

PICOGRAM And Abstracts

AMERICAN CHEMICAL SOCIETY Division of Agrochemicals 229th ACS National Meeting March 13 – 17, 2005, San Diego, CA



Spring 2005

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SYNTHESIS AND CHEMISTRY OF AGROCHEMICALS

Edited by Don R. Baker, Joseph G. Fenyes, George P. Lahm, Thomas P. Selby, and Thomas M. Stevenson This 30-chapter volume is a complete reference book that includes current updates and trends in the field of agrochemicals. Topics in the book include herbicides in agriculture, control of insects and acrids in agriculture, and control of fungal disease in agriculture. (ACS Symposium Series No. 800)

(An American Chemical Society Publication)

2001 368 pp. 0-8412-3783-2 \$120.00/\$72.00

ENVIRONMENTAL FATE AND SAFETY MANAGEMENT OF AGROCHEMICALS

Edited by **J. Marshall Clark**, University of Massachusetts, and **Hideo Ohkawa**, Kobe University

Environmental Fate and Safety Management of Ágrochemicals discusses residue analysis, environmental fate and safety management, environmental risk assessment, metabolism, resistance and management, and advances in formulation and application technology from the academic, government, and industry perspective.

(ACS Symposium Series No. 899) (An American Chemical Society Publication) 2005 384 pp.

0-8412-3910-X \$144.50/\$86.70

NEW DISCOVERIES IN AGROCHEMICALS

Edited by **J. Marshall Clark**, University of Massachusetts, and **Hideo Ohkawa**, Kobe University

New Discoveries in Agrochemicals discusses molecular and combinatorial chemistry techniques impacting the agrochemical sciences. Topics in this book include biopesticides and transgenic crops, combinatorial chemistry, mode of action, natural products, green chemistry, and human vector control.

(ACS Symposium Series No. 892) (An American Chemical Society Publication) 2004 440 pp.

0-8412-3903-7 145.00/**87.00**

ENVIRONMENTAL FATE AND EFFECTS OF







PESTICIDES

Edited by **Joel R. Coats**, *Iowa State University*, and **Hiroki Yamamoto**, *Shimane University*

Synthesis and Properties of Silicones and Silicone-Madified Materials includes sections on synthesis, characterization, elastomers and reinforcement, surfaces and interfaces, copolymers, and reinforcing fillers. The book also reviews recent academic and technological developments behind silicones and silicone-modified materials. And finally, it includes sections on synthesis, characterization, elastomers and reinforcement, surfaces and interfaces, copolymers, and reinforcing fillers.

(ACS Symposium Series No. 853)

(An American Chemical Society Publication) 2003 320 pp. 0-8412-3722-0 \$145.00/\$87.00

ENVIRONMENTAL IMPACT OF FERTILIZER ON SOIL AND WATER

Edited by **William L. Hall Jr.**, and **Wayne P. Robarge** Fertilizers contribute to the variety, abundance, and low cost of food stuffs available to the public. However, fertilizer misuse can lower air, soil, and water quality. Regulators are scrutinizing fertilizers now more than ever because of their impact on the environment. This book provides an analysis of perchlorate in highly dissolved solid matrices and health issues of trace metals in fertilizers. This book focuses on nutrient impacts to water and the environment.

 ACS Symposium Series No. 872)
 (An American Chemical Society Publication)

 2003
 296pp.

 0-8412-3811-1
 \$125.00/\$75.00

PESTICIDE ENVIRONMENTAL FATE

Bridging the Gap Between Laboratory and Field Studies Edited by **Warner Phelps**, **Kim Winton**, and

William R. Effland

This book examines types of bridging studies currently being performed to help facilitate the transition from laboratory studies to field studies in support of pesticide registration. It includes discussions of modeling, variation in field sample profiles, bound vs. available residues, bare ground studies vs. cropped studies, the role of macropores in the field, pipe studies, hop plot studies, the tracking of material balance, and data interpretation. (ACS Symposium Series No. 813)

(An American Chemical Society Publication) 2002 248 pp. **0-8412-3726-3** 146.45/**87.87**



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HOSPITALITY COMMITTEE REPORT

Coffee Lounge-Philadelphia

Nine hundred fifty dollars were donated by six companies in support of the coffee lounge in Philadelphia. We thank them for their generosity. The friendly and hospitable reputation that our technical sessions enjoy throughout the Society is largely thanks to our sponsors – our fine members also help.

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Our Tuesday evening Social Hour, arranged by Barefoot & Jenkins, Ballmasters of Renown, must have been a great success; when I returned to my hotel I had to get a cab back to the Courtyard Marriott to get my valise. Our 2004 Coffee Lounge Chair, David Smith, is unable to continue in his office, so Spittler (c'est moi) is back in the trenches. Again, we are seeking one or two young, enthusiastic, funaphilic co-chairs to join the Hospitality Committee. Help promote wildlife, ours. Thank you.

Jeff Jenkins and Terry Spittler, Hospitality Co-chairs.



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MESSAGE FROM THE CHAIR

Allan Felsot, AGRO Chair 2005

This spring we assemble in San Diego, California for the 229th national meetings of the American Chemical Society and the Division of Agrochemicals (March 13-17, 2005). Many of us will welcome the break from cold and wet weather for sun and warmer temperatures. San Diego is California's second largest city and it has the diversity of recreation, arts, and business opportunities to match its size. Speaking of diversity, at this spring's ACS meetings, AGRO continues its distinguishing characteristic of highly diversified and interdisciplinary research interests with a Sunday to Thursday program packed with symposium that should interest everyone.

Discussions in our business meetings have centered on the trends in our membership as influenced by industry consolidation and the greatly expanded number of professional societies and other meetings for presenting our research efforts. One theme that always emerges is the importance of including students and recent graduates. I'm pleased to report that our Graduate Education programs—the Agrochemical Graduate Student Research Poster Competition and the Young Scientist's Research Recognition Award and Symposium—are alive and well and garnering success in attracting participation of younger scientists. At the Philadelphia meetings during Fall, 2004, the poster competition had 13 student participants. At the San Diego meeting, we will have an all day symposium with 15 student and post-doctoral associate speakers. The subject matter is highly diverse with papers being presented on everything from synthesis, natural products, pest control, toxicology, and environmental chemistry. We are now having a lot of participation by people interested in fertilizer and soil chemistry, as well as our traditional interests in pesticides.

In San Diego we will honor Dr. Robert Krieger with the ACS International Award for Research in Agrochemicals sponsored by BASF Corporation. During Bob's very diverse and long career he has become the most prominent scientist assessing worker and residential pesticide exposure using empirical studies. Bob has not slowed down in his current position at the University of California-Riverside. Both the symposium in his honor (starting Monday morning) as well as paper contributions from his colleagues will illustrate the state-of-the art in exposure assessment research and applications for risk characterization.

One of the themes that the current ACS president has expounded upon is change and where we will be in the year 2015. I think our programs have always reflected underlying changes, and we have responded with topical symposia on current events and future prognostications. Our predilection to be on top of things is again reflected in our meetings this spring. You have heard about genomics and the evolving focus to proteomics. AGRO is ahead of the curve now with perhaps the first ACS symposium on metabolomics, the next wave in research towards understanding how our genes and gene products are integrated to make cells and tissues function. One web site defines metabolomics as "the quantitative measurement of all low molecular weight metabolites in an organism's cells at a specified time under specific environmental conditions." Metabolomics research is ideally oriented to understanding how environmental conditions and stimuli change plant and animal physiology. Pertinently, scientists associated with AGRO have for a long time been interested in metabolites of pesticides, but our more contemporary focus on biopesticides, natural products, and host-plant resistance has the potential to make our division an important venue for discussion in this rapidly growing discipline. Please take time to see some of the talks in the Metabolomics symposium that will be held on Wednesday.

Our colleagues in the Fertilizer subdivision have organized another "state-of-the-art" symposium focusing on organic agriculture. Organic agriculture is growing at a very rapid rate and finding a very successful market niche in larger cities. Only recently has the scientific method been rigorously applied to solving pest control problems and answering questions about nutrient utilization and how plant physiology (and thus metabolomics!) might be affected by alternative agronomic practices. The full day "Organic Farming and Nutrients" symposium contains a diversity of topics and will be held on Tuesday.

In San Diego we will have several other symposia and contributed posters/papers that cover a wide variety of interests. Our Program Chair, Don Wauchope has carried on successfully the tradition of organizing a diverse program. Please take a minute to view the program on the ACS web site. You can easily access the San Diego programming information through a link on the refurbished AGRO web site at URL http://membership.acs.org/a/agro/. Also, the AGRO web site has a direct link to the national ACS portal that will allow you to click on the national meetings site where you can register for San Diego and book a hotel.

One goal for the refurbished AGRO web site is to be dynamic and up-to-date. We will have links to meetings most relevant to our members, as well as downloadable copies of the Picogram. Please contact me at afelsot@tricity.wsu.edu for your suggestions for improving the site or additions to the site.

As we look ahead past 2005 and into the future our current ACS president, Bill Carroll has made a commitment to producing a report on where the society will be in 2015. He has recognized the tremendous consolidations in the chemical industry but also the great emphasis on interdisciplinary research. We've already talked about these themes and need to express our ideas more formally. I intend to email some of you for ideas that we can forward to Bill for incorporation into the report on "Enterprise 2015".

The new ACS President-Elect is E. Ann Nalley from Cameron University, a moderately sized academic institution in Lawton, OK. She has a long history of service to ACS and seems especially interested in ACS' role in improving science education. In addition to education as one of her focused themes for 2006, she has spoken of the promise of nanotechnology. "Nano" this and "nano" that is the new buzz prefix, but I remind you once again that we in AGRO have been ahead of the curve. After all, we've been studying new molecules with biological activities in the nanomolar range for some time now. We're analyzing nanogram per liter concentrations and feeding our information to risk managers worried about nano effects on hormonal signaling and control systems.

I hope you share my vision of our Division as a place where progressive, future-looking scientists will have a place to meet, communicate, and share new big ideas about ever smaller things. We are as strong as your commitment. I thank all of Councilors, Executive Committee members, and Committee Chairs for their service. I especially thank our treasurer Terry Spittler and secretary Aldos Barefoot who work behind the scenes to serve our Division all year long. We also appreciate the work of Laura McConnell, our Picogram Editor and force behind ensuring that your presentation abstracts are published in a publicly accessible format (see the AGRO web site for electronic access). I also extend my appreciation to our coffee/social Patrons and Picogram Advertisers from the various private enterprises that support agrochemical sciences and technology. Finally, to this list of thanks I want to include Judy Ruppert from Washington State University who took over maintenance of the AGRO web site from Laura and refurbished it into a meeting place for all of our members. Please visit.

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Dr. Robert Krieger has conducted a program of excellence in assessing and reducing exposures and risks associated with the use of pesticides, and communicating this information to student, professional, and lay audiences. He and his many collaborators have defined the principles and developed the methodology needed for conducting exposure studies that underpin the assessment, reduction, and communication of risks. His work with exposure to soil fumigants and chemicals used for orchard pest control, particularly organophosphates, typifies his accomplishments. The results have been used in setting regulations, in extension courses he and others have given for pesticide formulators, applicators, and field workers, and in responding to concerns from urban and rural populations. His firm belief that effective risk management requires accurate determination of dose and time to evaluate the health significance of chemical exposures permeates his research

in the 'Personal Chemical Exposure Program' which he established and directs at the University of California. Research focuses on the development and use of advanced analytical methodology to identify fate and movement of pesticide residues from environmental compartments to children and adults. Indoor, turf, and field settings have been included. In agriculture this research has supported development of exposure-based reentry times, as opposed to adverse effect based reentry times used prior to implementation of the risk assessment process. Effective reentry times require accurate human exposure data and clear definition of work tasks so that short-term and long-term adverse effects can be considered. He continues to investigate the relationship between dislodgeable foliar residues and the bioavailability of those residues to harvesters based upon biomonitoring of urine and blood. A linear plant exposure chamber was developed for use in predictive structure-activity relationships. His research explores chemical transferability of chemical residues with respect to chemical (active ingredients as well as adjuvants) as well as from physical (adsorption, particularly cuticular waxiness in the case of plants) characteristics. Recent human studies have included assessment of the effects of perspiration on skin absorption, transfer and absorption of pyrethroids from indoor carpeting, human perchlorate exposure from food and water, and an exposure assessment of triclopyr and 2,4-D herbicides during backpack application in forestry.

Bob is a Cooperative Extension Toxicologist in the Department of Entomology, University of California, Riverside. He holds a B.S. in Chemistry from Pacific Lutheran University (1967) and a Ph.D. from Cornell University (1970) where he was a student in the Department of Entomology and an NIEHS Trainee in Environmental Toxicology. He has held tenured academic

appointments at University of California, Davis (1971-1980) and in the Washington-Oregon-Idaho Regional Veterinary Medical Education Program (1981-1986) where he was Professor of Veterinary and Comparative Toxicology. In 1986 he became a staff toxicologist and later Branch Chief of Worker Health and Safety, California Department of Food and Agriculture (now California EPA). Krieger served two major Washington, D.C. consulting firms (1991-94) in exposure and risk assessment before returning to the University of California as an extension Toxicologist (1994-present) specializing in pesticide exposure assessment and worker health and safety. He has taught toxicology at both the undergraduate and graduate levels and received several teaching awards including the Society of Toxicology's Education Award.

He has organized and participated in numerous symposia of ACS, IUPAC, the Society of Toxicology, and other scientific societies, and authored/coauthored over 250 published papers, book chapters, and abstracts, including serving as editor for the comprehensive Handbook of Pesticide Toxicology, issued in 2001. He has trained a generation of environmental toxicology students who hold important positions in academia, government, and industry. Bob resides in Riverside, CA, with his wife Lee and son William.





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and

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Cordially invite you to attend a banquet in honor of the Winner of The Division's International Award for Research in Agrochemicals

Robert I. Krieger

Department of Entomology Personal Chemical Exposure Program University of California, Riverside

Time & Location: Monday March 14, 2005 6-9PM Tom Ham's Lighthouse Restaurant, San Diego

RSVP TO: Don Wauchope, (229) 386-3892, don@tifton.usda.gov Please indicate entrée selection 1. Filet of halibut 2. Chicken Florentine 3. 9 oz. Prime Rib

Details: Reception and Social Hour 6-7 (cash bar); Dinner 7-9 Price \$41.50 includes salad, entree and dessert plus soft drink, taxes and gratuity. Liquor or wine extra.

Directions to restaurant: Restaurant is at the western tip of Harbor Island. From the Convention Center head north on Harbor drive and follow towards the Airport. Turn left at Harbor *Island* Drive, and then right when you come to the water. Follow road to the circle at the end.



YOUNG SCIENTIST PRE- & POST-DOCTORAL RESEARCH AWARD & SYMPOSIUM



AGROCHEMICALS DIVISION with Sponsorship by Dow AgroSciences

The 2005 awardees highlighted below will present their work during the annual Young Scientists Recognition Symposium at the 229th ACS National Meetings in San Diego, CA. Their awards will be presented to them during the Agrochemicals Division social hour on Tuesday evening. The symposium will also feature presentations by 13 other outstanding graduate students and post-doctoral associates on Sunday morning starting at 9:00 AM in the Horton Grand Hotel. The speakers (and affiliations) include Luis Avila (Texas A&M), Johan Desaeger (Univ. of Georgia), Anubha Goel (Univ. of Maryland), Hope Harris (USDA-ARS, Oxford, MS), Michelle Hladik (Johns Hopkins), Kevin Kelley (Univ. of Illinois), Jianhang Lu (Univ. Calif.-Riverside), Konstantinos Makris (Univ. of Texas-San Antonio), Zachary Parisa (Mississippi State), Joshua Seil (Minot State Univ.), Steven Symington (Univ. Massachusetts), Jianguo Tan (Michigan State), Kelly Tindall (Louisiana State Univ.), Jason Woodward (Univ. of Georgia), and Xiaofei Zhang (Univ. Calif-Riverside). The presentations will include a wide diversity of topics (synthesis, environmental chemistry, pest control, toxicology) and cover all types of agrochemicals. Link to the national meetings website through the AGRO website at http://membership.acs.org/a/agro/ to view the Agrochemicals Division programming for San Diego and please plan to attend the symposium.

Michelle Hladik, runner-up winner for 2005, entered the paper *Occurrence and Treatment of Neutral Chloroacetamide Degradates in Midwestern U.S. Drinking Water*. Michelle conducted the research in the laboratory of Dr. Ann Roberts at Johns Hopkins University. Congratulations to Michelle and Dr. Roberts for important research that contributes to an extensive picture on a wide array of herbicide degradates that occur in drinking water supplies before and after treatment.

Jianguo Tan is the 2005 first-place winner with his entry *Decreased Nicotinic Sensitivity to Imidacloprid as a Resistance Mechanism in the Colorado Potato Beetle, Leptinotarsa decemlineata (Say).* Jianguo conducted his research in the lab of Dr. Robert Hollingworth at Michigan State University. Congratulations to Jianguo and Dr. Hollingworth for elucidating a new toxicodynamic mechanism that helps explain development of resistance to chloronicotinyl insecticides.

Awardees will receive a cash award, award plaques, and travel reimbursements to the San Diego meetings. All other presenters will receive a travel stipend from AGRO. The Agrochemicals Division would greatly appreciate your efforts to encourage students and post-doctoral research associates to apply for future award competitions. Further information about the Young Scientist Pre- and Post-Doctoral Research Award and application information for next year can be obtained from Dr. Allan Felsot at Washington State University (phone: 509-372-7365; fax: 372-7460; email: afelsot@tricity.wsu.edu) or by visiting the Division of Agrochemicals web site (http://membership.acs.org/a/agro/). Applications will be accepted until November 5, 2005 for consideration of the year 2006 award to be presented at the spring meeting of the American Chemical Society in Atlanta, Georgia, March 26-30, 2006.



YOUNG SCIENTIST PRE- & POST-DOCTORAL RESEARCH AWARD & SYMPOSIUM



AGROCHEMICALS DIVISION with Sponsorship by Dow AgroSciences Co-sponsored by the ACS Younger Chemists Committee 231st ACS NATIONAL MEETING, Atlanta, GA, March 26-30 2006

| Who is qualified to enter competition? Pre- & post-doctoral students Only work conducted primarily at U. S. institutions | Winner and runner-up will receive: Cash award (\$750 & \$500) and plaque Travel costs to meeting (up to \$600) Partial meeting per diem costs 3 years free AGRO membership |
|---|--|
| NAME | DATE |
| Current affiliation including address, phone & fax num | ber, and email: |
| Place where research was conducted if different from a | bove: |
| Date work was completed: D | ate of expected/actual degree: |
| Briefly describe your contribution to the work: | |
| | |
| SIGNATURES: Applicant | |
| Major Professor/Supervisor | |
| Will you present this paper even if you do not receive a | n award: YES NO |
| WITH THIS APPLICATION FORM INCLUDE TO 1. An extended abstract of your presentation (4 pages of describes the nature of the work (hypothesis, method) | |

- significance for the field of agrochemicals.
- 2. An abstract of 150 words (submit directly to <u>http://oasys.acs.org/oasys.htm</u>); this short abstract will be printed in the Agrochemicals Division biannual publication, PICROGRAM.

MAIL OR FAX THIS SIGNED APPLICATION, & FAX OR EMAIL EXTENDED ABSTRACT TO:

Dr. Allan Felsot, Washington State University, FEQL, 2710 University Dr., Richland, WA 99354 (Phone: 509-372-7365; Fax: 509-372-7460; email: afelsot@tricity.wsu.edu)

****Deadline for submittal of application materials:** November 5, 2005.

NOTE: Two awards will be made based on the merits of the submitted applications. Applicants not winning the awards will be invited to present their research in the Young Scientist's Recognition Symposium and will be eligible to receive a small travel grant.

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CALL FOR APPLICANTS AGROCHEMICAL EDVCATION AWARDS

FINANCIAL SUPPORT FOR GRADUATE STUDENT RESEARCH POSTER PRESENTATIONS NATIONAL AMERICAN CHEMICAL SOCIETY MEETING AUGUST 28 - SEPTEMBER 1, 2005

Graduate students conducting research related to agrochemicals (pesticides, pest management chemicals, fertilizers, livestock drugs, etc.) are invited to apply for competitive travel grants to present research posters at the 2005 American Chemical Society (ACS) Meeting in New York City. Each selected student will receive one year ACS membership and \$600 each to help defray travel costs. Posters will be displayed in a special section of the Agrochemical Division's Poster Session and at the ACS Sci-Mix. The first, second and third place winners will receive an additional cash award at the Agrochemical Division's Social Mixer. Potential areas of agrochemical related research include (but are not limited to): discovery, synthesis, metabolism, regulation, registration, biotechnology, delivery, risk assessment, resistance, residues, mode of action and/or environmental fate.

To apply, graduate students should submit the following by April 23, 2005:

- 1) Abstract and presenter information to the agrochemical division, graduate student research symposium at http://oasys.acs.org/oasys.htm If students are not selected for an award, they will have the opportunity to withdraw their abstract.
- 2) A two page extended abstract which includes an overview of the research justification, experimental approach, research findings and significance of findings. Please include phone, mailing address and e-mail.
- 3) A short letter of nomination from faculty advisor.

Items 2 and 3 should be submitted as MS Word or Word Perfect files to john.j.johnston@aphis.usda.gov To submit hard copies or for additional information, please contact Dr. John Johnston, USDA National Wildlife Research Center, 4101 LaPorte Ave, Fort Collins, CO 80521, 970-266-6082.

AWARDS COMMITTEE REPORT

Robert I. Krieger, Department of Entomological Sciences, University of California, Riverside will receive the International Award for Research in Agrochemicals at the San Diego ACS meeting. This Award is sponsored by BASF Corporation. The award presentation will take place first thing Monday morning, followed by a 2-day symposium on minimizing exposures and understanding risks in the use of pesticides organized by Nancy Ragsdale and Jim Seiber. Don Wauchope organized the award dinner, which will be held Monday evening. Don should be contacted for information/reservations for the dinner (don@tifton.usda.gov, 229-386-3892).

Janice Chambers, Mississippi State University, will receive the International Award for Research in Agrochemicals at the Fall ACS meeting, to be held in Washington, D.C. This Award is sponsored by DuPont Crop Protection. A symposium around the general topic of pesticide biochemistry and toxicology is being organized by Ernie Hodgson.

Nominations for the 2006 International Award for Research in Agrochemicals received prior to the December, 2004, deadline are currently being considered by the Awards Committee. The Awards Committee is accepting new awards nominations for the International Award for Research in Agrochemicals and for the Division Fellow Award. The nomination forms for both are found in the Picogram. Please consider nominating a deserving colleague. The deadline for the International Award is December 31, and for the Fellow Award is May 31 each year.

Respectfully submitted James N. Seiber, Chair AGRO Awards Committee January 10, 2004



PAST WINNERS OF THE ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS CO-SPONSORED BY BASF COMPANY (SPRING) AND DUPONT CROP PROTECTION (FALL)

| 1992-Fall | Dr. Bruce Hammock, Univ. of Calif., Davis, | 1999-Fall | Dr. James Seiber, University of Nevada, Reno |
|-------------|---|-------------|--|
| | CA | 2000-Spring | Dr. George P. Georghiou, University of |
| 1993-Spring | Dr.Morifuso Eto, Kyushu Univ., Fuoka, Japan | | California, Riverside |
| 1994-Fall | Dr. Toshio Fujita, Kyoto Univ. Kyoto, Japan | 2000-Fall | Dr. Herbert B. Scher, Zeneca |
| 1995-Spring | Dr. Mohyee Eldefrawi, U. Of Maryland, | 2001-Spring | Dr. Donald Crosby, University of California, |
| | Baltimore | | Davis |
| 1995-Fall | Dr. Koji Nakanishi, Columbia Univ., New | 2001-Fall | Dr. Ralph Mumma, Penn State |
| | York | 2002-Spring | Dr. Keith Solomon, University of Guelph, |
| 1996-Spring | Dr. Günther Voss, Ciba, Basel, Switzerland | | Ontario, Canada |
| 1996-Fall | Dr. Klaus Naumann, Bayer, Leverkusen, | 2002-Fall | Dr. Marinus Los, American Cyanamid |
| | Germany | 2003-Spring | Dr. Bob Hollingworth, Michigan State Univ |
| 1997-Spring | Dr. Fritz Führ, Jülich, Germany | 2003-Fall | Dr. Hideo Ohkawa, Kobe University, Japan |
| 1997-Fall | Dr. Izuru Yamamoto, Univ. of Tokyo, Japan | 2004-Spring | Dr. Stephen Duke, USDA-ARS, Oxford, MS |
| 1998-Spring | Dr. George Levitt, DuPont, Wilmington, DE | 2004-Fall | Dr. John Marshall Clark, University of |
| 1998-Fall | Dr. Leslie Crombie, Univ. of Nottingham, | | Massachusetts |
| | England | | |
| 1999-Spring | Dr. Don Baker, Zeneca, Richmond, CA | | |
| | | | |

PAST AWARDEES OF THE BURDICK AND JACKSON INTERNATIONAL AWARD:

- 1969 Prof. John E. Casida, University of California, Berkley, CA.
- 1970 Prof. Richard D. O'Brien, Cornell University, Ithaca, NY.
- 1971 Prof. Robert L. Metcalf, University of Illinois, Urbana, IL.
- 1972 Prof. Ralph L. Wain, Wye College, University of London, England
- 1973 Dr. Hubert Martin, British Crop Protection Council, England.
- 1974 Prof. T. Roy Fukuto, University of California, Riverside, CA.
- 1975 Dr. Michael Elliot, Rothamsted Experiment Station, England
- 1976 Dr. Morton Beroza, U.S.D.A.-A.R.S. (retired).
- 1977 Prof. Francis A. Gunther, University of California, Riverside, CA.
- 1978 Dr. Julius J. Menn, Stauffer Chemical, CA.
- 1979 Mr. Milton S. Schecter, U.S.D.A. (retired).

- 1980 Dr. Minuro Nakajima, Kyoto University, Kyoto, Japan.
- 1981 Dr. Philip C. Kearney, U.S.D.A., Beltsville, MD.
- 1982 Dr. Jack R. Plimmer, U.S.D.A., Beltsville, MD.
- 1983 Dr. Karl Heinz Buechel, Bayer AG, Germany.
- 1984 Dr, Jacques Jean Martel, Roussel Uclaf, Paris, France.
- 1985 Dr. Junshi Miyamoto, Sumitomo Chemical Co., Japan.
- 1986 Dr. James Tumlinson, U.S.D.A., Gainesville, FL.
- 1987 Prof. Fumio Matsumura, Michigan State U., East Lansing, MI.
- 1988 Dr. Ernest Hodgson, North Carolina State U., Raleigh, NC.
- 1989 Dr. Toshio Narahashi, Northwestern University, Chicago, IL.
- 1990 Dr. David Schooley, University of Nevada, Reno, NV.
- 1991 Dr. Stuart Frear, U.S.D.A. Fargo, ND.

PAST AWARDEES OF THE STERLING B. HENDRICKS MEMORIAL LECTURSHIP: SPONSORED BY USDA-ARS AND AGROCHEMICALS DIVISION

- 1981 Norman E. Borlaug, Nobel Laureate and Director of International Maize and Wheat Improvement Center, Mexico City.
- 1982 Warren L. Butler, Professor of Biology and Past Chairman, Biology Department, University of California at San Diego.
- 1983 Melvin Calvin, Nobel Laureate and University Professor of Chemistry, University of California at Berkeley.
- 1984 Frederick Ausubel, Professor of Genetics, Harvard Medical School and Massachusetts General Hospital.
- 1985 Alan Putnam, Professor, Department of Horticulture and Pesticide Research Center, Michigan State University.
- 1986 Ralph Hardy, President, Boyce Thompson Institute for Plant Sciences, Cornell University, and Deputy Chairman, BioTechnica International.
- 1987 Mary-Dell Chilton, Director of Biotechnology Research for Ciba-Geigy Corporation, Research Triangle Park, North Carolina.
- 1988 Bruce N. Ames, Chairman, Department of Biochemistry, University of California at Berkeley.
- 1989 Sanford A. Miller, University of Texas Health Science Center at San Antonio.
- 1990 Roy L. Whistler, Emeritus Professor of Purdue University.
- 1991 Peter S. Eagleson, Professor of Civil Engineering, Massachusetts Institute of Technology.

- 1992 John E. Casida, Professor of Chemistry and Toxicology, University of California at Berkeley.
- 1993 Philip H. Abelson, Deputy Editor, *Science*, and Scientific Advisor to AAAS.
- 1994 Wendell L. Roelofs, Liberty Hyde Bailey Professor of Insect Biochemistry, Cornell University.
- 1995 Winslow R. Briggs, Director Emeritus, Department of Plant Biology, Carnegie Institution of Washington.
- 1996 Hugh D. Sisler, Professor Emeritus, Department of Plant Biology, University of Maryland.
- 1997 Ernest Hodgson, Head, Department of Toxicology, North Carolina State University.
- 1998 Martin Beroza, Chief, Organic Chemicals Synthesis Laboratory, Agricultural Research Service.
- 1999 Bruce D. Hammock, Professor, Department of Entomology, University of California at Davis.
- 2000 William S. Bowers, Professor, Department of Entomology and Chemical Ecology at the University of Arizona.
- 2001 Malcolm Thompson, Research Chemist, USDA/ARS Beltsville, MD
- 2002 Ervin E. Leiner, Professor Emeritus, Biochemistry Department, University of Minnesota.
- 2003 Dr. Kriton Kleanthis Hatzios, VA Agric. Exper. Station
- 2004 Dr. Robert L. Buchanan, Food & Drug Administration

MESSAGE FROM THE PROGRAM CHAIR

Don Wauchope

The San Diego program is barely put to bed and the Washington DC program OASYS will open in a few weeks—not much time to catch our breath!

Here's the San Diego schedule:

| PROGRAM | ORGANIZER(S) | Sun | Mon | Tue | Wed | Thu |
|--|---|-------------|-------------|------------|----------|----------|
| AGRO Business Meeting | A. Felsot, A. Barefoot | 5-10 EVE | | | | |
| Young Scientist' Research Recognition Award Symposium | A. Felsot | AM PM | | | | |
| Robert Krieger ACS International Award for Research in Agrochemicals Symposium | N. Ragsdale, J. Seiber | | AM PM | AM | | |
| Organic Farming and Nutrients: Productivity, Value and Food Safety | W. Hall | | AM PM | | | |
| Award Symposium Dinner | D. Wauchope | | 6-8 EVE | | | |
| SCI-MIX | D. Wauchope | | 8-10 EVE | | | |
| Agricultural Chemistry in the Classroom: Solutions for Global Environmental Issues | Joint with CHED: at Holiday Inn on the Bay | | | PM | | |
| GENERAL POSTERS | D. Wauchope | | | PM | | |
| AGRO/AGFD SOCIAL | J. Jenkins | | | 6-8 EVE | | |
| Applications of Metabolomics in Agriculture | W. Ridley, J. Seiber | | | | AM PM | |
| Monitoring and Analysis of Agricultural Products Impacting Air, Water and Soil | W. Hall, W. Robarge | | | | AM | |
| GENERAL PAPERS | D. Wauchope | | | | PM | AM PM |

As Allan says, as usual we offer a heterogeneous (that is to say, multidisciplinary) collection of really interesting presentations and posters. Be sure to look through the titles in the GENERAL POSTERS and GENERAL PAPERS—there is a remarkable collection of intriguing items there!

