



Non-Targeted Analysis of Water

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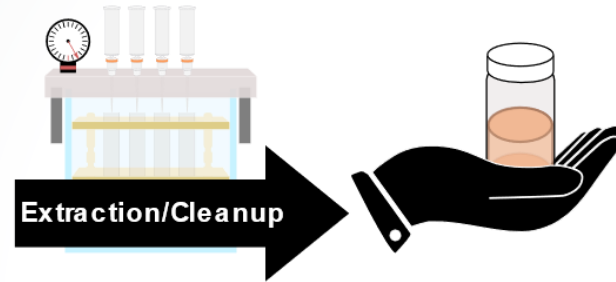
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- Continuous development of emerging compounds requires open-ended screening techniques to detect new contaminants of concern
- Need for comprehensive, quantitative, multimedia approach to screening
- Continued identification of emerging chemical species
- Research focus on improvements to NTA methods
 - Increased accuracy/reproducibility
 - Methods formalization/transfer
 - Automation/Library building
 - Quantitation

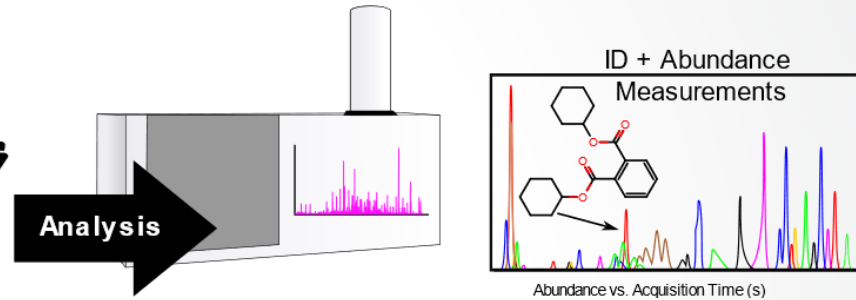
Media Sample



Sample Extract



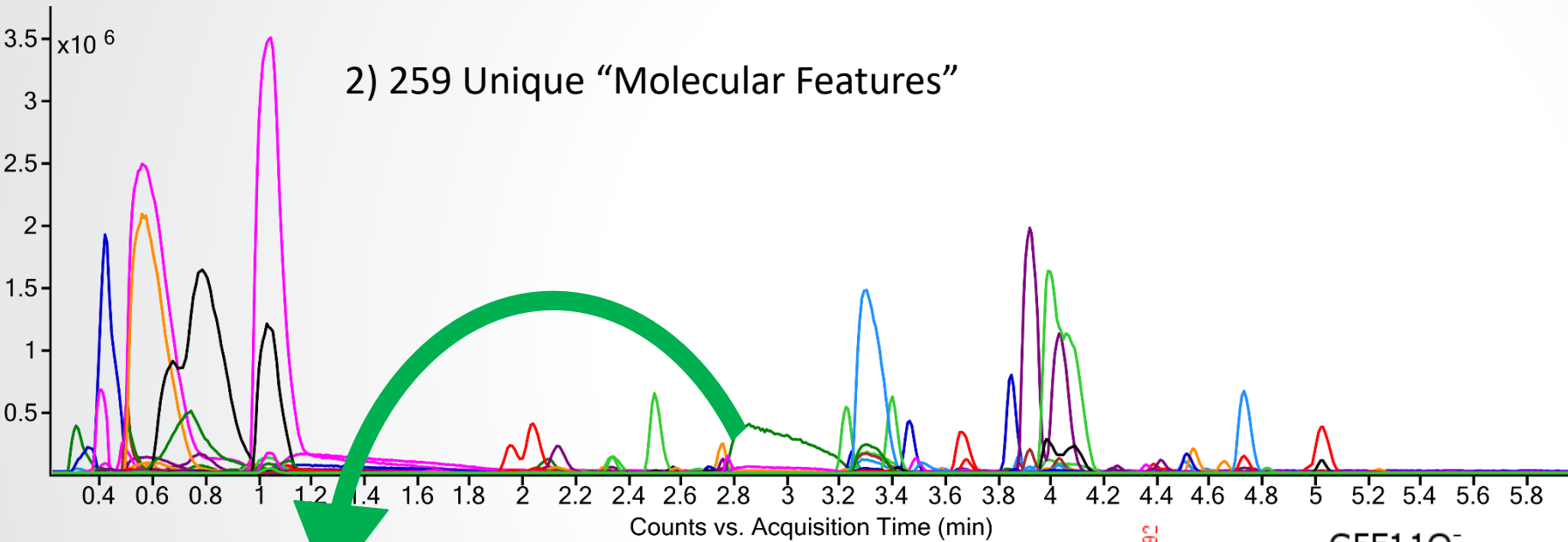
MS Analysis



- Samples prepared consistent with existing water methods (e.g. EPA 533)
- Analysis by high-resolution mass spectrometry to collect non-targeted abundance data and structural information vis MS/MS
- Screening against chemical lists (e.g. Comptox Dashboard) and software assisted manual examination to determine compounds of concern
- (Semi-)quantitative estimates of abundance and relative concentration trends for monitoring

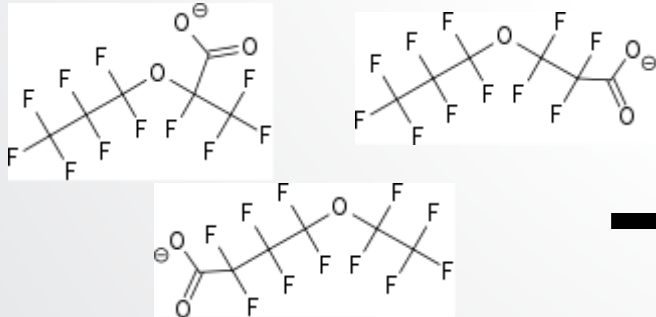
