

Your Name: _____



Unraveling the Exposome

Organized by

Jarod Grossman & Anthony Macherone
Agilent Technologies

32nd Sanibel Conference on Mass Spectrometry
January 23 – 26, 2020
South Seas Island Resort, Captiva, FL

Thank you to our sponsors!



Agilent Technologies

ThermoFisher
S C I E N T I F I C

Speakers – please arrive ½ hour before your session begins to load your presentation

THURSDAY, JANUARY 23

4:00 - 7:00 pm **Setup all posters, Captiva West**

6:00-7:00 pm **Registration**

7:00 – 7:10 pm **Opening Remarks**, Jarod Grossman and Anthony Macherone
Captiva East

7:10 - 8:10 pm
Keynote Lecture
Captiva East

7:10-8:10 pm **Using the Blood Exposome to Discover Causes of Chronic Human Diseases;**
Stephen M. Rappaport, *University of California, Berkeley*

8:10-10:00 pm
Reception
Captiva West

**The following students received an ASMS Student Travel Award.
Congratulations!**

Emmalyn Dupree
Clarkson University

Cassandra Herbert
University of Cincinnati

Sathisha Kamanna
Indian Institute of Science

Jeremy Koelmel
Yale University

Iqbal Mahmud
Univ. of Florida

Ons Ousji
UQAM

Leah Schneider
University of North Texas

Xinyue Zhang
Stanford University

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FRIDAY, JANUARY 24

7:00 - 8:30 am **Continental Breakfast, Captiva West**

8:30-10:15 am
The Utility of the Exposome
Captiva East

- 8:30-9:15 am **Keynote Lecture: Using High-Throughput Non-Targeted Analysis to Map the Exposome;** Jon Sobus, *U.S. EPA*
- 9:15-9:45 am **Exposomics to Study Health and Disease;** Doug Walker, *Mount Sinai School of Medicine*
- 9:45-10:15 am **NIH/NIEHS Vision and Strategies to Characterize the Exposome;** David Balshaw, *NIEHS*
- 10:15-10:45 am **Coffee Break, Captiva West**

10:45 am - 12:15 pm
Sources of Exposure

- 10:45-11:15 am **Epigenetics and Fetal Development: Recent Updates and Challenges Surrounding PFAS Exposure;** Jacqueline Bangma, *University of North Carolina*
- 11:15-11:45 am **The Human Toxome Meeting the Exposome: How Mechanistic Toxicology Helps Making Sense of Omics Data;** Andre Kleensang, *Johns Hopkins University School of Public Health*
- 11:45-12:15 pm **Assessment of Food Contaminants in Biological Matrices: From Targeted Towards Exposome-Scale Approaches;** Benedikt Warth, *University of Vienna*
- 12:15-12:30 pm **Group Photo**
- 12:30 - 1:30 pm **Group Lunch,** provided by ASMS
Sand Dollar Plaza

1:30-2:30 pm
The Microbiome

- 1:30-2:00 pm **Integrating Multi-“Omics”- Mass Spectrometry-Based Methods to Characterize Oral Carcinogenesis;** Silvia Balbo, *University of Minnesota*
- 2:00-2:30 pm **Insect and Animal Models to Study the Microbiome;** Justin Cross, *Memorial Sloan Kettering Cancer Center*
- 2:30 – 7:00 pm **Free Time**

Speakers – please arrive ½ hour before your session begins to load your presentation

