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LCMS-2050 Liquid Chromatograph Mass Spectrometer

Application News

Analysis of 28 Common PFAS Compounds using the Compact Single Quadrupole LCMS-2050

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User Benefits

- Can quantitatively acquire LCMS data of individual PFAS compounds with a straightforward workflow.
- Sensitive analysis of PFAS targets detected down to 0.5 ng/mL.
- Fast and accurate separation with a compact, single quadrupole detector — the Shimadzu LCMS-2050.
- Simultaneous analysis in SIM and scan modes allows monitoring of suspected degradation or transformation products.

■ Introduction

The growing concern of per- and polyfluoroalkyl substances (PFAS) in the environment has driven the need for quick, inexpensive measurement of PFAS for evaluating PFAS removal by novel treatment technologies, monitoring of remediation projects, or added capability to detect emerging contaminants. Most PFAS applications require the sensitivity and specificity of the triple quadrupole mass spectrometer; however, this presents significantly higher maintenance costs in a much larger laboratory footprint. The compact, affordable LCMS-2050 single quadrupole mass spectrometer can be easily integrated into existing laboratories for measurement of PFAS in diverse samples where adherence to regulated methods (e.g., EPA 533, 537.1, and 1633) is not required, or samples where expected concentrations are larger than sub ppb levels.

■ Methods

The 28 PFAS standards were purchased through Wellington Laboratories using two mixes (PFAC-MXJ and PFAC-MXH) at concentrations ranging from 1 to 20 µg/mL. The standards were further diluted in 50:50 methanol:water with 0.1% acetic acid to create the calibration curve standards. The calibration standards were acidified because previous studies have shown that it helps maintain better peak shape for PFAS analysis. A C18 column was used for the chromatographic separation, and the LCMS-2050 interface parameters were optimized accordingly (Table 1). The Shimadzu Nexera™ LC and the LCMS-2050 were set up for PFAS analysis using a delay column (Figure 1). The delay column was critically important for the prevention of native PFAS in the mobile phases and the system from interfering with the sample analysis.

A DUIS™ ionization source, which is the default ionization source for the LCMS-2050 that combines ESI and APCI techniques, was used for the analysis. A scan event with a *m/z* range of 50 - 750 was set up to monitor the standards. In the same acquisition, selected ion monitoring (SIM) channels were also set up for each PFAS analyte for the ease of quantitation. The Shimadzu LabSolutions™ software was used to automatically generate the *m/z* ions based on the chemical formula in the acquisition method. All listed PFAS analytes were measured using the [M-H]- ion based on the chemical formula (Table 2).

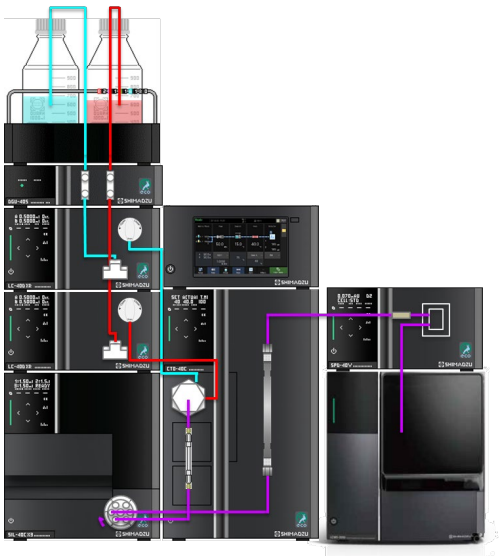

Fig. 1 The delay column setup in the system for PFAS analysis

Table 1. Nexera LC and LCMS-2050 parameters for PFAS analysis

System	: Nexera X3
Delay column	: Shim-pack™ GIST C18 (50 mm × 3.0 mm I.D., 5 µm)*1
Analytical column	: Shim-pack Velox™ SP-C18 (50 mm × 2.1 mm I.D., 2.7 µm)*2
Temperature	: 40 ˚C
Injection volume	: 1 µL
Mobile phases	: A: 5 mM ammonium acetate in Water B: Methanol
Flow rate	: 0.4 ml/min
Time program (%B)	: 2 % (0 min) → 20 % (0.21 min) → 55 % (7 min) → 75 % (12 min) → 98 % (13-14 min) → 2 % (14.1-18 min)
System	: LCMS-2050 (DUIS Negative)
Nebulizing gas	: 2 L/min
Drying gas	: 5 L/min
Heating gas	: 7 L/min
DL temp	: 300 ˚C
Heat block temp	: 250 ˚C
Interface temp	: 400 ˚C
Scan range	: *m/z* 50-750
SIM events	: 28

