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LCMS-8050RX High Performance Liquid Chromatograph Mass Spectrometer

Application News

# Simultaneous Analysis of 40 PFAS Components in Drinking Water Using a Triple Quadrupole LC/MS/MS

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## User Benefits

- Enables analysis of 40 PFAS components within 20 minutes and simultaneous analysis of multiple components without sensitivity loss.
- Enables quantitative analysis of concentrations as low as 0.2 ng/L (in water samples) for PFOA, PFOS, PFHxS, and others.
- Consistent and accurate results can be obtained with good recovery rates and reproducibility data for recovery tests.

## ■ Introduction

Perfluoroalkyl and polyfluoroalkyl substances (PFAS) offer broad versatility for a wide range of applications. Due to their structural stability and resistance to decomposition, they easily accumulate in the environment and are suspected to be harmful for humans. Due to concerns about their environmental impacts, the U.S. Environmental Protection Agency (EPA) and the European Chemicals Agency (ECHA) have been implementing measures to strengthen PFAS-related regulations in recent years. Consequently, efforts to comply with such PFAS regulations have been increasing every year, and the list of compounds governed by such regulations continues to grow. That makes it increasingly useful to apply an analytical method that can reliably analyze all the various PFAS substances at the same time.

This article describes the results from simultaneously analyzing 40 PFAS components (Table 1) as target compounds after automatic sample preparation. Good results were obtained from measuring standard solutions and recovery tests of drinking water samples.

Table 1 List of Compounds

| No. | Compound | Type | No. | Compound | Type |
|---|---|---|---|---|---|
| 1 | PFBA | Target | 33 | 11Cl-PF3OUdS | Target |
| 2 | PFPeA | Target | 34 | 3:3 FTCA | Target |
| 3 | PFHxA | Target | 35 | 5:3 FTCA | Target |
| 4 | PFHpA | Target | 36 | 7:3 FTCA | Target |
| 5 | PFOA | Target | 37 | PFEESA | Target |
| 6 | PFNA | Target | 38 | PFMPA | Target |
| 7 | PFDA | Target | 39 | PFMBA | Target |
| 8 | PFUnA | Target | 40 | NFDHA | Target |
| 9 | PFDoA | Target | 41 | 13C4-PFBA | EIS |
| 10 | PFTrDA | Target | 42 | 13C5-PFPeA | EIS |
| 11 | PFTeDA | Target | 43 | 13C5-PFHxA | EIS |
| 12 | PFBS | Target | 44 | 13C4-PFHpA | EIS |
| 13 | PFPeS | Target | 45 | 13C8-PFOA | EIS |
| 14 | PFHxS | Target | 46 | 13C9-PFNA | EIS |
| 15 | PFHpS | Target | 47 | 13C6-PFDA | EIS |
| 16 | PFOS | Target | 48 | 13C7-PFUnA | EIS |
| 17 | PFNS | Target | 49 | 13C2-PFDoA | EIS |
| 18 | PFDS | Target | 50 | 13C2-PFTeDA | EIS |
| 19 | PFDoS | Target | 51 | 13C3-PFBS | EIS |
| 20 | 4:2FTS | Target | 52 | 13C3-PFHxS | EIS |
| 21 | 6:2FTS | Target | 53 | 13C8-PFOS | EIS |
| 22 | 8:2FTS | Target | 54 | 13C2-4:2FTS | EIS |
| 23 | PFOSA | Target | 55 | 13C2-6:2FTS | EIS |
| 24 | NMeFOSA | Target | 56 | 13C2-8:2FTS | EIS |
| 25 | NEtFOSA | Target | 57 | 13C8-PFOSA | EIS |
| 26 | NMeFOSAA | Target | 58 | D3-NMeFOSA | EIS |
| 27 | NEtFOSAA | Target | 59 | D5-NEtFOSA | EIS |
| 28 | NMeFOSE | Target | 60 | D3-NMeFOSAA | EIS |
| 29 | NEtFOSE | Target | 61 | D5-NEtFOSAA | EIS |
| 30 | HFPO-DA | Target | 62 | D7-NMeFOSE | EIS |
| 31 | ADONA | Target | 63 | D9-NEtFOSE | EIS |
| 32 | 9Cl-PF3ONS | Target | 64 | 13C3-HFPO-DA | EIS |

