Poster #	Author	Institution	Title	Abstract
1	Ana Carolina Alves dos Santos	Concordia University	Steroid and contraceptive analysis in human serum using LC-MS/MS and LC-HRMS	Steroids play a role in many physiological and pathophysiological processes in the human body. Therefore, measuring steroid levels is important to understand the mechanisms of their regulation to define the best therapeutic targets, and monitor disease severity, response to treatment or prognosis. This need has motivated us to develop a sensitive and selective method by LC-MS/MS for targeted analysis of corticoids, estrogens, androgens, progestogens and selected contraceptives, and by LC-HRMS for untargeted steroid/contraceptive profiling. The method comprises a 3-step liquid-liquid extraction (LLE) with methyl tert-butyl ether, followed by derivatization using dansyl chloride or Girard-P reagent to profile estrogens and dehydroepiandrosterone, respectively. LLE approach outperformed simple acetonitrile solvent precipitation. The completeness of the derivatization reactions was assessed, as well as the suitability of selected labelled internal standards for expanded steroid profiling. Chromatographic separation of analytes of interest including isomers was achieved by biphenyl reversed-phase chromatography with a total analysis time of 28 minutes. The performance of acetic acid and ammonium fluoride mobile phase additives was evaluated. Final validated method is applicable for comprehensive steroid measurement in serum from both men and women, including post-menopausal women and older men with lower hormone levels and for monitoring contraceptive levels.
3	Ashley Zubkowski	University of Alberta	Metabolomic comparison of blood stability methods during shipment	Human blood samples are fundamental to many metabolomics studies, but collection, storage and shipment methods can vary widely. Previously, we determined that collection methods (capillary vs. venous) and freshly collected sample types (plasma vs. serum) did not significantly differ in metabolomic profiles. Before analysis, many samples are shipped for multiple days under various conditions. Dried blood spots (DBS) have become increasingly popular for simple shipping, but a regulated shipment temperature (frozen vs. room temperature) has not been established. The shipping variation effects on these samples have not been studied extensively, and it is challenging to compare quantitative metabolite values under different conditions. In the present study, blood samples from 5 healthy volunteers were collected through fingerstick, Tasso and a venous blood draw. Dried spots from capillary and venous collections, blood extracts and liquid samples were analyzed after 3-day periods stored at various temperatures. Analysis was completed through quantitative liquid chromatography-tandem mass spectrometry (LC-MS/MS). The LC-MS/MS analysis measured 1000 biomedically relevant metabolites (including amino acids, acylcarnitines, lipids, organic acids, etc.). This study aims to determine if shipment temperature alters metabolite profiles in various sample preparations. Preliminary data indicates a change in metabolites under various temperature storage conditions but not between collection methods.
4	Charles Viau	McGill University	Optimization a Biphasic Extraction Method for Metabolomics Study of Islet Cells	Diabetes is a common metabolic disease in the Western world, affecting over 10% of US adults. Here, we developed an extraction protocol for both untargeted metabolomics and lipidomics analysis optimized from a small quantity of pancreatic material (200 islets, or 2,000 Islet Equivalents (IEQs)) exposed to low glucose (LG) versus high glucose (HG) (n=8). Using methyl-tert-butyl ether (MTBE), methanol and water at a ratio of 3.6:1.2:1, 5,000 and 3,000 features were obtained in positive and negative modes from the non-polar phase, whereas 2,500 features were detected in each the positive and negative modes analyses from the polar phase. Although no clear separation was observed between LG- versus HG- exposed islet samples using the complete set of features, lipidomics (non-polar phase) analysis in positive and negative modes, revealed intra- and inter-individual differences in lipid profiles, and metabolomics (polar phase)

				analysis showed the same trend. LC-MS/MS analysis annotated putative lipids (diacylglycerols and triacylglycerols, octadecanoids and glycerophosphocholines) and metabolites (purines, arginine) involved in islet cell function. This work lays the foundation for an improved understanding of diabetes etiology with a minimal amount of starting sample.
5	Dorsa Yahya Rayat	University of Alberta	Using Digital Wearable Data to Infer an Individual's Metabolomic Profile	Targeted metabolomics and digital wearable technologies offer the possibility of quantitatively monitoring the effects of dietary or lifestyle interventions. By comparing the outputs of these two methods of physiological assessment, it may be possible to correlate metabolomic measurements with digitally acquired data. In this "N-of-one" study, a healthy 25-year-old female participant was monitored using multiple wearable digital monitoring devices to measure body temperature, blood pressure, blood glucose, etc. The subject also underwent multiple physical and mental performance assessment tests while altering diets (Fast food, Mediterranean, and Keto diet) as a lifestyle intervention over an 8-week period. Blood and urine samples were collected during the diet periods. These samples were analyzed using a quantitative MS-based metabolomic assay that measures 636 different endogenous metabolites and an additional 220 metabolite ratios and sums. Analysis of the digital wearable data led to the identification of a number of diet-induced, digitally-defined physiological states (good/poor mental performance, good/poor sleep, high/low energy, high/low heart rate, healthy/sick, etc.) These digitally defined states were then correlated with the metabolomic data collected during these states. This work led to the identification of consistent metabolomic profiles that correlated with digitally measured physiological states – independent of the diet. These data suggest that it may be possible to use digital wearables to infer an individual's metabotype.
