such as paraoxon when delivered directly into the lung and bode well for the use of a non-invasive and consumer-friendly method of rHuBChE delivery as a human pretreatment to counteract OP and carbamate toxicity.

AGRO 296

Development of a generic seed treatment exposure database

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The treatment of seeds such as corn, soybeans, and cereals with insecticides and fungicides is growing in importance in North American agriculture. Seed treatment promotes greater plant growth in the period following planting and reduces the amount of pesticide required per acre. In determining the exposure and potential risks to individuals involved in seed treatment and in the planting of treated seed, the US Environmental Protection Agency (EPA) and Canada's Pest Management Regulatory Agency (PMRA) rely on exposure studies conducted with variable methodology and often using equipment that are no longer relevant. The Agricultural Handlers Exposure Task Force (AHETF) is a consortium of 28 member agrochemicals companies and 10 participating companies developing a database comprised of modern occupational exposure studies involving the treatment of seed in commercial facilities and on-farm operations and also to farmers planting treated seed. AHETF has been working with EPA and PMRA in the analysis and evaluation of these data to create a generic exposure database to estimate dermal and inhalation exposure to workers accurately. This will allow for high confidence regulatory decisions regarding seed treatment pesticide products.

AGRO 297

Acute nondietary exposure assessment

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Non-dietary exposure assessments are commonly treated as seasonal, repeated exposure estimates and are compared to subchronic points of departure in pesticide risk assessments. These seasonal exposures are combined with chronic dietary (food and drinking water) estimates for aggregate exposure assessments. Assessment of acute single day non-dietary exposures coupled with acute dietary components have been assessed in US EPA cumulative exposure assessments for organophosphate, carbamate, and pyrethroid insecticides using a variety of models and data sources. Criteria for consideration of acute non-dietary assessments on a chemical or scenario basis will be presented in this session.

AGRO 298

Considerations for estimating pesticide volatilization fluxes from various crops

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One goal of every field pesticide volatility flux study should be to measure as many environmental parameters as possible to aid in the development of models to predict volatilization fluxes for current-use pesticides from all crops grown throughout the country. Such a database and modeling effort does not currently exist. The transfer of pesticides from soil, field crops, and orchards to the atmosphere is governed primarily by the chemical characteristics of the pesticide and by the atmospheric turbulence generated by wind moving over that surface. If the source strength is known, estimating volatilization flux is a function of wind speed gradients and atmospheric stability. Knowing the source strength, however, requires an understanding of how the pesticide moves through the soil, crop, or orchard to the surface and is critical in modeling the volatilization process. Modeling efforts need to be verified with actual field data, but currently available pesticide flux data are limited and mostly from fallow soil. Canopy structures, function, and microclimates within most field crops and orchards are very complex. Understanding their complexity is critical to being able to model pesticide movement through the canopies. Knowledge and understanding of the physical and physiological attributes of plant canopies, their spatial and temporal variability, and wind speed and temperature gradients within the canopies are also needed. In addition, how the pesticide is distributed within the canopy as well as how it interacts with leaves, stems, branches, and soil are important parameters. This presentation will discuss the field measurements needed to develop a robust model to estimate pesticide volatilization fluxes from various crops, then using these field data to fine-tune the model in order to predict the next field experiment, and continuing in an iterative manner until the model can reliably predict volatilization fluxes from any crop type or surface.

AGRO 299

Volatility and air dispersion modeling considerations for assessing bystander exposure and risk from semivolatiles applied to crops and orchards

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Assessing the inhalation risk of semi-volatile pest control products requires knowledge of the rate of evaporation (flux) of the chemical, the extent of off-site movement of the chemical, and the inhalation toxicity of the chemical. Numerous direct micro-meteorological methods as well as an indirect method have been used to estimate the flux of chemicals, primarily soil fumigants, from fallow soil. Since most pest control products are applied directly to field crops and orchards, it is necessary to adapt the current methods to take into account the competing processes at the plant surface including plant uptake, sorption to plant leaves and stems, formulation type, and canopy architecture. Currently, there is no model that can take into account these factors and reliably predict evaporation from a crop canopy. Once the evaporation rate of the chemical from the plant canopy has been adequately characterized, either experimentally or using a model, it can be used as an input to an appropriate air dispersion model to predict off-site movement. Air dispersion models have been used extensively to predict off-site movement of soil applied fumigants, but their use in modeling off-site movement of semi-volatile chemicals from a plant canopy has been limited. Modeling off-site movement from a crop or orchard canopy needs to take into consideration parameters including the height of the canopy and the effect of the canopy on the roughness boundary layer. The air dispersion model also requires meteorological data from representative geographies where the crops of interest are grown. Valid exposure estimates must then be coupled with appropriate inhalation toxicity data which also presents unique challenges for compounds with low vapor pressure.

AGRO 300

Understanding the origin of aerosols at the urban-regional interface

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Atmospheric particles (aerosols) are a major component of urban and regional air pollution, causing more than a million premature deaths annually, reducing visibility (haze), distorting the radiative energy budget of the lower atmosphere and surface, and modifying cloud nucleation, precipitation, and lifetimes. While some of these are emitted directly and their sources are relatively easy to identify (e.g., dust, soot, and some organics), many are produced in the atmosphere by condensation of gases formed as products of photochemical reactions among the numerous pollutant and natural compounds present in the atmosphere. This second category, which includes sulfates, nitrates, and most organics, can be much more difficult to attribute to specific sources. Urban plumes, with their reactive nitrogen oxides and hydrocarbons, can continue to generate particles for several days downwind. Recent studies suggest that they can interact with rural emissions (e.g., isoprene and terpenes from forests and agriculture) to increasethe regional particle burden substantially. Field measurements and modeling studies are begun to reveal the complex formation, properties, and removal processes for these aerosols.