*1 P/N：227-30015-03
*2 P/N : 227-32003-02

■ Results and Discussion

The compact, single quadrupole LCMS-2050 was used to separate and quantify 28 commonly studied PFAS in neat standards (see **Table 2**). The limits of quantitation (LOQ) were in the low ng/mL concentration range with %accuracy between 80 – 120% and %RSD area < 12%. Representative LOQ chromatograms of each analyte are shown in **Figure 3**. This result showcased the ability of a compact LCMS system for PFAS quantitation with a user-friendly software interface for optimization and data analysis. The inclusion of the scan event did not hinder the separation and quantitation of the PFAS, which demonstrates the additional benefit of scanning for degradation products and obtaining additional mass information which can only be achieved by a mass spectrometer.

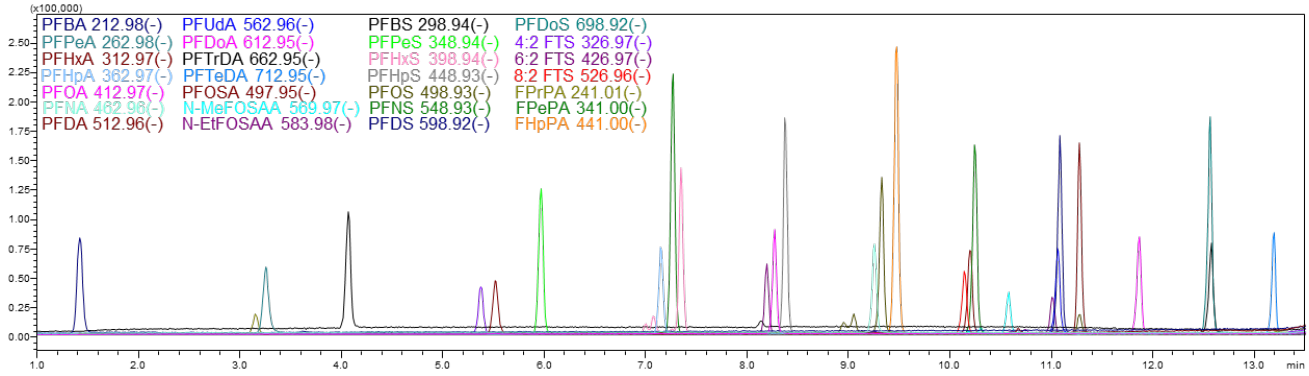

Fig. 2 Representative chromatogram of the 28 PFAS analytes at the highest calibration standard (20 to 200 ng/mL) by SIM acquisition.

Table 2. Calibration curve of the 28 PFAS measured using the C18 column (n=4). All analytes were measured in negative mode using SIM. LOQ defined as the low end of the linear range with S/N>10.

PFAS	$[M-H]^-$	Linear Range (ng/mL)	R^2	Accuracy (%)	LOQ %RSD (Area)
PFBA	212.98	2.0 - 80	0.998	85.5 - 108.6	7.5
PFPeA	262.98	1.0 - 40	0.999	88.0 - 109.3	2.1
PFHxA	312.97	0.5 - 20	0.999	90.2 - 107.6	6.6
PFHpA	362.97	0.5 - 20	0.999	84.0 - 115.1	6.9
PFOA	412.97	0.5 - 20	0.999	85.5 - 111.2	7.7
PFNA	462.96	0.5 - 20	0.999	87.8 - 111.1	3.4
PFDA	512.96	0.5 - 20	0.999	86.1 - 108.5	4.3
PFUdA	562.96	0.5 - 20	0.999	85.0 - 109.6	7.6
PFDoA	612.95	0.5 - 20	0.999	91.4 - 113.0	2.2
PFTrDA	662.95	0.5 - 20	0.999	86.3 - 111.7	8.4
PFTeDA	712.95	0.5 - 20	0.999	86.6 - 112.3	7.7
PFOSA	497.95	0.2 - 20	0.999	87.3 - 114.2	7.5
N-MeFOSAA	569.97	1.0 - 20	0.998	81.9 - 116.0	3.2
N-EtFOSAA	583.98	1.0 - 20	0.999	90.4 - 113.4	5.6
PFBS	298.94	0.5 - 20	0.999	89.0 - 112.6	6.0
PFPeS	348.94	0.2 - 20	0.999	85.7 - 109.1	8.1
PFHxS	398.94	0.2 - 20	0.999	84.6 - 109.3	6.5
PFHpS	448.93	0.1 - 20	0.999	82.0 - 113.1	5.7
PFOS	498.93	0.5 - 20	0.999	87.0 - 115.7	8.1
PFNS	548.93	0.2 - 20	0.999	85.5 - 111.2	4.7
PFDS	598.92	0.2 - 20	0.999	82.5 - 115.1	4.8
PFDoS	698.92	0.2 - 20	0.999	81.1 - 109.8	5.4
4:2 FTS	326.97	2.0 - 80	0.999	85.9 - 111.6	2.6
6:2 FTS	426.97	2.0 - 80	0.994	90.0 - 119.0	3.3
8:2 FTS	526.96	2.0 - 80	0.999	81.5 - 116.0	5.9
FPrPA	241.01	2.0 - 40	0.999	88.2 - 111.3	8.8
FPePA	341.00	1.0 - 200	0.999	83.3 - 112.4	8.9
FHpPA	441.00	1.0 - 200	0.999	86.5 - 114.5	4.8