2) 259 Unique "Molecular Features"

- 1) Data Generation
- 2) Feature Finding
- 3) Formula Assignment
 - 3a) Structural Assignment
 - 3b) Structure Confirmation
- 4) Quantitation?
 - 4a) Relative Quant
 - 4b) Absolute Quant

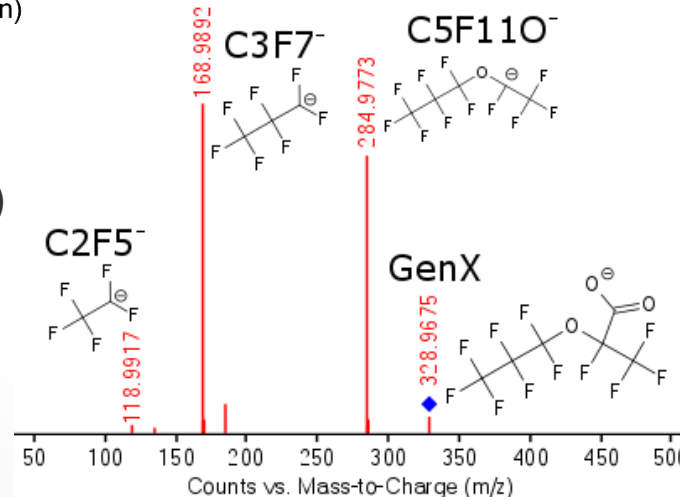


3) C₆HF₁₁O₃

3a)



3b)





Current Status

- First detection of emerging PFAS in NJ ([DOI: 10.1126/science.aba7127](https://doi.org/10.1126/science.aba7127)) and validation of point-of-entry water treatment ([DOI: 10.1021/acs.estlett.0c00640](https://doi.org/10.1021/acs.estlett.0c00640))
 - Ongoing exposure and tox measures.
- Multiple State/Regional Partnerships for PFAS screening
 - R1/NH, R2/NJ+NY, R3/WV+PA, R4/NC, R5/MI
 - Screening for emerging PFAS, legacy precursors, transformation products
- NTA working group tools for studies (<https://nontargetedanalysis.org/>)
- Evaluating method extensions
 - Improved quantitative estimates
 - Instrumentation installation/training in additional labs (ORD/Narragansett, R5)



Contributors

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**Supported by Chemical Safety for Sustainability and
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