SHIMADZU
Excellence in Science

Liquid Chromatograph Mass Spectrometer LCMS-8060NX

Application News

Determination of various PFAS in drinking water using on-line SPE coupled to LC-MS/MS

Anja Grüning
Shimadzu Europa GmbH

User Benefits

- Single vendor solution for UHPLC and MS system
- Quantification of 44 PFAS in ng/L range using an on-line SPE approach
- All PFAS requested by the EU directive 2020/2184[1] on the quality of water intended for human consumption are covered

■ Introduction

Perfluoroalkyl and polyfluoroalkyl substances (PFAS) refer to a class of more than 4000 individual chemicals that have been widely used since the 1950s, e.g. as fire retardants, food packaging materials or non-stick coatings. These compounds offer heat-resistant, and oil- and water-repellant properties as well as chemical and thermal stability, resistance to UV light and weathering. Due to their anthropogenic origin, PFAS cannot be degraded, and hence they accumulate and can now be detected ubiquitously in the environment. Since drinking water is considered to be an important source of human PFAS intake, testing drinking water for PFAS levels has been essential for several years now.

This Application News demonstrates the determination of all PFAS requested in the EU directive 2020/2184[1] on the quality of water intended for human consumption in an appropriate concentration range. Furthermore, the analysis includes 24 additional PFAS and 22 internal standard using the same method based on an on-line SPE approach which omits additional sample preparation steps.

■ Materials and Methods

Fast, sensitive and robust LC-MS/MS systems provide the basis for routine analysis in drinking water laboratories. For the described application, a Shimadzu LCMS-8060NX triple-quadrupole mass spectrometer coupled with a Nexera™ X3 UHPLC system was used (Figure 1, Figure 3).

44 PFAS standards and one IS-mixture (ISO 21675-LSS) were purchased (Wellington Laboratories / neochema). Stock solutions of these PFAS were diluted with methanol and combined to a single standard mixture with a final a concentration of 1ng/µL for each compound. Further dilutions of this mixture were produced and spiked into Evian water to prepare calibration samples in drinking water in the concentration range from 0.5 ng/L to 100 ng/L. Bottled Evian water was chosen as dinking water matrix as no noticeable PFAS could be detected in the blank. All samples (except blanks) were spiked with IS to a final concentration of 20 ng/L.

No further sample preparation is required. 1 mL of sample is injected directly on a SPE-trap column.

Analysis was performed within 15 minutes using MRM acquisition with at least two transitions for each compound (except PFBA, PFMPA, PFMBA, HPFHpA where only one transition is available). Analytical conditions are listed in Table 1. The optimized MRM transitions are summarized in Table 2.

Since PFAS can be present in reagents, glassware, pipettes, tubing, degassers and other parts from the LC-MS/MS instrument, the use of a solvent delay column is necessary. Small C18 columns are placed between mixer and autosampler respectively between mixer and valve to delay possible PFAS contaminations and separate them from sample-derived PFAS.

To minimize adsorption of (especially long chain) PFAS to the surface LabTotal Vials (P/N 227-34001-01) with PP-caps, with aluminium septa (P/N 961-10030-31) were used.

Figure 1 LCMS-8060NX coupled to a Nexera™ X3 system

Table 1 Analytical conditions

Mass Spectrometer	: LCMS-8060NX
Ionization	: Electrospray Ionization (ESI), negative
Interface Voltage	: -1 kV
Focus Voltage	: -2 kV
Heating Gas	: 15 L/min
DL Temp.	: 150 ˚C
Interface Temp.	: 300 ˚C
Nebulizing Gas	: 3 L/min
Drying Gas	: 3 L/min
Heat Block	: 400 ˚C
Dwell-/Pause-time	: 4 (3 for IS) / 1 msec
CID	: 270 kPa
UHPLC	: Nexera X3
Pump A (Analytical)	: 2 mM ammonium acetate in H_2O
Pump B (Analytical)	: 10 mM ammonium acetate in Methanol
Pump C (Trap)	: H_2O + modifier (sample loading)
Pump D (Trap)	: Methanol (washing of SPE and delay column)
Analytical column	: Shim-pack™ Scepter 1.9 µm, C18-120, 2.1 x 50 mm
Delay column	: Shim-pack™ GIST HP 3 µm, C18-AQ, 3 x 30 mm
Trap column	: EVOLUTE® Express ABN on-line SPE cartridge
Injection Volume	: 1000 µL
Cooler temperature	: 15 ˚C
Column Oven	: 50 ˚C