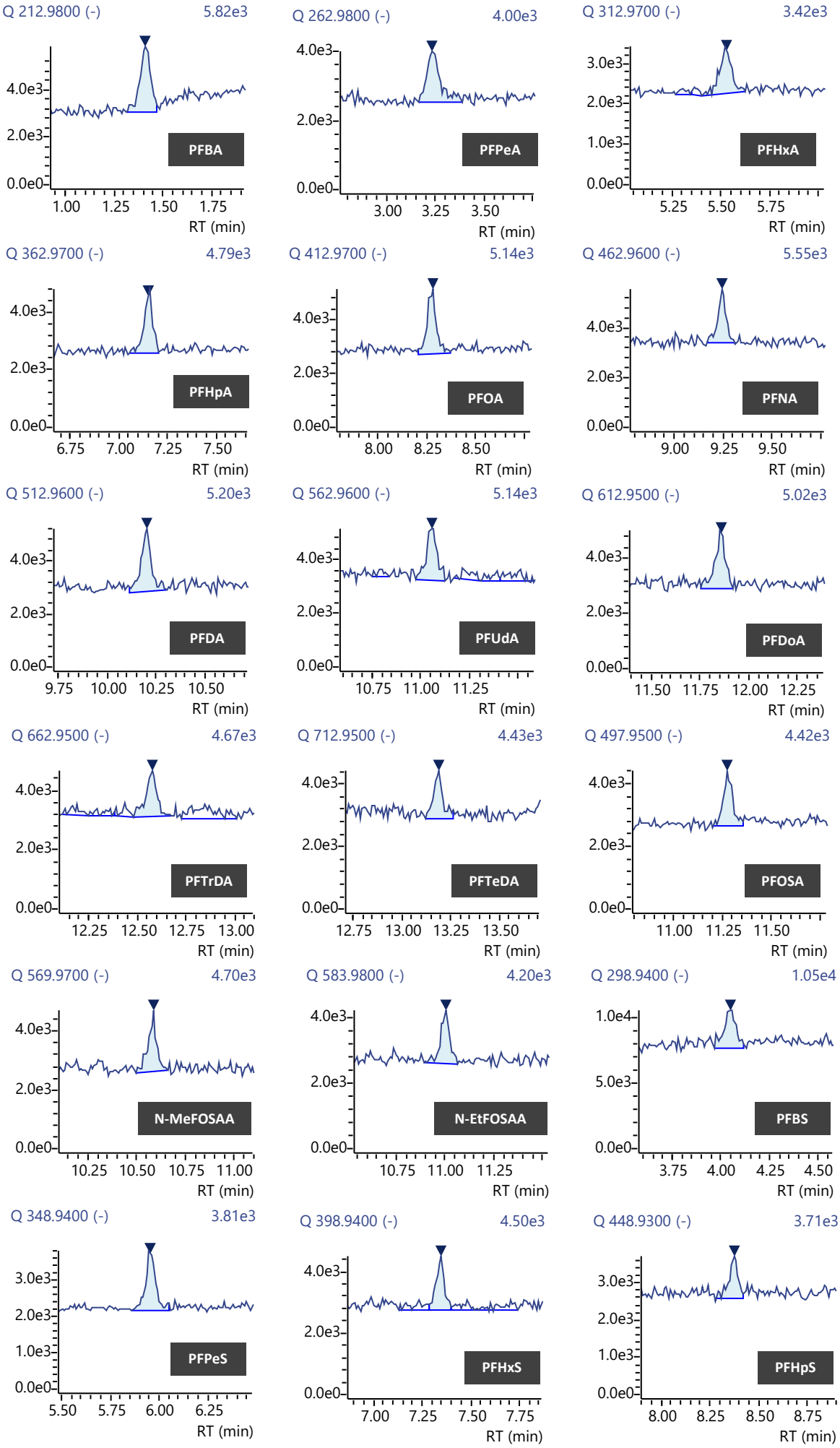

Fig. 3 Representative chromatogram at LOQ for each PFAS standard. See Table 2 for LOQs.

