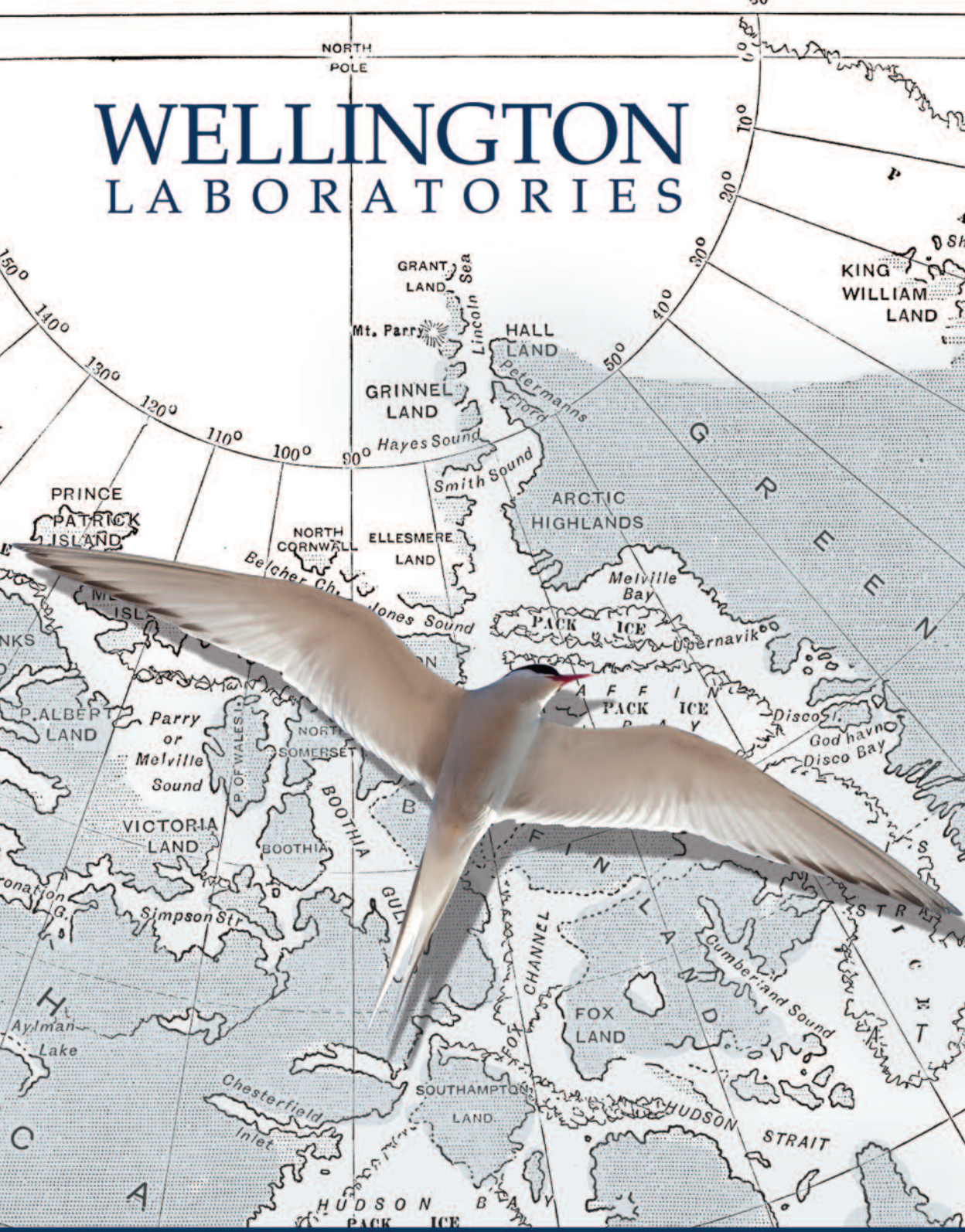


# WELLINGTON LABORATORIES



QUICK REFERENCE GUIDE:  
PERFLUOROALKYL COMPOUNDS



# GUIDELINES FOR THE USE AND HANDLING OF WELLINGTON'S FLUORINATED PRODUCTS

## HAZARDS

Our products are polyfluorinated alkyl compounds offered as solutions in organic solvents such as methanol, isopropanol and nonane.

