THE 2ND ANNUAL

# Ohio Mass Spectrometry and Metabolomics Symposium

THE OHIO STATE UNIVERSITY

MAY 16 – 17, 2018
BLACKWELL INN
THE OHIO STATE UNIVERSITY

# Agenda Overview

THE 2ND ANNUAL

## Ohio Mass Spectrometry and Metabolomics Symposium

### Wednesday, May 16

| | |
|---|---|
| 7:30-8:30 a.m. | **Registration** |
| 8:30-8:40 a.m. | **Welcoming Remarks**<br>Blackwell Inn Ballroom (2nd Floor) |
| 8:40-10:45 a.m. | **Plenary Session I: NMR and MS-based Metabolomics**<br>Blackwell Inn Ballroom |
| 10:45-11:15 a.m. | **BREAK** |
| 11:15-12:15 p.m. | **Metabolomics and Mass Spectrometry Oral Presentations**<br>*Session IA*<br>Blackwell Inn Ballroom<br>*Session IB*<br>140 Pfahl Hall |
| 12:15-12:35 p.m. | **BREAK and Lunch Pickup** |
| 12:35-1:15 p.m. | **Lunch & Learn Session 1: Sponsored by Agilent**<br>Blackwell Inn Ballroom |
| 1:15-2:15 p.m. | **Breakout Sessions**<br>**"Preparing for a Career in Industry"**<br>Blackwell Inn Ballroom<br>**"Making your Science Accessible" & TED-style Talks**<br>140 Pfahl Hall |
| 2:15-2:45 p.m. | **BREAK (Exhibitors and Networking)** |
| 2:45-4:50 p.m. | **Plenary Session II: Food and Nutritional Metabolomics**<br>Blackwell Inn Ballroom |
| 5-7 p.m. | **Poster & Networking Reception**<br>Blackwell Inn and Pfahl Hall |

### Thursday, May 17

| | |
|---|---|
| 8-8:30 a.m. | **Registration and Networking** |
| 8:30-10:35 a.m. | **Plenary Session III: Advances in Mass Spectrometry**<br>Blackwell Inn Ballroom |
| 10:35-10:50 a.m. | **BREAK** |
| 10:50-12:10 p.m. | **Metabolomics and Mass Spectrometry Oral Presentations**<br>*Session IIA*<br>Blackwell Inn Ballroom<br>*Session IIB*<br>140 Pfahl Hall |
| 12:10-12:25 p.m. | **BREAK and Lunch Pickup** |
| 12:25-1:05 p.m. | **Lunch & Learn Sessions**<br>*Session II: Sponsored by Waters*<br>Blackwell Inn Ballroom<br>*Session III: Sponsored by Bruker*<br>140 Pfahl Hall |
| 1:05-1:35 p.m. | **Break: Poster Voting & Networking** |
| 1:35-3:40 p.m. | **Plenary Session IV: Multi-Omics for Health**<br>Blackwell Inn Ballroom |
| 3:40-3:45 p.m. | **Poster Awards & Closing Remarks**<br>Blackwell Inn Ballroom |

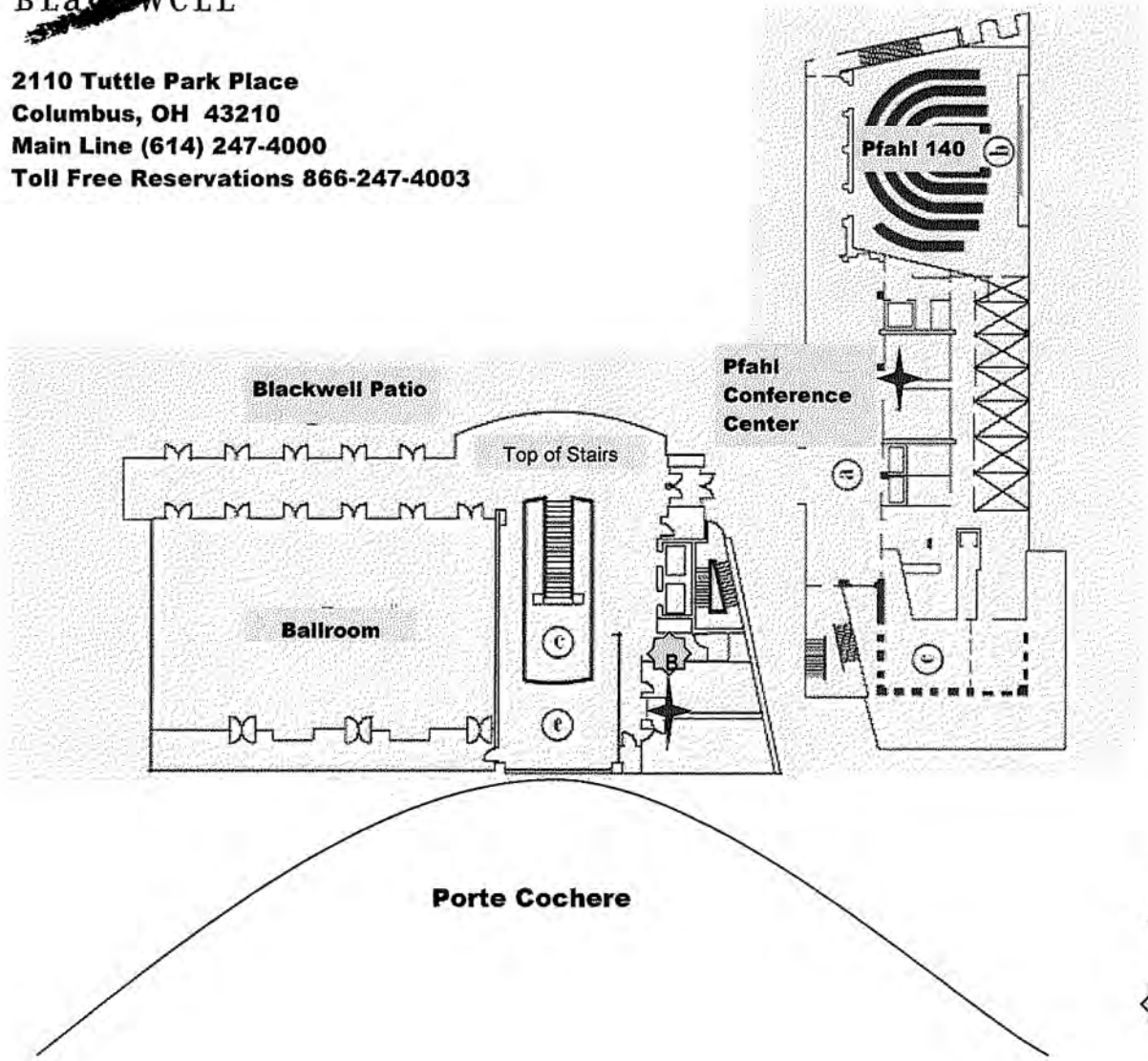
# Contents



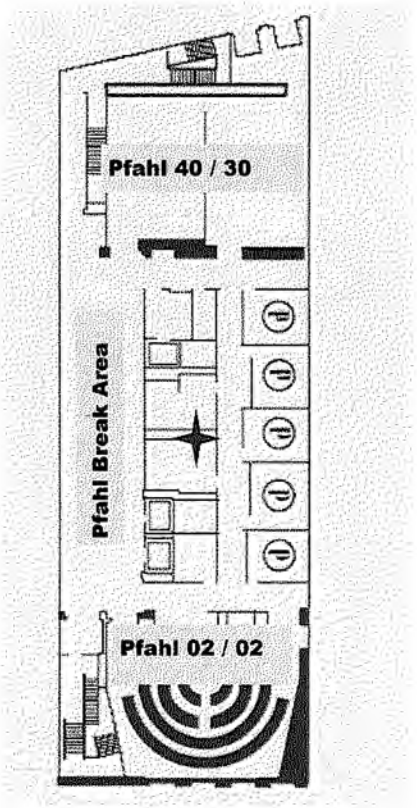
the BLACKWELL

**2110 Tuttle Park Place**
**Columbus, OH 43210**
**Main Line (614) 247-4000**
**Toll Free Reservations 866-247-4003**

**Pfahl Conference Center**
**First Floor**




**Pfahl Conference Center**
**Second/Third Floor**




**Restrooms**

**Business Center**

WELCOME FROM THE PLANNING COMMITTEE FOR:

