



Innovative Omics

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PFAS 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 FluoroMatch Suite which covers:
 - Removing any contamination from analyzed blanks
 - Finding all molecular features including non-PFAS features (unannotated)
 - Annotation using multiple lines of evidence
 - Retention time trends across PFAS sub-classes (homologous series detection)
 - Mass to charge trends across sub-classes (homologous series detection)
 - Fragmentation presence
 - Fragmentation library match (we include over 15,000 candidates in our extensive PFAS library developed in collaboration with the EPA)
 - Isotopic ratio analysis (Kaufmman analysis)
 - Formula prediction
- Manually review of data in FluoroMatch Visualizer to compile a list of confident PFAS annotations and definite PFAS which have no annotations
- Brief report of results (3-10 pages), describing our methods, which PFAS were discovered, our confidence in each PFAS discovered and the evidence for each structure determination and a brief literature review connecting those PFAS discovered to other carpeting and dust studies if desired.
- 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

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