## ■ LCMS-8050RX

Samples were analyzed using a triple-quadrupole mass spectrometer, LCMS-TQ8050RX (Fig. 1). The LCMS-TQ RX series offer the same high sensitivity and high-speed performance achieved by previous models with UF technology, but they also include the new CoreSpray technology, which generates a more uniform nebulizer flow and provides more consistent measurements.

Fig. 1 LCMS-8050RX

## ■ Sample Preparation

Drinking water samples were pretreated by adding 20 µL of an internal standard solution (EIS) and then using an anion exchange solid phase column for solid phase extraction. The eluate from the solid phase column was concentrated by a factor of 1000 by drying with nitrogen gas stream and then bring the volume to 0.5 mL with methanol for analysis. The sample preparation process is shown in Fig. 2. In this case, AquaTrace automatic solid phase extraction system from GL Sciences was used to perform all steps, from conditioning to concentrating automatically.

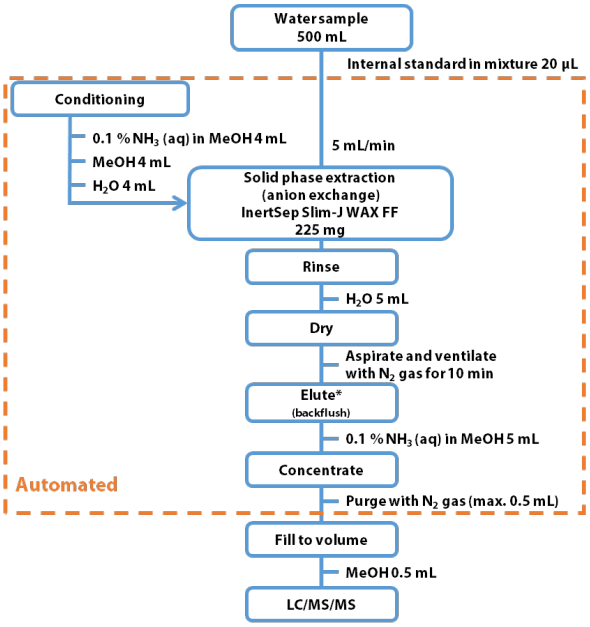


Fig. 2 Pretreatment Process Flow

(* The solid phase column was manually inverted for elution by backflushing.)

## ■ Analytical Conditions

The HPLC and MS analytical conditions are shown in Table 2. Measuring PFAS requires particular care due to the risk of contamination from the system, the mobile phase, and other sources.

For this article, a delay column was installed between the mixer and autosampler to inhibit the effects of PFAS contamination from the system. A reagent intended for PFOS/PFOA analysis was used in the mobile phase.

Table 2 Analytical Conditions

| UHPLC (Nexera™-X3 System) | | MS (LCMS-8050RX) | |
|---|---|---|---|
| Analytical Column: | Shim-pack™ GIST-HP C18 (50 mm × 2.1 mm I.D., 3 µm, P/N: 227-30039-02) | Ionization: | ESI (Negative mode) |
| | | Mode: | MRM |
| Solvent Delay Column: | Shim-pack GIST C18 (50 mm × 2.1 mm I.D., 5 µm, P/N: 227-30015-03) | Probe Voltage: | -1 kV |
| | | Nebulizing Gas: | 3 L/min |
| Mobile Phase A: | 2 mM Ammonium Acetate in 5 % (v/v) Acetonitrile in reagent water | Drying Gas Flow: | 5 L/min |
| | | Heating Gas Flow: | 15 L/min |
| Mobile Phase B: | Acetonitrile | DL Temp.: | 200 °C |
| Gradient Program: | B 5 % – 22 % (2.3 – 5.8 min) – 50 % (8.5 – 10.5 min) – 75 % (12.0 – 13.0 min) – 80 % (13.5 min) – 95 % (13.51 – 16.5 min) – 5 % (16.51 – 20.00 min) | Block Heater Temp.: | 300 °C |
| | | Interface Temp.: | 190 °C |
| | | Probe Position: | +1 mm |
| Flowrate: | 0.4 mL/min | MRM Transition: | Refer to Table 3 |
| Column Temp.: | 40 °C | | |
| Injection Volume : | 2 µL | | |
| Run Time: | 20 min | | |