# The 2nd Annual Ohio Mass Spectrometry and Metabolomics Symposium

***The 2nd Annual Conference on Foods and Nutritional Metabolomics for Health***
***&***
***The 15th Annual Ohio Mass Spectrometry Symposium***

Dear 2018 Conference Participant,

Building on the success of last year's conference, it is with great pleasure that we welcome you to the 2nd Annual Ohio Mass Spectrometry and Metabolomics Symposium, a joint meeting of the *2nd Annual Conference on Foods and Nutritional Metabolomics for Health and the 15th Annual Ohio Mass Spectrometry Symposium*! This year, we offer plenary sessions in *Food and Nutritional Metabolomics, Multi-omics for Health, Advances in Mass Spectrometry*, and *NMR and MS-based Metabolomics*, with presentations by internationally recognized researchers in these fields. Student and postdoctoral researchers from the Ohio Valley region will have the opportunity to present their work through oral and poster presentations. This year we offer two new interactive breakout sessions: *Preparing for a Career in Industry* will give students an opportunity to learn from our industry sponsor panelists and will promote industry-student networking and *Making Your Science Accessible*, an interactive presentation by Articulation, will show researchers how to make their presentations more engaging, with several TED-style Foods for Health Discovery Talks serving as examples. In addition, we have planned for several opportunities to network with academic and industry partners working in the rapidly developing fields of metabolomics and mass spectrometry. We hope you leave the conference feeling inspired to begin or continue your work in these vital fields.

We would like to thank all of our generous sponsors as well as our media partners, The Metabolomics Society and the journal *Metabolites*, for their support. We would also like to thank the Ohio State University Discovery Themes Initiative for their targeted investment in Food and Nutritional Metabolomics for Health (learn more at discovery.osu.edu/ffh).

We look forward to a great symposium!

Sincerely,

- **Besma Abbaoui**, Program Manager, OSU Foods for Health
- **Kamal Aboshamaa**, Executive Director, OSU Foods for Health
- **Matt Bernier**, Research Associate, OSU CCIC Mass Spectrometry & Proteomics Facility
- **Sophie Harvey**, Research Associate, OSU CCIC Mass Spectrometry & Proteomics Facility
- **Arpad Somogyi**, Associate Director, OSU CCIC Mass Spectrometry & Proteomics Facility
- **Laura VanArsdale**, Project Coordinator, OSU Foods for Health
- **Vicki Wysocki**, Ohio Eminent Scholar, Professor, Director of OSU Campus Chemical Instrument Center

# Sponsors

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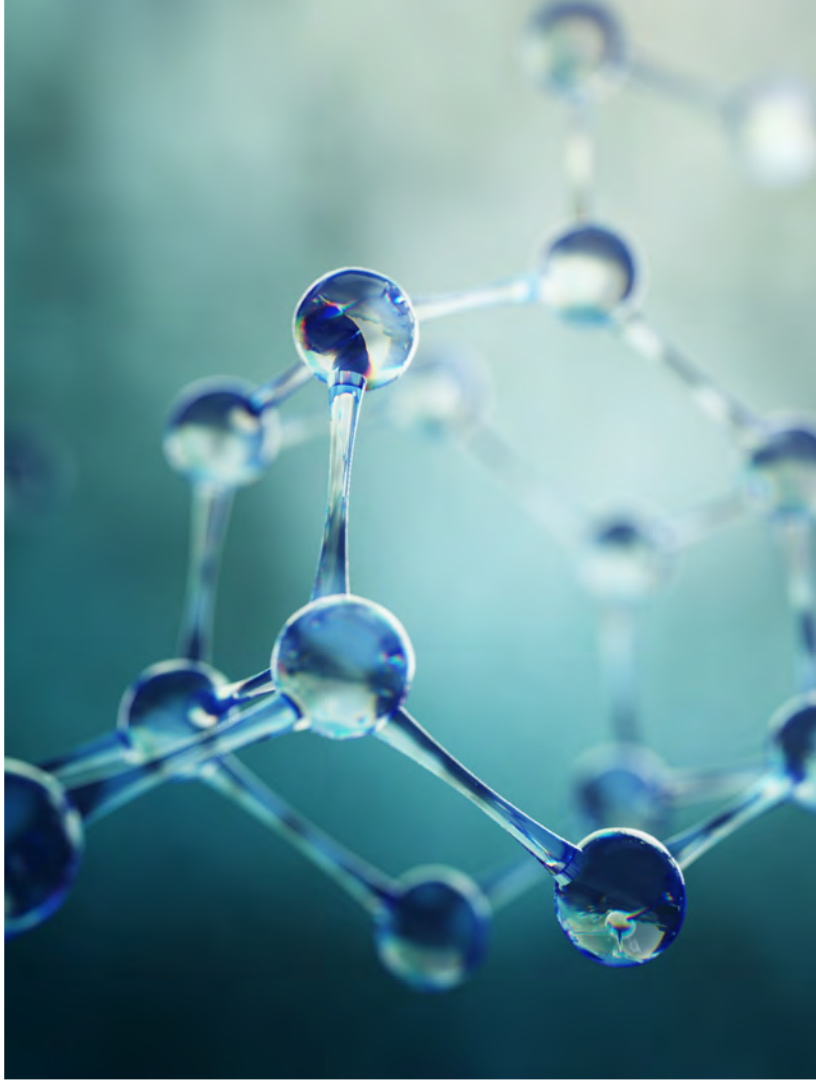
## MEDIA PARTNERS

METABOLOMICS SOCIETY


*Metabolites* (ISSN 2218-1989) is an open access journal of metabolism and metabolomics, published quarterly online by MDPI. Manuscripts are peer-reviewed and a first decision provided to authors approximately 19.5 days after submission; acceptance to publication is undertaken in 4 days (median values for papers published in this journal in first half of 2017). Currently, Metabolites is indexed by **PubMed**, PubMed Central, **Scopus** and ESCI (Web of Science).



# Conference Agenda

## WEDNESDAY, MAY 16

7:30-8:30 a.m.

**Registration and Networking** *(breakfast available)*
Blackwell Inn Ballroom (2nd Floor)

8:30-8:40 a.m.

**Welcoming Remarks**
**Dr. Randy Moses**
*Interim Senior Vice President for Research, Professor of Electrical and Computer Engineering*
Blackwell Inn Ballroom (2nd Floor)

8:40-10:45 a.m.

**Plenary Session I: NMR and MS-based Metabolomics**
Blackwell Inn Ballroom

**Plenary Chair:**
**Dr. Rafael Brüschweiler, The Ohio State University**
*Professor of Chemistry & Biochemistry, Ohio Research Scholar, CCIC-NMR Executive Director*

**Keynote Speaker:**
**Dr. Robert Powers, University of Nebraska-Lincoln**
*Professor of Chemistry*
"Metabolomics: A Tool for Drug Discovery, Disease Diagnosis and Systems Biology"

**Invited Speakers:**
**Dr. Emmanuel Hatzakis, The Ohio State University**
*Assistant Professor of Food Science & Technology*
"Monitoring Food Quality and Producing Value-Added Products from Food Waste Using NMR-based Approaches"

**Dr. Bo Zhang, The Ohio State University**
*Post-Doctoral Researcher, Department of Chemistry & Biochemistry*
"Application of a Combined NMR/MS Metabolomics Approach to Study the Impact of EPA on the Bioaccessibility, Cell Uptake and Metabolism of β-carotene"

**Dr. Jiangjiang (Chris) Zhu, Miami University**
*Assistant Professor, Department of Chemistry & Biochemistry*
"A Metabolomics Investigation of the Reciprocal Interaction between Polyphenols and Human Gut Microbiota"

10:45-11:15a.m.

