

## Application News

Liquid Chromatograph Mass Spectrometer LCMS-8060RX

### Quantitative Analysis of Selected Per- and Polyfluoroalkyl Substances (PFAS) in Cosmetic Products by LC-MS/MS

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#### User Benefits

- ◆ Accurate quantification of multiple PFAS in complex cosmetic matrices is possible using LC-MS/MS with internal-standard calibration.
- ◆ QuEChERS extraction combined with SPE cleanup provides effective matrix removal, enabling reliable PFAS analysis in diverse cosmetic products.
- ◆ The PFAS-targeted method can be expanded to include additional PFAS compounds as analytical requirements evolve.

#### Introduction

Per- and polyfluoroalkyl substances (PFAS) are a diverse group of synthetic chemicals that have been intentionally used in certain cosmetic products because of their unique physicochemical properties and functional characteristics, including water and oil resistance, conditioning, and film formation<sup>1</sup>. These properties can contribute to the performance and sensory characteristics of cosmetic products. However, concerns regarding the persistence and potential environmental and health impacts of certain PFAS have increased the need for reliable analytical methods to identify and quantify these compounds in cosmetic products<sup>2</sup>. This Application News presents a workflow for the quantitative analysis of selected PFAS in cosmetic products using Shimadzu's LCMS-8060RX triple quadrupole mass spectrometer coupled with the Nexera™ LC-40 ultra-high-performance liquid chromatography system (Fig. 1).



Fig. 1 Shimadzu Nexera™ X3 coupled with LCMS-8060RX

#### Sample Preparation and Analysis Conditions

The reference standards were procured from Wellington Laboratories with below catalogue numbers:

Isotope Dilution Standard PDS:- EPA-533ES

Native Analyte Primary Dilution Standard:- EPA-533PAR

Six different types of cosmetic samples namely, foundation, sunscreen, lip balm, lipstick, moisturizing cream and serum cream were collected from a local supplier.

Calibration standards were prepared in a methanol/acetonitrile mixture (90:10, v/v) over a concentration range of 0.5-25 µg/L and analyzed under the specified LC-MS/MS conditions (Table 1).

PFAS contamination can originate from commonly used laboratory materials, including certain pipette tips, sticky notes, vial caps containing LDPE or PTFE (Teflon), and various plastic consumables. To minimize background contamination from these unavoidable sources, the Nexera LC-40 system was equipped with a PFAS-Free Kit, which includes PFAS-free mobile phase tubing, a PFAS-free in-line filters, and a delay column. The delay column effectively separates background PFAS originating from the

LC system and laboratory materials from the PFAS present in the sample, thereby improving analytical accuracy and confidence in trace-level quantification. The system was used for the identification and quantification of PFAS in cosmetic products.

Table 1 Analysis Conditions of Nexera and LCMS-8060RX

|                   |                                                                     |
|-------------------|---------------------------------------------------------------------|
| System            | : Nexera X3                                                         |
| Column            | : Restek Ultra IBD<br>(100 mm × 2.1 mm I.D., 3 µm) <sup>*1</sup>    |
| Temperature       | : 45 °C                                                             |
| Injection volume  | : 5 µL (Co-Injection 15 µL Water)                                   |
| Mobile phases     | : 10 mM ammonium acetate in Water<br>10 mM ammonium acetate in MeOH |
| Flow rate         | : 0.3 mL/min                                                        |
| Time program (%B) | : 5 % (0 min- 4 min) → 90 % (23-25 min) →<br>5 % (25.1-30 min)      |
| System            | : LCMS-8060RX (ESI Negative)                                        |
| Nebulizing gas    | : 3 L/min                                                           |
| Drying gas        | : 5 L/min                                                           |
| Heating gas       | : 15 L/min                                                          |
| DL temp           | : 150 °C                                                            |
| Heat block temp   | : 250 °C                                                            |
| Interface temp    | : 100 °C                                                            |

