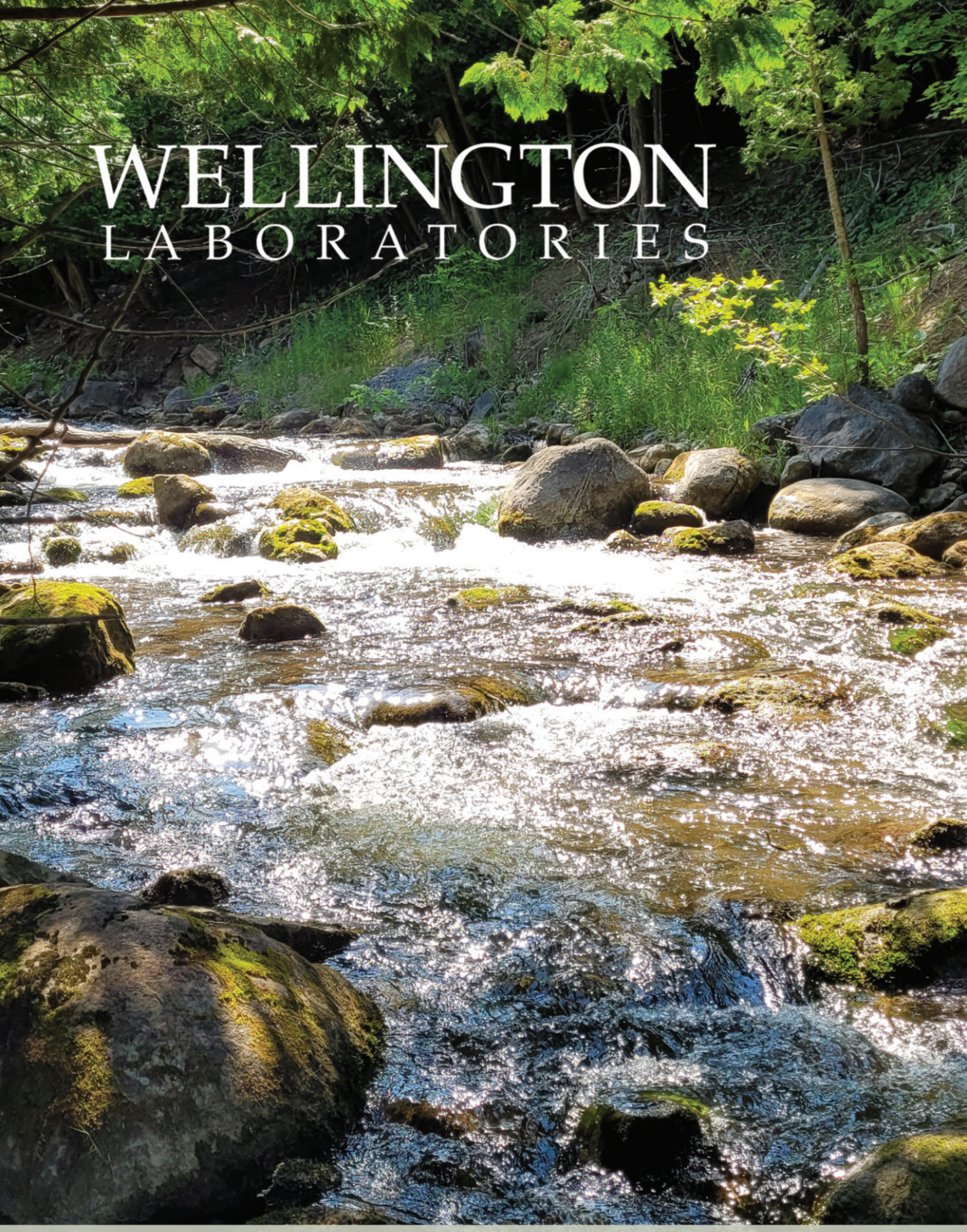


WELLINGTON
LABORATORIES

QUICK REFERENCE GUIDE:
PERFLUOROALKYL AND POLYFLUOROALKYL SUBSTANCES

GUIDELINES FOR THE USE AND HANDLING OF WELLINGTON'S PFAS PRODUCTS

HAZARDS

Our products are perfluoroalkyl and polyfluoroalkyl substances (PFAS) offered as solutions in organic solvents such as methanol and isopropanol. Although the maximum concentration is 50.0 µg/mL, that is 0.005% (w/v), these compounds must be considered toxic and should be handled accordingly. As with all of our products, due care should be exercised to prevent human contact and ingestion. The absence of a toxicity warning for any of our products must not be interpreted as an indication that there is no possible health hazard.