**BREAK**

11:15-12:15 p.m.

**Parallel Oral Presentation Sessions**

**Session IA: Oral Presentations**
Blackwell Inn Ballroom
Moderated by: **Dr. Ken Riedl**, The Ohio State University, Acting Director, Senior Research Scientist Nutrient and Phytochemical Analytics Shared Resource

- ***Cheng Wang, The Ohio State University***
  "Accurate Identification of Known and Unknown Metabolites in Gallbladder Bile by Multidimensional NMR and Customized Metabolite Database"
- ***Sichaya Sittipod, The Ohio State University***
  "A Flavoromics Approach in Determining Key Chemical Markers in Coffee Beans that have Significant Impact on Coffee Brew Flavor Quality"
- ***Rebecca Kimmelfield, The Ohio State University***
  "Identification of Pseudomonas spp. VOCs for Use in Biocontrol of Nematodes"

**Session IB: Oral Presentations**
140 Pfahl Hall
Moderated by: **Dr. Matthias Klein**, The Ohio State University, Assistant Professor of Foods Science and Technology

- ***Savannah Snyder, The University of Akron***
  "Elucidation of Engine Oil Deposits by Mass Spectrometry Methods"
- ***Priti Thakur, University of Cincinnati***
  "Improving RNA Modification Mapping through Generation of Overlapping Digestion Products"
- ***Andrew Norris, The Ohio State University***
  "Surface-Induced Dissociation Ion Mobility Mass Spectrometry and Crosslinking Reveals Different Quaternary Structures of Anthranilate Synthase Homologs"

12:15-12:35 p.m. **BREAK (lunch pickup)**

12:35-1:15 p.m. **Lunch & Learn Session: Sponsored by Agilent Technologies**
***Steven Fischer, Agilent Technologies***
"Investigation of Pyrazinamide Mechanism of Action for Tuberculosis Using Metabolomics"
The Blackwell Inn, Ballroom (2nd Floor)

1:15-2:15 p.m. **Parallel Breakout Sessions**
**I. "Preparing for a Career in Industry" Panel with Industry Representatives and Industry-Student Networking**
Blackwell Inn Ballroom

**II. "Making your Science Accessible" Presentation and Foods for Health TED-style Talks**
140 Pfahl

2:15-2:45 p.m. **BREAK (Exhibitors and Networking)**

2:45-4:50 p.m. **Plenary Session II: Food and Nutritional Metabolomics**
Blackwell Inn Ballroom

**Plenary Chair:**
**Dr. Joshua Blakeslee, The Ohio State University**
*Associate Professor of Horticulture and Crop Sciences, Director of the OARDC Metabolite Analysis Cluster (OMAC)*

**Keynote Speaker:**
**Dr. Colin Kay, North Carolina State University**
*Associate Professor of Food, Bioprocessing and Nutrition Sciences, Plants for Human Health Research Institute*
"Establishing The Utility of Microbial-derived Biosignatures of Dietary Phytochemicals"

**Invited Speakers:**
**Dr. Verena Kriechbaumer, Oxford Brookes University**
*Vice Chancellor's Research Fellow in Biology, Department of Biological and Medical Sciences*
"The Odd One Out: Arabidopsis Reticulon 20 has a Role in Lipid Regulation"

**Dr. Richard Bruno, The Ohio State University**
*Professor of Human Nutrition*
"Evaluation of Dysregulated Vitamin E Pharmacokinetics Along the Gut-Liver Axis in Adults with Metabolic Syndrome Using an Orally Administered Stable Isotope"

**Dr. Jessica Cooperstone, The Ohio State University**
*Assistant Professor of Horticulture & Crop Sciences and Food Science & Technology*
"Using Metabolomics to Understand Chemical Changes and Bioactivity of Black Raspberries through Thermal Processing and Storage"

5-7 p.m. **Posters & Networking Reception**
Blackwell Inn

*continued on next page...*

# Conference Agenda

## THURSDAY, MAY 17

8-8:30 a.m. **Registration and Networking** *(breakfast available)*

8:30-10:35 a.m. **Plenary Session III: Advances in Mass Spectrometry**
Blackwell Inn Ballroom

**Plenary Chair:**
**Dr. Amanda Hummon, The Ohio State University**
*Associate Professor of Chemistry & Biochemistry*

**Keynote Speaker:**
**Dr. Jonathan Sweedler, The University of Illinois at Urbana-Champaign**
*Professor of Chemistry, Editor-in-Chief of Analytical Chemistry*
"From Mass Spectrometry Imaging to MS of Individual Cells: Measuring Neurochemical Changes in the Brain"

**Invited Speakers:**
**Dr. Arpad Somogyi, The Ohio State University**
*Associate Mass Spec and Proteomics Facility Director*
"Untargeted and Targeted Metabolomics Projects in the CCIC MSP Facility: Challenges and Solutions"

**Katelyn Ludwig, The Ohio State University**
*Doctoral Student, Department of Chemistry & Biochemistry*
"Calcitriol Supplementation Causes Decreases in Tumorigenic Proteins and Different Proteomic and Metabolomic Signatures in Right versus Left-Sided Colon Cancer"

**Dr. Hao Chen, Ohio University**
*Professor, Department of Chemistry & Biochemistry*
"Mass Spectrometric Study of Electrochemistry and Organometallic Chemistry"

10:35-10:50 a.m. **BREAK**

10:50-12:10 p.m. **Parallel Oral Presentation Sessions**

**Session IIA: Oral Presentations**
Blackwell Inn Ballroom
Moderated by: **Dr. Kerry Rouhier**, Kenyon College, Associate Professor of Chemistry

- ***Miranda Gardner, The Ohio State University***
  "Multiomic Approach to Characterize Sperm Maturation"
- ***Alecia Blaszczak, The Ohio State University***
  "Weight Loss in Mice and Its Impact on Adipose Tissue Inflammation and Visceral Adipocyte Metabolomics"
- ***Mengxuan Jia, The Ohio State University***
  "Protein-Protein Interaction Specificity for Computationally Designed Hetero-Dimers: Ion Exchange Chromatography (IEX) Coupled to Native Mass Spectrometry (MS)"
- ***Geoffrey Sasaki, The Ohio State University***
  "Green Tea Reduces Metabolic Endotoxemia in Nonalcoholic Steatohepatitis in Association with Altered Relative Abundance of Bile Acids and Phosphatidylcholine Metabolites"

**Session IIB: Oral Presentations**
140 Pfahl Hall
Moderated by: **Dr. Yan Zhang**, The Ohio State University, Assistant Professor of Biomedical Informatics

- ***Qiongqiong Wan, The Ohio State University***
  "Integrated Mass Spectrometry Platform Enables Picomole-Scale Real-time Electrosynthetic Reaction Screening and Discovery"
- ***Kevin Endres, The University of Akron***
  "Determining Covalently Crosslinked Polymer Connectivities by ASAP-MS"
- ***Samantha Hinckley, The Ohio State University***
  "Interrogating the Conformation of HIV-1 Gag and its Stoichiometry of Binding to Genomic RNAs"
- ***Manasses Jora, University of Cincinnati***
  "Differentiating Positional Isomers of Nucleoside Modifications by Higher-Energy Collisional Dissociation Mass Spectrometry"

12:10-12:25 p.m. **BREAK (lunch pickup)**

12:25-1:05 p.m. **Parallel Lunch & Learn Sessions**

**Lunch & Learn Session A: Sponsored by Waters Corporation**
***Dr. Suraj Dhungana, Waters Corporation***
"Untargeted Lipid Profiling in Differentially Activated Macrophages"
Blackwell Inn, Ballroom (2nd Floor)