## ■ Measuring Standard Solutions

The standard solutions that were prepared with CS1 to CS7 concentrations are listed in Table 3 (The equivalent concentrations in water sample). The successive five injections were made per concentration. The MRM chromatograms for CS1 of the 40 target PFAS compounds are shown in Fig. 3, and the CS1 and CS3 area repeatability values are shown in Fig. 4. For CS1, the repeatability was less than 20 % (%RSD of area values) for 87.5 % of the compounds. For CS3, the repeatability decreased to less than 10 % (%RSD of area values) for all compounds.

Note: The area values for target compounds were calculated as the total of both linear and branched-chain compounds.

In this case, calibration curve linearity was evaluated based on the accuracy (%RSD) of the response factor (RF) over the entire calibration curve, as specified in EPA Method 1633.[1)] RF values were calculated using Eq. 1, and the results are shown in Fig. 5. The RF accuracy (RF %RSD) values were less than 20 % for all of the 40 PFAS components, which is a good result. Furthermore, RF accuracy (RF %RSD) values were less than 10 % for 34 of the components.

$$RF = \frac{\text{Target Compound Area}}{\text{EIS Area}} \times \frac{\text{EIS Concentration Injected}}{\text{Target Compound Concentration Injected}}$$

Eq. 1 Formula for RF Calculation

Table 3-1 Quantitation Ion, Reference Ion and Concentrations of Standard Solutions (Target)

