THE 3rd ANNUAL

Ohio Mass Spectrometry and Metabolomics Symposium

THE OHIO STATE UNIVERSITY

OCTOBER 1 – 2, 2019
BLACKWELL INN
THE OHIO STATE UNIVERSITY

Agenda Overview

THE 3rd ANNUAL

Ohio Mass Spectrometry and Metabolomics Symposium

Tuesday, October 1

8:15-8:45 a.m.	**Registration for Workshop Participants** Blackwell Inn Ballroom lobby (2nd floor)	
8:45-12 p.m.	**Parallel Pre-Symposium Workshops** **Metabolomics** Blackwell Inn Ballroom	**Native Mass Spectrometry** 140 Pfahl Hall
11:15 a.m.-12:15 p.m.	**Symposium Registration** Blackwell Inn Ballroom lobby (2nd floor)	
12:15-12:50 p.m.	**Parallel Lunch & Learn Sessions** **Sponsored by Agilent** Blackwell Inn Ballroom	**Sponsored by Waters** 140 Pfahl Hall
1:00-1:10 p.m.	**Welcoming Remarks: Dr. Morley Stone** Blackwell Inn Ballroom	
1:10-1:45 p.m.	**Plenary Speaker: Dr. Nathalie Agar** Blackwell Inn Ballroom	
1:45-2:15 p.m.	**Flash Talks I** Blackwell Inn Ballroom	
2:15-2:40 p.m.	**BREAK (Exhibitors and Networking)**	
2:40-3:40 p.m.	**Oral Presentations** Blackwell Inn Ballroom	
3:40-4:10 p.m.	**Flash Talks II** Blackwell Inn Ballroom	
4:10-5:00 p.m.	**Keynote Lecture: Dr. Pieter Dorrestein** Blackwell Inn Ballroom	
5:00-6:00 p.m.	**Reception** Blackwell Patio (2nd Floor)	

Wednesday, October 2

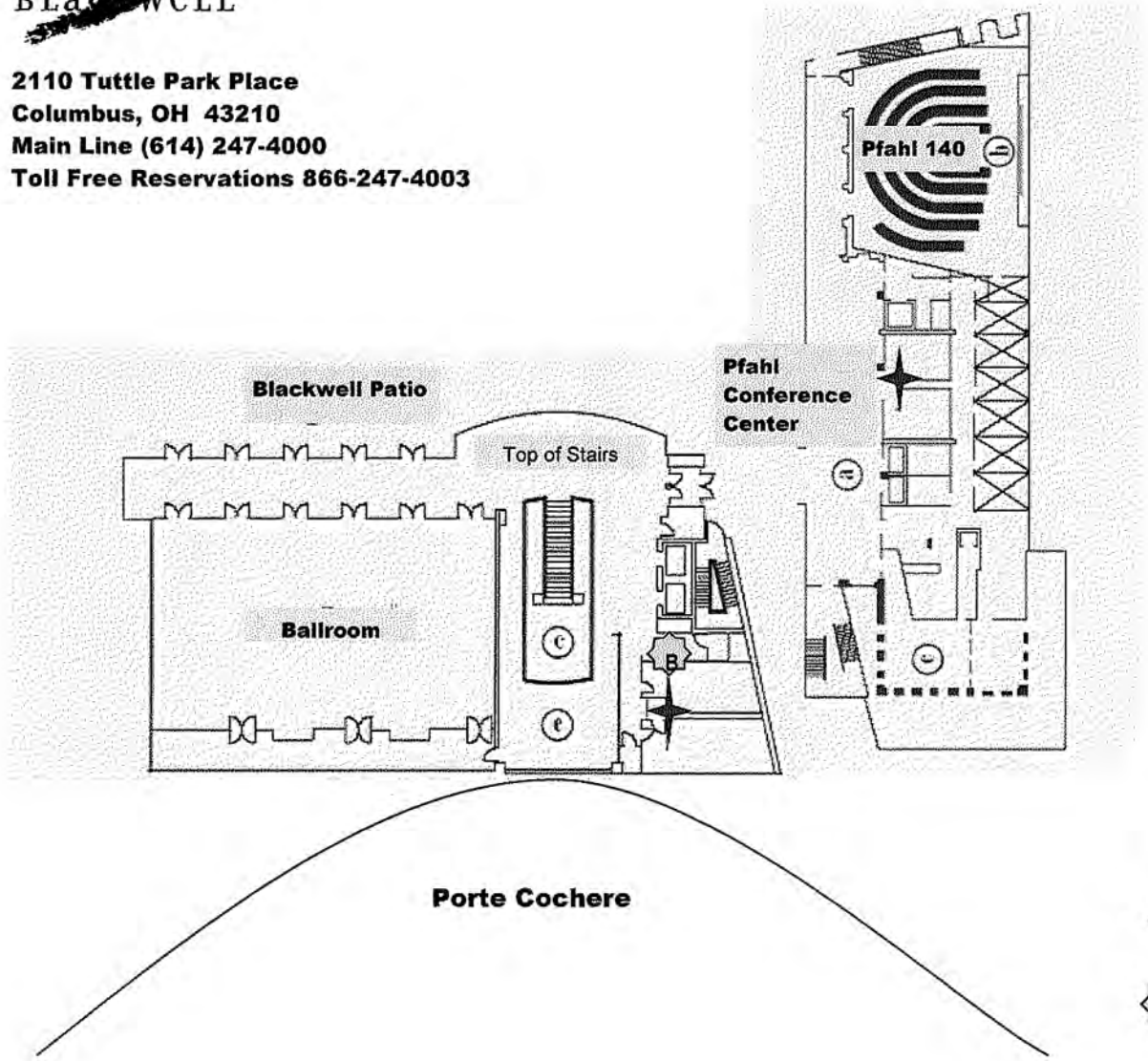
8:30-9:05 a.m.	**Plenary Speaker: Dr. Ian Lewis** Blackwell Inn Ballroom	
9:05-10:05 a.m.	**Oral Presentations** Blackwell Inn Ballroom	
10:05-10:15 a.m.	**BREAK**	
10:15-11:45 a.m.	**Poster Session (Exhibitors and Networking)** Blackwell Patio (2nd Floor)	
11:45-11:55 a.m.	**Lunch Pickup**	
11:55 a.m.-12:30 p.m.	**Parallel Lunch & Learn Sessions** **Sponsored by SCIEX** Blackwell Inn Ballroom	**Sponsored by Metabolon** 140 Pfahl Hall
12:30-1:05 p.m.	**Student-Industry Networking Session** Blackwell Inn Ballroom	
1:05-1:25 p.m.	**BREAK (Networking and Exhibitors)** Blackwell Inn Ballroom Lobby	
1:25-2:00 p.m.	**Plenary Speaker: Dr. Susan Sumner** Blackwell Inn Ballroom	
2:00-3:00 p.m.	**Oral Presentations** Blackwell Inn Ballroom	
3:00-3:05 p.m.	**Student Poster Awards & Closing Remarks** Blackwell Inn Ballroom	

Contents

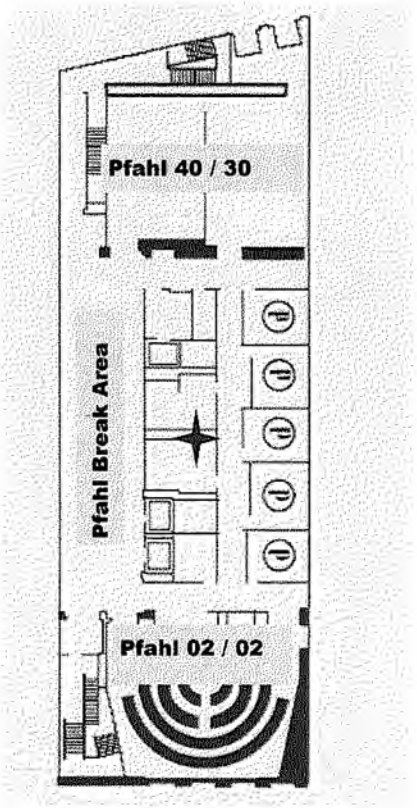
the BLACKWELL

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 3rd Annual Ohio Mass Spectrometry and Metabolomics Symposium

The 16th Annual Ohio Mass Spectrometry Symposium
&
The 3rd Annual Conference on Food and Nutritional Metabolomics for Health

Dear OMSMS 2019 Participant,

It is with great pleasure that we welcome you to the 3rd Annual Ohio Mass Spectrometry and Metabolomics Symposium! We strive to provide an excellent opportunity for academic and industrial researchers to present their findings, share information, discuss research challenges with colleagues, and spark new collaborations in the rapidly advancing fields of mass spectrometry and metabolomics.