**Lunch & Learn Session B: Sponsored by Bruker Daltonics**
***Dr. Mike Easterling, Bruker Daltonics***
**"**Enabling Next Generation Metabolomics by Going Beyond the Molecular Realm"
140 Pfahl Hall

1:05-1:35 p.m. **Break: Poster Voting & Networking**

1:35-3:40 p.m. **Plenary Session IV: Multi-Omics for Health**
Blackwell Inn Ballroom

**Plenary Chair:**
**Dr. Ewy Mathé, The Ohio State University**
*Assistant Professor of Biomedical Informatics*

**Keynote Speaker:**
**Dr. Debashis Ghosh, Colorado School of Public Health**
*Professor and Chair of Biostatistics and Informatics*
"Kernel Machine Methods for High-throughput Biological Data"

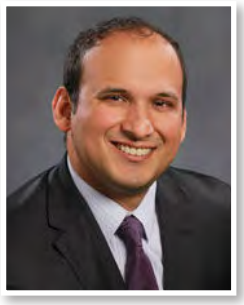
**Invited Speakers:**
**Dr. Brian Ahmer, The Ohio State University**
*Associate Professor of Microbial Infection & Immunity*
"Impacts of Salmonella Infection on the Chemical and Biological Landscape of the Gut"

**Dr. Jalal Siddiqui, The Ohio State University**
*Post-Doctoral Researcher, Department of Biomedical Informatics*
"Integrating Metabolomics and other Omics Data via Linear Modeling and Comprehensive Pathway Analysis"

**Dr. Michael Bailey, The Ohio State University and Nationwide Children's Hospital**
*Associate Professor of Pediatrics, Principal Investigator in the Center for Microbial Pathogenesis at The Research Institute at NCH*
"Assessing the Colonic Microbiome and Metabolome to Understand Stressor-Induced Immunomodulation"

3:40-3:45 p.m. **Poster Awards & Closing Remarks**
Blackwell Inn

# Keynote Speakers



## DEBASHIS GHOSH

Debashis Ghosh, PhD, is Professor and Chair of the Department of Biostatistics and Informatics at the Colorado School of Public Health. Dr. Ghosh previously was at the University of Michigan and Penn State University. Dr. Ghosh has spent the last eighteen years working on the development of statistical methods for bioinformatics and genomics, primarily with applications to biomedical research funded by the National Institutes of Health and the National Science Foundation. More recently, he has developed recent interests in the areas of causal inference and neuroimaging. He has published over 190 papers in a broad variety of areas of collaborative and methodological research that have appeared in high-profile journals including Biometrika, Bioinformatics, Journal of the American Statistical Association, Journal of the Royal Statistical Society Series B, Nature and the New England Journal of Medicine. In 2015, he edited Integration of 'Omics Data (Cambridge University Press) with George Tseng (Pittsburgh) and Jasmine Zhou (USC). He was previously chair of the Biostatistical Methods Research and Design (BMRD) and is currently co-editor of Biometrics, a leading methodological journal in biostatistics.

## COLIN KAY

Collin Kay is an associate professor in the Department of Food, Bioprocessing and Nutrition Sciences at the North Carolina State University's Plants for Human Health Research Institute. Dr. Kay's research is centered around establishing the metabolism of dietary phytochemicals and the potential impact this has on their biological activity, particularly with respect to disorders and diseases associated with aging. His research core is focused on the development of targeted methodologies for the identification of microbial-derived biosignatures of polyphenol consumption. This core is supported by a program of human clinical research, involving pharmacokinetic analysis and screening of vascular and immune activity.

## ROBERT POWERS

Dr. Robert Powers is a professor of Chemistry at the University of Nebraska-Lincoln. His research program centers around the development of NMR metabolomics techniques, biomarker discovery, disease diagnosis and the application of bioinformatics for the analysis of the metabolome. He has applied his methodology to study (i) S. epidermidis and S. aureus adaptability and viability, (ii) antibiotic activity and resistance in tuberculosis and Mycobacterium smegmatis, (iii) drug activity in Aspergillus nidulans, (iv) identified biomarkers for MS, (v) the role of MUC1 and ketone bodies in pancreatic cancer, and (vi) the molecular mechanism of neurotoxins in Parkinson's disease and drug resistance in pancreatic cancer.

## JONATHAN SWEEDLER

Jonathan Sweedler received his Ph.D. in Chemistry from the University of Arizona in 1988, spent several years at Stanford before moving to the University of Illinois at Urbana-Champaign in 1991 where he has been ever since. At Illinois, he is currently the James R. Eiszner Family Endowed Chair in Chemistry, Director of the School of Chemical Science, and affiliated with the Institute of Genomic Biology and the Beckman Institute for Advanced Science and Technology. His research interests focus on developing new approaches for assaying small volume samples using metabolomics and peptidomics. He has used these tools to characterize small molecules and peptides in a range of animal models across the metazoan and in samples as small as individual cells and cellular domains. Recent work includes the development of a series of high throughput mass spectrometry approaches for characterizing tens of thousands of individual cells. Sweedler, with large international teams of biologists and technologists, has performed comprehensive interrogation of the genome, transcriptome and peptidome in a range of animal models to uncover signaling peptides and pathways involved in wide range of functions and behaviors. Sweedler has published more than 400 manuscripts and presented 500 invited lectures. He has received numerous awards including the ACS Award in Analytical Chemistry and the ANACHEM Award. He is currently the Editor-in-Chief for *Analytical Chemistry*.

# Plenary Session Abstracts

## PLENARY SESSION I: NMR AND MS-BASED METABOLOMICS

**Plenary Chair: Dr. Rafael Brüschweiler, The Ohio State University**
*Professor of Chemistry & Biochemistry, Ohio Research Scholar, CCIC-NMR Executive Director*

### Keynote Presentation:

**Dr. Robert Powers, University of Nebraska-Lincoln**
*Professor of Chemistry*
**Metabolomics: a tool for drug discovery, disease diagnosis and systems biology**
Metabolomics is an invaluable tool of systems biology and has made significant contributions to a diverse number of fields, such as drug discovery, disease diagnosis, and personalized medicine. Unlike other OMICs techniques, an observed difference in the metabolome is directly correlated with a relevant biological response (a *change in the biological activity of protein*). The metabolome captures how the system responds to drug treatment, disease state, environmental stress or genetic modification. As a consequence, the application of metabolomics has increased exponentially over the last decade. A diseased-centered systems biology approach to drug discovery provides a unique infrastructure to identify novel druggable targets and therapeutic agents to increase the efficiency and success rate of drug discovery. One important component of this approach is the use and development of NMR and MS based metabolomics techniques to monitor the *in vivo* activity and selectivity of potential drugs. Similarly, metabolomics can be used to monitor disease development, identify *in vivo* mechanisms of action for novel drugs, and evaluate mechanisms of drug resistance. Additionally, metabolomics may be an invaluable approach to easily and rapidly diagnose human disease and assist in personalized medicine by monitoring a patient's response to a particular treatment. Our metabolomics technology, including our MVAPACK metabolomics software platform, PCA/PLS-DA utilities, and protocols for integrating NMR and MS data, sample preparation and metabolite identification will be discussed. Also, our analysis of the mechanism of action and resistance of TB and cancer drugs, and metabolic processes related to pancreatic cancer, Parkinson's disease and a potential diagnostic tool for multiple sclerosis will be presented.

### Invited Speakers:

**Dr. Emmanuel Hatzakis, The Ohio State University**
*Assistant Professor of Food Science & Technology*
**"Monitoring Food Quality and Producing Value-Added Products from Food Waste Using NMR-based Approaches"**
Despite its strengths, NMR spectroscopy is an underutilized method in the field of food science. The combination of NMR with statistical analysis can be an efficient tool for the comparison of spectral patterns and the identification of chemical compounds, thus providing invaluable information for the evaluation of foods and the development of new products. We used Magnetic Resonance and metabolomics for the determination of several bioactive molecules in coffee and for understanding the impact of various processing on its composition. In addition, NMR plays a crucial role in monitoring the production of value-added products from food wastes. Using spent coffee grounds, we produced molecules that can be used as precursors for manufacturing bioplastics and we revealed the structure and properties of a novel natural colorant produced from avocado seeds.

