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Per- and polyfluorinated alkyl compound (PFAS) analysis in cosmetics using high resolution accurate mass spectrometry

SCIEX The Power of Precision

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Introduction

This poster describes a non-targeted method to improve the characterization of PFAS in cosmetic products to increase our knowledge of cosmetics as potential PFAS exposure sources. The enhanced MS/MS spectral sensitivity of the ZenoTOF 7600 system improves compound confirmation through better library matching and identification using diagnostic fragment ions.

Targeted analytical methods typically monitor ~20-30 PFAS compounds which represent a small fraction of the estimated 5000 PFAS used in commercial products. Further, targeted methods are limited by the availability of analytical standards. Non-targeted methods, using MS/MS fragmentation patterns from accurate mass spectrometry, can be used to confirm the identity of suspected PFAS.

SCIEX ZenoTOF 7600 system

Figure 1. The entire PFAS life cycle can influence human exposure, including personal care products such as cosmetics.

Methods

- A diverse range of cosmetic products was purchased including foundations, concealers, and creams. All products contained some PFAS compounds.
- Samples were extracted by sonication in basic methanol. The samples were then cleaned with ENVI-Carb SPE cartridges and the extracts were concentrated under N_2 gas.
- Chromatography was performed using an ExionLC AD system modified to replace fluoropolymer tubing with PEEK. The delay and analytical columns used were the Phenomenex Luna Omega PS C18 column. Mobile phases were water and methanol, both modified with 10mM ammonium acetate. A 12 min gradient was used with a 10 µL injection volume.
- Samples were analyzed on the ZenoTOF 7600 system using negative mode electrospray ionization. Data were collected using data-dependent acquisition (DDA) with Zeno trap pulsing turned on and MS/MS triggered for the top 30 precursor ions using collision-induced dissociation (CID).

MS/MS library matching to confirm PFAS detection in cosmetics

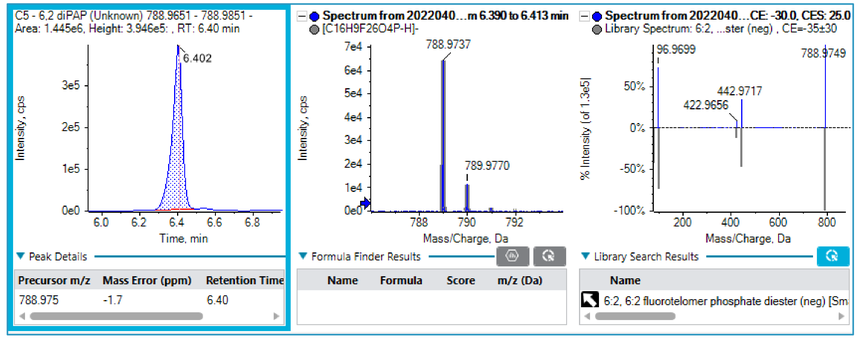


Figure 2. Detection of 6:2 diPAPs in a cosmetic sample. Compound confirmation achieved through excellent precursor mass error (left panel), good isotope pattern match (middle panel) and MS/MS spectrum match to SCIEX Fluorochemical High Resolution MS/MS library.

- Suspect screening list built from legacy PFAS and PFAS reported in cosmetics
- Detection criteria: Precursor mass error (<5 ppm), isotope pattern match, MS/MS library match based on "fit" score (>70)
- Confirmed detection of 6:2 diPAPs in most samples

Compound confirmation using diagnostic MS/MS fragments

- 4:2/6:2 diPAP detected with good precursor mass error
- No MS/MS library spectrum available
- Experimental MS/MS showed diagnostic loss of 4:2 and 6:2 side-chains, and subsequent loss of $[HF]^-$

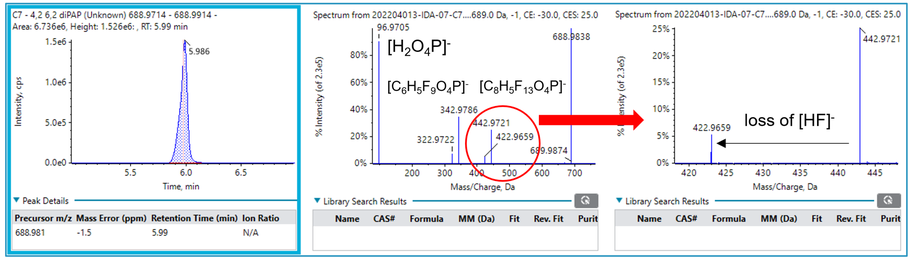
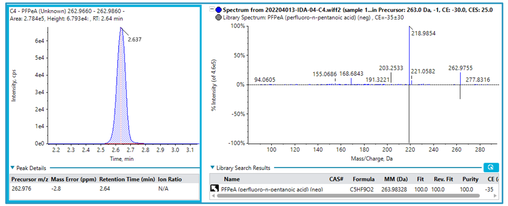


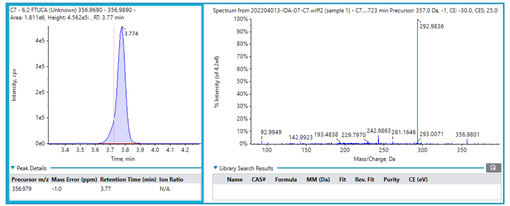
Figure 3. Detection of 4:2/6:2 diPAPs in a cosmetic sample. Compound confirmation shown by excellent precursor mass error (left panel), and diagnostic fragments based on MS/MS of analogous diPAP compounds (right panels).

Additional PFAS detected

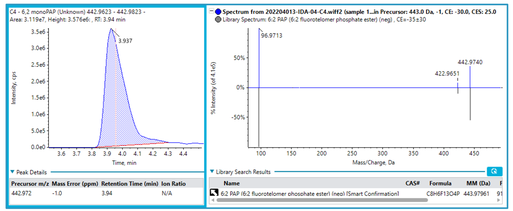
1. Perfluorinated carboxylic acids (PFCAs)



2. Fluorotelomer saturated and unsaturated acids (FTCAs and FTUCAs)



3. Mono-PAPs



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