Although the maximum concentration is 50 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.**

## **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 using NIST-traceable weights.

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 NIST-traceable.

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

## **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 GC/MS and/or LC/MS.
- ii) monitoring the solutions during storage by GC/MS and/or LC/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.

## Summary of LC/MS/MS Tune Parameters and Transitions

### Perfluoroalkylcarboxylic Acids

| Compound    | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|-------------|--|------------------|----------|----------------|---------------------|-------------------|
| PFBA        | C <sub>4</sub> HF <sub>7</sub> O <sub>2</sub>  | 214.0396         | 10       | 8              | 213                 | 169               |
| PFBA [M+4]  | <sup>13</sup> C <sub>4</sub> HF <sub>7</sub> O <sub>2</sub>                                | 218.0090         | 10       | 8              | 217                 | 172               |
| PFPeA       | C <sub>5</sub> HF <sub>9</sub> O <sub>2</sub>  | 264.0474         | 10       | 9              | 263                 | 219               |
| PFPeA [M+3] | <sup>13</sup> C <sub>3</sub> <sup>12</sup> C <sub>2</sub> HF <sub>9</sub> O <sub>2</sub>   | 267.0244         | 10       | 9              | 266                 | 222               |
| PFPeA [M+5] | <sup>13</sup> C <sub>5</sub> HF <sub>9</sub> O <sub>2</sub>                                | 269.0091         | 10       | 9              | 268                 | 223               |
| PFHxA       | C <sub>6</sub> HF <sub>11</sub> O <sub>2</sub>   | 314.0552         | 10       | 9              | 313                 | 269               |
| PFHxA [M+2] | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>4</sub> HF <sub>11</sub> O <sub>2</sub>  | 316.0399         | 10       | 9              | 315                 | 270               |
| PFHxA [M+5] | <sup>13</sup> C <sub>5</sub> <sup>12</sup> C <sub>1</sub> HF <sub>11</sub> O <sub>2</sub>  | 319.0169         | 10       | 9              | 318                 | 273               |
| PFHpA       | C <sub>7</sub> HF <sub>13</sub> O <sub>2</sub>   | 364.0630         | 15       | 11             | 363                 | 319               |
| PFHpA [M+4] | <sup>13</sup> C <sub>4</sub> <sup>12</sup> C <sub>3</sub> HF <sub>13</sub> O <sub>2</sub>  | 368.0324         | 15       | 11             | 367                 | 322               |
| PFOA        | C <sub>8</sub> HF <sub>15</sub> O <sub>2</sub>   | 414.0708         | 15       | 11             | 413                 | 369               |
| PFOA [M+2]  | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>6</sub> HF <sub>15</sub> O <sub>2</sub>  | 416.0555         | 15       | 11             | 415                 | 370               |
| PFOA [M+4]  | <sup>13</sup> C <sub>4</sub> <sup>12</sup> C <sub>4</sub> HF <sub>15</sub> O <sub>2</sub>  | 418.0402         | 15       | 11             | 417                 | 372               |
| PFOA [M+8]  | <sup>13</sup> C <sub>8</sub> HF <sub>15</sub> O <sub>2</sub>                               | 422.0096         | 15       | 11             | 421                 | 376               |
| PFNA        | C <sub>9</sub> HF <sub>17</sub> O <sub>2</sub>   | 464.0786         | 15       | 11             | 463                 | 419               |
| PFNA [M+5]  | <sup>13</sup> C <sub>5</sub> <sup>12</sup> C <sub>4</sub> HF <sub>17</sub> O <sub>2</sub>  | 469.0404         | 15       | 11             | 468                 | 423               |
| PFNA [M+9]  | <sup>13</sup> C <sub>9</sub> HF <sub>17</sub> O <sub>2</sub>                               | 473.0098         | 15       | 11             | 472                 | 427               |
| PFDA        | C <sub>10</sub> HF <sub>19</sub> O <sub>2</sub>  | 514.0864         | 15       | 13             | 513                 | 469               |
| PFDA [M+2]  | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>8</sub> HF <sub>19</sub> O <sub>2</sub>  | 516.0711         | 15       | 13             | 515                 | 470               |
| PFDA [M+6]  | <sup>13</sup> C <sub>6</sub> <sup>12</sup> C <sub>4</sub> HF <sub>19</sub> O <sub>2</sub>  | 520.0405         | 15       | 13             | 519                 | 474               |
| PFUdA       | C <sub>11</sub> HF <sub>21</sub> O <sub>2</sub>  | 564.0942         | 15       | 13             | 563                 | 519               |
| PFUdA [M+2] | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>9</sub> HF <sub>21</sub> O <sub>2</sub>  | 566.0789         | 15       | 13             | 565                 | 520               |
| PFUdA [M+7] | <sup>13</sup> C <sub>7</sub> <sup>12</sup> C <sub>4</sub> HF <sub>21</sub> O <sub>2</sub>  | 571.0407         | 15       | 13             | 570                 | 525               |
| PFDoA       | C <sub>12</sub> HF <sub>23</sub> O <sub>2</sub>  | 614.1020         | 20       | 13             | 613                 | 569               |
| PFDoA [M+2] | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>10</sub> HF <sub>23</sub> O <sub>2</sub> | 616.0867         | 20       | 13             | 615                 | 570               |
| PFTrDA      | C <sub>13</sub> HF <sub>25</sub> O <sub>2</sub>  | 664.1098         | 22       | 15             | 663                 | 619               |
| PFTeDA      | C <sub>14</sub> HF <sub>27</sub> O <sub>2</sub>  | 714.1176         | 15       | 14             | 713                 | 669               |
| PFHxDA      | C <sub>16</sub> HF <sub>31</sub> O <sub>2</sub>  | 814.1332         | 25       | 15             | 813                 | 769               |
| PFODA       | C <sub>18</sub> HF <sub>35</sub> O <sub>2</sub>  | 914.1488         | 25       | 15             | 913                 | 869               |