\*1 P/N: 9175312

#### Sample Preparation

Approximately 1.0 g of the cosmetic sample was weighed into a PFAS free 50 mL centrifuge tube. The internal standard (ISTD) was spiked at 5 ng/mL, followed by the addition of 10 mL of acetonitrile containing 1% acetic acid. The sample was shaken for 5 min and then sonicated for 30 min. Subsequently, 10 mL of water was added, and the mixture was shaken for 1 min. QuEChERS buffer (SHIMSEN QuEChERS Extraction Salts; Part No: 380-00149) was then added, and the sample was thoroughly shaken and vortexed. The mixture was centrifuged at 5000 rpm for 5 min, and 5 mL of the upper organic layer was transferred into a 15 mL centrifuge tube. The dSPE (SHIMSEN QuEChERS II; Part No: 380-00990-20) was added to the extract, followed by shaking and centrifugation at 5000 rpm for 10 min. An aliquot of 2.5 mL of the resulting extract was transferred to a 50 mL centrifuge tube and diluted with water to a final volume of 25 mL.

For the SPE cleanup, the Biotage EVOLUTE® PFAS 533 500 mg/6 mL (604-00500-C-533) cartridge was placed in a positive-pressure manifold for sample cleanup<sup>3</sup>. The cartridge was sequentially conditioned with 5 mL of methanol followed by 5 mL of 0.1 M phosphate buffer (pH 7). The entire diluted extract was then passed through the SPE cartridge under positive pressure. The analytes were eluted by adding 5 mL of the elution solvent (ammonium hydroxide in methanol) and allowing it to pass slowly through the cartridge into a polypropylene tube. The elution process was repeated, and a total of 10 mL of eluate was collected. The eluate was evaporated to dryness under a

stream of nitrogen at 50 °C. The dried residue was finally reconstituted in 0.5 mL of methanol/acetonitrile (90:10, v/v) for LC-MS/MS analysis.

## ■ Results and Discussion

### Calibration and Linearity

Calibration curves for the 29 PFAS were established using mixed calibration standards over the concentration range of 0.5–25 ng/mL. Quantification was performed using the internal standard calibration method with isotopically labeled internal standards, where the response ratio of each target PFAS to its corresponding internal standard was used for calibration. Excellent linearity was obtained, with coefficient of determination ( $R^2$ ) > 0.99 for all targeted PFAS across the calibration range. Accuracy was within 80–120% for the calibration standards. The calibration results, along with the detection limits (LOD) and quantitation limits (LOQ) calculated from the signal-noise ratio, are summarized in Table 2. Fig. 2 shows the calibration curves for four representative native PFAS compounds along with their corresponding QC (5 ng/mL) plots across the linearity range. Fig. 3 shows the chromatograms of the four representative PFAS at 1 ng/mL and 5.0 ng/mL, respectively.

### QC Performance

A QC standard was analyzed periodically throughout the analytical sequence to monitor the stability of the LC-MS/MS system and the quantitative performance of the method. The QC results demonstrated accuracy within 80–120% for all target PFAS throughout the analytical sequence, except for 11CI-PF3OUdS, which showed an accuracy of 77% in the final QC injection as shown in Table 3. Overall, the QC results demonstrated acceptable analytical performance and confirmed the suitability of the method for quantitative analysis of PFAS in cosmetic samples.

### Quantitative Analysis of Cosmetic Samples

The developed method was applied to the quantitative determination of PFAS in cosmetic samples. Both unspiked and spiked samples were analyzed to evaluate the method's applicability to complex cosmetic matrices. Overall, acceptable recoveries were obtained for most PFAS; however, FOSA showed lower recovery in foundation, lip balm, and sunscreen samples, while 9CI-PF3ONS showed higher recovery in liquid lipstick. These variations may be attributed to matrix effects associated with the non-matrix-matched calibration. The quantitative results and recovery data are summarized in Table 3 and Fig. 4.