FRIDAY, JANUARY 24

7:00 – 8:00 pm

Submitted Talks

Captiva East

Three Short Talks, 12 minutes each followed by 3 minutes for Q&A

Six Highlight Talks, 3 minutes each

- 7:00 – 7:15 pm **Poster #1; Untargeted Profiling of Serum Metabolites, Nutrients, and Toxins in an Exposomic Investigation of the Isle of Wight Multigenerational Birth Cohort;** Thilani M Anthony; *Michigan State University, East Lansing, MI*
- 7:15 – 7:30 pm **Poster # 9; Systemic Effects of Gamma Ionizing Radiation in Radiation Sensitive Tissues;** Srujana Golla; *Icahn School of Medicine at Mount Sinai, New York, NY*
- 7:30 – 7:45 pm **Poster # 13; Automated PFAS Annotation Using FluoroMatch: Application to Sources of PFAS Exposure;** Jeremy Koelmel; *Yale University, New Haven, CT*
- Highlight Talks*
- 7:45 – 7:48 pm **Poster #3; Are we Doing Non-Targeted Analysis Right? A Progress Report from the Benchmarking and Publications for Non-Targeted Analysis Working Group;** Stephan A Baumann; *Agilent Technologies, Inc., Alpharetta, GA*
- 7:48 – 7:51 pm **Poster #7; Improvements in Gas Chromatography Mass Spectrometry-Based Non-Targeted Analysis Workflows through Integration of Supervised Learning Techniques for Signal Quality Assessment;** Kristin A Favela; *Southwest Research Institute, San Antonio, TX*
- 7:51 – 7:54 pm **Poster #15; Technology Developments in Fourier Transform Mass Spectrometry Imaging for Model Organism Exposomic Studies;** Franklin E. Leach III; *University of Georgia, Athens, GA*
- 7:54 – 7:57 pm **Poster # 17; A Landscape of Fusobacterium-Modulated Metabolism in Oral Cancer;** Iqbal Mahmud; *Department of Pathology, Immunology and Laboratory Medicine, Gainesville, FL*
- 7:57 – 8:00 pm **Poster # 19; Identification of Glucuronidated Biotransformation Products in Fish Exposed to Wastewater Effluent using Untargeted High-Resolution Mass Spectrometry;** Jonathan D. Mosley; *Center for Environmental Measurement & Modeling, U.S. Environmental Protection Agency, Athens, GA*
- 8:00 – 8:03 pm **Poster #23; Simplifying Non-Target Analysis and Improving Peak Match Confidence with Gas Chromatography - High Resolution-TOFMS and Improved Data Processing Strategies;** Todd Richards; *LECO Corporation, St Joseph, MI*

8:00-10:00 pm

**Poster Session I & Reception
Odd-Numbered Posters Present**

Captiva West

Speakers – please arrive ½ hour before your session begins to load your presentation

SATURDAY, JANUARY 25

7:00 - 8:30 am **Continental Breakfast, Captiva West**

8:30-10:30 am Measuring the External Exposome I <i>Captiva East</i>

8:30-9:00 am **Keynote Lecture: Non-Targeted Analysis: Environmental Chemistry in the Age of Computational Mass Spectrometry**; Lee Ferguson, *Duke University*

9:00-9:30 am **The Placental Exposome**; Alex Chao, *ORISE U.S. EPA*

9:30-10:00 am **The DBP Exposome: Uncovering the Ubiquitous and Mostly Unknown Exposure in Drinking Water**; Susan Richardson, *University of South Carolina*

10:00-10:30 am **The Dental Exposome**; Manish Arora, *Icahn School of Medicine at Mt. Sinai*

10:30-10:45 am **Coffee Break, Captiva West**

10:45-11:45 am Measuring the External Exposome II
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10:45-11:15 am **Utilizing LC-IMS-MS for the Untargeted Analysis of PerFluoroAlkyl Substances (PFAS) in Environmental and Biological Samples**; Erin Baker, *North Carolina State University*

11:15-11:45 am **Using Metabolomics to Characterize the Exposome**; David Graham, *Johns Hopkins University School of Medicine*

11:45-1:30 pm **Lunch on your own**

Speakers – please arrive ½ hour before your session begins to load your presentation

SATURDAY, JANUARY 25

1:30-3:00 pm
Open-Access Resources for Toxicity/Exposure Predictions and Feature Identification
Captiva East

1:30-2:30 pm **Keynote Lecture: Comptox Chemicals Dashboard**, Antony Willams, *US EPA*

2:30-3:00 pm **Exposure Data and Gap-filling Methods**; Katherine Phillips, *US EPA*

3:00 - 3:15 pm **Coffee Break**

3:15-4:45 pm
The Exposome and the Public

3:15-3:45 pm **Toxicity and Exposure Models**; John Wambaugh, *US EPA*

3:45-4:15 pm **P2i™ and Exposome (Preconception to infancy)**; David Humphrey, *The Forum Institute*

4:15-4:45 pm **Improving Maternal Health Outcomes**; Jeannie Conry, *FIGO*

4:45 -7:00 pm **Free Time**

Speakers – please arrive ½ hour before your session begins to load your presentation