The Young Scientists' Award Presentations include papers on pest control and toxicology, synthesis, and environmental Chemistry. The Krieger Award Symposium has three packed

sessions on exposure assessment, biomonitoring, environmental monitoring and mitigation. The FERT section has sessions on nutrients and organic farming, and a very timely session on atmospheric and soil monitoring technologies. Bill Ridley's "Metabolomics" symposium includes sessions on "Challenges of Metabolomics in agriculture" and "State of the science of Agricultural Metabolomics"—just look at the titles to see how broadly this new technology is already being applied in agriculture.

Finally, note that several of our AGRO folks are journeying over to the "Holiday Inn by the Bay" to take part in a Chemical Education Division Seminar "Agricultural Chemistry in the Classroom: Solutions for Global Environmental Issues" Check out the titles—hot topics! These should be very well attended, and offer a chance for AGRO to tell its story to an unusual audience.

My only regret is that, once again, the GENERAL PAPERS have been placed at the end of the week. This is a shame because these are where the new science comes from! The ACS rules for program scheduling just about require this for our smaller Spring program. HOWEVER: in Washington we have SIXTEEN specific symposia —probably thirty sessions—to schedule and obviously symposia are going to have to be scheduled on Sunday and Thursday. Any volunteers?



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AGRO CALL FOR PAPERS

230TH ACS NATIONAL MEETING WASHINGTON, DC, AUGUST 28-SEPTEMBER 1, 2005

We have sixteen specific symposia as well as general sessions planned for Washington, DC. See Calls for Papers elsewhere in this issue for some of these, but here is a complete listing.

This listing was constructed for *C&E NEWS's* Preliminary Program announcement and Call for Papers. WE ARE NOT LIMITED TO THESE SYMPOSIA—it is still possible to put another one together, but I need to hear from any prospective Organizers SOON.

Almost all of these Symposia will be listed as accepting "contributed papers" and Organizers are responsible for reviewing all submissions. If you are interested in volunteering a paper--or receiving an invitation-- CONTACT THE ORGANIZERS.

For general questions: call Don Wauchope, Program Chair, Southeast Watershed Research Laboratory, USDA-Agricultural Research Service, POB 748, Tifton, GA 31794, don@tifton.usda.gov, Phone: 229-386-3892 (Fax 229-386-7215)

(Q)SAR in Today's Agrochemistry Cosponsored with COMP

Organizer: Bob Clark, Tripos, Inc, 1699 S. Hanley Rd., St. Louis, MO 63144, bclark@tripos.com, Phone: 314-951-3365 (Fax 314-647-9241)

Agrochemical Education Awards For Graduate Student Travel: Research Poster Presentations

Organizer:John J. Johnston, Chemistry Project Leader, USDA/National Wildlife Research Center, 4101 LaPorte Avenue, Fort Collins, CO 80521, john.j.johnston@aphis.usda.gov, Phone: 970-266-6082 (Fax 970-266-6089)

Agrochemical Residue & Metabolism Chemistry

Organizers: Teresa A. Wehner, Pharmacokinetics & Drug Metabolism, Merial Ltd, 631 Route 1 South, North Brunswick, NJ 08902, teresa.wehner@merial.com, Phone: 732-729-5713 (Fax 732-729-5824); John J. Johnston, Chemistry Project Leader, USDA/National Wildlife Research Center, 4101 LaPorte Avenue, Fort Collins, CO 80521, john.j.johnston@aphis.usda.gov, Phone: 970-266-6082 (Fax 970-266-6089); David Smith, Biosciences Research Laboratory, USDA-ARS, P.O. Box 5674, University Station, Fargo, ND 58105, smithd@fargo.ars.usda.gov, Phone: 701-239-1238 (Fax (701) 239-1430)

Biochemical Toxicology of Agrochemicals: Symposium in Honor of Janice Chambers, ACS International Awardee for Research in Agrochemicals

Organizer: Ernest Hodgson, Department of Environmental and Molecular Toxicology, North Carolina State University, 850 Main Campus Drive, Raleigh, NC 27695, ernest_hodgson@ncsu.edu, Phone: 919-515-5295 (Fax 919-513-1012)

Control of Invasive Species: Regulatory Concerns and Achievements

Organizer: Anne Leslie, ARK Enterprises, Inc, 6024 Telegraph Rd, Alexandria, VA, VA 22310-2117, aleslieipm@aol.com, Phone: 703-960-0095

General Oral Presentations

Organizer: Don Wauchope (vide ante)

General Posters *Organizer*: Don Wauchope (*vide ante*)

Modern Chiral Pesticides: Enantioselectivity And Its Consequences

Organizers: Wayne Garrison, Ecosystems Research Division, US EPA, NERL, 960 College Station Road, Athens, GA 30605, garrison.wayne@epamail.epa.gov, Phone: (706)355-8219 (Fax (706)355-8202); Ron Williams, Syngenta Crop Protection, 410 Swing Road, Greensboro, NC 27409, ron.williams@syngenta.com, Phone: 336 632 7785

Organophosphate-Induced Chronic Neurotoxicity

Organizer: Mohamed B. Abou-Donia, Duke University Medical Center, Durham, NC 27710, donia@duke.edu, Phone: 919-684-2221 (Fax 919-681-8224)

Symposium: The Continuum of Biological Pest Control

Organizer: Paul L. Zubkoff, Biopesticides and Pollution Prevention Division 7511C, U.S. Environmental Protection Agency, 1200 Pensylvania Ave NW, Washington, DC 20460-0001, zubkoff.paul@epa.gov, Phone: 703-308-8694 (Fax 703-308-7026)

Synthesis of Agrochemicals: Good Ideas that Never Made it to Products

Organizers: John W. Lyga, Agricultural Products Group, FMC Corporation, P. O. Box 8, Princeton, NJ 08543, john_lyga@fmc.com, Phone: 609-951-3046 (Fax 609-951-3835); George Theodoridis, Agricultural Products Group, FMC Corporation, P.O. Box 8, Princeton, NJ 08543, george_theodoridis@fmc.com

Translation of Pesticidal Activity from Lab to Greenhouse to Field

Organizers: John W. Lyga, Agricultural Products Group, FMC Corporation, P. O. Box 8, Princeton, NJ 08543, john_lyga@fmc.com, Phone: 609-951-3046 (Fax 609-951-3835); George Theodoridis, Agricultural Products Group, FMC Corporation, P.O. Box 8, Princeton, NJ 08543, george_theodoridis@fmc.com

Turfgrass: Pesticide Exposure Assessment and Predictive Modelling Tools *Cosponsored with Turf Umbrella Workgroup*

Organizers: Mary Nett, Water Quality Consulting, 3360 Ash Hopper Lane, Colorado Springs, CO 80906, MNett_WQC@msn.com, Phone: 719-282-3113 (Fax 719-623-0559); Joseph H. Massey, Mississippi State University, Mississippi State, MS, jmassey@pss.msstate.edu, Phone: (Fax N/A); Mark Carroll, University of Maryland, College Park, MD, mc92@umail.umd.edu, Phone: (Fax N/A); Pamela J. Rice, USDA-Agricultural Research Service, St. Paul, MN, price@soils.umn.edu

Workshop: The Fate of Turfgrass Nutrients and Plant Protection Chemicals in the Urban Environment Cosponsored with RISE (Responsible Industry for a Sound Environment) Organizers: Mary Nett, Water Quality Consulting, 3360 Ash Hopper Lane, Colorado Springs, CO 80906, MNett_WQC@msn.com, Phone: 719-282-3113 (Fax 719-623-0559); Brian Horgan, University of Minnesota, St. Paul, MN, Bphorgan@umn.edu, Phone: (Fax N/A); A. Martin Petrovic, Cornell University, Ithaca, NY, AMP4@Cornell.edu, Phone: (Fax N/A); Jim Skillen, RISE, Washington, DC, jskillen@pestfacts.org

FERTILIZER (FERT) SUBDIVISION SYMPOSIA

Organizers:

Bill Hall, IMC Global, 3095 Country Road 640 West, Mulberry, FL 33860,
wlhall@imcglobal.com, Phone: 963-428-7161 (Fax 963-428-7398)
W. C. Herz, Scientific Programs, The Fertilizer Institute, 820 First Street, N.E, Washington, DC 20002, wcherz@tfi.org, Phone: 202-515-2706
Wayne P. Robarge, North Carolina State University, 3406 Williams Hall, Raleigh, NC 27695-

7619, wayne robarge@ncsu.edu Phone: 919-515-1454 (Fax 919-515-2167)

National/Regional Air Monitoring Programs Impacting Agriculture (Continued)

New Nutrient & Soil Amendment Products Impacting Agricultural Production & the Environment

Homeland Security & Agriculture: Managing Agricultural Inputs and Assuring Food Safety Cosponsored with AGFD

Water Quality Protection at the Watershed Scale: Monitoring & Trading, Are They Working? *Cosponsored with ENVR*

| Program Chair: | D. Wauchope | (229)-386-3892 | Biotechnology: | J. Seiber J. Nelson | (702)-784-6460 (301)-405-3919 |
|--------------------------------|-----------------|----------------|----------------|------------------------|----------------------------------|
| Vice Chair | L. McConnell | (301)-504-6298 | | W.P. Ridley | (314)-694-8441 |
| Synthesis-Special Topics | J. Fenyes | (901)-278-0330 | Resistance: | T.M. Brown | (803)-656-5038 |
| Standing Program: | D. Baker | (510)-231-1093 | | J. Nelson | (301)-405-3919 |
| Residues-Special Topics | J.J. Johnston | (970)-266-6082 | Toxicology: | J.M. Clark | (413)-545-1052 |
| Standing Program: | T.A. Wehner | (732)-729-5713 | | J. Coats | (515)-294-4776 |
| Metabolism-Special | H. Cutler | (770)-986-3240 | Regulation | N. Ragsdale | (301)-504-4509 |
| Topics | | | - | - | |
| Standing Program: | D. Smith | (701)-239-1238 | Special | J.M. Clark | (517)-545-1052 |
| | M.G. Beconi- | (616)-385-5597 | Conferences | | |
| | Barker | | | | |
| Analytical: | R. Grazzini | (841)-231-8032 | ACS Awards | J. Seiber | (510)-559-5600 |
| - | | | Symposia | | |
| Environmental | R. Honeycutt | (336)-294-5559 | | | |
| | J. Seiber | (702)-784-6460 | Young | A. Felsot | (509)-372-7365 |
| | A. Felsot | (509)-375-9365 | Scientists | | |
| | | | Award | | |
| Mode of Action | R. Hollingworth | (517)-533-9430 | | | |
| | J.M. Clark | (413)-545-1052 | | | |

AGROCHEMICALS DIVISION PROGRAMMING CONTACTS

FERTILIZER & SOIL CHEMISTRY SUBDIVISION NEWS

Have you thought about the FERTILIZER & SOIL CHEMISTRY subdivision lately? Do you know that your subdivision is becoming a leader in addressing critical issues such as perchlorate, agriculture and the environment; trace metals and sustainable agriculture; agriculture and air quality; homeland security? Do you know that your subdivision brings together regulatory agencies, stakeholders, and leaders in cutting edge science to discuss/debate issues of concern regarding the current and future use of fertilizers? Do you know that your subdivision is working to publish several of its symposiums on the above subjects? So, if you didn't know, now you do. Better still, why not actively support these efforts and become or renew (if it's been awhile) your membership, and then attend our sessions at the national meetings. Joining is easy (and inexpensive) - just check the appropriate box on the application form included with this issue of PICOGRAM and send it to the indicated address. Now that you have joined, get involved! We need your ideas, your leadership to help organize future symposiums. Our tentative schedule till Spring 2006 is listed below, but nothing after September 2005 is cast in stone. Have a more regional interest or issue you want to address? Great! We are searching for ways to have the subdivision more involved with regional ACS meetings, or other scientific societies. Your participation will make a difference. See you in San Diego!

Future subdivision activities and program topics are listed below: Metals Forum IV & ACS FERT Division Metals Analysis Workshop-Phoenix, AZ Feb. 23-25, 2005

229th Annual National Meeting- San Diego, CA, March 13-17, 2005

- National/Regional Air Monitoring Programs Impacting Agriculture
- Organic Farming and Nutrients Productivity, Value, and Food Safety (Joint with AGFD)
- Innovative Technologies for Production & Analysis of Specialty Fertilizers & Pesticides (Joint with AGRO)

FERT Division Metals Analysis Workshop- Raleigh, NC, Spring, 2005

230th - Washington, DC, August 28 - September 1, 2005

- National/Regional Air Monitoring Programs Impacting Agriculture Cont.
- Water Quality Protection at the Watershed Scale: Monitoring & Trading, Are They Working? (Joint with ENV)

- New Nutrient & Soil Amendment Products Impacting Agricultural Production & the Environment
- Homeland Security & Agriculture: Managing Agricultural Inputs and Assuring Food Safety (Joint with AGFD)

231st - Atlanta, GA, March 26-30, 2006

• Agriculture and Nutrient Recycling Technology – Efficiency, Necessity and Economics

- U.S. Fertilizer Production Challenges of Operating in a Global Marketplace
- Mineral Nutrition And Plant Disease Interactions And Effects
- Agriculture and Adjacent Ecosystems Can Both Be Protected? (Joint with ENV)

• New Techniques and Instrumentation Used In Fertilizer and Soil Analysis (Joint with ANYL)

232nd - San Francisco, CA, September 10-14, 2006

Open for suggestions

Take part in the revitalization of FERT division by joining our division and attending upcoming programs. Please let me, or any FERT officer listed below know how we can be more responsive to your needs.

| Wayne Robarge Subdivision Chair | Bill Herz Chair Elect/Program | Vice Chair | Herb McKinnon Secretary |
|--|---|---------------|--|
| wayne_robarge@ncsu.edu 919-515-1454 | Chair wcherz@tfi.org 202-515-2706 | Open | hmackin1@tampabay.rr.com 813-989-2267 |







THE CONTINUUM OF BIOLOGICAL PEST CONTROL

American Chemical Society 230th National Meeting Washington, DC August 28 - September 1, 2005

The Agrochemicals Division is pleased to sponsor a symposium addressing the scientific and regulatory issues pertaining to biological pest control.

The aim of this symposium is to provide a forum for chemists, biologists and others who participate in the development of pest control strategies that are alternatives to practices that may be deleterious to populations and/or the environment. Participation from industry, foundations, academia, civic organizations, and government agencies is encouraged.

Some suggested topics are:

Natural products as biopesticides Microbial biopesticides Plant incorporated protectants Pheromones Fermentation products

Presentations on applications (laboratory, greenhouse, field) and demonstration projects (public areas, parks, schools) are welcome.

To submit proposed papers or posters, please contact:

Paul L. Zubkoff
U.S. Environmental Protection Agency
Biopesticides and Pollution Prevention Division 7511C
1200 Pennsylvania Avenue NW, Washington DC 20460
703-308-8694 zubkoff.paul@epa.gov



CALL FOR PAPERS



AGRICULTURAL DISCOVERY SYMPOSIUM

American Chemical Society 230th National Meeting Washington, DC August 28 - September 1, 2005

Continuation of the Successful Agrochemical Symposium first presented at the Philadelphia ACS meeting in 2004 (see note below)

$\label{eq:constraint} \begin{array}{l} Topic \ 1-Translation \ of \ pesticidal \ activity \ from \ lab \ to \ greenhouse \ to \ field \end{array}$

Relevant papers would include chemistry, ADMET, biochemistry research, etc., leading to a better understanding of the issues involved with loss in activity going from lab assays to advanced testing in the greenhouse and field.

Topic 2 – Synthesis of Agrochemicals; Good ideas that never made it to products

Relevant papers would include any chemistry work done in the field of Agricultural Discovery that was based on a good hypothesis or lead but for one reason or another never made it. It could have stopped at any stage of optimization but should be complete enough to have tested the original idea or validated the initial lead activity.

The full day symposium will include oral papers, a poster session, and a panel discussion. If you are interested in leading or participating in the panel discussion contact the symposium organizers;

John W. Lyga (john_lyga@fmc.com) and George Theodoritis (george_theodoritis@fmc.com) ; FMC Agricultural Products Group, Discovery Research, P.O.Box 8, Princeton, New Jersey, 08543

(papers presented in this Symposium at both the Philadelphia and Washington meetings will be included in an ACS symposium series recently accepted for publication by ACS Books)







AGROCHEMICAL RESIDUE & METABOLISM CHEMISTRY

American Chemical Society 230th National Meeting Washington, DC August 28 - September 1, 2005

The Autumn 2005 Agrochemical Residue & Metabolism Chemistry Symposium will focus on the determination of agrochemicals (herbicides, insecticides, fertilizers, pheromones, livestock drugs, etc.), metabolites and degradation products in a wide variety of matrices. Presentations describing techniques, equipment, supplies, data analysis, etc. to improve method limits of detection, sample throughput, isolation, identification, etc. are especially welcome. Presentations describing the results of agrochemical metabolism, environmental fate or field residue studies are also encouraged. Oral presentations will be 20-25 minutes in length followed by a 5 to 10 minute period for questions, comments and discussion.

Abstracts should be submitted to the division of Agrochemicals, Agrochemical Residues and Metabolism at http://oasys.acs.org/oasys.htm no later than MAY 1st. For additional information contact:

Dr. John J. Johnston, USDA National Wildlife Research Center (970) 266-6082 email: john.j.johnston@aphis.usda.gov ,

Dr. David Smith, USDA/ARS Biosciences Research Laboratory, (701) 239-1238 email: smithd@fargo.ars.usda.gov

Dr. Teresa Wehner, Merial Ltd., (732) 729-5713 email: teresa.wehner@merial.com


CALL FOR PAPERS



MODERN CHIRAL PESTICIDES: ENANTIOSELECTIVITY AND ITS CONSEQUENCES

American Chemical Society 230th National Meeting Washington, DC August 28 - September 1, 2005

Purpose of Symposium: Many of the currently registered and developmental stage pesticides are chiral and exist as two (or more) enantiomers. Quite often, these enantiomers exhibit significant differences in biological activity towards the target species. In order to achieve the best possible level of environmental and human health protection, while also maintaining the desired crop protection benefits, the agrochemical industry has introduced a number of single- or enriched-enantiomer products. As advances in synthesis and purification have made such products economically feasible, reductions in pesticide use rates have been achieved while maintaining the desired level of efficacy. The goal of this symposium is the presentation of research on the development, registration, environmental impact, and use of single- or enriched-enantiomer pesticide products. Presentations on the benefits, economic drivers and regulatory factors governing the production and use of chiral pesticides are encouraged to provide relevant, societal context for the environmental assessments.

Possible Topics (although not limited to the following):

- * Methods for separation and analysis of enantiomers of pesticides in environmental samples
- * Occurrence of pesticide enantiomers in the environment and humans
- * Microbial degradation of pesticide enantiomers with emphasis on selectivity
- * Enantioselective effects of such pesticides on environmental species
- * Economic factors relating to the manufacture and use of single- or enriched-enantiomer pesticides
- * Regulatory assessment of single- and enriched-enantiomer pesticide products

For additional information contact the organizers:

Wayne Garrison, U.S.Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division, 960 College Station Rd., Athens, GA 30621. Phone: 706 355 8219; email: garrison.wayne@epa.gov

Ron Williams, Syngenta Crop Protection, 410 Swing Road, Greensboro, NC 27409, Phone: 336 632 7785 Email: ron.williams@syngenta.com





CALL FOR PAPERS

ADVANCES IN PESTICIDE ENVIRONMENTAL FATE AND EXPOSURE ASSESSMENTS

American Chemical Society 230th National Meeting Washington, DC August 28 - September 1, 2005

The Agrochemicals Division is pleased to sponsor a symposium addressing the advances made in assessment of pesticide environmental fate and exposure. The focus of this symposium is on advances in environmental fate research, data requirements, study designs, modeling, and monitoring that affect pesticide environmental risk assessments.

Some suggested topics are:

- **Data Requirements:** changes in regulatory requirements and evaluations to meet the objectives of environmental risk assessments, study guidelines, global guideline harmonization, minor-use product requirements, requirements by state regulatory agencies
- **Research on pesticide transformation:** degradation through hydrolysis, photolysis, metabolism in soil and aquatic systems, characterization and effect of biological activity in soil, kinetic analysis of degradation and dissipation rates, small scale outdoor studies, evaluation of major and relevant metabolites
- **Research on mobility and sorption:** model inputs, aged sorption, column leaching, lysimeters, field-scale experiments, run off
- Field Studies: study designs, use of data, comparisons of lab and field data, use of field data in aquatic and terrestrial risk assessments
- **Modeling:** drift models, scenario development, groundwater and aquatic exposure models, watershed models, tiered approach, comparison of US, EU and PMRA modeling approach, role of GIS in exposure assessment

To submit proposed papers or posters, please contact one of the co-organizers: Ellen Arthur, Bayer CropScience (ellen.arthur@bayercropscience.com; 913-433-5328); Patricia Rice, BASF Corporation (ricep@basf-corp.com; 919-547-2668); Pamela Rice, USDA-ARS (pamrice@umn.edu; 612-624-9210); Dan Dyer, Bayer CropScience; Aldos Barefoot, DuPont; K. Balu, Waterborne Environmental Inc.; Glenn Miller, University of Nevada.

(Abstracts should be submitted by April 1, 2005)

OFFICERS AND COMMITTEES OF THE DIVISION OF AGROCHEMICALS

AGRO Division Officers

Dr. Allan Felsot, **Division Chair** Dr. Donald Wauchope, **Program Chair** Dr. Laura L. McConnell, **Vice Chair** Dr. Aldos C. Barefoot, **Secretary**

Dr. Terry Spittler, **Treasurer**

Dr. Wayne Robarge, **Chair Elect** William Herz, **Vice Chair** Herb MacKinnon, **Secretary**

Phone (509) 372-7365

Fax 5 (509) 372-7460

(229) 386-3892 (229)-3 (301)-504-6298 (301)-5 (302)-451-5856 (302)-3

(229)-386-7215 (301)-504-5048 (302)-351-6656 (315) 787-2320 email

afelsot@tricity.wsu.edu

mcconnel@ba.ars.usda.gov

wayne robarge@ncsu.edu

hmackin1@tampabay.rr.com

aldos.c.barefoot@usa.dupont.com

don@tifton.usda.gov

tds2@cornell.edu

wcherz@tfi.org

Dr. Matthew Brooks

Dr. Marty Kovacs

Dr. Teresa Wehner

Dr. Paul Zubkoff

Dr. Ann Lemley

2005-2007

FERT Subdivision Officers

(919) 515-1454 (202) 515-2706 (813)-989-2267

(315) 787-2283

Executive Committee

2003-2005

Dr. Todd Anderson Dr. Kevin Armbrust Dr. Jeff Jenkins Dr. Laura McConnell Dr. Scott Senseman Dr. Luis Ruzo

2004-2007

Dr. Barrington Cross, Councilor Dr. Judd Nelson, Alt. Councilor Division Committees

Dr. Rodney Bennett, **Chair** Dr. Allan Felsot, **Co-Chair** Dr. Don Baker Dr. John M. Clark Dr. Joel Coats Dr. Barry Cross

Mr. William Hall, **Chair** Dr. Wayne Robarge Ms. Michelle Nutting

Dr. Jeanette Van Emon, **Chair** Dr. Jeff Jenkins

Dr. Randy Weintraub, **Co-Chair** Dr. Christopher Peterson, **Co-Chair** 2004-2006 Dr. Randy Weintraub Dr. Jeff Bloomquist Dr. John Clark Dr. Kenneth Racke Dr. Pamela Rice

Councilors

2005-2008 Dr. Joel Coats, Councilor Dr. Nancy Ragsdale, Alt. Councilor

AGRO Program Committee

(610) 878-6476 (610) 878-6475 (509) 372-7365 (509) 372-7460 Dr. Allan Felsot Dr. Rick Grazzini Dr. Robert Hollingworth Dr. Mark S. Lee rodney.bennett@cerexagri.com afelsot@tricity.wsu.edu Dr. Judd Nelson Dr. James Seiber Dr. David J. Smith

FERT Program Committee

(863)-428-7161 Dr. Gary Pierzynski Wlhall@imcglobal.com Mr. William Herz

Nominating Committee

(702)798-2154 (702)798-2243 Dr. Terry Spittler vanemon.jeanette@epa.gov

Membership Committee

610-878-6472 662-338-3104 610-878-6475 662-338-3101

randy.weintraub@cerexagri.com cjpeterson@fs.fed.us

/lhall@imcglobal.com

Dr. Barry Cross, Chair

Dr. Terry Spittler, Ex Officio Dr. Don Baker Dr. Ralph Mumma

Dr. James Seiber, Chair Dr. John Casida Dr. Bruce Hammock Dr. Robert Hollingworth Dr. Ralph Mumma

Dr. Laura McConnell, Chair Dr. Judd Nelson

Dr. Terry Spittler, Coffee Hour Dr. Aldos Barefoot, Social Hour Dr. Jeff Jenkins, Social Hour

Finance Committee

(814) 272-1039 (814) 272-1019 Dr. Willis Wheeler

bcross@weidel.com ROM1@psu.edu Dr. Willa Garner

Awards Committee

(510)-559-5600 jseiber@pw.usda.gov Dr. Ernest Hodgson Dr. Fritz Fuehr Dr. Jim Tumlinson Dr. Nancy Ragsdale Dr. Willis Wheeler Dr. Izuru Yamamoto

Publications Committee

(301)504-6298 (301)504-5048 Dr. Terry Spittler Dr. John Clark

mcconnel@ba.ars.usda.gov

Hospitality Committee

| (315) 787-2283 | (315) 787-2320 | tds2@cornell.edu |
|----------------|----------------|---------------------------------|
| (302)-451-5856 | (302)-451-5941 | aldos.c.barefoot@usa.dupont.com |
| (541)737-5993 | (541) 737-5001 | jeffrey.jenkins@orst.edu |

Special Committees

By-laws Committee (925) 254-108

Dr. Don Baker, Chair

Committee on Patron Relations

(510) 741-3000 (510) 741-3030 l.ruzo@ptrlwest.com

Dr. Luis Ruzo, Chair Mr. Paul Giesler

Dr. John M. Clark, Chair Dr. Robert Hollingworth

Future Special Conference Committee (413) 545-1052

Public Relations Committee

| Dr. Jeff Jenkins , Chair | (541) 737-5993 | (541) 737-5001 | jeffrey.jenkins@orst.edu | | | |
|--|---------------------|----------------|--------------------------------|--|--|--|
| Dr. James Seiber | Dr. Ann Lemley | | | | | |
| Education Committee | | | | | | |
| Dr. John Johnston, Chair | (970)266-6082 | (970)266-6089 | John.J.Johnston@aphis.usda.gov | | | |
| Dr. John Bourke, Investment | | | | | | |
| Coordinator | | | | | | |
| Dr. Allan S. Felsot, Young Scientist | (509)372-7365 | (509)372-7460 | afelsot@tricity.wsu.edu | | | |
| Recognition Coordinator | | | | | | |
| Dr. John M. Clark | Dr. Joel Coats | | Dr. Barry Cross | | | |
| Dr. Vincent Hebert | Dr. Ann Lemley | | Dr. Glenn Miller | | | |
| Dr. Judd O. Nelson | Dr. Jack R. Plimmer | | Dr. Nancy Ragsdale | | | |
| Dr. William Ridley | Dr. David Barneko | W | Dr. J. Harold Falls | | | |
| Long Range Planning Committee (Ad Hoc) | | | | | | |
| Dr. Don Wauchope | (229) 386-3892 | (229) 386-7215 | don@tifton.usda.gov | | | |
| Dr. Rod Bennett | Dr. Allan Felsot | | Dr. Dave Barnakow | | | |

MINUTES FROM THE AGROCHEMICAL DIVISION COMBINED GOVERNANCE MEETING ACS 228th ACS Annual Meeting - Philadelphia

ACS 228th ACS Annual Meeting - Philadelphia Sunday, August 22, 2004, 5:00 p.m. - 10:05 p.m. Chair, Agrochemicals Division – Rodney Bennett

Program Planning

Rod Bennett called the meeting to order at 5:00 pm. Members in attendance introduced themselves, and Rod passed around a sign up sheet. The sign-up sheet is retained in the archives. Rod asked for volunteers for the AGRO desk to answer questions about the division, sell books, and seek new members. The meeting continued with a presentation on programming.

Philadelphia Update - Allan Felsot

There are 159 papers & posters in 9 subject symposia with at least 2 sessions each. For comparison, there are 321 papers in Environmental Chemistry and 189 papers in Agricultural & Food Chemistry. The program includes the International Award Symposium in honor of John Clark, a standing symposium on "Agrochemical Residues & Metabolism", a general paper session (6 papers) and general poster session (30 posters). The Graduate Student Research Poster Competition has13 posters, and FERT organized a workshop onTrace Metal Analysis in Fertilizer. AGFD designated "Is Organic Food Healthier than Conventional Food" a symposium of interest, and ENVR designated

"Metals Contamination in Agricultural Products & Soils: Methodology, Monitoring, Regulation, and Remediation" and "Perchlorate Contamination and Remediation in Agricultural Products and Soils" as symposia of interest. The Sterling Hendricks Memorial Lectureship Award will be presented to R.L. Buchanan. The lecture is part of the AGFD symposium: Advances in Microbial Food Safety: New Challenges to Public Health from a Food Safety Perspective

San Diego Program - 229th ACS Natl Meeting, March 13-17, 2005 - Don Wauchope The International Award symposium for Bob Krieger will be part of a two day risk assessment symposium planned by Nancy Ragsdale, Jim Seiber, Rich Fenske, and A. Felsot. Will Ridley and Jim Seiber will organize a symposium on Metabolonomics (1 - 1.5 days). The program will include the Young Scientists Research Recognition Award Symposium, general papers and posters.