| No. | Compound | Sample Type | ISTD Group | Retention Time | Quantitation Ion *m/z* | Reference Ion *m/z* | Concentration (ng/L in water sample) | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 | CS7 |
| 1 | PFBA | Target | 1 | 2.024 | 213.00 > 169.00 | — | 0.8 | 2 | 5 | 10 | 20 | 50 | 250 |
| 2 | PFPeA | Target | 2 | 3.57 | 263.00 > 219.00 | 263.00 > 69.00 | 0.4 | 1 | 2.5 | 5 | 10 | 25 | 125 |
| 3 | PFHxA | Target | 3 | 4.906 | 312.95 > 269.00 | 312.95 > 119.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 4 | PFHpA | Target | 4 | 7.708 | 362.95 > 319.00 | 362.95 > 169.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 5 | PFOA | Target | 5 | 8.64 | 412.95 > 369.00 | 412.95 > 169.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 6 | PFNA | Target | 6 | 9.119 | 462.95 > 418.95 | 462.95 > 219.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 7 | PFDA | Target | 7 | 9.511 | 512.95 > 468.95 | 512.95 > 219.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 8 | PFUnA | Target | 8 | 9.901 | 562.95 > 518.95 | 562.95 > 269.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 9 | PFDoA | Target | 9 | 10.461 | 612.95 > 568.95 | 612.95 > 319.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 10 | PFTrDA | Target | Avg. of 9 and 10 | 11.345 | 662.95 > 618.95 | 662.95 > 168.90 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 11 | PFTeDA | Target | 10 | 12.237 | 712.95 > 668.95 | 712.95 > 168.90 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 12 | PFBS | Target | 11 | 4.841 | 298.95 > 79.95 | 298.95 > 98.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 13 | PFPeS | Target | 12 | 7.766 | 348.95 > 79.95 | 348.95 > 98.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 14 | PFHxS | Target | 12 | 8.776 | 398.95 > 79.95 | 398.95 > 98.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 15 | PFHpS | Target | 13 | 9.294 | 448.95 > 79.95 | 448.95 > 98.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 16 | PFOS | Target | 13 | 9.709 | 498.95 > 79.95 | 498.95 > 98.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 17 | PFNS | Target | 13 | 10.2 | 548.95 > 79.95 | 548.95 > 98.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 18 | PFDS | Target | 13 | 10.956 | 598.90 > 79.95 | 598.90 > 98.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 19 | PFDoS | Target | 13 | 12.524 | 698.90 > 79.95 | 698.90 > 98.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 20 | 4:2FTS | Target | 14 | 4.404 | 326.95 > 306.95 | 326.95 > 80.90 | 0.8 | 2 | 5 | 10 | 20 | 50 | 250 |
| 21 | 6:2FTS | Target | 15 | 8.398 | 426.95 > 406.95 | 426.95 > 80.90 | 0.8 | 2 | 5 | 10 | 20 | 50 | 250 |
| 22 | 8:2FTS | Target | 16 | 9.323 | 526.95 > 506.95 | 526.95 > 80.90 | 0.8 | 2 | 5 | 10 | 20 | 50 | 250 |
| 23 | PFOSA | Target | 17 | 11.438 | 497.95 > 77.95 | 497.95 > 477.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 24 | NMeFOSA | Target | 18 | 13.178 | 511.95 > 219.00 | 511.95 > 169.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 25 | NEtFOSA | Target | 19 | 13.475 | 526.00 > 219.00 | 526.00 > 169.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 26 | NMeFOSAA | Target | 20 | 9.491 | 569.95 > 418.95 | 569.95 > 482.95 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 27 | NEtFOSAA | Target | 21 | 9.647 | 584.00 > 418.95 | 584.00 > 526.00 | 0.2 | 0.5 | 1.25 | 2.5 | 5 | 12.5 | 62.5 |
| 28 | NMeFOSE | Target | 22 | 13.016 | 616.00 > 59.00 | — | 2 | 5 | 12.5 | 25 | 50 | 125 | 625 |
| 29 | NEtFOSE | Target | 23 | 13.305 | 630.00 > 59.00 | — | 2 | 5 | 12.5 | 25 | 50 | 125 | 625 |
| 30 | HFPO-DA | Target | 24 | 5.693 | 285.00 > 169.00 | 285.00 > 185.00 | 0.8 | 2 | 5 | 10 | 20 | 50 | 250 |
| 31 | ADONA | Target | 24 | 8.209 | 376.95 > 251.00 | 376.95 > 85.00 | 0.8 | 2 | 5 | 10 | 20 | 50 | 250 |
| 32 | 9Cl-PF3ONS | Target | 24 | 10.032 | 530.90 > 350.95 | 532.90 > 352.95 | 0.8 | 2 | 5 | 10 | 20 | 50 | 250 |
| 33 | 11Cl-PF3OUdS | Target | 24 | 11.728 | 630.90 > 450.95 | 632.90 > 452.95 | 0.8 | 2 | 5 | 10 | 20 | 50 | 250 |
| 34 | 3:3 FTCA | Target | 2 | 2.937 | 241.00 > 177.00 | 241.00 > 117.00 | 1 | 2.5 | 6.25 | 12.5 | 25 | 62.5 | 312.5 |
| 35 | 5:3 FTCA | Target | 3 | 6.076 | 341.00 > 237.00 | 341.00 > 217.00 | 5 | 12.5 | 31.25 | 62.5 | 125 | 312.5 | 1563 |
| 36 | 7:3 FTCA | Target | 3 | 8.952 | 441.00 > 317.00 | 441.00 > 337.00 | 5 | 12.5 | 31.25 | 62.5 | 125 | 312.5 | 1563 |
| 37 | PFEESA | Target | 3 | 5.943 | 314.95 > 135.00 | 314.95 > 82.95 | 0.4 | 1 | 2.5 | 5 | 10 | 25 | 125 |
| 38 | PFMPA | Target | 2 | 2.681 | 228.95 > 85.00 | — | 0.4 | 1 | 2.5 | 5 | 10 | 25 | 125 |
| 39 | PFMBA | Target | 2 | 3.916 | 278.95 > 85.00 | — | 0.4 | 1 | 2.5 | 5 | 10 | 25 | 125 |
| 40 | NFDHA | Target | 3 | 4.715 | 294.95 > 201.00 | 294.95 > 85.00 | 0.4 | 1 | 2.5 | 5 | 10 | 25 | 125 |