SATURDAY, JANUARY 25

7:00 – 8:00 pm

Submitted Talks

Captiva East

Three Short Talks, 12 minutes each followed by 3 minutes for Q&A

Five Highlight Talks, 3 minutes each

- 7:00 – 7:15 pm *Poster # 18; **Metabolic Changes in Response to a High Fat High Cholesterol Dietary Exposure Reveals Atherosclerosis Biomarkers in Liver**; Biswapriya Biswavas Misra; *Wake Forest School of Medicine, Winston-Salem, NC**
- 7:15 – 7:30 pm *Poster # 26; **Targeted and Untargeted Interrogation of the Human Serum Albumin Cys34 Adductome for Quantification and Discovery of Environmental Exposures**; Joshua W Smith; *Johns Hopkins University, Baltimore, MD**
- 7:30 – 7:45 pm *Poster # 28; **Deep Sequencing Revealed Potential Microbial Exposure in Hospital Air**; Xinyue Zhang; *Stanford University, Palo Alto, CA**
- Highlight Talks*
- 7:45 – 7:48 pm *Poster # 4; **Sick Building Syndrome: A Bottom-Up Evaluation of Anthropogenic Compounds Found in Common Household Dust**; Stephan A Baumann; *Agilent Technologies, Inc., Santa Clara, CA**
- 7:48 – 7:51 pm *Poster # 16; **Validating Medication Use via Metabolomics Analysis in Clinical Trials: How the Exposome Enhances Precision Medicine**; Jia Li; *University of Alabama, Birmingham, AL**
- 7:51 – 7:54 pm *Poster # 20; **Liquid Chromatography-Ion Mobility-High Resolution Mass Spectrometry for Analysis of Pollutants in Indoor Dust: Identification and Predictive Capabilities**; Lauren Mullin; *Waters Corporation, Milford, MA**
- 7:54 – 7:57 pm *Poster # 22; **Environmental Electrophiles: Relevance of Exposures through Drinking Water Treated with Chemical Oxidants**; Carsten Prasse; *Johns Hopkins University, Baltimore, MD**
- 7:57 – 8:00 pm *Poster # 24; **Simultaneous Analysis of Multiple Classes of Organic Compounds Using SIFT-MS**; Mitch Rubenstein; *US Air Force, Dayton, OH**

8:00-10:00 pm

Poster Session II & Reception

Even-Numbered Posters Present

Captiva West

Speakers – please arrive ½ hour before your session begins to load your presentation

SUNDAY, JANUARY 26

7:00 - 8:30 am **Continental Breakfast**, *Captiva West*

<p>8:30-10:00 am The Future of the Exposome <i>Captiva East</i></p>

8:30-9:00 am **Systems Biology and the Exposome**; Gary Miller, *Columbia University*

9:00-9:30 am **Understanding the Relationship between the Environment and Metabolism: Opportunities and Challenges for the Omic Sciences**; Gary Patti, *Washington University in St. Louis*

