Summary of Metabolic Data Acquisition & Analysis Timeline

Sample Preparation Extraction

Mouse livers are pulverized into granules in liquid nitrogen. Each liver is weighed for sample normalization by weight and small polar molecule extraction is used to extract samples for mass spectrometer analysis
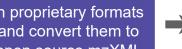
Experimental Optimization

Metabolites are highly diverse unlike proteins and successful detection of complex chemistry requires optimization of experimental protocol

Raw Data Acquisition and Conversion

Take the raw machine level intensities stored in proprietary formats and convert them to open source mzXML or mzML format to allow preprocessing using Matlab

Preprocessing

Detection of ion features is across of the data set generated is done in Matlab which detects, quantifies and aligns peaks throughout the samples

Centroiding and Quality Control

The aligned peaks are centroided, and corrected for bias from the instrument or batch effects. Data imputation may be performed to extract data from low intensity peaks.

Annotation

Annotate molecules that have been detected using search engines of libraries of known molecules and adducts in Online databases

Univariate Statistics

Determine whether ion are differentially represented in different Age and Diet cohorts. Parametric and Non-parametric test for significant differences employed

Multivariate Statistics

In order to extract information from the set with thousands of ion measurements: Clustering, classification and Dimension reduction and visualization used to summarize data and determine relationships within

Metabolic Network and Enrichment

Using Metabolic Network analysis to investigate correlation networks, various effects on pathways in order to determine structural an causal relations in the metabolic data

QTL Mapping, Biomarker detection MultiOmics Integration

In a refined set of target pathways performed QTL and biomarker analysis using multiomics data sets in order to enrich and validate observations in the metabolic level