This year's program will provide opportunities to advance your knowledge of developments in Advanced Ionization Techniques and Instrumentation, Native MS-Guided Structural Biology, Metabolomics, and Personalized Nutrition. We offer presentations by internationally recognized researchers; keynote speaker Pieter Dorrestein (University of California-San Diego) will illustrate the tremendous potential for mass spectrometry data to understand the chemistry of life, and Natalie Agar (Harvard Medical School), Ian Lewis (University of Calgary), and Susan Sumner (University of North Carolina-Chapel Hill) will present plenary talks in mass spectrometry and metabolomics. Sponsored Lunch and Learn speakers will provide additional opportunities to learn about advances in these fields. Established researchers, students and postdoctoral researchers will present their work through oral and poster presentations, and flash talks. Two pre-symposium workshops will provide introductions to *Metabolomics* and *Native Mass Spectrometry*. We hope you will take advantage of opportunities for networking, with an evening reception, a *Student-Industry Networking* session, and networking breaks. We hope you will leave the conference with new knowledge, new connections, and a renewed sense of possibility.

We would like to thank all of our generous sponsors, who make OMSMS possible. Please visit our exhibitor tables and be sure to thank our sponsors when you have an opportunity.

We would also like to thank Ohio State for continued investment and support of the Campus Chemical Instrument Center (ccic.osu.edu) and the Foods for Health initiative (discovery.osu.edu/ffh). We are excited to share new advances and resources available through the new NIH P41 Resource for Native MS-Guided Structural Biology (nativems.osu.edu).

We look forward to a great symposium!

Sincerely,

Vicki Wysocki, Ohio Eminent Scholar, Professor, Director of OSU Campus Chemical Instrument Center

Devin Peterson, Professor, Director of Foods for Health, Director of Flavor Research Education Center

A Special Thanks to Our Generous Sponsors

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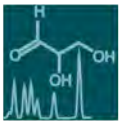


metabolites

an Open Access Journal by MDPI

Keynote Speaker

PIETER DORRESTEIN

Dorrestein is Professor at the University of California - San Diego. He is the Director of the Collaborative Mass Spectrometry Innovation Center and a Co-Director, Institute for Metabolomics Medicine in the Skaggs School of Pharmacy & Pharmaceutical Sciences, and Departments of Pharmacology and Pediatrics. Since his arrival to UCSD in 2006, Prof. Dorrestein has been pioneering the development of mass spectrometry methods to study the chemical ecological crosstalk between populations of microorganisms, including host interactions for agricultural, diagnostic and therapeutic applications. He participated in panels for the white house science and technology office of president on the launch of a national microbiome initiative and has been on panels for the National Academy of Sciences on the Chemistry of the Microbiome. He has co-authored over 220 publications and his work has been featured by the wall street journal, CNN, NYTimes, Fox, BBC and hundreds of other news outlets. He has been recognized with several awards, among them are awards from the Beckman foundation, V-foundation in cancer research, EUREKA award for unconventional and enabling research, Hearst Foundation, Pharmaceutical Research and Manufacturing Association research award and the Abel award in pharmacology. For a more detailed biography see http://www.nature.com/news/the-man-who-can- map-the-chemicals-all-over-your-body-1.20035

Plenary Speakers

NATHALIE Y.R. AGAR

Nathalie Y. R. Agar, Ph.D. is the founding Director of the Surgical Molecular Imaging Laboratory (SMIL) in the Department of Neurosurgery at Brigham and Women's Hospital, and Associate Professor of Neurosurgery and of Radiology at Harvard Medical School. Dr. Agar's multidisciplinary training includes a B.Sc. in Biochemistry, Ph.D. in Chemistry, and postdoctoral fellowships in Neurosurgery at McGill University, and BWH/HMS. Areas of research include surgical applications of mass spectrometry, pharmacometabolomics, and biomarker discovery. Her team works closely with surgeons at Brigham and Women's Hospital to develop mass spectrometry methods for rapid tissue characterization to aid in diagnoses of glioblastoma and breast cancer. The Agar Lab harnesses mass spectrometry imaging techniques to investigate drug distribution and metabolic response in tissue, particularly in brain, breast, and prostate cancer. The molecular signatures of tissue specimens are characterized to facilitate the discovery of disease specific biomarkers.

IAN LEWIS

Dr. Ian Lewis is an Assistant Professor and Alberta Innovates Translational Health Chair in the Department of Biological Sciences at the University of Calgary. Dr. Lewis earned a PhD in Biochemistry from the University of Wisconsin-Madison and completed his postdoctoral training at Princeton University. The Lewis laboratory specializes in unraveling the complex host-pathogen metabolic dynamics that occur during infections. To support this research, Dr. Lewis founded the Calgary Metabolomics Research Facility (CMRF), a unique microbiology, engineering, and analytical laboratory that was specifically designed for decoding microbial metabolism and translating these phenomena into practical tools for diagnosing and fighting infections. Dr. Lewis has recently launched the Alberta Precision Exchange https://albertaprecisionexchange.ca, an network of partners working with the Alberta Healthcare system to advance a suite of new diagnostic tools and treatment practices that may significantly reduce the number of people die from infections.

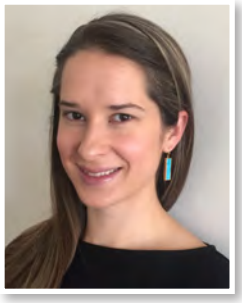
SUSAN SUMNER

Susan Sumner, PhD, is a Professor in the Department of Nutrition at the University of North Carolina at Chapel Hill (UNC-CH), where she is working to make Precision Nutrition a reality. The Sumner Lab at UNC Chapel Hill has served as the Eastern Regional Comprehensive Metabolomics Research Center (ERCMRC) since 2012, as an Untargeted Core for a NIEHS funded Children's Health Exposure Analysis Resource (CHEAR) Hub (PI, Tim Fennell) since 2015, and as the Untargeted Core for the NIDDK funded Nutrition Obesity Resource Core (NORC, Zeisel, PI) since 2017. Dr. Sumner earned a PhD in physical chemistry at North Carolina State University, and conducted a postdoctoral fellowship in the Heart, Lung, and Blood Institute at the National Institutes of Health. She serves on the Editorial Boards for Frontiers in Nutrition, Metabolomics, Metabolites, Environmental Health Perspectives, and was elected two terms to the Board of Directors of the Metabolomics Society.

Lunch and Learn Speakers

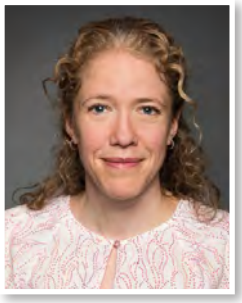
ANTHONY MIDEY

Anthony Midey is a Senior Application Support Scientist in the Biomedical Research group at Waters working in lipidomics, metabolomics, and Mass Spectrometry Imaging. He also supports direct sample analysis using techniques such as Desorption Electrospray Ionization (DESI) and Rapid Evaporative Ionization MS (REIMS). He has been supporting Waters applications for 4 years, with an extensive background in instrumentation and ion mobility spectrometry from 10 years in the instrument industry, with 55 publications in peer-reviewed journals and numerous conference presentations.