**Dr. Bo Zhang, The Ohio State University**
*Post-Doctoral Researcher, Department of Chemistry & Biochemistry*
**"Application of a Combined NMR/MS Metabolomics Approach to Study the Impact of EPA on the Bioaccessibility, Cell Uptake and Metabolism of β-carotene"**
There are two experimental analytical techniques forming the cornerstones of metabolome detection: nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS). There is still a lack of universal strategy for the integration of NMR and MS platforms, to capture the complementary information provided by each. Our groups develop and apply new experimental and computational tools to combine NMR and MS methods. Previously, the SUMMIT approach was applied to explore unknown metabolites in gall bile where NMR and MS data were collected with no sample separation. Currently, we are working on an enhanced version that introduces chromatography into the protocol, and have applied it to a nutritionally relevant model. The

carotenoid β-carotene is a lipophilic provitamin synthesized in orange and green fruits and vegetables. It serves as provitamin A, and its consumption is also associated with a decreased risk of certain chronic diseases. Long-chain omega-3 fatty acids (FA) may be directly obtained from dietary sources like cold-water fish, and are essential for human health. Due to the commensal health benefits of omega-3 FA and carotenoids, it is sensible to supplement them together. However, the acute effects of EPA on BC bioaccessibility and bioavailability are unknown. Therefore, we studied the direct interaction(s) between EPA and β-carotene, and the corresponding impact on their respective bioaccessibilities and bioavailabilities using an in vitro Caco-2 cell model, coupled with a targeted HPLC-PDA approach. Preliminary results indicate that EPA increases the micellarization of BC, although this increase does not translate into a subsequent increase in BC uptake by the Caco-2 cells. Using this biological model, we also performed combined HPLC-MS and NMR-based metabolomics and lipidomics analyses on the samples. The combined metabolomics approach provides enhanced identification and cross-system confirmation of metabolites, including metabolites of interest involved in the regulation of cell osmolality and lipid uptake.

**Dr. Jiangjiang (Chris) Zhu, Miami University**
*Assistant Professor, Department of Chemistry & Biochemistry*
**"A Metabolomics Investigation of the Reciprocal Interaction between Polyphenols and Human Gut Microbiota"**
There is a growing evidence to support the hypothesis that the gut microflora can metabolize plant-derived dietary compounds into metabolites with important biological activity, and these microbial metabolites may ultimately be the missing link that explains the widely acknowledged health benefits of diets high in compounds such as polyphenols. Recent studies have shown that consumption of polyphenol-rich drink, such as green tea and black tea, leads to several health benefits. However, a better effort is needed to systematically identify the variety of gut microbial metabolites produced during the polyphenol ingestion, the commensal microbes responsible for their production, and their potentially beneficial biological activities. This presentation will share some recent results from our lab to fill the current gaps in knowledge. We determined the abundance and variety of these gut microbial metabolites and how they individually and/or collectively might have biological signatures associated with improved measures of health and resilience. Various omics technologies, particularly targeted and untargeted metabolomics, were applied to detect and validate correlations between the chemical profile of microbial metabolites, the microbial population changes, and their biological profile of activities. We have demonstrated, in a human colonic model, the dramatic impact of green tea polyphenols to gut microbial population, diversity and metabolism. We also detected a group of polyphenols and their microbial metabolites and mapped their spatiotemporal distribution over two weeks of 'daily green tea consumption' in the human colonic model. The bioconversion of polyphenols to their microbial metabolites are monitored, both parent and microbial-derived polyphenols were tested for their bactericidal effects to pathogens. In conclusion, the presented study provided novel insight into how dietary components and the intestinal microbiota could interact to alter health outcomes via polyphenol microbial metabolites. This knowledge could be utilized to inform new dietary recommendations or to inspire new functional foods.

## PLENARY SESSION II: FOOD AND NUTRITIONAL METABOLOMICS

**Plenary Chair: Dr. Joshua Blakeslee, The Ohio State University**
*Associate Professor of Horticulture and Crop Sciences, Director of the OARDC Metabolite Analysis Cluster (OMAC)*

**Keynote Presentation:**

**Dr. Colin Kay, North Carolina State University**
*Associate Professor of Food, Bioprocessing and Nutrition Sciences, Plants for Human Health Research Institute*
**"Establishing The Utility of Microbial-derived Biosignatures of Dietary Phytochemicals"**
It is believed the discovery of microbial-derived biosignatures will translate into next-generation public health applications, such as diagnostics for monitoring clinical treatment or prevention strategies, and identifying metabolic health status. However, defining microbial-derived biosignatures of dietary phytochemicals requires significant clinical and analytical corroboration. Establishing any biomarker requires proof of analytical performance, mechanistic link between analyte and outcome, biological specificity, clinical predictive performance, and diagnostic value. Traditionally, biomarkers of nutrition status are single targets, yet microbial phytochemical biosignatures could theoretically comprise dozens of unique metabolites, and reflect host genetics, environmental exposure and microbiome. Unfortunately, microbial metabolites derived from the diet are often unidentified in untargeted metabolomics databases, and generally reported as unknown signals or background noise. Targeted approaches will therefore be required initially to establish biosignatures of major dietary phytochemicals, particularly in the case of polyphenols, which have considerable chemical and metabolic diversity. The major challenges in building targeted spectral libraries to distinguish unique polyphenol metabolites from other dietary substrates are a lack of commercial analytical standards and the significant numbers of small molecules and their isomers, which are common across differing food sources. Therefore, costly synthesis and labelling studies are

required to characterize unique biosignatures. Aside from significant hurdles in establishing biosignatures, there are many possible benefits. Biosignatures will: provide diagnostics for the prediction of metabotypes/metabolic phenotypes, dietary quality, metabolic and intestinal health; establish associations between intake and activity; establish authentication of dietary recall and food diary strategies in population research; aid in the identification of outliers or 'non-compliers' in clinical studies; and finally, aid in the identification of previously uncharacterized signals in untargeted metabolomics databases, fostering new discoveries from prior research assets.

## Invited Speakers:

**Dr. Verena Kriechbaumer, Oxford Brookes University**
*Vice Chancellor's Research Fellow in Biology, Department of Biological and Medical Sciences*
**"The Odd One Out: Arabidopsis Reticulon 20 has a Role in Lipid Regulation"**
The plant endoplasmic reticulum (ER) is a multifunctional organelle involved in a plethora of aspects of plant life. The plant cortical ER network has been shown to play numerous roles in production, folding and quality control of proteins, lipid biosynthesis and pathogen responses. The polygonal and highly dynamic network of the cortical ER consists of tubules and cisternae. Reticulons (RTN) are integral membrane proteins characterised by a reticulon homology domain comprising four transmembrane domains which results in the proteins sitting in the membrane in a W-topology. They are found in a wide range of eukaryotes and have been shown to localise to the ER in many species, including mammals, yeast and plants. Previous studies have demonstrated a role for reticulons in shaping the ER into tubules and constricting the ER membrane on overexpression. Here we report on a novel subgroup of reticulons with an extended N-terminal domain and in particular on arabidopsis reticulon 20 (RTN20). Using high resolution confocal microscopy we show that RTN20 is located in a unique punctate pattern on the ER membrane. Its closest homologue RTN19 labels the whole ER. Other than demonstrated for the other members of the reticulon protein family RTN20 and 19 do not display ER constriction phenotypes on over expression. We show that mutants in RTN20 or RTN19, respectively, display a significant reduction in sterol levels in roots indicating a role in lipid regulation. A third homologue in this family -3BETAHSD/D1- is unexpectedly localised to ER exit sites resulting in an intriguing location difference for the three proteins.