FERT Proposals

National/Regional Air Monitoring Programs Impacting Agriculture - Bill Hall, Wayne Robarge, Allan Felsot

Organic Farming & Nutrients--Productivity, Value & Food Safety - Bill Hall, joint with AGFD

Washington and Beyond - Allan Felsot, Don Wauchope, Bill Hall

Harmonization Issues in Regulation: Science & Global Politics Pest Management by Government Agencies Public Health Pest Control Issues – Paul Zubkoff Management of Contaminants in Public Water Supplies: Metals, Microbials, Agrochemicals Agrochemical Technology: What Will Be the State of the Art in 2015? Agrochemical Research, Extension & Education: Who will train the next generation? Environmental chemistry of chiral pesticides (Wayne Garrison) Turf Chemicals (2 symposia) Vertebrate Pest Control The role of Integrated Chemical Management in IPM: Antagonisms, Synergisms (Potentiation), & Resistance Management Forestry Pest Control & Management Chemicals Biotechnology's Next Generation of Crop Protection Characters Ten year retrospective on FQPA (during Washington DC 2005) Natural Plant Defenses

FERT Proposals for Washington

Assessing Effectiveness of Agricultural BMPs on Yields & the Environment Water Quality Protection at the Watershed Scale: Monitoring & Trading, Are They Working? New Nutrient & Soil Amendment Products Impacting Agricultural Production & the Environment Homeland Security & Agriculture: Managing Agricultural Inputs and Assuring Food Safety Bioavailability of Metals in Soil Workshop on Analysis of Metals

Atlanta

Issues in Sports Turf Management Future of Pest Control Cotton Production Fruit & Nuts Environmental Chemistry & Toxicology of Reduced Risk Pesticides Farewell Symposium for Methyl Bromide: Hello Replacements

Long Range Programming

Consumer exposure, Children's Health, Changes in pesticide use profiles, Stimulation of Pest Management Strategic Plans, Pest Control in Military Establishments/Areas, Emission from Ag facilities, Pest Control/Ag Issues by Tribes, Desperately Seeking Nothing (Analytical Detection at Ever Lower Levels--What Does It Mean?) Invasive Species (National Invasive Species Program)

Presentation by Bob Hausermann – ACS Books

Bob provided an update on the ACS books program. He noted that anything published by ACS must by copyrighted by ACS. A published pre-print cannot be published by a journal. ACS will begin asking OUP for a marketing plan for books. OUP publishes about 1000 books a year of which only 35 are ACS books. ACS also will ask for information on numbers sold, international sales and purchasers. Book chapters are not seen as cutting edge science and do not count as much as peer reviewed papers.

2006 IUPAC International Pesticide Congress and Other Special Programming John Clark reported that he had received one communication from the organizers and that plans were at an early stage.

Pan-Pacific Conference - 2004

John Clark reported that ACS Symposium Series had accepted both books from the conference for publication. Barry Cross discussed ACS support for the Pan-Pacific with Nancy Todd who indicated that ACS might be able to handle the conference in 2008. Barry will work on a proposal to submit to ACS. Barry noted that we will need an organizing committee and suggested adding a delegate from China.

<u>Mid-Atlantic Regional Meeting</u>, Rutgers, May 22-25, 2005, www.<u>marmacs</u>.org Rod Bennett proposed sponsoring the meeting and sending AGRO representatives. (See action under New Business)

Executive Committee

Update from the Chair

Rod gave a presentation to the Division Activity Committee on Saturday, August 21. He provided a brief history of the division, current membership status (see membership report), update on committee structure and membership and recent symposium topics. DAC noted that the division has been successful in its programming, symposia attract good audiences, and questioned by we continue to lose members. They suggested we look at ways to mold the division to attract more members. ACS is now willing to put more effort into small, special conferences. This may help the division with the Pan-Pacific Conference or retreats for programming planning.

The P2C2 conference will be October 3, 2004 in Charlotte and will focus on setting directions and planning. The merger with AICHE has been tabled. DAC asked for volunteers to join a liaison committee between local sections and national committees.

Secretary's Report - Aldos Barefoot

Al reported that he forwards membership lists for AGRO to membership chair and lists for FERT to subdivision officers. He worked with the membership chair to collect information from activity lists during the past two years. The secretary scheduled the business meeting and provided an agenda and announcement for distribution via the email list. He asked for reports in an electronic form prior to the meeting for display during the business meeting and to facilitate preparation of the minutes after the meeting.

Treasurer's Report - Terry Spittler

Terry provided a summary of the AGRO financial status. Assets have grown during the year as the stock market has recovered some of the ground lost in recent years. We continue to fund our activities from established income sources and are not relying on an endowment for operating expenses. Income from investments is used for educational grants.

Fertilizer Subdivision Report - Bill Hall, Herb MacKinnon

Bill reported that the FERT membership has stabilized. The sub-division applied for an ACS mini-grant to fund sponsorships at several conferences. FERT set up tables and booths as part of

the program to attract new members. FERT will publish three books from symposia organized for the Philadelphia meeting. They need a candidate for Chair after Wayne Robarge's term. The AGRO executive committee approved new officers for the subdivision as follows: Chair, Wayne Robarge; Vice-Chair, Bill Herz.

Councilor's Report - Joel Coats, Barry Cross

Electronic balloting is coming, but there are some difficulties. The M&E committee agreed to change the division annual report deadline. There is a new committee on ethics and new membership requirements for teachers. Grants for Academic Employment Initiative – none received by AGRO. There is a drive to consider offering membership to non-chemist scientists. There is some concern that it may be difficult to include non-chemist in ACS activities.

Membership Committee - Randy Weintraub, Chris Peterson

AGRO had a net loss of 102 members during 2003. The division lost 249 members and gained 147 new members for a 7% net loss. Chris sent questionnaires to all the people on the activity list to determine the reason people leave. Most people leaving AGRO leave ACS completely. The highest net losses are from industry, which accounts for 50% of the total net loss. Chris now sends welcome letters to ALL new members. Previously he had sent letters to people who sent in applications. He will need about 150 Picograms to send to new members. Chris proposed acknowledging new members in Picogram and putting membership applications of backs of symposium announcements. He suggested adding Fertilizers as a choice under "Major Interests" and increasing the visibility of "Free Fertilizer and Soil Science Subdivision Membership" on the application form.





** To April 30, 2004

Publications Committee - Laura McConnell

The PICOGRAM was successfully published for the Fall 2004 meeting with 6 half-page ads and 7 full-page ads. The Printing Center in Cornell, NY printed the PICOGRAM and mailed it out to our members. The full program with titles and abstracts was included again this issue, but the very large program required that some commonly included items were omitted (previous award recipient lists and ACS book titles and prices). The annual printing of the Division By-Laws was also included. The editor thanked Allan Felsot for proofing and editing the copy prior to submission to the printer and thanked the officers for updating the committee membership. Terry and Laura suggest that the program chair should be assigned to proofread the Picogram.

We are currently in negotiations with Washington State University web management group to take over responsibility for the AGRO website. The importance of our website is increasing each year, and improved functionality is required. This very large job should be handled by someone with excellent web design skills to reduce the amount of time involved in updating the web page. Allan's group will be able to handle this easily with minimal funding.

Jim Seiber reported that the number of manuscripts submitted to the Journal of Agricultural and Food Chemistry continues to increase. The number of agrochemicals papers is stable. The Journal needs reviewers. Don asked participants in the Watershed Modeling Symposium to submit papers to the Journal – eight papers will be submitted.

E-mail Communications System - Tim Ballard & Terry Spittler

Tim has taken over responsibility for the email system. He has located a programmer to work on a directory.

Awards Committee - Jim Seiber

BASF will sponsor the International Award for Bob Krieger in Spring 2005. DuPont will sponsor the International Award for Janice Chambers in Fall 2005. Don arranged the dinner for John Clark

Finance Committee - Barry Cross

Finances are stable. There will be more money from ACS and perhaps more money from books.

Hospitality Committee - David Smith, Jeff Jenkins

David has resigned from the committee. We need a replacement to organize the coffee fund. Six companies supported the coffee lounge in Philadelphia. Please take note of the sponsors listed on the board at the AGRO desk and thank them for their contributions. The Division Social Hour will be held on Tuesday, August 24, 2004 6-8 pm at the Courtyard Marriott.

Committee on Patron Relations (Luis Ruzo)

Luis reported that he has received contributions from 3 patrons and is not certain that others will continue to contribute.

Nominating Committee (Jeanette Van Emon (2005 election), Rodney Bennett (2006))

Jeanette informed us that our elections will be a bit late again this year. It has been difficult to find people willing to run for office.

Public Relations Committee - Jeff Jenkins

Press releases were sent to five news organizations to publicize the presentation of the International Award for Research in Agrochemicals to Dr. John Marshall Clark at the Philadelphia ACS meeting.

Don Wauchope suggested publicizing the graduate student awards by sending a press release to the ACS press office.

Education Committee - John Johnston

Graduate Research Poster Competition:

There were 13 entries for the Graduate Student Research Poster Competition.

John encouraged all members to interact with the students at the poster competition on Tuesday, the Sci Mix and the AGRO social. The next Graduate Student Research Poster Competition is scheduled for the Fall meeting in Washington, DC. The next Young Scientists Research Award will be presented at the March 13-17, 2005 meeting in San Diego. Applications should be sent to Allan Felsot by Nov. 1, 2004.

By-Laws Committee - Don Baker

Don continues to look for needed changes in the by-laws.

AGRO Division Procedures Manual - Nancy Ragsdale

The manual is in line for the next round of review. Don Wauchope will review it.

New Business

Allan Felsot proposed that AGRO contribute \$350 to the SETAC World Congress, which would allow us to set up a table and advertise our activities. Kevin Armbrust seconded the motion. The motion was amended to request a formal, written report from the AGRO representatives. The motion passed. Laura McConnell, Kevin, Allan and Joel Coats expressed interest in representing the division.

Rod Bennett proposed that AGRO contribute \$750 to the Mid-Atlantic regional meeting for a table. Al Barefoot seconded the motion. The motion passed.

Don Wauchope suggested that AGRO apply to ACS for funds to hold a retreate on programming and direction of the division. Rod Bennett moved that Don submit a grant request. Barry Cross seconded the motion, which passed unanimously.

Rod Bennett passed the gavel to Allan Felsot who takes over as Chair of the Division. Allan adjourned the meeting at 10:05 pm.

Respectfully submitted, Aldos C. Barefoot, Secretary

COUNCILOR REPORT ACS PHILADELPHIA 2004

ACS President Casey highlighted the accomplishments of the past year as the Academic Employment Initiative (AEI) in which over 120 candidates seeking faculty positions presented research posters at SCI-Mix and the presidential symposium on "the Changing Needs in Postdoctoral Education ". The importance of training scientists in biosciences materials science and nanoscience was emphasized. Related to this a Board Council Task Force on the Multidisciplinarity of chemistry will have recommendations by March 2005. Indeed, Madeline Jacobs ,ACS Executive CEO said "the challenge facing ACS today is to keep the core membership satisfied and to identify as quickly as possible a new value proposition for those ACS members of the future"

President Elect Bill Carroll's agenda for his term is via service, secondary education and chemical Enterprise in 2015 We learned that the ACS is planning for joint programs with AICHE as early as the Spring of 2006 in New Orleans.

In 2003 the ACS had a favorable budget variance of \$811,000, but still incurred a deficit of (\$64,000).

M&E reported that there were 14,189 attendees at the ACS Meeting in Anaheim, and at time of council meeting 13,805 were registered in Philadelphia. The advanced registration fee for 2005 will be \$295

A proposal for an ethics committee was voted on and recommended back to the Committee on Committees for further study

Council voted to accept three amendments to the ACS Constitution and Bylaws. Namely, a petition for electronic balloting, a petition to change divisions annual report date and a petition for the membership requirements for teachers.

ACS membership declined 1% as of June 30 2004

Of particular interest to our division was discussion about delays of visas to those seeking temporary visa to attend National Meetings. Program organizers will find a web site whose address is:

http://www.chemistry.org/portal/resources/ACS/ACSContent/international/visa app.doc In addition Kathleen Thompson ACS Staff will assist us if we have such problems. Parenthetically, our inability to get Chinese visas at the last Pan Pacific Conference in Hawaii detrimentally impacted on the number of speakers and attendees.

B.Cross

J.Coats

TREASURER'S REPORT

DIVISION OF AGROCHEMICALS - ACS ANNUAL MEETING, AUGUST 22, 2004 PHILADELPHIA

| DATE | 7/31/03 | 12/31/03 | 7/31/04 |
|-------------------------------|-----------|-----------|-----------|
| CHECKING ACCOUN T | \$ 33,453 | \$ 19,903 | \$ 31.856 |
| INVESTMENTS | | | |
| Spectrum Income (T. R. Price) | 158,577 | 171,247 | 172,999 |
| Prime Reserve (T. R. Price) | 30,884 | 30,952 | 16,015* |
| Educational Trust (Chase) | 345,783 | 392,028 | 394,441 |
| ACS Investment Pool | 17,141 | 18,905 | 19,391 |
| TOTAL INVESTMENTS | 557 385 | 613,132 | 604,847 |
| IOTAL INVESTIMENTS | 552,385 | 013,132 | 004,047 |
| TOTAL ASSETS | 585,838 | 633,035 | 636,703 |

*\$15,000 transferred to checking 5/04

Terry D Spittler - Treasurer

American Chemical Society DIVISION OF AGROCHEMICALS ABSTRACTS Final Program, 229th ACS National Meeting, in San Diego, CA, March 13-17, 2005 R. D. Wauchope, *Program Chair*

SOCIAL EVENTS: Award Banquet: Mon Social Hour: Tue

BUSINESS MEETING: Sun

SUNDAY MORNING Section A Horton Grand -- Regency B

Young Scientists Research Recognition Award Symposium Pest Control; Toxicology A. S. Felsot, *Organizer, Presiding*

8:55 — Introductory Remarks.

9:00—**1.** Drip fumigation for nematode control in multiple-cropped plasticulture vegetable systems. **J. A. Desaeger**

9:20—**2.** Effects of irrigation timing on the redistribution of fungicides applied to peanut foliage. **J. E. Woodward**, T. B. Brenneman

9:40 —3. Evaluation of the potential role of glufosinate-tolerant rice in integrated pest management strategies for rice water weevil. K. V. Tindall, M. J. Stout, B. J. Williams

10:00—**4.** Southern Pine Beetle over-wintering site detection by geo-referenced pheromone concentration analysis. **Z. A. Parisa**, W. E. Holmes, T. E. Nebeker

10:20 — Intermission.

10:40—**5.** Influence of moisture on the transferability and absorption of malathion. **X. Zhang**, R. I. Krieger

11:00—**6.** Comparative toxicity of commercially available pyrethroids at rat brain presynaptic nerve terminals. **S. B. Symington**, J. M. Clark

11:20—**7.** Decreased nicotinic sensitivity to imidacloprid as a resistance mechanism in the Colorado potato beetle, *Leptinotarsa decemlineata* (Say). **J. Tan**, D. Mota-Sanchez, V. L. Salgado, **R. M. Hollingworth**

11:40—**8.** Expression analysis of *GH3*, a gene induced in soybean leaves by plant growth regulator herbicides. **K. B. Kelley**, K. N. Lambert, A. G. Hager, D. E. Riechers

SUNDAY AFTERNOON

Section A Horton Grand -- Regency B

Young Scientists Research Recognition Award Symposium Synthesis; Environmental Chemistry

A. S. Felsot, Organizer, Presiding

1:30— Introductory Remarks.

1:35—**9.** Microwave assisted synthesis of novel formamide fungicides. M. M. Bobylev, **J. E.** Seil

1:55—**10.** Synthesis of quinolones with antimicrobial activity. **H. Harris**, K. M. Meepagala, D. E. Wedge, S. O. Duke

2:15—**11.** Quantification of polyacrylamide and evaluation of its environmental impacts. **J. Lu**, L. Wu

2:35—**12.** Phosphorus immobilization in micropores of drinking water treatment residuals: Implications for long-term stability. **K. C. Makris**, W. G. Harris, G. A. O'Connor, T. A. Obreza

2:55 — Intermission.

3:15—**13.** Imazethapyr photodegradation in rice paddy water. **L. A. Avila**, J. H. Massey, S. A. Senseman, K. L. Armbrust, S. Lancaster, G. N. McCauley, M. J. Chandler

3:35—**14.** Factors affecting the wet depositional flux of current use pesticides at a rural location on the Delmarva Peninsula. **A. Goel**, L. L. McConnell, A. Torrents

3:55—15. Occurrence and treatment of neutral chloroacetamide degradates in Midwestern U.S. drinking water. M. L. Hladik, E. J. Bouwer, A. L. Roberts

MONDAY MORNING

Section A Horton Grand -- Courtyard

ACS International Award for Research in Agrochemicals Sponsored by BASF Corporation: Symposium in Honor of Robert Krieger Award Session: Exposure Assessment

N. Ragsdale, Organizer J. N. Seiber, Organizer, Presiding

8:30 — Introductory Remarks.

8:45 —16. Chemical and pesticide exposures and a perspective on risk. R. I. Krieger

9:30—17. Pesticides in foods: Ensuring a safe food supply and promoting new pesticides within the context of international trade and new regulations. **B. J. Petersen**

10:00 — Intermission.

10:10 —18. Search for the causes of and solutions to worker reentry illnesses. H. N. Nigg

10:40—**19.** Cholinesterase assays as indicators of exposure. **B. W. Wilson**, J. D. Henderson, D. E. Arrieta

11:10 —20. In vivo percutaneous penetration in animal and man: Revelation and mystery. H. I. Maibach

11:40 —21. Testing for persistent organic pollutants in banked maternal serum specimens. W. M. Draper, J. Liang, M. Fowler, M. Kharrazi, P. Flessel, K. Perera

Section B Horton Grand -- Regency B

Organic Farming and Nutrients: Productivity, Value, and Food Safety B. Hall, *Organizer, Presiding*

8:30 — Introductory Remarks.

8:40—22. A critique of methodologies for the comparison of organic and conventional farming systems. **H. Lee**

9:10 —23. Release characteristics of organic and inorganic fertilizer nutrients. W. L. Hall Jr.

9:40—**24.** Estimating nitrogen availability from organic nutrient sources. **C. Cogger**, D. Sullivan, E. Gale, A. Bary, D. Hemphill

10:10 — Intermission.

10:30—**25.** Using vermicomposts in conventional and organic agricultural systems: Applications, markets, and regulations. **S. Subler**

11:00—**26.** Nutritional quality of crops grown with organic and conventional fertility management. **V. Worthington**

11:30—**27.** A two-year study of the effects of conventional and organic agriculture on quality and nutritive characteristics in tomatoes and peppers. **A. E. Mitchell**

MONDAY AFTERNOON

Section A Horton Grand -- Courtyard

ACS International Award for Research in Agrochemicals Sponsored by BASF Corporation: Symposium in Honor of Robert Krieger

Biomonitoring

J. N. Seiber, Organizer N. Ragsdale, Organizer, Presiding

1:30 — Introductory Remarks.

1:35—**28.** Indoor human Pyrethrins exposure: Contact, absorption, metabolism and urine biomonitoring. **S. Selim**, R. I. Krieger

2:00—**29.** Residential exposure to pesticides: Advances in exposure assessment and risk reduction. **R. A. Fenske**

2:25—**30.** Wet n' Wild: The influence of moisture on chemical transferability and human exposure. **R. L. Williams**

2:50 — Intermission.

3:05—**31.** Monitoring human exposure to pesticides using immunoassay. **S. J. Gee**, M. E. Koivunen, M. Nichkova, K. C. Ahn, D. Dosev, I. M. Kennedy, B. D. Hammock

3:30—**32.** Dosimetry and biomonitoring following golfer exposure to pesticides. **J. M. Clark**, R. A. Putnam

3:55 —**33.** Design and execution of a national study to monitor repeated measures of pesticide dose in turf applicators. **S. A. Harris**, K. A. Hurto, K. M. Wells, C. L. Forth

4:20—**34.** Measurement of pesticide exposure of suburban residents associated with the residential use of carbaryl. **C. Lunchick**, R. I. Krieger, F. Rice

Section B Horton Grand -- Regency B

Organic Farming and Nutrients: Productivity, Value, and Food Safety

B. Hall, Organizer B. Herz, Presiding

1:15 — Introductory Remarks.

1:20—**35.** Survey of perchlorate in leafy vegetables produced under conventional and organic systems in North America. **C. Sanchez**, J. Gibbs

1:50—**36.** Arsenic, poultry litter, and organic production regulations: A literature review. **B. C. Bellows**

2:20—**37.** Review of trace metal levels in organic and inorganic fertilizers. **W. L. Hall Jr.**, W. C. Herz

2:50 — Intermission.

3:10—**38.** A review of the process for evaluation and certification of inputs intended for use in the USDA National Organic Program. **A. B. Baker**

3:40—**39.** Exploring the limits of nitrogen percentages in composts and biofertilizers as measured by the US Composting Council's testing methods for determining stability and maturity values. **J. McNelly**

4:10—**40.** Regulatory aspects of organically derived nutrients. **M. Khosravifard MONDAY EVENING**

Section A Convention Center -- Sails Pavilion

Sci-Mix R. D. Wauchope, *Organizer*

8:00 - 10:00

49-50, 52-54, 56, 58-59, 61, 64-65, 68, 74, 77-78. See subsequent listings.

TUESDAY MORNING

Section A Horton Grand -- Courtyard

ACS International Award for Research in Agrochemicals Sponsored by BASF Corporation: Symposium in Honor of Robert Krieger

Environmental Measurements and Mitigation

N. Ragsdale, Organizer J. N. Seiber, Organizer, Presiding

8:45 — Introductory Remarks.

8:50 —41. Reducing spray drift to mitigate human exposure. D. K. Giles

9:15—**42.** Assessing exposure to agricultural fumigants in outdoor and indoor air environments. **J. E. Woodrow**, R. I. Krieger

9:40—**43.** Drift of insecticide residues from orchards: Empirical and modeling results for exposure assessment and risk management. **A. S. Felsot**

10:05 — Intermission.

10:20 — 44. Setting buffer zones for pesticide applications. T. A. Barry, B. R. Johnson, R. T. Segawa

10:45—**45.** Developing pesticide exposure mitigation strategies. **T. Thongsinthusak**, J. P. Frank

11:10—**46.** Integrated exposure analyses for pesticides: A retrospective. **D. J. H. Driver**, J. H. Ross

11:35 -47. A reality fix for risk managers. J. H. Ross, D. J. H. Driver

TUESDAY AFTERNOON

Section A Convention Center -- Hall D

General Poster Session R. D. Wauchope, *Organizer*

2:00 - 4:00

48. Synthesis and fungicidal activity of sulfonamide derivatives. **H. Takahashi**, T. Takeyama, T. Hamada, K. Yamagishi, M. Nishioka, H. Suzuki

49. A sustained-release, bio-absorbable, injectable gel formulation for delivery of doramectin to cattle for control of ticks and biting flies. **J. A. Klavons**, J. A. Miller, J. M. Pound, K. H. Lohmeyer

50. Thioacetals as novel inhibitors of Peptide Deformylase: Synthesis and data mining. M. H. Howard, **T. M. Cenizal**, R. Kucharczyk, S. Samajdar

51. Newly developed phenazine compounds may offer control of soil-borne plant pathogens. **D. Vukomanovic**

52. Decade of monitoring and studying the fate and transport of triazine herbicides in ground water and surface water. **E. A. Scribner**, E. M. Thurman, M. T. Meyer

53. Dialkylphosphates (DAPs) in fruit and vegetables confound biomonitoring in organophosphate risk assessment. **X. Zhang**, D. B. Barr, **J. H. Ross**, **R. I. Krieger**

54. Pesticide exposure assessment: Concurrent passive dosimetry and biological monitoring of triclopyr and 2,4-d exposures of a backpack applicator crew. **X. Zhang**, S. P. Acevedo, Y. Chao, T. M. Dinoff, R. L. Williams, R. I. Krieger

55. Pilot studies of indoor pyrethroid exposures of adults and their children using urine biomonitoring. **J. J. Keenan**, X. Zhang, G. Leng, R. I. Krieger

56. Reconnaissance data for glyphosate, other selected herbicides, and their degradation products in 51 streams in nine midwestern states, 2002. **E. A. Scribner**, W. A. Battaglin, M. T. Meyer

57. Concentration gradients of azinphos-methyl residues associated with spray drift and post-application volatilization at an apple orchard. **M. Tulio**, A. Felsot, Q. Macdonald

58. Evaluation of the stereoselectivity of fenthion sulfoxidation in fish. **O. Bawardi**, B. Furnes, D. Schlenk

59. Method development for pesticides analysis in breast milk using Stir Bar Sorptive Extraction

followed by TDU/GC/MS. B. A. Rocha-Gutierrez, W -Y. Lee

60. Allatotropin-increased biosynthesis of juvenile hormones (JH) from L-isoleucine and L-methionine by corpora allata of Manduca sexta. D. Schooley, **J. Seifert**

61. In vitro formation of guanosine adducts with pesticides. **D. W. Boerth**, M. Medeiros, D. Coulombe

62. Rice suspension cell culture as a tool for metabolism studies of non-radiolabelled penoxsulam and other N-triazolo[1, 5-c]pyrimidinylbenzene sulfonamides. **G. J. deBoer**, S. Thornburgh

63. Biocatalytic resolution of (RS)-HMPC acetate by immobilized Acinetobacter sp. cells expressing carboxylic esterase activity. **J -H. Xu**, Y. Chen, J. Pan

64. Cross-coupling reactions of 5- and 6-bromoquinazolin-2-ones: Synthesis of inhibitors of Peptide Deformylase. M. H. Howard, **T. M. Cenizal**, R. A. Coats, S. Samajdar

65. Detoxification of carbamate pesticides by halamine structures. **X. Fei**, T. Shibamoto, P. Gao, G. Sun

66. Evaluation of mutagenic activity caused by pesticides residues in corn, wheat, bean and chickpea by microsuspension in S. typhimurium TA98. **M. Aldana-Madrid**, N. Salazar-Lopez, F. Loarca-Piña, M. Silveira-Gramont

67. Study of organophosphate insecticides and biochemical indicators in blood and urine of urban adult males. **M. Aldana-Madrid**, E. Molina-Romo, G. Rodriguez-Olibarria, M. Silveira-Gramont

68. Application of a holistic approach in allelopathy research. **I. S. Fomsgaard**, P. Kudsk, E. Benfenati, S. Blümel, F. A. Macias, J. Fritz, D. Barcelo, O. Sakaliene, B. B. Mogensen, W. Oleszek, L. M. Hansen, S. K. Mathiassen, A. G. Mortensen, M. B. Gents, A. G. Understrup, S. T. Nielsen, S. S. Krogh, S. J. M. Mensz, T. Etzerodt, E. Lo Piparo, F. Fratev, T. Coja, J. Idinger, D. Chinchilla, D. Marin, J. M. G. Molinillo, A. Oliveros-Bastidas, A. M. Simonet, E. Eljarrat, L. Bonnington, M. Guillamon, M. Villagrasa, A. Taberner, T. Krongaard, J. Kus, S. Martyniuk, A. Stochmal

69. Modelling of degradation kinetics for the cereal allelochemical 2-benzoxazolinone (BOA) and its metabolites in soil. **A. G. Understrup**, S. Ravnskov, H. C. B. Hansen, I. S. Fomsgaard

70. Metolachlor, total coliforms and Escherichia coli dissipation in soil treated with biosolid. W. Mersie, **J. R. Moore**, C. G. McNamee, S. Pao, A. Atalay

71. Investigating the photostability of aphicidal benzamidazole and triazole analogs. **E. A. Bolessa**, S. D. Crawford, B. J. Dugan, J. W. Lyga, R. N. Henrie II, W. H. Yeager, Z. M. Elshenawy, H. R. Wendt, J. A. Argentine, D. M. Roush, F. J. Zawacki, W. D. Gravelle, L.

Varanyak, J. M. Willut, L. Dungan

72. Multiresidue analysis of seven anticoagulant rodenticides by LC/ES/MS/MS. L. J. Marek, W. C. Koskinen

73. Synthesis of conformationally restricted analogs of benzhydrolpiperidine and their insecticidal activity. **S. F. Ali**, I. R. Silverman, J. W. Lyga, L. LaFrance, K. G. Anouna

74. Improved synthesis of carbonated soybean oil in supercritical carbon dioxide. **K. M. Doll**, S. Z. Erhan

75. Pre-sowing irradiation of corn seeds. S. B. Karabaeva

76. The influence of mulching the soil with polyethylene film on agrochemical property of soil and chemical composition of tobacco. **T. C. Goziev**

77. Enzymatical hydrolysis investigation on the inclusion of chiral dichlorprop methyl ester in β -Cyclodextrins. Y. Wen, S. Zhou, **W. Liu**

78. Enantioselective degradations of (rac)-metolachlor and (s)-metolachlor in chinese soils. **W.** Liu, Y. Ma

79. Differential metabolism of benzhydrolpiperidines in the rat. **S. F. ElNaggar**, T. McLaughlin, R. W. Creekmore, R. Henrie, D. Wu, J. Wu

Agricultural Chemistry in the Classroom: Solutions for Global Environmental Issues *Cosponsored with CHED*

WEDNESDAY MORNING

Section A Horton Grand -- Courtyard

Applications of Metabolomics in Agriculture

Unique Challenges for Metabolomics in Agriculture J. N. Seiber, *Organizer* W. P. Ridley, *Organizer, Presiding*

8:30 — Introductory Remarks.

8:35—**80.** Integrated metabolite and transcript profiling for plant natural product pathway discovery and manipulation. **R. A. Dixon**, L. Achnine, B. Deavours, M. Farag, M. Naoumkina, L. W. Sumner

9:05—**81.** Potential and limitations of profiling methods for food safety assessment. **H. A. Kuiper**, E. J. Kok

9:35—**82.** Metabolic networks from Arabidopsis to woody plants ensure predictable orderedness in lignin/lignan/phenylpropanoid pathway metabolism. **N. G. Lewis**

10:05 — Intermission.

10:20 —83. Specialized metabolism in aromatic plants. D. R. Gang

10:50—**84.** Quantitating the natural variability in hybrid corn composition. **T. L. Reynolds**, J. Astwood, M. Nemeth, K. Glenn, W. Ridley

11:20 —85. Application of NMR-based metabolomics to environmental toxicology. **R. S.** Tjeerdema, M. R. Viant, C. A. Pincetich, E. R. Rosenblum

Section B Horton Grand -- Regency B

Local and Regional Monitoring and Analysis of Specialty and Agricultural Products Impacting Air, Water, and Soil

B. Hall, *Organizer* W. Robarge, *Presiding*

8:30 — Introductory Remarks.

8:35—**86.** Long term monitoring of ammonium in precipitation, the role of the National Atmospheric Deposition Network. **K. Karlin**, V. Bowersox, B. Larson

9:00—**87.** Monitoring atmospheric chemistry In an agricultural region using annular denuder technology. **W. Robarge**, J. Walker

9:25 —88. An assessment of ammonia emissions from alternative technologies for swine waste. W. Robarge, V. P. Aneja, P. Arya, L. Todd, K. Mottus

9:50—**89.** Determining ammonia dry deposition near a swine facility using low-cost passive samplers. **J. Walker**

10:15 — Intermission.

10:25—**90.** Regional off-target movement of auxin-type herbicides in the Pacific Northwest USA. **V. Hebert**, G. Amos, J. LePage, K. Holshue

10:50—**91.** Adaptation and application of LC/MS/MS in FMC's Environmental Sciences Laboratory. **A. W. Chen**

11:15—**92.** Environmentally friendly syntheses of pyridine mono- and dicarboxylic acids via permanganate oxidation. **Q. Zhang**, E. Meyer, M. W. Osborne, M. Marcenac

11:40—**93.** Desorption kinetics of chloroacetanilide and dinitroaniline herbicides from unsaturated soil in the presence of surfactants. **W. Yang**, B. A. Holmen

WEDNESDAY AFTERNOON

Section A Holiday Inn on the Bay -- Wicker

Applications of Metabolomics in Agriculture

State of the Science of Agricultural Metabolomics W. P. Ridley, *Organizer* J. N. Seiber, *Organizer, Presiding*

1:30 — Introductory Remarks.