Table 3-2 Quantitation Ion, Reference Ion and Concentrations of Standard Solutions (IS)

| No. | Compound | Sample Type | ISTD Group | Retention Time | Quantitation Ion *m/z* | Reference Ion *m/z* | Concentration (ng/L in water sample) | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 | CS7 |
| 41 | 13C4-PFBA | EIS | 1 | 2.025 | 217.00 > 172.00 | 217.00 > 172.00 | 80 | 80 | 80 | 80 | 80 | 80 | 80 |
| 42 | 13C5-PFPeA | EIS | 2 | 3.568 | 268.00 > 223.00 | 268.00 > 223.00 | 40 | 40 | 40 | 40 | 40 | 40 | 40 |
| 43 | 13C5-PFHxA | EIS | 3 | 4.904 | 318.00 > 273.00 | 318.00 > 120.00 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 44 | 13C4-PFHpA | EIS | 4 | 7.707 | 367.00 > 322.00 | 367.00 > 322.00 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 45 | 13C8-PFOA | EIS | 5 | 8.64 | 421.00 > 376.00 | 421.00 > 376.00 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 46 | 13C9-PFNA | EIS | 6 | 9.119 | 472.00 > 427.00 | 472.00 > 427.00 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 47 | 13C6-PFDA | EIS | 7 | 9.51 | 519.00 > 474.00 | 519.00 > 474.00 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 48 | 13C7-PFUnA | EIS | 8 | 9.899 | 570.00 > 525.00 | 570.00 > 525.00 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 49 | 13C2-PFDoA | EIS | 9 | 10.458 | 615.00 > 569.95 | 615.00 > 569.95 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 50 | 13C2-PFTeDA | EIS | 10 | 12.236 | 714.95 > 669.95 | 714.95 > 669.95 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 51 | 13C3-PFBS | EIS | 11 | 4.835 | 301.95 > 79.95 | 301.95 > 98.95 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 52 | 13C3-PFHxS | EIS | 12 | 8.775 | 401.95 > 79.95 | 401.95 > 98.95 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 53 | 13C8-PFOS | EIS | 13 | 9.71 | 506.95 > 79.95 | 506.95 > 98.90 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 54 | 13C2-4:2FTS | EIS | 14 | 4.405 | 329.00 > 308.95 | 329.00 > 80.90 | 40 | 40 | 40 | 40 | 40 | 40 | 40 |
| 55 | 13C2-6:2FTS | EIS | 15 | 8.397 | 428.95 > 408.95 | 428.95 > 80.90 | 40 | 40 | 40 | 40 | 40 | 40 | 40 |
| 56 | 13C2-8:2FTS | EIS | 16 | 9.323 | 528.95 > 508.95 | 528.95 > 80.90 | 40 | 40 | 40 | 40 | 40 | 40 | 40 |
| 57 | 13C8-PFOSA | EIS | 17 | 11.438 | 505.95 > 77.95 | 505.95 > 77.95 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 58 | D3-NMeFOSA | EIS | 18 | 13.174 | 515.00 > 219.00 | 515.00 > 168.90 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 59 | D5-NEtFOSA | EIS | 19 | 13.467 | 531.00 > 219.00 | 531.00 > 168.90 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 60 | D3-NMeFOSAA | EIS | 20 | 9.489 | 573.00 > 418.95 | 573.00 > 418.95 | 40 | 40 | 40 | 40 | 40 | 40 | 40 |
| 61 | D5-NEtFOSAA | EIS | 21 | 9.645 | 589.00 > 418.95 | 589.00 > 418.95 | 40 | 40 | 40 | 40 | 40 | 40 | 40 |
| 62 | D7-NMeFOSE | EIS | 22 | 12.997 | 623.05 > 59.00 | 623.05 > 59.00 | 200 | 200 | 200 | 200 | 200 | 200 | 200 |
| 63 | D9-NEtFOSE | EIS | 23 | 13.282 | 639.10 > 59.00 | 639.10 > 59.00 | 200 | 200 | 200 | 200 | 200 | 200 | 200 |
| 64 | 13C3-HFPO-DA | EIS | 24 | 5.688 | 287.00 > 169.00 | 287.00 > 185.00 | 80 | 80 | 80 | 80 | 80 | 80 | 80 |