■ Results

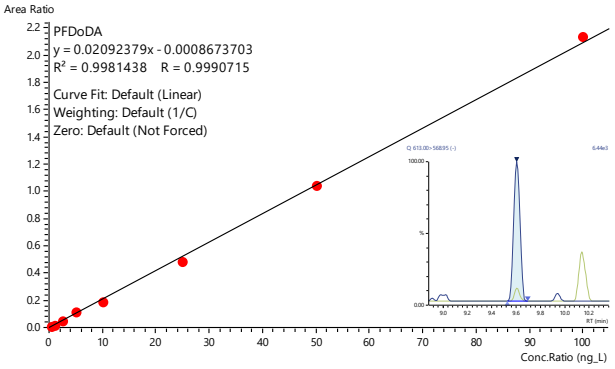
Calibration curves were calculated using weighted (1/conc) linear regression. The linearity ranges from 0.5 ng/L (resp. 1 or 2.5 ng/L) – 100 ng/L (50 ng/L for PFNS) with an R^2 of at least 0.99 for all PFAS. The lowest calibration point (0.5 ng/mL) can be determined in 77.3% of all PFAS (Table 2). Exemplary calibration curves and respective MRM-chromatograms at 1 ng/L are shown in Figure 2.

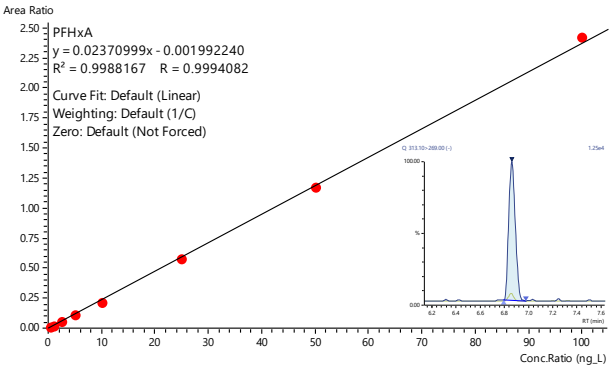
Two control samples at 5 ng/l and 25 ng/L were analyzed in three-fold to measure analytical reproducibility. The percentage relative standard deviation was typically lower than 20% (for >95% of the determined compounds resp. QCs) from these measurements (Table 3).

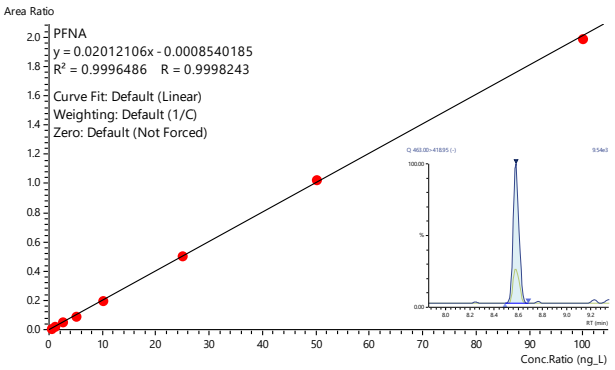
Table 2 MRM transitions and calibration information