1:35—**94.** Metabolomic assessment of a potato field trial: The metabolic composition of high fructan GM potatoes is equivalent to classic cultivars. **O. Fiehn**, J. Draper

2:05 —95. NMR profiling of transgenic peas. A. J. Charlton

2:35—**96.** Modification of potato alkaloids: A lesson in applied metabolomics. K. F. McCue, L. V. T. Shepherd, D. R. Rockhold, P. V. Allen, H. V. Davies, **W. R. Belknap**

3:05 — Intermission.

3:20—**97.** Application of metabolite profiling in rice. **K** -**H. Engel**, T. Frenzel, A. Miller, T. Frank, R. Roehlig

3:50—**98.** Natural variability of bioactive components in vegetable crops. **E. H. Jeffery**, J. A. Juvik

4:20 —99. Assessing metabolic health and dietary intervention. J. B. German

Section B Horton Grand -- Regency B

General Papers R. D. Wauchope, *Organizer* **1:30** — Introductory Remarks.

1:35—**100.** Knowledge of dynamic soil transformation processes: A key issue in the evaluation of defense properties of cereal benzoxazinoids. **I. S. Fomsgaard**, S. K. Mathiassen, P. Kudsk, A. G. Mortensen, C. Christophersen, T. Etzerodt, M. B. Gents, S. S. Krogh, S. J. M. Mensz, S. T. Nielsen, A. G. Understrup

2:00—**101.** Transport and degradation of glyphosate in a midwestern tile-drained watershed, Sugar Creek, Indiana. **M. Meyer**, J. W. Frey, E. A. Lee, K. Kuivila, M. Sandstrom

2:25—**102.** Assessing soil quality attributes by factor analysis with non-negativity constraints. **J. Lu**, L. Wu, A. C. Chang

2:50 — Intermission.

3:05 —103. Dissipation of thiobencarb and oxadiazon in soil. E. Hoque, R. M. Wilkins

3:30—**104.** Applying fluorescence spectra on identifying natural and man-made organic pollutants. **J -J. Horng**, C -L. Tang, B. H. Hsieh

THURSDAY MORNING

Section A Horton Grand -- Regency B

General Papers

R. D. Wauchope, *Organizer* K. M. Meepagala, *Presiding*

9:00 — Introductory Remarks.

9:05—105. Pharmacokinetics of intraruminally-dosed, 36Cl-labeled sodium chlorate in cattle. C. E. Oliver, D. J. Smith, R. C. Anderson, J. S. Caton

9:30—**106.** Residues and metabolism of 36Cl-labeled sodium chlorate in cattle. **D. J. Smith**, C. E. Oliver, R. C. Anderson, J. S. Caton

9:55—**107.** Development of a new method to quantify urinary concentrations of insecticides and herbicides in professional pesticide applicators. **F. Ciner**, T. R. Croley, S. A. Harris, C. D. Crawley

10:20 — Intermission.

10:35—**108.** Determination of urinary organophosphorus pesticide metabolites by automated solid phase extraction, post extraction derivatization, and GC-MS/MS. **G. K. H. De Alwis**, L. L. Needham, D. B. Barr

11:00—**109.** Surangin B: Interference with mitochondrial complex III and antifungal activity. **R. A. Nicholson**, Y. Deng

11:25—**110.** Evaluation of esterase activity for use in removal of pyrethroid-associated toxicity to Ceriodaphnia dubia and Hyalella azteca. **C. E. Wheelock**, J. L. Miller, M. Miller, B. M. Phillips, S. A. Huntley, S. Gee, R. S. Tjeerdema, B. D. Hammock

THURSDAY AFTERNOON

Section A Horton Grand -- Regency A

General Papers R. D. Wauchope, *Organizer* P. L. Zubkoff, *Presiding*

1:00 — Introductory Remarks.

1:05 —**111.** Natural products against Formosan Subterranean Termites (*Coptotermes Formosanus*). **K. M. Meepagala**, W. L. Osbrink, G. Sturtz, A. Lax, S. O. Duke

1:30 —112. Natural products as biopesticides: Botanical oils. P. L. Zubkoff

1:55 — Intermission.

2:10—**113.** Treatment of pesticide-contaminated soil with the ElectroChemical GeoOxidation process. **J. K. Wittle**, F. Doering

2:35—**114.** Novel formulations for control of immature mosquitoes. **R. Levy**, M. A. Nichols, W. R. Opp

3:00—**115.** Precision spray application for persistence and washoff studies of foliar pesticide residues: Method development. **R. D. Wauchope**, T. M. Webster, T. L. Potter, L. Wade

DIVISION OF AGROCHEMICALS

AGRO 1: Drip fumigation for nematode control in multiplecropped plasticulture vegetable systems

Johan AJ Desaeger, Department of Plant Pathology, University of Georgia, PO Box 748, Tifton, GA 31793, Fax: 229-386-7285, jdesaeger@tifton.uga.edu

Soil fumigation through drip irrigation systems is becoming a common practice among vegetable growers in the Southeastern US as a means to control soilborne pests and diseases. Most vegetable growers plant two to four crops on the same polyethylene mulch bed. Root-knot nematodes typically become a problem on second and later crops and practically can only be controlled by applying pre-plant pesticides through the drip tape. Metam sodium and emulsified 1,3-D + chloropicrin are the main fumigants that can be applied through the drip tape. Combinations of different fumigants (metam sodium + Telone) or of a fumigant + nematicide (oxamyl) significantly improved nematode control on a second crop, and increased yields from 20-75%. Drip fumigation also gave good control of root-knot nematodes on first crops, although phytotoxicity was a concern in spring. Plant-back periods in spring therefore may have to be extended to avoid plant damage.

AGRO 2: Effects of irrigation timing on the redistribution of fungicides applied to peanut foliage

Jason E. Woodward and Timothy B. Brenneman, Department of Plant Pathology, University of Georgia, Coastal Plain Experiment Station, 109 Plant Science Bldg, Tifton, GA 31793, Fax: 229-386-7285, jasonew@uga.edu

Studies in 2003 and 2004 compared the effects of irrigation timing on the redistribution of axozystrobin (Abound 2.08SC), flutolanil (Moncut 70 DF) and tebuconazole (Folicur 3.6F) on peanut. Irrigation (1.3 cm) was administered 0, 6, 12, 24, 48, and 96 hours after application, and non-irrigated plots served as controls. The design was a randomized complete block with seven replications. Foliar disease was significantly (P<0.05) higher for all fungicides for the 0 and 6 hour irrigation timings. A bioassay conducted on pods and leaves from three canopy levels showed a significant (P<0.05) increase in lesion area when irrigation was administered immediately after application. Pod colonization was less for all irrigation timings when compared to non-irrigated controls. Irrigation is required to maximize control of soilborne diseases; however, administering irrigation within 12 hours of fungicide applications may compromise foliar disease control.

AGRO 3: Evaluation of the potential role of glufosinate-tolerant rice in integrated pest management strategies for rice water weevil K.V. Tindall¹, M.J. Stout¹, and B.J. Williams², (1) Department of Entomology, LSU AgCenter, 402 Life Sciences Bldg, Baton Rouge, LA 70803, Fax: 318-435-2133, ktindall@agcenter.lsu.edu, (2) Northeast Research Station, LSU AgCenter

Glufosinate-tolerant rice with the genetic locus LLRICE62, was developed through recombinant DNA technology to be tolerant to glufosinate-ammonium via the insertion of the bialophos resistance (bar) gene. Glufosinate-tolerant technology can potentially affect management of the rice water weevil in three ways: by direct exposure of adults to glufosinate, indirectly through an herbicide-induced plant response, or indirectly by allowing floods to be delayed. Greenhouse studies were conducted to determine if glufosinate-treated and nontreated LLRICE62 rice were similar in their susceptibilities to infestations of rice water weevil. Additionally, the preference of rice water weevil adults for glufosinate-treated and non-treated LLRICE62 rice plants was examined. Direct toxicity of glufosinate to rice water weevil adults was also tested. Field experiments were conducted to examine effects of the use of glufosinate-tolerant technology on rice water weevils under field conditions. Currently, there are no data available examining how use of glufosinate-tolerant rice technology affects the most destructive insect pest of rice in the United States, the rice water weevil.

AGRO 4 : Southern Pine Beetle over-wintering site detection by geo-referenced pheromone concentration analysis Zachary A. Parisa¹, William E. Holmes², and T. E. Nebeker¹ (1)

Zachary A. Parisa', William E. Holmes', and T. E. Nebeker' (1) Department of Entomology, Mississippi State University, 157 Clay Lyle, MS State, MS 39769, Fax: 662-325-7807, zap2@msstate.edu, (2) Mississippi State Chemical Laboratory, Mississippi State University

This project tested the feasibility of locating southern pine beetle (SPB) over wintering spots by geo-referencing aggregation pheromone concentration levels throughout a forested environment. Research indicates that SPB populations are more susceptible to control methods during the late fall and winter months when beetles aggregate into densely populated over wintering spots. A method was developed using solid phase microextraction (SPME) combined with gas chromatography/ mass spectrometry (GC/MS). This method was used to detect and quantify beetle aggregation pheromones at locations in a pine forest during the fall months and through geostatistical analysis and identify the location of the pheromone source/ over wintering site. This method has proven capable of indicating with reasonable accuracy the source of pheromone emission.

AGRO 5: Influence of moisture on the transferability and absorption of malathion

Xiaofei Zhang and Robert I Krieger, Department of Entomology, Personal Chemical Exposure Program, University of California, Riverside, 900 University Ave, Riverside, CA 92521, Fax: 951-827-5803, zhangxiaofei@hotmail.com

In California, harvesting begins early in the morning when foliage is moist. We hypothesized that moisture might enhance the transferability of pesticides and influence harvester exposure. Twenty-four strawberry harvesters were randomly assigned to work either in the morning or afternoon in a malathion treated strawberry field followed by 2 days in untreated fields. This cycle was repeated two more times. Dislodgeable foliar residue (DFR), glove dosimetry, clothing dosimetry, and urine biomonitoring were performed. DFR decayed from 0.22 on Day 1 to 0.014 $\mu g/cm^2$ on Day 10 (T $_{1/2}$ = 52 h). Morning malathion sleeves residues were 4 to 9 times higher than afternoon residues. Glove residues were 3 to 12 times higher. Malathion biomarkers, however, were similar following AM or PM exposure. Therefore, foliage moisture increases malathion transferability but it was not associated with absorbed dose. These results weaken the association of passive dosimetry and biomonitoring in pesticide exposure assessment.

AGRO 6: Comparative toxicity of commercially available pyrethroids at rat brain presynaptic nerve terminals

Steven B Symington, Molecular and Cellular Biology Program, University of Massachusetts, 639 North Pleasant St., Morrill I, N418, Amherst, MA 01003, Fax: 413-577-4267, sbsyming@ent.umass.edu, and J. Marshall Clark, Department of Veterinary and Animal Sciences, University of Massachusetts

Published studies originally designed to assess the acute neurotoxicity of pyrethroids in mammals following intravenous administration are incomplete in regards to currently registered pyrethroids. There is evidence that other target sites, (voltage-sensitive calcium and chloride channels) may be involved with the development of the acute neurotoxic response. In this study, a comprehensive screen of commercially available pyrethroids on voltage-sensitive calcium channels was assessed using rat brain synaptosomes. The effects of these compounds on Ca²⁺ influx, membrane depolarization, and neurotransmitter release were determined using fluorescent assays for each of these endpoints. Our results indicate that a subset of the commercially available pyrethroids modify Ca²⁺ homeostasis and target voltage-sensitive calcium channels associated with the presynaptic nerve terminal, resulting in enhanced Ca2+ influx and neurotransmitter release. This intriguing observation opens up the possibility that the voltage-sensitive calcium channel may be target site for regulation by the EPA under the guidelines of the FQPA.

AGRO 7: Decreased nicotinic sensitivity to imidacloprid as a resistance mechanism in the Colorado potato beetle, *Leptinotarsa decemlineata* (Say)

Jianguo Tan¹, David Mota-Sanchez¹, Vincent L. Salgado², and Robert M. Hollingworth¹, (1) Department of Entomology and Center for Integrated Plant Systems, Michigan State University, 206 CIPS, East Lansing, MI 48824, Fax: 517-353-5598, tanj@msu.edu, rmholl@msu.edu, (2) Bayer CropScience AG

The development of resistance to imidacloprid (IMI) in eastern US populations of the Colorado potato beetle (CPB) threatens this critical use for neonicotinoid insecticides. Our previous pharmacokinetic studies with CPBs provided no explanation for the high resistance in adults (100-200-fold). IMI is toxic through effects on nicotinic acetylcholine receptors. We assessed the neural activity of IMI by recording spontaneous activity in the isolated central nervous system (CNS). The CNS from resistant CPBs required a 50-fold higher concentration of IMI to block spontaneous activity, indicating a probable change in the sensitivity of ne subtype of nicotinic receptor. Correspondingly, these insects show only a low level of resistance to nicotine and there were no differences in its neural effects between the two strains. This is the first report of nerve insensitivity as a mechanism of IMI-resistance in insects.

AGRO 8: Expression analysis of *GH3*, a gene induced in soybean leaves by plant growth regulator herbicides

Kevin B. Kelley, Kris N. Lambert, Aaron G. Hager, and Dean E. Riechers, Crop Sciences, University of Illinois, AW 101 Turner Hall, 1102 S. Goodwin Ave., Urbana, IL 61801, Fax: 217-333-5299, kelley@uiuc.edu

Symptoms resembling off-target plant growth regulator (PGR) herbicide injury are frequently found in soybean fields, but the causal agent is often difficult to identify. The expression of *GH3*, an auxin-regulated soybean gene, was quantified from soybean leaves injured by PGR and non-PGR herbicides using real-time RT-PCR to ascertain its suitability for detection of PGR herbicides as the cause of injury. *GH3* was highly induced by dicamba at 3 and 7 days after treatment (DAT), but induction was much lower at 17 DAT. *GH3* was also highly induced at 7 DAT by dicamba + diflufenzopyr, and to a lesser extent by clopyralid and 2,4-D. The non-PGR herbicides glyphosate, imazethapyr, and fomesafen did not induce *GH3* expression. GH3 protein expression in response to dicamba was also confirmed by immunoblotting. These results indicate that using the overexpression of auxin-responsive genes for detection of off-target PGR herbicide injury is feasible.

AGRO 9: Microwave assisted synthesis of novel formamide fungicides

Mikhail M. Bobylev and **Joshua E. Seil**, Department of Chemistry, Minot State University, 500 University Avenue West, Minot, ND 58707, Fax: 701-858-3163, mikhail.bobylev@minotstateu.edu, j_seil@hotmail.com

Formamides are a novel group of fungicides discovered by Bobylev et al. Some of these novel fungicides were obtained by reductive amination via Leuckart reaction, where formamide was used both as a reagent and a solvent. During the early development stage it was shown that the reaction proceeded at a reasonable rate only at the temperature range of 180-190°C, which corresponded to its vigorous boiling. Even at this elevated temperature the reaction required up to 1 hour to be completed. Temperatures higher than 190°C could not been used to accelerate the reaction because the reaction mixture quickly turned dark and a significant amount of tar formed. In this work, microwave assistance was investigated as a way to shorten the reaction time. It was found that the total time of the microwave assisted reaction was much shorter, typically about ten minutes, including the 30 seconds necessary to bring the reaction mixture to a boil. Microwave assisted Leuckart reaction appeared to be a fast and convenient procedure especially suitable for the preparation of a diverse series of analogs of novel formamide fungicides.

AGRO 10: Synthesis of quinolones with antimicrobial activity Hope Harris, United States Department of Agriculture, University of Mississippi, Natural Products Utilization Research Unit, Oxford, MS 38655, Kumudini M. Meepagala, USDA-ARS, Natural Product Utilization Research Unit, David E. Wedge, National Center for Natural Products Research, USDA-ARS, Natural Product Utilization Research Unit, and Stephen O. Duke, Natural Products Utilization Research Unit, US Department of Agriculture

The discovery of new antimicrobial agents that operate by a differing mode of action than that of existing antimicrobial agents while producing safer agrochemicals with less environmental and mammalian toxicity is of particular interest in agricultural research. Quinolones are antimicrobial agents effective in the treatment of some human illnesses; however, we found that several have significant antifungal activity against plant pathogenic fungi. These compounds inhibit DNA synthesis by promoting the cleavage of microbial DNA, resulting in rapid microbial death. Many plants belonging to the family Rutaceae contain diverse classes of secondary metabolites, including coumarins, flavanoids, furanocoumarins, and alkaloids. Two quinolone alkaloids (1-methyl-2-[6'-(3",4"-methylendioxyphenyl)hexyl]-4quinolone and 2-[4'-(3",4"methylenedioxyphenyl)butyl]-4-quinolone) were isolated from Ruta gravelones leaves which show promise as potential natural fungicides. After attempting several reaction schemes, the two quinolone alkaloids, as well as graveolin (1-methyl-2-phenyl-4-quinolone) and 1-methyl-2-(phenylmethyl)-quinolone, were successfully synthesized through an eight step process. The synthesized products were fungicidal in our bioassav.

AGRO 11: Quantification of polyacrylamide and evaluation of its environmental impacts

Jianhang Lu and Laosheng Wu, Department of Environmental Sciences, University of California-Riverside, 900 Univeristy Ave., Riverside, CA 92521, Fax: 951-827-3993, jianhang@ucr.edu

Polyacrylamide (PAM) treatment of irrigation water is a growing conservation technology in irrigated agriculture in recent years. With the increasing acceptance of this new technology, there is a need for methods to quantify PAM in soils and soil waters. In this work, a spectrophotometric method and a size exclusion chromatography method were developed to meet such a need. The spectrophotometric method was also further modified to be used for quantifying substrateborne PAM. By using these newly developed methods, several studies on the basic aspects of PAM application were carried out to assess the sorption and penetration of PAM in soils and the effects of PAM-use on sorption behaviors of herbicides. Results showed that: (1) PAM has very high sorption affinity on soils with its sorption isotherms being well described by the Langmuir equation; (2) PAM can penetrate into soils to a depth of 2-15 cm, deeper than it was commonly thought (1-2 mm of soil surface); and (3) PAM treatment can slightly slow down the sorption kinetics of herbicides, but has no significant effects on sorption amounts of herbicides.

AGRO 12: Phosphorus immobilization in micropores of drinking water treatment residuals: Implications for long-term stability Konstantinos C. Makris¹, Willie G. Harris², George A. O'Connor², and

Konstantinos C. Makris⁺, Willie G. Harris⁺, George A. O'Connor⁺, and Thomas A. Obreza², (1) Center for Water Research, University of Texas, San Antonio, 6900 N Loop 1604 W, San Antonio, TX 78249-0663, Fax: 210-458-5753, kcmakris@ufl.edu, (2) Soil and Water Science Department, Univ. of Florida

Drinking-water treatment residuals (WTRs) can immobilize excess soil phosphorus (P), but little is known about the long-term P retention by WTRs. To evaluate the long-term P sorption characteristics of one Feand one Al-based WTR, physicochemical properties pertinent to time-dependency and hysteresis of P sorption were assessed. Phosphorus sorption kinetics by the WTRs exhibited a slow phase that followed an initial rapid phase, as typically occurs with metal hydroxides. Phosphorus sorption maxima for both Fe- and Al-based WTRs exceeded 9,100 mg P kg⁻¹, and required a greater specific surface area (SSA) than would be available based on BET-N2 calculations. Electron microprobe analyses of cross-sectional, P-treated particles showed three-dimensional P sorption. Phosphorus-treated CO₂ SSAs were reduced by P treatment, suggesting P sorption by micropores (0.5-2 nm). Micropore-bound P should be stable and immobilized over long periods.

AGRO 13: Imazethapyr photodegradation in rice paddy water Luis A. Avila¹, Joseph H. Massey², Scott A. Senseman³, Kevin L. Armbrust⁴, Sarah Lancaster³, Garry N. McCauley⁵, and Mike J. Chandler³. (1) Soil and Crop Science, Texas A&M University, 2474, College Station, TX 77843-2474, lavila@ag.tamu.edu, (2) Mississippi State University, (3) Department of Soil and Crop Sciences, Texas Agricultural Experiment Station. Texas A&M University System, (4) Mississippi State Chemical Laboratory, Mississippi State University, (5) Texas Agricultural Experiment Station

With the introduction of imidazolinone tolerant rice varieties, imazethapyr has become a potential herbicide for red rice control in cultivated rice. Little is known about the behavior of this herbicide in the aquatic rice environment, particularly the effects of water quality. Since changes in turbidity, nutrients and other water quality parameters may affect the persistence of chemicals in an aquatic environment, data about imazethapyr dissipation in a rice field warrants further study. A laboratory experiment was conducted in 2004 to evaluate the photodegradation of imazethapyr in three rice paddy waters. Paddy water samples were collected from three locations, including Beaumont, TX (BM), Clarksdale, MS (CD) and Eagle Lake, TX (EL). Deionized water (DW) buffered at pH 7.0 was also included in the study as a control. All water samples were fortified with imazethapyr at 15 µg/ml and subjected to irradiation with UV lamps (100 W) for 0, 1, 2, 6, 12, 24, 48, 72 and 96 hours at 25°C in a growth chamber. The experiment was conducted as a randomized block design with four replications. To calculate half-life, for each water source the logarithm of the remaining herbicide concentration was plotted against time in hours. The slope of the line k (rate constant) was calculated using least square regression. Rate constants were compared between water samples using the Fisher's Protected LSD test at p≤0.05. The results showed that the halflife of imazethapyr was different among water samples. The order of imazethapyr photodegradation was DW = EL > BM = CD. Differences in degradation rates correlate well with the relative light attenuation of the water samples and to water pH.

AGRO 14: Factors affecting the wet depositional flux of current use pesticides at a rural location on the Delmarva Peninsula Anubha Goel, Department of Civil and Environmental Engineering, University of Maryland, 1173 Glenn L. Martin Hall, College Park, MD 20742, Fax: 301-504-5048, anubha@umd.edu, Laura L. McConnell, Agricultural Research Service, Environmental Quality Laboratory, U. S. Department of Agriculture, and Alba Torrents, Department of Civil and Environmental Engineering, University of Maryland College Park

Daily precipitation samples (204 samples from April-September, 2000-2003) were collected at a rural location on the Delmarva Peninsula, to study the effects of local agricultural activity and rainfall patterns on the wet deposition of pesticides used in this region. Of the three target compounds, chlorothalonil was the most frequently detected (in 90% of samples) followed by endosulfan (58%) and atrazine (49%). Concentrations and fluxes were typically high around application time. Endosulfan and chlorothalonil fluxes showed a significant positive correlation with sample volume (r = 0.42-0.46; α =0.05) whereas atrazine fluxes correlated with the frequency and timing of precipitation during corn planting. The nearby wetlands, which could be at risk from pesticide wet deposition, are more likely to receive the soluble herbicides in greater amount during rain events shortly after application. The more persistent insecticides and fungicides are likely to have a more diffuse and continuous deposition throughout the year.

AGRO 15: Occurrence and treatment of neutral chloroacetamide degradates in Midwestern U.S. drinking water

Michelle L. Hladik, Edward J. Bouwer, and A. Lynn Roberts, Department of Geography and Environmental Engineering, Johns Hopkins University, 3400 N Charles St., 313 Ames Hall, Baltimore, MD 21218

As some studies indicate that neutral chloroacetamide degradates can possess toxicity similar to the parent herbicides, their occurrence in drinking water supplies is of particular interest. Analyses of raw and finished drinking water samples obtained from 12 utilities in the Midwestern U.S. revealed 17 of 20 neutral degradates sought in the fall of 2003, and 19 of 20 neutral degradates in the spring of 2004. Median concentrations of neutral degradates in raw drinking water at both sampling periods were 10-100 ng/L; parent herbicide concentrations were 1-10 ng/L in the fall and 10-300 ng/L in the spring. Finished drinking water samples indicate little to no removal of the neutral degradates or parent herbicides in the fall, despite a diverse array of treatment processes. Finished drinking water samples in spring revealed significant average removals (~ 40%) of all neutral chloroacetamide degradates and parent herbicides in those treatment facilities that employed activated carbon.

AGRO 16: Chemical and pesticide exposures and a perspective on risk

Robert I. Krieger, Department of Entomology, Personal Chemical Exposure Program, Univ. California, Riverside, Citrus Ave, Riverside, CA 92521, Fax: 951-827-5803, bob.krieger@ucr.edu

Risk characterization is the latest means in product development and regulation to evaluate and regulate chemical technologies including pesticides. The strategy includes risk assessment, risk management, and risk communication-some collectively calls these processes "Risk Assessment." The process formalizes safety evaluations of food residues that have occurred for over 100 years, mixer/loader/applicator exposures during during the past 50 years, harvester field reentry during the past 30 years, and ever-present environmental residues since the general availability of gas liquid chromatography and other advanced techniques and publication of Silent Spring. Still more and more continues to be made of less and less since as analytical chemistry continues to record "findings" of trace analytes in diverse media-information that often exercises a strong role in defining the hazardousness of many aspects of modern life and public policy. Opinions vary, but fear (a real adverse effect) rather than confidence often comes from being better informed.

AGRO 17: Pesticides in foods: Ensuring a safe food supply and promoting new pesticides within the context of international trade and new regulations

Barbara J. Petersen, Exponent, Inc, 1730 Rhode Island Avenue, NW Suite 1100, Washington, DC 20036, Fax: 202-293-5377, bpetersen@exponent.com

Strategies have arisen for addressing the regulatory issues that arise with new types of pesticide chemistry, new forms of pesticides (including plant incorporated pesticides) and international trade in foods and pesticides. This paper will present a brief history of the risk assessment of pesticides and then explore in depth the current national methods for conducting refined risk assessments and new statistical tools that are being tested in the U.S. and Europe. The types of risk assessments that are needed for the final stage of tolerance reassessment under FQPA will be reviewed along with new methods and data that are needed to comply with the statute. The specific issues associated with conducting risk assessments for biotechnology derived pesticides will include case examples. The implications of the "vanishing" zero in terms of residues levels will also be discussed.

AGRO 18: Search for the causes of and solutions to worker reentry illnesses

Herbert N. Nigg, Citrus Research and Education Center, University of Florida, 700 Experiment Station Road, Lake Alfred, FL 33850, Fax: 863-956-4631, hnn@crec.ifas.ufl.edu

Worker reentry illnesses in the United States began after World War II when the use of the organophosphorus pesticides became widespread in agriculture. Early worker illnesses were related to the improper manufacture of these compounds but, in general, worker reentry illnesses were new and mysterious. The primary cause of worker reentry illnesses was discovered through science and intuition. This discovery led to research into the environmental chemistry of pesticides, work practices, dermal penetration of chemicals, field collection techniques and transfer mechanisms, culminating in the Worker Protection Standards and the Pesticide Handler Database. The history of this process, the political maneuvering, the players involved and the research they conducted are reviewed.



AGRO 19: Cholinesterase assays as indicators of exposure Barry W. Wilson, John D. Henderson, and Daniel E. Arrieta, Departments of Environmental Toxicology & Animal Science, University of California, 1 Shields Ave, Davis, CA 95616, Fax: 530-752-3394, bwwilson@ucdavis.edu

Red blood cell and serum acetvlcholinesterase and non-specific cholinesterase activities of humans and other animals are common surrogates for estimating the activity levels of the enzymes in brain and muscle of vertebrates and invertebrates. Such cholinesterase assays have been used to assess exposures to organophosphate and organocarbamate pesticides, chemical warfare agents and pharmaceuticals for many years utilizing colorimetric reagents, changes in pH and other stoichiometric methodologies. Recently, attention has been called to the lack of optimization of several common commercial methods resulting in steps to standardize the methods used to assess blood cholinesterases in California and other states. This paper compares methods of assessing blood cholinesterase levels used by commercial laboratories, the Department of Defense and research laboratories, illustrated with data from our own program. Advantages and disadvantages of ways to assess exposure to pesticides (such as blood cholinesterase methods, direct residue determinations and urinary metabolites) are presented. Although California and Washington are the only states currently requiring monitoring of occupational exposure to anticholinergic agents, the threat of chemical terrorism is leading to interest in establishing a national standard for clinical laboratories and the Department of Defense. Progress towards determining a normal human range of blood cholinesterases convertible between colorimetric and delta pH methods will be presented.

AGRO 20: In vivo percutaneous penetration in animal and man: Revelation and mystery

Howard I. Maibach, Department of Dermatology, University of California, San Francisco, 90 Medical Center Way, Surge Building, Room 110, Box 0989, San Francisco, CA 94143, Fax: 415-753-5304, himjlm@itsa.ucsf.edu

This presentation emphasizes clinical relevant issues requiring resolution:

•Local effects vs. blood and extracuteneous organ levels;

•Explanation of interindividual penetration differences in terms of new insights into s.c. structure and function;

 Advances in analytic chemistry permitting clinical resolution of previously unresolvable issues;

•In vivo assays in man – with direct readout.

AGRO 21: Testing for persistent organic pollutants in banked maternal serum specimens

William M. Draper, Jennifer Liang, Mary Fowler, Martin Kharrazi, Peter Flessel, and Kusum Perera, Sanitation and Radiation Laboratory, California Department of Health Services, 2151 Berkeley Way, Berkeley, CA 94704, Fax: 510-540-2053, wdraper@dhs.ca.gov

Human blood sera from the California Maternal Serum Expanded Alpha-Fetoprotein (XAFP) prenatal screening program were analyzed for persistent organic pollutants (POPs) in a pilot biomonitoring study. POPs, including DDT compounds, chlorobiphenyls (CBs) and brominated diphenyl ethers (BDE), were determined in the one to two mL specimens using a dual capillary column gas chromatographyelectron capture detector (GC-ECD) method developed for the study. Twenty-six target compounds were determined including 6 DDT compounds, 15 CB and 5 BDE congeners, BDE-47, -100, -99, -154, and -153. Analyses of a human serum standard reference material (SRM) established the method accuracy of 115 to 126% for 4,4'-DDE, 4,4'-DDT and the principal CBs (CB-138, -153, -170, -180, -187) at concentrations ranging from 0.09 and 6.6 ng/mL. Background correction was required, but only for CBs which averaged 546 pg s-CB (sum of congeners)/mL in reagent blanks. Among 40 XAFP specimens accessioned between May and June, 2002 in three southern California counties, 4,4'-DDE was detected in all with a range of 0.17 to 8.9 ng/mL -- 4,4'-DDT was detected in only two subjects. 2,2',4,4'-Tetrabromodiphenyl ether (BDE-47) was found in 55% of serum specimens, but only two maternal sera had elevated BDE consisting of

BDE-47, BDE-100, and BDE-153, and s-BDE of 1.4 and 1.9 ng/mL. This study demonstrates that chemical analysis of environmental contaminants in banked XAFP specimens is technically feasible. Chemical analysis of these specimens could provide chemical exposure information in population-based studies.