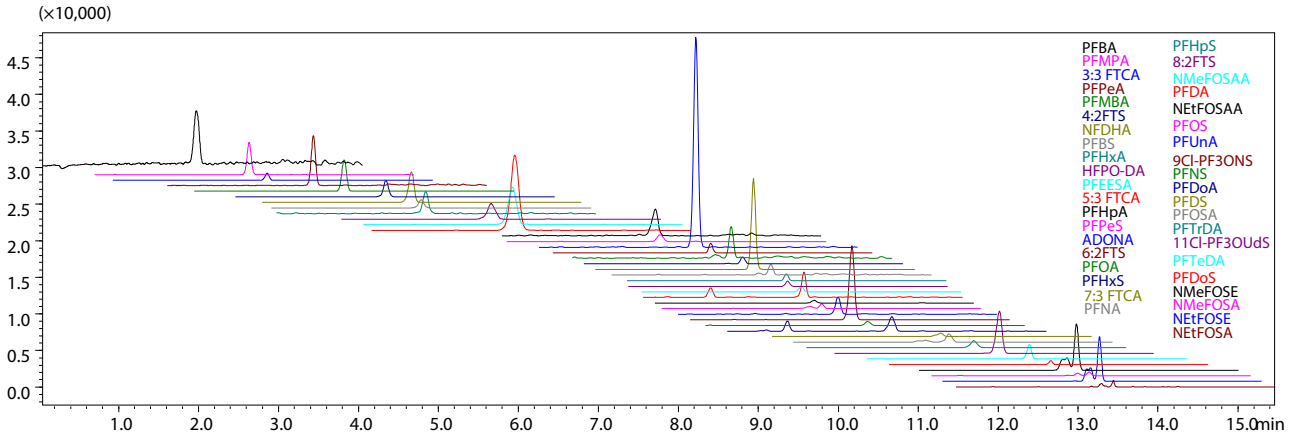


Fig. 3 MRM Chromatogram of PFAS (Target) at CS1


Fig. 4 CS1 and CS3 Area Repeatability (n = 5)

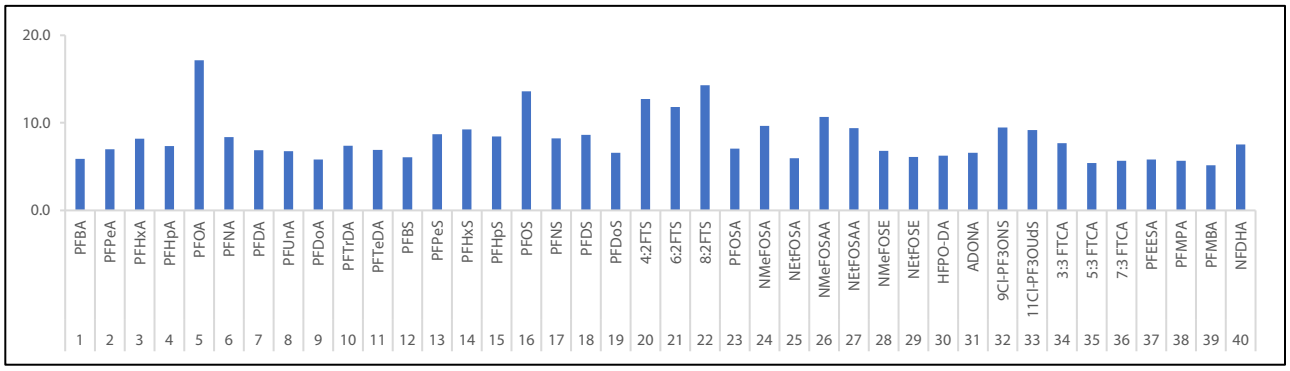


Fig. 5 RF Accuracy for CS1 to CS7 (n = 5 of Each Concentration)