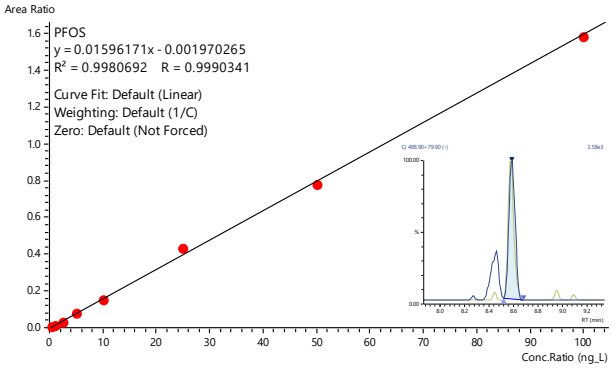
Acronym	Compound name	RT	Type	Quantifier	Qualifier	ISTD	Calibration range	Unit	R^2
10:2 FTS	1H,1H,2H,2H-perfluorododecane sulfonic acid	9.64	Target	627.00>607.00	627.00>80.90	PFDoDA-IS	1 - 100	ng_L	0.9953
11Cl-PF3OUdS	11-chloroeicosafluoro-3-oxaundecane-1-sulfonic acid	9.471	Target	630.90>451.05	630.90>82.95	PFDoDA-IS	0.5 - 100	ng_L	0.9958
3.7-DMPFOA	3,7-dimethylperfluorooctanoic acid	8.796	Target	469.00>269.00	469.00>219.05	PFNA-IS	0.5 - 100	ng_L	0.9975
4:2 FTS	1H, 1H, 2H, 2H-perfluorohexane sulfonic acid	6.806	Target	327.10>307.00	327.10>80.95	PFHxA-IS	0.5 - 100	ng_L	0.9995
6:2 FTS	1H, 1H, 2H, 2H-perfluorooctane sulfonic acid	8.112	Target	427.10>407.00	427.10>80.90	6:2 FTS-IS	0.5 - 100	ng_L	0.9994
6:2 FTS-IS		8.113	ISTD	428.90>408.90	428.90>80.95	----	----	ng_L	----
8:2 diPAP	8:2 Fluorotelomer phosphate diester	10.597	Target	989.10>543.15	989.10>96.95	8:2 diPAP-IS	2.5 - 100	ng_L	0.9914
8:2 diPAP-IS		10.596	ISTD	992.80>96.85	992.80>544.90	----	----	ng_L	----
8:2 FTS	1H, 1H, 2H, 2H-perfluorodecane sulfonic acid	8.996	Target	527.10>507.00	527.10>80.90	8:2 FTS-IS	1 - 100	ng_L	0.9989
8:2 FTS-IS		8.993	ISTD	529.00>508.95	529.00>80.95	----	----	ng_L	----
9Cl-PF3ONS	9-chlorohexadecafluoro-3-oxanone-1-sulfonic acid	8.826	Target	530.90>351.10	530.90>82.90	PFOS-IS	0.5 - 100	ng_L	0.9984
DONA	4,8-dioxa-3H-perfluorononanoic Acid	7.68	Target	377.10>251.00	377.10>84.95	PFHpA-IS	0.5 - 100	ng_L	0.9967
FOUEA/8:2 FTUCA	2H-perfluoro-2-decenoic acid	8.736	Target	457.10>393.20	457.10>343.05	FOUEA-IS	0.5 - 100	ng_L	0.9980
FOUEA-IS	2H,2H,3H,3H-perfluorundecanoic acid	8.735	ISTD	459.00>394.05	459.00>344.00	----	----	ng_L	----
H4PFUNA		9.133	Target	491.10>367.20	491.10>387.05	PFOS-IS	1 - 100	ng_L	0.9980
HPFHpA	7H-perfluorheptanoic acid	6.545	Target	345.10>281.00	----	PFHpA-IS	0.5 - 100	ng_L	0.9982
N-Et-FOSA	N-ethylperfluorooctanesulfonamide	10.167	Target	526.00>169.05	526.00>219.05	N-Et-FOSA-IS	0.5 - 100	ng_L	0.9995
N-Et-FOSAA	N-ethylperfluorooctanesulfonamidoacetic acid	9.345	Target	584.00>419.00	584.00>526.00	N-Et-FOSAA-IS	0.5 - 100	ng_L	0.9974
N-Et-FOSAA-IS		9.339	ISTD	589.00>419.10	589.00>530.90	----	----	ng_L	----
N-Et-FOSA-IS		10.163	ISTD	531.10>169.00	531.10>219.20	----	----	ng_L	----
