

Screening for Perfluoro acids using DART-MS

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October 2021

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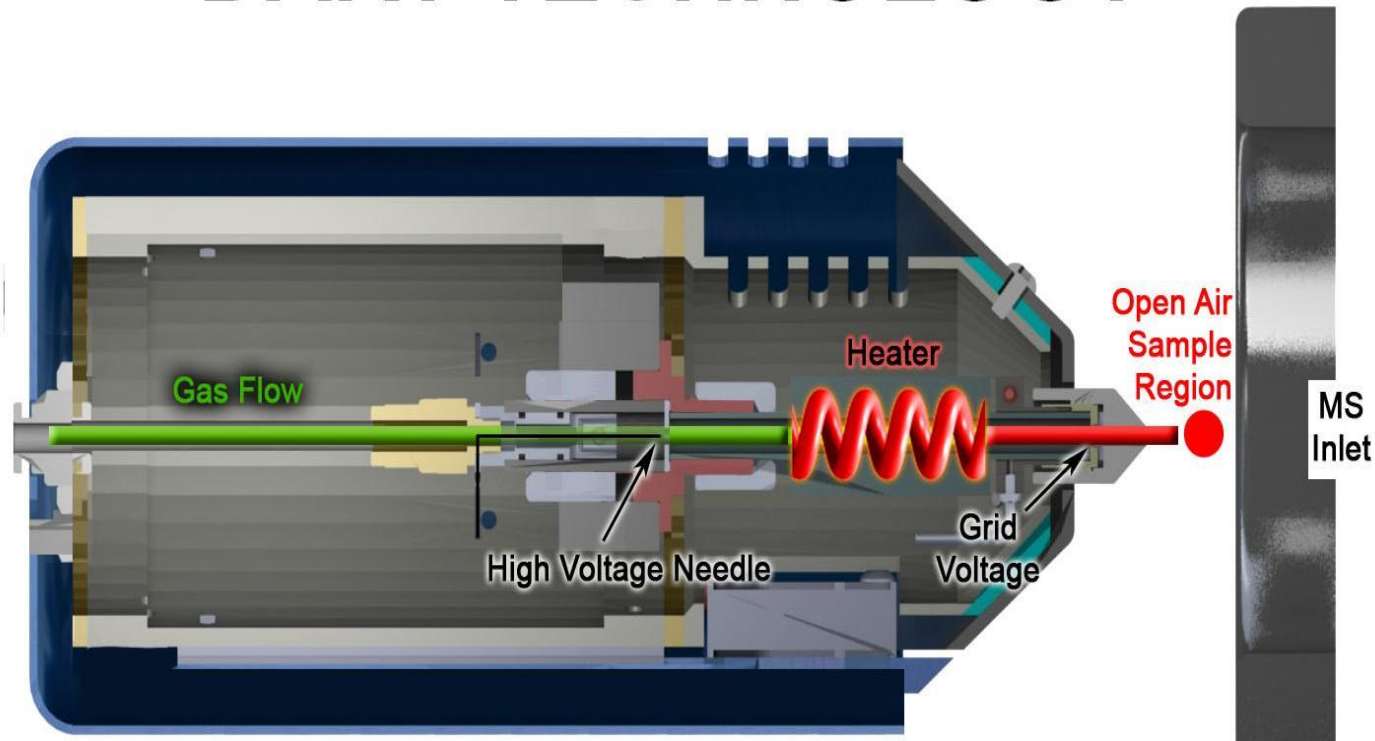
999 Broadway Suite 404 - Saugus, MA 01906 USA

