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Application News

High Performance Liquid Chromatograph Mass Spectrometer

An Ultra-high Sensitivity Analysis of 29 PFAS Compounds in Drinking Water by Direct Injection

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User Benefits

- The LCMS-8065XE enables highly sensitive and accurate analysis of 29 PFAS down to less than 1 ng/L.
- 29 PFAS can be analyzed in one cycle in 18 minutes without sample preconcentration.
- Good recovery of target PFAS is achieved in drinking water, enabling highly accurate quantification analysis.

■ Introduction

PFAS (Per- and Polyfluoroalkyl Substances) are synthetic fluorinated organic compounds. More than a few thousand compounds exist, each with a varied carbon chain length, functional groups, and structural isomers. Because of its useful qualities, such as their ability to repel water and their non-stickiness, PFAS are found in a wide range of consumer and industrial products, including firefighting foams and coatings. Their high stability and persistence raise concerns about their impact on human health and the environment. In recent years, regulations and studies regarding PFAS have been increasing globally. For example, the U.S. Environmental Protection Agency (EPA) has set a Maximum Contaminant Level (MCL) of 4 ng/L for PFOA and PFOS in drinking water. To improve the analysis of PFAS, more sensitive, accurate and faster methods are needed. This application introduces the ultra-high sensitivity analysis of 29 PFAS in drinking water by direct injection using the LCMS-8065XE (Fig. 1) and addresses the demands of testing laboratories for PFAS quantification.

Fig. 1 LCMS-8065XE

■ Analytical conditions

The HPLC and MS analytical conditions are shown in Table 1 and 2. The test compounds used were the 29 compounds included in methods EPA 533 and 537.1 for drinking water analysis. The LCMS-8065XE is equipped with a new ESI probe (StreamFocus) and a new collision cell (UFsweeper™ IV), providing more sensitive and accurate results in PFAS analysis. A delay column was installed between the mixer and autosampler to separate PFAS from the HPLC system and those in the sample. To ease the analysis, same type of column is used as delay and analytical columns.

Table 1 HPLC conditions

[HPLC conditions] (Nexera™ X3)	
Analytical column	: Shim-pack Scepter™ C18-120 *1 (50 mm x 3 mm I.D., 1.9 µm)
Delay column	: Shim-pack Scepter C18-120 *1 (50 mm x 3 mm I.D., 1.9 µm)
Mobile phases	: A) 2 mmol/L $AcONH_4$ in H_2O
	B) Methanol
Measurement time	: 18 min
Oven temperature	: 40 ˚C
Injection volume	: 20 µL

*1 P/N: 227-31013-01

Table 2 MS conditions

[MS conditions] (LCMS-8065XE)	
Ionization	: ESI (Negative)
Interface voltage	: -0.2 kV
Focus voltage	: 0 kV
Nebulizing gas flow	: 1.1 L/min
Drying gas flow	: 5 L/min
Heating gas flow	: 15 L/min
Interface temperature	: 200 ˚C
DL temp.	: 200 ˚C
Heat Block temperature	: 200 ˚C
MRM transitions	(refer to Table 3)

Table 3 MRM transitions

	Compound name	MRM transitions	Polarity
1	PFBA	213.00>169.00	—
2	PFPeA	263.00>219.00	—
3	PFHxA	312.95>269.00	—
4	PFHpA	362.95>319.00	—
5	PFOA	412.95>369.00	—
6	PFNA	462.95>418.95	—
7	PFDA	512.95>468.95	—
8	PFUnA	562.95>518.95	—
9	PFDoA	612.95>568.95	—
10	PFTrDA	662.95>618.95	—
11	PFTeDA	712.95>668.95	—
12	PFBS	298.95>79.95	—
13	PFPeS	348.95>79.95	—
14	PFHxS	398.95>79.95	—
15	PFHpS	448.95>79.95	—
16	PFOS	498.95>79.95	—
17	4:2FTS	326.95>306.95	—
18	6:2FTS	426.95>406.95	—
19	8:2FTS	526.95>506.95	—
20	NMeFOSAA	569.95>418.95	—
21	NEtFOSAA	584.00>418.95	—
22	HFPO-DA	285.00>169.00	—
23	ADONA	376.95>251.00	—
24	9Cl-PF3ONS	530.90>350.05	—
25	11Cl-PF3ONS	630.90>450.95	—
26	PFEESA	314.95>135.00	—
27	PFMPA	228.95>85.00	—
28	PFMBA	278.95>85.00	—
29	NFDHA	294.95>201.00	—

■ Sample preparation

The samples were prepared in H_2O/MeOH (50/50, v/v) without time consuming pretreatment such as solid-phase extraction. Internal standards were added to the samples to a concentration of 10 ng/L (20–40 ng/L for some compounds).

■ Method detection limit (MDL)

A PFAS mixed standard sample was prepared at a concentration of 1 ng/L. Seven replicates were analyzed and the MDLs were calculated. As summarized in Fig. 2, the MDLs for different classes of PFAS in the method, including carboxylic and sulfonic acids, ethers (carboxylic and sulfonic acids), FTSs, FOSAs, and FOSAAs, are less than 1 ng/L without the need of sample preconcentration.