AGRO 301

Agricultural influences on air quality from California's San Joaquin Valley to the Chesapeake Bay area

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Air quality continues to improve in many urban areas across the US, but progress in rural environments has been slower. Generally, areas at urban/rural interfaces experience some of the most persistent air quality problems. Mixing of urban NO_x emissions with agricultural volatile organic compound (VOC) emissions can lead to formation of ozone (O_3) and secondary organic aerosol (SOA). Transport of agricultural pesticides and inactive ingredients to unintended areas contributes to both atmospheric pollution and water quality issues. The focus of this paper will be based on three separate studies that demonstrate how increased knowledge of urban and agricultural emissions can enhance the accuracy of computational modeling and further our understanding of the affects of these emissions on air quality. In one study, detailed air quality model calculations were used to evaluate rigorously surface-level ozone concentrations from animal feed emissions and to compare this source to other leading VOC sources. Results demonstrated the effect of animal feed VOC emissions on actual ozone concentrations in the San Joaquin Valley (SJV) while at the same time evaluating the efficacy of VOC versus NO_x controls in the SJV. In a continuation of this study, the affect of NO_x emissions from animal these feed sources were considered and compared to NO_x emissions from urban sources. In the final study we untilized the Pesticide Emissions Model to generate emissions inventories that will feed directly into regional transportation models.

AGRO 302

Demonstration and evaluation of open-air tracer ratio flux measurements of methane and other trace gas emissions from pastured animals at low altitude, semi-tropical and higher altitude, semi-arid sites in Mexico

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Farm animals, especially ruminants, are recognized as important emissions sources of methane, a powerful greenhouse gas, as well as an important precursor of global tropospheric ozone, which is both a toxic air pollutant as well as a powerful greenhouse gas. As part of the 2013 Short-Lived Climate Forcing (SLCF) pollutant emissions characterization in Mexico, a mobile laboratory equipped with extensive real-time (1 s) trace gas sensors and quantitative tracer gas release equipment was deployed at two university-operated agricultural campuses, one in semi-tropical Martinez de la Torre (150 m a.s.l.) in the State of Veracruz and the second at a higher altitude and more arid site in Toluca (2,600 m a.s.l.) in the State of Mexico. Experiments were conducted on small pastured herds of both dairy and beef cattle. The open-air tracer ratio emissions flux measurement methods used will be described and the effectiveness and data quality of these novel open air tracer release methods will be evaluated. Additional experiments were conducted through the measurement of respiratory CO_2 and the concomitant methane released from individuals and small herds. These novel breath experiments reveal the dynamic variation in methane released during normal respiration versus rumination. Results from these respiratory and tracer release emissions flux measurements will be presented and compared with other methods of characterizing and quantifying trace gas releases from farm animals.

AGRO 303

Analysis and evaluation of measured trace gas emissions from farm animals in Mexico

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The recent 2013 Short-Lived Climate Forcing (SLCF) pollutant emissions characterization in Mexico obtained quantified trace gas emissions data from small pastured herds of dairy and beef cattle, as well as more limited data on goats, using novel, open-air tracer ratio methods. Data from cattle at two distinct sites, one in semi-tropical Martinez de la Torre (150 m a.s.l.) in the State of Veracruz and the second at a higher altitude and more arid site in Toluca (2,600 m a.s.l.) in the State of Mexico, will be compared. Data from cattle with diet variations, including a diet designed to suppress methanogenic bacteria, data from calves versus mature animals, and data from dairy versus beef animals will be discussed. Plans for ongoing work, including methods to incorporate these data into Mexico's national greenhouse gas emissions inventory, will be presented.

AGRO 304

Field evaluation of EPA approved PM_{10} and $PM_{2.5}$ ambient FRM samplers for determining emission concentrations from agricultural sources

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Agricultural operations across the United States are encountering difficulties in complying with the current air pollution regulations for particulate matter (PM). Typically emission concentration measurements from agricultural sources that are non-point sources are conducted in accordance with EPA's Federal Reference Method (FRM) PM_{10} and/or $PM_{2.5}$ ambient air samplers. The samplers use impactors or cyclones to separate out the particles larger than the size of interest. For example the purpose of the PM_{10} cyclone is to remove the particles larger than 10 µ; particles 10 µ and smaller pass onto the next stage of the

sampler. Laboratory tests and extensive field evaluations have been conducted to determine how well concentrations from the FRM ambient air samplers compare to a methodology that uses particle size analyses to determine the percent of particles less than the size of interest captured on a filter. The paper will summarize some of the key findings from this research.

AGRO 305

Field evaluation of EPA Method 201a (stack sampling methodology) for determining $PM_{2.5}$ and PM_{10} emission concentrations from an agricultural source

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Agricultural operations across the United States are encountering difficulties in complying with the current air pollution regulations for particulate matter (PM). Typically emission concentration measurements agricultural sources with exhaust stacks (point sources) are conducted in accordance with EPA's Method 201a. This method provides the protocols for determining $PM_{2.5}$, PM_{10}, and total particulate concentrations. Method 201a utilizes cyclones to separate out the particles larger than the size of interest. For example, the purpose of the PM_{10} cyclone is to remove the particles larger than 10 µ so; particles of 10 µ and smaller pass onto the next stage of the sampler. Laboratory tests and extensive field evaluations have been conducted to determine how well the Method 201a sizing cyclones work in agricultural environments where relatively large particles and fibers are present. The paper will summarize some of the key findings from this research.

AGRO 306

Oil and gas exploration impacts on air quality and their potential implications for agriculture

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The voracious demand for energy due to the growth of megacities has resulted in a rush to exploit unconventional resources such as shale deposits of oil and gas with fracking techniques. The environmental implications of this development have yet to be fully explored, including the impacts of oil and gas site emissions on air quality. Ozone and toxic air pollution from oil and gas activities may adversely affect both crops and livestock. A high resolution 3D Eulerian chemical transport model has been developed with the ability to simulate the near source air quality impacts of reactive species emitted by oil and gas facilities, as well as to infer the magnitude, timing, and location of facility emissions based on contemporary real-time measurements of ambient air pollution conducted outside facility fence lines. Applications of this model of interest to agriculturalists will be demonstrated. The possibility of expanding the model to include full multi-media (air, water, soil) simulation capabilities will also be discussed.

