

Materials List for:

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

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## Materials

Name	Company	Catalog Number	Comments
Acqity 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	
<b>Standard Solutions</b>			
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
<b>Software</b>			
Mass Profiler Professional	Agilent		Or open source software packages
Profinder	Agilent		Or open source software packages