6	Dr. Dipanjan Bhattacharyya	University of Alberta	Design of a portable, inexpensive, color based, user friendly metabolomics platform and its application in cancer screening and animal pregnancy	Metabolites can act as key biomarkers for various diseases and biological conditions. We have developed a unique metabolomics platform to quantify metabolites colorimetrically, which aims to be a replacement for more expensive or time-consuming assay techniques. The development of the platform has two distinct aspects: 1) development of colorimetric chemical or enzymatic assays and 2) design of an automated platform to perform chemistry along with a Red/Green/Blue (RGB) color sensor. This poster will highlight two key ongoing projects using this platform. The first is aimed at screening for colorectal cancer (CRC). We have developed novel colorimetric assays in human urine (e.g. kynurenine & N1, N12-diacetylspermine) which can accurately quantify the metabolites within the range of 0.25 µM - 25 mM. We designed a unique urine cleaning protocol using ion-exchange chromatography to improve assay sensitivity and consistency. The second one is a test to determine sheep pregnancy and litter size. For this application, a panel of five metabolites in sheep serum are assayed using the automated platform and colorimetric measurements are done using the color sensor. Overall, the development of these two projects that are so disparate in application and execution demonstrates the utility and versatility of this metabolomics sensor platform.
7	Eponine Oler	University of Alberta	MiMeDB: The Microbial Metabolome Database	MiMeDB is a new database containing detailed information about small molecule metabolites found in the human microbiome. It is intended to be used for applications in metabolomics, clinical chemistry, biomarker discovery and general education. The database is designed to contain and link metabolite data, microbe data, host data, health and bioactivity data, and exposure data. Many microbially produced chemicals play important roles in human health and disease, some offering protection against inflammation and cancer, while others cause damage to kidneys, the heart and brain. While all microbes synthesize primary metabolites required for their own survival, they also produce a variety of exotic compounds arising from their ability to grow on many unusual substrates or host-derived

				food sources. For instance, many of the metabolites produced by human microbes arise from the transformation of xenobiotics arising from human consumption such as food constituents, food additives, phytochemicals, drugs, cosmetics and other exogenous or man-made chemicals. Microbes also chemically transform many human metabolites as well as previously host-transformed xenobiotics. As a result, the human microbiome is believed to produce or process >55,000 different compounds – many of which affect human health, behavior and disease.
8	Erick Helmeczi	McMaster University	Peak Seeker: A Software Tool for the Rapid and Automated Pre-Processing of Serum Metabolomic Data Acquired by Multisegment Injection-Capillary Electrophoresis-Mass Spectrometry	Metabolomics is a rapidly growing field of discovery-based research which takes advantage of state-of-the-art analytical platforms to maximize metabolite coverage, data fidelity, and sample throughput. However, sample throughput, including data acquisition and data pre-processing, is typically the most demanding constraint in large-scale metabolomic studies required to meet project deadlines and keep costs down. In this case, multiplexed analyses based on multisegment injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS) greatly enhance sample throughput (3 min/sample) by allowing for the simultaneous analysis of up to 13 samples within a single analytical run with stringent quality control (QC). Nevertheless, automated data pre-processing in MSI-CE-MS remains a major hurdle given the lack of existing software tools compatible to reliable peak picking and integration of complex multiplexed metabolomic data sets. To this end, we have introduced a new open-source software in the R statistical environment referred to as Peak Seeker to enable the automated processing of serum metabolome data in MSI-CE-MS. Peak Seeker takes mzML files and user supplied tables of annotated serum metabolites and internal standards to perform mass calibration, electropherogram extraction, data smoothing, peak detection, and feature filtering. Data (peak areas and migration times) is exported in .csv files in suitable format for statistical analysis, and plots of annotated extracted ion electropherograms are conveniently exported for user review. In this work, we performed a rigorous validation of Peak Seeker by using it to automatically pre-process a panel of 50 serum metabolites from over 5,000 fasting serum samples, pooled QC samples, NIST SRM-1950 reference samples and calibration curves analyzed by MSI-CE-MS under positive ion mode conditions. We show that that this software dramatically reduces manual integration times by more than 99% (~125 days down to 1 day) while also achieving excellent peak annotation accuracy (median error < 0.25%) and excellent mutual agreement with manually processed data sets from an experienced analyst (average relative peak area bias < 2%). Upon the successful completion of our validation study, Peak Seeker will be released as open-source software and hosted on GitHub. This initiative aims to improve the accessibility and convenience of MSI-CE-MS technology to the broader metabolomics community in support of large-scale clinical and epidemiological studies.