AGRO 307

Air pollution in the metropolitan area of Buenos Aires: From emission inventories to air quality impacts

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In spite of being the twelfth largest megalopolis in the world and the third in Latin America, air quality information in the metropolitan area of Buenos Aires is still insufficient. In the last 10 years, we have undertaken a number of studies to address part of this gap in knowledge. Our series 1990-2011 of emission inventories of greenhouse gases (CO_2, CH_4, and N_2O) and commonly found air pollutants (CO, NO_x, SO2, VOCs, and particulate matter) constitute the first set of systematic estimates for this region. For mobile sources, our results highlight the role of older vehicle technologies accounting for almost 80% of the emissions of all species and allow identifying time-lags in technology penetration between developed and developing countries. We have used our CO emission estimates as input to regional air dispersion models as a first step to develop local chemical weather forecasting tools, while local government officers have used the inventories for decision making regarding traffic control and greenhouse gas mitigation options. Our group has also assessed key issues related to levels of crustal, toxic, and potentially toxic elements present in the local urban aerosol, analyzing the contribution of local and regional air pollution sources. We have paid particular attention to: traffic-related elements (Cu, Mo, Pb, Pt, Rh, Sb, Zn), black carbon, and the South Atlantic Ocean influence using sea salt as chemical marker. Regarding, environmental health, we have evaluated the health effects of climate and air pollution in the city through a time series analysis. We have shown that correlations exist between temperature changes and total cardiovascular and respiratory mortality; that about 4% extra deaths can be expected on the day following a 1 ppm increase in air pollution levels; and that the elderly are the most vulnerable, both to climate variables and pollution levels.

AGRO 308

Food commodity consumption data and new tools used by US EPA Office of Pesticide Programs

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The US EPA Office of Pesticide Programs (OPP) conducts dietary assessments for pesticides by combining data on pesticide concentrations in/on food commodities (e.g., apples) with data on consumption of these commodities. The consumption data were previously derived from the USDA Continuing Survey of Food Intakes by Individuals (CSFII). CSFII was replaced by the USDA What We Eat in America (WWEIA) survey in 1999, and is now conducted as part of the US National Health and Nutrition Examination Survey (NHANES). OPP recently shifted from CSFII to the WWEIA survey and now routinely uses the WWEIA data in its dietary assessments. In order to conduct these assessments, EPA has converted the foods reported “as eaten” in the WWEIA survey (e.g., lasagna) to their component ingredients (e.g.,

wheat flour, tomato, etc.) by means of recipe files developed for this purpose. OPP's dietary consumption data are public information and public availability, and have been recently enhanced through a collaborative effort between the University of Maryland and US FDA Joint Institute for Food Safety and Applied Nutrition (JIFSAN) with OPP. This effort has placed the data files on food commodity consumption and several web applications tools developed by JIFSAN on the web (http://fcid.foodrisk.org). These tools increase the availability and transparency of data used in dietary risk assessment and permits the public to perform simple queries of the data. The presentation will cover the US EPA Food Commodity Intake Database; the JIFSAN recipe search tool which permits the user to search (or reverse search) recipes; and the JIFSAN consumption calculator which enables customized analysis of WWEIA-FCID 2003-08. The results of some illustrative data analyses using these tools will also be demonstrated. Together, these data and tools open the public up to a wide range of information that is useful for exposure assessment and considerably eases its use and interpretation.

AGRO 309

What is the best use of available global data for regulatory assessments and harmonized Maximum Residue Limits (MRLs)?

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This talk begins with the premise that harmonized MRLs are advantageous for international relations and trade. The use of global information to inform MRL decisions, appropriate toxicological endpoints, and dietary assessments for a local regulatory decision is good stewardship in a world of expanding trade, but limited resources. Understanding how local use patterns (GAPs) fit within broader global uses and existing residue data is an important consideration for setting a harmonized MRL. In addition, information on observed residues from monitoring programs, processed product factors, market share or percent imports, and extrapolation of residues within crop groupings can ameliorate overly-conservative dietary risk assessments.

AGRO 310

Communicating the connection between MRLs and food safety

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North American consumers enjoy one of the safest, most abundant and varied food supplies in the word. The numerous food residue monitoring programs in US and Canada indicate extremely high level of compliance rate; nevertheless, food safety and potential risks from pesticide residues is an area of concern for many North American consumers. The perception held by not only general public, but also by many of our growers and exporters, is that Maximum Residue Limits are safety standards. Thus, North American harmonization of Maximum Residue Limits, which in some cases results in increased MRL values, is becoming an intensely debatable topic. There is a widely spread believe that increasing and harmonizing MRLs will result in exposure of the consumer to unsafe levels of pesticides. These ideas are not supported by scientific evidence and the framework for conducting consumer risk assessments. Thus, the issue is very complex and requires significant education efforts focused on decoupling of MRLs harmonization efforts and food safety concerns. The presentation will focused on several aspects of simple and clear communication messaging around food safety and Maximum Residue Limits.

AGRO 311

MRLs as potential barriers to innovation, trade, and food security

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Canola is a product of innovation and continues to succeed because of new innovations such as crop protection products. Canadian producers depend on exports and require effective and aligned regulatory systems in international markets for their livelihoods. This presentation will describe why effective regulation of crop protection products is so important for innovation, trade, and food security. It will outline why the current regulation of MRLs in key export markets creates risk for exporters and dissuades the industry from adopting new crop production technology. Providing examples from canola, the presentation will cover current needs for the canola industry and possible solutions to facilitate trade. It will also outline several initiatives undertaken by the canola value chain in Canada to manage risks associated with pesticide residue proactively.

AGRO 312

US citrus industry perspective on MRLs and trade

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The California citrus industry is a $1.5 billion industry that exports approximately 30 percent of its production. Moreover, revenue from exports represents approximately 40 percent of total sales revenue. Without strong export markets the California citrus industry cannot thrive. However, with recent liberalization of global tariffs chemical residue issues and phytosanitary regulations have become the dominant barrier to trade in citrus fruits and other specialty crops. This presentation will explain the critical role of maximum residue levels (MRLs) in facilitating trade of citrus and other export-oriented specialty crops and how cooperative efforts among specialty crop commodity organizations, registrants, and regulators can work together to provide important crop protection tools for growers and facilitate trade. Symposium participants outside the agricultural sphere may be interested in using this regulatory approach as a template for structuring regulatory-problem solving in other fields.

AGRO 313

Import tolerance approval process in Japan

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Japan's food self-sufficiency ratio for FY2011 was 39% on a calorie basis (MAFF, Aug. 2012), slowly declining continuously over decades. The modern Japanese diet relies heavily on the import of a large quantity of food from overseas. In light of the situation of imported foods, the Ministry of Health, Labour, and Welfare (MHLW) introduced the positive list system in 2006 and started to reinforce the import inspections such as residual agricultural chemical monitoring. Given the above, import tolerances are critical for both Japanese society and exporting countries, especially the US, China, Australia, Thailand, and Canada. This presentation will include the import tolerance requirements, such as scientific data and legal status in exporting countries, and pesticide registration process, focusing on how the import tolerances are approved in Japan. Potential challenges in the regulatory process for import tolerances in Japan will also be discussed.