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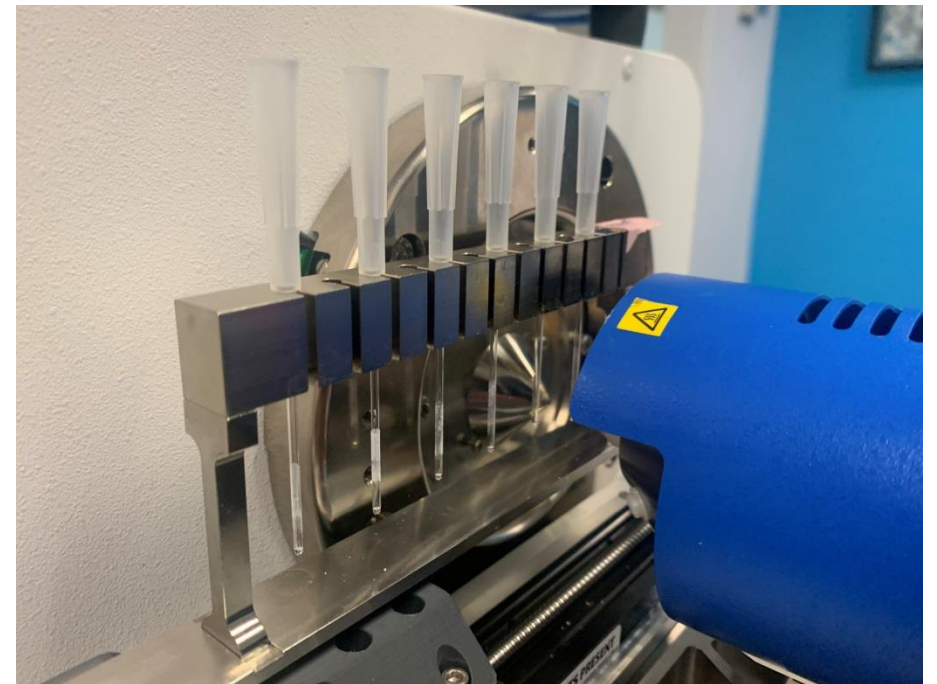
Bøgesvinget 8, DK-2740 Skovlunde, Denmark

DART Ionization Source

DART TECHNOLOGY



COATED GLASS CAPILLARY AUTOMATION MODULE



Mass spectrometer?

Of your choice:

- Unit res
 - Limited versatility
- High res MS/MS
 - Higher versatility
 - Everything comes at a price

PerFluoroAlkanoic Acids (PFAA) contamination

- From: <https://doi.org/10.1016/j.scitotenv.2020.140017>; *you have to pay for this article:*
PFA concentrations in soils: Background levels versus contaminated sites
- **Statements:**
 - PFA's are present in soils across the globe.
 - PFA's concentrations in soil range up to ppm levels at contaminated sites.
 - PFA's are retained at high concentrations in the vadose zone.

Protocol for PerFluoroAlkanoic Acids (PFAA) analysis

- **Article: Coated glass capillaries as SPME devices for DART mass spectrometry**, Cody and Maleknia, Rapid Commun Mass Spectrom., 2020;34:e8946)
- (www.doi.org/10.1002/rcm.8946), *this is the full article.*

Key points from article

- They utilized:
 - Dip glass tube into solution containing Hexadecylamine, let it dry.
 - Dip into sample and incubate-and-wait for minutes
 - Insert (or train robot to insert) the glass tubes in the DART and generate mass spectra
- **Analysis** using negative ion DART.
 - Results acquired in seconds per sample, with delay between, to avoid cross contamination

DART-MS Analysis essentials – and sensitivity

Article essentials:

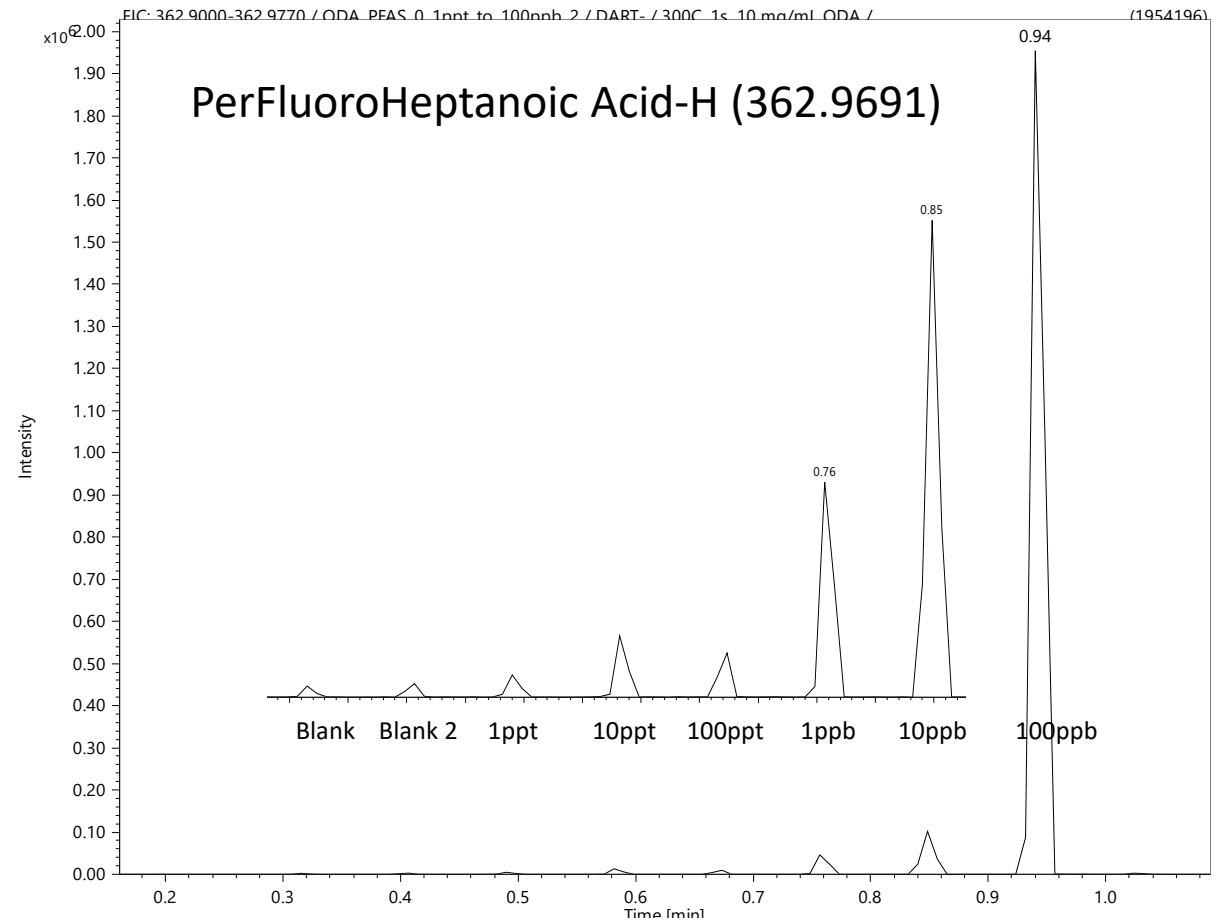
320°C chosen as the optimum temperature for desorption ionization.

Simple extraction from ground water (or the like) using hexadecylamine on a glass rod

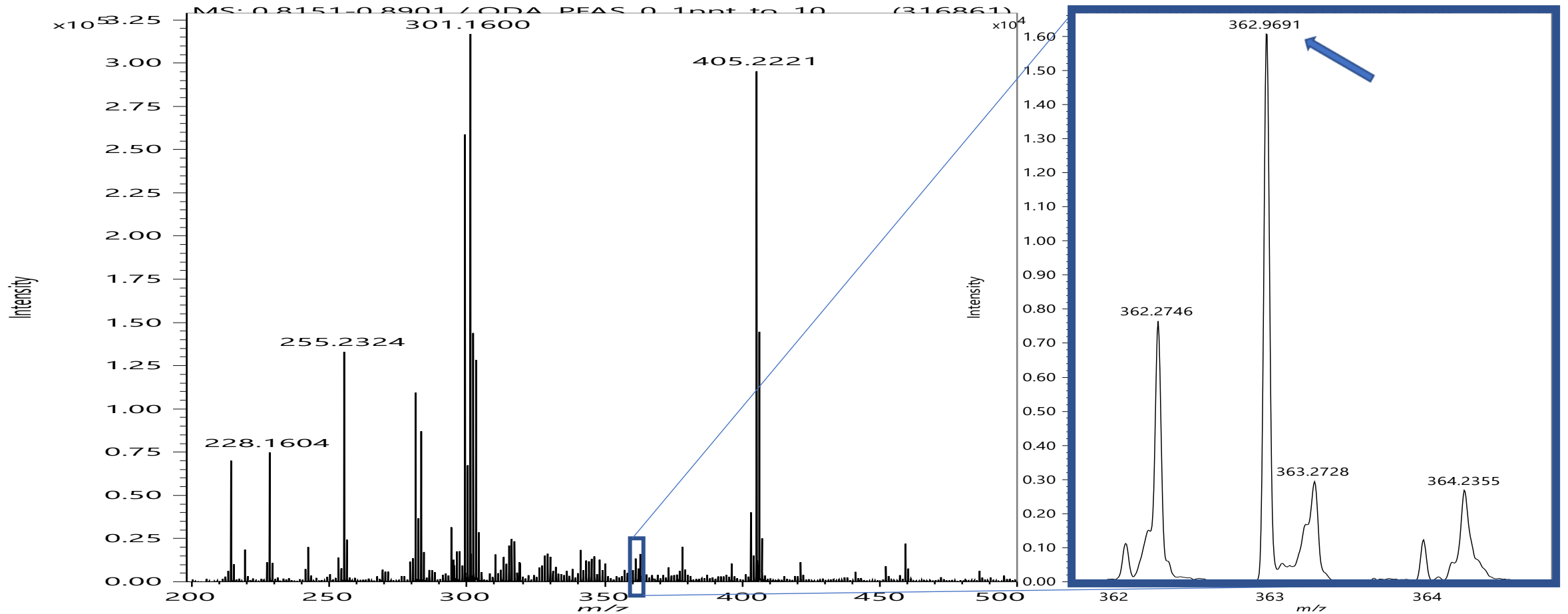
The method eliminates:

- solid phase extraction (SPE)
- organic solvents
- solvent dry down
- LC/MS analysis, as described in EPA methods.

Sensitivity; less than 1ppb

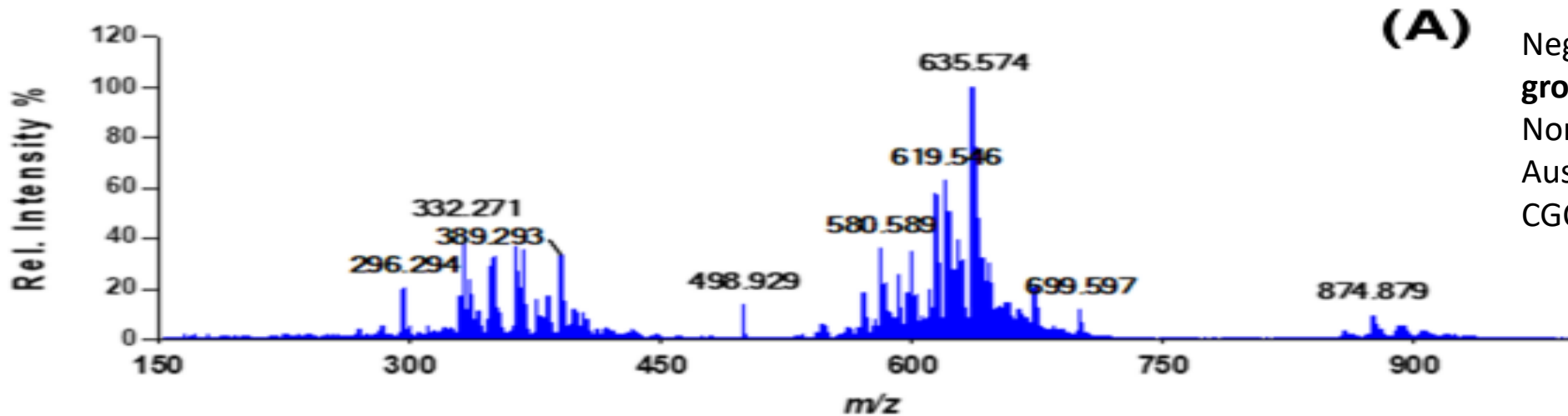


Negative Ion DART - 10ppb



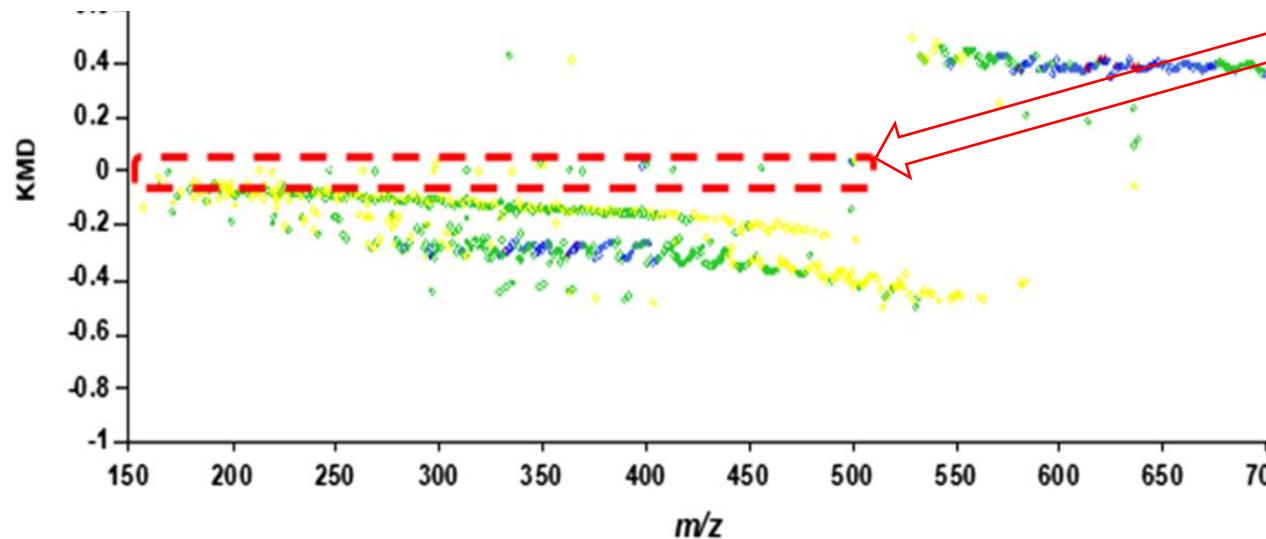
The full mass spectrum may be useful for potential detection of other contaminants while the partial mass spectrum documents both the deprotonated PFAS and its C¹³ containing isotope