9	Harrison Peters	University of Alberta	LC-Autofit: An LC-MS Analytical Suite	LC-Autofit is an in-house developed analytical tool and a webserver developed to analyse raw LC-MS data. This python-based program is developed as a flexible tool and can analyze different types of raw data. LC-Autofit is developed as an automated analytical suite. Users just need to drag and drop their raw unprocessed data on to the frontend and the tool will perform automatic peak picking and integration. Calculated results, including analyte concentration and LOD values, are displayed in both interactive graphs and tabular formats. LC-Autofit attempts to automatically perform peak picking, however the user is also able to make manual adjustments adjustments using the graphical user interface. The tool has three components: the main analytical code written in Python, the web server and graphical user interface written in Ruby on Rails (v6.1), and the display and graphing utilities written in Javascript. Currently,

				LC-Autofit is developed for targeted LC-MS Analysis, however we are working expanding LC-Autofit for untargeted analysis as well. Thus, LC-Autofit addresses the gap to serve the metabolomics community which requires a flexible fully automated and accurate analytical suite for LC-MS analysis.
10	Jessica Ewald	McGill University	Web-based tools for comprehensive multi-omics analysis	Multi-omics data promises to give more insight into biological processes than single omics data. When integrating details across omics layers, orthogonal information uncovers complementary biological processes, offering a more holistic view, while redundant information reduces false positives/negatives, giving more robust results. Recently, we have built web-based tools for multi-omics analysis. There are two main approaches for multi-omics integration, and we present one web-based tool for each: OmicsNet for knowledge-driven integration and OmicsAnalyst for data-driven integration. Knowledge-driven analysis first conducts independent analyses of each 'omics layer, resulting in a list of features of interest (signatures) for each. Next, the lists are integrated using a priori knowledge graphs. Converging biological processes and themes are identified from the merged lists using functional analysis. On the other hand, a data-driven approach conducts simultaneous analysis of multiple omics layers using advanced multivariate statistics to look for patterns of correlation or covariance across layers. Then, functional analysis is performed on the multi-omic signatures that drive the strongest trends to try and understand their biological meaning. Our overarching objective is to engage and empower researchers to leverage their domain expertise and reach deep insights of their multi-omics datasets.
11	Jiamin Zheng	University of Alberta	Comprehensive Targeted Exposome Assay for Serum Samples	Exposome, defined as the measure of exposures of an individual and how those exposures relate to health. Understanding how exposures from environment, diet, lifestyle impact health is more and more discussed now. A list of 200 analytes containing different classes of compounds, e.g., amino acid, organic acids, acylcarnitines, pollutants was chosen from a previous study for further quantitative method development. Here we presented a quantitative assay of the selected analytes as a customized exposome panel. It uses a combination of direct injection analysis mass spectrometry for accurate quantification of acylcarnitines, with a reverse-phase LC-MS/MS absolute quantification of all other classes of compounds. Two separate sample preparation involving two different pre-column derivatization reactions were developed for this assay: A) Phenylisothiocyanate (PITC) derivatization targeting amine-containing compounds and B) 3-nitrophenylhydrazine (3-NPH) derivatization targeting keto- and carboxyl-containing compounds. Isotopically-labeled internal standards are used for metabolite quantification. Calibration of metabolite concentration ranges was adjusted to fit the expected concentration levels. It has been fully validated for serum. Recovery rates of spiked samples with three different concentration levels are in the range of 80% - 120% with precision values within 20%. Moreover, it was specifically developed in a 96-well plate format, which enables high-throughput sample analysis.
12	Jun Han	University of Victoria	Targeted assay of 400 hydrophilic metabolites of major metabolic pathways by LC-MRM/MS	To provide reliable quantitation of >400 hydrophilic precursors, substrates, intermediates and enzyme cofactors in the metabolism of carbohydrates, amino acids, nucleotides, vitamins and fatty acids, we developed a targeted assay using complementary UPLC-MRM/MS methods. Hydrophilic metabolites in biological samples were extracted. After protein removal, four aliquots of each extractant and corresponding standard-substance solutions were analyzed by LC-MRM/MS, with or without pre-analytical derivatization. Stable isotope-labeling internal standards (SISs) or one-pot reaction generated chemical isotope-labeling internal standards (CILISs) were spiked to compensate for matrix effects. For assay of phosphometabolites, an iron-free LC-MRM/MS method was developed. To quantify 120 metabolites of amino acid metabolism, pre-analytical derivatization-LC-MRM/MS combined with the use of SISs and CILISs was employed and the method enabled separation of metabolite isomers. For

				sugars and organic acids, chemical isotope labelling using 12C6/13C6-3-nitrophenylhydrazine was validated for accurate quantitation. For additional polar metabolites, hydrophilic-interaction LC-MRM/MS was optimized for the chromatographic separations and MRM/MS detection. With the four LC-MRM/MS methods, the analytical sensitivity ranged from sub-femtomoles to low picomoles and good linearity of R(2) ≥0.999 was observed for all the metabolites. With multiple improvements of the experimental procedures, high precision and high accuracy of the quantitation were achieved for most of the metabolites.