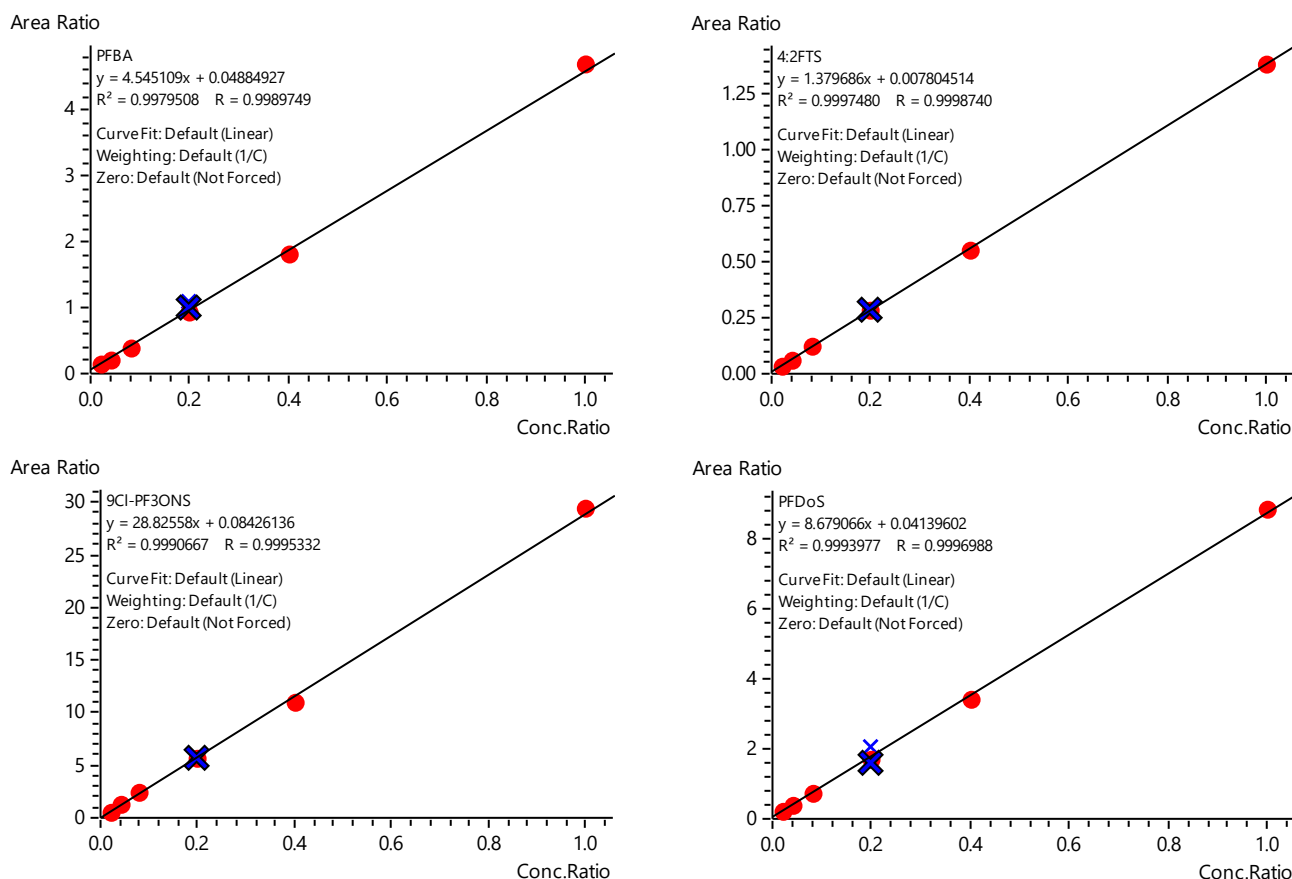


Fig. 2 Representative calibration curves for PFAS ranging from 0.5 ng/mL to 25 ng/mL.