AGRO 314

Responses of export-oriented tree fruit producers to the challenges of meeting MRL requirements around the world

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The tree fruit industry in the states of Idaho, Oregon, and Washington is the major source of fresh apples, pears, and cherries in the United States. Thirty percent of the total fresh crop from this region is exported to over 60 countries around the world. In the past decade, these individual family farmers, their pest control advisors, and the packing and sales agencies serving them have had to rethink orchard pest control strategies with the rise of MRL enforcement in their major markets around the world. The absence of coordinated information regarding pesticide application strategies to meet MRL requirements across all destination markets has created orchard management and marketing challenges for the industry and market penetration challenges for the crop protection chemical registrants when new active ingredients are introduced. A discussion of grower responses to the challenge and ideas for ways to improve decision-making are discussed.

AGRO 315

Challenges in establishing Maximum Residue Limits to support the export of raw agricultural commodities

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Maximum Residue Limits (Levels - MRLs) are regulatory standards established by governmental authorities for the purpose of regulating trace residues of agricultural chemicals that may occur in food commodities after the use of pesticides. This presentation will cover the challenges that industry member stakeholders face in obtaining MRLs in foreign markets to support the export of US commodities. Import tolerance applications, residue definitions, crop groupings, pesticide use patterns, and other factors will be discussed. Identification of the obstacles still affecting the establishment and harmonization of national/regional MRLs around the world is a first step in proposing possible solutions. Today's growers are doing a tremendous job of continuously increasing the quantity and quality of food needed to feed the ever-increasing world population. As such, they deserve national and international regulations which make it less burdensome and less risky to export their produce.

AGRO 316

Pyrethroid pesticides in municipal wastewater: A baseline survey of publicly-owned treatment works facilities in California

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In response to the 2006 California Department of Pesticide Regulation data re-evaluation, the Pyrethroid Working Group and Tri-TAC, representing publicly-owned treatment works (POTWs) developed a monitoring project for eight pyrethroid pesticides in influent, effluent, and biosolids. The project surveyed 32 POTWs between January and March 2013. At each location, samples of influent and effluent were collected as consecutive grab samples, and at sites that accommodated sampling of biosolids, this matrix was collected and composited. Two laboratories were used to analyze the biosolids samples as replicates and the effluent and influent samples as consecutive grabs (distinct samples). A pre-project intercomparison study was conducted to ensure sampling technique and comparability of the laboratories and methods. To maintain comparability with other pyrethroid pesticides data collected in the state of California, the project used the quality control criteria from the State of California's Surface Water Ambient Monitoring Program. Samples were analyzed using gas chromatography/mass spectrometry using a chemical ionization detector. Laboratory reporting limits ranged from 0.5 ng/L in the effluent to 80 ng/g in the biosolids. As predicted for a hydrophobic chemical, residues were greatest in the biosolids and lowest in the effluent. Of the eight pyrethroids monitored, permethrin was the dominant pyrethroid found followed by cypermethrin and bifenthrin.

AGRO 317

Analysis of pyrethroid insecticides in complex environmental samples using stable isotope labeled standards as surrogates

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Several synthetic pyrethroids have indoor, as well as lawn, garden, and external structural barrier uses. This broad range of use patterns may result in the presence of multiple pyrethroids in influent/effluent waters and biosolids from publicly-owned treatment works (POTWs). The presentation will describe an analytical approach to analyzing these complex matrices for eight representative pyrethroids, using the previously reported NCI-GC-MS instrumental analysis with D_6 stable isotope analogues as internal standards. Due to significant variability in the composition of biosolids from different POTWs, adding known amounts of surrogate compounds to each sample prior to extraction and then measuring recoveries in order to demonstrate acceptable method performance is highly desirable. The presentation will further describe the use of two selected D_6 analogues as surrogates that closely match the method behavior of the eight target analytes. Details of a recently-validated biosolids method now in routine use will be reported along with associated method performance and surrogate stable isotope analogue recovery data.

AGRO 318

Fate of pyrethroid pesticides through advanced wastewater treatment processes

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Pyrethoid pesticides are known to enter wastewater collection systems and wastewater treatment plants through direct and indirect disposal. The fate of pyrethroids passing through conventional wastewater treatment processes is not well understood and has been the subject of a series of recent studies conducted at the Sacramento Regional Wastewater Treatment Plant (SRWTP). The SRWTP provides wastewater treatment services for the urbanized areas of Sacramento County, on average treating 145 mgd of wastewater. A study of pyrethroid treatability was conducted as part of a demonstration-scale study for selecting advanced treatment processes for the SRWTP. The studies provided a unique opportunity to evaluate the performance

of several treatment process alternatives in removing pyrethroid pesticide residues. The advanced treatment processes studied included biological nutrient removal, membrane filtration, granular media filtration, ozonation followed by biologically-active media filtration, and three disinfection alternatives: chlorination, UV irradiation, and ozonation. Although conventional and advanced wastewater treatment processes were not designed to remove pyrethroid pesticide residues, the measured removals were significant. Treatment performance for all tested treatment processes and all pyrethroids will be presented.