NFDHA	Nonafluoro-3,6-dioxaheptanoic acid	6.75	Target	201.00>84.95	295.10>201.00	PFHxA-IS	0.5 - 100	ng_L	0.9980
N-Me-FOSA	N-methylperfluorooctanesulfonamide	9.976	Target	511.90>169.00	511.90>219.05	N-Me-FOSA-IS	0.5 - 100	ng_L	0.9956
N-Me-FOSAA	N-methylperfluorooctanesulfonamidoacetic acid	9.176	Target	569.90>418.95	569.90>512.15	N-Me-FOSAA-IS	0.5 - 100	ng_L	0.9973
N-Me-FOSAA-IS		9.168	ISTD	572.90>419.10	572.90>515.10	----	----	ng_L	----
N-Me-FOSA-IS		9.968	ISTD	515.00>169.00	515.00>219.00	----	----	ng_L	----
PEESA	Perfluoro(2-ethoxyethane)sulfonic acid	6.538	Target	315.00>135.00	315.00>82.90	PFHxA-IS	0.5 - 100	ng_L	0.9941
PFBA*	Perfluorobutanoic acid	4.759	Target	213.00>169.00	----	PFBA-IS	1 - 100	ng_L	0.9993
PFBA-IS		4.754	ISTD	216.90>172.00	----	----	----	ng_L	----
PFBS*	Perfluorobutane sulfonic acid	6.142	Target	299.00>79.90	299.00>98.90	PFBS-IS	0.5 - 100	ng_L	0.9996
PFBS-IS		6.139	ISTD	301.90>79.80	301.90>98.80	----	----	ng_L	----
PFDA*	Perfluorodecanoic acid	8.994	Target	513.00>469.00	513.00>219.05	PFDA-IS	0.5 - 100	ng_L	0.9975
PFDA-IS		8.997	ISTD	519.00>473.90	519.00>219.00	----	----	ng_L	----
PFDoA / PFDoDA*	Perfluorododecanoic acid	9.624	Target	613.00>568.95	613.00>169.10	PFDoDA-IS	0.5 - 100	ng_L	0.9981
PFDoDA-IS		9.619	ISTD	614.90>570.10	614.90>269.10	----	----	ng_L	----
PFDoS / PFDoDS*	Perfluorododecane sulfonic acid	9.853	Target	699.00>98.90	699.00>79.90	PFDoDA-IS	1 - 100	ng_L	0.9908
PFDS*	Perfluorodecane sulfonic acid	9.312	Target	598.80>79.95	598.80>98.85	PFDoDA-IS	1 - 100	ng_L	0.9995
PFHpA*	Perfluoroheptanoic acid	7.59	Target	363.10>319.00	363.10>169.00	PFHpA-IS	0.5 - 100	ng_L	0.9979
PFHpA-IS		7.591	ISTD	367.00>322.10	367.00>169.00	----	----	ng_L	----
PFHpS*	Perfluoroheptane sulfonic acid	8.167	Target	448.90>79.90	448.90>98.90	PFHxS-IS	0.5 - 100	ng_L	0.9981
PFHxA*	Perfluorohexanoic acid	6.886	Target	313.10>269.00	313.10>119.00	PFHxA-IS	0.5 - 100	ng_L	0.9988
PFHxA-IS		6.883	ISTD	317.90>273.00	317.90>120.10	----	----	ng_L	----
PFHxDA	Perfluorohexadecanoic acid	10.455	Target	813.00>769.00	813.00>169.00	PFHxDA-IS	2.5 - 100	ng_L	0.9943
PFHxDA-IS		10.454	ISTD	814.90>769.90	814.90>369.00	----	----	ng_L	----