AGRO 22: A critique of methodologies for the comparison of organic and conventional farming systems

Howard Lee, Hadlow College, Hadlow, Tonbridge, Kent TN11 0AL, United Kingdom, Howard.Lee@hadlow.ac.uk

The development of organic production systems in many parts of the world is an encouraging move towards more sustainable methods of food production. However, farmers and other stakeholders in the broader agricultural sector continue to demand objective and quantitative assessments of organic against conventional agriculture. It seems clear that the further development of organic farming will be assisted by such comparisons. But, how might organic farming be fairly, accurately and usefully compared with other production systems? This review critically assesses what has already been achieved and what might yet be done. Conclusions are that classic experimentation has a valuable part to play but that more qualitative assessment can also be useful and should be encouraged. Careful allowance should be made for major background differences in management when comparing, for example, financial profitability. Longer-term case studies, which try to monitor organic systems in their own right, should also be considered.

AGRO 23: Release characteristics of organic and inorganic fertilizer nutrients

William L. Hall Jr., Mosaic Phosphates, 3095 County Road 640 West, Mulberry, FL 33860, Bill.Hall@mosaicco.com

There are many sources of slow release nutrients in today's marketplace. As pressures increase to better manage fertility, the demand for slow release materials is likely to increase. These new materials will include recycled nitrogen, phosphate and other nutrients derived from manures, biosolids and composted wastes. Measurement of the slow release characteristics of such materials is therefore needed. Application of techniques to compare organic and inorganic sources of nutrients is examined. A nutrient release profile is generated by a procedure accelerating the natural release mechanism of most commercial materials and analyzing the extract by traditional methods. Since nitrogen and phosphate are the nutrients most commonly named as causes of degradation of water bodies in the US, these nutrients need the most effective management. The new procedure will allow manufacturers and regulators to assess the impact of these nutrients, and make quick judgments of their effectiveness.

AGRO 24: Estimating nitrogen availability from organic nutrient sources

Craig Cogger¹, Dan Sullivan², Eric Gale², Andy Bary¹, and Del Hemphill², (1) 7612 Pioneer Way East, Washington State University, Puyallup, WA 98371-4998, cogger@wsu.edu, (2) Oregon State University

Applying agronomic rates of organic nutrient sources is a challenge, because N availability varies widely, depending on the nutrient source and the environment. Field studies, lab incubations, and modeling were done to improve our estimates of N availability from a variety of organic amendments used by Northwest farmers. We evaluated 15 types of amendments, including composted and uncomposted poultry, dairy, and rabbit manures, and yard debris, along with other commercial and agricultural materials. Amendment C:N ratios ranged from 4:1 to 27:1 and first-year plant available N (PAN) ranged from –6 to 99% of total N. Amendments with C:N ratio >15:1 generally had <10% PAN, and would not be economical as sources of nitrogen. PAN increased linearly as C:N ratio decreased below 15:1. Lab incubations coupled with modeling predicted field results well (Model PAN = 1.06 * Field PAN +8.4, r^2 =0.74).

AGRO 25: Using vermicomposts in conventional and organic agricultural systems: Applications, markets, and regulations Scott Subler, Restoration Soil & Research Inc, 204 E. Calder Way, Suite 201, State College, PA 16801, Fax: 814-235-1629, ssubler@restorationsoil.com

Vermicomposts are stabilized organic materials produced by processing agricultural, domestic, or industrial organic wastes using composting worms. Recently, technologies have been developed to produce large commercial scale vermicomposts. Although vermicomposts are similar to composts in physicochemical characteristics, including nutrient and organic matter contents; they differ as a class from composts in several important ways impacting their use in conventional and organic soil fertility programs. They may be used as primary or supplemental nutrient sources in organic production systems. However, due to their unique microbiological activity, they may also be used in both systems to modify soil macroand micro-nutrient availability, increase nutrient efficiency, induce plant growth and immune responses through physiological mechanisms, promote soil aggregation, suppress plant pests and diseases, and promote the biodegradation of soil contaminants. Finding a good fit for vermicomposts regulatory frameworks, given their recent appearance in commercial agriculture and their multiple benefits, represents a significant challenge.

AGRO 26: Nutritional quality of crops grown with organic and conventional fertility management

Virginia Worthington, Nutrikinetics, 1900 L Street Northwest, Washington, DC 20036, nutrikin@sprynet.com

In the last 60 years, more than 40 studies have compared the nutrient content of crops grown using organic versus conventional fertility management. A review of these studies shows that organic and conventional crops differ with regard to nutrient content at least for some frequently studied nutrients. Specifically, organically fertilized crops had higher levels of vitamin C, magnesium, phosphorus and iron and lower levels of nitrates than comparable crops grown with conventional fertilizers. There was also a trend toward a lower protein content but better protein quality in organic versus conventionally fertilized crops. Furthermore, there was another trend showing higher concentrations of nutritionally significant minerals and lower concentrations of heavy metals in organically versus conventionally fertilized crops. The plant physiology and soil dynamics that would explain these findings are known. Differences in nutrient content could have significant public health consequences.

AGRO 27: A two-year study of the effects of conventional and organic agriculture on quality and nutritive characteristics in tomatoes and peppers

Alyson E. Mitchell, 106 Food Science and Technology, University of California, Davis, One Shields Avenue, Davis, CA 95616-8869, aemitchell@ucdavis.edu

Consumer awareness of the relationship between foods and health, together with environmental concerns, has led to an increased demand for organically produced foods. However, controversy remains regarding whether or not organic foods have a nutritional advantage as compared to their conventionally produced counterparts. Growth conditions such as soil minerals, water, light, as well as pressure from insects or microorganisms, can affect nutritionally relevant plant constituents. Organic produce may experience higher levels of plant stress, and reduced N availability, which may result in increased levels of defense-related secondary metabolites. In an on-going 3 year study, levels of ascorbic acid, total phenolics (TP), percentage of soluble solids, and the phenolic antioxidants quercetin, luteolin and kaempferol are being measured in tomatoes (Lycopersicon esculentum sp. Burbank and Ropreco) and peppers (Capsicum annuum sp. California Wonder sp. Excaliber) grown under defined organic and conventional conditions. To date, results demonstrate significantly higher levels of quercetin, TP, ascorbic acid and percent soluble solids in organic tomatoes.

AGRO 28: Indoor human pyrethrins exposure: Contact, absorption, metabolism and urine biomonitoring Sami Selim, Golden Pacific Laboratories, 4720 W Jenniffer Av, Fresno, CA 93722, Fax: 559-275-1810, sselim@gplabs.com, and Robert I. Krieger, Department of Entomology, University of California, Riverside

Naturally occurring pyrethrins (PY) are frequently formulated with piperonyl butoxide (PBO) and MGK 264 to enhance the activity of the insecticides. Products containing PY PBO and MGK 264 range from human pediculocides, to total release foggers, carpet sprays, and application to food crops. Because dermal contact and incidental ingestion are likely exposure pathways there is an interest in evaluating exposure to PY/PBO/MGK 264 from non-dietary, residential uses. This included the measurement of exposure to people who performed structured activities (Jazzercise™) on surfaces that have been treated with the pesticides. A critical part of this study is the concurrent measurement of surface levels of pesticide and biomonitoring of absorbed dose or other index of systemic exposure . Toward that goal, a dermal absorption study in normal male volunteers using ¹⁴C PI, the predominant isomer in PY, was initially performed. The dermal absorption was determined to be 0.22%. An oral administration of ¹⁴C PI was then conducted to identify and quantify the human biomarker, chrysanthemum dicarboxilic acid (CDCA) and to determine the relationship between the concentration of the biomarker in the urine and exposure to PI. A Jazzercise study on carpet was conducted following the use of total release foggers containing PY/PBO/MGK 264. Subjects wore whole body dosimeters or bathing suits during the exposure period. Samples including urine were collected and analyzed for PY/PBO/MGK 264 and urinary biomarker for PY (CDCA). Participants in whole body suits excreted 1.62 µg CDCA during a 5-day period, and those who wore swim suits excreted 13.7 µg CDCA. The exposure potential of PY foggers is well below levels of health or regulatory concern.

AGRO 29: Residential exposure to pesticides: Advances in exposure assessment and risk reduction

Richard A. Fenske, Environmental and Occupational Health Sciences, University of Washington, Health Sciences Bldg., F-233, Seattle, WA 98195, Fax: 206-616-2687, rfenske@u.washington.edu

Accurate assessments of human exposures following residential pesticide applications represent a challenge for exposure analysis. Exposure studies have relied on measurements of environmental pesticide concentrations, contact with pesticide residues during scripted activity scenarios, and pesticide metabolites in urine, or some combination of these approaches. This presentation provides a critical examination of the development of exposure assessment methods for several key residential exposure scenarios, noting advances in air, surface wipe, and biological sampling, as well as in our understanding of children's activities. Observational studies using biological measurements may reduce uncertainties in aggregate exposure estimates, but can also raise ethical concerns regarding the purposeful exposure of children to potentially hazardous levels of toxic chemicals. Recent actions to reduce risks have included regulatory decisions, voluntary withdrawal of product registrations, and application of the precautionary principle in environments such as public schools. Recommendations for improved exposure and risk reduction strategies will conclude the presentation.

AGRO 30: Wet n' Wild: The influence of moisture on chemical transferability and human exposure

Ryan L. Williams, Product Safety, Environmental and Regulatory Compliance, Clorox Services Company, 7200 Johnson Drive, Pleasanton, CA 94588, Fax: 925-425-4496, ryan.williams@clorox.com

Chemicals are frequently used to control insect pests in agricultural and urban environments. The identification and evaluation of potential determinants of human exposure are critical to conduct reliable and responsible human exposure assessments following chemical applications. Moisture has been evaluated as a potential determinant of exposure in a series of experimental studies. Evaluation of the influence of moisture on pesticide transferability and potential human exposure followed a residential application of chlorpyrifos (CP) and two subsequent water-only applications (24 and 48 hours) made to nylon carpet. Total chemical residue remained a stable source of CP, while transferable chemical residue measured using the California roller (Ross et al., 1991) declined rapidly following the CP and two water-only applications. The decline in transferable chemical residue correlated significantly with the percent carpet moisture. The effect of sweat on dermal absorption was evaluated in vitro using penetration-evaporation cells to measure percutaneous absorption. Cells received artificial sweat or were left "dry" prior to application of ¹⁴C-CP-treated carpet fiber. Sweat did not increase percutaneous absorption, but resulted in more radiolabel recovered after 24 hours from the epidermis and tape stripping the skin surface. The effect of sweat on absorbed dose in humans was evaluated with human volunteers that participated in a structured activity program (SAP). Participants (n = 20) performed a warm-up exercise to induce light sweating prior to a SAP on CP-treated nylon carpet (Ross et al., 1990; Krieger et al., 2001). Absorbed daily dosages (ADDs) were calculated using urinary biomonitoring of trichloropyridinol. Participation in the warm-up exercise prior to the exposure SAP resulted in an increased ADD of CP equivalents by approximately 50%. These measured ADD values were less than estimates of ADD made from CP deposition, the California roller, and clothing dosimeters worn by participants.

AGRO 31: Monitoring human exposure to pesticides using immunoassay

Shirley J. Gee1, Marja E. Koivunen¹, Mikaela Nichkova¹, Ki Chang Ahn¹, Dosi Dosev², Ian M. Kennedy², and Bruce D. Hammock¹, (1) Department of Entomology, University of California, Davis, 1 Shields Avenue, Davis, CA 95616, Fax: 530-752-1537, sjgee@ucdavis.edu, (2) Department of Mechanical and Aeronautical Engineering, University of California, Davis

To assess risk from exposure to pesticides it is imperative to measure the internal exposure and to determine the relationship between the internal exposure and potential health effects. One method for exposure assessment is to measure the amount of pesticide or pesticide metabolites in body fluids such as blood, urine and saliva. Comprehensive studies involving hundreds of samples result in high cost and time consuming analysis. One alternative analytical method for biomonitoring studies is immunoassay. Used extensively in clinical diagnostics, immunoassays are sensitive, selective and well suited to measurement in biological fluids. Recently conducted biomonitoring studies for paraquat and atrazine will be used to illustrate the strengths and weaknesses of the immunochemical method. Higher throughput and greater sensitivity are goals toward improving the utility of immunoassays for large-scale monitoring studies. Lanthanide oxide nanoparticles are promising fluorophores in biochemistry because of their large Stokes shift, sharp emission spectra, long lifetime and lack of photobleaching. The use of these nanoparticles in a multiplexed assay and for visualizing protein micropatterns as well as other strategies such as the adaptation of pesticide metabolite assays to an autoanalyzer using chemiluminescent acridinium labels and development of flow-through systems will also be presented.

AGRO 32: Dosimetry and biomonitoring following golfer exposure to pesticides

John M. Clark, Department of Veterinary & Animal Science, University of Massachusetts, N311 Morrill 1 Science Center, Amherst, MA 01003, Fax: 413-577-4267, jclark@ent.umass.edu, and Raymond A. Putnam, Environmental Toxicology and Risk Assessment Program, University of Massachusetts

Accurate assessment of exposure to golfers requires knowledge of the availability of pesticide residues following application, transfer and absorption processes of these residues, as well as major routes of entry into the body. Our past research used dislodgeable foliar and airborne pesticide residues to estimate pesticide exposure to golfers. This approach resulted in a highly useful screening tool to eliminate from further study any exposure scenarios that were deemed safe using USEPA Hazard Quotient criteria. Our research has established that there are airborne and dislodgeable foliar residues available for golfer exposure, and that not all of these exposures can be deemed "safe" using the USEPA Hazard Quotient (HQ). The present research

emphasizes dosimetry (measuring pesticide residues on cotton suits, gloves, and air samplers worn by golfers) and biomonitoring (measuring pesticide metabolites in urine of golfers) in conjunction with environmental monitoring to determine transfer and penetration factors. Three widely used insecticides, chlorpyrifos, cyfluthrin, and carbaryl were evaluated in over 150 rounds of golf. In all cases, exposure to these insecticides under worst case scenarios were significantly less than established acceptable daily dose (ADI) and OPP reference dose (RfD) criteria. These already low exposures were successfully mitigated using several management strategies.

AGRO 33: Design and execution of a national study to monitor repeated measures of pesticide dose in turf applicators

Shelley A. Harris¹, Kirk A. Hurto², Kristen M. Wells³, and Chris L. Forth², (1) Center for Environmental Studies & Department of Epidemiology and Community Health, Virginia Commonwealth University, Life Sciences Building, 1000 West Cary Street, Room 107, Richmond, VA 23248-3050, Fax: 804-828-1622, saharris@vcu.edu, (2) TruGreen Chemlawn, (3) Center for Environmental Studies, Virginia Commonwealth University

Epidemiologic studies designed to evaluate the effects of commonly used turf pesticides have limited power to detect health risks and may be subject to bias from exposure measurement error. To increase the accuracy and precision of dose estimation for both risk assessment and epidemiologic research, valid models must be developed. Further, repeated measures of exposures over time are necessary to estimate both inter- and intra-individual variation. To address some of these issues, a national study of TruGreen Chemlawn workers was initiated in 2003. The pilot study, conducted in Richmond, Virginia, collected 19 days of 24-hour urine samples from 20 individuals. In 2004, urine samples were collected from approximately 100 volunteers in the spring, summer and fall, from 5 locations across the country. The design of this study, the selection of pesticides, urine sampling methodology, and national locations, and preliminary questionnaire results will be described.

AGRO 34: Measurement of pesticide exposure of suburban residents associated with the residential use of carbaryl Curt Lunchick, Product Safety Management, Bayer CropScience, 2 T.W. Alexander Drive, Research Triangle Park, NC 27709, curt.lunchick@bayercropscience.com, Robert I. Krieger, Department of Entomology, University of California, Riverside, and Fred Rice, ABC Laboratories

The purpose of this study was to characterize the potential absorbed doses of carbaryl to homeowners and residents during and following the residential application of carbaryl by measuring 1-naphthol metabolite levels in the applicator, spouse, and children of representative families that use pesticides. Non-professional adult and child volunteers were used to measure carbaryl absorbed doses during and after application of Sevin GardenTech Ready-To-Spray, a formulation of carbaryl. Ten families were monitored in Missouri and 13 families were monitored in California. Activities outside the residence in or near the treated areas for the applicator, spouse, and children were monitored on the day of application (Day 0), and days 1 to 3 postapplication. Urine samples were collected from participants beginning two days before the application through three days after application. Each urine sample was a 24-hour composite, resulting in six 24-hour urine samples from each participant. Pre-application levels of 1naphthol, corrected to carbaryl, ranged from 0.005 µg/kg to 12.5 µg/kg among the study participants. For the Missouri sites, the mean carbaryl dose was 19 µg/kg in applicators. Daily carbaryl dose levels ranged from 0.005 to 4.9 µg/kg in spouses, 0.005 to 61 µg/kg in children age 4 - 12 years, and 0.25 to 12.6 µg/kg in children age 13 - 17 years. For the California sites, the mean carbary dose was 6.2 µg/kg in applicators. Daily carbaryl dose levels ranged from 0.005 to 8.2 in spouses, 0.005 to 12.6 µg/kg in other adult residents, 0.005 to 446 µg/kg in children age 4 - 12 years, and 0.005 to 58 µg/kg in children age 13 - 17 years.



AGRO 35: Survey of perchlorate in leafy vegetables produced under conventional and organic systems in North America Charles Sanchez and John Gibbs, University of Arizona, Tucson, AZ 85721, sanchez@Ag.arizona.edu

Trace levels of perchlorate have been found in lettuce (Lactuca sativa L.) irrigated with Colorado River water. Recently a North American survey to evaluate the occurrence of perchlorate in leafy vegetables produced outside the Lower Colorado River region was conducted. Conventionally and organically produced lettuce and other leafy vegetable samples were collected from fields and farmers markets in California, New Mexico, Colorado, Michigan, Ohio, New York, Quebec, and New Jersey. Samples were shipped to our laboratory on dry ice and kept frozen until freeze-dried. Samples were prepared by grinding and hot water extraction, then analyzed by ion chromatography. Results show 17% of the conventionally produced samples and 31% of the organically produced samples had quantifiable levels of perchlorate. Most samples were collected from areas with no known contamination from munitions or aerospace related industries. Additional work is needed to identify possible anthropogenic and natural sources of perchlorate entering the food chain.

AGRO 36: Arsenic, poultry litter, and organic production regulations: A literature review

Barbara C. Bellows, P.O. Box 3838, National Center for Appropriate Technology, Butte, MT 59702, barbarab@ncat.org

Most of the arsenic used as an antibiotic in commercial broiler production ends up in the litter. Using this litter as a soil amendment is not prohibited by the National Organic Program, but µ205.203(c) of the Rule requires that "the producer must manage plant and animal materials to maintain or improve soil organic matter content in a manner that does not contribute to contamination of crops, soil, or water by plant nutrients, pathogenic organisms, heavy metals, or residues of prohibited substances." A comprehensive literature of poultry litter practices in organic agriculture and arsenic reactions in soil environments indicates that poultry litter applied at agronomic levels, using good soil conservation practices, generally will not raise arsenic concentrations sufficiently over background levels. However, recent studies show that more than 70% of the arsenic in uncovered piles of poultry litter can be dissolved by rainfall and potentially leach into lakes or streams.

AGRO 37: Review of trace metal levels in organic and inorganic fertilizers

William L. Hall Jr., Mosaic Phosphates, 3095 County Road 640 West, Mulberry, FL 33860, Bill.Hall@mosaicco.com, and W. C. Herz, Scientific Programs, The Fertilizer Institute

Trace metal levels of materials applied to soils is a health and ecological concern. The possibility of trace metals in organic materials such as manures, biosolids and compost exists due to the recycling and concentration of the nutrients in these products. Additionally, recycling and addition or contamination of trace metals can take place in inorganic mineral fertilizers. Recently a survey of trace metals monitoring programs of the state regulatory programs in the US was conducted. The data and results of this survey will compare the trace metals in both organic and inorganic products to assess their relative safety and compliance to regulatory limits. Statistical evaluations will be used to assess the relative confidence and ability of the monitoring data to be used for regulatory purposes. As new methodologies are developed to analyze and monitor metal levels in the future, the current data can serve as a baseline for future comparisons.

AGRO 38: A review of the process for evaluation and certification of inputs intended for use in the USDA National Organic Program AM Brian Baker, OMRI, Box 11558, Eugene, OR 97440, Fax: 541-343-8971, bb@omri.org

The Organic Materials Review Institute (OMRI) is an independent reviewer of products intended for use in certified organic production, handling, and processing. OMRI provides guidance on the suitability of material inputs under the USDA National Organic Program (NOP) standards. The process of evaluation, suitability and certification will be presented with details on the procedures for application, evaluation, and approval. Products that apply for certification are evaluated and classified, then placed in various categories. The use and application of products is determined based on the category (allowed and regulated) in which they are placed. A survey of some of the products that are, and are not, included in the approved listings will also be presented. As the NOP becomes more widely used and accepted as an agricultural production option, the role and service provided by OMRI and the process for evaluation of program inputs will become even more important.

AGRO 39: Exploring the limits of nitrogen percentages in composts and biofertilizers as measured by the US Composting Council's testing methods for determining stability and maturity values

Jim McNelly, Renewable Carbon Management, LLC, 44 28th Ave N Suite J, Saint Cloud, MN 56303, rcm@composter.com

Composting has been long recognized as a method of stabilizing otherwise undesirable organic materials into value-added soil amendments. Recently, the US Composting Council's Testing Methods for Evaluating Composting and Compost (TMECC) Laboratory Methods has more clearly defined previously vague definitions such as "stability" and "maturity" of various composts and bionutrients. Stability is often determined by reduction of vectors (diseases, odors, and pests); whereas maturity is often determined by seed germination, oxygen uptake and off-gassing of ammonia. Although uncomposted biofertilizers are similar to composts in organic matter content, they differ from composts in characteristics and form of nitrogen. Most mature compost products are limited to 1% to 1.5% nitrogen while unstable chicken manure, for example, can contain 8% nitrogen. Uncomposted or unstable biofertilizers can be phytotoxic to plants, seeds and nitrate sensitive ornamentals. Using new techniques nitrogen levels in finished composts can now approach 5% while maintaining safe nitrogen release rates.

AGRO 40: Regulatory aspects of organically derived nutrients Maryam Khosravifard, Room A-472, California Department of Food and Agriculture, 1220 N Street, Sacramento, CA 95814, mkhosrav@cdfa.ca.gov

Fertilizing materials derived from organic fertilizers are subject to individual state's fertilizer laws and regulations. The Association of American Plant Food Control Officials (AAPFCO) has defined organic fertilizers, natural organic fertilizer, natural fertilizer, and organic base fertilizers. California and other states utilize these definitions to approve product labels with organic claims. The Organic Trade Association has raised concerns that the AAPFCO definitions are in conflict with the United States Department of Agriculture, National Organic Program (USDA NOP) recognized organic materials for organic production. Organic growers may be confused by this inconsistency and can lose their certifications because products that are not in compliance with USDA NOP but meet AAPFCO definitions get labeled as organic. The AAPFCO Terms and Definition's Committee is in the process of reviewing proposed definitions by the Organic Trade Association to address their concerns. Harmonizing these terms will be an important step in gaining consensus on the use and regulation of these products.

AGRO 41: Reducing spray drift to mitigate human exposure Durham K Giles, Biological & Agricultural Engineering Department, University of California, Davis, One Shields Avenue, UCD, Davis, CA 95616, Fax: 530-752-2640, dkgiles@ucdavis.edu

Spray draft is composed of droplets that fail to deposit on the target surfaces or fail to remain within the application site; these droplets are primarily those lacking sufficient velocity, momentum and kinetic energy for deposition. Most often, the lack of deposition originates in the production of droplets that are excessively small in relation to the gravitational and other forces driving deposition. Other factors contributing to spray drift are low droplet velocities, sparse capture efficiency of the targets, adverse weather conditions or improper equipment. This presentation will review the fundamental physics of spray drift and illustrate how understanding and manipulation of the physical processes can mitigate human exposure to spray drift. The interaction and linkage between the physics of spray drift and basic toxicological analysis will be addressed.

AGRO 42: Assessing exposure to agricultural fumigants in outdoor and indoor air environments

James E. Woodrow, Center for Environmental Sciences and Engineering, University of Nevada, Mail Stop 199, 1664 North Virginia Street, Reno, NV 89557, Fax: 775-784-1142, jwoodrow@unr.nevada.edu, and R. I. Krieger, Department of Entomology, Personal Chemical Exposure Program, University of California-Riverside

Because of ongoing concerns over exposure to agricultural fumigants, techniques have been developed for determining their volatilization losses from target sites and subsequent movement into non-target areas. These techniques include aerodynamic and flux chamber methods for determining volatilization losses as well as monitoring procedures for measuring downwind concentrations in both outdoor and indoor air environments. As a complementary approach, computer based models can also be used to estimate losses and downwind concentrations, using field and chemical property data as input. Taken together, these measurement and modeling techniques provide a quantitative and reasonable approach to determining the magnitude of various exposures to fumigants under typical use conditions as well as for evaluating ways to minimize those exposures. This presentation will summarize the results of a number of studies concerned with exposures to agricultural fumigants and it will include descriptions of the various measurement and modeling techniques that have been used and can be used for exposure assessment.

AGRO 43: Drift of insecticide residues from orchards: Empirical and modeling results for exposure assessment and risk management

Allan S. Felsot, Department of Entomology, Washington State University, 2710 University Drive, Richland, WA 99352, Fax: 509-372-7460, afelsot@tricity.wsu.edu

Insecticides are the most intensely used pest control agents in orchard fruit production. Application is typically by use of axial fan airblast sprayers that disperse the insecticide through the canopy but also tend to project the spray over the canopy. Over several decades, suburban residential developments nearby orchards have placed consumers closer to sources of sprayed insecticide residues. Studies are needed to characterize the magnitude of drift downwind and upwind of orchards so that potential exposures to bystanders are estimated and health risks are minimized. We have characterized deposition of residues associated with drift during both commercial and experimental orchard applications. We have also begun to examine airborne residues for improving complete exposure estimates. The model AgDrift has also been used to generate estimates of ground deposited residues along transects extending away from the outside row of an orchard. Modeled estimates were sometimes similar to measured residues but on other occasions they significantly underestimated downwind residue deposition. Nevertheless, modeled estimates have been changed to whole body dose deposition equivalences at downwind distances and used to determine toxicologically relevant buffer zones between new residential developments and nearby established orchards.

AGRO 44: Setting buffer zones for pesticide applications Terrell A. Barry, Bruce R. Johnson, and Randall T. Segawa, Department of Pesticide Regulation, California Environmental Protection Agency, 1001 I Street, Sacramento, CA 95814, Fax: 916-324-4088, tbarry@cdpr.ca.gov, rsegawa@cdpr.ca.gov

California's Department of Pesticide Regulation (DPR) has found that inhalation exposure to some pesticides can pose an unacceptable risk to human health. DPR uses air monitoring data and computer modeling to estimate exposures, and if necessary develop buffer zones to control exposure. Monitoring provides a snapshot of air concentrations in the area surrounding specific pesticide applications. DPR uses monitoring data in conjunction with the Industrial Source Complex-Short Term (ISCST) model to estimate air concentrations under a variety of conditions. If the monitoring data and computer modeling indicate unacceptable air concentrations in the vicinity of pesticide applications, DPR uses the ISCST model to determine the appropriate size and duration of buffer zones. These techniques will be illustrated using methyl bromide as an example.

AGRO 45: Developing pesticide exposure mitigation strategies Thomas Thongsinthusak and Joseph P. Frank, Worker Health and Safety Branch, California Department of Pesticide Regulation, 1001 I Street, P.O. Box 4015, Sacramento, CA 95812, Fax: 916-445-4280, tthongsinthusak@cdpr.ca.gov

As part of the regulatory process, DPR develops mitigation strategies when risk assessments identify unacceptable pesticide exposure levels. These strategies must not only reduce exposures to acceptable levels, they must also be practical and enforceable. Typical mitigation measures can include additions or changes to personal protective equipment, additional engineering controls, buffer zones, lengthened reentry times, or restrictions on use. This presentation will provide general considerations in developing mitigation strategies for handlers (application related exposures) and reentry workers (post-application exposures). Mitigation strategies will be discussed for EPTC and methyl bromide. While exposure issues were addressed with a simple label change for EPTC, the strategies necessary to address methyl bromide exposures were far more complex. They included a multistage process that started with use-specific permit conditions, followed by the development of new regulations intended to address field fumigation applications. DPR's mitigation strategies involve intra- and interdepartmental, as well as public participation.

AGRO 46: Integrated exposure analyses for pesticides: A retrospective

Dr. Jeffrey H. Driver and J. H. Ross, infoscientific.com, Inc, 10009 Wisakon Trail, Manassas, VA 20111, Fax: 703-392-0648, ddriver448@aol.com

The Food Quality Protection Act (FQPA) of 1996 required the U.S. Environmental Protection Agency to begin routinely evaluating potential "integrated" or "total" exposure to pesticides. Under FQPA this was defined as multi-route, multi-pathway aggregate and cumulative exposures to pesticides with agricultural and other (e.g., professional and consumer) uses. A constellation of science and policy-related activities were subsequently initiated, including the development of models to provide probabilistic simulations of potential aggregate and cumulative exposures and associated human health risks. The aggregate and cumulative modeling experience has helped to identify key model input data needs, sources of existing data, and sources of uncertainty, prompting additional or confirmatory data. The probabilistic modeling endeavors have intended to provide more realistic demographic, geographic and temporal integration of potential aggregate and cumulative exposures to the U.S. population and relevant subgroups of particular interest (e.g., females of reproductive age, children), and have also prompted a wealth of science policy dialogue in the U.S. and abroad. This presentation will provide a retrospective of exemplary exposure data and assessment methods development efforts, and comment on key lessons learned via predictive modeling case studies including those associated with the Cumulative and Aggregate Risk Evaluation System (CARES, version 2.0) under stewardship via the Research Foundation of the International Life Sciences Institute, Washington, D.C.

AGRO 47: A reality fix for risk managers

J. H. Ross and Dr. Jeffrey H. Driver, infoscientific.com, Inc, 5233 Marimoore Way, Carmichael, CA 95608, Fax: 916-486-6181, john@infoscientific.com

Risk assessment is the process of comparing hazard to exposure. Often risk managers are faced with making a decision on the basis of risk assessments that are purposefully biased by the Precautionary Principle. To help risk managers maintain perspective we have summarized comparisons between models and measurements. A comparison of risks between the most used pharmaceuticals and the default criteria applied to pesticides reveals that many pharmaceuticals could not qualify as pesticides. A compilation of the top 10 causes of

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mortality and morbidity in agriculture shows that pesticides don't usually make the list. Comparing results of water modeling versus USGS monitoring finds that the models consistently overestimate pesticide water concentrations by 10-fold or more. We compare dietary exposure estimates to biomonitoring that integrates exposure from all routes and find that our best stochastic models while still slightly biased are approaching reality, yet ~10,000 people in the US die from microorganisms in food each year. Moreover, models of residential dermal exposure currently overestimate total absorbed dose by an average of 19-fold. The most common causes of excessive residential and agricultural handler dose estimates are discussed. Risk managers can get the big picture by assuring themselves that risk estimates were made under realistic conditions. FQPA requires aggregate exposure from all routes and pathways and sometimes to perform cumulative assessments with chemicals having the same mode of action. There is a continuing need to reassess risk assessment defaults and models not for their ability to satisfy the Precautionary Principle but to pass the laugh test.

