Innovative Omics

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Lipidomics Training

Installation, application, and troubleshooting all necessary software prior to visit
Includes virtual support with installation and testing prior and 10 hours of support post onsite visit
Includes 40-50 onsite training hours (5 days over 1-2 weeks)
Any prereleases (e.g., new modifications to FluoroMatch Visualizer, PFAS Transformation Product Libraries, and training videos for interpreting 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:

1) Overview of mass spectrometry and non-targeted mass spectrometry (with a special focus on lipidomics):

- Presentation and discussion covering the basics of mass spectrometry: retention time, mass spectra, tandem mass spectra, and ways of examining this data (mass defect plots, fragment screening, etc.)
- Introduction to lipidomics screening and non-targeted workflows
- Use of Vendor and open-source software (e.g., MZMine if desired) for examining raw data (formula prediction, annotation, export, layouts, sequence upload…)

2) Acquisition workflows:

- Training and discussion on the best acquisition workflow for your applications with the downstream data-processing algorithms in mind (parameters for AIF, DDA, Full-Scan…)
- Choosing acquisition parameters, run sequence, proper blanks, and some QA/QC
- Using our LipidPioneer software: Quickly predict lipid masses for examining EIC traces in real time (DOI: 10.1007/s13361-016-1579-6)

3) Advanced acquisition workflows:

- **Training and application of our intelligent acquisition workflows** to double molecular coverage by improving MS/MS coverage.* Includes installation and training on software for improving this coverage. This software covers intelligent iterative inclusion and iterative exclusion approaches (**IE-Omics, over 215 citations**: https://pubs.acs.org/doi/10.1007/s13361-017-1608-0).
- **Training on our IonDecon software for integration of all-ions** Expand molecular coverage even further (in complex samples even by 2-3x) by improving MS/MS coverage.* Includes installation and training on IonDecon software for improving this coverage (https://pubs.acs.org/doi/10.1021/jasms.3c00244).

4) Successful **installation, setup, and training on lipidomics annotation software**:

LipidMatch Flow and/or Modular, over 350 citations (doi: 10.1186/s12859-017-1744-3): LipidMatch Flow covers data-conversion, feature finding, alignment and gap filling, blank filtration, annotation, combining positive and negative mode data. The Modular version is for those who have their own peak picking algorithms, and want to annotate their resulting feature tables.

LipidMatch Visualizer: Visualization and validation of lipid annotations using mass defect plots, retention time vs *m/z* plots, MS/MS review, and more.

LipidMatch Normalizer (doi: 10.1007/s13361-016-1579-6): Normalization of feature intensities to class specific lipid internal standards for relative quantitation.

Training and combining annotations from multiple software including MS-DIAL/vendor software.

Collaboration with peak picking and optimization of MZMine workflows (or other workflows)

Collaborations on the **development of new lipidomics libraries for your specific applications**, including oxidized lipids. These libraries will be integrated into the annotation software either for public use or for your use only. Free - (if provided annotated spectra of multiple lipid standards).

5) Statistics and data-visualizations using Metaboanalyst and FluoroMatch Visualizer

6) Collaborations on the **development of new lipid libraries for your specific applications**. These libraries will be integrated into the annotation software.

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