13	Le Chang	McGill University	mGWAS-Explorer 2.0: a Web-Based Platform for Prioritizing Metabolites with Causal Impact on Diseases	Background: This study presents the development and utility of mGWAS-Explorer version 2.0, an enhanced web-based platform for comprehensive analyses of results from metabolome genome-wide association studies (mGWAS). The primary aim was to facilitate the identification of causal relationships between metabolites and disease phenotypes to advance the understanding of molecular disease etiology. The platform implements Mendelian randomization (MR) to infer causal relationships, utilizing genetic variants as instrumental variables, reducing confounding and reverse causation risks. Methods: mGWAS-Explorer 2.0 incorporates three key features: (i) two-sample Mendelian randomization for causal inference; (ii) phenome-wide MR analysis of the metabolome; (iii) evidence triangulation via semantic triples. The platform utilizes a knowledgebase consisting of significant SNP-metabolite associations from 65 mGWAS and complete summary statistics from the IEU OpenGWAS database. The "PheMR" module offers pre-calculated results from phenome-wide MR analysis, evaluating 825 metabolites' causal effects on 236 phenotypes. This analysis identified 1243 significant metabolite-trait associations, including novel ones, which are integrated into mGWAS-Explorer 2.0 for quick data querying. Additionally, the platform supports triangulation of MR causal estimates with semantic triples extracted from literature. Conclusions: We developed mGWAS-Explorer 2.0 to enable users to investigate potential causal relationships between metabolites and diseases. The utility of the platform is demonstrated in three case studies. The tool is freely accessible at www.mgwas.ca.
14	Lei Xu	McGill University	Integrating Analytics and Bioinformatics for Exposomics	Exposomics is a rapidly evolving research area that seeks to comprehensively investigate the relationships between environmental exposures and phenotypes over a defined time-period. At the downstream of the omics cascade and capturing both host response and environmental exposure, metabolomics is poised to play a pivotal role in exposomics studies. Here we introduce a novel bioinformatics workflow designed to facilitate the exploration and elucidation of exposure-phenotype interactions based on LC-MS metabolomics. In this workflow, the linear model and correlation analysis are first applied to identify potential relationships between exposures and phenotypes. Subsequently, a highly sensitive and efficient peak detecting algorithm has been developed to detect exposures and their related biotransformation products. Finally, we combined targeted and global untargeted analysis to perform comprehensive metabolomics, which enabled us to identify additional metabolites that may play important roles in exposure-phenotype interactions. We are currently validating our workflow using the African E-waste exposomics study consisting of 500 plasma and urine metabolomics samples collected from a cohort of 200 individuals. We expect that this workflow will be a valuable tool for the study of exposure-phenotype interactions, and ultimately contribute to the development of more effective prevention and intervention strategies.
17	Mathew Johnson	University of Alberta	A Quantitative, High-Throughput	The Metabolomics Innovation Centre (TMIC) specializes in quantitative metabolomics assays for human, animal, plant, and microbial samples. The recently developed TMIC MEGA assay uses a combination of

			Assay for Measuring Metabolites in Urine and Feces	direct injection (DI) mass spectrometry with a reverse-phase LC-MS/MS to identify up to 1000 metabolites along with another 400 metabolite sums and ratios. It combines the derivatization and extraction of analytes, with selective mass-spectrometric detection using multiple reaction monitoring (MRM) pairs. Two separate panels involving two different precolumn derivatization reactions were developed for this assay: Panel A - Phenylisothiocyanate (PITC) derivatization targeting amine-containing compounds and Panel B - 3-nitrophenylhydrazine (3-NPH) derivatization targeting keto- and carboxyl-containing compounds. Isotopically-labeled internal standards are used for metabolite quantification. This custom assay is designed to be used for the targeted identification and quantification of up to 1000 metabolites across 21 chemical classes including amino acids and derivatives, biogenic amines, organic acids, nucleotides/nucleosides, ketone and keto acids, indole derivatives, vitamins and derivatives, sulfates, dipeptides and 11 different classes of lipids. The recovery rates of spiked urine samples with three different concentration levels are in the range of 80% to 120% with satisfactory precision values of less than 20%. This assay, validated specifically for urine samples, was used to successfully analyze human urine with results closely matching those reported in the literature as well as measured by our other in-house assays.