AGRO 48: Synthesis and fungicidal activity of sulfonamide derivatives

Hiroaki Takahashi¹, Toshiaki Takeyama¹, Toshimasa Hamada¹, Kazuhiro Yamagishi², Masanori Nishioka², and Hiroyuki Suzuki², (1) Chemical Research Laboratories, Nissan Chemical Industries, LTD, 722-1, Tsuboi-cho, Funabashi-shi, Chiba 274-8507 Japan, Funabashi 274-8507, Japan, Fax: 81-47-467-5307, takahashih@nissanchem.co.jp, (2) Biological Research Laboratories, Nissan Chemical Industries, LTD

Fungicidal activity against Oomycetes was observed in 1-{1-[(dimethylamino)sulfonyl](1,2,4-triazole-3-yl)}sulfonyl derivatives. Especially, a series of substituted indoles showed potent activity. After the optimization of substituents on the indole ring, 1-{1-[(dimethylamino)sulfonyl](1,2,4-triazole-3-yl)}sulfonyl-3-bromo-6-fluoro-2-methylindole was found to exhibit the highest activity among the derivatives. The compound has been developed for agricultural use under the code number NC224, which has good efficacy against vine downy mildew, potato late blight and other plant diseases caused by Oomycetes. Control of those diseases was achiveved at 60-100 g a.i./ha in the field trials. NC224 belongs to the chemical class of sulfonamides. {1-[(dimethylamino)sulfonyl](1,2,4-triazole-3-yl)}sulfonyl chloride was used as the key intermediate for synthesis of NC224. In this presentation, the structure-activity relationship of the derivatives will also be discussed.



AGRO 49: A sustained-release, bio-absorbable, injectable gel formulation for delivery of doramectin to cattle for control of ticks and biting flies

Jerome A. Klavons, J. Allen Miller, J. Mathews Pound, and Kimberly H. Lohmeyer, Knipling-Bushland U.S. Livestock Insects Research Laboratory, Agricultural Research Service, U.S. Department of Agriculture, 2700 Fredericksburg Rd., Kerrville, TX 78028, Fax: 830-792-0314, jerry.klavons@ars.usda.gov

The availability of systemically active pesticides that are effective in controlling livestock pests at dosages in the microgram per kilogram range provides a unique opportunity for the development of delivery systems heretofore impossible. We have developed bio-absorbable injectable microspheres using poly-(lactic/glycolic acid) copolymers for the delivery of avermectins to livestock for ectoparasite control. However, the process of producing the microsphere formulation in the laboratory is time consuming and expensive. The objective of this study was to develop a less labor intensive and more cost effective injectable

gel formulation for extended delivery of doramectin to cattle for control of ticks and biting flies such as horn flies. Hereford steers were treated with 5 cc subcutaneous injections of the doramectin formulation at dosages of 600 μ g/kg, 1200 μ g/kg, or gel only. Blood samples were taken weekly both for feeding of adult horn flies and for HPLC determination of serum concentration. Adult lone star ticks were placed on the animals inside stockinet sleeves at 2 week intervals. The number of engorging females, their individual weights, the weights of individual egg masses, and percent hatch were determined. The duration of treatment efficacy against adult horn flies and lone star ticks feeding on the blood of treated animals will be presented. In addition, the pharmacokinetics of the drug in the serum, as determined by HPLC analyses, will be shown.

AGRO 50: Thioacetals as novel inhibitors of peptide deformylase: Synthesis and data mining

Michael H. Howard¹, **Teodorica M. Cenizal**¹, Roman Kucharczyk², and Susanta Samajdar³, (1) Chemical Discovery, DuPont Crop Protection Products, P. O. Box 30, Newark, DE 19714, Fax: 302-366-5738, Michael.H.Howard-1@USA.dupont.com, teodorica.m.cenizal@usa.dupont.com, (2) DuPont Crop Protection, (3) Syngene International Pvt Ltd

Thioacetals of levulinic acid are a novel class of soybean peptide deformylase (PDF2) inhibitors. *In-vitro* screening of a diverse set of small molecules that represent biologically active chemical space led to the discovery of thioacetals (I), where Ar represents aryl substituents. The analogs of the acid displayed inhibition against PDF2, but did not display any whole organism activity. Data mining around this structure led to the discovery of a trithiane with the levulinic acid side chain (II, R=H) that, while inactive against PDF2, exhibited a broad spectrum of herbicidal activity. An analog synthesis program was designed around the trithiane backbone, varying the substituents and the length of the levulinic acid side chain to explore the structure activity relationship and to optimize herbicidal activity.



AGRO 51: Newly developed phenazine compounds may offer control of soil-borne plant pathogens

Dragic Vukomanovic, Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, N. Darmouth, MA 02747, Fax: 508-999-9167, dvukomanovic@umassd.edu

It has been well documented that some phenazine compounds, isolated from Pseudomonas aeruginosa and other environmental Pseudomonas species, are effective in suppressing a variety of plant diseases like: "wheat leave disease" caused by Septoria tritici, "take-all disease" in wheat caused by Gaeumannomyces graminis, "black root rot disease" in tobacco caused by Thielaviopsis basciola, "damping-off disease" in many plants caused by Rhizoctonia solani, "wilt disease" in cotton, etc. Our studies have shown the isolated phenazine compounds and newly synthesized phenazines exhibit a broad-spectrum of antimicrobial activity (the MIC90 in the range of 0.8 to 3.1 µg/mL) that may be useful in controlling plant pathogens. We have developed an efficient method of synthesis of phenazines which has dramatically reduced the cost, eliminated use of toxic solvents and significantly increased the yield. The method is a coupling reaction of benzofuroxane derivatives with quinones, naphthohydroquinones, α - and β -naphthols, phenols, benzoquinons and 1,4-naphthoginones. Synthesis, purification, structural elucidation as well as susceptibility testing of the new phenazines will be presented.

AGRO 52: Decade of monitoring and studying the fate and transport of triazine herbicides in ground water and surface water Elisabeth A. Scribner, E.M. Thurman, and Michael T. Meyer, Organic Geochemistry Research Group, U.S. Geological Survey, U.S. Geological Survey, 4821 Quail Crest Place, Lawrence, KS 66049, scribner@usgs.gov

Nonpoint-source contamination of water resources from triazine herbicides has been a major water-quality issue during the past decade (1990s) in the United States (US). Investigation of ground water and surface water have been carried out by the US Geological Survey to identify the relationship between land use, ground-water age, and concentration and occurrence of herbicides and their degradation products in ground water and to determine the geographic and seasonal distribution of herbicides in surface water. The result of these studies is that a clear understanding exists of the aquatic transport and partial fate of the triazine herbicides and their degradation products in the environment. Increased knowledge of the transport and fate of the triazines was an important goal of the monitoring effort of the past decade in addition to providing the data for monitoring exposure and toxicity of the triazines in the aquatic environment.

AGRO 53: Dialkylphosphates (DAPs) in fruit and vegetables confound biomonitoring in organophosphate risk assessment Xiaofei Zhang¹, Dana B Barr², J. H. Ross³, and Robert I Krieger¹, (1) Department of Entomology, Personal Chemical Exposure Program, University of California, Riverside, 900 University Ave, Riverside, CA 92521, Fax: 951-827-5803, zhangxiaofei@hotmail.com, bob.krieger@ucr.edu, (2) National Center for Environmental Health, Centers for Disease Control and Prevention, (3) infoscientific.com, Inc, 5233 Marimoore Way, Carmichael, CA 95608, Fax: 916-486-6181, iross@infoscientific.com

Organophosphorous (OP) insecticide metabolism in treated produce yields residues that can confound human exposure biomonitoring. OP metabolism in humans also produces the dialkylphosphates (DAPs) urinary biomarkers. Therefore dosage cannot be reliably estimated from urinary DAPs. DAPs were measured in 44 kinds of produce. Fruit and vegetable samples (153) positive for 1 or more OPs were selected from the channels of trade. All OPs were below established residue tolerances. Produce was also analyzed for 6 DAPs. Each sample contained 1 or more DAPs and 91 of 153 (60%) samples contained more DAPs than OP. Mole ratios DAPs:OP ranged from 0.02 to 73 (median, 1.7; geometric mean, 1.4). Preformed DAPs represent false positives when OP exposure is estimated from low-level urinary DAPs in children and adults. Occupational exposures are larger than environmental exposures and unlikely to be significantly inflated by preformed DAPs in food.

AGRO 54: Pesticide exposure assessment: Concurrent passive dosimetry and biological monitoring of triclopyr and 2,4-D exposures of a backpack applicator crew

Xiaofei Zhang, Sandra P. Acevedo, Yingfu Chao, Travis M. Dinoff, Ryan L. Williams, and Robert I Krieger, Department of Entomology, Personal Chemical Exposure Program, University of California, Riverside, 900 University Ave, Riverside, CA 92521, Fax: 951-827-5803, zhangxiaofei@hotmail.com

This study concerned the consistency of exposure monitoring strategies for workers using backpack sprayers in forestry. Eight applicators applied triclopyr and 2,4-D for weed control. Tier 1 data were derived from default assumptions and generic databases. Using coveralls, triclopyr and 2,4-D exposures were 2.50 ± 1.55 and 0.75 ± 0.52 mg equiv/day. Tier 2 measurements using whole body dosimeters were 0.22 ± 0.23 and 0.14 ± 0.17 mg equiv/day, respectively. Gloves, socks, and face/neck wipes contributed negligibly to the estimate. Complete urine samples were also analyzed for triclopyr and 2,4-D. The absorbed doses and dosages were $5.2 \pm 4.3 \ \mu g$ equiv/day and $0.072 \pm 0.057 \ \mu g$ equiv/kg-day (triclopyr); $3.8 \pm 3.4 \ \mu g$ equiv/day and $0.052 \pm 0.044 \ \mu g$ equiv/kg-day (2,4-D). Clothing penetration was 11% and 20%; dermal absorption was 3.6%/24 h and 4.2%/24 h, respectively. Exposure estimates from coveralls were more than 2 orders of magnitude greater than biomonitoring estimates.

AGRO 55: Pilot studies of indoor pyrethroid exposures of adults and their children using urine biomonitoring

James J Keenan¹, Xiaofei Zhang1, Gabriele Leng², and Robert I Krieger¹, (1) Department of Entomology, Personal Chemical Exposure Program, University of California, Riverside, 900 University Ave, Riverside, CA 92521, jkeen001@ucr.edu, (2) Bayer Industry Services

Pyrethroid exposure following use of total release foggers under normal use conditions was measured using cyfluthrin, pyrethrin, and cypermethrin. Pyrethroid biomarkers are rapidly excreted in the urine of adults and children and can be used to estimate absorbed dose. Metabolites were readily measurable in urine during the 7-day post-application period. Samples were taken in the a.m. and p.m. of study days (24 hour samples in some households). Concentrations were corrected for creatinine. Children excreted 7-day totals of 29.7 and 21.6 nmol/kg in a.m. and p.m. samples respectively, while adults excreted 2.3 and 4.3 nmol/kg. These data reveal significantly higher metabolite concentrations in subjects under the age of eighteen. Further studies will explore the availability of surface pyrethroid deposits and the influence of route of exposure on the nature of urinary metabolites of cypermethrin. These exposures are below known LOAELS and regulatory NOAELs for these insecticides.

AGRO 56: Reconnaissance data for glyphosate, other selected herbicides, and their degradation products in 51 streams in nine midwestern states, 2002

Elisabeth A. Scribner, William A. Battaglin, and Michael T. Meyer, Organic Geochemistry Research Group, U.S. Geological Survey, U.S. Geological Survey, 4821 Quail Crest Place, Lawrence, KS 66049, Fax: 785-832-3500, scribner@usgs.gov

Since 1989, the U.S. Geological Survey has conducted periodic reconnaissance studies of streams in the Midwestern United States to determine the geographic and seasonal distribution of herbicide compounds. These studies show that peak herbicide concentrations tend to occur during the first post-emergence runoff after herbicide application and that herbicide flushes can occur during runoff for several weeks to months following application. Glyphosate use significantly increased in the past five years by 127% while acetochlor use decreased by 16%, alachlor use decreased by 78%, atrazine use decreased by 13%, cyanazine use decreased by 100% (to zero), and metolachlor use decreased by 56%. In 2002, water samples were collected during two post-herbicide-application runoff events and one harvest-season runoff event. Results are compared with findings from samples collected from the same sites periodically since 1989. In general, concentrations of acetochlor have increased while concentrations of alachlor, atrazine, and metolachlor have decreased. Prior glyphosate data is unavailable.

AGRO 57: Concentration gradients of azinphos-methyl residues associated with spray drift and post-application volatilization at an apple orchard

Melissa Tulio, Allan Felsot, and Quentin Macdonald, Department of Entomology, Washington State University, Richland, WA 99352, Fax: 509-372-7460, Itulio@tricity.wsu.edu

Air and ground deposition samples were collected during the application of azinphos-methyl (AZM) (formulated as Guthion Solupak, 50% AI; 1.12 kg Al/ha) to a commercial orchard in eastern Washington. Upwind and downwind air samples were collected periodically along transects using high volume samplers over the next 72 hours after application. Filter paper fitted in front of a cartridge containing polyurethane foam plugs (PUFs) trapped the particulate portion of the sprayed AZM, and the PUFs collected the vapor phase portion. Silica gel deposition plates were used to collect AZM that was deposited on the ground along upwind and downwind transects both inside and outside of the orchard. Results from the deposition plates were compared to deposition estimates predicted by the orchard module of the model AgDRIFT. Residues of AZM were observed in upwind air and ground samples. The greatest proportion of AZM in the air samplers was collected on the filter paper, but the ratio of particulate phase to air phase AZM decreased in samples taken after 24 h.

AGRO 58: Evaluation of the stereoselectivity of fenthion sulfoxidation in fish

Ola Bawardi, Bjarte Furnes, and Daniel Schlenk, Department of Environmental Sciences, University of California Riverside, 2217 Geology Building, Riverside, CA 92521, Fax: 951-787-3993, obawardi@yahoo.com

The objective of this study is to examine the enantioselective sulfoxidation of fenthion in liver microsomes of various fish species (rainbow trout, hybrid striped bass, tilapia). Microsomes from striped bass, trout, and tilapia primarily formed (+) sulfoxides in approximately 65% enantiomeric excess. Enzyme inhibitors lubrol (cytochrome P450) and methimazole (Flavin Monooxygenases) were used to determine sulfoxide relative contributions from each enzyme system. In striped bass microsomes, P450 was responsible for 74% of sulfoxide formation. Co-incubation with methimazole or lubrol in trout liver microsomes enhanced sulfoxide formation. Salt water treatments which typically induce FMOs, did not significantly alter enantioselectivity or rates of fenthion sulfoxidation, even though toxicity tests indicated that saline environments enhanced the toxicity of fenthion in trout. These results indicated either the formation of additional metabolites of fenthion or the contribution of additional oxygenases to S-oxidation.

AGRO 59: Method development for pesticides analysis in breast milk using stir bar sorptive extraction followed by TDU/GC/MS Beatriz A. Rocha-Gutierrez, Department of Chemistry, University of Texas at El Pso, 500 W. University Ave., El Paso, TX 79968, Fax: 915-747-5748, brocha@utep.edu, and Wen-Yee Lee, Department of Chemistry, University of Texas at El Paso

Pesticides are substances intended for preventing, destroying, repelling, or mitigating any pest. However, persistent organochlorine (OC) pesticides are found to be bioaccumulated and biomagnified in the food chain. They pose a risk of causing adverse effects on biological species including humans. Ongoing studies of OC pesticides are focused on their fate and transport in the environment, and the impact on the ecosystem and human health. The study objectives were to analyze OC pesticides in breast milk, and to evaluate the possible health impact on women in El Paso, Texas. To determine OC pesticides in human breast milk, stir bar sorptive extraction (SBSE) was carried out. Whereas an analytical process normally requires time-consuming steps, SBSE is environmentally friendly (uses only methanol and water as solvents), and it is a simple, cost-effective, and rapid technique alternative compared to the traditional liquid extraction methods. SBSE uses a stir bar coated with 1 mm of polydimethylsiloxane (PDMS) as extraction medium to concentrate non-polar analytes from polar matrices. After extraction, the stir bar was removed from the solution and placed in a thermal desorption unit (TDU), thermally desorbed and injected directly into the GC/MS. Optimization of OC pesticides extraction and analyses will be reported.

AGRO 60: Allatotropin-increased biosynthesis of juvenile hormones (JH) from L-isoleucine and L-methionine by corpora allata of Manduca sexta

David Schooley, Department of Biochemistry, University of Nevada, Mail Stop 330, Howard Medical Sciences, Room 160, Reno, NV 89557, schooley@unr.edu, and **Josef Seifert**, Plant and Environmental Protection Sciences, University of Hawaii, 402 Gilmore Hall, Honolulu, HI 96822, Fax: 808-956-2428, josef@hawaii.edu

Understanding control of JH biosynthesis may lead to development of chemicals which can block it. We investigated in vitro allatotropinincreased biosynthesis of JH from L-³H-methionine and L-¹⁴C-isoleucine by corpora allata (CA) of Manduca sexta. CA of one-day old female moths were incubated with these precursors for two hours. ¹⁴C-labeled 2-keto-3-methylvaleric acid, 2-methylbutyric acid, tiglic acid, acetic acid and propionic acid (catabolites of isoleucine produced by the CA) were then assayed by HPLC. ³H- and ¹⁴C-labeled JH were determined after separation by TLC. Acetate and propionate were found in 7 to 200 fold higher abundance than the remaining acids. The amount of JH produced in response to allatotropin is linearly correlated to the amount of labeled acetate and propionate secreted by the glands into the medium. While there is variation between different glands in rates of both stimulated and basal JH production, allatotropin at 1 μ M gave a steady ~4-fold increase in JH production. The amount of acetic and propionic acids secreted by CA is considerably in excess of the amount of JH produced. These data suggest that allatotropin stimulates incorporation of isoleucine catabolites in JH biosynthesis.

AGRO 61: In vitro formation of guanosine adducts with pesticides Donald W. Boerth, Melissa Medeiros, and Danielle Coulombe, Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, North Dartmouth, MA 02747, Fax: 508-999-9167, dboerth@umassd.edu

Earlier ³²P post-labeling studies have demonstrated the presence of elevated levels of DNA adducts in a variety of crop plants after treatment with pesticides. Evidence was found for both direct adducts with the pesticide or its metabolites, as well as indirect adducts with 4hydroxy-2-nonenal and 2-hexenal from oxidative stress. In this study we have investigated the propensity for direct formation of DNA adducts with a diverse set of pesticide molecules. Guanosine was chosen as the mononucleoside base because it is usually the most reactive of the DNA bases. Pesticide treatment of guanosine was performed in phosphate buffered solutions of aqueous methanol or isopropanol. Adducts were identified by reverse phase HPLC. A companion molecular modeling study, utilizing semi-empirical, ab initio, and density functional methodologies, was carried out to determine reaction sites on the guanosine and pesticide molecules. Intermolecular interaction energies were computed to ascertain the relative potential for reaction between centers on each pair of molecules. Putative adduct structures were proposed.

AGRO 62: Rice suspension cell culture as a tool for metabolism studies of non-radiolabelled penoxsulam and other N-triazolo[1, 5-c]pyrimidinylbenzene sulfonamides

Gerrit J. deBoer and Scott Thornburgh, Discovery Research, Dow AgroSciences, Indianapolis, IN 46268, gjdeboer@dowagro.com

Rice selectivity was observed in a number of N-triazolo[1, 5c]pyrimidinylbenzene sulfonamides leading to an aggressive synthesis effort to generate a rice selective herbicide with attributes clearly superior to commercial standards. In the early stages of a project, the generation of radioactive labels of numerous experimental compounds is not possible. The rice suspension culture used for these studies proved to be very useful in evaluating the pathways of detoxification for a series of early stage N-triazolo[1, 5-c]pyrimidinylbenzene sulfonamide leads including penoxsulam without a radiolabel. The selectivity handle for all the chemicals studied was the O-demethylation of a methoxy in the 5-position of the heterocycle. This pathway is identical to what is observed for the sulfonylurea bensulfuron-methyl in rice plants. The rice suspension culture was also validated by comparison to the metabolism of radioactive penoxsulam and to whole plant data.

Figure 1 Structure of Penoxsulam.

AGRO 63: Biocatalytic resolution of (RS)-HMPC acetate by immobilized *Acinetobacter* sp. cells expressing carboxylic esterase activity

Jian-He Xu, Ya Chen, and Jiang Pan, State Key Laboratory of Bioreactor Engineering, East China University of Science and Technology, 130 Meilong Road, P.O. Box 283, Shanghai 200237, China, Fax: +86-21-6425-2250, jianhexu@ecust.edu.cn

Kinetic resolution of (R,S)-HMPC, 4-hydroxy-3-methyl-2-(2'-propenyl)-2-


cyclopentenone, a key chiral intermediate for the production of prallethrin insecticides, was successfully carried out by enantioselectivite hydrolysis of (RS)-HMPC acetate using calcium alginate gel-entrapped cells of Acinetobacter sp. CGMCC 0789. When the effect of different cosolvents was investigated, it was found that isopropanol could markedly enhance the activity and enantioselectivity of the immobilized cells. The optimum concentration of isopropanol was 10% (v/v) where immobilized cells still showed good operational stability. After 10 cycles of reaction, no significant loss of the enzyme activity was observed. The catalytic specificity constants (Vmax/Km) for both enantiomers of the substrate were determined with partially purified enzyme, giving 0.0184 and 0.671 h⁻¹ for the (S)- and (R)-ester, respectively.

AGRO 64: Cross-coupling reactions of 5- and 6-bromoquinazolin-2-ones: Synthesis of inhibitors of peptide deformylase

Michael H. Howard¹, **Teodorica M. Cenizal**¹, Reed A. Coats², and Susanta Samajdar³, (1) Chemical Discovery, DuPont Crop Protection Products, P. O. Box 30, Newark, DE 19714, Fax: 302-366-5738, Michael.H.Howard-1@USA.dupont.com,

teodorica.m.cenizal@usa.dupont.com, (2) DuPont Crop Protection, (3) Syngene International Pvt Ltd

2-(5-Bromo-2-oxo-1,4-dihydro-2H-quinazolin-3-yl)-N-hydroxy-acetamide (Apfel, C.; et al. J. Med. Chem. 2001, 44, 1847) has been reported as an inhibitor of bacterial peptide deformylase. We have found that this compound, and the corresponding N-acetic acid, are potent inhibitors of plant PDF as well. To explore the SAR around plant PDF activity, particularly around the inhibitor P1' pocket and the metal binding group, we prepared a series of 5- and 6-alkyl and aryl substituted dihydroquinazolin-2-ones as well as acetic acid side chain derivatives. The former could in some cases be synthesized by Suzuki and Sonogashira coupling reactions of (5- and 6-bromo-2-oxo-1,4-2Hquinazolin-3-yl)-acetic acid ethyl ester. In other cases, the cross coupling reactions were performed on earlier intermediates in the synthetic sequences.



AGRO 65: Detoxification of carbamate pesticides by halamine structures

Xin Fei, Division of Textiles and Clothing, University of California, Davis, One Shields Avenue, Davis, CA 95616, Fax: 530-752-7584, xfei@ucdavis.edu, Takayuki Shibamoto, Department of Environmental Toxicology, University of California, Pengfei Gao, National Personal Protective Technology Laboratory, National Institute for Occupational Safety and Health, and Gang Sun, Division of Textiles and Clothing, University of California at Davis

Halamines are compounds containing N-Cl or N-Br structures and widely used as disinfectants for swimming pools and recreation water. These compounds are able to oxidize many toxic compounds including pesticides. In recent years, halamine containing fabrics possessing durable and rechargeable biocidal properties were developed. A preliminary study of using the halamine fabrics in detoxifying certain pesticides has produced some interesting results, showing that several carbamates were decomposed rapidly by contact. Recent developments in halamine materials have resulted in fabrics containing different halamine structures such as imide, amide, and amine halamine, in order of oxidative reactivity. This reactivity will also affect the power of detoxification of toxic chemicals. In order to systematically understand the detoxifying mechanisms of halamine fabrics, we have performed a pesticide detoxifving study using different halamine compounds. This presentation will discuss our latest results in this study.

AGRO 66: Evaluation of mutagenic activity caused by pesticides residues in corn, wheat, bean and chickpea by microsuspension in S. typhimurium TA98

ML Aldana-Madrid¹, NJ Salazar-Lopez², FG Loarca-Piña³, and MI

Silveira-Gramont¹, (1) Departamento de Investigación y Posgrado en Alimentos, Universidad de Sonora, Professor, Rosales y Transversal s/n, Col. Centro, Hermosillo, Sonora 83000, Mexico, Fax: (662)259 2208, laldana@guayacan.uson.mx, (2) MD, (3) Universidad Autonoma de Queretaro, Professor

The objective of this study was to evaluate the mutagenic potential of the pesticide concentrations detected in corn, wheat, bean, and chickpea grains stored in the State of Sonora, by microsuspension assay, using *Salmonella typhimurium* tester strain TA98. Malathion and chlorpyrifos were mutagenic in the absence of the microsomal fraction (S9), suggesting a potential direct mutagenic behaviour of these pesticides. In the presence of S9, malathion (50 and 100 ng/tube) residual concentrations found in the analysed grains do not seem to induce damage to the genetic material.

AGRO 67: Study of organophosphate insecticides and biochemical indicators in blood and urine of urban adult males ML Aldana-Madrid, ED Molina-Romo, G Rodriguez-Olibarria, and MI Silveira-Gramont, Departamento de Investigacion y Posgrado en Alimentos, Universidad de Sonora, Professor, Rosales y Transversal s/n, Col. Centro, Hermosillo, Sonora 83000, Mexico, Fax: (662)259 2208, laldana@guayacan.uson.mx

The effect of the exposure to organophosphate insecticides (diazinon, parathion, malathion and chlorpyrifos) was evaluated measuring insecticide presence in blood and urine, as well as biochemical indicators in urban adult males from Caborca, Sonora. One group of 24 was exposed to agricultural related pesticides (EG), and a control group (CG) of 18, with no apparent exposure to chemicals. Results showed differences between the two groups (p<0.05) in the hemoglobin concentration (CHCM) and in red cell distribution width (RDW). In the EG the highest concentrations were: Chlorpyrifos 80.9 ppb, malathion 909 ppb, and parathion 284.3 ppb. All blood samples were over the daily reference dose for parathion, and only 8.3% for malathion. The CG has the highest blood concentration of diazinon (7.9 ppb). There was a significant relationship between malathion and transaminases (r=0.97) in EG groups. Some other indicators showed an increase with the total amount of insecticides in blood.

AGRO 68: Application of a holistic approach in allelopathy research

Inge S. Fomsgaard¹, Per Kudsk¹, Emilio Benfenati², Sylvia Blümel³, Francisco A. Macias⁴, Johann Fritz⁵, Damia Barcelo⁶, Ona Sakaliene⁷, Betty B. Mogensen⁸, Wieslaw Oleszek⁹, Lars M. Hansen¹, Solvejg K. Mathiassen¹, Anne G. Mortensen¹, Mia B. Gents¹, Anders G. Understrup¹, Susan T. Nielsen¹, Stine S. Krogh¹, Susanne J.M. Mensz¹, Thomas Etzerodt¹, Elena Lo Piparo², Filip Fratev², Tamara Coja³, Jacqueline Idinger³, David Chinchilla⁴, David Marin⁴, Jose M. G. Molinillo⁴, Alberto Oliveros-Bastidas⁴, Ana M. Simonet⁴, Ethel Eljarrat⁶, Lea Bonnington⁶, Miriam Guillamon⁶, Marta Villagrasa⁶, Andreu Taberner⁶, Teddy Krongaard⁸, Jan Kus⁹, Stefan Martyniuk⁹, and Anna Stochmal⁹, (1) Department of Crop Protection, Danish Institute of Agricultural Sciences, Research Centre Flakkebjerg, Slagelse DK-4200, Denmark, Fax: +45 58113301, Inge.Fomsgaard@agrsci.dk, (2) Laboratory of Environmental Chemistry and Toxicology, Istituto di Ricerche Farmacologische "Mario Negri", Milan, Italy, (3) Institute for Phytomedizin, Österreichische Agentur für Gesundheit und Ernährungssicherheit, Vienna, Austria, (4) Department of Organic Chemistry, Facultad de Ciencas, University of Cadiz, Spain, (5) Department IFA-Tulln Umweltbiotechnologie, Universität für Bodenkultur Wien, Vienna, Austria, (6) Environmental Chemistry, IIQAB-CSIC, Barcelona, Spain, (7) Lithuanian Institute of Agriculture, Vilnius, Lithuania, (8) Department of Atmospheric Environment, National Environmental Research Institute, Roskilde, Denmark, (9) Department of Biochemistry and Crop Quality, Institute of Soil Science and Plant Cultivation, Pulawy, Poland

A new holistic approach on research into allelopathy was launched in the FATEALLCHEM project. The project was financed by the European Commission with a total budget of 2.7 mill EUR (www.fateallchem.dk and http://europa.eu.int/comm/research/quality-oflife/ka5/en/01967.html) and dealt with benzoxazinoids from cereals. When using cereals as catch crops and green manure, the allelopathic properties of the cereals could now be much more extensively exploited, choosing varieties with optimal production of benzoxazinoids and optimizing the time of sowing in relation to the formation of bioactive metabolites. The project showed that future assessments of an extensive use of allelopathic crops must include the development of validated analytical methods, considerations of relevant concentrations, studies on soil transformation, ecotoxicological studies on individual compounds and mixtures, evaluation on human and mammal toxicity and joint effect studies on weeds, fungi and pests. This poster only presents selected results.