AGRO 319

Potential influence of pyrethroids, metals, sediment characteristics, and water quality conditions on benthic communities in Cache Slough California in 2012

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Tasks conducted at twelve sites in Cache Slough California during both spring and fall of 2012 were: (1) collect and identify benthic macroinvertebrates; (2) measure TOC, grain size, bulk metals, simultaneously extracted metals (SEM) and acid volatile sulfides (AVS), 8 pyrethroids and basic water quality parameters; and (3) use univariate and stepwise multiple regressions to determine the relationship between various benthic metrics and TOC, grain size, metals (bulk metals and SEM/AVS), and pyrethroids. A total of 54 different tolerant benthic taxa were collected from the twelve Cache Slough sites during the spring, and 43 different tolerant taxa were collected during the fall. The highest number of metals threshold effects levels (TEL) exceedances for the twelve sites with both seasons combined in descending order was: 24 for nickel; 21 for chromium; 19 for copper; 12 for arsenic; 6 for mercury; and 2 for cadmium. Sediment pyrethroid toxic units (TUs) for the sum of pyrethroids based on *Hyalella* were calculated. The sum of pyrethroid TUs was slightly greater than 1 (1.07 - 1.97) at four upstream sites sampled during the spring. However, for the fall sampling the sum of pyrethroid TUs was less than 0.5 at all twelve sites which suggests no toxicity due to pyrethroids. The benthic metrics % Collectors/Filterers & Collectors/Gatherers appeared to be directly related to arsenic in the sediments. The metric Abundance was also inversely related to TOC and % silt. Multivariate canonical correlation analysis showed that samples with sandier sediments tended to have benthic communities that were more diverse. No significant relationships were detected between the benthic principal components and the principal components associated with metals or pyrethroids. Results from this limited data set suggest that sediment characteristics are a more important factor than toxicant concentrations in the sediments for the benthic communities of Cache Slough.

AGRO 320

Pyrethroid monitoring of the Lower American River in California (USA)

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The Lower American River starts below Folsom Dam (Folsom Lake) and runs 49.2 km to the river's confluence with the Sacramento River. This portion of the river is very wide and shallow and moves swiftly as it passes through an urbanized area; it is buffered by riparian parks, cycle paths, and is used extensively for recreation. The majority of the flow in this section of the river throughout the year is a controlled discharge from the Folsom Dam. Local storm drains, small ephemeral channels and an extensive network of organized storm drain collection and pump stations discharge excess rainfall from surrounding urban and suburban environments into the Lower American River channel. The current study was designed to systematically investigate the nature, timing, likelihood, and scale of potential pyrethroid detections. This objective was accomplished through (1) various rainfall event-driven sampling studies during the 2011-2012 and 2012-2013 rainy seasons and (2) a robust, multi-site, spatio-temporal transect study, appropriate for investigating a river system of this size and scale. Results demonstrate that pyrethroid residues have generally been low and infrequent.

AGRO 321

Overview of updates to US EPA Office of Pesticide Programs dietary models and Residential SOPs

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In 2012, the US EPA Office of Pesticide Programs (OPP) issued an updated version of the Dietary Exposure Evaluation Model-Food Commodity Intake Database (DEEM-FCID)/Calendex software and revised Standard Operating Procedures for Residential Pesticide Exposure Assessment (Residential SOPs). The DEEM-FCID/Calendex software has been updated to incorporate food consumption data from the National Health and Nutrition Examination Survey/What We Eat in America (NHANES/WWEIA) dietary survey for the years 2003-2008 and updated crop groups. OPP can use the DEEM-FCID model to estimate dietary intake of pesticides and the Calendex model to evaluate exposure to chemicals resulting from residues in food, drinking water, and/or residues in or around the residence. Additionally, OPP has collaborated with the University of Maryland/US FDA's Joint Institute for Food Safety and Applied Nutrition (JIFSAN) to share data files on food commodity consumption and several dietary-exposure related web applications tools developed by JIFSAN on the web (http://fcid.foodrisk.org). The 2012 Residential SOPs “are instructions for estimating exposure resulting from the most common non-occupational pesticide uses including lawn and garden care, foggers, and pet treatments” that provide “background, data analysis, and assessment characterization” for residential assessments. This presentation will provide an overview of: (1) updates to the DEEM-FCID/Calendex models, how OPP is using the models, and an introduction to the new features (eating occasions, etc.); (2) updates to crop groupings; (3) a brief

introduction to the JIFSAN website and tools; and (4) updates to the Residential SOPs and how OPP is applying them in risk assessments.

AGRO 322

Use of open literature toxicity and epidemiology studies in regulatory decision making

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Information relevant for regulatory decision making can come from a variety of sources. In addition to studies conducted to fulfill data requirements, often publications available in the open literature can provide valuable information. A recent document from US EPA Office of Pesticide Programs (OPP) entitled *Guidance for Considering and Using Open Literature Toxicity Studies to Support Human Health Risk Assessment* provides direction to OPP scientists in selection and utilization of relevant publications for use in risk assessments. The purpose of this presentation is to provide an overview of the US EPA guidance, highlight additional opportunities for consideration in determining how information from disparate sources should be utilized in a regulatory context, and provide perspective on challenges unique to human research. In particular, because the use of human epidemiology studies for decision making is often particularly challenging, additional detailed and unambiguous guidance should be provided on how this type of information should be evaluated and utilized. In addition, rigorous methods and tools should be provided to enable a consistent, transparent, and uniform evaluation approach. Having such methodologies in place *a priori* is critical in reducing bias that could occur during the review process. Additionally, providing examples would assist in illustrating how the guidance provided should be applied. It would also be valuable for the Agency to implement test cases in which the same chemical is evaluated by multiple reviewers independently to determine if the process outlined is reproducible. Once in place, these guidelines should be communicated to journal editors so that researchers are encouraged to provide sufficient data with their manuscript submissions. In summary, while the guidance document provides a good starting point for the discussion of how literature studies should be utilized in risk assessment, there are several aspects that merit further detailed guidance and dialogue within the scientific community.

AGRO 323

Impact of recent changes in pesticide exposure assessment procedures on dietary, residential, and aggregate exposure estimates

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In 2012, the US Environmental Protection Agency Office of Pesticide Programs adopted changes to the methods and models used to estimate dietary and residential exposures to pesticides for regulatory purposes. Dietary exposures to pesticides resulting from the consumption of treated foods are still estimated using the Dietary Exposure Evaluation Model with Food Consumption Intake Database (DEEM-FCID), but EPA replaced the food consumption data from the Continuing Survey of Food Intakes by Individuals (CSFII) conducted by the US Department of Agriculture (USDA) during 1994-1996, and 1998 with more recent data collected through the National Health and Nutrition Examination Survey/What We Eat in America (NHANES/WWEIA) in 2003-2008. The presentation will compare dietary exposure estimates generated using the CSFII and NHANES/WWEIA data. A variety of dietary exposure assessments will be examined, ranging from simple Tier 1 tolerance-level assessments to highly-refined assessments incorporating monitoring data and Monte Carlo modeling. Also in 2012, EPA released revised Standard Operating Procedures for Residential Pesticide Exposure Assessments (SOPs). The revised SOPs represent a major expansion and update of prior SOPs, and new models and default assumptions result in changes to exposure estimates for pesticide products used in and near residences. The presentation will also compare exposure estimates using the former and revised SOPs for select products. Aggregate (dietary + residential) exposure assessments are impacted by the changes to the dietary model and revised SOPs, and the extent of this impact will be discussed. Finally, drinking water will be considered through the use of various data sources from modeled to monitored values.