IEVA ROZNERE

Ieva Roznere, PhD, is a research associate in the department of Evolution, Ecology, and Organismal Biology at The Ohio State University. She is an aquatic ecologist interested in how environmental stress affects freshwater mussel physiology. Dr. Roznere's research focuses on how metabolism and gene expression change when freshwater mussels are subjected to stressors such as translocation to different habitats, food limitation, and exposure to contaminants. She collaborates with U.S. Fish and Wildlife Service, Ohio Division of Natural Resources, Metro Parks, and The Columbus Zoo and Aquarium. She received her B.S. from Binghamton University and her Ph.D. from The Ohio State University.



JULIE ST-PIERRE

The central research focus of the St-Pierre laboratory is the understanding of metabolic adaptation to physiological and pathological conditions. They are particularly interested in the plasticity of mitochondrial functions and how they contribute to overall energy homeostasis. During the last decade, her team contributed significantly to understanding the role of the master regulators PGC-1s in cancer, with a particular focus on poor outcome breast cancers. We showed that PGC-1alpha plays a key role in setting the metabolic state of poor outcome breast cancers and that it promotes breast cancer growth. Recently, we focused our investigation of the role of PGC-1s in breast cancer progression and we are pursuing research projects on metabolic adaptations fueling metastasis and therapeutic resistance. The St-Pierre laboratory is enriched by numerous national/international collaborations that complement our own expertise in metabolism. Dr. St-Pierre received her PhD at Cambridge University and was Postdoctoral Fellow at Cambridge University, Harvard Medical School, and University of Montreal, and was previously Assistant and Associate Professor at McGill University.

BALJIT K. UBHI

Baljit is currently responsible for the global metabolomics & lipidomics business at SCIEX and is based on the West Coast in California, USA. Baljit joined SCIEX in Europe in November 2011 after finishing her Ph.D. studies at the University of Cambridge, where she applied metabolomics & lipidomics to disease biomarker research in the group of Dr Julian Griffin. Prior to this, she held a research scientist position in the metabolic profiling group at GlaxoSmithKline R&D in the UK where she evaluated biomarkers for the effects of drug toxicity in support of drug candidate selection and development. In her time at SCIEX Baljit has been significantly involved in a new product development working closely with the marketing, product management, R&D and applications teams as well as many other responsibilities.

Symposium Agenda

TUESDAY, OCTOBER 1

PRE-SYMPOSIUM WORKSHOPS

8:15-8:45 a.m.

Registration for Workshop Participants
The Blackwell Inn, Ballroom lobby (2nd floor)

8:45-12:00 p.m.

Parallel Pre-Symposium Workshops

Introduction to Metabolomics
This "primer" workshop will highlight fundamental points of metabolomics data collection and interpretation, including LC-MS and NMR data collection, deconvolution, statistical analysis, and unknown identification.
The Blackwell Inn, Ballroom (2nd floor)

Presented by:

- **Dr. Rachel Kopec**, The Ohio State University
  Assistant Professor, Human Nutrition
- **Dr. Jessica Cooperstone**, The Ohio State University
  Assistant Professor, Horticulture and Crop Science, Food Science and Technology
- **Dr. Djawed Bennouna**, The Ohio State University
  Postdoctoral Researcher, Human Nutrition
- **Dr. Ewy Mathé**, The Ohio State University
  Assistant Professor, Biomedical Informatics
- **Dr. Emmanuel Hatzakis**, The Ohio State University
  Assistant Professor, Food Science & Technology

Introduction to Native Mass Spectrometry
Resource for Native MS-Guided Structural Biology presents an introduction to native MS methods used to help solve structural biology questions. Workshop topics include preparation/online separations, spray and instrument conditions, ion mobility, activation methods, and case studies.
140 Pfahl Hall

Presented by:

- **Dr. Florian Busch,** The Ohio State University
  Research Associate, Resource for Native MS-Guided Structural Biology, CCIC
- **Dr. Sophie Harvey,** The Ohio State University
  Research Associate, Resource for Native MS-Guided Structural Biology, CCIC
- **Dr. Dalton Snyder,** The Ohio State University
  Research Associate, Resource for Native MS-Guided Structural Biology
- **Alyssa Stiving**, The Ohio State University
  Graduate Research Assistant, PhD Candidate, Wysocki Group, Resource for Native MS-Guided Structural Biology
- **Zachary VanAernum**, The Ohio State University
  Graduate Research Assistant, PhD Candidate, Wysocki Group, Resource for Native MS-Guided Structural Biology
- **Dr. Vicki Wysocki,** The Ohio State University
  Professor, Chemistry and Biochemistry; Ohio Eminent Scholar; Director, Campus Chemical Instrument Center; Director, Resource for Native MS-Guided Structural Biology

SYMPOSIUM (DAY ONE)

11:15 a.m.-12:15 p.m.

Registration (Exhibitors and Networking)
Lunch pickup begins at 11:45 a.m.
The Blackwell Inn, Ballroom lobby (2nd floor)

12:15-12:50 p.m.

Parallel Lunch & Learn Sessions

Lunch and Learn: Sponsored by Agilent
Dr. Julie St-Pierre, University of Ottawa
Professor, Biochemistry, Microbiology and Immunology
"Integrated metabolomics analyses to uncover metabolic vulnerabilities in cancer"
The Blackwell Inn, Ballroom (2nd Floor)

Lunch and Learn: Sponsored by Waters
Dr. Anthony Midey, Waters Corporation
Senior Application Support Scientist, Biomedical Research Group
"Spatial visualization of metabolite and lipid markers using MS imaging"
140 Pfahl Hall

1:00-1:10 p.m.

Welcoming Remarks
Dr. Morley Stone, The Ohio State University
Senior VP for Research, Office of Research
The Blackwell Inn, Ballroom (2nd Floor)

1:10-1:45 p.m.

Plenary Speaker
Dr. Nathalie Agar, Brigham and Women's Hospital, Harvard Medical School
Director, Surgical Molecular Imaging Laboratory (SMIL); Associate Professor of Neurosurgery and Radiology
"Mass spectrometry imaging applications to support clinical decision making"
The Blackwell Inn, Ballroom (2nd Floor)

1:45-2:15 p.m.

Flash Talks I
The Blackwell Inn, Ballroom (2nd Floor)

2:15-2:40 p.m.

BREAK (Exhibitors and Networking)
The Blackwell Inn, Ballroom Lobby (2nd Floor)

2:40-3:00 p.m.

Oral Presentation
Dr. Fernando Tobias, The Ohio State University
Postdoctoral Researcher, Hummon Group, Chemistry and Biochemistry
"Untargeted spatial lipidomics of colon carcinoma spheroids using a LC-QTOF platform"
The Blackwell Inn, Ballroom (2nd Floor)

3:00-3:20 p.m.

Oral Presentation
Suji Lee, The Ohio State University
PhD Candidate, Badu Group, Chemistry and Biochemistry
"An ultra-sensitive paper-based diagnostic platform of detecting colorectal cancer via mass spectrometry"
The Blackwell Inn, Ballroom (2nd Floor)

3:20-3:40 p.m.

Oral Presentation
Dr. Michael Freitas, The Ohio State University
Director, CCC Proteomics Shared Resource; Associate Professor, Molecular Virology, Immunology and Medical Genetics, Biomedical Informatics
"A data science perspective on transparent and reproducible analysis of complex omic data"
The Blackwell Inn, Ballroom (2nd Floor)

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Symposium Agenda

3:40-4:10 p.m.
Flash Talks II
The Blackwell Inn, Ballroom (2nd Floor)

4:10-5:00 p.m.
Keynote Lecture
Dr. Pieter Dorrestein, University of California-San Diego
Professor, Skaggs School of Pharmacy and Pharmaceutical Sciences, Departments of Pharmacology and Pediatrics; Director, Collaborative Mass Spectrometry Innovation Center; Co-Director, Institute for Metabolomics Medicine
"Connecting the world's mass spectrometry data to understand the chemistry of life – a Big Data strategy"
The Blackwell Inn, Ballroom (2nd Floor)

5:00-6:00 p.m.
Reception
Blackwell Patio (2nd Floor)

WEDNESDAY, OCTOBER 2

SYMPOSIUM (DAY TWO)

