

Materials List for:

Identifying Per- and Polyfluorinated Chemical Species with a Combined Targeted and Non-Targeted-Screening High-Resolution Mass Spectrometry Workflow

James McCord¹, Mark Strynar²

¹Oak Ridge Institute for Science and Education, National Exposure Research Laboratory, U.S. Environmental Protection Agency

²National Exposure Research Laboratory, U.S. Environmental Protection Agency

Correspondence to: Mark Strynar at strynar.mark@epa.gov

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Materials

Name	Company	Catalog Number	Comments
Acquity ultra-high performance liquid chromatography system	Waters Corporation		Modified with PFCs analysis kit (176001744); equivalent UPLC system is acceptable if PFAS background is checked and confirmed to be low
Ammonium acetate	Fluka	17836	Mass spectrometry grade>99% pure
Ammonium Hydroxide	Sigma-Aldrich	338818	
Balance	Mettler	AB204S	
BEH C18 reverse phase UPLC column, 2.1×50 mm, 1.7 μm	Waters Corporation	186002350	
Dual piston syringe pump	Waters Corporation	SPC10-C	
Glacial Acetic Acid	Sigma-Aldrich	ARK2183	
Glass Microfiber Filters	Whatman	1820-070	
High density polyethylene sample bottle	Nalgene	2189-0032	
High Resolution Mass Spectrometer	Various		Mass Spectrometer should be capable of providing accurate mass to <10ppm and collecting MS/MS data. Agilent 6530 qTOF and Thermo Fisher Orbitrap Fusion were used in this work
Methanol	Sigma-Aldrich		
Nitric Acid (35% w/w)	Thermo Fisher Scientific	SVCN-5-1	Can be prepared in house using concentrated nitric acid and reagent water
Polypropylene Buchner funnel	ACE Glass	12557-09	
Polypropylene centrifuge tube and cap	BD Falcon	352096	
Polypropylene Vacuum Flask (1 L)	Nalgene	DS4101-1000	
Quattro Premier XE triple quadrupole mass spectrometer	Waters Corporation		Equivalent triple-quadrupole or better system can be used instead, should provide high sensitivity and stability for targeted analysis
Reagent Water			Any source determined to be PFAS free
Sodium Acetate	Sigma-Aldrich	W302406	

TurboVap nitrogen evaporator	Caliper Life Sciences	103198	Equivalent systems or rotary vacuum evaporator may be used instead
Weak anion exchange SPE cartridge (Oasis WAX Plus)	Waters Corporation	186003519	
Standard Solutions			
2,3,3,3-Tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)propanoic acid (HFPO-DA)	Wellington	HFPO-DA	
Additional targeted compound standards of interest			to be determined based on preliminary analysis and standard availability
Mass labeled HFPO-DA	Wellington	M2HFPO-DA	
Native PFCA/PFAS Mixture (2 ug/mL)	Wellington	PFAC-MXA	or PFAC-MXB; or individually prepared mixture containing compounds of interest
Stable Isotope Labeled PFCA/PFAS Mixture (2 ug/mL)	Wellington	MPFAC-MXA	or MPFAC-MXB; or individually prepared mixture containing compounds of interest as appropriate for Native PFASs
Software			
Mass Profiler Professional	Agilent		Or open source software packages
Profinder	Agilent		Or open source software packages