19	Reza Maulana	Concordia University	Evaluation of Ionic Liquids in Dispersive Liquid-Liquid Microextraction Format for Lipidomics	In recent years, ionic liquids (ILs) have emerged as a popular alternative for organic solvents due to their unique properties and customizable selection of cations and anions, dubbing them as designer solvents. Currently, there is limited information about the performance of ionic liquids in biological matrices. Due to their customizability and selectivity, ionic liquids have good potential for extracting biological analytes such as lipids and metabolites. Here, the extraction selectivity of two ionic liquids, 1-hexyl-3-methylimidazolium hexafluorophosphate ([C6MIM][PF6]) and trihexyl(tetradecyl)phosphonium hexafluorophosphate ([P6,6,6,14][PF6]), was evaluated in dispersive liquid-liquid microextraction (IL-DLLME) format for selected lipids. Methanol was used as dispersing solvent. The resulting supernatants were analyzed using liquid chromatography-mass spectrometry (LC-MS). The results showed similar selectivity of [P6,6,6,14][PF6] and [C6MIM][PF6] towards lipid extraction. In standard solutions, both ionic liquids caused significant ion suppression of glycerolipids and glycerophospholipids, with [P6,6,6,14][PF6] having stronger ion suppression than [C6MIM][PF6]. The ionic liquids showed selective recovery of very polar lipids where by 17:0 LPC was fully recovered by the ionic liquids but other lipids such as 17:0 PE and 19:0 PC was not extracted. In plasma, [P6,6,6,14][PF6] and [C6MIM][PF6] showed similar selectivity towards glycerolipids, glycerophospholipids, and sphingolipids.
20	Rui Qin	University of Alberta	Biomarker discovery with chemical isotope labeling LC-MS metabolomics	Untargeted metabolomics, aiming to characterize and quantitate a broad spectrum of metabolites in biological samples, has become an important tool in the discovery of biomarkers for environmental exposures and diseases. The chemical isotope labeling (CIL) LC-MS method developed by our group significantly improves the sensitivity and metabolite coverage in untargeted metabolomics, enhancing our potential in identifying genuine biomarkers. Here, we present a biomarker discovery workflow integrated with our CIL LC-MS pipeline. This biomarker discovery workflow features 1) high versatility in model/feature selection and 2) multiple panels of biomarker candidates based on different statistical metrics, including a combined candidate panel to minimize false discovery. We tested our pipeline on samples from several rheumatoid arthritis (RA) cohorts and showed that the combined biomarker panel had consistently better predictive performance, compared to biomarkers identified by individual

				conventional feature selection methods such as the top-K feature selection method. We provide proof-of-concept evidence that CIL LC-MS is a powerful method in high-throughput metabolite biomarker discovery.
23	Tanisha Jean Shiri	McGill University	Global isotope labeling metabolomics reveals favorable metabolic interactions of aging C. elegans with its native microbiome member Chryseobacterium sp.	Aging is the system wide loss of homeostasis eventually leading to death. As the microbiome actively evolves with its aging host, it also directly affects aging via modulation of metabolites that affect important cellular functions. The widely used model organism C. elegans exhibits high selectivity towards its native microbiome members some of which even exhibit detrimental effects such as Chryseobacterium sp. The ability of Chryseobacterium sp. to improve the lifespan of C. elegans and to promote the production of Vitamin B6 in the co-colonizing member Comamonas sp. are some of its favorable features. Studying the global metabolic effects of Chryseobacterium sp. throughout the lifecycle of C. elegans could provide further insights into mutualistic interactions of such pathogenic bacteria with their host. Microbial cells grown on U-13C glucose were fed to C. elegans to track the differentially active pathways within the host. We repurposed certain MetaboAnalyst features for the streamlined analysis of isotope labeling data along with added features to extract the enrichment of isotopologues within pathways. In addition to the upregulation of biosynthesis and detoxification pathway intermediates, we found that Chryseobacterium sp. upregulates the glyoxylate shunt in mid-adult worms which is linked to the upregulation of trehalose, an important metabolite for desiccation tolerance in older worms.
24	Yao Lu	McGill University	MicrobiomeNet: a comprehensive database for understanding microbial interactions and systems biology	The past decade has seen tremendous growth of studies on microbial interactions, as well as their associations with host genetics and environmental factors. Curating and organizing this large amount information into user-friendly and computable formats have the great potential to enable discovery of important ecological patterns, functional insights, and translational applications. Here we introduce MicrobiomeNet, a comprehensive database to investigate potential microbial interactions from three different perspectives: (1) metabolic interactions: a collection of ~ 6000 microbial genome-scale metabolic models (GEMs) and KEGG metabolic network of ~8000 microorganisms to study and visualize microbial interactions at metabolic level across different taxonomic levels; 2) ecological community interactions: a comprehensive microbial association networks containing >50,000 interactions curated from ~100 studies; and 3) semi-structured functional groups: library of >5,000 taxon sets curated from ~1000 literatures accompanied with their metadata and attributes. Users can easily query and compare results from different studies as well as to annotate and update the information. MicrobiomeNet supports interactive network visualization and network-based analysis allowing users to intuitively explore community structures and functional motifs. It also supports regression-based analysis to dynamically predict metabolic potentials for given community structures. Together with MicrobiomeAnalyst, MicrobiomeNet aims to provide a FAIR-compliant web-based resource to help improving our understanding of how different microbial relationships affect the ecosystem at both community and metabolic levels.