AGRO 69: Modelling of degradation kinetics for the cereal allelochemical 2-benzoxazolinone (BOA) and its metabolites in soil Anders G. Understrup¹, Sabine Ravnskov¹, Hans Christian Bruun Hansen², and Inge S. Fomsgaard¹, (1) Department of Crop Protection, Danish Institute of Agricultural Sciences, Research Centre Flakkebjerg, Slagelse DK-4200, Denmark, Anders.Understrup@agrsci.dk, (2) Chemistry Department, The Royal Veterinary & Agricultural University

Defense compounds in cereals (benzoxazinoids) have been shown to possess allelopathic effects. Studies of the degradation kinetics for allelochemicals and the metabolites provide necessary information in estimating the exploitability of these compounds, as the weed reducing effects and the risk of leaching to aquatic environments are dependent on the half-lives of benzoxazinoids and their metabolites in soil. The determination of compound half-lives is a novel approach in the allelochemical literature. Modelling of the kinetics is performed according to the "Guidance Document of Estimating Persistence and Degradation Kinetics from Environmental Fate Studies in EU registration", a guidance document prepared by the FOCUS group in the European Commission. This poster presents results of the modelling of degradation data from the allelochemical 2benzoxazolinone (BOA) and its metabolites in soil. The research was part of the FATEALLCHEM project, financed by the European Commission (www.fateallchem.dk and

http://europa.eu.int/comm/research/quality-of-life/ka5/en/01967.html)

AGRO 70: Metolachlor, total coliforms and *Escherichia coli* dissipation in soil treated with biosolid

Wondi Mersie, **Jonathan R. Moore**, Clyde G. McNamee, Steven Pao, and Asmare Atalay, Virginia State University, P.O. Box 9061, Petersburg, VA 23806, Fax: 804-524-5950

The effect of rainfall on the release of metolachlor, Escherichia coli, and coliforms from Bojac sandy loam soil treated with a biosolid (sewagesludge) was investigated. Rainfall at 65 mm h⁻¹ for 45 min was simulated on aluminum tilted beds (3 m long by 0.9 m wide) filled with Bojac sandy loam soil containing a biosolid. Aqueous surface runoff, leachate and soil samples were collected and analyzed. The average concentration of metolachlor was greater in surface runoff than in leachates. However, there was no difference in total coliform and E. coli counts in surface runoff and leachate samples. Biosolid incorporation in Bojac soil reduced total volume of surface runoff by increasing water infiltration as compared to beds without the biosolid. The reduction of metolachlor concentration after rain simulation in soil with and without biosolid was 64 and 54%, respectively. Metolachlor metabolite, oxanilic acid (OA) was detected in greater quantity in soil with biosolid than without. The reduction in concentration of metolachlor could be due to removal by runoff, retention by soil and degradation during the seven day period between herbicide application and rainfall simulation. Biosolid incorporation increased the retention and dissipation of metolachlor.

AGRO 71: Investigating the photostability of aphicidal benzamidazole and triazole analogs

Evon Anthony Bolessa¹, Scott D. Crawford¹, Benjamin J. Dugan¹, John W. Lyga¹, Robert N. Henrie II¹, Walter H. Yeager¹, Zeinab M. Elshenawy¹, Harvey R. Wendt¹, Joseph A. Argentine¹, David M. Roush², Frank J. Zawacki¹, William D Gravelle¹, Linda Varanyak¹, James M. Willut¹, and Leo Dungan¹, (1) Agricultural Products Group, FMC Corporation, P.O. Box 8, Princeton, NJ 08543, Fax: (609) 951 3330, evon_bolessa@fmc.com, (2) Agrochemical Products, FMC Corporation The photostability of a series of benzamidazoles (1) and triazoles (2) was evaluated using a Suntest TM apparatus. The photostability of the benzamidazoles (1) varied from excellent to modest depending on the substituents (R1, R2, R3 and X). The analogs with X = N showed greater photostability while those with X = O were usually photolabile. The triazoles (2) also showed photostability that varied from excellent to poor and the stability seemed to be sensitive to the substituents (X, R1 and R2).



AGRO 72: Multiresidue analysis of seven anticoagulant rodenticides by LC/ES/MS/MS

LeEtta J. Marek, Laboratory Services Division, Minnesota Department of Agriculture, 90 West Plato Blvd, St. Paul, MN 55107, Fax: 651-297-8787, Leetta.Marek@state.mn.us, and William C. Koskinen, Soil and Water Management Research, USDA-Agricultural Research Service

Mice and rat populations are commonly controlled by two classes of rodenticide anticoagulants, coumarins and indandiones. However, poisoning of nontarget animals also often occurs. For cases such as these, a rapid, multiresidue method, which provides positive confirmation for both classes of anticoagulant rodenticides, is needed by diagnostic laboratories. A method was developed for the determination of seven anticoagulent rodenticides, coumafuryl, pindone, warfarin, diphacinone, chlorophacinone, bromadiolone, and brodifacoum by high performance liquid chromatography/electrospray/mass spectrometry (LC/ES/MS/MS). Separation was performed using a Zorbax RX-C8 (2.1 x 150 mm x 5 µm) column. The mobile phase gradient elution was 60% 10 mM ammonium acetate:40% methanol (v:v) from 0 to 4 min. increasing to 50%, to 70% and to 90 % methanol at 9, 14, and 18 min, respectively, with a total run time of 24 min. Detection was by MS/MS with electrospray ionization in negative mode. Confirmation was by retention time, m/z of molecular ion and two parent daughter transitions. Recoveries from selected matrices ranged from 70-100%. Detection limits were as low as 1-5 ng/g. The developed method was rapid and provided the simultaneous quantification and confirmation of the seven anticoagulant rodenticides.

AGRO 73: Synthesis of conformationally restricted analogs of benzhydrolpiperidine and their insecticidal activity

Syed F. Ali¹, I. Robert Silverman¹, John W. Lyga¹, Lou LaFrance², and K. G. Anouna¹, (1) Agricultural Products Group, FMC Corporation, Box 8, Princeton, NJ 08543, Fax: 609-951-3603, syed_f_ali@fmc.com, (2) Medicinal Chemistry, 3-Dimensional Pharmaceuticals, Inc

Benzhydrolpiperidines (1, m = 0) are a new class of insecticides, which provide excellent control of a broad range of Lepidoptera. Early in the project we were interested in exploring modifications to the piperidine ring and the effects on insect activity. We were especially interested in the conformationally restricted analogs, azabicyclic 3.2.1 octanes (1, n = 2) and 3.3.1 nonanes (1, n = 3). We will present the synthesis and biological activity of these new azabicyclic insecticides.





AGRO 74: Improved synthesis of carbonated soybean oil in supercritical carbon dioxide

Kenneth M. Doll, Food and Industrial Oil, USDA-ARS-NCAUR, 1815 N. University St., Peoria, IL 61604, Fax: 309-681-6340, dollkm@ncaur.usda.gov, and Servim Z. Erhan, Oil Chemical Research, NCAUR, ARS, USDA

Carbonates from oleochemical origin have shown recent promise for use in the cosmetics, filter, and detergent industries. Carbonates may also form building blocks for polymeric materials. Especially of interest are cyclic carbonates, which upon addition with an amine, form a nonisocyanate urethane. Many traditional preparations of carbonates are expensive and involve environmentally unfriendly phosgene, or metal catalysis. However, it is possible to use a simple base catalyst to directly add carbon dioxide to an epoxide. We have synthesized and characterized carbonated soybean oil from commercially available epoxidized soybean oil using a tetrabutylammonium bromide catalyst. Our synthesis takes advantage of the higher density of super critical carbon dioxidee, as compared to the gas, to considerably reduce the time required for the reaction. Fully epoxidized product could be produced in 40 hours at 100 $^{\circ}$ C (1500 PSI of CO₂), as opposed to the 70 hours reported in the literature.

AGRO 75: Pre-sowing irradiation of corn seeds

Sora B. Karabaeva, Department of Plants Studies, Samarkand Agricultur Institute, 3,Ulugbek street,Samarkand, Samarkand 703030, Uzbekistan, Fax: 998-662-312199, S_narpay@mail.ru

Specific influence of an ionizing radiation on biological objects is related to high energy of quanta and elementary particles, which significantly exceeds the bonding energy of orbital electrons in atoms, as well as the energy of chemical bonds that leads to appearance of highly reactive molecules (ions, free radicals). The highly-reactive ions, free radicals, and variously excited molecules, which appear in a biological object directly at the moment of irradiation, are initiators of primary radiationchemical processes. These processes change the structural and metabolic organization of cells and tissues that leads through a series of intermediate stages to formation of the radiobiological effect. Relatively small doses of irradiation are used for stimulation of development, rise of product, and alteration of regular processes in organisms. At the present time the pre-sowing gamma-irradiation of seeds of various agricultural crops has been widely introduced to agricultural practice providing significant profit. We have carried out a three-year study of the gamma-irradiation of corn seeds, and its influence on silage output. The irradiation dose for the corn seeds was 3.5 krad. The results showed an increase in yield (from 16 % to 20%), concentration of carotins (22%) and proteins (35%) in silage mass, and a higher stability of the irradiated plants to various diseases. Moreover, the method of presowing-irradiation accelerated harvest (8-10 days), which has significant economic impor-tance.

AGRO 76: The influence of mulching the soil with polyethylene film on agrochemical property of soil and chemical composition of tobacco

Toshniyoz Ch. Goziev, Biology, Samarkand State University, University Blvd., 15, Samarkand 703004, Uzbekistan, Fax: 998-662 312199, goziev@rambler.ru

Soil temperature and humidity can be increased by mulching the soil with polyethylene film. Increases in the temperature and humidity of soil stimulate microbiological processes. To study these problems the field experiences in Zarafshan valley of Uzbekistan have been put. Tobacco has been planted under the mulched soil with polyethylene film. The results of experiences show, that mulching the soil with polyethylene film increases the content of mobile nutritious substances ammonium, nitrate and mineral nitrogen. So, in the control 1.06 numbers the content of mineral nitrogen in arable layer was 65,4 mg/kg, in subarable - 47,6 mg/kg, in mulched variant accordingly -76,0 and 58,4 mg/kg. In other terms of the analyses was the same appropriateness too. It is connected to increase of the temperature of soil and preservation of moisture in mulching of the soil. In consequence of it the processes ammoniafication and nitrification are made active. In the mulching of soil the content of mobile phosphorus, especially in top horizons of the

soil is increased. It was observed in all terms of vegetation. Hence, mulching the most of all influences the top horizon of soil. The increase of temperature and humidity of soil promotes the increase of solubility phosphates in soil. Besides increase of the microbiological activity results in increase of the content mobile phosphates. Mulching has raised the exchange content of potassium in soil. Hence, mulching of soil raises the content of mobile nutritious substances. It has resulted in increase of the content of in plants - nitrogen, phosphorus and potassium. Alongside with it in tobacco the amount of nicotin, watersoluble carbohydrates and proteins raises. Thus mulching the soil with polyethylene film improves agrochemical composition of soil and plants.

AGRO 77: Enzymatical hydrolysis investigation on the inclusion of chiral dichlorprop methyl ester in β -cyclodextrins

Yuezhong Wen1, Shanshan Zhou¹, and **Weiping Liu**², (1) Institute of Environmental Science, Zhejiang University, P.O. Box 1707, hangzhou 310027, China, Fax: 86-571-8696-8420, (2) Research Center of Green Chirality, Zhejiang University of Technolgy, College of Biological and Environmental Engineering, Hangzhou 310032, China, Fax: 86-571-8696-8420, wliu@zjut.edu.cn

The effect of β -cyclodextrins (β -CDs) on the enzymatic hydrolysis of chiral dichlorprop methyl ester (DCPPM) has been specifically studied. Four kinds of β-cyclodextrins (β-cyclodextrin, partly methylated-CD (PM-CD), hydroxypropyl-cyclodextrin (HP-CD) and carboxymethylcyclodextrin (CM-CD)) were used. Compared with 100% DCPPM in the absence of β -cyclodextrins, the activity of lipase decreased with the increase of β-cyclodextrin and PM-β-cyclodextrin. However, CM-βcyclodextrin stimulated the lipase activity. The inhibition effect of β cyclodextrin and PM-β-cyclodextrin on the hydrolysis of DCPPM is affected by many factors other than degree of the methylation blocking the active site of lipase. UV-Vis and Fourier transform infrared (FTIR) spectroscopy studies of the complexation of aqueous DCPPM with β-CDs provide fresh insight into the molecular structure of the complex and explain the effects of β-CDs on enzymatical hydrolysis of chiral DCPPM. Data showed that inclusion complexes had formed by complexation of the CM-CD with DCPPM and the solubility of DCPPM was increased in water, which leaded to the increased lipase activity.

AGRO 78: Enantioselective degradations of (rac)-metolachlor and (S)-metolachlor in Chinese soils

Weiping Liu, Research Center of Green Chirality, Zhejiang University of Technology, College of Biological and Environmental Engineering, Hangzhou 310032, China, Fax: 571-8696-8420, wliu@zjut.edu.cn, and Yun Ma, Institute of Environmental Science, Zhejiang University

Racemic metolachlor is currently being replaced by herbicidal-active (S)-metolachlor, an enantiomer of metolachlor with specific stereo configuration at the asymmetrically substituted carbon atom in the alkyl moiety. In this study, the dissipation of (rac)-metolachlor and (S) metolachlor in soil was evaluated using achiral HPLC and chiral GC methods. Because of the presence of two chiral elements (asymmetrically substituted carbon and chiral axis), the baseline separation of metolachlor enantiomers was not achieved. The obtained results showed that (S)-metolachlor degrades faster than (rac)metolachlor in Chinese soils. After a 42-day incubation, 73.4% of (rac)metolachlor and 90.0% of (S)-metolachlor were degraded, respectively. Howerer, the degradation process in sterilized soil showed no enantioselectivity due to the absence of biological processes. The results indicate that enantioselective degradations may greatly affect the environmental fate of metolachlor and should be considered when the environmental behavior of these compounds is assessed.

AGRO 79: Differential metabolism of benzhydrolpiperidines in the rat

Shaaban F ElNaggar¹, Theresa McLaughlin², R. William Creekmore¹, Robert Henrie¹, Diana Wu³, and Jinn Wu³, (1) Environmental Sciences, FMC Corporation, PO Box 8, Princeton, NJ 08543, Fax: 609-951-3670, shaaban_elnaggar@fmc.com, (2) Finnigan Mass Spectrometry, Thermo Electron Corporation, (3) XenoBiotic Laboratories, Inc

Benzhydrolpiperidines, Compounds 1 and 2 (Figure 1), two analogues of FMC insecticide candidates were evaluated to determine their

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mammalian metabolism and disposition profiles. Their ¹⁴C-radiolabeled isotopes were studied in the rat following oral administration at a rate of 5 mg/kg of rat body weight. Elimination of the N-ethyl analogue was quite different from that of the N-methyl analogue. The N-ethyl moiety containing a beta-carbon position, provided an extended metabolic site, that was readily metabolized to highly polar functions, alcohol and carboxylate groups, resulting in a facile conjugation and elimination of the chemical and its metabolites. On the other hand, the N-methyl analogue underwent N-demethylation resulting in minor polarity alteration and relatively slower elimination rate.



(Figure 1)

AGRO 80: Integrated metabolite and transcript profiling for plant natural product pathway discovery and manipulation Richard A. Dixon, Lahoucine Achnine, Bettina Deavours, Mohamed Farag, Marina Naoumkina, and Lloyd W. Sumner, Plant Biology Division, Samuel Roberts Noble Foundation, 2510 Sam Noble Parkway, Ardmore, OK 73401, Fax: 580-224-6692, radixon@noble.org

The rich diversity of chemical structures found in the plant kingdom arises in large part from a limited number of basic chemical scaffolds (eg. terpene, polyketide) that are modified by a limited number of chemical substitution types (hydroxylation, glycosylation, acylation, prenylation, O-methylation, etc). Much of the diversity is brought about by the substrate- and/or regio-specificities of the substitution enzymes. In contrast to the large collections of gene sequence and transcript level data available on-line. little detailed information exists on the plant (secondary) metabolome. Promiscuity of substrate specificity in vitro may complicate attempts to assign functions to genes of secondary metabolism accessible to researchers through various cDNA library collections. Using the isoflavonoid and triterpene pathways in Medicago species as examples, we describe how integrated metabolite and transcript profiling approaches can aid functional genomics, help explain metabolic regulation, and provide tools for assessing the impacts of genetic modifications in plant secondary metabolism.

AGRO 81: Potential and limitations of profiling methods for food safety assessment

Harry A. Kuiper and Esther J. Kok, RIKILT Institute of Food Safety, Wageningen University&Research Centre, Bornsesteeg 45, 6708 PD Wageningen, NV, Fax: 31 317 417717, harry.kuiper@wur.nl

Non-targeted profiling methods like gene expression technology, proteomics and hyphenated analytical techniques have been proposed as tools to characterise the safety of foods. In particular attention is paid to the identification of unintended alterations the composition of genetically modified (GM) food crops as result of the genetic modification and its consequences for human/animal safety. The feasibility and limitations of the use of microarray technology proteomics and nuclear magnetic resonance (NMR) to detect possible altered gene expression patterns as result of genetic modification will be evaluated, and results from the European Thematic Network on the Safety Assessment of Genetically Modified Food Crops (ENTRANSFOOD, GMOCARE) will be presented. Results from microarray analysis and metabolite profiling indicate that these technologies may successfully be applied to screen for intended and unintended side-effects of breeding processes, while the use of proteomics demands further development. The set up of interconnected data bases containing compositional profiles obtained under varying developmental stages and environmental conditions, is essential for routine use of these techniques for safety assessment purposes.

AGRO 82: Metabolic networks from *Arabidopsis* to woody plants ensure predictable orderedness in lignin/lignan/phenylpropanoid pathway metabolism

N.G. Lewis, Institute of Biological Chemistry, Washington State University, PO Box 646340, Pullman, WA 99164-6340, Fax: 509-335-8206, lewisn@wsu.edu

The application of genomic, proteomic, metabolomic, computational and structural biology analyses to wild type, mutant and transgenic plant lines has markedly altered how we study, for example, phenylpropanoid metabolism and growth/development in vascular plants. Using the phenylpropanoid pathway as a model system (together with related metabolic cross-talk), we describe the predictability of modulating various steps on overall metabolism, ranging from phenylalanine ammonia lyase to dirigent protein mediated coupling (and analogous processes) leading to the lignans, lignins and associated metabolites. The recently developed approaches amenable to the identification of such biochemical network systems are comprehensively defined as is the fully explicable nature of the biochemical processes involved. The widely claimed but unproven random coupling model (now recently designated as "combinatorial" biochemistry) leading to lignins/lignans is discussed, and the limitations revealed. Interestingly, the latter model has been entirely lacking in any biochemical characterization including identification of a single new enzyme/protein.

AGRO 83: Specialized metabolism in aromatic plants

David R. Gang, Department of Plant Sciences and Bio5 Institute, University of Arizona, 303 Forbes Building, Tucson, AZ 85721-0036, Fax: 520-621-7186, gang@ag.arizona.edu

Aromatic plants like sweet basil (Ocimum basilicum L.), ginger (Zingiber officinale Rosc.) and turmeric (Curcuma longa L.) produce a diverse set of metabolites, well known for their bioactive properties. For example, the curcuminoids and gingerols, found in the rhizome tissue of turmeric and ginger possess anti-inflammatory and other pharmacological properties. Eugenol and related phenylpropenes are important components of many economically important herbs and spices (such as sweet basil and cloves) and are highly valued as flavoring/fragrance additives and for their biological properties. Because of these properties, these plants have been used for millennia as spices and as important elements in traditional Indian and Chinese medicine, and now as important parts of modern herbal remedies that are designed to reduce inflammation, treat nausea and fight infections. Despite their importance to human health, the biochemical pathways that produce the important bioactive compounds in these aromatic plant species have only recently been investigated. We have created an aromatic plant EST database from selected lines and tissues of sweet basil, ginger and turmeric, and have used this database to identify several genes involved in the production of important specialized metabolites in these plants. We are also producing cDNA microarrays to characterize the expression profiles of genes with known and unknown function, in various tissues and at various stages of development, coupled to analysis of LC/MSand GC/MS-based metabolic profiling with the goal of identifying other genes involved in production and regulation specific metabolite production.

AGRO 84: Quantitating the natural variability in hybrid corn composition

Tracey L Reynolds, J Astwood, M Nemeth, K Glenn, and W Ridley, Product Safety Center, Regulatory Science, Monsanto Company, 800 N Lindbergh Blvd-O3A, St Louis, MO 63167, tracey.l.reynolds@monsanto.com

It is generally assumed that the composition of corn grain is fairly constant. To test this view, and to understand base-line variability in grain composition, 7 hybrid corn varieties grown at 4 different locations were analyzed for a range of metabolites. Of the 4935 hybrid-to-hybrid comparisons, 40% were found to be statistically significantly different (p<0.05). Comparisons were also made of any one hybrid to itself at each site to assess the effects of environment on corn composition. Of the 1974 comparisons, 22% were found to be statistically significantly different (p<0.05). In total, all of the differences in analyte levels found



in this study emphasize the importance of genetic background and environment as important determinants of biochemical composition and allows one to better understand the natural range of these components.

AGRO 85: Application of NMR-based metabolomics to environmental toxicology

Ronald S. Tjeerdema¹, Mark R. Viant², Christopher A. Pincetich¹, and Eric R. Rosenblum¹, (1) Department of Environmental Toxicology, University of California, Davis, One Shields Avenue, Davis, CA 95616-8588, Fax: 530-752-3394, rstjeerdema@ucdavis.edu, (2) School of Biosciences, The University of Birmingham

NMR-based metabolomics is proving to be a powerful technique for characterization of organism health and the metabolic perturbations that result from exposure to hazardous chemicals or natural stress factors in the environment. Recently, the approach was used to determine the actions of several pesticides on the developing life stages of chinook salmon and medaka. Following chemical exposure, survivors were flash frozen, subjected to perchloric acid extraction, and lyophilized. Proton NMR spectra of the reconstituted extracts were acquired and analyzed using principal components analysis, enabling visualization of the biochemical changes that occur at each developmental stage. Observed differences in the metabolic responses to the pesticides at different developmental stages are most likely an indication of their different biochemical modes of action. Detailed results will be presented to provide an example of the potential of NMR-based metabolomics to characterize organism health and the deleterious metabolic impacts that can result from chemical exposure.

AGRO 86: Long term monitoring of ammonium in precipitation, the role of the National Atmospheric Deposition Network Karen Karlin, Van Bowersox, and Bob Larson, Illinois State Water Survey, National Atmospheric Deposition Network, 2204 Griffith Dr, Champaign, IL 61820, kharlin@uiuc.edu

The National Atmospheric Deposition Program's National Trends Network (NTN) has measured the acids, nutrients, and base cations in U.S. precipitation for more than two decades. Researchers use NTN data to determine the role of wet deposition for monitoring chemical changes in the environment. The NTN has over 250 precipitationmonitoring stations throughout the continental US, the Virgin Islands, Puerto Rico, Hawaii, and Alaska. Precipitation scavenges airborne gases and particles, which are affected by emissions, chemical transformations, and weather, NTN data indicate that significant changes have occurred in precipitation chemistry, particularly for the ammonia/ammonium system and important related chemical species. Ammonium concentrations have increased in precipitation over the last 20 years at the majority of NTN stations. The largest ammonium increases are in the midwestern states. This presentation will discuss the NTN, its role in monitoring precipitation chemistry, and the trends observed for ammonium levels in precipitation over the last 20 years. AGRO 87: Monitoring atmospheric chemistry In an agricultural region using annular denuder technology

Wayne Robarge, Department of Soil Science, North Carolina State University, Raleigh, NC 27695-7619, wayne_robarge@ncsu.edu, and John Walker, National Risk Management Research Laboratory, U.S. Environmental Protection Agency

An increase in the density of animal feeding operations can impact air quality within a rural region. Ambient monitoring of ammonia and speciated inorganic PM2.5 and its acid precursors using annular denuder technology was conducted at 3 sites with widely differing local ammonia emissions in eastern North Carolina. Annual average ammonia concentrations were approximately 5 micrograms per meter cubed at distances beyond 1 km from animal operations. Total concentrations of ammonium-based PM2.5 were 8.7 micrograms per meter cubed in an area with relatively high ammonia emissions compared to 5.3 micrograms per meter cubed at a low ammonia emissions coastal site. Inorganic aerosol formation in the region of highest emissions is acid-gas limited, and sulfate aerosol exhibits a higher degree of neutrality than displayed at the coastal site. Although labor intensive, annular denuder technology provides an assessment of ambient atmospheric chemistry necessary for understanding the impact of agricultural operations on a regional basis.

AGRO 88: An assessment of ammonia emissions from alternative technologies for swine waste

Wayne Robarge¹, Viney P. Aneja², Pal Arya², Lori Todd³, and Kathleen Mottus³, (1) Department of Soil Science, North Carolina State University, Raleigh, NC 27695-7619, wayne_robarge@ncsu.edu, (2) Dept. of Marine, Earth & Atmospheric Sciences, North Carolina State U, (3) Department of Environmental Sciences and Engineering, University of North Carolina at Chapel Hill

In 2001, a multi-institutional research science team, Project OPEN (Odor, Pathogens, and Emissions of Nitrogen) was funded to conduct evaluations of "Environmentally Superior Technologies" (EST) for handling swine waste. Presented here is the approach adopted by Project OPEN to evaluate the ability of the ESTs to reduce ammonia emissions. The approach adopted had to allow comparison of measurements differing in space and time. The approach does NOT contrast absolute measurements. Rather, relative emissions of N as ammonia (%E) from baseline farms (conventional technology) are compared to those measured for EST sites, after suitable corrections for differences in animal numbers, feed composition, housing ventilation, N excreted, size of lagoons, and weather parameters. The numerical difference between %E values serves as the index calculated for comparison between ESTs. Although not optimal in design, the approach has proven successful in identifying alternative technologies that have succeeded in substantially eliminating or reducing atmospheric emissions of ammonia.

AGRO 89: Determining ammonia dry deposition near a swine facility using low-cost passive samplers

John Walker, National Risk Management Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC 27711

Domestic animals are the largest source of atmospheric ammonia, comprising approximately 40% of natural and anthropogenic emissions combined, while synthetic fertilizers and agricultural crops contribute an additional 23% of emissions. Within and downwind of mixed agricultural regions, ammonia plays a significant role in the formation of inorganic PM2.5, and deposition of nitrogen to terrestrial and aquatic systems. This project investigates the dry deposition of ammonia near a swine production facility in eastern North Carolina. Passive samplers are used to measure weekly-integrated ammonia concentrations along horizontal gradients from the lagoon/housing complex out to a distance of 500 m. Dry deposition is estimated using a resistance model that accounts for vegetation and soil compensation points as well as cuticular and stomatal uptake. Results indicate dry deposition rates ranging from 200 kg NH₃-N per ha per yr within 25 m of the lagoon/housing complex to 5 kg NH₃-N per ha per yr at a distance of 500 m.

AGRO 90: Regional off-target movement of auxin-type herbicides in the Pacific Northwest USA

Vincent Hebert, Entomology Department, Food and Environmental Quality Laboratory, Washington State University, 2710 University Drive, Richland, WA 99352, Fax: 509-372-7460, vhebert@tricity.wsu.edu, Gail Amos, Pesticide Management Division, Washington State Department of Agriculture, Jane LePage, Food and Environmental Quality Laboratory, Washington State University, and Kenneth Holshue, Environmental Sciences and Regional Planning, Washington State University-TriCities

Grape vineyards, especially in regions of mixed cereal and field crop production have historically been exposed to auxin-type herbicides, presumably from a combination of local spray drift and regional offtarget movement. The combined efforts among affected grape and cereal grain commodity groups, regulatory agencies, and land grant university research has significantly reduced the severity and number of reported auxin-type herbicide injuries over the past fifty years. These efforts have lead to the banning of dust and volatile ester formulations, restricting the timing of low volatile ester formulations, and prohibiting applications when physical drift is likely. Unfortunately, episodic vine injuries from regional off-target herbicide movement remains severe and occasionally causes economic losses to the grape industry. Our recent WSU air and vine injury monitoring programs further underscore the chronic nature of regional off-target movement of this class of herbicides to vineyards throughout the Columbia River and Walla Walla Valleys. The auxin-type herbicides will remain important agrochemical tools for economically managing broadleaf weeds in cereal grains and field crops. To minimize future injury to non-target sensitive crops, all stakeholders must continue to work together. Cooperation among commodity grower groups and policy harmonization among state agricultural departments in the Pacific Northwest should be encouraged. Meanwhile, applied field research should also continue to assist stakeholders in characterizing potential sources of local, regional, and long-range transport of chlorophenoxy herbicides and taking necessary steps to more effectively mitigate non-target crop injury of these highly active herbicides.

AGRO 91: Adaptation and application of LC/MS/MS in FMC's Environmental Sciences Laboratory

Audrey W. Chen, Environmental Sciences, FMC Corporation, P. O. Box 8, Princeton, NJ 08543, Fax: 609-951-3670, audrey chen@fmc.com

Since the Micromass Quattro LC/MS/MS was installed in FMC's lab three years ago, most of the trace FMC agrochemicals in environmental, crop, and biological sample matrices have been routinely analyzed by this instrument. The greatest advantage of this instrument over the conventional GC is that LC/MS/MS can shorten the time for method development, sample preparation and analysis. The labor-intensive chemical derivatizations to reduce the compound polarity and sample clean-up procedures for GC at ppb levels, particularly for the conjugated metabolites, can be reduced considerably or eliminated. FMC's current analysis of agrochemicals by the LC/MS/MS, including parent and metabolite compounds, will be summarized. Some of the compound's chemical and physical properties, which determine the instrument sensitivity will be discussed. Ionization suppression and enhancement due to matrix effects are common phenomena. The possible means to eliminate them will be discussed. Sensitivity comparison by GC and LC/MS/MS for some compounds will also be demonstrated. The ion source, another crucial part that determines the instrument sensitivity, from different products will be compared. The sensitivity comparison of several newly designed LC/MS/MS products will be presented as well. Other than trace analysis in environmental, crop, and biological samples, FMC's LC/MS/MS has been used in support of other agrochemical development areas including metabolism, analytical, formulations, toxicology, risk exposure, and other non-crop applications. Furthermore, it has supported the discovery areas, such as crop and soil efficacy trials for the pipeline compounds. LC/MS/MS can promptly provide invaluable preliminary data, which can then be used to identify the most promising candidate compounds for further advanced development.

AGRO 92: Environmentally friendly syntheses of pyridine monoand dicarboxylic acids via permanganate oxidation Qiuhua Zhang, Eric Meyer, Mike W. Osborne, and Marie Marcenac, Technology, Carus Chemical Company, 1500 8th St, LaSalle, IL 61301, Fax: 815 224-6896

Pyridinecarboxylic acids and their derivatives are important intermediates in pharmaceutical, agrochemical and fine chemical industries. In this work, a series of pyridinecarboxylic acids and dicarboxylic acids with high purity and high yield are synthesized from permanganate oxidation of corresponding picolines, lutidines, and ethylmethylpyridine in aqueous solution at 70 - 85°C. Reaction parameters are optimized. The yields are >75% and > 64% for pyridinecarboxylic acids and pyridinedicarboxylic acids, respectively. The processes are simplified to synthesize high purity products (> 99%). Large crystals of pyridinedicarboxylic acids are produced via temperature-controlled acidification and crystallization, which is one of the most crucial steps in production scale-up. Products are analyzed on HPLC, GC-MS, and SEM. The manganese oxide by-product from permanganate oxidation is successfully recycled in KMnO₄ manufacturing, or modified to oxidatively/catalytically active manganese dioxide, therefore no solid waste is generated. The overall processes are environmentally friendly, economic, and versatile in a large class of

organic syntheses by permanganate oxidation.