AGRO 324

What if there was no USDA Pesticide Data Program? Advantages and rigor of the US EPA tiered process for risk assessment

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Today, US agriculture benefits greatly from a robust, tiered, risk assessment process for consumer dietary exposure which is in place for US EPA Office of Pesticide Programs (OPP). The OPP tiered process is data-driven and is supported by up-to-date government residue monitoring data for the most-commonly consumed foods performed under the USDA Pesticide Data Program (PDP). This process is so integral to the pesticide registration process and the fulfillment of the Food Quality Protection Act (FQPA), which requires collection of pesticide residue data, that it is often taken for granted within the US. This presentation will illustrate, through concrete examples, the current advantages of the OPP refined dietary assessment in support of US agriculture, and particularly of minor crop agriculture. This highly refined approach will be contrasted with dietary assessment practices in other countries, which generally allow for fewer refinements, and also with the less refined US EPA OPP screening level approach for drinking water exposure assessment. This presentation will highlight the vital role of the PDP monitoring data in development of realistic and highly-refined risk assessments supporting US agriculture.

AGRO 325

Improving the estimation of drinking water exposure in dietary risk assessment

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This presentation introduces a conceptual tiered approach to estimation of agricultural chemical residues in the drinking water component of a dietary risk assessment. Passage of the Food Quality Protection Act of 1996 required the US EPA to reassess tolerances and reregister all active ingredients. Since FQPA was adopted, the US EPA human health risk assessment considers the combined exposure potential from

all routes, such as residue from food intake, drinking water, and non-occupational exposures. A tiered process has evolved for the analysis of exposure from food in a dietary risk assessment. Early tiers feature maximum exposure estimates assuming high levels of product use and consumption. More realism is introduced through inclusion of actual residue data from surveys of commodities and probabilistic assessment of exposure potential. In contrast, the assessment of exposure potential from drinking water for dietary risk assessment has not evolved considerably. The modeling tools for estimation of residues in surface water adjacent to a farm field are used to produce estimates of potential residues in reservoirs. Modeling with scenarios and input parameters consistent with a high risk for leaching are used to produce a deterministic evaluation of potential residues in groundwater. The groundwater and surface water values are used as estimates for drinking water exposure. The refinement of drinking water exposure requires monitoring, and for a few chemicals the monitoring data available is extensive. Extensive monitoring is not always practical, and statistical analysis of the available data suggest that monitoring programs can be more pragmatically designed with targeted programs that consider the temporal and spatial sampling requirements to achieve a desirable predictive power. We propose that the lessons learned since FQPA was implemented be applied in developing an approach to estimation of exposure from drinking water that is analogous to the approach used in estimation of potential exposure from food.

AGRO 326

Pesticide dietary exposure and risk assessment: Incorporating monitoring data to address controversial issues

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Public attention has frequently been drawn to pesticide residues in foods. Concerns are often raised regarding the origin of foods (domestic vs. imported), the method of production (conventional vs. organic), and potential risks associated with specific foods (the “Dirty Dozen”). Consumers have frequently been advised to limit their consumption of imported fruits and vegetables, to seek out organic foods when available, and specifically to avoid purchasing conventional forms of many common fruits and vegetables. Existing federal pesticide residue monitoring data from the US Food and Drug Administration and the US Department of Agriculture were incorporated into the exposure and risk assessment processes to examine the appropriateness of such consumer recommendations. Results indicated that while consumption of neither imported nor domestic fruits and vegetables triggered health concerns, typical dietary exposure to pesticides was frequently greater from consumption of domestic fruits and vegetables. Organic foods were associated with lower levels of pesticides, although residues were frequently detected. An examination of the foods considered by some to represent the most-highly contaminated fruits and vegetables indicated that exposures to the most-commonly detected pesticides on these commodities represented only tiny fractions of levels considered to be of concern and that exposures would frequently need to be one million times higher to reach levels that caused no effects in laboratory animals undergoing long-term toxicity testing.

AGRO 327

FQPA and health effects

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The Food Quality Protection Act of 1996 (FQPA) requires a default 10x factor to be added to the traditional interspecies and intraspecies uncertainty factors, resulting in an initial 1000-fold UF in deriving the acute and chronic RfD's. This FQPA factor is retained if there are (a) “Residual concerns for susceptibility given the available evidence on pre- and postnatal toxicity” or (b) “Residual concerns or uncertainties in the exposure assessment” (US EPA, 2002). In practice, the FQPA factor has been reduced to "1" for over 90% of approximately 352 pesticides listed in EPA's Human Health Benchmarks for Pesticides (http://iaspub.epa.gov/apex/pesticides/f?p=HHBP:home). This talk focuses on a weight-of-evidence approach US EPA OPP uses to evaluate the potential for pre- and postnatal toxicity and the completeness of the toxicology databases. Specifically, US EPA considers human epidemiology and animal published literature on developmental toxicity and mode of action in its deliberation of residual concerns for infants and children. Criteria are needed for evaluating developmental studies that have not been conducted according to general principles outlined by GLP and EPA test guidelines.

AGRO 328

EU update on dietary risk assessment: An industry perspective

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In 2005, the EUMRL regulation 396/2005 was published, and it includes the legal obligation to consider aggregate and synergistic effects during MRL setting for pesticides. The requirement is also part of the EU Regulation 1107/2009. In the past seven years, the European Food Safety Authority (EFSA) and institutions such as RIKILT (Wageningen, NL) have initiated multiple projects in order to fulfill this requirement. The projects include the definitions of cumulative assessments groups, the collection of appropriate consumption data, the publication of guidance documents, and the development of an appropriate IT tool for performing probabilistic dietary risk assessments. Most of the projects are well advanced; due to high pressure and public concerns on cocktail effects, first assessments can be expected in 2013/2014. In the presentation, the different initiatives will be briefly summarized. Furthermore, an outlook on future needs from industry perspective will be provided.