8:30-9:05 a.m.
Plenary Speaker
Dr. Ian Lewis, University of Calgary
Assistant Professor, Biological Sciences; Alberta Innovates Translational Health Chair
"Harnessing metabolomics to combat infectious diseases"
The Blackwell Inn, Ballroom (2nd Floor)

9:05-9:25 a.m.
Oral Presentation
Dr. Xiaowei Sun, The Ohio State University
Postdoctoral Researcher, Zhu Lab, Human Nutrition
"Investigating the metabolic impact of green tea extract and its major constitutes on gut microbial metabolism in obese mice model"
The Blackwell Inn, Ballroom (2nd Floor)

9:25-9:45 a.m.
Oral Presentation
Zachary Konkel, The Ohio State University
Graduate Fellow, Translational Plant Sciences
"Structure-guided targeting of psilocybin gene homolog metabolites: a novel a utonomous approach"
The Blackwell Inn, Ballroom (2nd Floor)

9:45-10:05 a.m.
Oral Presentation
Dr. Angela Di Capua, The Ohio State University
Postdoctoral Researcher, Wysocki Group, Chemistry and Biochemistry
"Application of omics and native mass spectrometry approaches to understand Salmonella pathogenesis"
The Blackwell Inn, Ballroom (2nd Floor)

10:05-10:15 a.m.
BREAK

10:15-11:45 a.m.
Poster Session (Exhibitors and Networking)
Blackwell Patio (2nd Floor)

11:45-11:55 a.m.	**Lunch Pickup**
11:55 a.m.-12:30 p.m.	**Parallel Lunch & Learn Sessions** **Lunch and Learn: Sponsored by SCIEX** **Dr. Baljit Ubhi, SCIEX** *Application Scientist, Metabolomics & Lipidomics* "Novel approaches to quantitative metabolomics" The Blackwell Inn, Ballroom (2nd Floor) **Lunch and Learn: Sponsored by Metabolon** **Dr. Ieva Roznere, The Ohio State University** *Research Associate, Evolution, Ecology, and Organismal Biology* "Using metabolomics in freshwater mussel conservation" 140 Pfahl Hall
12:30-1:05 p.m.	**Student-Industry Networking Session** A panel of industry representatives from Abbott, Agilent, Metabolon, SCIEX, and Waters will provide insight into how to prepare for and find opportunities in industry. Moderated by Jeremy Hale, Center for Career and Professional Success. The Blackwell Inn, Ballroom (2nd Floor)
1:05-1:25 p.m.	**BREAK (Networking and Exhibitors)** The Blackwell Inn, Ballroom (2nd Floor)
1:25-2:00 p.m.	**Plenary Speaker** **Dr. Susan Sumner, University of North Carolina-Chapel Hill** *Professor, Nutrition* "The exposome meets precision nutrition" The Blackwell Inn, Ballroom (2nd Floor)
2:00-2:20 p.m.	**Oral Presentation** **Michael Dzakovich, The Ohio State University** *PhD Candidate, Cooperstone Lab, Horticulture and Crop Science* "Exploring natural variation in tomato steroidal glycoalkaloids: Using small tomatoes to answer big questions" The Blackwell Inn, Ballroom (2nd Floor)
2:20-2:40 p.m.	**Oral Presentation** **Wen Cong, The Ohio State University** *PhD Candidate, Flavor Research and Education Center, Food Science and Technology* "Identification of consumer liking markers in whole wheat bread using flavoromics" The Blackwell Inn, Ballroom (2nd Floor)
2:40-3:00 p.m.	**Oral Presentation** **Dr. Pan Deng, University of Kentucky** *Postdoctoral Researcher, Animal and Food Sciences, Superfund Research Center* "Dietary inulin decreases circulating ceramides by suppression of neutral sphingomyelinase expression and activity" The Blackwell Inn, Ballroom (2nd Floor)
3:00-3:05 p.m.	**Student Poster Awards & Closing Remarks** The Blackwell Inn, Ballroom (2nd Floor)

Abstracts

INVITED ABSTRACTS

Mass spectrometry imaging applications to support clinical decision making

Nathalie Y.R. Agar, PhD
Department of Neurosurgery, Brigham and Women's Hospital, Harvard Medical School

Mass spectrometry provides multiple options for the direct characterization of tissue to support surgical decision-making, and provides significant insight in the development of drugs targeting tumors of the central nervous system (CNS). Using an array of mass spectrometry (MS) applications, we rapidly analyze specific tumor markers ranging from small metabolites to proteins from surgical tissue for rapid diagnosis and surgical guidance. Using similar clinical protocols, we visualize drug and metabolites penetration in brain tumor tissue and correlate with tumor heterogeneity and response to support drug development.

Connecting the world's mass spectrometry data to understand the chemistry of life – a Big Data strategy

Pieter Dorrestein, PhD
Skaggs School of Pharmacy and Pharmaceutical Sciences, Departments of Pharmacology and Pediatrics; Collaborative Mass Spectrometry Innovation Center; Institute for Metabolomics Medicine, *University of California-San Diego*

Imagine if we could figure out the chemical composition of any sample and understand their relationships of the molecules to all other samples in seconds – akin to a Google search but instead of using a text we use mass spectrometry information. This is now beginning to be possible. The foundation for such infrastructure is being created through community wide knowledge capture and analysis tool development. In this lecture I will discuss the steps we have taken with building such community tools. This infrastructure is now used by 78,000 people worldwide. I will showcase how world-wide users are applying these tools in understanding the role of the microbiome in health and disease via reuse of public data, including non-clinical data. We have processed 100,000s of datasets and from this I will show representative examples associated with ecological questions, early therapeutic discovery, disease, sleep deprivation, personal care, malnutrition but also several single patient case studies, including a single patient phage therapy treatment but also how useful it is to enable rapid turn around of the analysis in a clinical setting.

Harnessing metabolomics to combat infectious diseases
Ian Lewis, PhD
Dept. of Biological Sciences, University of Calgary
The global rise in the prevalence of antibiotic resistant organisms is an imminent threat to global health and is projected to lower North American life expectancies by over a decade. Diagnostic technology could play a pivotal role in fighting antimicrobial resistance by enabling clinicians to make timely, evidence-based, decisions regarding the type antibiotics to prescribe to each patient. Unfortunately, it currently takes 2-5 days to identify microbial pathogens and measure their susceptibility to antimicrobials – a timeline that directly contributes to preventable deaths. To address this, the Lewis Research Group has recently developed a suite of metabolomics-based tools that can identify bloodstream and urinary tract infections in a fraction of the time required by more traditional approaches. The key to this transformative technology is a new metabolomics strategy that tracks the metabolic preferences of microbes. The presentation will discuss this new strategy and the potential role metabolomics could play in shaping global health.

The exposome meets precision nutrition
Susan Sumner, PhD
Nutrition Research Institute, University of North Carolina at Chapel Hill, NC 28081
The use of metabolomics in precision medicine often involves the development of biomarkers to detect, stage, and monitor disease, as well as to determine individuals' responses to drug treatments. Similarly, in the field of precision nutrition, individuals' have different nutrient requirements, and individuals' respond differently to nutrient intake. Lifestyle factors (e.g., stress, smoking, physical activity), use of medications or illicit drugs, dietary intake, and exposure to environmentally relevant chemicals are all part of our Exposome, and can lead to perturbations in endogenous metabolism to create new endogenous Exposomes. Genetics, polymorphisms, and metabolic individuality all contribute to the adverse or positive responses of an individual to the exposures they encounter. The intersection between genomics, metabolomics, and the environment (e.g., foods, nutrients, chemicals, drugs, lifestyle factors) are important to inform the development of nutritional intervention at the individual level. This section will cover examples of the challenges of Exposome Research to inform Precision Nutrition [U2CES026544; 1U24DK097193].

