

Application Note

Emerging Contaminant of Concern - Perfluorinated Compounds (PFOS/PFOA)

Waters Corporation



This is an Application Brief and does not contain a detailed
Experimental section.

Abstract

Recent research has provided evidence that perfluorinated compounds (PFCs), such as perfluorooctanesulfonic acid (PFOS) and perfluorooctanoic acid (PFOA), are persistent organic pollutants and are ubiquitous in the environment.

Benefits

Analytical method for perfluorinated compounds (PFCs)

Introduction

Recent research has provided evidence that perfluorinated compounds (PFCs), such as perfluorooctanesulfonic acid (PFOS) and per-fluorooctanoic acid (PFOA), are persistent organic pollutants and are ubiquitous in the environment. Because PFCs may be toxic and have bioaccumulative properties, there is growing interest in the development of analytical methods for PFCs in the environment.

Experimental

UPLC conditions

Instrument:	ACQUITY UPLC System
Column:	ACQUITY UPLC BEH C ₁₈ , 1.7 μm, 2.1 x 50 mm,
Flow Rate:	0.40 mL/min
Injection Volume:	10 μL [full loop injection mode]
Column Temp:	40 °C
Mobile Phase:	A: 20 mM ammonium acetate in water/acetonitrile [90:10]

B: Methanol/acetonitrile [60:40]

Gradient: 15% – 95% B over 8 minutes

Curve: Linear

MS conditions

Instrument: Quattro Premier XE

Ionization Mode: ESI -

Capillary Voltage: 3 kV

MS Mode: MRM

Desolvation Temp: 350 °C

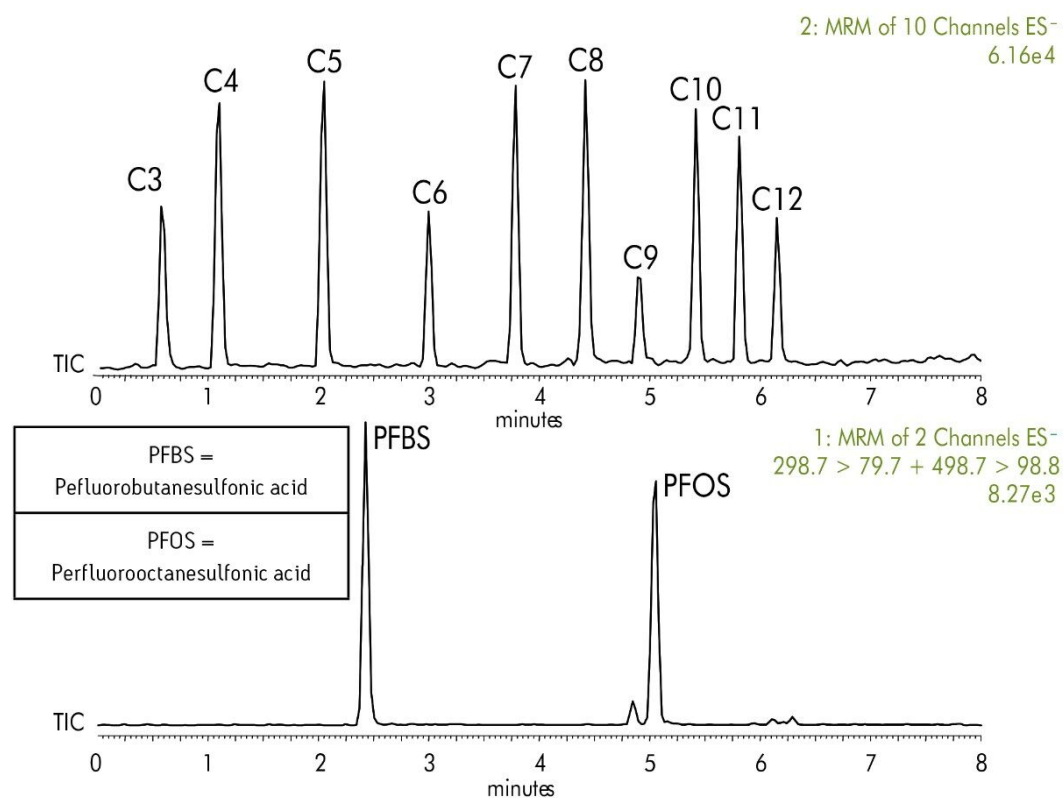
Source Temp: 150 °C

PFC	MRM Transition	Cone (V)	Collision (eV)
PFBS	299>80	40	30
PFOS	499>80	50	40
C3	163>119	20	13
C4	213>169	15	10
C5	263>219	15	9
C6	313>269	15	12