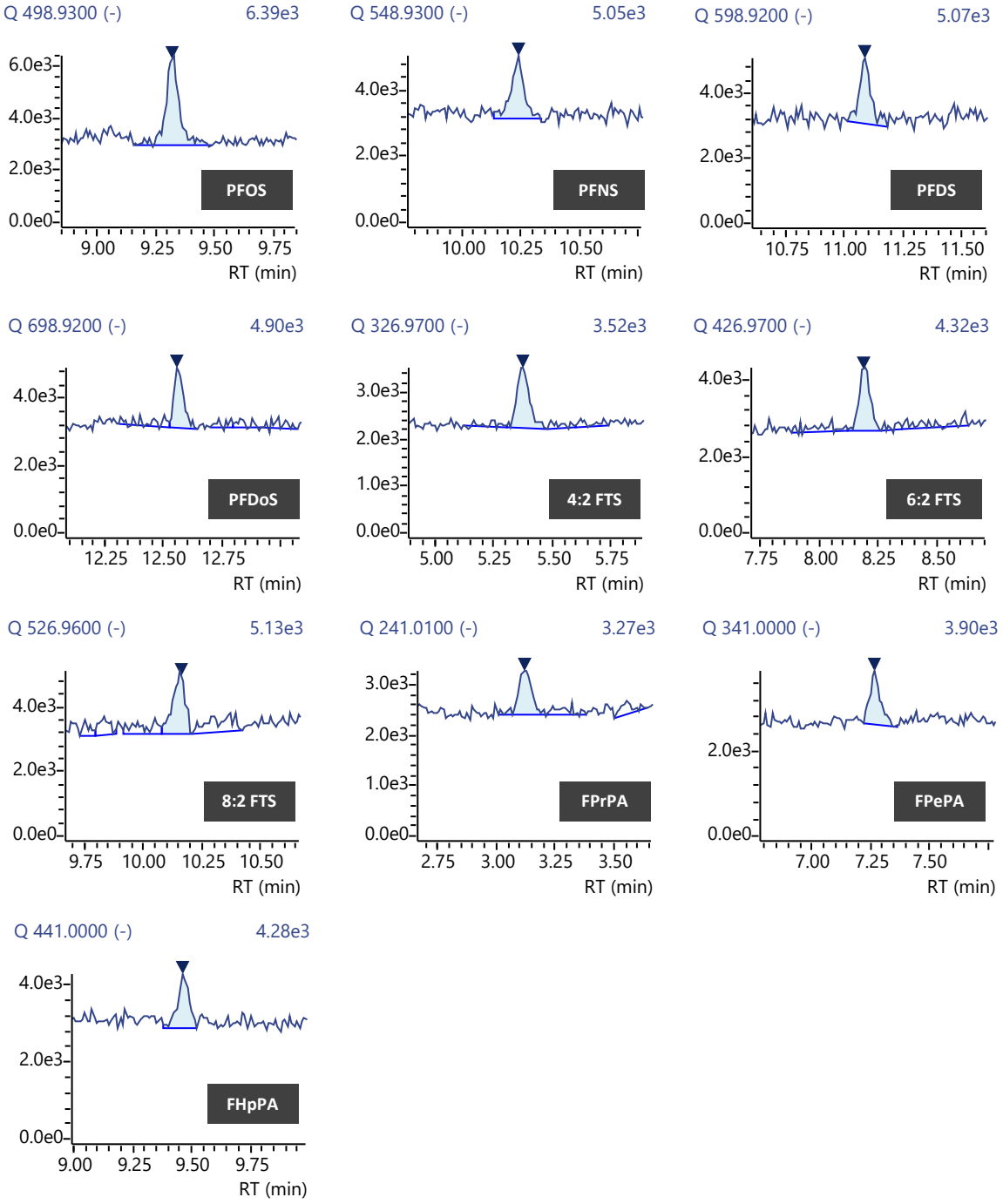

Fig. 3 (continued) Representative chromatogram at LOQ for each PFAS standard. See Table 2 for LOQs.

■ Conclusion

The Shimadzu LCMS-2050 compact single quadrupole mass spectrometer was successfully employed for the accurate separation and quantitation of 28 commonly studied PFAS. These results demonstrate the accessible, effective, and cost-effective Shimadzu LCMS-2050 for measuring PFAS for applications such as determining PFAS removal by current and novel treatment technologies.

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