

Innovative Omics
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## **PFAS 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 PFAS):
  - 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 PFAS non-targeted workflow
  - 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
- 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: doi: 10.1007/s13361-017-1608-0).
  - Training on IonDecon 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.
- 4) Successful installation, setup, and training on FluoroMatch PFAS software:

FluoroMatch Flow and FluoroMatch Modular:

 Training covers data-conversion, feature finding, alignment and gap filling, blank filtration, and annotation.

- Either in one simple user-friendly workflow, or integrating your own data-processing workflows
- Reviewing of data from first project in FluoroMatch Visualizer and working through any issues and aiding in interpretation
- Lifetime access to latest FluoroMatch software pre-release
- 5) Successful installation, setup, and training on vendor or other solutions and integration into the FluoroMatch workflow:
  - Includes Compound Discoverer, Agilent Profinder, MZMine, ...
  - Reviewing of data from first project and working through any issues and aiding in interpretation
- 6) Collaborations on the **development of new PFAS libraries for your specific applications.** These libraries will be integrated into the annotation software.
- 7) Virtual setup of software and methods, trouble shooting of errors, pre- and post- 1 hour meets covering all aspects above, training on new releases, walking through actual experimental data, help with manuscript writeup, etc.: 10 virtual hours:

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