Innovative Omics
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Lipidomic non-targeted data analysis and summarization of results

The following are things we can cover, depending on the user needs not all aspects may need to be covered and more attention can be given to other aspects:

Non-targeted mass spectrometry data-processing

- Processing of data in LipidMatch Flow which covers:
  - Detecting and aligning all molecular features (deisotoping, gap-filling, etc.)
  - Removing any features which are contamination from extraction blanks
  - Annotation using MS/MS rule-based library match (we include over 200,000 lipid candidates in our extensive library developed over the last 10 years with <5% false positive rate)
  - Combining positive and negative polarity data

- Manual review of data in LipidMatch Visualizer to compile a list of confident lipid annotations (increases confidence to nearly 0% false positive rate, unless noted specifically, and at least doubles the number of annotations including additional lipids such as fatty acids which do not fragment well):
  - Retention time trends across lipid sub-classes (homologous series detection)
  - Mass to charge trends across sub-classes (homologous series detection)
  - Fragmentation presence
  - Isotopic Pattern and Formula prediction

- Normalization / semi-quantification of the lipid values using internal standards

- Brief report of results (3-10 pages), describing our methods, which lipids were discovered, our confidence in each lipid discovered and the evidence for each structure determination

- Other services included:
  - Compilation of figures in PowerPoint or as a PDF containing all evidence used
  - Excel sheet with all resulting data and evidence
  - Up to 3 hours of consulting time to meet about the report and go over the results / train on how to use various tools

*Actual improved coverage in annotation depends on instrument acquisition methods, spectral density (complexity of sample), and application.