## ■ Recovery Test

Target compounds were spiked to the drinking water samples to prepare the respective concentrations. These are shown in Table 4 and are marked as "High" and "Low." Next, the samples were pretreated according to the process in Fig. 2. The quantitation values for PFAS in samples were calculated from Eq. 2. The RF values calculated from Eq. 1 were used for it. As shown in Table 4, for samples with low spike concentrations, recovery rates ranged from 70 to 130 % for 90 % of the compounds, and repeatability was less than 20 %RSD for 95 % of the compounds. For samples with high spike concentrations, recovery rates ranged from 70 to 130 % for 97.5 % of the compounds, and repeatability was less than 13 %RSD for all compounds. These were good results, and they confirmed that drinking water samples can be analyzed accurately.

## ■ Conclusion

LCMS-8050RX provided ample sensitivity for analyzing 40 PFAS components at less than 1/10 of the final maximum contaminant levels (final MCLs) that are specified by the EPA (4 ng/L PFOA, 4 ng/L PFOS, 10 ng/L PFHxS, 10 ng/L PFNA, and 10 ng/L HFPO-DA).

Good recovery rates and reproducibility results were achieved even when evaluating recoveries with 1/4 of the final MCL concentrations.

The above results demonstrate that LCMS-8050RX can be used to simultaneously and accurately analyze 40 PFAS components in drinking water samples.

$$\text{Conc.}\left(\mathrm{ng/L}\right)=\frac{\text{Area of Target Compounds in Sample}}{\text{EIS Area}}\times\frac{\text{EIS Concentration Injected}}{\text{Avg. RF for Standard Solution}}$$