**Dr. Richard Bruno, The Ohio State University**
*Professor of Human Nutrition*
**"Evaluation of Dysregulated Vitamin E Pharmacokinetics Along the Gut-Liver Axis in Adults with Metabolic Syndrome Using an Orally Administered Stable Isotope"**
Dietary recommendations for α-tocopherol, the only essential form of vitamin E, are challenging to meet from food alone. Indeed, >92% of Americans fail to meet recommendations, and α-tocopherol status is likely further compromised by inflammatory responses occurring in metabolic syndrome (MetS). It is therefore important to establish the extent to which MetS increases dietary α-tocopherol requirements due to underlying inflammation that likely impairs α-tocopherol trafficking and metabolism along the gut-liver axis. Our approach entailed a randomized cross-over study in MetS and age- and gender-matched healthy adults in which they ingested encapsulated hexadeuterium-labeled ($d_6$)-*RRR*-α-tocopherol (15 mg) with dairy milk beverages containing 0-8 g fat. Pharmacokinetics of $d_6$-α-tocopherol and its physiologic metabolite $d_6$-α-CEHC (carboxyethyl-hydroxychromanol) were then assessed for 72 h using LC-MS. MetS adults had increased circulating oxidized LDL and pro-inflammatory cytokines in association with metabolic endotoxemia. Plasma $d_6$-α-tocopherol absorption, $C_{max}$, and bioavailability ($AUC_{0\text{-}72\ h}$) were significantly lower in MetS adults regardless of dairy milk fat content. Their isolated chylomicrons and VLDL also had lower $d_6$-α-tocopherol enrichment, suggesting impaired intestinal and hepatic trafficking of α-tocopherol. MetS adults also had lower circulating and urinary $d_6$-α-CEHC, suggesting inadequate α-tocopherol status to activate P450-mediated metabolism of α-tocopherol. Pharmacokinetic parameters of both $d_6$-α-tocopherol and $d_6$-α-CEHC were correlated with inflammatory responses. Thus, MetS adults have higher dietary requirements to offset inflammatory stress responses that limit α-tocopherol bioavailability by decreasing intestinal absorption and hepatic secretion. This presentation will therefore discuss the potential mechanisms by which MetS impairs α-tocopherol status, and implications for achieving optimal health.

**Dr. Jessica Cooperstone, The Ohio State University**
*Assistant Professor of Horticulture & Crop Sciences and Food Science & Technology*
**"Using Metabolomics to Understand Chemical Changes and Bioactivity of Black Raspberries through Thermal Processing and Storage"**
Pre-clinical and clinical studies have implicated black raspberries (BRBs) and their associated phytochemicals in the modulation of several chronic diseases, including oral and aerodigestive cancers. Most research on the health benefits of BRBs is conducted using freeze-dried or minimally processed products, yet BRBs are typically consumed as thermally processed goods like jams and syrups. Here, we used UHPLC-QTOF-MS untargeted metabolomics to profile global chemical changes that result from 1) thermal processing of BRB powder into a nectar

and 2) its subsequent storage. Stored samples were then applied to SCC-83-01-82 premalignant oral epithelial cells and anti-proliferative activity was assessed. A total of 547 chemical features were found to differ by at least two-fold ($P$<0.05) between raw BRB powder and nectar, including 170 features unique to the nectar. Some of these were identified as key degradation products of anthocyanins along with several other proposed phenolic degradants. Of high-abundant features, key BRB phytochemicals including quercetin derivatives, procyanidin monomers and dimers, and some phenolic acids were stable to thermal processing, while the ellagitannin profile was differentially modulated. Interestingly, minimal differences were noted in anti-proliferative activity when raw and stored nectar extracts were applied *in vitro*, despite large chemical changes. As proof of concept, cyanidin-3-*O*-rutinoside and its degradation product, protocatechuic acid, were administered in different ratios maintaining an equimolar dose, and anti-proliferative activity was maintained. This demonstrates that single, isolated phytochemicals do not explain the complete bioactivity of a complex food product, and the utility of metabolomics to profile global chemical changes in food.

## PLENARY SESSION III: ADVANCES IN MASS SPECTROMETRY

**Plenary Chair: Dr. Amanda Hummon, The Ohio State University**
*Associate Professor of Chemistry & Biochemistry*

### Keynote Presentation:

**Dr. Jonathan Sweedler, The University of Illinois at Urbana-Champaign**
*Professor of Chemistry, Editor-in-Chief of Analytical Chemistry*
**"From Mass Spectrometry Imaging to MS of Individual Cells: Measuring Neurochemical Changes in the Brain"**
In the postgenomic era, one expects the suite of chemical players in a brain region to be known and their functions uncovered. However, many neurochemicals remain poorly characterized and for those that are known, their localization, dynamics and function are oftentimes unknown. We have created new approaches for assaying the chemical content within targeted brain regions and from individual brain cells. The approaches described here include mass spectrometry imaging (MSI) and single cell measurements from the hippocampus of a range of animals to follow neurochemical changes as a function of age, learning and diet. For MSI, tissue slices are treated with derivatizing agents and other compounds to enhance the detection of specific metabolite classes and then imaged with MS. Using these approaches, we can measure lipids, fatty acids and neurotransmitters, among others. MSI is robust enough to provide statistical significant changes in transmitters and other molecules as a function of animal diet; we have validated the MSI results using follow-up LC-MS measurements from the same brain regions, demonstrating the ability to perform quantitative animal comparisons via MSI. For single cell measurements, the cells of interest are scattered across a microscope slide, the exact cell positions determined via optical microscopy, and mass spectra are acquired only at the cell positions. The single cell assays allow differences in the metabolome and peptidome from supposedly homogeneous populations of cells to be explored. By obtaining information from tens of thousands of individual cells, rare cells are found and unusual neurochemicals are discovered. For select cells, follow-up capillary electrophoresis-mass spectrometry is performed. Several applications of single cell mass spectrometry are highlighted from the discovery of unusual metabolites to characterizing the neuropeptides and hormones in single cells. Our overarching goal is to uncover the complex chemical mosaic of the brain and pinpoint key cellular players in a range of physiological and pathological processes.

### Invited Speakers:

**Dr. Arpad Somogyi, The Ohio State University**
*Associate Mass Spec and Proteomics Facility Director*
**"Untargeted and Targeted Metabolomics Projects in the CCIC MSP Facility: Challenges and Solutions"**
Identifying unknown metabolites (untargeted analysis) by HPLC-MS/MS methods has been an active area of research for many years. In spite of significant improvements and success there is still a lot to do to further improve sample preparation techniques, ionization efficiencies, chemical composition determination, structure identification, and metabolite search programs. In the current presentation, we will show some demonstrative examples to the necessity of using ultrahigh resolution mass spectrometry (such as Orbitrap or FT-ICR analyzers) to reliably identify chemical compositions. We will show the usefulness of using van Krevelen diagrams, Kendrick masses, and degree of unsaturation to characterize very complex, multicomponent samples. In most of the cases, both positive and negative ion modes, as well as different ionization techniques, such as ESI and LDI are desirable for the characterization of complex metabolomics mixtures. Collaborations with colleagues from other fields, most notably from NMR, are helpful to provide complementary and supportive information regarding structural details. A few examples will also be shown for quantitative (targeted) metabolomics obtained on our Quantiva QqQ instrument. Quantification of small ions (m/z < 120) is sometimes challenging due to the ion discrimination on the

QqQ instrument. Examples include, but not limited to both untargeted and targeted metabolomics studies: E-Coli metabolites, the study on the relationship between cardiovascular disease and diabetes, low and high fat diet lipidomics, humic acid mixtures, and TMA/TMAO quantitative analyses. We are grateful to all our collaborators who will be credited in the presentation.