Abstracts

LUNCH AND LEARN ABSTRACTS

Spatial visualization of metabolite and lipid markers using MS imaging

Anthony Midey, PhD
Biomedical Research Group, Waters Corporation

Mass spectrometry imaging (MSI) extends the discovery process of identifying key markers in lipidomics and metabolomics to include spatial distribution information, increasing the understanding of how different mechanisms proceed. Understanding where metabolites are located and how their distributions evolve offers keen insights into disease pathology, drug targets, drug treatments, and other processes. Desorption electrospray ionization (DESI) for source sampling and ionization provides a label-free method for MSI under ambient conditions with no sample preparation for direct analysis. Adding ion mobility complementary structure/shape pre-separation prior to MS analysis in MSI resolves isobaric mass peaks, isomers, and extends peak capacity. An overview of how DESI, ion mobility, and mass spectrometry imaging work and what tools are available will provide the basis for a review of applications in lipidomics, metabolomics, and drug metabolism and kinetics (DMK), including direct monitoring of metabolism in cell cultures.

Integrated metabolomics analyses to uncover metabolic vulnerabilities in cancer

Shawn McGuirk[1], Yibo Xue[1], Mathieu Vernier[1], Kaiqiong Zhao[3,4], Geneviève Morin[1], Celia MT Greenwood[3,4,5,6], Vincent Giguère[1], Sidong Huang[1], Julie St-Pierre[1,2]
[1]Department of Biochemistry, Rosalind and Morris Goodman Cancer Research Centre, McGill University, Montreal, QC, Canada, H3G 1Y6; [2]Department of Biochemistry, Microbiology, and Immunology, University of Ottawa, Ottawa, ON, Canada, K1H 8M5;[3]Department of Epidemiology, Biostatistics and Occupational Health, McGill University, Montreal, QC, Canada, H3A 1A2;[4]Lady Davis Institute, Jewish General Hospital, Montreal, QC, Canada, H3T 1E2;[5]Department of Human Genetics, McGill University, Montreal, QC, Canada, H3A 0C7;[6]Gerald Bronfman Department of Oncology, 5100 de Maisonneuve Blvd. West, Suite 720. Montreal, Quebec H4A 3T2

Development of chemotherapy resistance is a critical barrier in cancer treatment. Increased reliance on mitochondrial metabolism has been described as a distinctive characteristic of resistant cancers, however it is unknown whether enhanced oxidative metabolism is an intrinsic property or whether the metabolic signature of resistant cancers is dependent on the therapeutics. Here we show that two anthracyclines, doxorubicin and epirubicin, elicit distinct primary metabolic vulnerabilities in human breast cancer cells. Doxorubicin-resistant cells rely on glutamine to drive oxidative phosphorylation and *de novo* glutathione synthesis, while epirubicin-resistant cells display markedly increased bioenergetic capacity and mitochondrial ATP production. Targeting the global metabolic regulator PGC-1α abrogated growth and survival of doxorubicin- and epirubicin-resistant cells, as it controls both drug-specific metabolic vulnerabilities. Overall, our work reveals that targeting global regulators of metabolism like PGC-1α may provide an effective strategy to overcome resistance to multiple therapeutic agents.

Using metabolomics in freshwater mussel conservation

Ieva Roznere, PhD
Department of Evolution, Ecology, and Organismal Biology, The Ohio State University

Freshwater mussels are the most endangered group of animals in North America. As numbers of freshwater mussels continue to decline, conservation efforts are more critical than ever in order to protect existing populations. Freshwater mussels are often translocated between habitats or into captivity for purposes such as propagation, basic research, or as temporary refugia. Although translocation is an important tool that is increasingly used in wildlife conservation and management, it often results in increased mortality and reduced growth. Despite the necessity, there is limited knowledge of mussel health and the effects of environmental stressors on mussel physiology. I leverage the power of metabolomics to better understand the physiology of these animals and how they respond to environmental stress, such as translocation. Adult *Amblema plicata* were translocated from the Muskingum River to the Columbus Zoo and Aquarium Freshwater Mussel Conservation and Research Center and to Big Darby Creek. Hemolymph samples were taken from wild and translocated mussels every few months for one year. Samples were analyzed by Metabolon, Inc. using GS-MS and LC-MS and approximately 100 metabolites were identified. Glucose and lipid metabolism remained similar among groups but differences were observed in altered amino acid and nucleotide metabolism. The results are indicative of a general stress response, which is evident after a year post-translocation. The mussels in our research center were also subjected to a separate food limitation study. Because metabolite production is closely associated with environmental conditions, studying changes in these biological molecules is especially helpful in understanding how animals react to environmental stressors. In this presentation I will discuss the insights gained from using metabolomics to study freshwater mussel physiology and how this research helps to improve ongoing and future conservation efforts.

Novel approaches to quantitative metabolomics

Baljit Ubhi, PhD
Global Metabolomics & Lipidomics Applications, SCIEX

The major challenge in the field of metabolomics is to accurately identify and quantify hundreds of metabolites within a single analytical run. The ability to measure biologically relevant metabolites and quantitate them in complex matrices has always been a major objective in any Omics lab. Therefore the flexibility of an analytical platform to offer the flexibility of quantitative and qualitative workflows is deemed critical. These workflows can be delivered these objectives. Recently variable window SWATH acquisition has shown to identify a higher number of metabolites compared to the traditional Data Dependent Acquisition (DDA) approach, thus enabling broader metabolome coverage. Using MS/MS fragments for metabolite quantitation provides better selectivity, and ultimately increased sensitivity. Variable window SWATH Acquisition provides quality quantitative data for metabolites in complex matrix. Targeted workflows on QTRAP technology have shown increased metabolite coverage (by upto 50%) by utilizing low flow rates, through the M5 microflow platform. Quantitation of large panels of metabolites (n=310) and lipid molecular species (n=1500) is possible given the speed of the QTRAP platform in a single analytical run. Given the overlap of MRMs in the small molecule space, the TRAP allows a user to run added confirmatory experiments for qualitative data review through library matching workflows. All of these workflows will be demonstrated during this presentation.

Abstracts

OSU CORE FACILITY ABSTRACTS

The OSU CCIC Mass Spectrometry and Proteomics Facility

Árpád Somogyi[1], Liwen Zhang[1], Andrew Reed[1], Florian Busch[1,4], Nan Kleinholz[1], Sophie Harvey[1,4], Matt Bernier[1], Michael Freitas[2], Vicki H. Wysocki[3,4]

[1]OSU CCIC MSP Facility, [2] SBS-Cancer Biology and Genetics, OSU, [3] Department of Chemistry and Biochemistry, OSU, [4]Resource for Native MS-Guided Structural Biology, 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, and a vi) Bruker timsTOF Pro nanospray ion mobility MS/MS system. Representative examples for collaborative projects and services will be shown in the presentation.

Shared 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

The shared NMR facility at the Ohio State University (OSU) houses 9 state-of-the-art high-field NMRs from Bruker Biospin with 5 instruments at 800 MHz and above. The 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. CCIC NMR also develops the public suite of web servers (COLMAR) for the automated analysis of multidimensional NMR spectra for the accurate identification and quantification of metabolites in complex biological mixtures. CCIC NMR instruments and staff 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.

Resource for Native Mass Spectrometry Guided Structural Biology

Árpád Somogyi[1], Sophie Harvey[1,3], Florian Busch[1,3], Dalton Snyder[3], Vicki H. Wysocki[1,2,3]

[1]OSU CCIC MSP Facility, [2] Department of Chemistry and Biochemistry, [3]Resource for Native MS-Guided Structural Biology, OSU.

The Resource for Native Mass Spectrometry Guided Structural Biology (nMS➔SB) was established in 2018 with a 6.8M P41 grant from the NIH National Institute of General Medical Sciences. As a national Biomedical Technology Research Resource, our mission is to develop improved native MS as a routine tool and disseminate the technology to the biomedical research community through vendor partnerships and training. We are building an integrated MS-based workflow for intact, native complexes, i.e. "complex-down" characterization, with state-of-the-art instrumentation and software that can answer structural biology questions. An integrated workflow for native MS will define the m/z of the intact complex, m/z of subcomplexes, stoichiometry, heterogeneity, connectivity of partners, topology, conformational diversity, collision cross sections, and relative subunit binding strengths of intact, native protein complexes with high sensitivity and throughput. The Resource works with investigators across

the nation and globe on challenging biomedical projects that have both biomedical significance and substantial technical structural characterization challenges. These Driving Biomedical Projects, ranging from viral hemorrhagic fevers and HIV to cataract formation and neurological disorders, are integrated with Technology Research and Development projects and serve as the drivers and testbeds of developing technologies. Collaboration and Service Projects show investigators how developed technologies can begin to answer their questions for structural biology. Technology Research and Development is fostered by collaborations with Software Consultants, Technology Partners, and National Lab Partners.