### Perfluoroalkylsulfonates

| Compound      | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|---------------|--|------------------|----------|----------------|---------------------|-------------------|
| KPFBS         | C <sub>4</sub> F <sub>9</sub> SO <sub>3</sub> K  | 338.1901         | 40       | 25             | 299                 | 99                |
| NaPFHxS       | C <sub>6</sub> F <sub>13</sub> SO <sub>3</sub> Na  | 422.0972         | 50       | 30             | 399                 | 99                |
| NaPFHxS [M+3] | <sup>13</sup> C <sub>3</sub> <sup>12</sup> C <sub>3</sub> F <sub>13</sub> SO <sub>3</sub> Na | 425.0743         | 50       | 30             | 402                 | 99                |
| NaPFHxS [M+4] | C <sub>6</sub> F <sub>13</sub> S <sup>18</sup> O <sub>2</sub> <sup>16</sup> ONa              | 426.0968         | 50       | 30             | 403                 | 103               |
| NaPFHpS       | C <sub>7</sub> F <sub>15</sub> SO <sub>3</sub> Na  | 472.1050         | 60       | 35             | 449                 | 99                |
| KPFOS         | C <sub>8</sub> F <sub>17</sub> SO <sub>3</sub> K   | 538.2214         | 60       | 40             | 499                 | 99                |
| NaPFOS        | C <sub>8</sub> F <sub>17</sub> SO <sub>3</sub> Na  | 522.1129         | 62       | 40             | 499                 | 99                |
| NaPFOS [M+4]  | <sup>13</sup> C <sub>4</sub> <sup>12</sup> C <sub>4</sub> F <sub>17</sub> SO <sub>3</sub> Na | 526.0823         | 62       | 40             | 503                 | 99                |
| NaPFOS [M+8]  | <sup>13</sup> C <sub>8</sub> F <sub>17</sub> SO <sub>3</sub> Na                              | 530.0517         | 62       | 40             | 507                 | 99                |
| NaPFDS        | C <sub>10</sub> F <sub>21</sub> SO <sub>3</sub> Na   | 622.1285         | 70       | 50             | 599                 | 99                |
| NaPFDoS       | C <sub>12</sub> F <sub>25</sub> SO <sub>3</sub> Na   | 722.1441         | 80       | 50             | 699                 | 99                |

