P-17	Automated System for High Throughput Targeted Metabolomic Analysis

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In the context of industrial synthetic biology, high throughput targeted metabolic analysis of the diverse chemical space of products and pathway intermediates enables rapid cycles of strain optimization to improve or troubleshoot pathway bottlenecks. We have developed a metabolomics pipeline that combines a software tool for Automated Method Prediction (AMP), a high throughput MS system for data acquisition and an automated data processing system. Given a specific set of metabolic targets for each sample, AMP selects the smallest set of analytical methods (from a predefined set of 8) based on physicochemical properties of the targets. The LC-MS system is capable of processing samples at approximately 2 minute per sample and automatically switching between multiple methods via column and solvent selection valving. The current LC-MS method set includes 8 methods. Acquired data is analyzed and scored using an automated process to generate a standardized output which is transferred to a LIMS system for use in evaluating and informing strain optimization processes. The system we have developed represents a significant advance for both increasing throughput of metabolomics measurements and reducing the amount of expert time-intensive work involved in method selection and data processing. The current system was developed for accelerating microbial strain optimization for industrial chemical production but has potential for advancing high throughput metabolomics measurements in other contexts as well.

P-18	Automatic CCS and MS/MS Library Creation and Application for Large Scale Metabolic and Lipidomic Profiling

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Metabolomics and Lipidomics involve identification and quantification of chemical fingerprint of cellular processes within a biological system. Precise identification is a major challenge since polar metabolites and lipids are chemically and structurally diverse and span a wide mass range. Chromatographic separation does not typically resolve all components, and often lacks retention time reproducibility. The addition of ion mobility, a gas phase separation of ion, increases peak capacity, selectivity, and can potentially resolve isomeric/isobaric. Benefits of collision cross-section (CCS) library obtained from mobility drift times together with accurate tandem mass spectrometry data (MS/MS) of human metabolites/lipids, will be shown to be an additional source of reference to aid metabolite and lipid identification. ESI and MALDI-MS were used to measure ion drift-times on Synapt G2-Si and Vion time-of-flight (TOF) high resolution mass spectrometers. IM was used to measure CCS values in both positive and negative ESI modes in three differently laboratories. The preliminary data showed excellent correlation (median centering < 2%). A tandem mass spectrum of each ionised metabolite/lipid was also acquired and added to the scientific database. A sub-set of the CCS values were verified a Vion instrument to show the across instrument transferability of CCS, and on a MALDI-IM-MS to demonstrate the ionization independence of CCS measurements. Utility of CCS library is demonstrated using an analysis of human plasma sample. Spiked metabolite/lipid standards were identified using a combination of accurate mass measurements and CCS values. The addition of CCS measurements improved the confidence in identification compared to traditional analytical approaches

P-19	Speaq2: Large scale NMR metabolomics data analysis made easy

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Introduction Many present day metabolomics experiments rely on both LC-MS and NMR spectrometry data to fully quantify the available information. NMR tools often lack the automation potential of current advanced LC-MS tools as manual intervention is still required in certain steps. This is a consequence of the fact that most workflows rely on interval methods, such as binning/bucketting, to process these spectra. This approach effectively summarizes the spectra and allows easier data processing and statistics. However, several problems are introduced, both in pre-processing and in the subsequent analysis, that compromise the automation potential. What we did We present a new user-friendly workflow for the analysis of NMR spectra that uses wavelets to fully automate the process of converting raw spectra to peaks, which are then aligned and grouped into features. Since wavelets are also often used in peak picking for LC-MS data (to convert spectra into peaks with minimal information loss) this method advances the integration of LC-MS and NMR data. A crucial aspect is that this is not just another NMR data analysis tool but it can be used to improve other tools that rely on the binning method or tools that start with already processed spectra into peak lists. By using the wavelet based method the quality of these peak lists can be improved. The framework is validated by replicating the results of two papers demonstrating the speed, user-friendliness, minimal user interaction and improved results. Can I use it? The algorithms are made available in the speaq2 R-Package.