Nutrient and Phytochemical Analytics Shared Resource (NPASR)

Ken Riedl, PhD, Acting Director

Department of Food Science & Technology; OSU Comprehensive Cancer Center

NPASR brings world class expertise in applying LCMS technologies to measure key bioactives and biomarkers in foods and biologics. We excel at targeted and untargeted metabolomics for biomarker identification, quantification, and metabolite discovery. Metabolomics experiments (targeted and untargeted) provide broad metabolite coverage to aid in identifying new relationships between metabolites and associations with clinical metadata. We have particular experience in targeted and untargeted metabolomics supporting a 'Crops to Clinic' approach in which dietary interventions are used 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 lipidomics delivering >1,000 lipid species over 13 classes with our Lipidyzer platform and smaller focused LCMS panels to recover less abundant classes like eicosanoids.

OARDC Metabolite Analysis Cluster (OMAC)

Blakeslee, J.J.[1,2]

[1]Department of Horticulture and Crop Science, Ohio Agricultural Research and Development Center (OARDC), The Ohio State University

[2]OARDC 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 simultaneously 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, microbial cells or cellular exudates, food and beverage samples, 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. Compounds in which the facility specializes include: terpenoids, phytohormones, organic acids, sugars/polysaccharides, lipid signaling molecules and membrane components, plant secondary metabolites, neurotransmitters, nucleotides. protein purification and enzyme characterization, plant secondary/specialized metabolism. OMAC also provides services in the areas of metabolic engineering of plant, microbial, and cellular systems; detection of herbicide and pesticides; protein purification and enzymatic assay development; kinase/phosphatase assay development; and the biochemical dissection of cellular signaling and organismal stress responses.

Posters

Submitted abstracts are available at ***go.osu.edu/omsms***

(1) A deeper dive into HILIC chromatography
Scott Abernathy, Peter A. Lobue, Patrick A. Limbach
University of Cincinnati

(2) Optimization of sample preparation method for proteomics analysis of gut microbiota
Maryam Baniasad[1], Yongseok Kim[1], Anice Sabag-Daigle[2], Brian Ahmer[2], Vicki H. Wysocki[1]
[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210
[2]Department of Microbial Infection and Immunity, The Ohio State University, Columbus, OH 43210

(3) The effects of doxorubicin-based chemotherapy and omega-3 supplementation on the mouse brain lipidome
Djawed Bennouna[1], Melissa Solano[16], Tonya S. Orchard[1], A. Courtney DeVries[2,3], Maryam Lustberg[4], Rachel E. Kopec[1,5*]
[1]Department of Human Sciences, Human Nutrition Program, The Ohio State University, Columbus, OH
[2]Department of Neuroscience, College of Medicine, The Ohio State University,Columbus, OH
[3]Rockefeller Neuroscience Institute, West Virginia University, WV
[4]Department of Internal Medicine, College of Medicine, The Ohio State University, Columbus, OH
[5]Foods for Health Discovery Theme, The Ohio State University, Columbus, OH
[6]Medical Dietetics, College of Medicine, The Ohio State University, Columbus, OH

(4) Linking genomics and metabolomics for nutrition-driven germplasm improvement of apples
Emma Bilbrey,[1] Emmanuel Hatzakis,[2] Diane Miller,[1] Jonathan Fresnedo Ramirez,[1] Jessica Cooperstone[1,2]
[1]Horticulture and Crop Sciences and [2]Food Science and Technology, The Ohio State University, Columbus, OH.

(5) Metabolome-based genome wide association profiling of innate immunity in rice
Joshua Blakeslee[1,2], Bai, P.[3], Liu, Y.[3], Lin, Y.[1], Bernier, M.C.[4], Wang, G.L.[3]
[1]Department of Horticulture and Crop Science, The Ohio State University, Wooster, OH
[2]OARDC Metabolite Analysis Cluster, The Ohio State University, Columbus, OH
[3]Department of Plant Pathology, The Ohio State University, Columbus, OH
[4]Campus Chemical Instrumentation Center, The Ohio State University, Columbus, OH

(6) Development and validation of a sensitive LC-MS/MS method for quantifying dynorphin B
Karthik Chandu[1]; Tony L Sahley[2]; Michael D Hammonds[2]; Masaru Miyagi[3]; David J Anderson[1]
[1]Department of Chemistry; Cleveland State University, Cleveland, OH; [2]School of Health Sciences; Cleveland State University, Cleveland, OH; [3]Department of Pharmacology; Case Western Reserve University, Cleveland, OH

(7) Untargeted metabolomic profiling of early diet energy intake in C57BL/6N mice indicates tentative differences correlated with diet and colon region
Haley Chatelaine[1]; Kyle Spencer[2]; Cynthia Ramazani[2,3]; Susan Olivo-Marston[4]; Emmanuel Hatzakis[5,6]; Ewy Mathe[2,7,8]; Rachel E. Kopec[1,6]
[1]Human Nutrition Program, The Ohio State University, Columbus, OH; [2]Department of Biomedical Informatics, The Ohio State University; [3]Indiana State University; [4]Division of Epidemiology, College of Public Health, The Ohio State University; [5]Department of Food Science and Technology, The Ohio State University; [6]Foods for Health and Metabolomics Discovery Theme, The Ohio State University, Columbus, OH; [7]Comprehensive Cancer Center, The Ohio State University; [8]Translational Data Analytics Institute, The Ohio State University

(8) Characterization and differentiation of bispecific antibody chain pairing variants by native and ion mobility mass spectrometry
Chen Du[1], Zac VanAernum[1], Monita Muralidharan[1], Wendy Sandoval[2] and Vicki H. Wysocki[1]
[1]The Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH
[2]Departments of Proteomics & Biological Resources, Genentech, Inc., South San Francisco, CA

(9) Modification mapping of large subunit ribosomal RNA through overlapping digestion products
Mariana Estevez, Priti Thakur, Peter Lobue, Patrick Limbach, Balasubrahmanyam Addepalli
Rieveschl Laboratories for Mass spectrometry, University of Cincinnati, Cincinnati, Ohio

(10) Discrimination of differently pasteurized orange juices and identification of marker compounds using untargeted UHPLC-IMS-qToF-MS
Lara Etzbach, Svenja Treu, Fabian Weber, Andreas Schieber
Institute of Nutritional and Food Sciences, Molecular Food Technology, University of Bonn, Endenicher Allee 19b, 53115 Bonn, Germany

(11) Modulating the chemical micro-environment of dried blood spheroids for long-term storage of labile organic molecules and biomarkers
Benjamin S. Frey, Deidre E. Damon, and Abraham K. Badu-Tawiah*
The Ohio State University, Columbus, OH

(12) Identification of compounds that contribute to the bitterness perception of coffee brew
Chengyu Gao, Devin G Peterson
Department of Food Science and Technology, The Ohio State University

(13) A multi-omics approach to investigate the role of EZH2 in chromatin remodeling, cell proliferation and tumorigenesis
Miranda L. Gardner[1,2], Michael A. Freitas[1,2]
[1]Ohio State Biochemistry Program, The Ohio State University, Columbus Ohio
[2]Department of Cancer Biology and Genetics, The Ohio State University Wexner Medical Center, Columbus Ohio

(14) Tomato steroidal glycoalkaloids are absorbed, metabolized, and stored in pigs
Mallory Goggans[1], Michael Dzakovich[2], David Francis[2], Sheila Jacobi[3], Jessica Cooperstone[1,2]
[1]The Ohio State University Department of Food Science and Technology
[2]The Ohio State University Department of Horticulture and Crop Science
[3]The Ohio State University Department of Animal Sciences