NOTE:
THESE MATERIALS SHOULD ONLY BE USED BY PERSONNEL TRAINED IN THE HANDLING OF HAZARDOUS CHEMICALS.
ALL PROCEDURES SHOULD BE PERFORMED IN A FUME HOOD AND SUITABLE GLOVES, EYE PROTECTION AND CLOTHING SHOULD BE WORN AT ALL TIMES.

RECEIPT, INSPECTION, HANDLING AND STORAGE

Unless crystalline material is provided, all of our reference standard solutions are shipped in flame-sealed, pre-scored amber glass ampoules. Upon receipt, inspect the ampoules for breakage and leakage and then store them upright in a refrigerator until needed.

Prior to opening, allow the solution to drain into the bottom of the ampoule, lightly tapping the ampoule if necessary. Using the plastic ampoule collar provided, hold the ampoule upright and snap the top off, breaking away from the body. Transfer the solution to an amber glass container with a glass stopper for storage.

ADDITIONAL HANDLING SUGGESTIONS SPECIFIC TO THE COMPOUND WILL BE PROVIDED WITH THE CERTIFICATE OF ANALYSIS.

The SRM transitions presented in this guide are meant as starting points only.
Further optimization is recommended.

DISPOSAL

All waste materials generated during the use of these solutions should be treated as hazardous in accordance with national and regional regulations. A licensed disposal company should be employed.

ACCURACY

Each of our stock solutions is prepared from crystalline material that has been well characterized as to its structure and purity. The crystalline material is weighed using microbalances that are externally calibrated and traceable to an ISO/IEC 17025 accredited laboratory.

Solutions are prepared by completely dissolving the crystalline material in ultrapure, distilled-in-glass solvents. The volumetric flasks used for this purpose, and the pipets used for subsequent preparation of dilutions and mixtures, are all of class A tolerance and traceable to an ISO/IEC 17025 accredited laboratory.

The maximum percent relative combined uncertainty for solution preparation is calculated to be ± 5%.

INTERLABORATORY CERTIFICATION

Wellington has contributed standards to various independent interlaboratory testing studies. Since 2005, our standards have been tested in several international round-robins. Data from these studies is available upon request.

Wellington plans to continue participating in independent interlaboratory studies to confirm the accuracy of our reference standard solutions.

EXPIRY DATE/SHELF LIFE

In order to accurately determine the shelf life of our products, testing must reveal degradation or loss in concentration of the particular analyte. Most of these fluorinated compounds are presumed to be stable based on current scientific literature. However, many of these compounds have never been offered as solutions and therefore may have degradation pathways that have not been previously observed.

Consequently, we continue to monitor the stability of these compounds by:
i) comparing freshly prepared solutions to older solutions by LC/MS and/or GC/MS.
ii) monitoring the solutions during storage by LC/MS and/or GC/MS.

Thus, our stability studies are still ongoing. In the absence of a “true expiry date”, we consider that our reference solutions retain their accuracy for a period of at least 2 years from delivery in the unopened ampoule.

Certified System™
Quality
ISO 9001

Reporting Adjustment for PFAS Analytes in Salt Form

Salts are acceptable starting materials for stock standards provided that the measured mass is corrected for the salt content as per the equation and methods cited below:

$$mass(acid\ form) = mass(salt)\ x\ \frac{MW acid}{MW salt}$$

U.S. EPA Method 537.1
Determination of Selected Per- and Polyfluorinated Alkyl Substances in Drinking Water by Solid Phase Extraction and Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS) – November 2018

U.S. EPA Method 533
Determination of Per- and Polyfluoroalkyl Substances in Drinking Water by Isotope Dilution Anion Exchange Solid Phase Extraction and Liquid Chromatography/Tandem Mass Spectrometry – November 2019

Commonly Used Units of Measure

wt/wt basis				wt/vol basis			
ppm	mg/kg	µg/g	ng/mg	**ppm**	mg/L	µg/mL	ng/µL
ppb	µg/kg	ng/g	pg/mg	**ppb**	µg/L	ng/mL	pg/µL
ppt	ng/kg	pg/g	fg/mg	**ppt**	ng/L	pg/mL	fg/µL
ppq	pg/kg	fg/g	ag/mg	**ppq**	pg/L	fg/mL	ag/µL

