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Outline for the workshop - Advancing metabolomics with high performance GCMS - practices and opportunities

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Learn how to perform a GCMS metabolomics analysis. The Metabolomics GCMS Workshop will cover the entire process of executing an analysis using GCMS. The participant will be exposed to what is necessary to achieve successful analysis of samples from a metabolomic study. Where possible examples and discussion will be based on examples form recent research papers and data or recommendations from global experts. The participant will be introduced to some of the sample preparation and derivatization schemes used for samples and the caveats and advantages of each. The various analytical options for mass spectrometry including quadrupoles, time-of-flight and hybrids will be discussed and will include the advantages of accurate mass anlaysis. The choice of appropriate GC conditions will be a topic including some key attributes for the GC as well as the choice of column and other sample introduction practices. Typical and ideal system performance will be addressed. The advantages and disadvantages of each will be examined including data output advantages and how their inherent capabilities affect their utility in the analysis of metabolomic samples. Data processing including peak finding and integration as well as library and data base matching will be discussed with the benefits of spectral features discussed. The use of unique workflows to demonstrate the identification of unknowns, a key bottleneck in metabolomic analysis will be discussed with examples of analyte identification. Finally, the analysis of the output data including data alignment, comparative analysis and other tools available will be touched upon. The intent of this Workshop is an introduction to the techniques and practices.

1. Why GCMS? –
   a. Busting some myths
2. Sample Preparation for GCMS
   a. Analyte extractions
3. Good Derivatization Practices
   a. Derivatization
   b. Automation
4. Column Considerations
5. Quantitation
   a. External standardization
   b. Internal Standardization
   c. Isotope consideration
   d. Tracer Studies
6. Available GCMS Platforms
   a. Quadrupoles
   b. Time of Flight
   c. Ion Traps
   d. Q-Tofs
   e. High Resolution Time of Flight
   f. Two Dimensional GC
7. Ionization
   a. Electron Ionization
   b. Chemical Ionization
   c. Other Ionizations
8. Dealing with Unknown Analytes
9. Data Analysis and Workflows for Metabolomics
10. Study Examples

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