28	Paulina de la Mata	University of Alberta	EVALUATION OF EXTRACTION SYSTEMS FOR SOIL AND SHALE SAMPLES BY GC×GC-TOFMS	New environmental contaminants are always emerging, and there is a need for improved methods for the comprehensive non-target analysis of environmental samples. Herein, we apply GC×GC-TOFMS for the routine analysis of soil and shale samples. Typically, certified contract laboratories use solvents as the primary extraction method to perform environmental analyses of organic contaminants. However, these liquid-liquid extraction systems do not cover all chemical families, and the analytical methods used are generally targeted methods relying on GC-MS(/MS). Herein, we compare various extraction solvents as well as a Thermal Desorption, as a solvent-less, “green” method. The extraction capabilities were evaluated using a framework derived from multiple sources. The framework includes the ASTM E1412-19

				protocol for ignitable liquid residues, the list of toxic substances managed under Canadian Environmental Protection Act, and various other literature sources to determine ions of interest for non-targeted analysis. A set of mixed soil and sand samples with presumed environmental contamination were selected for analysis using the proposed methods. Data was collected by GC×GC-TOFMS. Seven different solvents were tested; hexane, methyl tert-butyl ether, toluene, ethyl acetate, hexane/acetone and t-butyl alcohol/acetone (50:50 v:v), and compared against the solvent-less TD method.
29	Sheri Schmidt	University of Alberta	Headspace Analysis of Disinfection By-products in Drinking Water using DHS and SPME with GC×GC-TOFMS	During the disinfection process for drinking water, dangerous pathogens are removed, often by chlorination. However, chlorine can react with natural organic matter (NOM) often present in the source water feeding the treatment plant. During treatment to remove pathogens, NOM such as polysaccharides, humic and fulvic substances, and amino acids can react with chlorine to form halogenated disinfection by-products (DBPs), of which the trihalomethanes (THMs) are well known. Chronic exposure to THMs, even at trace levels, has been linked to cancer in humans, and DBPs have been an area of active research for decades. In this study, methods for analyzing water samples for DBPs using GC×GC-TOFMS were explored. Using GC×GC-TOFMS in conjunction with SPME should result in methods capable of improved detection limits identification power over established GC methods. This, in turn, will permit studies to track lower concentrations of THMs and other DBPs and support ongoing research into reactions driving the generation of DBPs.
32	Ryland Giebelhaus	University of Alberta	Profiling and Characterizing the Volatile Exposome with Wristband-Based Passive Samplers and GC×GC-MS	We are exposed to hundreds of volatile chemicals every day, varying in their concentration and effect on human physiology. Current air monitoring technology focuses on measuring particulate matter (PM2.5), or detecting specific gases including CO2, CO, and CH4. While these are important metrics for assessing air quality, they do not profile the entire volatile exposome. To sample the entire volatile exposome, tools such as sorbent traps and solid phase micro extraction are employed. These tools are expensive and may not represent an individual's exposome. O'Connell et al. reported the use of silicone wristbands as personal passive samplers to profile exposures. Wristband passive samplers (WPS) are inexpensive, reusable, and worn by participants, providing a more representative profile of the exposome. Characterization of WPS is done with gas chromatography mass spectrometry (GC-MS), which allows for the detection and identification of chemicals captured by the WPS. Here, we describe the development of a protocol employing comprehensive two-dimensional gas chromatography mass spectrometry (GC×GC-MS) to characterize the WPS. GC×GC-MS has more peak capacity, higher sensitivity, selectivity, and resolution over GC-MS, due to the two chromatographic dimensions. We deployed WPS with GC×GC-MS characterization to monitor exposure events in different worksites and households for different individuals.
33	Andrea Velasco Suarez	University of Alberta	Method Optimization for the analysis of Particle-Phase and Volatile Organic Compounds of Tobacco and Cannabis Joints Using a Smoking Cycle Simulator	Tobacco cigarette smoking is a well-known health hazard, and with the legalization of cannabis in several countries, there is an increasing need to study the effects of cannabis consumption as well. Comprehensive chemical analysis of the particulate and volatile fractions of tobacco and cannabis smoke is crucial for understanding the associated health risks from these exposures. While there are multiple smoking machines available on the market, all designs have aspects that are concerning from a point of view of carryover and the ability to accurately collect both VOCs and particles. Herein we present a modified commercial smoking machine that permits the sampling of both phases without cross-contamination. Briefly, air drawn through a cigarette/joint is directed through a particle filter as normal, before being drawn through a glass chamber with two outlets. A valve after the chamber permits control of the flow of volatiles between the main chamber (waste) and a slower stream which is directed to thermal desorption

				sampling tube. This setup allows for the effective fractionation of mainstream smoke into particle and volatile phases, while minimizing the potential carryover of components from one experiment to the next.
