

Electronic Supplementary Information

Comparison of solvent extraction and thermal desorption methods for determination of volatile polyfluorinated alkyl substances in the urban atmosphere

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1. Isotopically labeled standards

Table A1. Analytes, acronyms, purity, and vendor information of isotopically labeled standards.

Analyte	Acronym	Purity	Vendor
2-perfluorobutyl-[1,1,2,2- ² H ₄]-ethanol	d ₄ -4:2 FTOH	> 98%	Wellington Laboratories, Canada
2-perfluorohexyl-[1,1- ² H ₂]-[1,2- ¹³ C ₂]- ethanol	¹³ C ₂ , d ₂ -6:2 FTOH	> 98%	Wellington Laboratories, Canada
2-perfluorooctyl-[1,1- ² H ₂]-[1,2- ¹³ C ₂]- ethanol	¹³ C ₂ , d ₂ -8:2 FTOH	> 98%	Wellington Laboratories, Canada
2-perfluorodecyl-[1,1- ² H ₂]-[1,2- ¹³ C ₂]- ethanol	¹³ C ₂ , d ₂ -10:2 FTOH	> 98%	Wellington Laboratories, Canada
N-methyl-d ₃ -perfluoro-1- octanesulfonamide	d ₃ -NMeFOSA	> 98%	Wellington Laboratories, Canada
N-ethyl-d ₅ -perfluoro-1-octanesulfonamide	d ₅ -NEtFOSA	> 98%	Wellington Laboratories, Canada

2. GC–MS parameters

Table A2. Retention times (on a 60 meter HP-INNOWAX column), molecular weights, and ions monitored for GC–MS analysis of targeted PFASs in PCI mode.

Analyte	Retention time (min)	Molecular weight	PCI Ions monitored m/z
4:2 FTOH	13.6	264	227, 265 ^a
6:2 FTOH	15.5	364	327, 365 ^a , 393
8:2 FTOH	17.3	464	427, 465 ^a , 493
10:2 FTOH	18.7	564	527, 565 ^a , 593
NMeFOSA	24.5	513	514 ^a
NEtFOSA	23.8	527	528 ^a
NMeFOSE	26	557	540 ^a , 558
NEtFOSE	26.1	571	554 ^a , 572
d ₄ -4:2 FTOH ^b	13.3	268	230, 269 ^a
¹³ C ₂ , d ₂ -6:2 FTOH ^b	15.4	368	331, 369 ^a , 397
¹³ C ₂ , d ₂ -8:2 FTOH ^b	17.2	468	431, 469 ^a , 496
¹³ C ₂ , d ₂ -10:2 FTOH ^b	18.8	568	531, 569 ^a , 597
d ₃ -NMeFOSA ^b	24.4	516	517 ^a
d ₅ -NEtFOSA ^b	23.7	532	533 ^a
7:1 FA ^c	16.6	400	381, 401
11:1 FA ^c	19.6	600	581, 601

^a Quantification Ion

^b Mass-labeled Surrogate Standard

^c Internal Standard