

MANA 2021
Oral Sessions
October 19 – 20

Tuesday October 19
1:00 – 2:40 pm

Biomedical 1		Computational	Food/Nutrition
1:00	Priyanka Baloni , Institute for Systems Biology <i>Multiomic analyses of sphingolipid pathway identifies potential drugs for Alzheimer's disease</i>	Hayden Johnson , Univ Memphis <i>Robust and reproducible time-domain NMR metabolomics of hepatic tissues using CRAFT</i>	Jacob Folz , UC Davis <i>In-vivo sampling of healthy human intestinal tract regions using a novel ingestible sampling device with comprehensive metabolomics</i>
1:25	Abigail Leggett , Ohio State Univ <i>Unique metabolite and pathway differences between planktonic and biofilm states in Pseudomonas aeruginosa by NMR-based metabolomics</i>	Yuri Corilo , PNNL <i>CoreMS: Mass Spectrometry software framework and acquisition-time data analysis</i>	Robert Hood , Emory <i>Pesticide residue intake from fruits and vegetables and alterations in the serum metabolome of women undergoing infertility treatment</i>
1:40	Nicole Prince , Harvard Univ <i>Steroid metabolite profiles at age 1 are indicative of immune-related outcomes in children through age 6</i>	Xinmeng Li , Tufts <i>Exploring improved graph neural networks with topic modeling and attention for spectra prediction</i>	Rosalie Zhong , Ohio State Univ <i>A metabolomics approach to iron chlorophyll derivative identification from kale leaf (Brassica oleracea L. var. sabellica) following moderate electric field (MEF) treatment</i>
1:55	Si Wu , Stanford Univ <i>Integrated multi-omics analysis of thyroid cancer reveals key molecular pathways involved in tumor formation and metastasis</i>	Gayatri Iyer , Univ of Michigan <i>Applications of data-driven network analysis in metabolomics and lipidomics data</i>	Haley Chatelaine , Ohio State Univ <i>¹H-NMR and LC-MS untargeted metabolomic profiling of mouse colon in response to probiotic yogurt consumption</i>
2:10	Oana Zeleznik , Harvard Univ <i>Metabolomics within-person stability over 10 years among women in two large datasets</i>	Yujue Wang , Rutgers <i>AccuCor2: isotope natural abundance correction for dual-isotope tracer experiments</i>	Michael Dzakovich , Ohio State Univ <i>Dietary tomato phytochemicals impact the mouse liver transcriptome and metabolome</i>
2:25	Oliver Fiehn , UC Davis <i>A Metabolome Atlas of the Aging Mouse Brain</i>	Yue Wu , Univ of Georgia <i>Automatic NMR spectral decomposition through computational fitting of time-domain signals</i>	Sneha Couvillion , PNNL <i>Multi-platform fecal metabolomics and lipidomics reveals significant differences between vegan and omnivore diets</i>

Wednesday October 20

12:00 – 1:40 pm

Agriculture, Ecology, & the Environment		Biomedical #2	Metabolite ID
12:00	Oliver Baars , North Carolina State Univ <i>Root exudation of secondary metabolites by three tomato varieties in response abiotic and biotic stressors</i>	Laura-Isobel McCall , Univ of Oklahoma <i>Chemical cartography-based metabolomics to guide rational drug development</i>	Vasuk Gautam , Univ Alberta <i>NP-MRD: The World's Largest NMR Database for Natural Products</i>
12:25	Christopher Anderton , PNNL <i>High spatial resolution laser ablation electrospray ionization mass spectrometry for target single cell analysis and imaging application</i>	Fouad Choueiry , Ohio State Univ <i>Metabolomics integration with gene expression profiling elucidates IL411 as modulator of ibrutinib resistance in ABC-diffuse large B cell lymphoma</i>	Jessica Bade , PNNL <i>Drift time shift modeling in IMS-MS/MS fragmentation matching</i>
12:40	Amanda Bayless , NIST <i>The Influence of Caging on the Dreissenid Mussel Metabolome</i>	Xin Ma , Georgia Tech <i>Ultrahigh resolution imaging mass spectrometry reveals lipidome alterations in early-stage ovarian cancer</i>	Goncalo Gouveia , Univ of Georgia <i>Building a fraction library for metabolomics</i>
12:55	Maris Cinelli , Michigan State Univ <i>Discovery of indole-tropane hybrid alkaloids from Datura stramonium</i>	Rachel Kelly , Harvard Univ <i>Metabo-endotypes, Multi-Omic Endotypes and Precision Medicine: An Example from Asthma</i>	Wenyun Lu , Princeton Univ <i>Experimental approaches for confident annotation of ammonium adducts in LC-HRMS metabolomics data</i>
1:10	Pawanjit Kaur Sandhu , Clemson Univ <i>Mapping the cellular physiology of glyphosate resistance in Palmer amaranth using global metabolomic approaches</i>	Boryana Petrova , Harvard Univ <i>Untargeted Metabolomics of the Maternal Immune Activation Brain Model Pathogenicity</i>	David Degnan , PNNL <i>Evaluating retention index score assumptions refined existing metrics for GC-MS small molecule identification</i>
1:25	Vidya Suseela , Clemson Univ <i>Utilizing phytometabolome to visualize the parasitic and mutualistic phenotypes of arbuscular mycorrhizal fungi</i>	Hannah Heath , Cal Poly San Luis Obispo <i>Metabolomics profiling in plasma distinguish metabolic alterations across pregnancy in women with gestational diabetes: A case-control time-course analysis</i>	Brady Anderson , Univ of Michigan <i>Improved Untargeted Metabolomics Compound Identification and Annotation by Using Longer Gradients, Increased Sample Loading, and Iterative Acquisition</i>