Conversion Factors

Prefix	Symbol	Factor	Fraction	
centi	c	10^{-2}	= 1/100	part per hundred
milli	m	10^{-3}	= 1/1,000	part per thousand
micro	µ	10^{-6}	= 1/1,000,000	part per million (ppm)
nano	n	10^{-9}	= 1/1,000,000,000	part per billion (ppb)
pico	p	10^{-12}	= 1/1,000,000,000,000	part per trillion (ppt)
femto	f	10^{-15}	= 1/1,000,000,000,000,000	part per quadrillion (ppq)
atto	a	10^{-18}	= 1/1,000,000,000,000,000,000	part per quintillion
zepto	z	10^{-21}	= 1/1,000,000,000,000,000,000,000	part per sextillion
yocto	y	10^{-24}	= 1/1,000,000,000,000,000,000,000,000	part per septillion

The masses utilized to calculate the molecular weights stated in this reference guide are as follows:

^{12}C or C = 12.0107 (representing the average atomic mass of carbon)

^{13}C = 13.003355	O = 15.9994	N = 14.0067	Na = 22.9898
^{18}O = 17.9992	H = 1.00794	F = 18.9984	K = 39.0983
^{2}H = 2.0141	S = 32.065	P = 30.97376	Cl = 35.453

Summary of PFAS Analyte Information

Perfluoroalkanesulfonates (PFSAs)

Compound	Molecular Formula	Molecular Weight Salt	Molecular Weight Acid	ESI- SRM Transition 1	ESI- SRM Transition 2
NaPFPrS	$C_3F_7SO_3Na$	272.0739	250.0920	249 > 80	249 > 99
KPFBS	$C_4F_9SO_3K$	338.1899	300.0995	299 > 80	299 > 99
NaPFBS [M+3]	$^{13}C_3{}^{12}CF_9SO_3Na$	325.0594	303.0775	302 > 80	302 > 99
NaPFPeS	$C_5F_{11}SO_3Na$	372.0889	350.1070	349 > 80	349 > 99
KPFHxS	$C_6F_{13}SO_3K$	438.2049	400.1145	399 > 80	399 > 99
NaPFHxS	$C_6F_{13}SO_3Na$	422.0964	400.1145	399 > 80	399 > 99
NaPFHxS [M+3]	$^{13}C_3{}^{12}C_3F_{13}SO_3Na$	425.0744	403.0925	402 > 80	402 > 99
NaPFHxS [M+4]	$C_6F_{13}S^{18}O_2ONa$	426.0960	404.1141	403 > 84	403 > 103
NaPFHpS	$C_7F_{15}SO_3Na$	472.1039	450.1220	449 > 80	449 > 99
KPFECHS	$C_8F_{15}SO_3K$	500.2231	462.1327	461 > 381	461 > 99
NaCl-PFOS	$C_8ClF_{16}SO_3Na$	538.5660	516.5841	515 > 80	515 > 99
KPFOS	$C_8F_{17}SO_3K$	538.2199	500.1295	499 > 80	499 > 99
NaPFOS	$C_8F_{17}SO_3Na$	522.1114	500.1295	499 > 80	499 > 99
NaPFOS [M+4]	$^{13}C_4{}^{12}C_4F_{17}SO_3Na$	526.0820	504.1002	503 > 80	503 > 99
NaPFOS [M+8]	$^{13}C_8F_{17}SO_3Na$	530.0526	508.0708	507 > 80	507 > 99
NaPFNS	$C_9F_{19}SO_3Na$	572.1189	550.1370	549 > 80	549 > 99
NaPFDS	$C_{10}F_{21}SO_3Na$	622.1264	600.1445	599 > 80	599 > 99
NaPFUdS	$C_{11}F_{23}SO_3Na$	672.1339	650.1520	649 > 80	649 > 99
NaPFDoS	$C_{12}F_{25}SO_3Na$	722.1414	700.1595	699 > 80	699 > 99
NaPFTrDS	$C_{13}F_{27}SO_3Na$	772.1489	750.1670	749 > 80	749 > 99

Chloroperfluoroalkyl Ether Sulfonates (Cl-PFESA)

Compound	Molecular Formula	Molecular Weight Salt	Molecular Weight Acid	ESI- SRM Transition 1	ESI- SRM Transition 2
9Cl-PF3ONS	$C_8F_{16}ClSO_4K$	570.6739	532.5835	531 > 351	531 > 83
11Cl-PF3OUdS	$C_{10}F_{20}ClSO_4K$	670.6889	632.5985	631 > 451	631 > 83

Perfluoroalkyl Ether Sulfonate (PFESA)

Compound	Molecular Formula	Molecular Weight Salt	Molecular Weight Acid	ESI- SRM Transition 1	ESI- SRM Transition 2
PFEESA	$C_4F_9SO_4K$	354.1893	316.0989	315 > 135	315 > 69

Fluorotelomer Sulfonates (X:2FTS)