AGRO 329

Cumulative risks: When do they add up? Using the Maximum Cumulative Ratio (MCR) to understand risks from concurrent exposures to multiple chemicals

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Human and environmental receptors are co-exposed to multiple synthetic chemicals from multiple sources. The question has been raised whether chemical-by-chemical assessments of risk underestimate the total toxicity to individuals. This talk presents a simple screening tool, the Maximum Cumulative Ratio (MCR), which can be used to prioritize cumulative exposures to chemicals, including pesticides, for human and ecological receptors. MCR values, along with a measurement of cumulative hazard such as the

Hazard Index (HI) have shown a consistent pattern. Specifically, for any population of receptors exposed to multiple chemicals from one or more sources, the individuals with the largest HI values tend to have risks that are dominated by a single chemical (MCR values close to 1). This suggests that receptors with the largest cumulative stresses are more likely due to a single chemical (either from high toxicity or high exposures), rather than multiple chemicals operating in combination. This further implies that chemical-by-chemical approaches are protective for the majority of cumulative and aggregate exposures. These studies also demonstrated the ability of the MCR to identify certain exposures whose cumulative risks could be missed using chemical-by-chemical approaches under certain conditions. The MCR and the HI provide a basis for risk management of cumulative exposures. Cumulative exposures can be divided into four groups based upon MCR and HI values, Group I, where one or more individual compounds have hazard quotient values greater than 1; Group II, where there is low concern for cumulative effects; Group IIIA, where cumulative exposures are a concern but one chemical is the clear driver; and Group IIIB, where information on mode of action is needed for refining the assessment. Using this approach, assessors can identify exposures where chemical-by-chemical approaches would have missed cumulative toxicity, and whether there are specific groups of chemicals that warrant additional investigation.

AGRO 330

Can the oxidative stress responses in pine needles be used as reliable biomarkers to assess exposure to POPs?

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Anthropogenic contaminants can be transported in the atmospheric. Passive air sampling is increasingly being recognized as an effective approach for measuring the atmospheric contamintants including the relative concentrations of Persistent Organic Pollutants (POPs): organochlorine pesticides (OCPs), polychlorinated biphenyls (PCBs), and polybrominated diphenyls ethers (PBDEs). Pine needles accumulate POPs in their tissues and integrate contaminants over a long time. POPs are able to generate reactive oxygen species (ROS), but the organisms have evolved systems of antioxidant defense. This project seeks to study the combined effects of environmental pollutants on oxidative stress biomarker systems to determine whether some of those changes could be used as reliable biomarkers to assess the end results of exposure to POPs. Pine needles were used to evaluate longitudinal and latitudinal POPs levels in the atmosphere of Patagonia, Argentina. Levels of lipid peroxidation, GST activity, and total antioxidant capacity (ACAP) were also evaluated. HCHs, endosulfans, DDTs, PCBs, and PBDEs congeners were determined. The Rio Negro watershed, characterized by an intensive fruit production, showed the highest POPs levels with a predominance of endosulfans (51-90%) as result of its unrestricted use, followed by DDE and low proportion of PCBs and PBDE; concomitantly high ACAP and GST activity were quantified. A decrease gradient in POPs and biomarkers levels from west to east was observed, indicating a direct relation between both parameters. An increasing latitudinal gradient (20-440 ng/g lipid weight) to the southeast station (Rio Gallegos) with a predominance of DDTs (30%), PCBs (35%) and PBDEs was observed but the non-direct relationship with biomarkers would be influenced by other factors, both biochemicals or environmental conditions in biomarker responses to POPs. Thus, the biomarkers selected would be a useful tool in the atmospheric pollution assessment by POPs, but more studies considering pine needle lipid classes and a range of temperature among stations should be performed.

AGRO 331

Design and performance of a study for the determination of trichlorofon transferrable residues from turf and residues in air

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Lawn protection products can potentially result in both transferrable residues on turf and volatile residues in air. A study was performed to measure the transferrable and volatile residues of trichlorofon and the related primary metabolite dichlorvos (DDVP) following a liquid application to turf with and without irrigation. This presentation will cover the study design, sample collection and analysis, and the nature of dissipation for both trichlorofon and dichlorvos under typical use conditions.

AGRO 332

Brominated flame retardants in the Great Lakes atmosphere

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Due to environmental concerns, the use of most polybrominated diphenyl ethers (PBDEs) was banned by the European Union and phased out in the United States in 2004. Perhaps as a result, there seems to be a shift to using non-regulated flame retardants, and several “new” flame retardants have been recently detected in the environment. Here we present temporal and spatial trends in PBDEs, decabromodiphenylethane (DBDPE), 1,2-*bis*(2,4,6-tribromophenoxy)ethane (TBE), hexabromobenzene (HBB), and pentabromoethylbenzene (PBEB) concentrations in air (vapor and particle phases) and in precipitation at the five United States Integrated Atmospheric Deposition Network sites located in the Great Lakes basin. These samples were collected from January 2005 to December 2009, inclusive. Overall, Chicago and Cleveland had the highest concentrations of PBDEs in both air and precipitation, suggesting a strong urban atmospheric source of these pollutants. This urban effect could also be observed at the rural Sturgeon Point site. The other two remote sites, Sleeping Bear Dunes and Eagle Harbor, have the lowest concentrations of these contaminants. Following this pattern, TBE and DBDPE have highest levels at urban Chicago and Cleveland. The spatial pattern for HBB and PBEB was surprising: the highest levels of these compounds were detected at the rural site in Sturgeon Point and at the remote site in Eagle Harbor, respectively. The sources of HBB and PBEB at these sites are not known. The temporal trends of PBDEs, DBDPE, HBB, PBEB, and TBE were investigated using harmonic regression applied to concentrations in all three phases at all the sites combined together, which allowed us to examine the overall temporal behavior of these compounds in the Great Lakes region.