PFHxS*	Perfluorohexane sulfonic acid	7.637	Target	398.90>79.95	398.90>98.90	PFHxS-IS	0.5 - 100	ng_L	0.9985
PFHxS-IS		7.636	ISTD	402.00>79.90	402.00>98.80	----	----	ng_L	----
PFMBA	Perfluoro-4-methoxybutanoic acid	6.265	Target	279.10>84.95	----	PFPeA-IS	0.5 - 100	ng_L	0.9987
PFMPA	Perfluoro-3-methoxypropanoic acid	5.209	Target	228.90>84.95	----	PFBA-IS	0.5 - 100	ng_L	0.9995
PFNA*	Perfluorononanoic acid	8.606	Target	463.00>418.95	463.00>219.00	PFNA-IS	0.5 - 100	ng_L	0.9996
PFNA-IS		8.605	ISTD	471.90>427.00	471.90>223.00	----	----	ng_L	----
PFNS*	Perfluorononane sulfonic acid	8.984	Target	549.10>79.90	549.10>98.90	PFUnDA-IS	0.5 - 50	ng_L	0.9947
PFOA*	Perfluorooctanoic acid	8.144	Target	413.20>369.00	413.20>169.05	PFOA-IS	0.5 - 100	ng_L	0.9967
PFOA-IS		8.142	ISTD	421.00>376.10	421.00>172.00	----	----	ng_L	----
PFOcDA / PFODA	Perfluorooctadecanoic acid	10.75	Target	913.00>868.95	913.00>169.00	PFHxDA-IS	1 - 100	ng_L	0.9965
PFOS*	Perfluorooctane sulfonic acid	8.606	Target	498.90>79.90	498.90>98.90	PFOS-IS	0.5 - 100	ng_L	0.9981
PFOSA / FOSA	perfluorooctane sulfonamide	9.313	Target	497.90>77.90	497.90>478.15	FOSA-IS	0.5 - 100	ng_L	0.9974
PFOSA-IS		9.312	ISTD	505.90>78.00	505.90>172.00	----	----	ng_L	----
PFOS-IS		8.603	ISTD	506.90>79.90	506.90>98.80	----	----	ng_L	----
PFPeA / PFPA*	Perfluoropentanoic acid	5.94	Target	263.10>219.00	263.10>69.10	PFPeA-IS	0.5 - 100	ng_L	0.9991
PFPeA-IS		5.946	ISTD	267.90>223.00	267.90>69.10	----	----	ng_L	----
PFPeS / PFPS*	Perfluoropentane sulfonic acid	6.992	Target	349.20>79.95	349.20>98.95	PFHxS-IS	0.5 - 100	ng_L	0.9978
PFTeDA	Perfluorotetradecanoic acid	10.096	Target	713.00>669.05	713.00>169.05	PFTeDA-IS	0.5 - 100	ng_L	0.9967
PFTeDA-IS		10.102	ISTD	714.90>670.00	714.90>368.90	----	----	ng_L	----
PFTrDA*	Perfluorotridecanoic acid	9.878	Target	663.00>619.00	663.00>169.00	PFDoDA-IS	0.5 - 100	ng_L	0.9988
PFTrDS*	Perfluorotridecane sulfonic acid	10.067	Target	749.00>99.10	749.00>79.90	PFDoDA-IS	1 - 100	ng_L	0.9915
PFUnDA*	Perfluoroundecanoic acid	9.332	Target	563.00>518.95	563.00>269.05	PFUnDA-IS	0.5 - 100	ng_L	0.9947
PFUnDA-IS		9.333	ISTD	570.00>524.90	570.00>268.90	----	----	ng_L	----
PFUnS / PFUnDS*	Perfluoroundecane sulfonic acid	9.601	Target	649.00>79.95	649.00>98.95	PFDoDA-IS	0.5 - 100	ng_L	0.9962