9:30-10:00 am **The Future of the Exposome**; Jenna Hua, *Million Marker*

10:00-10:15 am **Coffee Break**, *Captiva West*

10:15-11:00 am **Closing Remarks**, Jarod Grossman and Anthony Macherone

POSTERS

Captiva West Ballroom

Setup up all posters by 7:00 pm on Thursday

ODD-numbered posters present during the Friday Poster Session

EVEN-numbered posters present during the Saturday Poster Session

- 1 **Untargeted Profiling of Serum Metabolites, Nutrients, and Toxins in an Exposomic Investigation of the Isle of Wight Multigenerational Birth Cohort;** Thilani M Anthony¹; Wilfried J. J. Karmaus²; Su Chen³; Susan Ewart⁴; Syed Hasan Arshad^{5, 6, 7}; John W Holloway⁸; Hongmei Zhang²; A. Daniel Jones¹; ¹*Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, Michigan;* ²*Division of Epidemiology, Biostatistics, and Environmental Health, School of Public Health, University of Memphis, Memphis, Tennessee;* ³*Department of Mathematical Sciences, University of Memphis, Memphis, Tennessee;* ⁴*Department of Large Animal Clinical Sciences, College of Veterinary Medicine, Michigan State University, East Lansing, Michigan;* ⁵*Clinical and Experimental Sciences, Faculty of Medicine, University of Southampton, Southampton, United Kingdom;* ⁶*The David Hide Asthma and Allergy Research Centre, Isle of Wight, United Kingdom;* ⁷*NIHR Respiratory Biomedical Research Unit, University Hospital Southampton, Southampton, United Kingdom;* ⁸*Human Development and Health, University of Southampton, Southampton, United Kingdom*
- 2 **Nontarget Screening for Comprehensive Characterization of Chemical Exposure: GCxGC-HRMS with Complimentary Ionization Techniques;** Viatcheslav Artaev; *LECO Corporation, St Joseph, MI*
- 3 **Are we Doing Non-Targeted Analysis Right? A Progress Report from the Benchmarking and Publications for Non-Targeted Analysis Working Group;** Stephan A Baumann; *Agilent Technologies, Inc., Alpharetta, GA*
- 4 **Sick Building Syndrome: A Bottom-Up Evaluation of Anthropogenic Compounds Found in Common Household Dust;** Marcus Kim¹; Stephan A Baumann¹; Dayue Shang²; ¹*Agilent Technologies, Inc., Santa Clara, CA;* ²*Environment Canada, North Vancouver, BC*
- 5 **Quantifying Microplastic Hazard and Exposure in the Human Fetal Environment;** Zoe Coates Fuentes¹; Douglas I Walker¹; ¹*Icahn School of Medicine at Mount Sinai, New York, NY*
- 6 **Effects to the Human Proteome Due to Legacy Chemical Exposure in the Great Lakes;** Emmalyn Dupree¹; Bernard Crimmins¹; Thomas Holsen¹; James Pagano²; Brooke Thompson³; Krista Christensen³; Michelle Raymond³; Jonathan Meiman³; Costel C Darie¹; ¹*Clarkson University, Potsdam, NY;* ²*SUNY Oswego, Oswego, NY;* ³*Wisconsin Department of Health Services, Madison, WI*
- 7 **Improvements in Gas Chromatography Mass Spectrometry-Based Non-Targeted Analysis Workflows through Integration of Supervised Learning Techniques for Signal Quality Assessment;** Kristin A Favela¹; Michael J Hartnett¹; Andrew J Schaub¹; Jake A Janssen¹; Adam K Van Horn¹; Steven R Westbrook¹; David W Vickers¹; Keith S Pickens¹; ¹*Southwest Research Institute, San Antonio, TX*
- 8 **Protein Adducts in Newborn Dried Blood Spots are Associated with Exposure to PM2.5 and Ozone during Pregnancy;** William Funk¹; Nathan Montgomery¹; Anny Xiang²; Rob Mcconnell³; Ting Chow²; ¹*Northwestern University, Chicago, IL;* ²*Southern California Permanente Medical Group, Pasadena, CA;* ³*University of Southern California, Los Angeles, CA*
- 9 **Systemic Effects of Gamma Ionizing Radiation in Radiation Sensitive Tissues;** Srujana Golla¹; Douglas I Walker¹; Frank Gonzalez²; ¹*Icahn School of Medicine at Mount Sinai, New York, NY;* ²*National Cancer Institute, NIH, Bethesda, MD*
- 10 **LC-MS Based Detection of Ribonucleoside Changes upon Benzo[A]Pyrene Exposure;** Cassandra Herbert; *University of Cincinnati, Cincinnati, OH*