Eq. 2 Formula for Calculating PFAS Quantitation Values in Sample

Table 4 Recovery Test Results

| No. | Compound | Low (n = 3) | | | | High (n = 3) | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | Spiked Concentration (ng/L) | Avg. Concentration (ng/L) | Avg. Recovery Rate (%) | Repeatability (%) | Spiked Concentration (ng/L) | Avg. Concentration (ng/L) | Avg. Recovery Rate (%) | Repeatability (%) |
| 1 | PFBA | 4 | 5.2 | 130 | 0.7 | 20 | 18.9 | 95 | 0.8 |
| 2 | PFPeA | 2 | 2.2 | 112 | 3.4 | 10 | 10.0 | 100 | 1.5 |
| 3 | PFHxA | 1 | 1.2 | 121 | 6.5 | 5 | 4.7 | 93 | 3.7 |
| 4 | PFHpA | 1 | 1.2 | 124 | 2.6 | 5 | 5.1 | 102 | 3.3 |
| 5 | PFOA | 1 | 1.1 | 113 | 9.3 | 5 | 4.7 | 95 | 4.5 |
| 6 | PFNA | 1 | 1.3 | 132 | 5.2 | 5 | 5.2 | 105 | 5.8 |
| 7 | PFDA | 1 | 1.3 | 126 | 6.7 | 5 | 5.4 | 107 | 3.0 |
| 8 | PFUnA | 1 | 1.1 | 107 | 4.9 | 5 | 4.7 | 94 | 0.9 |
| 9 | PFDoA | 1 | 1.2 | 115 | 2.8 | 5 | 4.7 | 94 | 6.2 |
| 10 | PFTrDA | 1 | 1.0 | 103 | 5.9 | 5 | 4.8 | 96 | 1.5 |
| 11 | PFTeDA | 1 | 1.0 | 100 | 4.7 | 5 | 4.7 | 94 | 4.4 |
| 12 | PFBS | 1 | 1.2 | 122 | 12.1 | 5 | 5.3 | 106 | 3.7 |
| 13 | PFPeS | 1 | 0.8 | 82 | 6.6 | 5 | 3.6 | 73 | 4.5 |
| 14 | PFHxS | 1 | 0.9 | 90 | 10.4 | 5 | 4.2 | 85 | 3.5 |
| 15 | PFHpS | 1 | 1.0 | 100 | 6.2 | 5 | 4.6 | 93 | 2.6 |
| 16 | PFOS | 1 | 1.4 | 140 | 16.0 | 5 | 4.4 | 88 | 1.5 |
| 17 | PFNS | 1 | 0.8 | 80 | 20.8 | 5 | 3.9 | 78 | 5.3 |
| 18 | PFDS | 1 | 0.7 | 74 | 9.7 | 5 | 3.5 | 70 | 5.6 |
| 19 | PFDoS | 1 | 0.7 | 69 | 7.5 | 5 | 2.8 | 57 | 2.7 |
| 20 | 4:2FTS | 4 | 4.5 | 113 | 5.3 | 20 | 20.2 | 101 | 0.7 |
| 21 | 6:2FTS | 4 | 4.9 | 124 | 8.2 | 20 | 20.3 | 102 | 1.2 |
| 22 | 8:2FTS | 4 | 4.3 | 107 | 13.8 | 20 | 19.5 | 97 | 5.8 |
| 23 | PFOSA | 1 | 1.2 | 120 | 9.1 | 5 | 4.9 | 98 | 4.1 |
| 24 | NMeFOSA | 1 | 1.2 | 120 | 6.0 | 5 | 5.4 | 108 | 11.0 |
| 25 | NEtFOSA | 1 | 1.0 | 97 | 7.5 | 5 | 5.0 | 101 | 3.1 |
| 26 | NMeFOSAA | 1 | 1.1 | 112 | 1.9 | 5 | 5.1 | 103 | 6.0 |
| 27 | NEtFOSAA | 1 | 1.0 | 98 | 24.4 | 5 | 5.4 | 108 | 12.2 |
| 28 | NMeFOSE | 10 | 11.0 | 110 | 5.8 | 50 | 48.5 | 97 | 1.2 |
| 29 | NEtFOSE | 10 | 11.1 | 111 | 1.3 | 50 | 48.1 | 96 | 1.8 |
| 30 | HFPO-DA | 4 | 4.5 | 112 | 4.8 | 20 | 22.0 | 110 | 0.6 |
| 31 | ADONA | 4 | 4.8 | 121 | 2.3 | 20 | 21.5 | 107 | 1.0 |
| 32 | 9Cl-PF3ONS | 4 | 4.9 | 123 | 1.0 | 20 | 22.0 | 110 | 1.6 |
| 33 | 11Cl-PF3OUdS | 4 | 3.8 | 94 | 6.8 | 20 | 15.7 | 79 | 3.9 |
| 34 | 3:3 FTCA | 5 | 5.0 | 101 | 7.3 | 25 | 23.2 | 93 | 3.2 |
| 35 | 5:3 FTCA | 25 | 21.8 | 87 | 4.0 | 125 | 90.1 | 72 | 3.2 |
| 36 | 7:3 FTCA | 25 | 20.1 | 80 | 3.4 | 125 | 87.4 | 70 | 1.8 |
| 37 | PFEESA | 2 | 2.2 | 111 | 1.2 | 10 | 9.7 | 97 | 2.6 |
| 38 | PFMPA | 2 | 2.5 | 123 | 2.2 | 10 | 10.6 | 106 | 0.6 |
| 39 | PFMBA | 2 | 2.0 | 100 | 3.2 | 10 | 8.8 | 88 | 1.3 |
| 40 | NFDHA | 2 | 2.5 | 124 | 1.0 | 10 | 10.6 | 106 | 1.1 |

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**Reference**

1) EPA Method 1633
Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous, Solid, Biosolids, and Tissue Samples by LC-MS/MS
https://www.epa.gov/system/files/documents/2024-01/method-1633-final-for-web-posting.pdf

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