

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



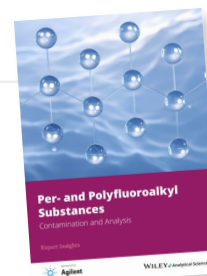
Conclusions



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

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

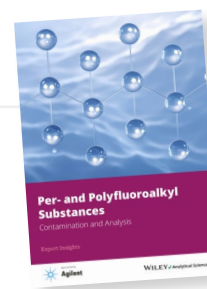
Tissue-specific distribution

3

Newer PFAS replacements

4

Organ-specific half-life data



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Agilent Equipment Used

Agilent 6495 LC/TQ



WILEY Analytical Science