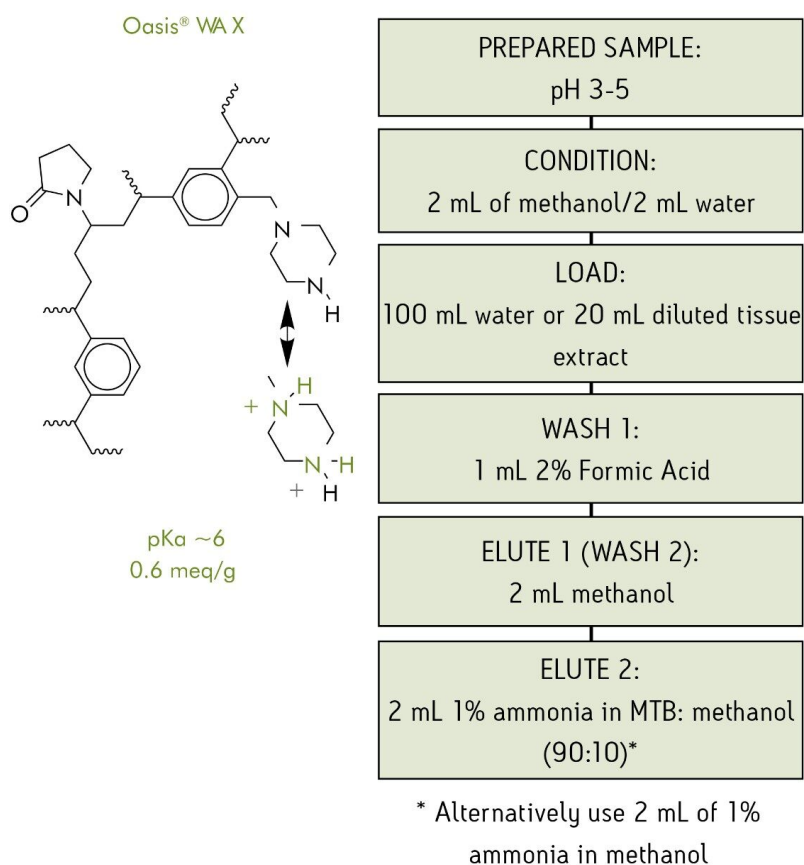
PFC	MRM Transition	Cone (V)	Collision (eV)
C7	363>319	15	10
C8	413>369	15	10
C9	463>419	15	10
C10	513>469	15	10
C11	563>519	15	10
C12	613>569	15	10

Optimized MRM transition parameters.

C3 = Perfluoropropanoic acid	C7 = Perfluoroheptanoic acid	C10 = Perfluorodecanoic acid
C4 = Perfluorobutyric acid	C8 = Perfluorooctanoic acid	C11 = Perfluoroundecanoic acid
C5 = Perfluoropentanoic acid	C9 = Perfluorononanoic acid	C12 = Perfluorododecanoic acid
C6 = Perfluorohexanoic acid		



UPLC-MS/MS of 12 PFCs spiked at 10 µg/kg in chicken liver.



Oasis WAX Sorbent and SPE protocol for water and tissue.

Sample preparation

Method 1: Water

Water samples [100 mL] were spiked with the appropriate compounds, adjusted to pH 3 with formic acid, and then processed by SPE. The SPE eluate [Elute 2] was collected in polypropylene test tubes, diluted with 2 mL of 2% aqueous formic acid and brought to 5 mL with water. Alternatively, the eluate may be evaporated and reconstituted in mobile phase prior to analysis, but polypropylene labware should be used exclusively.

Method 2: Tissues

A 1 mL aliquot of supernatant was diluted to 20 mL with water and the pH was adjusted to 4–5 using 2% formic acid. This solution was then loaded on an Oasis WAX cartridge. SPE eluates were evaporated and reconstituted in 1 mL of mobile phase [polypropylene labware].

Results and Discussion

Recovery from Drinking Water [%]

Spike Level μ g/L	C11	PFBS	PFOS	C3	C4	C5	C6	C7	C8	C9	C10
0.1	101	122	109	108	119	97	184	107	83	121	101
0.3	94	110	117	95	132	105	110	119	126	137	118
0.7	119	102	98	91	107	93	118	100	78	103	126
1	117	113	94	128	106	98	130	100	88	100	110
4	84	104	86	101	99	99	102	102	92	115	99
10	101	104	100	98	101	100	87	89	82	103	99

Recovery of PFCs from drinking water.

References

1. Environmental System Solutions 720001601EN
2. Analysis of Perfluorinated Compounds (PFCs) on the ACQUITY UPLC System and the Quattro Premier XE in ES-MS/MS 720001761EN
3. Separation of Branched PFOS Isomers by UPLC with MS/MS Detection 720001694EN
4. Oasis WAX Sorbent for UPLC/MS Determination of PFOS and Related Compounds in Water and Tissue

720001817EN

5. Analysis of Perfluorinated Compounds using UPLC and MS/MS Detection 720001848EN

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ACQUITY UPLC System <<https://www.waters.com/514207>>

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