(15) Improved high-throughput targeted lipidomic analysis with sMRM Pro Builder
Santosh Kapil Kumar Gorti[1], Sean Seymour[2], Mackenzie J Pearson[1], Christie Hunter[3] and Paul RS Baker[3]
[1]SCIEX, 500 Old Connecticut Rd, Framingham, CA, [2]Seymour data science, CA, [3]SCIEX, 1201 Radio Rd, Redwood City

(16) Are steroidal glycoalkaloids imparting bitterness in tomato?
Jordan L. Hartman[1], Michael P. Dzakovich[1], David M. Francis[1], Jessica L. Cooperstone[1, 2]
[1]The Ohio State University Department of Horticulture and Crop Science
[2]The Ohio State University Department of Food Science and Technology

(17) Benzo(a)pyrene and its interactions with modified RNA
Cassandra Herbert, Balasubrahmanyam Addepalli, Patrick A. Limbach
University of Cincinnati

(18) Novel standardized metabolomics/lipidomics analysis tool for comprehensive targeted profiling
Timothy Hyde', Hai Pham Tuan; Ulf Sommer, Svenja Heischmann, Doreen Kirchberg, Xenia Iwanowa, Radu Talmazan, Barbara Wolf, Martin Buratti, Rosa Argamasilla Martinez, Cornelia Röhring, Therese Koal
BIOCRATES Life Sciences AG, Eduard-Bodem-Gasse 8, 6020 Innsbruck, Austria

Posters

(19) Enzymatic and chemical hydrolysis in the identification of sugars in citrus pectin using ^{1}H and ^{13}C NMR
Jennifer Janovick; Emmanuel Hatzakis
Department of Food Science and Technology, The Ohio State University

(20) Detection and discovery of ribonucleosides by higher-energy collisional dissociation mass spectrometry (HCD MS)
Manasses Jora, Peter A. Lobue, Robert L. Ross, Ningxi Yu, Ruoxia Zhao, Balasubrahmanyam Addepalli and Patrick A. Limbach
Rieveschl Laboratories for Mass Spectrometry, Department of Chemistry, University of Cincinnati, Cincinnati OH 45221

(21) A pilot study of untargeted urine metabolomics in sarcoma patients treated with HD-AIM
Garrett Kinnebrew[1], James Chen[1,2], David Liebner[1,2], Ewy Mathe[1]
[1] Department of Biomedical Informatics, College of Medicine, The Ohio State University, Columbus, OH 43210, USA.
[2] Department of Internal Medicine, Division of Medical Oncology, The Ohio State University, Columbus, OH 43210, USA.

(22) Putting together the pieces of archaeal RNase P
Stella M. Lai[1-3], Venkat Gopalan[1,2], and Vicki H. Wysocki[1-3]
Department of Chemistry and Biochemistry[1], Center for RNA Biology[2], and Resource for Native Mass Spectrometry-Guided Structural Biology[3]
The Ohio State University, Columbus, OH 43210

(23) Using multiple ionization techniques to understand dissolved organic matter (DOM) oxidation by permanganate
Juliana R. Laszakovits[1], Arpad Somogyi[2], Allison A. MacKay[1]
[1]Department of Civil, Environmental, and Geodetic Engineering, The Ohio State University
[2]Campus Chemical Instrument Center: Mass Spectrometry and Proteomics, The Ohio State University

(24) Evaluation of sample processing parameters for optimized 2D NMR metabolomics experiments
Courtney E. Littlefield, Matthias S. Klein
Department of Food Science and Technology, The Ohio State University, 2015 Fyffe Road, Columbus OH 43210

(25) Metabolomic analysis of an endophytic *Streptomyces sp.* from the liverwort *Bazzania trilobata*
Preston K. Manwill[1], Zach Shank[1], Choon Yong Tan[1], Hee-Byung Chai[1], Thomas Wieboldt[2] and Harinantenaina L. Rakotondraibe[1]
Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University[1]; Department of Biological Sciences, Virginia Polytechnic Institute and State University[2]

(26) Identifying urinary biomarkers of tomato consumption using untargeted metabolomics
Jenna Miller,[1] David Francis[2], Earl Harrison[3], Janet Novotny[4], Jessica Cooperstone,[1,2]
[1]Food Science and Technology, [2]Horticulture and Crop Sciences, [3]Human Sciences, Human Nutrition, The Ohio State University, Columbus, OH; and [4]USDA Agricultural Research Service, Beltsville Human Nutrition Research Center, Beltsville, MD

(27) Subunit interaction of glutathionylated human hemoglobin probed by surface-induced dissociation/ion mobility mass spectrometry
Monita Muralidharan[1], Amit Kumar Mandal[2], Vicki H. Wysocki[1]
[1] Department of Chemistry and Biochemistry and Resource for Native Mass Spectrometry Guided Structural Biology, Ohio State University, Columbus, Ohio 43210, United States
[2]Clinical Proteomics Unit, St. John's Research Institute, Bangalore, 560034, India

(28) Comparison of strategies for the enrichment of cross-linked peptides
Andrew Norris, Florian Busch, Vicki Wysocki
The Ohio State University Department of Chemistry and Biochemistry

(29) AcquireX... A deep Dive into the sea of metabolic features
Ioanna Ntai, Tatjana Talamantes, Sven Hackbusch, Amanda Souza
Thermo Fisher Scientific, San Jose, CA

(30) Modifying a 15T FT-ICR platform for native mass spectrometry applications
Erin M. Panczyk[1,2], Dalton T. Snyder[2], Arpad Somogyi[2,3], Desmond A. Kaplan[4], Mark E. Ridgeway[5], Melvin A. Park[5], and Vicki H. Wysocki[1,2,3]
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[3]Campus Chemical Instrument Center, Mass Spectrometry and Proteomics Facility, The Ohio State University, Columbus, OH 43210
[4]KapScience, Tewksbury, MA, 01876
[5]Bruker Daltonics Inc., Billerica, MA, 01821

(31) MDM2 copy number aberrations alter ceramide glycosylation in liposarcoma tumors, impacting drug response
Andrew Patt (andrew.patt@osumc.edu)[1,2#], Bryce Demoret (bryce.demoret@osumc.edu)[3#], Andrew Patterson (adp117@psu.edu)[4], Philip Smith (pbs13@psu.edu)[5], Ewy Mathé (ewy.mathe@osumc.edu)[1*], James L Chen (james.chen@osumc.edu)[3*]
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[2] Biomedical Sciences Graduate Program, The Ohio State University, Columbus, Ohio, United States of America
[3] Department of Internal Medicine, The Ohio State University, Columbus, OH, USA.
[4] Department of Veterinary and Biomedical Sciences, The Pennsylvania State University, University Park, PA, United States of America
[5] The Huck Institutes of the Life Sciences, The Pennsylvania State University, University Park, PA, 16802-4400, USA.

(32) Development of gradient chromatofocusing -mass spectrometry in the determination of protein isoforms
Sreenivasavi Rayaprolu, David J Anderson
Cleveland State University

(33) Mass spectrometry-based detection of genetically variable peptides: An alternative to DNA typing
Andrew J. Reed[1], Maryam Baniasad[1], Stella M. Lai[1], Liwen Zhang[1], Florian Busch[1], Vicki H. Wysocki[1], Myles W. Gardner[2], F. Curtis Hewitt[2], and Michael A. Freitas[1]
[1]The Ohio State University, Columbus, OH, [2]Signature Science, LLC, Austin, TX

(34) Assessment of the effects of black raspberry phytochemicals on the mechanisms of allergic contact dermatitis
Nathan Ryan[1], Kelvin Anderson[1], Arham Siddiqui[1], Travis Pero[1,2], Annalise Celano[3,4], Jessica Cooperstone Ph.D[3,4], Steve Oghumu[1] Ph.D
[1] Department of Pathology, The Ohio State University Wexner Medical Center
[2] College of Dentistry, The Ohio State University
[3] Department of Horticulture and Crop Science, College of Food, Agricultural and Environmental Sciences, The Ohio State University
[4] Department of Food Science and Technology, College of Food, Agricultural and Environmental Sciences, The Ohio State University