The MDLs for PFOA and PFOS were 0.48 ng/L and 0.45 ng/L, respectively, an order of magnitude lower than the MCL and required by EPA. These MDLs are suitable to address the PFAS testing needs within the countries in the European Union and under the Water Framework Directive, where local limits are under development and the strictest being <1 ng/L.

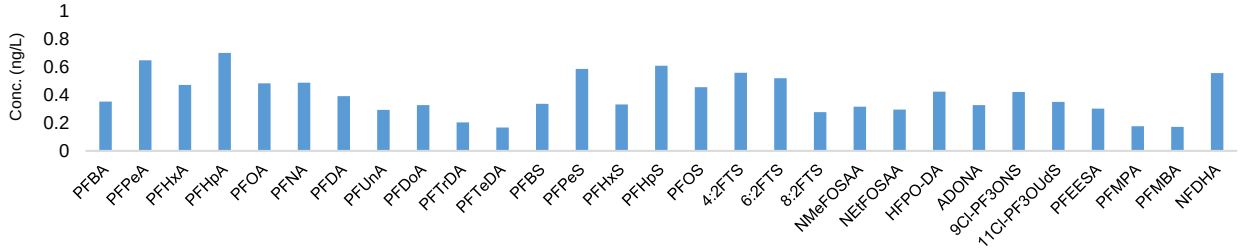

Fig. 2 MDL (99% confidence interval) of the target compound

■ Calibration curve and MRM chromatogram

A series PFAS mixed standard samples (7) were prepared so that the target compounds were in the range of 1-100 ng/L to create a calibration curve. As an example, Fig. 3 shows the calibration curves for PFOA and PFOS, as well as the MRM chromatogram at 1 ng/L, the lowest point of the calibration range.

The calibration curves showed good linearity for both PFOA and PFOS, with the accuracy of each calibration point being within the range of 80-120%. Furthermore, the accuracy of each calibration point for the other target compounds was within the range of 70-130%.

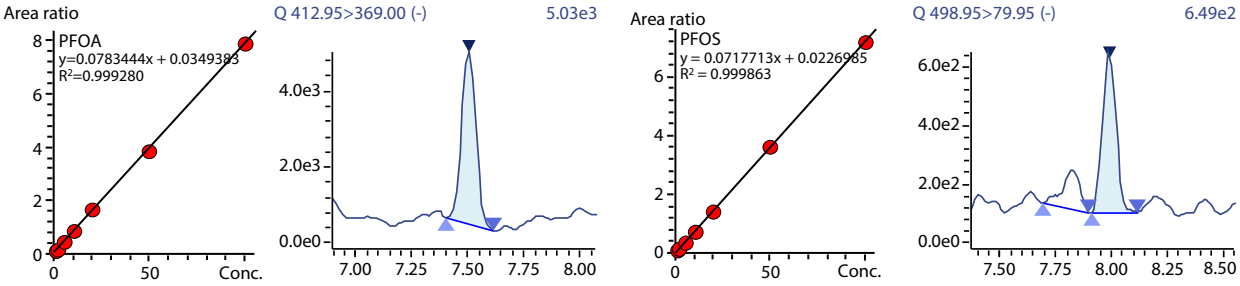

Fig. 3 Calibration curves and MRM chromatograms of PFOA（left) and PFOS（right）

■ Recovery test in drinking water

Following the method described above, the drinking water samples were diluted with MeOH (50/50, v/v) before analysis. The samples were fortified with a PFAS standard at a concentration of 4 ng/L of each compound. PFBA and PFHxA were quantified in the drinking water samples, recovery was calculated by subtracting the concentration detected in the drinking water. Fortified samples were analyzed 7 times. Each sample showed excellent recovery in the range of 80-120% for all tested compounds with reproducibility of within 20% (Fig. 4).

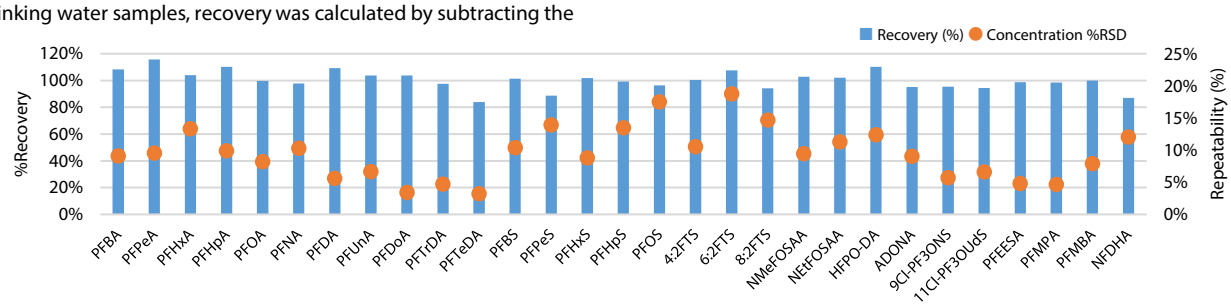

Fig. 4 Recovery and reproducibility of drinking water spiked with 4 ng/L (n=7)

■ Conclusion

- 29 of PFAS in drinking water were measured with high sensitivity (<1 ng/L) by direct injection method using the LCMS-8065XE.
- Good recovery and reproducibility were obtained in drinking water samples, confirming that this analytical method can deliver accurate quantification for PFASs in drinking water.

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