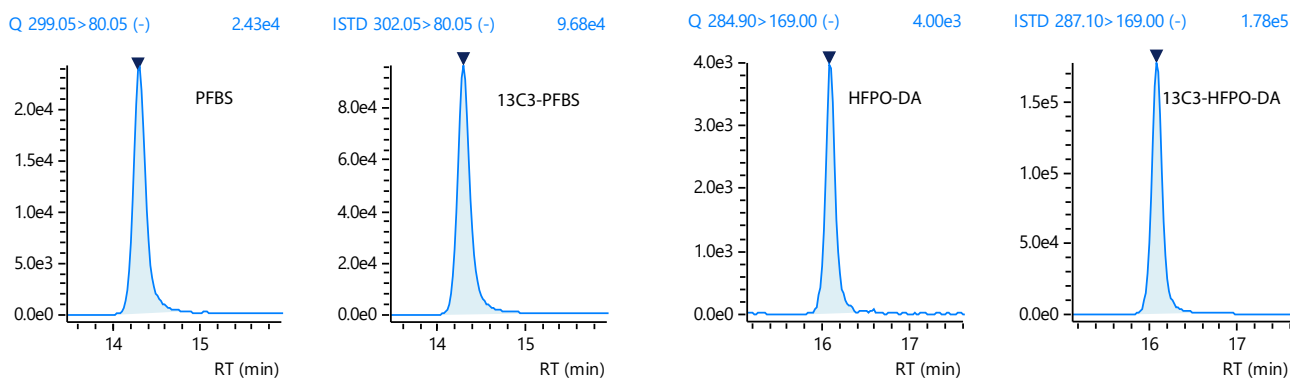


Fig. 3 Representative chromatograms of native PFAS and their corresponding internal standards at 1.0 ng/mL and 5.0 ng/mL, respectively

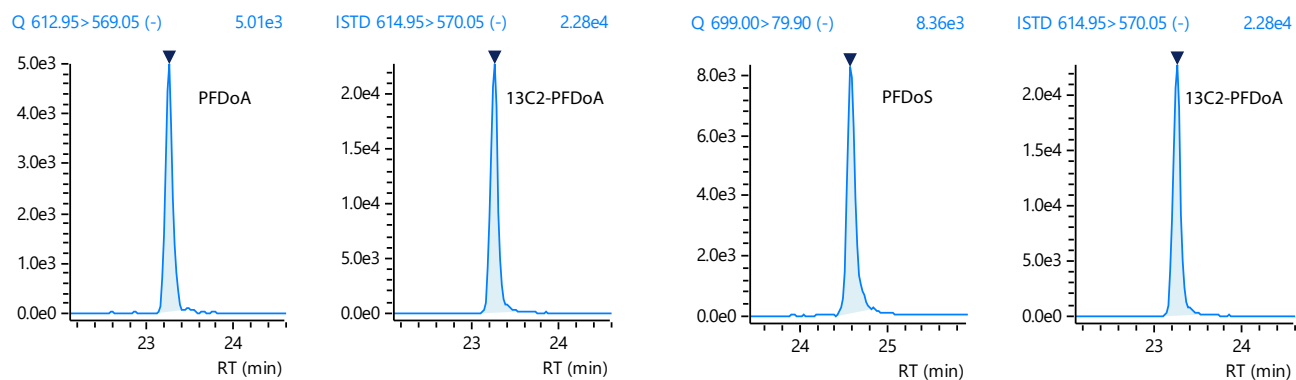


Fig. 3 Representative chromatograms of native PFAS and their corresponding internal standards at 1.0 ng/mL and 5.0 ng/mL, respectively

Table 2 Summary of PFAS with respect to linearity, accuracy, detection limit and quantitation limit.