Compound	Molecular Formula	Molecular Weight Salt	Molecular Weight Acid	ESI- SRM Transition 1	ESI- SRM Transition 2
4:2FTS	$C_6H_4F_9SO_3Na$	350.1346	328.1527	327 > 307	327 > 81
4:2FTS [M+2]	$^{13}C_2{}^{12}C_4H_4F_9SO_3Na$	352.1199	330.1380	329 > 81	329 > 309
6:2FTS	$C_8H_4F_{13}SO_3Na$	450.1496	428.1677	427 > 407	427 > 81
6:2FTS [M+2]	$^{13}C_2{}^{12}C_6H_4F_{13}SO_3Na$	452.1349	430.1530	429 > 81	429 > 409
8:2FTS	$C_{10}H_4F_{17}SO_3Na$	550.1646	528.1827	527 > 507	527 > 81
8:2FTS [M+2]	$^{13}C_2{}^{12}C_8H_4F_{17}SO_3Na$	552.1499	530.1680	529 > 81	529 > 509
10:2FTS	$C_{12}H_4F_{21}SO_3Na$	650.1796	628.1977	627 > 607	627 > 81

Summary of PFAS Analyte Information

Perfluoroalkylcarboxylic Acids (PFCA)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
PFBA	$C_4HF_7O_2$	214.0383	213 > 169	-
PFBA [M+3]	$^{13}C_3{}^{12}CHF_7O_2$	217.0163	216 > 172	-
PFBA [M+4]	$^{13}C_4HF_7O_2$	218.0090	217 > 172	-
PFPeA	$C_5HF_9O_2$	264.0458	263 > 219	263 > 69
PFPeA [M+3]	$^{13}C_3{}^{12}C_2HF_9O_2$	267.0238	266 > 222	266 > 70
PFPeA [M+5]	$^{13}C_5HF_9O_2$	269.0091	268 > 223	268 > 70
PFHxA	$C_6HF_{11}O_2$	314.0533	313 > 269	313 > 119
PFHxA [M+2]	$^{13}C_2{}^{12}C_4HF_{11}O_2$	316.0387	315 > 270	315 > 119
PFHxA [M+5]	$^{13}C_5{}^{12}C_1HF_{11}O_2$	319.0166	318 > 273	318 > 120
PFHpA	$C_7HF_{13}O_2$	364.0608	363 > 319	363 > 169
PFHpA [M+4]	$^{13}C_4{}^{12}C_3HF_{13}O_2$	368.0315	367 > 322	367 > 169
PFOA	$C_8HF_{15}O_2$	414.0683	413 > 369	413 > 169
PFOA [M+2]	$^{13}C_2{}^{12}C_6HF_{15}O_2$	416.0537	415 > 370	415 > 169
PFOA [M+4]	$^{13}C_4{}^{12}C_4HF_{15}O_2$	418.0390	417 > 372	417 > 169
PFOA [M+8]	$^{13}C_8HF_{15}O_2$	422.0096	421 > 376	421 > 172
T-PFOA	$C_8F_{15}O_2NH_4$	431.0989	413 > 369	413 > 169
PFNA	$C_9HF_{17}O_2$	464.0758	463 > 419	463 > 219
PFNA [M+5]	$^{13}C_5{}^{12}C_4HF_{17}O_2$	469.0391	468 > 423	468 > 219
PFNA [M+9]	$^{13}C_9HF_{17}O_2$	473.0097	472 > 427	472 > 223
PFDA	$C_{10}HF_{19}O_2$	514.0833	513 > 469	513 > 219
PFDA [M+2]	$^{13}C_2{}^{12}C_8HF_{19}O_2$	516.0687	515 > 470	515 > 219
PFDA [M+6]	$^{13}C_6{}^{12}C_4HF_{19}O_2$	520.0393	519 > 474	519 > 219
PFUdA	$C_{11}HF_{21}O_2$	564.0908	563 > 519	563 > 269
PFUdA [M+2]	$^{13}C_2{}^{12}C_9HF_{21}O_2$	566.0762	565 > 520	565 > 269
PFUdA [M+7]	$^{13}C_7{}^{12}C_4HF_{21}O_2$	571.0394	570 > 525	570 > 270
PFDoA	$C_{12}HF_{23}O_2$	614.0983	613 > 569	613 > 269
PFDoA [M+2]	$^{13}C_2{}^{12}C_{10}HF_{23}O_2$	616.0837	615 > 570	615 > 269
PFTrDA	$C_{13}HF_{25}O_2$	664.1058	663 > 619	663 > 269
PFTeDA	$C_{14}HF_{27}O_2$	714.1133	713 > 669	713 > 369
MPFTeDA [M+2]	$^{13}C_2{}^{12}C_{12}HF_{27}O_2$	716.0987	715 > 670	715 > 369
PFHxDA	$C_{16}HF_{31}O_2$	814.1283	813 > 769	813 > 369
MPFHxDA [M+2]	$^{13}C_2{}^{12}C_{14}HF_{31}O_2$	816.1137	815 > 770	815 > 369
PFODA	$C_{18}HF_{35}O_2$	914.1433	913 > 869	913 > 369