AGRO 333

Airborne steroids and growth promoters near concentrated animal feeding operations

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In order to increase the amount of affordable animal protein in the human diet, chemicals to promote growth and prevent disease are often used in animal feeding operations. A large proportion of cattle and swine at feeding operations within the USA are raised in arid or semi-arid areas. Particulate matter (PM) in the vicinity of concentrated animal feeding operations in these dry areas contain synthetic and natural anabloic steroids, as well as other growth promoters. $PM_{2.5}$, PM_{10}, and total suspended particulates were collected near several feeding operations. Trenbolone, estradiol, and melengestrol were among the analytes detected in these PM fractions. Temporal profiles of growth promoters within PM revealed interesting patterns. The management of feeding operations appears to affect the constituents sorbed to PM. As cities in the USA encroach into agricultural areas, these compounds may reach major metropolitan areas. Also, as the need for animal protein increases globally, the confluence of animal feeding areas and major metroplitan areas is likely to become more common. As such, it is critical to understand environmental and health risks to allow proper resource management. The data within this presentation will form the basis of an exposure assessment for PM associated growth promoters.

AGRO 334

Examining the fate and transport of α- and β-endosulfan in the atmosphere of South Florida

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Agricultural activity in the South Florida region occurs in close proximity to both urban and natural areas like Biscayne and Everglades National Parks. One possible transport mechanism for pesticides into these sensitive ecosystems is release to the atmosphere after application. The process is enhanced in this region due to the calcareous soils, frequent rainfall, and high humidity and temperatures. Endosulfan is a widely-used pesticide with high toxicity to aquatic organisms. Air samples were collected over a five-year period (2001 to 2006) at a site within the agricultural community of Homestead, Florida and at sites located in Biscayne and Everglades National Parks (NPs). Mean gas-phase air concentrations of α-endosulfan were 17 ± 19 ng m^{-3} at Homestead, 2.3 ± 3.6 ng m^{-3} at Everglades NP, and 0.52 ± 0.69 ng m^{-3} at Biscayne NP. Examination of spatial and temporal trends indicated that endosulfan emissions from agricultural areas around Homestead influenced air concentration observations at the NP sites. Results of an intensive sampling campaign during the larger study indicated the highest total endosulfan concentrations at the NP sites were observed on days when air parcels were predicted to move from Homestead agricultural area towards the sampling locations. The α-endosulfan fraction (α/(α+β)) was used to examine the contribution of pesticide drift versus volatilization to the overall residue level. The median α-fraction observed during periods of high agricultural activity at Homestead and Everglades NP was 0.84 and 0.88, respectively, and during periods of low agricultural activity the median at Homestead was 0.86, indicating contributions from drift. The median α-fraction at Everglades NP was 1.0 during periods of low agricultural activity, while Biscayne NP was 1.0 year round indicating air concentrations are primarily influenced by regional volatilization.

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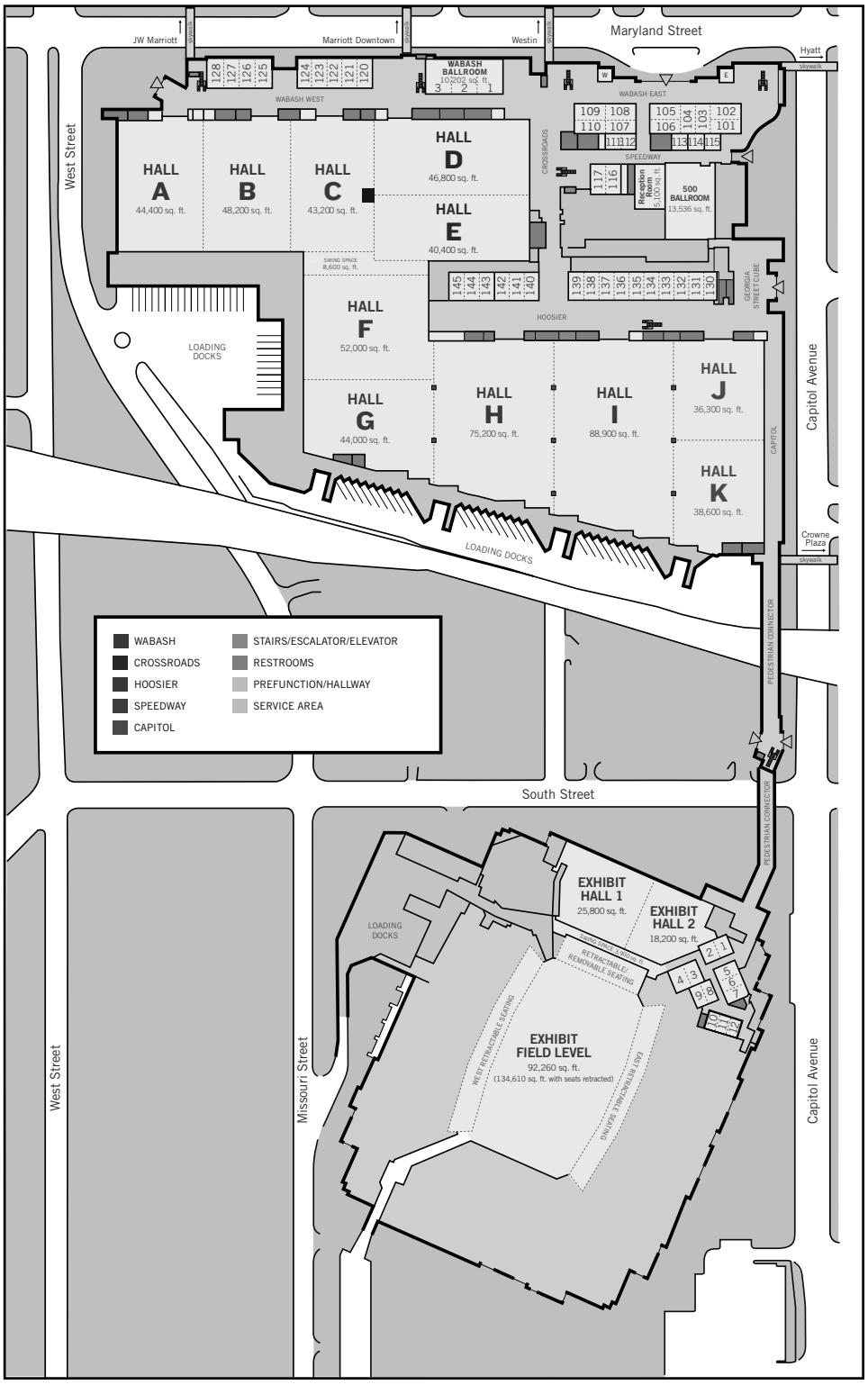

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