Posters

(35) Assessment of dietary compliance and catechin/catechin-derived microbial metabolite pharmacokinetic responses in obese and healthy individuals following consumption of a novel green tea extract-rich confection
Geoffrey Y. Sasaki,[1] Allison L. Barnes,[2] Meghan McErlean,[3] Yael Vodovotz,[4] Richard S. Bruno[1]
[1]Human Nutrition Program, [2]School of Health and Rehabilitation Sciences, [3]Biological Sciences Program, [4]Department of Food Science and Technology, The Ohio State University, Columbus, Ohio

(36) A second-generation device for surface-induced dissociation of protein complexes in a 15 T FT-ICR mass spectrometer
Dalton T. Snyder[1]; Erin Panczyk[1,3]; Arpad Somogyi[1,2]; Desmond Kaplan[4]; Vicki Wysocki*[1,2,3]
[1]Resource for Native MS Guided Structural Biology
[2]Campus Chemical Instrument Center, Mass Spectrometry and Proteomics
[3]Department of Chemistry and Biochemistry
The Ohio State University, Columbus OH, USA 43210
[4]KapScience LLC, Tewksbury, MA, USA 01876

(37) The effect of diet on the metabolome and microbiome of the colon in a lifetime obesity murine model
Kyle Spencer[1], Haley Chatelaine[2], Cynthia Ramazami[1,3], Susan Olivo-Marston[8], Emmanuel Hatzakis[6,7], Rachel Kopec[2,6], Ewy Mathé[1,4,5]
[1]Department of Biomedical Informatics, The Ohio State University; [2]Human Nutrition Program, The Ohio State University, Columbus, OH; [3]Indiana State University; [4]Comprehensive Cancer Center, The Ohio State University; [5]Translational Data Analytics Institute, The Ohio State University; [6]Foods for Health and Metabolomics Discovery Theme, The Ohio State University, Columbus, OH; [7]Department of Food Science and Technology, The Ohio State University; [8]Division of Epidemiology, College of Public Health, The Ohio State University

(38) Using metabolomics to classify the underlying effects of multi-nutrient supplementation in ADHD Youth
Madeline Stern[1], Leanna Perez[1], L. Eugene Arnold[2], Irene Hatsu[1], Rachel Kopec[1,3]
[1]Human Nutrition Division, The Ohio State University, United States of America
[2] Department of Psychiatry & Behavioral Health, Ohio State University, Columbus, Ohio
[3]Foods for Health and Metabolomics Discovery Theme, The Ohio State University

(39) Metabolite profiling and authentication of pomegranate juice using high-resolution NMR spectroscopy and chemometrics.
Fenfen Tang[1] , Emmanuel Hatzakis[1]
1 Department of Food Science and Technology, The Ohio State University, Columbus, OH

(40) Probing the mechanism of inhibition for inhibitors of metallo-β-lactamase VIM-2
Caitlyn A. Thomas, Zishuo Cheng, Kundi Yang, Elle Hellwarth, Sarah Fullington, Cole Yurkiewicz, Faith Baxter, Michael W. Crowder
Miami University

(41) In vitro evaluation of apple pomace as a source of prebiotics: an NMR metabolomics approach
Kathryn Williamson[1], Emmanuel Hatzakis[1,2]
[1]Department of Food Science and Technology, The Ohio State University
[2]Discovery Themes, The Ohio State University

(42) Iron chlorophyllin metabolites in simulated digestion and Caco-2 human small intestinal cell model
Siqiong Zhong[1], Rachel Kopec[1,2]
[1]Human Nutrition Program, Department of Human Sciences, The Ohio State University, Columbus, OH
[2]Foods for Health and Metabolomics Discovery Theme, The Ohio State University, Columbus, OH

Thank You

TO OUR POSTER JUDGES!

Randy Arnold, SCIEX
Stephan Baumann, Agilent
Matt Bernier, Campus Chemical Instrument Center
Josh Blakeslee, Horticulture and Crop Science
Florian Busch, Campus Chemical Instrument Center
Timothy Chapman, Abbott
Jessica Cooperstone, Horticulture and Crop Science
Sagar Deshpande, Food Science and Technology
Diana Forero Arcila, Food Science and Technology
Krystyn Gumpper, Internal Medicine
Sophie Harvey, Campus Chemical Instrument Center
Amanda Hummon, Chemistry and Biochemistry
Sanja Ilic, Human Sciences
Matthias Klein, Food Science and Technology
Tom Knobloch, Public Health
Rachel Kopec, Human Sciences
Francisco (Pakito) Martinez, Metabolon
Anthony Midey, Waters
Steve Oghumu, Pathology
Quang Son Pham, Abbott
Ken Riedl, Food Science and Technology
Mei Shotts, Abbott
Baljit Ubhi, SCIEX
Yael Vodovotz, Food Science and Technology
Chris Weghorst, Public Health
Liwen Zhang, Campus Chemical Instrument Center
Chris Zhu, Human Sciences
Ouliana Ziouzenkova, Human Sciences

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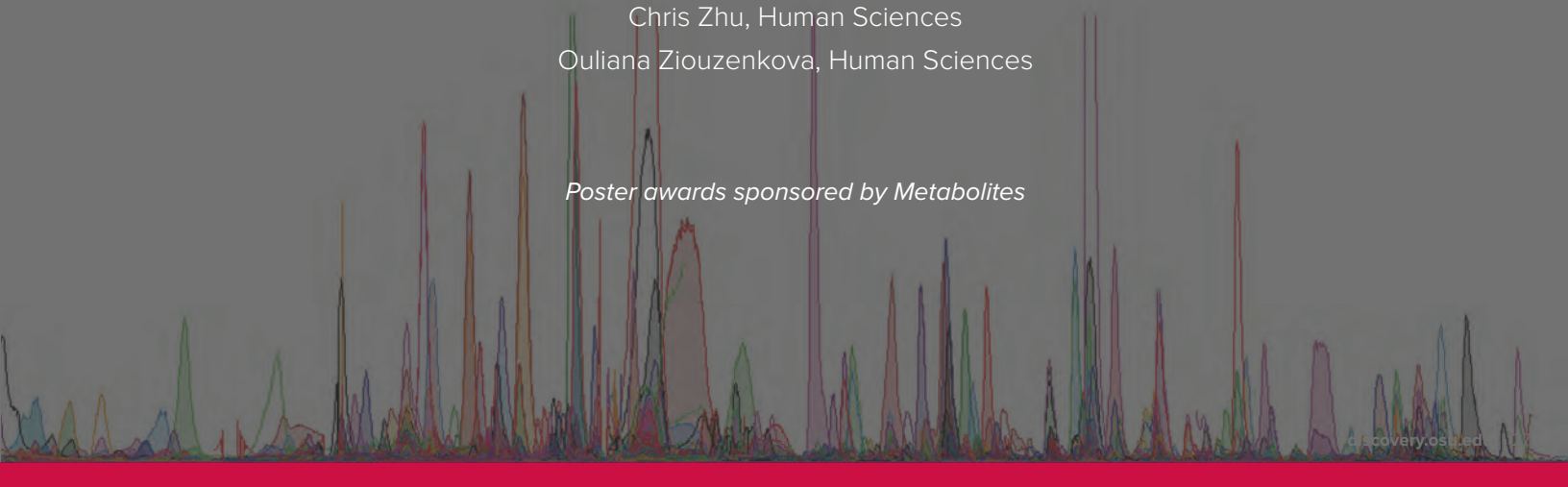

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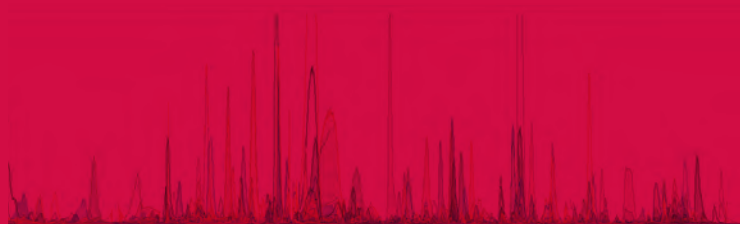

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& Metabolomics Symposium

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