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- 11 **Investigation and Characterization of the Jumping Translocation Breakpoint (JTB) Protein using Mass Spectrometry based Proteomics;** Madhuri Jayathirtha¹; Devika Channaveerappa¹; Kangning Li¹; Costel C. Darie¹; ¹*Clarkson University, Potsdam, NY*
- 12 **Mass Spectrometry-Based Proteomics and Metabolomics Analysis for the Detection of Biological and Disease Progression Markers;** Sathisha Kamanna; *Flinders University, Adelaide, Australia*
- 13 **Automated PFAS Annotation Using FluoroMatch: Application to Sources of PFAS Exposure;** Jeremy Koelmel, Matthew Paige, Paul Stelben, Elizabeth Lin, Juan Aristizabal, John Bowden, Krystal Pollitt; *Yale University, New Haven, CT*
- 14 **Automatically Classifying Airborne Exposures Using Gas Chromatography High Resolution Mass Spectrometry of Passive Samplers, Neural Networks, and EPA Compound Databases;** Jeremy Koelmel¹; Alex Chen¹; Alexander Aksenov²; Elizabeth Lin¹; Fiona O'brien¹; Jieqiong Zhou¹; Koustav Ganguly³; Swapna Upadhyay³; Kirill Veselkov⁴; Vasilis Vasiliou¹; Krystal G. Pollitt¹; ¹*Yale University, New Haven, CT*; ²*University of California, San Diego, CA*; ³*Karolinska institutet, Solna, Sweden*; ⁴*Imperial College London, South Kensington, United Kingdom*
- 15 **Technology Developments in Fourier Transform Mass Spectrometry Imaging for Model Organism Exposomic Studies;** Heather Flanagan-Steet¹; Donald F. Smith²; Richard Steet¹; Franklin E. Leach III³; ¹*Greenwood Genetic Center, Greenwood, SC*; ²*National High Magnetic Field Laboratory, Tallahassee, FL*; ³*University of Georgia, Athens, GA*
- 16 **Validating Medication Use via Metabolomics Analysis in Clinical Trials: How the Exposome Enhances Precision Medicine;** Jia Li¹; Landon S. Wilson¹; Amie Mclain¹; Rebecca Howell¹; Taylor F. Berryhill¹; Ceren Yazar¹; Stephen Barnes¹; ¹*University of Alabama, Birmingham, AL*
- 17 **A Landscape of Fusobacterium-Modulated Metabolism in Oral Cancer;** Iqbal Mahmud¹; Sasanka Sekhar Chukkapalli²; Ann Progulsk-Fox³; Timothy J. Garrett⁴; ¹*Department of Pathology, Immunology and Laboratory Medicine, Gainesville, Florida*; ²*Department of Periodontology, Gainesville, FL*; ³*Department of Oral Biology, University of Florida, Gainesville, FL*; ⁴*Department of Pathology, Immunology and Laboratory Medicine, Gainesville, FL*
- 18 **Metabolic Changes in Response to a High Fat High Cholesterol Dietary Exposure Reveals Atherosclerosis Biomarkers in Liver;** Biswapriya Biswavas Misra^{1,2}; Clayton S. Bloszies³; Sobha R. Puppala^{1,2}; Anthony G. Comuzzie^{2,4}; Michael C. Mahaney⁵; John L. Vandenberg⁵; Laura A. Cox^{1,2,6}; Oliver Fiehn^{3,7}; Michael Olivier^{1,2,6}; ¹*Center for Precision Medicine, Department of Internal Medicine, Section on Molecular Medicine, Wake Forest School of Medicine, Winston-Salem, NC*; ²*Department of Genetics, Texas Biomedical Research Institute, San Antonio, TX*; ³*West Coast Metabolomics Center, UC Davis Genome Center, Davis, CA*; ⁴*The Obesity Society, Silver Spring, MD*; ⁵*South Texas Diabetes and Obesity Institute and Department of Human Genetics, The University of Texas Rio Grande Valley School of Medicine, Brownsville, TX*; ⁶*Southwest National Primate Research Center, Texas Biomedical Research Institute, San Antonio, TX*; ⁷*Department of Molecular and Cellular Biology, University of California, Davis, CA*

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EVEN-numbered posters present during the Saturday Poster Session