**Katelyn Ludwig, The Ohio State University**
*Doctoral Student, Department of Chemistry & Biochemistry*
**"Calcitriol Supplementation Causes Decreases in Tumorigenic Proteins and Different Proteomic and Metabolomic Signatures in Right versus Left-Sided Colon Cancer"**
Vitamin D deficiency is a common problem in the northern hemisphere where UVB rays from the sun do not readily penetrate the atmosphere for many months of the year. The active metabolite of vitamin D is 1α,25$(OH)_2D_3$, known as calcitriol. Colorectal cancer is unique in that there is a sidedness to the cancer. The right-sided colon is composed of the ascending and transverse colon. The left-sided colon is composed of the descending and sigmoidal colon. Metadata analysis has confirmed that there are differences between left- and right-sided colon cancer, including incidence and prognosis. We are interested in treating left and right-sided colorectal cancer cell cultures with calcitriol and doing proteomic and metabolomics analysis. In this work, we treat DLD-1 right-side colon cancer cells and HCT116 left-side colon cancer cells with calcitriol to examine proteomic and metabolomics changes that occur on the different sides of the colon We use ultraperformance liquid chromatography-tandem mass spectrometry (UPLC-MS/MS) to survey the proteins and metabolites at a global level. Our results show that left-sided colon cancer treated with calcitriol has a substantially greater number of changes in both the proteome and the metabolome than right-sided colon cancer. We found that calcitriol treatment in both right-sided and left-sided colon cancer causes a downregulation of ribosomal protein L37 and protein S100A10. Both of these proteins are heavily involved in tumorigenesis, suggesting a possible mechanism for the correlation between low vitamin D levels and colon cancer.

**Dr. Hao Chen, Ohio University**
*Professor, Department of Chemistry & Biochemistry*
**"Mass Spectrometric Study of Electrochemistry and Organometallic Chemistry"**
Electrochemistry coupled with mass spectrometry (EC/MS) is a powerful means for identifying the products or intermediates of electrochemical reactions, which is not only useful for redox reaction mechanism elucidation but also leads to many valuable bioanalytical applications. The versatility of EC/MS stems from two facts. First, MS can serve as a sensitive and general detector for electrochemical cells and can provide molecular weight information about analyte of interest. In addition, tandem MS analysis can be used for structural determination based on ion dissociation. Second, electrochemical conversion can improve analyte ionization efficiency or provide desired modification to the analyte prior to MS analysis. Attracted by the complementary nature of these two techniques, the marriage of EC and MS appears quite attractive and appealing. In this talk, I will focus on the development of electrochemical mass spectrometry using ambient ionization methods such as desorption electrospray ionization (DESI) and its applications for proteomics study. The study of organometallic reaction mechanism using mass spectrometry will also be presented.

## PLENARY SESSION IV: MULTI-OMICS FOR HEALTH

**Plenary Chair: Dr. Ewy Mathé, The Ohio State University**
*Assistant Professor of Biomedical Informatics*

### Keynote Presentation:

**Dr. Debashis Ghosh, Colorado School of Public Health**
*Professor and Chair of Biostatistics and Informatics*
**"Kernel Machine Methods for High-throughput Biological Data"**
In this talk, I will discuss a class of statistical methods for high-dimensional data that are termed kernel machines. While they have been popularized in the machine learning and have found tremendous utility in various genomics contexts recently, in fact the mathematics that underlies the procedures date back to over 100 years ago. In this talk, I will give a brief history of the development of kernel machines and show that one key property that arises is that of a metric. Given the availability of a metric for any particular data structure, a straightforward development of theory for testing for associations using kernel machines is available. The methodology is fairly generic and can be applied to a wide variety of fields. In this talk, we will describe applications of kernel machines to problems in multivariate genomic data fusion, metabolomics and neuroimaging problems.

## Invited Speakers:

**Dr. Brian Ahmer, The Ohio State University**
*Associate Professor of Microbial Infection & Immunity*
**"Impacts of *Salmonella* Infection on the Chemical and Biological Landscape of the Gut"**
Salmonellosis is one of the most significant food-borne diseases affecting humans and agriculture. *Salmonella enterica* induces inflammation of the host intestinal tract to disrupt the normal microbiota. *Salmonella* thrives on the nutrients that are no longer consumed by the microbiota. Known *Salmonella* nutrient sources include 1,2-propanediol, which is a product of the microbiota; ethanolamine, which is derived from damaged cells; glucarate and galactarate which are derived from Nos2-mediated oxidation of glucose and galactose; and fructose-asparagine which is derived from the diet. We are using several omics approaches to identify all of the major nutrient sources utilized by *Salmonella* in the inflamed gut, and to identify the microbes that compete for those nutrients. Using non-targeted metabolomics we observe these known nutrients increasing in abundance in *Salmonella*-infected mice intestines compared to uninfected intestines. Using metatranscriptomics we also observe transcripts of these same nutrient utilization systems during infection. We have also identified many other previously unknown changes in this environment. For example, amino acids are metabolized by the Stickland reaction in the healthy intestine. Metagenomics analysis reveals that the primary organisms involved in this metabolism include members of the families Lachn.

**Dr. Jalal Siddiqui, The Ohio State University**
*Post-Doctoral Researcher, Department of Biomedical Informatics*
**"Integrating Metabolomics and other Omics Data via Linear Modeling and Comprehensive Pathway Analysis"**
Metabolomics data are increasingly integrated with other omics data, including the transcriptome and microbiome. To facilitate integration, we have developed IntLIM (Integration through LInear Modeling) to uncover gene-metabolite pairs that are significantly correlated in one phenotype and oppositely or not correlated in another. While this approach does not model the complexities of biochemical reactions (reaction rates and mechanisms), co-regulated genes and metabolites tend to be associated with functional roles and our approach can thus help identify putative gene-metabolite associations for experimental testing. To better interpret the biological significance of identified phenotype-specific pairs, we perform pathway enrichment analysis, which includes clustering of significant pathways by content overlap, using our comprehensive database RaMP (Relational database of Metabolomics Pathways). RaMP integrates KEGG, HMDB, Reactome, and WikiPathways, and thus contains up-to-date and comprehensive annotations for genes and metabolites. To this point, we applied IntLIM to metabolomics and transcriptomics data from tumor (N=61) and adjacent non-tumor (N=47) breast tissue from a previously published breast cancer study. By running IntLIM on all possible gene-metabolite pairs (N=6,908,412 models), we uncovered 2,842 tumor-dependent pairs (FDR p-value < 0.05 and Spearman correlation difference > 0.5). Using RaMP, we find these gene-metabolite pairs enriched for pathways involved in nucleotide metabolism, cell cycle, and WIF signaling. We are now expanding IntLIM's functionalities to allow for integration of a broader range of multi-omics data. As an example, we applied IntLIM to microbiome and metabolomics data from a murine study on farnesoid receptor (FXR) signaling and a clinical colorectal cancer study. By running IntLIM, we were able to respectively identify 4 (N=2,356 models; FDR p-value < 0.20 and Spearman correlation above 90$^{th}$ percentile) and 28 (N=30,210 models; FDR p-value < 0.10 and Spearman correlation above 90$^{th}$ percentile) phenotype-dependent microbe-metabolite pairs. IntLIM (https://github.com/Mathelab/IntLIM) and RaMP (https://github.com/Mathelab/RaMP-DB) are publicly available and contain user-friendly web interfaces.

**Dr. Michael Bailey, The Ohio State University and Nationwide Children's Hospital**
*Associate Professor of Pediatrics, Principal Investigator in the Center for Microbial Pathogenesis at The Research Institute at NCH*
**"Assessing the Colonic Microbiome and Metabolome to Understand Stressor-Induced Immunomodulation"**
Exposure to stressful stimuli is known to affect the composition of the gut microbiota, and an increasing number of studies have linked the gut microbiota to stressor-induced changes in immune system activity and behavioral responses. However, mechanisms by which alterations in the gut microbiota may impact the immune system are not well understood. We have been incorporating colonic metabolome data (generated using NMR spectroscopy or LC-MS/MS) into our studies assessing colonic microbiota (using 16S rRNA gene sequencing) to begin to determine whether microbial-produced metabolites may mediate the link between the gut microbiota and stressor-induced immunomodulation. This presentation will describe our approach to use the machine learning algorithm, random forest, along with Boruta feature selection to identify microbes and metabolites that are different in human patients or laboratory rodents. Data from a rodent study will be presented in which reductions in multiple B1, B3, and B6 vitamers were identified in the colons of mice exposed to a social stressor. Interestingly, feeding mice a prebiotic diet (containing galactooligosaccharide, polydextrose, and sialyllactose) increased colonic B vitamers and prevented the effects of the stressor on immune system reactivity. These effects were directly correlated with significant increases in the abundance of bacteria in the genus *Bifidobacterium* that are known producers of B vitamins. When considered together, these results suggest that stressor-induced changes in *Bifidobacterium* abundances contribute to immunomodulation through changes in B vitamin production. This study demonstrates the usefulness of "multi-omic" approaches to identify interactions between colonic microbes, metabolites, and host physiology.