AGRO 93: Desorption kinetics of chloroacetanilide and dinitroaniline herbicides from unsaturated soil in the presence of surfactants

Wenli Yang and Britt A Holmen, Environmental Engineering Program, University of Connecticut, 261 Glenbrook Road, Storrs, CT 06269, Fax: 860-486-2298, wenli@engr.uconn.edu

Chloroacetanilide and dinitroaniline herbicides are common preemergence herbicides. After field application, the partitioning of herbicides between soil and the ambient atmosphere depends on environmental conditions. Surfactants are important components in herbicide formulations that improve the performance of the active ingredients. However, to our knowledge, little has been reported about the influence of surfactants on the soil-air desorption processes of herbicides. Quantifying and modeling herbicide desorption kinetics in the presence of surfactants is important for understanding and controlling the transport and fate of herbicides in the environment. Desorption experiments were conducted in soil-gas flow systems at constant temperature (25 °C) and relative humidity (40%). Two surfactants, one anionic and one nonionic, were examined with seven herbicides representing two families-chloroacetanilides and dinitroanilines. Connecticut clay loam soil was spiked with pure herbicide or a herbicide-surfactant mixture and was allowed to air dry prior to loading into a stainless steel filter holder. Clean, particle-free air was pulled through the soil, and gaseous herbicides desorbed from the soil were collected on polyurethane foam (PUF) plugs. The PUF and soil samples were extracted by supercritical fluid extraction (SFE) and analyzed by GC/MS to quantify herbicide concentration in the gas and soil phases, respectively, as a function of exposure time up to 400 hours. Metolachlor and pendimethalin air-soil desorption was 3 to 4 times faster when the herbicides were in a surfactant mixture. The effects of surfactants on the relationships between desorption behavior and herbicide physicochemical properties (e.g., vapor pressure and octanol-water partition coefficient) will be discussed.

AGRO 94: Metabolomic assessment of a potato field trial: The metabolic composition of high fructan GM potatoes is equivalent to classic cultivars

Oliver Fiehn, UC Davis Genome Center, UC Davis, Health Sci Drive, Davis, CA 95616, ofiehn@ucdavis.edu, and John Draper, Institute of Biological Sciences, University of Wales

There is concern that genetic engineering may allow the introduction of unforeseen traits into crops, causing them to contain undesirable metabolites. Substantial equivalence is used to structure the safety assessment of GM foods. As test case for a strategy combining analytics and statistical metrics for assessing compositional similarity, we compared field-grown tubers from six conventional potato cultivars and six experimental genotypes bioengineered to contain high levels of fructans. A hierarchical mass spectrometry-based metabolomics approach is described which utilizes firstly a rapid metabolite fingerprinting technique to assess overall compositional similarity followed by comprehensive metabolite profiling where there is evidence for unexpected differences. We show that high fructan GM potatoes do not exhibit unexpected compositional alterations and suggest that this approach has value for future food safety assessments. These findings were reproduced in two years with large climatic differences in the four weeks prior to harvest

AGRO 95: NMR profiling of transgenic peas

Adrian J. Charlton, Central Science Laboratory, Department for Environment, Food and Rural Affairs, Sand Hutton, York YO41 1LZ, United Kingdom, Fax: +44-0-1904-462133, adrian.charlton@csl.gov.uk

Recent metabolomic studies have focused on detecting pleiotropic (unintended) effects of transgene insertion in plants. Manipulation of the genome through genetic engineering can lead to perturbation of metabolic pathways other than those intended. Additionally, environmental factors and natural genetic diversity often alter the distribution of metabolites. Studies of natural diversity and environmental effects have been undertaken in order to evaluate the



significance of metabolic changes due to transgene insertion. An NMR study of the metabolome of *Pisum* is presented. Pea plants (n≈1300) grown over three years, form the basis for the most extensive metabolomic study of this agriculturally relevant crop. Leaves and seeds were harvested from 21 *Pisum* genotypes and from a recombinant inbred population. *Pisum sativum* cv. Puget was used to study environmentally induced diversity in the metabolome. This information is being used to set into context changes in the metabolome produced by genetic modification.

AGRO 96: Modification of potato alkaloids: A lesson in applied metabolomics

Kent F. McCue¹, Louise V.T. Shepherd², David R. Rockhold¹, Paul V. Allen¹, Howard V. Davies², and **William R. Belknap**¹,(1) Western Regional Research Center, USDA Agricultural Research Service, Albany, CA 94710, Fax: 510-559-5775, kmccue@pw.usda.gov, wrb@pw.usda.gov, (2) Quality, Health & Nutrition Programme, Scottish Crop Research Institute

Potatoes contain steroidal glycoalkaloids (SGAs), undesirable bitter metabolites whose accumulation is subject to environmental, physical and genetic variation. Two major triglycosylated SGAs α -chaconine and α -solanine have been the targets of genetic down regulation. Using members of the steroidal alkaloid glycosyl transferase (SGT) gene family we have analyzed the effects of antisense down regulation of the pathway at multiple steps. The resulting transgenic plants have been analyzed for SGA profiles as well as additional non-specific metabolic perturbations and variations as a result of the genetic transformation regeneration process. What we have observed is that feedback regulation between products of the pathway and the biosynthetic enzymes has resulted in compensation of end products or intermediates resulting in a net zero effect on total levels of SGAs in antisense tubers.

AGRO 97: Application of metabolite profiling in rice

Karl-Heinz Engel¹, Thomas Frenzel², Andreas Miller¹, Thomas Frank¹, and Richard Roehlig¹, (1) Chair of General Food Technology, Technical University Munich, Am Forum 2, Freising D-85350, Germany, Fax: +49-8161-714259, K.H.Engel@wzw.tum.de, (2) Landesuntersuchungsamt Sachsen

A gas chromatographic metabolite profiling method for screening of a broad spectrum of compounds has been developed using rice as model crop. The approach is based on a fractionation which allows nontargeted investigation of major and minor rice constituents. Software tools for comparative analysis of metabolite profiling data were developed. They allow transfer of normalized datasets into databases and automated unbiased comparison of chromatograms. Application of the metabolite profiling methodology to the analysis of genetically modified and conventional rice revealed the suitability of the approach to detect statistically significant differences between metabolite levels in different genotypes. The usefulness of databases established through investigation of conventional rice cultivars for assessment of differences in metabolite profiling data is demonstrated.

AGRO 98: Natural variability of bioactive components in vegetable crops

E.H. Jeffery, University of Illinois, Department of Food Science and Human Nutrition, 905 S. Goodwind Ave, Urbana, IL 61081, Fax: 217-265-0925, ejeffery@uiuc.edu, and John A Juvik, Department of Natural Resources and Environmental Sciences, University of Illinois

Variability in content of bioactive components within food plants has proven a substantial hindrance to interpretation of epidemiological studies of diet and chronic disease incidence, to the study of safety and efficacy of bioactive components within whole foods, and to providing consumer varietal and dose recommendations. Establishing component databases is crucial for eventual control of this variability. Traditionally, growers have chosen varieties based on crop production factors, cosmetic product appeal and pest control. Without information on content of bioactive food components within available varieties, the grower cannot use this as a factor in deciding which variety to grow. In general, variability in bioactive food component concentrations is regulated by environmental and genetic factors and by their interaction. This information can also be used to develop strategies for enhancing vegetable health promotion through genetic manipulation and/or management of the crop's growing environment and processing conditions.

AGRO 99: Assessing metabolic health and dietary intervention J. Bruce German, Department of Food Science & Technology, University of California at Davis, Cruess Hall, One Schields Avenue, Davis, CA 95616-8598, Fax: 530-752-4759

The knowledge, technologies and research strategies emerging from genomics sciences are changing agriculture and providing opportunities to improve food. The varying needs for different dietary components among different people and situations can be matched to the varying compositions, functions and actions of foods. Human health assessment will increasingly require the accurate, comprehensive measurement of individual metabolism through the new field of metabolomics. The capability to measure and model lipid species in human blood comprehensively provides the means to distinguish various metabolic features of health. Identifying the components and bio-actions of foods is also being enabled by these new tools. Milk evolved with the Darwinian pressure to nourish, protect and support mammalian infants, and new analytical tools are revealing the means by which these benefits are achieved. Food processing is taking advantage of the broader biological understanding of commodities to bioguide commodity components towards more targeted food compositions, functions and delights.

AGRO 100: Knowledge of dynamic soil transformation processes: A key issue in the evaluation of defense properties of cereal benzoxazinoids

Inge S. Fomsgaard¹, Solvejg K. Mathiassen¹, Per Kudsk¹, Anne G. Mortensen¹, Carsten Christophersen², Thomas Etzerodt¹, Mia B. Gents¹, Stine S. Krogh¹, Susanne J.M. Mensz¹, Susan T. Nielsen¹, and Anders G. Understrup¹, (1) Department of Crop Protection, Danish Institute of Agricultural Sciences, Research Centre Flakkebjerg, Slagelse DK-4200, Denmark, Fax: +45 58113301, Inge.Fomsgaard@agrsci.dk, (2) Department of Chemistry, University of Copenhagen, Denmark During the last decades there has been an increasing focus on the prospects of exploiting the defense properties of secondary metabolites from agricultural crops as an alternative strategy for controlling weeds, insects and diseases. Defense properties (allelopathic properties) of cereal benzoxazinoids have been investigated thoroughly. In this presentation it will be shown that a complex pattern of benzoxazinoids and their microbial transformation products can be found in soil depending on the initial concentration of benzoxazinoids in plants, soil or test media. Some of the transformation products showed much more pronounced biological activity than the parent compounds from wheat. Conclusions in earlier published studies, in which the effect of cereal benzoxazinoids on weeds or soil-borne diseases have been studied without any focus on the transformation that occurred during the time of study, must now be revised. The research was part of the FATEALLCHEM project, financed by the European Commission (www.fateallchem.dk and http://europa.eu.int/comm/research/quality-oflife/ka5/en/01967.html)

AGRO 101: Transport and degradation of glyphosate in a midwestern tile-drained watershed, Sugar Creek, Indiana Michael Meyer, Jeffrey W. Frey, Edward A. Lee, Kathryn Kuivila, and Mark Sandstrom, U.S. Geological Survey, 4821 Quail Crest PI, Lawrence, KS 66049, mmeyer@usgs.gov

Concentrations of glyphosate and aminomethylphosphonic acid (AMPA) ranged from less than 0.01 to more than 400 μ g/L in overland-flow, tile-drain, surface-water, and wet deposition (rainfall) samples collected between May and September 2004 at a row-crop field planted in glyphosate-resistant soybeans. Concentrations of glyphosate and AMPA ranged from a maximum of approximately 20 to 450 and 3 to 30 μ g/L, respectively, in overland-flow samples. Concentrations of glyphosate and AMPA ranged from less than 0.01 to 5 and 0.01 to 2.6 μ g/L, respectively, in tile-drain samples and surface water from a drainage ditch adjacent to the farm. Glyphosate and AMPA were

detected at concentrations of less than 2 μ g/L in 11 wet deposition samples collected between May and September. Spatial and temporal variations in concentrations of glyphosate and AMPA also were observed in pre- and post-application 45-cm deep soil cores divided into 15-cm intervals.

AGRO 102: Assessing soil quality attributes by factor analysis with non-negativity constraints

Jianhang Lu, Laosheng Wu, and Andrew C. Chang, Department of Environmental Sciences, University of California-Riverside, 900 University Ave., Riverside, CA 92521, Fax: 951-827-3993, Jianhang@ucr.edu

Assessment of soil quality is of great importance for both agricultural production and environmental protection. A model of factor analysis with non-negativity constraints is developed to assess soil quality attributes. The model is solved by the positive matrix factorization (PMF) algorithm. Mathematically, it finds a set of factors in nonnegativity constrained factor spaces based on the least squares principle. Comparing to customary factor analysis through eigenanalysis, the model produces strict non-negative factor loadings and scores, which are physically meaningful and thus are easy to interpret. Preliminary results from a case study on soil quality assessment of a long-term reclaimed wastewater-irrigated cropland and a corresponding control field showed that: (1) in both fields, more than 90% of the total variances of 24 measured soil quality attributes (8 physical attributes, 13 chemical attributes, and 3 biological attributes) can be accounted for by two major factors; (2) the two factors show the characteristics of fine and coarse components of the soils, respectively; (3) long-term irrigation with wastewater appears to alter the distribution of micronutrient metals like Cr, Cu, Ni, and Zn between the fine and coarse components of the soils, though their concentrations and spatial distribution (as indicated by their mean values and standard deviations) are both close in the two fields. Detailed interpretation of the model results is currently underway. Overall, the model is able to extract information that was not obtainable from a former study with traditional statistical methods, including customary factor analysis.

AGRO 103: Dissipation of thiobencarb and oxadiazon in soil Enamul Hoque, School of Biology, University of Newcastle upon Tyne, Kings Walk, Newcastle upon Tyne NE1 7RU, United Kingdom, Fax: 44-191 222-5228, Enamul.Hoque@ncl.ac.uk, and Richard M Wilkins, Department of Agricultural and Environmental Science, Newcastle University

Thiobencarb and oxadiazon are pre-emergence soil-applied herbicides now used in tropical countries to control rice weeds. Thiobencarb (S-4chlorobenzyl diethylthiocarbamate) and oxadiazon (5-tert-butyl-3-(2,4dichloro-5-isopropoxyphenyl)-1,3,4-oxadiazol-2 (3H)-one) were used for the dissipation studies in soils. Laboratory studies were conducted at an incubation temperature of 25 C and 40% MHC (moisture holding capacity) in two Bangladeshi soils (Silmondy and Sonatala soil series) and one UK soil (Hallsworth). To increase the microbial activity in the stored soils, glucose was added at a rate of 8mg g⁻¹. Following treatment with glucose (7days) separate aliquots of various soils (80g) were treated with thiobencarb and oxadiazon at a rate of 50mg Kg-1and were incubated at 250°C for 90 days. Moisture content was monitored weekly and maintained at 40% MHC. Soil samples (5g) were extracted with hexane (10 mL) with shaking (250 rpm) for 24 hours. The extracts were analysed by High Performance Liquid Chromatography (HPLC). The minimum detection limit for both herbicide was 0.5 µg g Experiments were conducted both in glucose treated and non-treated soils. Dissipation of thiobencarb was found to be much more rapid in glucose treated soils than untreated soils due to enhanced microbial activity, while oxadiazon suffered no significant degradation in either treated or untreated soil samples.

AGRO 104: Applying fluorescence spectra on identifying natural and man-made organic pollutants

Jao-Jia Horng¹, C-L. Tang², and B.H. Hsieh², (1) Department of Safety, Health, and Environment, National Yulin University of Science and Technology, 123 University Road Section 3, Douliou 640, Taiwan, Fax: 886-5-532-6202, horngjj@yuntech.edu.tw, (2) Department of Safety, Health and Environment, National Yulin University of Science and Technology

Using Fluorescence spectra to detect or analyze natural organics was studied by many researchers on natural chemicals appearing in river basins and estuaries. By comparing the excitation and emission (EX-EM) fluorescence spectra, this study could distinguish organic pollutants from various sources, such as domestic wastewater, industrial wastewater, animal farm wastewater, run off, and ground waters. These chemicals were natural or man-made sources, such as humic acids, alcohol ethoxylates (from detergents), tyrosine, urea, urine, chlorophyll, and several antibiotics. Several visual computation algorithms were developed to identify these fluorescence spectra. With minimum or no preparation of water samples, the detection limits for different chemicals were varied from ppms to 10 ppbs with relatively good correlation (r² 0.82 to 0.99). Further applications will apply this method to determine the pollutants from swine farm wastewater. It is expected that these results might serve as one of the environmental forensic tools to determine the possible sources of natural and human pollutants in non-point source pollution in agriculture or animal farming.

AGRO 105: Pharmacokinetics of intraruminally-dosed, ³⁶Cllabeled sodium chlorate in cattle

Christy E. Oliver¹, David J. Smith², Robin C. Anderson³, and J. S. Caton¹, (1) Department of Animal and Range Sciences, North Dakota State University, P. O. Box 5727 University Station, Fargo, ND 58105-5727, christy.oliver@ndsu.edu, (2) Biosciences Research Laboratory, USDA ARS, (3) USDA-ARS

Six ruminally cannulated Loala cattle (3 steers, 3 heifers; 151 ± 36 kg) received 1 of 3 sodium chlorate levels (21, 42, or 63 mg/kg BW) in 4 intraruminal boluses over 24 hours. Blood and serum were collected by jugular catheter at h 0, 0.5, 1, 2, 4, 6, 8, 8.5, 9, 10, 12, 14, 16, 16.5, 17, 18, 20, 22, 24, 24.5, 25, 26, 28, 30, 32, 36, 40, 44, and 48 relative to first dose. Total radioactivity of whole blood and serum was measured by liquid scintillation counting. Serum chlorate was assayed by passing diluted serum through an AgNO3 column to precipitate chloride; chlorate content of eluent was determined by liquid scintillation counting. Peak total radioactivity occurred between h 30 and 36 and was dose dependent in whole blood (low: 48 ppm; medium: 83 ppm; high: 97 ppm) and serum (low: 54 ppm; medium: 99 ppm; high: 118 ppm); higher serum radioactivity concentrations indicate that chlorate/chloride do not concentrate in the blood cell fraction. Serum chlorate peaked between 1 to 2 hours post dosing and then returned to baseline between dosing times in all but the high dose. Peak serum chlorate levels were dose dependent (low: 5.6 ppm; medium: 12.0 ppm; high: 20.5 ppm). Half-lives of chlorate absorption (0.5 to 1 h) and elimination (4 to 6 h) were estimated. Chlorate is rapidly eliminated from the circulation, but chloride concentrates in blood. Intraruminally-dosed chlorate is rapidly absorbed, mostly as chloride; the chlorate fraction is quickly eliminated from blood.

AGRO 106: Residues and metabolism of 36CI-labeled sodium chlorate in cattle

David J. Smith1, C. E. Oliver2, R. C. Anderson1, and J. S. Caton3. (1) Biosciences Research Laboratory, USDA-ARS, 1605 Albrecht Boulevard, Fargo, ND 58105-5674, Fax: 701-239-1430, smithd@fargo.ars.usda.gov, (2) North Dakota State University, (3) Department of Animal and Range Sciences, North Dakota State University

Inclusion of an experimental sodium chlorate product (ECP) in the diets of cattle, sheep, swine, and poultry decreases gastrointestinal concentrations of *Salmonella* species and enteropathogenic *E. coli* strains, without adversely affecting normal microflora. The selectivity of sodium chlorate is due to the presence of assimilatory nitrate reductase in target organisms and its absence in non-target bacteria. Intracellular nitrate reductase co-metabolizes chlorate to the bactericidal agent chlorite. The objective of this study was to assess the effect of sodium chlorate dose on metabolism, residues, and excretion in cattle. Six Loala steers and heifers (151 ± 36 kg) on a forage-corn diet were trained to metabolism crates, and dosed intra-ruminally with 0.5X, X, and 1.5X levels of ³⁶Cl-labeled ECP (0.091 µCi/mg), where X is



equivalent to a dose known to have in vivo efficacy. The daily dose equivalent was administered intraruminally at 0, 8, 16, and 24 hours in equal aliquots, and animals were slaughtered 24 hours later. Total radioactive residues in urine and tissues were composed only of sodium chloride and sodium chlorate. No sodium chlorite was measured in urine or tissues. Maximum chlorate residues in liver, kidney, and adipose tissue were 5.9, 21.1, and 4.5% of provisional safe tissue concentrations (STC) of chlorate provided by the US FDA CVM. In skeletal muscle, chlorate residues were 6.9, 34.7, and 117% of the provisional FDA STC, for the 0.5X, X, and 1.5X doses, respectively. These data suggest that further development of the ECP as a feed additive for cattle is warranted.

AGRO 107: Development of a new method to quantify urinary concentrations of insecticides and herbicides in professional pesticide applicators

Frederic Ciner, Commonwealth of Virginia, Division of Consolidated Laboratory Services &, Center for Environmental Studies, Virginia Commonwealth University, 1000 West Cary Street, Room 105, Richmond, VA 23284-3050, Fax: (804) 828-1622, Frederic.Ciner@dgs.virginia.gov, Timothy R. Croley, Division of Consolidated Laboratory Services, Commonwealth of Virginia, Shelley A. Harris, Center for Environmental Studies & Department of Epidemiology and Community Health, Virginia Commonwealth University, and Charlene D. Crawley, Department of Chemistry, Virginia Commonwealth University

To assess health risks associated with pesticide exposures, robust, high-throughput, and sensitive methods for the determination of multiple pesticides in urine are necessary. The objective of this work was to develop a new method to quantify in urine a mixture of insecticides and herbicides, as part of a national occupational dose monitoring study including over 120 subjects. Of interest were the herbicides dicamba mecoprop (MCPP), 4-chloro-2-methylphenoxyacetic acid (MCPA), and 2,4-D and the insecticides, imidacloprid and bifenthrin, and their metabolites, 6-chloronicotinic acid (6-CNA) and 2-methyl-3phenylbenzoic acid (MPA), respectively. Analyses were performed using solid-phase extraction (SPE) followed by positive/negative ion electrospray ionization HPLC/MS/MS. Separation was performed using an Agilent 1100 HPLC with the mobile phase consisting of 0.1% formic acid:0.1% formic acid in ACN. Gradient separation was used (total run time of 16 minutes) on a 150 x 2 mm x 4 µm Phenomenex Synergi RP-18 column. A Bruker Esquire 3000plus quadraupole ion trap mass spectrometer was utilized for MS/MS determination of analytes. A timesegmented acquisition was utilized in the analyses. Measured concentration of analytes from over 1000 24-hour urine samples will be used to predict the total absorbed dose following multiple exposures to multiple pesticides. Data obtained in this bio-monitoring study also will be used to develop recommendations to reduce occupational exposures and the analytical method will allow for cost-effective followup of the cohort over time.

AGRO 108: Determination of urinary organophosphorus pesticide metabolites by automated solid phase extraction, post extraction derivatization, and GC-MS/MS

G.K. Hemakanthi De Alwis, Larry L Needham, and Dana B. Barr, Division of Laboratory Sciences, Centers for Disease Control and Prevention, 4770 Buford Highway. NE, Mailstop F-17, Atlanta, GA 30341, Fax: 770-488-0142, hdd9@cdc.gov

Organophosphorus (OP) pesticides account for about half of the insecticides used in the United States. They are primarily used in agriculture on crops but are also used in residential settings for pest control. Exposure of the general population to these pesticides occurs primarily from ingestion of food products or from residential use. The majority of the OP pesticides used in the United States are metabolized to up to three of six common urinary dialkyl phosphate metabolites. Quantification of these metabolites provides information on cumulative exposure to all OP pesticides. For simultaneous measurement of urinary OP metabolites, we developed an accurate, sensitive and selective method with limits of detection in the low nanogram per milliliter (ng/mL) range. This novel method involves automated solid phase extraction of human urine, followed by post extraction

derivatization of the OP metabolites with 1-chloro-3-iodopropane and analysis by isotope dilution-gas chromatography-mass spectrometry. This method allows for the unattended extraction of urine samples with a concomitant increase in sample throughput.

AGRO 109: Surangin B: Interference with mitochondrial complex III and antifungal activity

Russell A. Nicholson and Yanshen Deng, Department of Biological Sciences, Simon Fraser University, 8888 University Drive, Burnaby, BC V5A 1S6, Canada, Fax: 604-291-3496, nicholso@sfu.ca

Our previous investigations have found that surangin B (a coumarin from the roots of Mammea longifolia) blocks electron transport in bovine heart mitochondria at complexes II, III and IV. Difference spectra of reduced complex III equilibrated with surangin B were found to closely parallel those of the Qi site blocker antimycin A but not those obtained with the Qo site-selective inhibitors myxothiazol and famoxadone. Investigation of functional interference with complex III by surangin B used the electron acceptor 2-nitrosofluorene. These experiments demonstrated that like antimycin A, surangin B acts as a selective blocker of electron diversion to 2-nitrosofluorene through Qi within complex III. The release of neurotransmitter amino acids from synaptosomes evoked by surangin B was reduced by N,N,N',N'tetramethyl-p-phenylenediamine, suggesting that blockade of complex III in intraterminal mitochondria contributes to this effect. Mycelial growth and spore germination assay results indicate that surangin B may have potential in control of certain fungi associated with plants.

AGRO 110: Evaluation of esterase activity for use in removal of pyrethroid-associated toxicity to Ceriodaphnia dubia and Hyalella azteca

Craig E. Wheelock¹, Jeff L. Miller², Mike Miller², Bryn M. Phillips³, Sarah A. Huntley³, Shirley Gee⁴, Ronald S. Tjeerdema⁵, and Bruce D. Hammock⁶, (1) Department of Entomology and Cancer Reseach Center, University of California Davis, Briggs Hall, One Shields Ave, Davis, CA 95616, and Kyoto University, Ugi, Kyoto 611-0011, Japan, Fax: 530-752-1537, craig@kuicr.kyoto-u.ac.jp, (2) AQUA-Science, (3) Environmental Toxicology, University of California Davis, (4) Department of Entomology, University of California, (5) Department of Environmental Toxicology, University of California, Davis, (6) Department of Entomology and Cancer Resarch Center, University of California Davis

Current analytical techniques for pyrethroid detection in receiving waters are labor intensive, time consuming, and expensive. The use of toxicity identification evaluation (TIE) techniques is an efficient routine method to detect and identify toxicants in receiving waters. However current TIE methods do not include protocols for pyrethroid detection. Previous work reported that carboxylesterase activity successfully detected and remediated pyrethroid-associated toxicity. This project expanded upon these studies and examined the efficacy of the esterase treatment. The esterase successfully removed permethrinand bifenthrin-associated toxicity in river water (up to 1,000 and 600 ng/L, respectively) and pore water (up to 200 and 60 ng/L, respectively) using both Ceriodaphnia dubia and Hyallela azteca. Catalytically active enzyme is required to achieve full efficacy, but some non-specific protein effects were observed. Carboxylesterase activity appears to be a viable and useful treatment step for the detection of pyrethroidassociated toxicity in a variety of bioassays and TIE methods.

AGRO 111: Natural products against Formosan Subterranean Termites (Coptotermes formosanus)

Kumudini M. Meepagala¹, Weste L. Osbrink², George Sturtz³, Alan Lax², and Stephen O. Duke⁴, (1) USDA-ARS, Natural Product Utilization Research Unit, University of Mississippi, University, MS 38677, Fax: 662-915-1035, kmeepaga@olemiss.edu, (2) USDA-ARS, SRRC-FSRU, (3) Aromagen, (4) USDA- ARS, Natural Products Utilization Research Unit

The Formosan subterranean termite, *Coptotermes formosanus*, is among the most devastating termite pests. This pest costs an estimated one billion dollars a year in the United States alone. In our efforts in search for effective, environmentally friendly, termite control agents we have screened some plant extract derived natural products. Secondary metabolites are produced by plants as part of the natural defense mechanism. They play a role in defending the plants from insects, fungi, bacteria and other plants. We have postulated that this is one area to explore in order to search for such termite control agents. Among the natural products that we have tested, vulgarone B (isolated from *Artemisia douglasiana*), apiol (isolated from *Ligusticum hultenii*), and cinicin (isolated from *Centurea maculosa*) caused significantly higher mortalities compared to untreated controls in our bioassay. These compounds are present in significantly high levels in the plants from which they have been isolated and also possess other biological activities such as phytotoxic and antifungal properties. We continue to explore these compounds and their derivatives for possible use in termite control.

AGRO 112: Natural products as biopesticides: Botanical oils

Paul L. Zubkoff, Biopesticides and Pollution Prevention Division 7511C, U.S. Environmental Protection Agency, 1200 Pensylvania Ave NW, Washington, DC 20460-0001, Fax: 703-308-7026

Of the natural products that have pesticidal activities, many botanical oils, including some that are widely utilized as foods or in the preparation of foods, are registered as biopesticides. For this presentation, the chemical characteristics and compositions of some oils are reviewed as 3 groups, each with generally similar compositions and a fourth group which is very different: (a) glycerides of fatty acids; (b) essential oils; (c) citrus oils and (d) special cases. The compositions of these oils are discussed as a possible aid for identifying other natural substances that may have potential as biochemical pesticides.

AGRO 113: Treatment of pesticide-contaminated soil with the ElectroChemical GeoOxidation process

J. Kenneth Wittle, Electro-Petroleum, Inc, 996 Old Eagle School Rd., Wayne, PA 19087, Kwittle@electropetroleum.com, and Falk Doering, ElectroChemical Processes, LLC

ElectroChemical GeoOxidation (ECGO) is an electrochemical process that has been used extensively in Europe to treat soils contaminated with industrial chemicals such as PAHs, chlorinated hydrocarbons and BTEX. The process has not however been used in the treatment of pesticide contaminated farmland. EPI and ecp initiated a project to demonstrate that the ECGO can reduce the concentration of intractable pesticides from soil collected from agricultural soil. Two soil samples were collected from "contaminated farmland" and sent to the EPI test facility in Butte, MT where the soils were subjected to the ECGO treatment. At the EPI test facilities approximately one cubic yard of soil is used in the testing program. The contaminants of interest included 2,3-D; bentazon; dinoseb; chlorothalonil; metribuzin and metolachlor. The decrease in concentration with time was tracked during treatment. A steady decrease in the concentration was observed over the treatment period. The results will be presented

AGRO 114: Novel formulations for control of immature mosquitoes

Richard Levy, Michael A. Nichols, and William R. Opp, LCMCD Technology Development Center, PO Box 60005, Fort Myers, FL 33906, Fax: (239) 693-5011, levy@lcmcd.org

Novel controlled delivery and surface film technologies were developed. Matricap® controlled delivery single and joint-action granular formulations of biolarvicides and/or insect growth regulators were evaluated against freshwater and/or salt marsh mosquito larvae. Results of a series of bioassays indicated the potential for sustained long-term larval control from a single granular application. Comparative bioassays against 1st to 4th instar larvae and pupae of freshwater and salt marsh mosquito species with two experimental surface films and a commercial surface film were also evaluated. Results indicated that the larvicidal and pupicidal action of the experimental surface films were significantly faster than the commercial surface film. Additional tests showed the efficacy of aqueous joint-action admixtures of the experimental surface films and commercial products. Field evaluations with the controlled delivery and surface film formulations are in progress. AGRO 115: Precision spray application for persistence and washoff studies of foliar pesticide residues: Method development R. Don Wauchope, Southeast Watershed Research Laboratory, USDA-Agricultural Research Service, POB 748, Tifton, GA 31794, Fax: 229-386-7215, don@tifton.usda.gov, Theodore M. Webster, Crop Protection and Management Research Unit, USDA- Agricultural Research Service, Thomas L. Potter, Southeast Watershed Research Laboratory, USDA-ARS, and Laura Wade, Science Department, Crisp County Public Schools

Pesticide spray concentrations in the plant canopy are typically difficult to measure because of large variation in deposition from the typical sprayer. This high variability is a serious problem because a good description of the fate of pesticide residues on plant foliage residues is a fundamental need for predicting food residues and the environmental fate of many pesticides. One approach to this problem is to develop a high precision technique for measuring deposition of pesticide spray solutions on specific locations within the plant canopy. We are investigating a technique that uses a soluble fluorescent dye and digital graphic image analysis along with washoff experiments using both classical residue analysis and fluorescence spectrometry. Preliminary results suggest that we are able to precisely characterize absolute deposit amounts and their variability from point to point in a plant canopy, and as a consequence we are able to measure washoff and foliar persistence of deposits with much greater precision than previously reported.

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E. Marketing

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