Hexafluoropropylene Oxide Dimer Acid

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
HFPO-DA	$C_6HF_{11}O_3$	330.0527	285 > 169	329 > 285
HFPO-DA [M+3]	$^{13}C_3{}^{12}C_3HF_{11}O_3$	333.0307	287 > 169	332 > 287

Summary of PFAS Analyte Information

Per- and Polyfluoroalkyl Ether Carboxylic Acids (PFECA)

Compound	Molecular Formula	Molecular Weight Salt	Molecular Weight Acid	ESI- SRM Transition 1	ESI- SRM Transition 2
NaDONA	$C_7HF_{12}O_4Na$	400.0510	378.0692	377 > 251	377 > 85
PF4OPeA	$C_4HF_7O_3$	-	230.0377	299 > 85	299 > 185
PF5OHxA	$C_5HF_9O_3$	-	280.0452	279 > 85	279 > 235
3,6-OPFHpA	$C_5HF_9O_4$	-	296.0446	295 > 201	201 > 85

Perfluoroalkanesulfonamides (FASA)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
FBSA	$C_4H_2F_9NO_2S$	299.1148	298 > 78	298 > 119
N-MeFBSA	$C_5H_4F_9NO_2S$	313.1414	312 > 219	312 > 112
N-EtFBSA	$C_6H_6F_9NO_2S$	327.1679	326 > 219	326 > 126
FPeSA	$C_5H_2F_{11}NO_2S$	349.1223	348 > 78	348 > 119
FHxSA	$C_6H_2F_{13}NO_2S$	399.1298	398 > 78	398 > 169
FHpSA	$C_7H_2F_{15}NO_2S$	449.1373	448 > 78	448 > 169
FOSA	$C_8H_2F_{17}NO_2S$	499.1448	498 > 78	498 > 169
FOSA [M+8]	$^{13}C_8H_2F_{17}NO_2S$	507.0860	506 > 78	506 > 172
N-MeFOSA	$C_9H_4F_{17}NO_2S$	513.1714	512 > 219	512 > 169
N-MeFOSA [M+3]	$C_9{}^2H_3HF_{17}NO_2S$	516.1898	515 > 219	515 > 169
N-EtFOSA	$C_{10}H_6F_{17}NO_2S$	527.1979	526 > 219	526 > 169
N-EtFOSA [M+5]	$C_{10}{}^2H_5HF_{17}NO_2S$	532.2287	531 > 219	531 > 169
FDSA	$C_{10}H_2F_{21}NO_2S$	599.1598	598 > 78	598 > 169

Perfluoroalkanesulfonamidoethanols (N-MeFASE and N-EtFASE)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
N-MeFBSE	$C_7H_8F_9NO_3S$	357.1939	356 > 122	356 > 80
N-EtFBSE	$C_8H_{10}F_9NO_3S$	371.2205	370 > 136	370 > 80
N-MeFOSE	$C_{11}H_8F_{17}NO_3S$	557.2239	556 > 122	556 > 80
N-MeFOSE [M+7]	$C_{11}{}^2H_7HF_{17}NO_3S$	564.2670	563 > 126	563 > 80
N-EtFOSE	$C_{12}H_{10}F_{17}NO_3S$	571.2505	570 > 136	570 > 80
N-EtFOSE [M+9]	$C_{12}{}^2H_9HF_{17}NO_3S$	580.3059	579 > 142	579 > 80

Perfluorooctanesulfonamidoacetic Acids (FOSAA)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
FOSAA	$C_{10}H_4F_{17}NO_4S$	557.1809	556 > 498	556 > 419
N-MeFOSAA	$C_{11}H_6F_{17}NO_4S$	571.2074	570 > 419	570 > 483
N-MeFOSAA [M+3]	$C_{11}{}^2H_3H_3F_{17}NO_4S$	574.2259	573 > 419	573 > 515
N-EtFOSAA	$C_{12}H_8F_{17}NO_4S$	585.2340	584 > 419	584 > 526
N-EtFOSAA [M+5]	$C_{12}{}^2H_5H_3F_{17}NO_4S$	590.2648	589 > 419	589 > 531