34	Chu-Fan Wang	University of Alberta	Segment Scan Mass Spectral Acquisition for Increasing Metabolite Detectability in Chemical Isotope Labeling LC-MS Metabolome Analysis	We report a segmented-spectrum scan method using Orbitrap MS in chemical isotope labeling (CIL) LC-MS for improving metabolite detection efficiency. In this method, the full m/z range is divided into multiple segments with the scanning of each segment to produce multiple narrow-range spectra during the LC data acquisition. Various experimental conditions, including automatic gain control (AGC) values, mass resolutions, segment widths, number of segments and total data acquisition time in LC run, have been examined to arrive at an optimal setting in segment scan for increasing the number of detectable metabolites while maintaining the same analysis time as in full scan. The optimal method used a segment width of 120-m/z with 60k resolution for a 16-min CIL LC-MS run. Using dansyl labeled human urine samples as an example, we demonstrated that this method could detect 5867 peak pairs or metabolites, compared to 3765 peak pairs detectable in full scan, representing a 56% gain. Out of 5867 peak pairs, 5575 (95.0%) could be identified or mass-matched. Relative quantification accuracy and precision were not affected by segment scan. This work shows a remarkable increase in metabolomic coverage achievable by detecting co-eluting metabolites using segment scan Orbitrap MS in CIL LC-MS.
35	Cyrene Catenza	University of Alberta	Comprehensive metabolomic analysis of single-spheroids based on chemical isotope labeling liquid chromatography-mass spectrometry	Untargeted cellular metabolomics involves the study of an entire set of metabolites and their roles in biochemical reactions. This can reveal important links between pathways that occur within a living cell, which may provide information about the underlying causes of different diseases. However, due to the large chemical diversity of metabolites, it is impossible to profile the entire metabolome using a single method. Chemical isotope labeling (CIL) is a technique that alters the properties of metabolites to increase their detectability using reverse-phase LC-MS. The CIL LC-MS method targeting the amine/phenol submetabolome was applied to analyze single spheroids, and approximately 1000 metabolites were detected in single-spheroid samples. In addition, this method was used to elucidate the possible mechanism of action of anticancer drugs, and it successfully distinguished anticancer-treated spheroids from untreated spheroids. Lastly, by monitoring the levels of significantly changed metabolites, we were able to identify the possible pathways that were significantly affected by the drugs. The next step of this project is to apply other CIL LC-MS methods targeting other submetabolomes to analyze single spheroids. And with this, we hope to cover approximately 95% of a single spheroid's metabolome.
37	Zhan Cheng	University of Alberta	Development of Chemical Isotope Labeling Liquid Chromatography Orbitrap Mass Spectrometry for Comprehensive Analysis of Dipeptides in rice wines	In recent years, the biological functions of dipeptides have attracted attention, such as their inhibition of human dipeptidyl peptidase IV, angiotensin-converting enzyme, and antioxidative properties. With 20 types of alpha-amino acids, there are 400 possible dipeptide combinations that possess a wide range of physiochemical properties. Therefore, accurate identification and quantification of each dipeptide remains challenge. In this study, we have developed a chemical isotope labeling (CIL) liquid chromatography high-resolution tandem mass spectrometry approach for comprehensive profiling and accurate quantification of dipeptides. We constructed a CIL standard library consisting of retention time, MS, and MS/MS information of a complete set of 400 dansyl-dipeptides to facilitate rapid dipeptide identification. For qualitative analysis, data-dependent acquisition was carried out to enhance the reliability of dipeptide identification. As examples of applications, we successfully identified 321 dipeptides in rice wines. For quantitative analysis, we demonstrated that the intensity ratios of the peak pairs from 96% of the detectable dansyl-dipeptides in a 1:1 mixture of 12C- and 13C-labeled rice wine samples were within

				±20% of an expected value of 1.0. Furthermore, more than 90% of dipeptides were detected with a relative standard deviation of less than 10%, indicating good performance of relative quantification.