| Sr.No. | Name         | Type   | RT min. | Linearity range ng/mL | R <sup>2</sup> | Accuracy (%) | ISTD Name    |
|--------|--------------|--------|---------|-----------------------|----------------|--------------|--------------|
| 1      | PFBA         | Target | 3.02    | 0.5 - 25              | 0.9980         | 97.53        | 13C4-PFBA    |
| 2      | PFPeA        | Target | 8.67    | 0.5 - 25              | 0.9993         | 96.55        | 13C5-PFPeA   |
| 3      | PFBS         | Target | 14.28   | 0.5 - 25              | 0.9980         | 93.65        | 13C3-PFBS    |
| 4      | 4:2FTS       | Target | 14.70   | 0.5 - 25              | 0.9997         | 98.87        | 13C2-4:2FTS  |
| 5      | PFHxA        | Target | 15.46   | 0.5 - 25              | 0.9989         | 95.5         | 13C5-PFHxA   |
| 6      | HFPO-DA      | Target | 16.07   | 0.5 - 25              | 0.9996         | 98.45        | 13C3-HFPO-DA |
| 7      | PFPeS        | Target | 17.26   | 0.5 - 25              | 0.9983         | 94.80        | 13C4-PFHpA   |
| 8      | ADONA        | Target | 17.59   | 0.5 - 25              | 0.9988         | 95.56        | 13C4-PFHpA   |
| 9      | PFHpA        | Target | 17.93   | 0.5 - 25              | 0.9992         | 96.06        | 13C4-PFHpA   |
| 10     | PFHxS        | Target | 18.93   | 0.5 - 25              | 0.9995         | 97.61        | 13C3-PFHxS   |
| 11     | 6:2FTS       | Target | 19.21   | 0.5 - 25              | 0.9997         | 97.95        | 13C2-6:2FTS  |
| 12     | PFOA         | Target | 19.40   | 0.5 - 25              | 0.9993         | 96.01        | 13C8-PFOA    |
| 13     | PFHpS        | Target | 20.21   | 0.5 - 25              | 0.9996         | 99.68        | 13C9-PFNA    |
| 14     | PFNA         | Target | 20.57   | 0.5 - 25              | 0.9995         | 97.30        | 13C9-PFNA    |
| 15     | 9Cl-PF3ONS   | Target | 21.15   | 0.5 - 25              | 0.9991         | 95.64        | 13C8-PFOS    |
| 16     | PFOS         | Target | 21.30   | 0.5 - 25              | 0.9996         | 97.54        | 13C8-PFOS    |
| 17     | FOSA         | Target | 21.42   | 0.5 - 25              | 0.9977         | 93.78        | 13C8-PFOS    |
| 18     | 8:2FTS       | Target | 21.57   | 0.5 - 25              | 0.9996         | 99.29        | 13C2-8:2FTS  |
| 19     | PFDA         | Target | 21.57   | 0.5 - 25              | 0.9987         | 95.71        | 13C6-PFDA    |
| 20     | PFNS         | Target | 22.25   | 0.5 - 25              | 0.9992         | 99.52        | 13C7-PFUnA   |
| 21     | PFUnA        | Target | 22.45   | 0.5 - 25              | 0.9989         | 95.04        | 13C7-PFUnA   |
| 22     | 11Cl-PF3OUdS | Target | 22.67   | 0.5 - 25              | 0.9993         | 95.89        | 13C7-PFUnA   |
| 23     | PFDS         | Target | 23.11   | 0.5 - 25              | 0.9992         | 97.97        | 13C2-PFDoA   |
| 24     | PFDoA        | Target | 23.24   | 0.5 - 25              | 0.9987         | 95.92        | 13C2-PFDoA   |
| 25     | 10:2 FTS     | Target | 23.38   | 0.5 - 25              | 0.9988         | 96.44        | 13C2-PFDoA   |
| 26     | PFUdS        | Target | 23.87   | 0.5 - 25              | 0.9992         | 98.35        | 13C2-PFDoA   |
| 27     | PFDoS        | Target | 24.56   | 0.5 - 25              | 0.9994         | 97.35        | 13C2-PFDoA   |
| 28     | PFTTrDS      | Target | 25.17   | 0.5 - 25              | 0.9989         | 96.59        | 13C2-PFDoA   |