Summary of PFAS Analyte Information

Fluorotelomer Alcohols (X:2FTOH)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
4:2 FTOH	$C_6H_5F_9O$	264.0889	263 > 203	263 > 245
4:2 FTOH [M+4]	$C_6{}^2H_4HF_9O$	268.1135	266 > 204	266 > 225
5:2 sFTOH	$C_7H_5F_{11}O$	314.0964	293 > 119	293 > 236
6:2 FTOH	$C_8H_5F_{13}O$	364.1039	363 > 303	363 > 255
6:2 FTOH [M+2]	$^{13}C_2{}^{12}C_6H_5F_{13}O$	366.0892	365 > 305	365 > 256
6:2 FTOH [M+4]	$^{13}C_2{}^{12}C_6{}^2H_2H_3F_{13}O$	368.1015	367 > 306	367 > 256
7:2 sFTOH	$C_9H_5F_{15}O$	414.1114	393 > 219	393 > 169
8:2 FTOH	$C_{10}H_5F_{17}O$	464.1189	463 > 403	463 > 355
8:2 FTOH [M+2]	$^{13}C_2{}^{12}C_8H_5F_{17}O$	466.1042	465 > 405	465 > 356
8:2 FTOH [M+4]	$^{13}C_2{}^{12}C_8{}^2H_2H_3F_{17}O$	468.1165	467 > 406	467 > 356
10:2 FTOH	$C_{12}H_5F_{21}O$	564.1339	563 > 503	563 > 455
10:2 FTOH [M+4]	$^{13}C_2{}^{12}C_{10}{}^2H_2H_3F_{21}O$	568.1315	567 > 506	567 > 456

Fluorotelomer Carboxylic Acids (FTCA)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
3:3 FTCA	$C_6H_5F_7O_2$	242.0915	241 > 177	241 > 117
5:3 FTCA	$C_8H_5F_{11}O_2$	342.1065	341 > 237	341 > 217
7:3 FTCA	$C_{10}H_5F_{15}O_2$	442.1215	441 > 337	441 > 317
6:2 FTCA	$C_8H_3F_{13}O_2$	378.0874	377 > 293	377 > 63
6:2 FTCA [M+2]	$^{13}C_2{}^{12}C_6H_3F_{13}O_2$	380.0727	379 > 294	379 > 64
8:2 FTCA	$C_{10}H_3F_{17}O_2$	478.1024	477 > 393	477 > 63
8:2 FTCA [M+2]	$^{13}C_2{}^{12}C_8H_3F_{17}O_2$	480.0877	479 > 394	479 > 64
10:2 FTCA	$C_{12}H_3F_{21}O_2$	578.1174	577 > 493	577 > 63
10:2 FTCA [M+2]	$^{13}C_2{}^{12}C_{10}H_3F_{21}O_2$	580.1027	579 > 494	579 > 64

Fluorotelomer Unsaturated Carboxylic Acids (FTUCA)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
6:2 FTUCA	$C_8H_2F_{12}O_2$	358.0811	357 > 293	357 > 243
6:2 FTUCA [M+2]	$^{13}C_2{}^{12}C_6H_2F_{12}O_2$	360.0664	359 > 294	359 > 244
8:2 FTUCA	$C_{10}H_2F_{16}O_2$	458.0961	457 > 393	457 > 343
8:2 FTUCA [M+2]	$^{13}C_2{}^{12}C_8H_2F_{16}O_2$	460.0814	459 > 394	459 > 344
10:2 FTUCA	$C_{12}H_2F_{20}O_2$	558.1111	557 > 493	557 > 119
10:2 FTUCA [M+2]	$^{13}C_2{}^{12}C_{10}H_2F_{20}O_2$	560.0964	559 > 494	559 > 119

Sodium Perfluoroalkyl Phosphinates (X:XPFPi)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
6:6PFPi	$C_{12}F_{26}PO_2Na$	724.0492	701 > 401	701 > 63
6:8PFPi	$C_{14}F_{30}PO_2Na$	824.0642	801 > 501	801 > 401
8:8PFPi	$C_{16}F_{34}PO_2Na$	924.0792	901 > 501	901 > 63

Summary of PFAS Analyte Information

Perfluoroalkylphosphonic Acids (PFAPA)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
PFHxPA	$C_6H_2F_{13}PO_3$	400.0312	399 > 79	-
Cl-PFHxPA	$C_6H_2ClF_{12}PO_3$	416.4858	415 > 79	-
PFOPA	$C_8H_2F_{17}PO_3$	500.0462	499 > 79	-
Cl-PFOPA	$C_8H_2ClF_{16}PO_3$	516.5008	515 > 79	-
PFDPA	$C_{10}H_2F_{21}PO_3$	600.0612	599 > 79	-