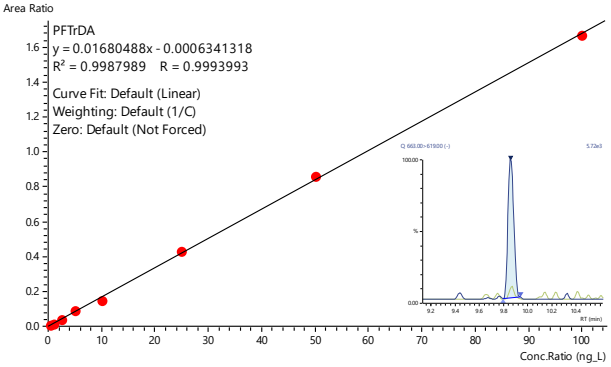
* PFAS requested in EU directive 2020/2184[1] on the quality of water intended for human consumption

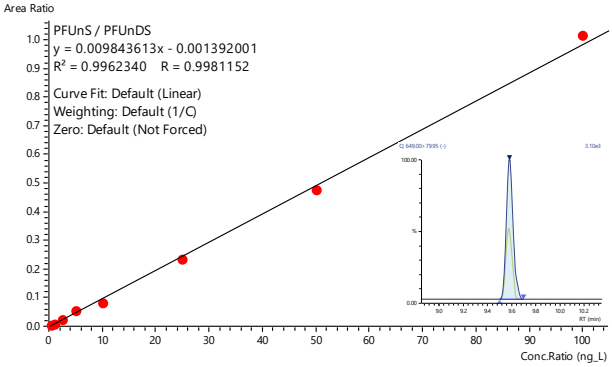


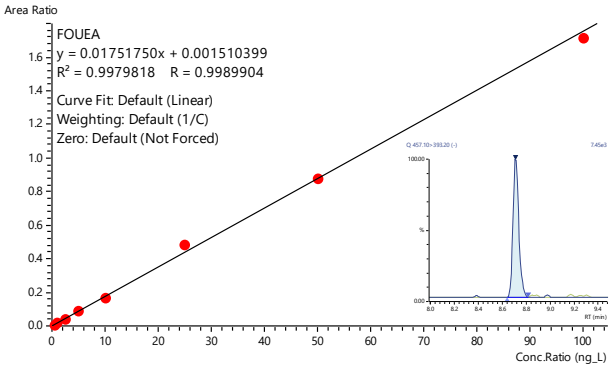


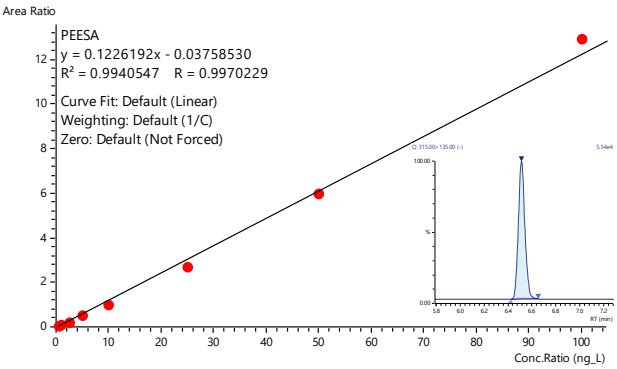


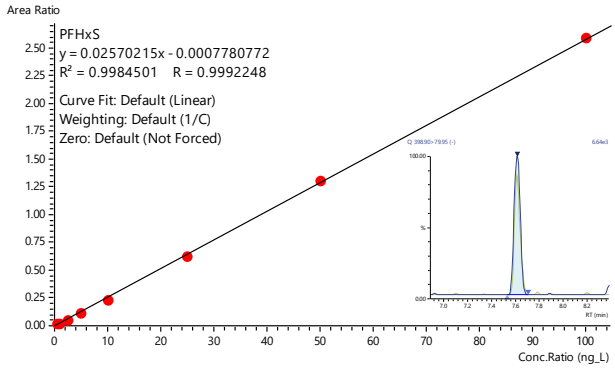












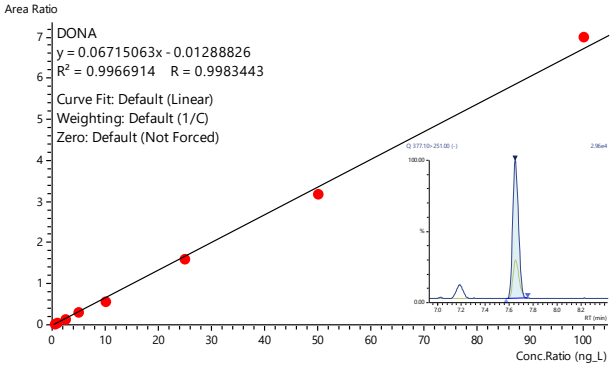


Figure 2 Exemplary calibration curves ranging from 0.5– 100 ng/L and a typical chromatogram at 1 ng/L level

Table 3 Reproducibility of QC samples

	10:2 FTS		11Cl-PF3OUdS		3.7-DMPFOA		4:2 FTS		6:2 FTS		8:2 diPAP		8:2 FTS		9Cl-PF3ONS		DONA		FOSA		FOUEA	
	QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low	
	5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L	
	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy
QC L1	5.31	106.23	5.19	103.81	4.77	95.3	4.72	94.32	4.98	99.55	3.61	72.1	6.9	137.93	4.98	99.55	4.67	93.36	4.6	91.96	4.02	80.45
QC L2	5.46	109.24	4.62	92.33	4.08	81.59	4.73	94.56	4.75	95.07	4.45	89.06	5.43	108.58	4.29	85.86	4.78	95.53	4.78	95.55	4.65	92.94
QC L3	5.04	100.72	4.11	82.14	4.37	87.5	4.57	91.48	5.55	110.98	4.71	94.15	5.53	110.58	4.29	85.79	4.48	89.52	4.68	93.59	4.87	97.48
Mean		105.39		92.76		88.13		93.46		101.87		85.1		119.03		90.4		92.81		93.7		90.29
SD		4.32		10.84		6.88		1.71		8.21		11.54		16.4		7.92		3.04		1.79		8.82
%RSD		4.1		11.68		7.8		1.83		8.06		13.56		13.78		8.77		3.28		1.92		9.76
	QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high	
	25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L	
	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy
QC H1	26.11	104.45	21.67	86.68	19.91	79.63	25.11	100.44	26.79	107.17	26.08	104.3	25.13	100.54	24.43	97.71	23.23	92.92	25.59	102.35	24.58	98.33
QC H2	28.41	113.64	24.83	99.33	21.29	85.16	24.93	99.71	26.17	104.69	20.85	83.42	26.86	107.44	24.36	97.43	24.12	96.49	25.52	102.09	25.1	100.42
QC H3	21.79	87.16	20.43	81.71	21.28	85.11	25.78	103.1	25.34	101.36	19.04	76.15	28.41	113.63	21.26	85.05	25.08	100.31	23.74	94.97	25.88	103.53
Mean		101.75		89.24		83.3		101.09		104.4		87.96		107.2		93.4		96.57		99.8		100.76
SD		13.45		9.09		3.18		1.78		2.92		14.61		6.55		7.23		3.7		4.19		2.62
%RSD		13.22		10.18		3.82		1.76		2.79		16.61		6.11		7.74		3.83		4.2		2.6