DART-MS Screening Capability – PFAA in water

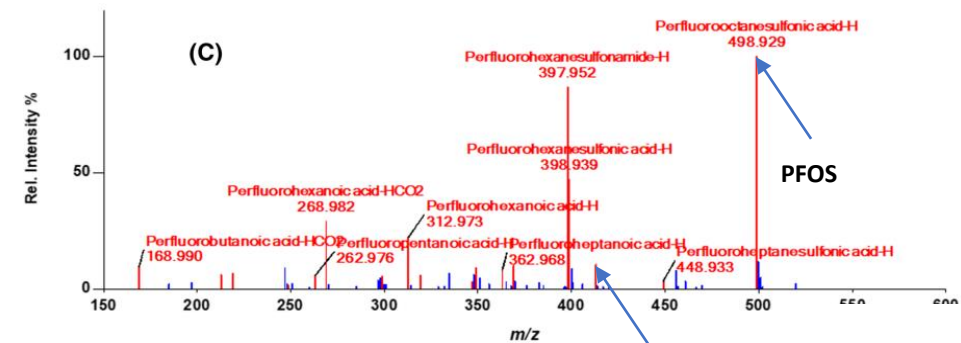


(A)

Negative ion DART-MS of **ground water** from Northern Queensland, Australia processed using CGC (Fig 4a ref. RCMS)



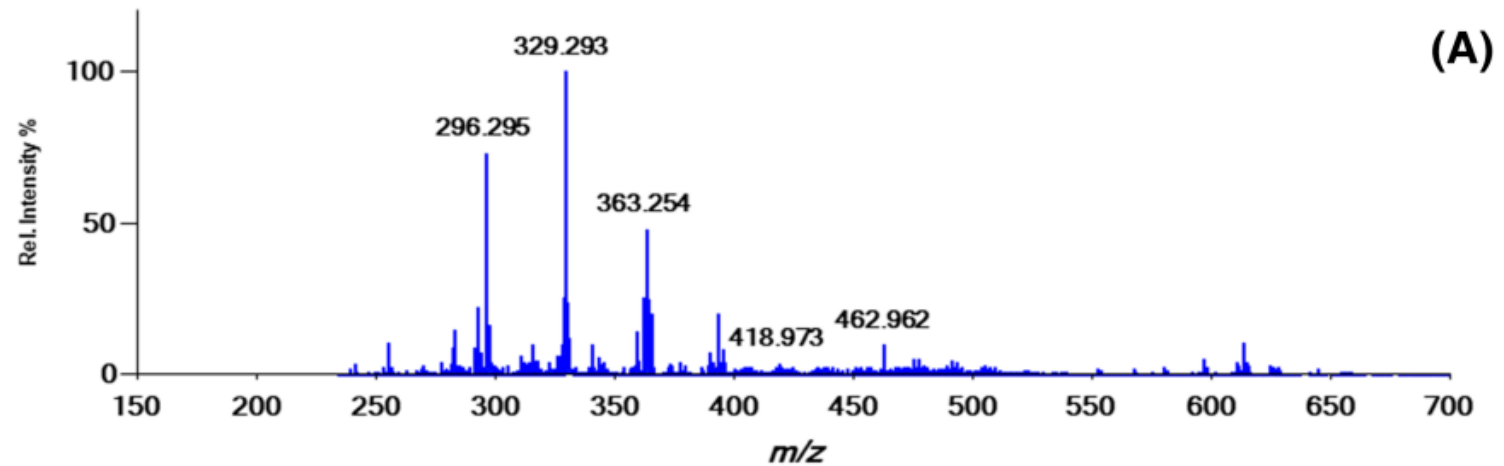
Kendrick mass defect plot using CF₂ as the base unit. **Peaks corresponding to PFAs** isolated from the area marked in red are subsequently labelled