Polyfluoroalkyl Phosphate Mono-Esters (PAP)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
6:2PAP	$C_8H_4F_{13}PO_4Na_2$	488.0475	443 > 97	443 > 79
6:2PAP [M+2]	$^{13}C_2{}^{12}C_6H_4F_{13}PO_4Na_2$	490.0328	445 > 97	445 > 79
8:2PAP	$C_{10}H_4F_{17}PO_4Na_2$	588.0625	543 > 97	543 > 79
8:2PAP [M+2]	$^{13}C_2{}^{12}C_8H_4F_{17}PO_4Na_2$	590.0478	545 > 97	545 > 79

Polyfluoroalkyl Phosphate Di-Esters (diPAP)

Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
6:2diPAP	$C_{16}H_8F_{26}PO_4Na$	812.1543	789 > 97	789 > 443
6:2diPAP [M+4]	$^{13}C_4{}^{12}C_{12}H_8F_{26}PO_4Na$	816.1249	793 > 97	793 > 445
6:2/8:2diPAP	$C_{18}H_8F_{30}PO_4Na$	912.1693	889 > 97	889 > 443
8:2diPAP	$C_{20}H_8F_{34}PO_4Na$	1012.1843	989 > 97	989 > 543
8:2diPAP [M+4]	$^{13}C_4{}^{12}C_{16}H_8F_{34}PO_4Na$	1016.1549	993 > 97	993 > 545

Polyfluoroalkyl Phosphate Esters (SAmPAP)

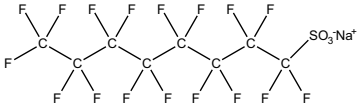
Compound	Molecular Formula	Molecular Weight	ESI- SRM Transition 1	ESI- SRM Transition 2
SAmPAP	$C_{12}H_9F_{17}NO_6PSNa_2$	695.1941	650 > 526	650 > 97
diSAmPAP	$C_{24}H_{18}F_{34}N_2O_8PS_2Na$	1226.4475	1203 > 526	1203 > 169

Cationic/Zwitterionic PFAS

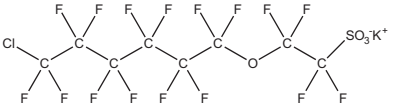
Compound	Molecular Formula	Molecular Weight	ESI+ SRM Transition 1	ESI+ SRM Transition 2
N-AP-FHxSA	$C_{11}H_{13}F_{13}N_2O_2S$	484.2773	485 > 85	485 > 58
N-TAmP-FHxSA	$C_{12}H_{15}F_{13}N_2O_2S$	498.3039	499 > 60	499 > 73
N-CMAmP-6:2FOSA	$C_{15}H_{19}F_{13}N_2O_4S$	570.3666	571 > 104	571 > 58
5:3FTB	$C_{12}H_{14}F_{11}NO_2$	413.2275	414 > 58	414 > 104
5:1:2FTB	$C_{12}H_{13}F_{12}NO_2$	431.2179	432 > 58	432 > 104

Structures of Commonly Analyzed PFAS

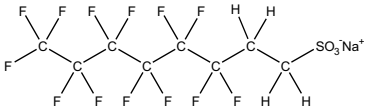
PFSA (example = PFOS)



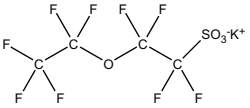
Cl-PFESA (example = 9Cl-PF3ONS)



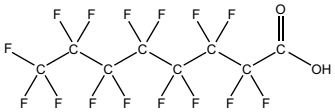
X:2FTS (example = 6:2FTS)



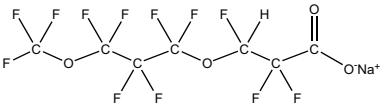
PFESA (example = PFEESA)



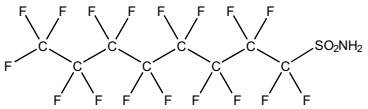
PFCA (example = PFOA)



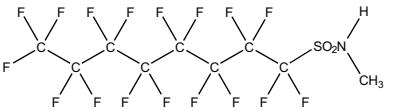
PFECA (example = NaDONA)



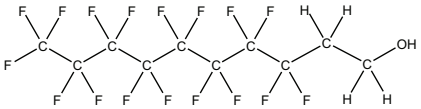
FASA (example = FOSA)



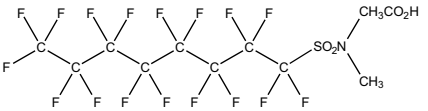
N-alkylFASA (example = N-MeFOSA)