- 19 **Identification of Glucuronidated Biotransformation Products in Fish Exposed to Wastewater Effluent using Untargeted High-Resolution Mass Spectrometry;** Jonathan D. Mosley¹; Marina G. Evich¹; Ioanna Ntai²; Jenna E. Cavallin³; Dan L. Villeneuve³; Gerald T. Ankley³; Timothy W. Collette¹; ¹*Center for Environmental Measurement & Modeling, U.S. Environmental Protection Agency, Athens, GA;* ²*Thermo Fisher Scientific, San Jose, CA;* ³*Center for Computational Toxicology & Exposure, U.S. Environmental Protection Agency, Duluth, MN*
- 20 **Liquid Chromatography-Ion Mobility-High Resolution Mass Spectrometry for Analysis of Pollutants in Indoor Dust: Identification and Predictive Capabilities;** Lauren Mullin¹; Robert Dilorenzo²; Karl Jobst³; Robert Plumb¹; Eric Reiner⁴; Leo W.Y. Yeung⁵; Ingrid Ericson Jogsten⁵; ¹*Waters Corporation, Milford, MA;* ²*Department of Physiology and Experimental Medicine, The Hospital for Sick Children, Mouse Imaging Centre, Toronto, Ontario;* ³*Memorial University of Newfoundland, St. John's, NL;* ⁴*Ontario Ministry of the Environment, Conservation and Parks, Toronto, Ontario;* ⁵*MTM Research Centre, Örebro University, Örebro, Sweden*
- 21 **Studying the Metabolism of Bisphenol A Analogs by LC-HRMS/MS';** Ons Ousji¹; Lekha Sleno¹; ¹*University of Quebec in Montreal, Montreal, QC*
- 22 **Environmental Electrophiles: Relevance of Exposures through Drinking Water Treated with Chemical Oxidants;** Carsten Prasse¹; Zhuoyue Zhang¹; ¹*Johns Hopkins University, Baltimore, MD*
- 23 **Simplifying Non-Target Analysis and Improving Peak Match Confidence with Gas Chromatography - High Resolution-TOFMS and Improved Data Processing Strategies;** Todd Richards¹; James Carlson¹; Joseph E. Binkley¹; ¹*LECO Corporation, St Joseph, MI*
- 24 **Simultaneous Analysis of Multiple Classes of Organic Compounds Using SIFT-MS;** Mitch Rubenstein¹; Anthony V. Qualley²; ¹*US Air Force, Dayton, OH;* ²*UES, Dayton, OH*
- 25 **Development and Validation of a Dietary Biomarker Panel Reflecting Multiple Foods;** Nanna Vidkjaer; Alastair Ross; Carl Brunius; Rikard Landberg; Otto Savolainen; *Chalmers University of Technology, Gothenburg, Sweden*
- 26 **Targeted and Untargeted Interrogation of the Human Serum Albumin Cys34 Adductome for Quantification and Discovery of Environmental Exposures;** Joshua W Smith¹; Robert N O'Meally²; Derek Ng³; Thomas W Kensler^{1,4}; Robert N Cole²; John D Groopman¹; ¹*Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD;* ²*Department of Biological Chemistry, School of Medicine, Johns Hopkins University, Baltimore, MD;* ³*Department of Epidemiology, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD;* ⁴*Translational Research Program, Fred Hutchinson Cancer Research Center, Seattle, WA*
- 27 **Top-Down Proteomics Reveals Alterations in Liver Protein Profiles of C57Bl/6 Mice Exposed to Traffic-Generated Emissions and a High Fat Diet;** Leah J Schneider¹; Rachel Koerber¹; Joann Lucerno¹; Jacob McDonald²; Amie Lund¹; ¹*University of North Texas, Denton, TX;* ²*Lovelace Biomedical and Environmental Research Institute, Albuquerque, NM*

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EVEN-numbered posters present during the Saturday Poster Session

- 28 **Deep Sequencing Revealed Potential Microbial Exposure in Hospital Air;** Xinyue Zhang¹; Chao Jiang¹; Michal Snyder^{1,2}; ¹*Stanford University, Palo Alto, CA*; ²*Stanford Center for Genomics and Personalized Medicine, Palo Alto, CA*
- 29 **Proteomic Analysis of Human Breast Milk to Reveal Potential Protein Biomarkers for Breast Cancer;** Danielle Whitham¹; Roshanak Aslebagh¹; Devika Channaveerappa¹; Brian Penetcost²; Kathleen F. Arcaro²; Costel C. Darie¹; ¹*Clarkson University, Potsdam, NY*; ²*University of Massachusetts, Amherst, MA*
- 30 **A Permethrin Metabolite is Associated with Adaptive Immune Responses in Gulf War Illness;** Utsav Joshi¹; Jim E Evans¹; Sarah Oberlin¹; Teresa Darcey¹; Adam Cseresznye¹; Andrew Keegan¹; Fiona Crawford¹; Michael Mullan¹; Laila Abdullah¹; ¹*Roskamp Institute, Sarasota, FL*