## Summary of LC/MS/MS Tune Parameters and Transitions

### Perfluorooctanesulfonamides

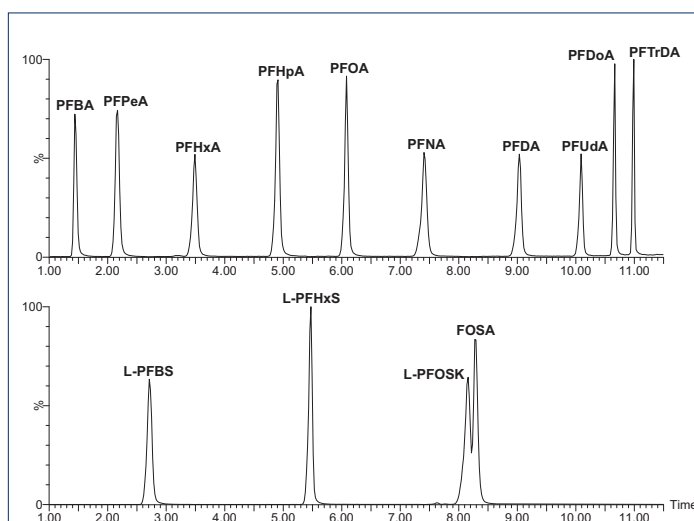
| Compound       | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|----------------|--|------------------|----------|----------------|---------------------|-------------------|
| FOSA           | C <sub>8</sub> H <sub>2</sub> F <sub>17</sub> NO <sub>2</sub> S                | 499.1462         | 40       | 30             | 498                 | 78                |
| FOSA [M+8]     | <sup>13</sup> C <sub>8</sub> H <sub>2</sub> F <sub>17</sub> NO <sub>2</sub> S  | 507.0851         | 40       | 30             | 506                 | 78                |
| N-MeFOSA       | C <sub>9</sub> H <sub>4</sub> F <sub>17</sub> NO <sub>2</sub> S                | 513.1731         | 45       | 25             | 512                 | 169               |
| N-MeFOSA [M+3] | C <sub>9</sub> <sup>2</sup> H <sub>3</sub> HF <sub>17</sub> NO <sub>2</sub> S  | 516.1913         | 45       | 25             | 515                 | 169               |
| N-EtFOSA       | C <sub>10</sub> H <sub>6</sub> F <sub>17</sub> NO <sub>2</sub> S               | 527.2000         | 40       | 25             | 526                 | 169               |
| N-EtFOSA [M+5] | C <sub>10</sub> <sup>2</sup> H <sub>5</sub> HF <sub>17</sub> NO <sub>2</sub> S | 532.2303         | 40       | 25             | 531                 | 169               |

### Perfluorooctanesulfonamidoethanols

| Compound       | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|----------------|--|------------------|----------|----------------|---------------------|-------------------|
| N-MeFOSE       | C <sub>11</sub> H <sub>8</sub> F <sub>17</sub> NO <sub>3</sub> S               | 557.2263         | 40       | 35             | 556                 | 122               |
| N-MeFOSE [M+7] | C <sub>11</sub> <sup>2</sup> H <sub>7</sub> HF <sub>17</sub> NO <sub>3</sub> S | 564.2694         | 40       | 35             | 563                 | 126               |
| N-EtFOSE       | C <sub>12</sub> H <sub>10</sub> F <sub>17</sub> NO <sub>3</sub> S              | 571.2532         | 40       | 33             | 570                 | 136               |
| N-EtFOSE [M+9] | C <sub>12</sub> <sup>2</sup> H <sub>9</sub> HF <sub>17</sub> NO <sub>3</sub> S | 580.3086         | 40       | 33             | 579                 | 142               |