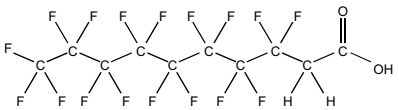
FTOH (example = FOET / 8:2 FTOH)



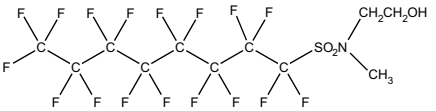
N-alkylFASAA (example = N-MeFOSAA)



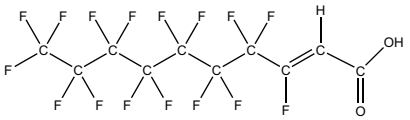
FTCA (example = FOEA / 8:2 FTCA)



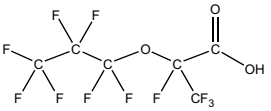
N-alkylFOSE (example = N-MeFOSE)



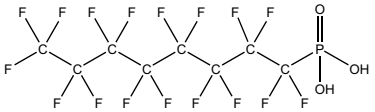
FTUCA (example = FOUEA / 8:2 FTUCA)



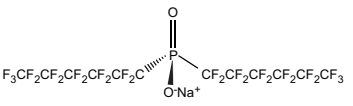
Dimer Acid (example = HFPO-DA)



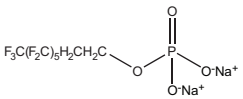
PFAPA (example = PFOPA)



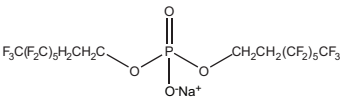
X:XPFPi (example = 6:6PFPi)



PAP (example = 6:2PAP)



diPAP (example = 6:2diPAP)



Typical HPLC/UPLC Flow Rates

Column ID (mm)	Particle Size 5 µm	Particle Size 3 µm	Particle Size 2 µm	Particle Size sub 2 µm*
1.0	0.05 mL/min	0.07 mL/min	0.10 mL/min	0.15 mL/min
2.1	0.2	0.3	0.5	0.4 - 0.6
3.2	0.5	0.7	1.0	0.8
4.6	1.0	1.5	2.0	1.0

*Flow rate may be limited by column back pressure.

Common Buffers

Buffer Type	pKa	Buffer pH Range	Examples
Acetate	4.8	3.8 - 5.8	Ammonium Acetate Acetic Acid Sodium Acetate
Ammonia	9.2	8.2 - 10.2	Ammonium Hydroxide Ammonium Phosphate (mono- and di-basic) Ammonium Carbonate
Borate	9.2	8.2 - 10.2	Sodium Borate Boric Acid
Carbonate	10.2	9.2 - 11.2	Ammonium Carbonate Ammonium Bicarbonate
Citrate	3.1 4.7 5.4	2.1 - 4.1 3.7 - 5.7 4.4 - 6.4	Trisodium Citrate Diammonium Citrate Triammonium Citrate Citric Acid
Formate	3.8	2.8 - 4.8	Ammonium Formate Formic Acid
Phosphate	2.1 7.2 12.3	1.1 - 3.1 6.2 - 8.2 11.3 - 13.3	Potassium Phosphate Monobasic Potassium Phosphate Dibasic Potassium Phosphate Tribasic Phosphoric acid

Conversion Factors for Units of Pressure Measurement

	PSI	*bar*	*torr*	*kPa*	*atm*	*inches Hg*	*kg/cm²*
PSI=	1	0.06895	51.713	6.8948	0.068	2.0359	0.0703
bar=	14.5038	1	751.88	100	0.9869	29.5300	1.0197
torr=	0.0193	0.00133	1	0.1330	0.00132	0.0394	0.00136
kPa=	0.1450	0.0100	7.52	1	0.00987	0.2962	0.0102
atm=	14.696	1.0133	760	101.32	1	29.921	1.0332
inches Hg=	0.49612	0.03376	25.400	3.376	0.0334	1	0.0345
kg/cm²=	14.223	0.9806	735.5	98.06	0.967	28.958	1

Grow with us

The popularity of our Reference and Handling Guide for Halogenated Aromatic Compounds prompted us to introduce this *Quick Reference Guide for Perfluoroalkyl and Polyfluoroalkyl Substances (PFAS)*. A full *Reference and Handling Guide for PFAS* containing information on stability, analytical challenges, and recommended storage is available on our website.

If you have any comments or suggestions for future reference guides, or if you would like to receive additional copies, please contact Wellington Laboratories at the address below.

345 Southgate Drive,
Guelph, Ontario, Canada
N1G 3M5

Phone: (519) **822-2436**
Toll-free: **1-800-578-6985**
Fax: (519) **822-2849**
Email: **info@well-labs.com**
Internet: **www.well-labs.com**