Per- and polyfluoroalkyl substances (PFAS)

Determination in shellfish by liquid chromatography coupled to accurate mass spectrometry

Piva, E. *et al.* 2022 https://doi.org/10.1002/dta.3282

"...a rise in emerging chemicals that can't be monitored with conventional methods, means we should explore alternative monitoring techniques."

Tarun Anumol, Ph.D.
Global Director, Environmental Market, Agilent Technologies

Study – Analyzed PFAS levels in mussel, clam and oyster samples

Study

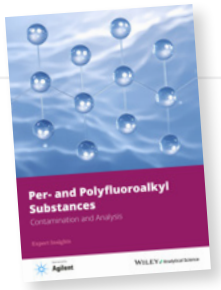
- Used liquid chromatography and mass spectrometry (LC/MS) with Agilent 1290 Infinity II LC coupled to a 6546 quadrupole-time-of-flight mass spectrometer
- LC/Q-TOF method used a library of 150 PFCA and PFSA compounds for non-targeted analysis

Results

- Every sample showed detectable PFAS
- Of 12 PFAS detected, 7 PFAS were quantified (0.03-0.57 ng/g)
- PFAS higher in Mediterranean than Pacific or Atlantic clams
- N-MeFOSA, N-EtFOSA, N-MeFOSAA identified – possible new PFAS precursors
- LC/MS/MS and LC/Q-TOF used for improved PFAS detection

Conclusions

- LC/Q-TOF method is effective in detecting linear and branched PFAS in shellfish at ng/g concentration
- Method can also identify PFAS precursors e.g. 6:2 FTS and N-MeFOSAA in Mediterranean clams and mussels



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Agilent Equipment Used

Agilent 6546 LC/Q-TOF and 1290 Infinity II HPLC

WILEY Analytical Science

Abbreviations: Gen X – hexafluoropropylene oxide dimer acid **FTS** – fluorotelomer perfluoroalkyl sulfonic acids **LC/MS/MS** – liquid chromatography mass spectrometry **N-MeFOSA and N-EtFOSA** – perfluorooctane sulfonamides **N-MeFOSAA** – perfluorooctane sulfonamide acetic acid **PFAS** – per- and polyfluoroalkyl substances **PFCA** – perfluoroalkyl carboxylic acids **PFSA** – perfluoroalkyl sulfonic acids **PFOS** – perfluorooctane sulfonate **Q-TOF** – quadrupole time-of-flight spectrometer

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Dietary Uptake and Depuration Kinetics of

Perfluorooctane Sulfonate, Perfluorooctanoic Acid, and Hexafluoropropylene Oxide Dimer Acid (GenX) in a Benthic Fish

Hassell, K.L. *et al.* 2019 • https://doi.org/10.1002/etc.4640

"We are still at the tip of the iceberg in terms of information on PFAS occurrence and toxicity studies. Information is available for only a handful of them, but it's prudent to monitor as many as possible now for baseline levels."

Tarun Anumol, Ph.D.
Global Director, Environmental Market, Agilent Technologies

Study on benthic fish on the Werribee River, Australia looked at:
PFAS depuration and accumulation • PFAS contaminations

Study

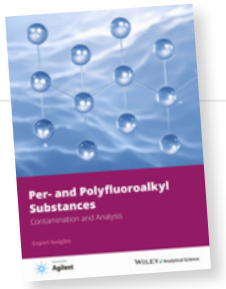
- 40 male and 8 female adult blue spot gobies
- Uniform food ingestion rates
- 11 week experiment
- Ultra-high performance LC/MS/MS used to analyze body samples
- Low limits of reporting for:
  - PFOA
  - Linear PFOS
  - Linear+branched PFOS
  - GenX

Results

- Accumulation of PFOA, linear PFOS and linear+branched PFOS
- Steady-state concentration reached after 14 days
- Depuration rate faster for PFOA compared to PFOS
- Indication of different depuration kinetics for PFOS isomers
- GenX (PFOS replacement) did not accumulate

Research priorities

1. Specific PFOS isomers (branched and linear)
2. Tissue-specific distribution
3. Newer PFAS replacements
4. Organ-specific half-life data



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Agilent Equipment Used

Agilent 6495 LC/TQ

WILEY Analytical Science

Abbreviations: Gen X – hexafluoropropylene oxide dimer acid **LC/MS/MS** – liquid chromatography mass spectrometry **PFAS** – per- and polyfluoroalkyl substances **PFOA** - perfluorooctanoic acid **PFOS** – perfluorooctane sulfonate

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