### Perfluorooctanesulfonamidoacetic acids

| Compound        | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|-----------------|--|------------------|----------|----------------|---------------------|-------------------|
| FOSAA           | C <sub>10</sub> H <sub>4</sub> F <sub>17</sub> NO <sub>4</sub> S                             | 557.1829         | 35       | 25             | 556                 | 498               |
| N-MeFOSAA       | C <sub>11</sub> H <sub>6</sub> F <sub>17</sub> NO <sub>4</sub> S                             | 571.2098         | 35       | 20             | 570                 | 419               |
| N-MeFOSAA [M+3] | C <sub>11</sub> <sup>2</sup> H <sub>3</sub> H <sub>3</sub> F <sub>17</sub> NO <sub>4</sub> S | 574.2280         | 32       | 20             | 573                 | 419               |
| N-EtFOSAA       | C <sub>12</sub> H <sub>8</sub> F <sub>17</sub> NO <sub>4</sub> S                             | 585.2367         | 35       | 20             | 584                 | 419               |
| N-EtFOSAA [M+5] | C <sub>12</sub> <sup>2</sup> H <sub>5</sub> H <sub>3</sub> F <sub>17</sub> NO <sub>4</sub> S | 590.2670         | 32       | 20             | 589                 | 419               |



The LC/MS/MS parameters presented were determined using a Micromass Quattro micro API MS and are meant as starting points only. *Further optimization is recommended.*

## Summary of LC/MS/MS Tune Parameters and Transitions

### Fluorinated Telomer Alcohols

| Compound        | Molecular Formula   | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|-----------------|---|------------------|----------|----------------|---------------------|-------------------|
| 4:2 FTOH        | C <sub>6</sub> H <sub>5</sub> F <sub>9</sub> O  | 264.0907         | 15       | 12             | 263                 | 203               |
| 4:2 FTOH [M+4]  | C <sub>6</sub> <sup>2</sup> H <sub>4</sub> HF <sub>9</sub> O  | 268.1150         | 15       | 12             | 266                 | 204               |
| 6:2 FTOH        | C <sub>8</sub> H <sub>5</sub> F <sub>13</sub> O   | 364.1063         | 13       | 9              | 363                 | 303               |
| 6:2 FTOH [M+4]  | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>6</sub> <sup>2</sup> H <sub>2</sub> H <sub>3</sub> F <sub>13</sub> O  | 368.1032         | 13       | 9              | 367                 | 306               |
| 7:2 sFTOH       | C <sub>9</sub> H <sub>5</sub> F <sub>15</sub> O   | 414.1141         | 20       | 14             | 393                 | 219               |
| 8:2 FTOH        | C <sub>10</sub> H <sub>5</sub> F <sub>17</sub> O  | 464.1220         | 14       | 12             | 463                 | 403               |
| 8:2 FTOH [M+4]  | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>8</sub> <sup>2</sup> H <sub>2</sub> H <sub>3</sub> F <sub>17</sub> O  | 468.1188         | 14       | 12             | 467                 | 406               |
| 10:2 FTOH       | C <sub>12</sub> H <sub>5</sub> F <sub>21</sub> O  | 564.1376         | 13       | 11             | 563                 | 503               |
| 10:2 FTOH [M+4] | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>10</sub> <sup>2</sup> H <sub>2</sub> H <sub>3</sub> F <sub>21</sub> O | 568.1344         | 13       | 11             | 567                 | 506               |