# OSU Core Facility Abstracts

**The New State-of-the-Art CCIC-NMR Facility at The Ohio State University**

Alexandar L Hansen, Chunhua Yuan, Dawei Li, Lei Bruschweiler-Li, Tanya Whitmer, Christopher P Jaroniec, Rafael Brüschweiler
*Campus Chemical Instrument Center, NMR Facility, The Ohio State University, Columbus, OH*

Over the past few years, the shared NMR facility at the Ohio State University (OSU) has seen an expansion with new instruments and update of existing instruments housing now 9 high-field NMRs from Bruker Biospin with 5 instruments at 800 MHz and above. The new Campus Chemical Instrument Center (CCIC) NMR facility has unique capabilities in solution NMR, with 5 instruments equipped with cryoprobes (including TCI, TXO, and QCI probes) and automated, temperature-controlled sample changers (SampleJet and SampleCase), fast-MAS solid-state NMR, Dynamic Nuclear Polarization (DNP), and micro-imaging. These instruments support a wide range of research interests at OSU, in the state of Ohio, and beyond. Here we present an overview of current capabilities highlighting several ongoing projects.

**The OSU CCIC Mass Spectrometry and Proteomics Facility**

Árpád Somogyi[1], Liwen Zhang[1], Cindy James[1], Nan Kleinholz[1], Sophie Harvey[1], Matt Bernier[1], Michael Freitas[2], Vicki H. Wysocki[3]
*[1] OSU CCIC MSP Facility, [2] SBS-Cancer Biology and Genetics, OSU, [3] Department of Chemistry and Biochemistry, OSU*

The Mass Spectrometry and Proteomics Facility (MSP) is part of OSU's Campus Chemical Instrument Center (CCIC) and serves a wide variety of research groups from OSU, other universities and industry nationwide. MSP provides considerable expertise in bottom up and top down proteomics, quantitative proteomics analysis, untargeted (qualitative) and targeted (quantitative) metabolomics analyses (including lipid analyses), and the analysis of complex organic and inorganic matter and synthetic polymers. The MSP houses state-of-the-art mass spectrometry instrumentation to support research needs of all investigators at the State of Ohio Consortium. Modern high performance instruments that are house in the core include: i) a Thermo Orbitrap Fusion tandem HPLC MS/ MS system, ii) a Thermo Quantiva QQQ HPLC MS/MS, iii) a Bruker 15 T SolariX XR FT-ICR ultrahigh resolution instrument, iv) a Thermo QE Plus HPLC MS/MS system, and v) an Agilent 4650 HPLC MS Q-TOF. Representative examples for collaborative projects and services will be shown in the presentation.

**Nutrient and Phytochemical Analytics Shared Resource**

Ken Riedl, Jinshan Lin, Leslie Rankin
*Department of Food Science & Technology; OSU Comprehensive Cancer Center*

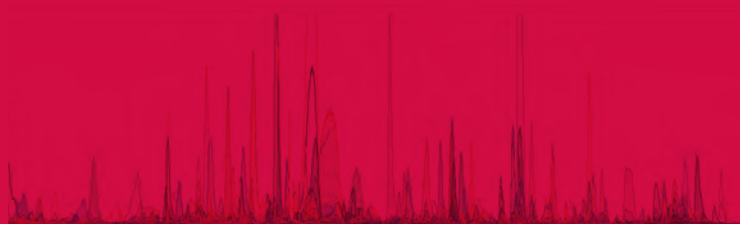
Our core (NPASR) brings world class expertise and cutting edge LCMS instrumentation to analytical exploration of foods and biologics. We excel at targeted and untargeted metabolomics for biomarker identification, quantification, and metabolite discovery. Metabolomics is an experimental capability providing unrivaled depth of metabolite coverage to enhance scientific rigor of investigations and competitiveness of grants. We have particular experience in targeted and untargeted metabolomics in support of a 'Crops to Clinic' approach with dietary interventions for cancer prevention, and provide analytical support for the OSU Discovery Themes - Foods for Health. NPASR service goals: provide investigators with bioanalytical method development and quantitative analyses of nutrients and phytochemicals in foods and their metabolites in biological samples, enhance understanding of the role of dietary compounds in cancer prevention and control, metabolite and biomarker discovery through untargeted LCMS metabolomics techniques, and offer broad quantitative targeted lipidomics with our Lipidyzer platform.

**OARDC Metabolite Analysis Cluster (OMAC)**

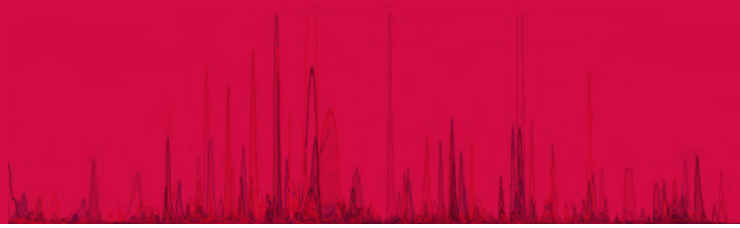
Lin, Y. 1,2, Lin, J. 2, Chanon, A. 2, Blakeslee, J.J. 1,2
*1Department of Horticulture and Crop Science, Ohio Agricultural Research and Development Center (OARDC), The Ohio State University; 2OARDC Metabolite Analysis Cluster, Department of Horticulture and Crop Science, OARDC The Ohio State University*

The OARDC Metabolite Analysis Cluster (OMAC) is a metabolomics facility located in the Ohio Agricultural Research and Development Center (OARDC), at The Ohio State University. The facility is focused on using the tools of metabolomics to dissect biochemical and physiological responses and metabolic partitioning. One area of expertise is using multiple analytical platforms (LC-MS/MS, GC-MS, HPLC, FPLC, TLC, and zonal capillary electrophoresis) to generate "metabolic fingerprints" of compounds and pathways involved in plant cells/tissues/organs, food and beverage samples, microbial cells or cellular exudates, and/or animal tissue or fluid samples. In sample analyses, we focus on using multiple analytical approaches in parallel to allow the breadth of a broad spectrum metabolomic approach, while still retaining the sensitivity and low limit of detection of a targeted metabolomic approach. To enable these assays, we have developed tools and techniques allowing the micro- extraction and quantification of low-volume or low-mass samples. OMAC also assists researchers in the development of procedures for the extraction and analysis of their compounds of interest. Areas of specialization of the facility include: phytohormone and membrane biochemistry, protein purification and enzyme characterization, plant secondary/specialized metabolism, metabolic engineering, metabolic profiling, detection of herbicide and pesticides, biochemical dissection of cellular signaling and organismal stress responses.

# Notes



# Notes



# DISCOVERY AT OHIO STATE

The 2nd Annual Ohio Mass Spectrometry &
Metabolomics Symposium

A Joint Meeting of:
The 2nd Annual Conference on Food and Nutrition Metabolomics for Health
& The 15th Annual Ohio Mass Spectrometry Symposium

Foods for Health Discovery Theme
**discovery.osu.edu/ffh**

Campus Chemical Instrument Center
**ccic.ohio-state.edu**

THE OHIO STATE UNIVERSITY