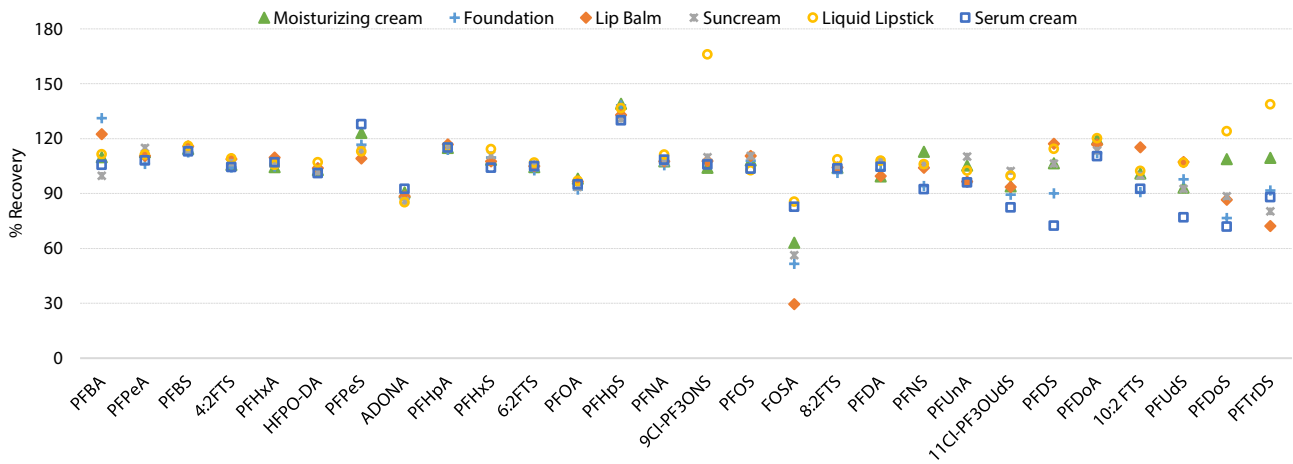


Fig. 4 Percentage recovery of PFAS in cosmetic samples at a spiking concentration of 25 ng/mL.

Table. 3 Summary of PFAS with respect to linearity, accuracy, detection limit and quantitation limit.

| Name         | Foundation     | Lip balm       | Sunscreen      | Liquid lipstick | Serum cream    | Moisturizing cream |
|--------------|----------------|----------------|----------------|-----------------|----------------|--------------------|
|              | Conc. in ng/mL | Conc. in ng/mL | Conc. in ng/mL | Conc. in ng/mL  | Conc. in ng/mL | Conc. in ng/mL     |
| PFBA         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFPeA        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFBS         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| 4:2FTS       | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFHxA        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| HFPO-DA      | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFPeS        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| ADONA        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFHpA        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFHxS        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| 6:2FTS       | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFOA         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFHpS        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFNA         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| 9CI-PF3ONS   | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFOS         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| FOSA         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| 8:2FTS       | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFDA         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFNS         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFUnA        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| 11CI-PF3OUdS | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFDS         | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFDoA        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| 10:2 FTS     | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFUdS        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFDoS        | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |
| PFTTrDS      | <LOQ           | <LOQ           | <LOQ           | <LOQ            | <LOQ           | <LOQ               |

## Conclusion

The developed workflow provides a simple and effective approach for the extraction and quantitative analysis of PFAS in cosmetic products. The QuEChERS-based extraction combined with SPE cleanup provides effective matrix reduction, although it does not eliminate matrix-related effects. The cleanup helps minimize matrix components that can contribute to ion suppression and contamination of the LC-MS/MS ion source. The use of PFAS-free materials throughout the analytical workflow further minimizes the risk of background contamination.

Combined with the high sensitivity of the LCMS-8060 RX, the developed workflow demonstrated good analytical performance for the targeted PFAS compounds in cosmetic matrices.

The developed sample preparation protocol can be extended to HRMS platforms such as the LCMS-9050 for non-targeted PFAS analysis, enabling the screening and identification of a broader range of PFAS beyond the targeted compounds evaluated in this study.

## References

- 1) FDA, 2025 — supports intentional use of PFAS in cosmetics and their functional properties. The FDA report is based on U.S. cosmetic product-listing data and found 51 intentionally added PFAS across 1,744 formulations.
- 2) United States Environmental Protection Agency, Increasing Our Understanding of the Health Risks from PFAS and How to Address Them.  
<https://www.epa.gov/pfas/increasing-our-understanding-health-risks-pfas-and-how-address-them>
- 3) Method 533: Determination of Per- and Polyfluoroalkyl Substances in Drinking Water by Isotope Dilution Anion Exchange Solid Phase Extraction and Liquid Chromatography/Tandem Mass Spectrometry.

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