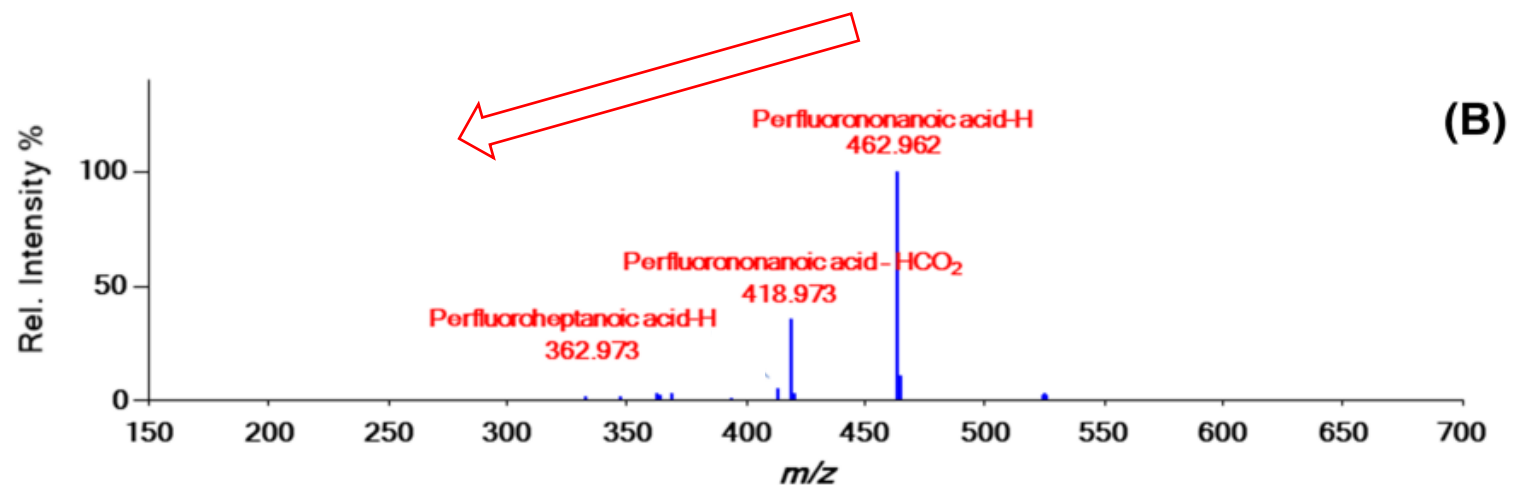
(C)

DART-MS Screening Capability – PFAA in aqueous extract from soil

Negative ion DART-MS of **aqueous extract of a soil** sample taken adjacent to an airbase in Portsmouth NH, USA (Fig 5a ref. RCMS) presents a complex mass spectrum containing many ions



Perfluoroacid peak isolated from the CF₂ **Kendrick mass defect plot** simplifies the identification of the fluorine containing peak enabling rapid screening for any related molecules



Final words:

- PFAA's in soil probably demand a lot of attention in the future.
- Simple extraction method permits screening of aqueous samples for PFAA's without neither SPE nor LC/MS/MS.
- Water and water-from-soil samples have been analyzed using the screening method.
- The method permits high throughput (12 samples per 10 minutes).
- We may perform demo analyses for you – to test your application, or you may loan an instrument.
- Thank you for your attention