39	Deema Qasrawi	McGill University-Lady Davis Institute	Comparison of HILIC and C18-based Liquid Chromatography-Mass Spectrometry Methods for Targeted Lipidomics Analysis of Human Plasma	Background Lipids are essential building blocks of cells, serving crucial roles as integral components of cellular signaling pathways and metabolism. Lipidomics involves identifying and quantifying lipids in biological samples. This study assessed the utility and feasibility of two platforms for targeted lipidomics: hydrophilic interaction liquid chromatography (HILIC) and reversed-phase C18 chromatographic separation with multiple reaction monitoring (MRM)-based assays. Both approaches were applied for human plasma (BioIVT) samples and have been recently introduced by Sciex and Agilent for quantifying a broad range of lipids. Our study adopted both assays to compare their effectiveness. Methods In this study, we added a deuterated lipid internal standards (Avanti EquiSPLASH®) mixture, and the lipids were extracted using a modified Bligh-Dyer protocol. Chromatographic separation was performed using the HILIC-MRM based targeted analysis using SCIEX 6500+ QTRAP mass spectrometry (MS). Another set of samples was extracted using the Butanol: Methanol (BuMe) method, and chromatographic separation was performed using the C18-MRM based targeted analysis using Agilent 1290/6495A. Triplicate samples were injected using both approaches, and cross validation was performed to assess the performance of the two methods. Results The HILIC chromatography-based method separated lipids according to their polar groups. This method provided chromatographic separation of different lipid classes, which were eluted and grouped in a similar retention time range. On the other hand, the C18-based method separates lipids based on their hydrophobicity and proved to be an effective and straightforward approach for targeted lipidomics analysis. Combining both methods enabled the comprehensive profiling of a large panel of lipid species. This approach allowed for detecting a broad range of lipids in different samples with high reproducibility and precision.
40	Tingting Zhao	University of British Columbia	De Novo Cleaning of Chimeric MS/MS Spectra for LC-MS/MS-Based Metabolomics	Experimental tandem mass spectra (MS/MS) generated in liquid chromatography-tandem mass spectrometry analysis (LC-MS/MS) are often contaminated by fragments from other coeluting precursors of similar m/z values. These contaminated MS/MS spectra, called chimeric MS/MS spectra, hinder the application of MS/MS-based metabolite annotation and unknown identification. In this work, we developed a de novo MS/MS purification workflow, termed DNMS2Purifier, to automatically identify and remove contamination fragments in experimental MS/MS spectra. Using chemical standards, we explored the characteristics of true and false (or contamination) fragments in chimeric MS/MS spectra and trained an XGBoost model to identify true and false fragments. Incorporating the trained model, we constructed an automated bioinformatic platform, DNMS2Purifier for metabolic features in metabolomics studies. DNMS2Purifer was evaluated on a metabolomics dataset generated with different precursor isolation windows. It successfully captured the increase in false fragments with the increased isolation window. In a real experimental metabolomics study, DNMS2Purifier also improved MS/MS spectral quality and led to better molecular networking outcomes.

41	Ying Chen	University of British Columbia	Development of Bioinformatic Solutions to Enable Hair-Based Exposome Research	Hair is an underexplored matrix for studying exposomics, serving as a record of chemicals deposited on its surface. However, the lack of a comprehensive database and annotation pipeline has hindered the use of hair. To address these challenges, a comprehensive database of hair metabolomes and exposomes was developed. The database systematically compiles all reported hair chemicals through text-mining and manually includes chemicals with a high likelihood of being deposited on the surface of hair. HairDB contains 4191 unique chemicals from 9214 articles, 172 of which were further categorized as biomarkers. Next, I developed a novel bioinformatic pipeline enabling the study of unknown exposome utilizing a software called BUDDY. Out of the 26119 features detected, 316 were annotated, 4270 were predicted with formula using BUDDY. Global optimization of chemical annotation was applied to detect 1755 potential transformations, with 579 being between identified metabolic features and those with predicted molecular formulas through known chemical reactions. Using HairDB, 43 unique metabolites were found with corresponding literature. The predicted molecular formulas were also used to search HairDB, resulting in 275 hits. The development of HairDB and the annotation pipeline for hair metabolome offer valuable resources for researchers in the fields of metabolomics and exposomics.
42	Brian Low	University of British Columbia	Closing the Knowledge Gap on Post-Acquisition Sample Normalization for Untargeted Metabolomics	Post-acquisition sample normalization is a critical step in untargeted metabolomics to minimize sample-to-sample variation. This biological variation must be removed prior to downstream processing to allow for fair comparisons between treatment groups to reveal more interesting biological variation that can allow for better understanding of diseases. Using the improper normalization method may also potentially introduce artifacts which can lead to misleading biological interpretations. Thus, it is important to choose the right method. Various normalization algorithms have been proposed over the past few years, but it remains unclear as to which method performs the best. In this work, we use simulations and experimental datasets to benchmark the following normalization methods: sum, median, probabilistic quotient normalization (PQN), maximal density fold change (MDFC), quantile, and the class-specific quantile methods. We investigate the influence of data structure and missing values on normalization performance and address the limitations of each method. Our results show that MDFC consistently outperforms the other methods in terms of estimating the true dilution factor and reducing the intragroup variation in both our simulated and experimental data.