	H4PFUNA		HPFHpA		PFDoS		PFTrDS		N-Et-FOSA		N-Et-FOSAA		NFDHA		N-Me-FOSA		N-Me-FOSAA		PEESA		PFBA	
	QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low	
	5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L	
	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy
QC L1	5.21	104.23	5.23	104.52	4.56	91.14	4.17	83.31	4.86	97.25	4.22	84.31	4.63	92.68	4.56	91.22	4.83	96.64	4.29	85.71	4.75	94.96
QC L2	4.82	96.45	5.33	106.7	4.07	81.3	5.92	118.41	4.54	90.86	4.8	95.96	4.67	93.32	5.25	104.93	5.27	105.45	4.42	88.45	4.86	97.29
QC L3	5.57	111.42	4.92	98.37	4.22	84.33	3.88	77.54	4.24	84.87	3.62	72.41	4.29	85.78	5.1	102	6.04	120.77	4.36	87.23	4.53	90.58
Mean		104.03		103.19		85.59		93.08		90.99		84.23		90.59		99.38		107.62		87.13		94.28
SD		7.49		4.32		5.04		22.12		6.19		11.77		4.18		7.22		12.21		1.37		3.4
%RSD		7.2		4.19		5.89		23.76		6.81		13.98		4.61		7.27		11.34		1.58		3.61
	QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high	
	25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L	
	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy
QC H1	27.56	110.24	26.32	105.26	21.13	84.52	20.06	80.26	24.91	99.63	24.67	98.68	24.04	96.16	24.63	98.53	27.48	109.94	21.6	86.41	25.02	100.09
QC H2	25.61	102.43	26.94	107.75	24.8	99.19	19.47	77.89	26.51	106.05	21.96	87.86	23.64	94.57	25.58	102.32	24.1	96.39	22.57	90.27	24.36	97.45
QC H3	24.41	97.65	27.49	109.97	17.95	71.82	21.95	87.78	23.24	92.94	27.96	111.84	24.43	97.73	21.9	87.58	24.8	99.21	22.86	91.45	24.09	96.37
Mean		103.44		107.66		85.18		81.98		99.54		99.46		96.15		96.15		101.85		89.38		97.97
SD		6.36		2.35		13.7		5.17		6.56		12.01		1.58		7.66		7.15		2.64		1.91
%RSD		6.14		2.19		16.08		6.3		6.59		12.08		1.64		7.96		7.02		2.95		1.95

	PFBS		PFDA		PFDoDA		PFDS		PFHpA		PFHpS		PFHxA		PFHxDA		PFHxS		PFMBA		PFMPA	
	QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low	
	5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L	
	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy
QC L1	4.71	94.2	5.26	105.22	5.01	100.29	5.01	100.1	4.91	98.21	5.13	102.62	4.81	96.29	3.13	62.53	4.65	92.93	4.7	94.09	4.69	93.73
QC L2	4.97	99.45	5.72	114.45	4.93	98.7	6.32	126.32	4.66	93.28	4.99	99.73	4.7	94.03	4.78	95.55	4.86	97.2	4.66	93.29	4.92	98.41
QC L3	4.6	92.07	5.29	105.88	4.1	81.9	6.85	137.01	4.5	89.93	5.02	100.39	4.45	89.06	3.06	61.24	4.81	96.17	4.97	99.3	4.85	96.97
Mean		95.24		108.52		93.63		121.14		93.81		100.91		93.13		73.11		95.43		95.56		96.37
SD		3.8		5.15		10.19		18.99		4.16		1.51		3.7		19.44		2.23		3.26		2.4
%RSD		3.99		4.74		10.88		15.67		4.44		1.5		3.97		26.6		2.34		3.42		2.49
	QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high	
	25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L	
	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy
QC H1	24.31	97.23	23.81	95.22	24.84	99.37	24.35	97.39	24.46	97.84	25.69	102.75	23.93	95.7	23.96	95.82	24.97	99.9	25.4	101.59	25.6	102.38
QC H2	24.92	99.69	27.11	108.43	24.84	99.35	28.56	114.23	25.97	103.86	24.81	99.22	24.39	97.54	24.88	99.51	24.94	99.75	25.02	100.08	25.23	100.92
QC H3	23.97	95.89	26.51	106.05	21.72	86.86	24.29	97.17	26.63	106.54	25.64	102.55	24.14	96.57	24.16	96.64	25.54	102.15	24.38	97.52	25	100
Mean		97.6		103.24		95.19		102.93		102.75		101.51		96.61		97.33		100.6		99.73		101.1
SD		1.93		7.04		7.21		9.79		4.45		1.98		0.92		1.94		1.35		2.06		1.2
%RSD		1.97		6.82		7.58		9.51		4.33		1.95		0.95		1.99		1.34		2.06		1.19

	PFNA		PFNS		PFOA		PFODA		PFOS		PFPeA		PFPeS / PFPS		PFTeDA		PFTrDA		PFUnDA		PFUnS / PFUnDS	
	QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low		QC low	
	5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L		5 ng/L	
	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy
QC L1	4.68	93.6	4.72	94.32	4.65	92.96	3.93	78.6	4.15	82.93	4.69	93.86	4.62	92.35	4.65	92.93	4.64	92.84	4.25	85.01	4.12	82.47
QC L2	4.78	95.64	5.56	111.23	4.92	98.38	5.92	118.39	4.87	97.4	4.76	95.21	4.68	93.68	3.67	73.33	4.18	83.7	4.24	84.76	3.51	70.23
QC L3	4.45	89.1	5.65	112.91	4.78	95.54	5.34	106.85	5.3	106.06	4.83	96.53	4.97	99.34	3.85	77.05	3.93	78.69	4.71	94.22	2.84	56.84
Mean		92.78		106.15		95.62		101.28		95.46		95.2		95.13		81.1		85.08		88		69.85
SD		3.35		10.28		2.71		20.47		11.69		1.34		3.71		10.41		7.17		5.39		12.82
%RSD		3.61		9.69		2.84		20.21		12.24		1.4		3.9		12.84		8.43		6.13		18.35
	QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high		QC high	
	25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L		25 ng/L	
	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy	Conc.	Accuracy
QC H1	21.94	87.75	27.02	108.1	24.01	96.06	24.63	98.51	25.73	102.94	25.35	101.42	23.74	94.96	25.32	101.29	24.77	99.08	25.75	103.02	22.83	91.33
QC H2	24.48	97.93	26.94	107.75	23.77	95.06	28.41	113.63	25.38	101.52	24.92	99.68	24.11	96.43	23.47	93.88	23.64	94.56	24.69	98.77	25.7	102.81
QC H3	24.36	97.45	27.99	111.94	22.88	91.52	26.33	105.3	24.68	98.73	24.75	98.99	25.88	103.52	19.6	78.39	22.32	89.28	23.37	93.48	17.16	68.63
Mean		94.38		109.26		94.21		105.82		101.06		100.03		98.31		91.19		94.31		98.42		87.59
SD		5.74		2.33		2.39		7.57		2.14		1.25		4.58		11.68		4.91		4.78		17.39
%RSD		6.09		2.13		2.53		7.16		2.12		1.25		4.66		12.81		5.2		4.85		19.86

Figure 3 Scheme of the Nexera™ on-line SPE LCMS-8060NX system

■ The Package

❑ *Main Unit*

LCMS-8060NX:	TQ Mass spectrometer
Nexera X3:	Liquid chromatograph CBM-40 DGU-405 2x LC-40D X3 LC-40B X3 SIL-40C X3 CTO-40S 2x Reservoir Tray

❑ *Accessory*

Valve:	FCV-0206H3
Mixer:	2x Mir20 µL
Loop:	1 mL

❑ *Main Consumables*:

Shim-pack Scepter C18
(50 mm x 2.1 mm I.D., 1.9 µm; P/N 227-31012-03)

Shim-pack GIST HP C18-AQ (2x)
(30 mm x 3.0 mm I.D., 3 µm; P/N 227-30766-01)

EVOLUTE® Express ABN on-line SPE cartridge (Biotage)
(30 mm x 2.1 mm I.D; P/N OSPE-620-32150)

Shimadzu LabTotal Vial for LC/LCMS
(P/N 227-34001-01)

PP-caps, with aluminium septa
(P/N 961-10030-31)
(This part number is available in the EU area only. If you are in another territory, please contact for your Shimadzu local office)

❑ *Software and Libraries*

LabSolutions LCMS

LabSolutions Insight

■ Conclusions

This application note describes an on-line SPE LC-MS/MS method to monitor 44 PFAS and 22 internal standards in drinking water. Using the LCMS-8060NX coupled with a Nexera UHPLC system equipped for on-line SPE a highly robust and sensitive method for routine PFAS analysis in drinking water which omits additional sample preparation steps is demonstrated.

■ References

1. DIRECTIVE (EU) 2020/2184 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2020 on the quality of water intended for human consumption

05-SCA-210-065-EN First Edition: Mar. 2022

Shimadzu Corporation
www.shimadzu.com/an/

SHIMADZU Europa GmbH,
www.shimadzu.eu