### Fluorinated Telomer Acids

| Compound       | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|----------------|--|------------------|----------|----------------|---------------------|-------------------|
| 6:2 FTA        | C <sub>8</sub> H <sub>3</sub> F <sub>13</sub> O <sub>2</sub>   | 378.0899         | 15       | 15             | 377                 | 293               |
| 6:2 FTA [M+2]  | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>6</sub> H <sub>3</sub> F <sub>13</sub> O <sub>2</sub>  | 380.0746         | 15       | 15             | 379                 | 294               |
| 8:2 FTA        | C <sub>10</sub> H <sub>3</sub> F <sub>17</sub> O <sub>2</sub>  | 478.1055         | 14       | 15             | 477                 | 393               |
| 8:2 FTA [M+2]  | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>8</sub> H <sub>3</sub> F <sub>17</sub> O <sub>2</sub>  | 480.0902         | 14       | 15             | 479                 | 394               |
| 10:2 FTA       | C <sub>12</sub> H <sub>3</sub> F <sub>21</sub> O <sub>2</sub>  | 578.1211         | 15       | 15             | 577                 | 493               |
| 10:2 FTA [M+2] | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>10</sub> H <sub>3</sub> F <sub>21</sub> O <sub>2</sub> | 580.1058         | 15       | 15             | 579                 | 494               |
| 3:3 FTA        | C <sub>6</sub> H <sub>5</sub> F <sub>7</sub> O <sub>2</sub>  | 242.0933         | 15       | 8              | 241                 | 177               |
| 5:3 FTA        | C <sub>8</sub> H <sub>5</sub> F <sub>11</sub> O <sub>2</sub>   | 342.1089         | 15       | 10             | 341                 | 237               |
| 7:3 FTA        | C <sub>10</sub> H <sub>5</sub> F <sub>15</sub> O <sub>2</sub>  | 442.1245         | 15       | 10             | 441                 | 337               |

### Fluorinated Telomer Unsaturated Acids

| Compound        | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|-----------------|--|------------------|----------|----------------|---------------------|-------------------|
| 6:2 FTUA        | C <sub>8</sub> H <sub>2</sub> F <sub>12</sub> O <sub>2</sub>   | 358.0835         | 14       | 21             | 357                 | 293               |
| 6:2 FTUA [M+2]  | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>6</sub> H <sub>2</sub> F <sub>12</sub> O <sub>2</sub>  | 360.0682         | 14       | 21             | 359                 | 294               |
| 8:2 FTUA        | C <sub>10</sub> H <sub>2</sub> F <sub>16</sub> O <sub>2</sub>  | 458.0991         | 14       | 21             | 457                 | 393               |
| 8:2 FTUA [M+2]  | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>8</sub> H <sub>2</sub> F <sub>16</sub> O <sub>2</sub>  | 460.0838         | 14       | 21             | 459                 | 394               |
| 10:2 FTUA       | C <sub>12</sub> H <sub>2</sub> F <sub>20</sub> O <sub>2</sub>  | 558.1147         | 14       | 21             | 557                 | 493               |
| 10:2 FTUA [M+2] | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>10</sub> H <sub>2</sub> F <sub>20</sub> O <sub>2</sub> | 560.0995         | 14       | 21             | 559                 | 494               |

### Fluorinated Telomer Sulfonates

| Compound | Molecular Formula   | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|----------|---|------------------|----------|----------------|---------------------|-------------------|
| 4:2 FTS  | C <sub>6</sub> H <sub>4</sub> F <sub>9</sub> SO <sub>3</sub> Na   | 350.1354         | 25       | 20             | 327                 | 307               |
| 6:2 FTS  | C <sub>8</sub> H <sub>4</sub> F <sub>13</sub> SO <sub>3</sub> Na  | 450.1510         | 25       | 20             | 427                 | 407               |
| 8:2 FTS  | C <sub>10</sub> H <sub>4</sub> F <sub>17</sub> SO <sub>3</sub> Na | 550.1666         | 25       | 25             | 527                 | 507               |

## Summary of LC/MS/MS Tune Parameters and Transitions

### Perfluoroalkylphosphonic acids

| Compound  | Molecular Formula   | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|-----------|---|------------------|----------|----------------|---------------------|-------------------|
| PFHxPA    | C <sub>6</sub> H <sub>2</sub> F <sub>13</sub> PO <sub>3</sub>   | 400.0331         | 40       | 35             | 399                 | 79                |
| PFOPA     | C <sub>8</sub> H <sub>2</sub> F <sub>17</sub> PO <sub>3</sub>   | 500.0487         | 40       | 35             | 499                 | 79                |
| PFDPA     | C <sub>10</sub> H <sub>2</sub> F <sub>21</sub> PO <sub>3</sub>  | 600.0643         | 45       | 35             | 599                 | 79                |
| Cl-PFHxPA | C <sub>6</sub> H <sub>2</sub> ClF <sub>12</sub> PO <sub>3</sub> | 416.4877         | 40       | 35             | 415                 | 79                |

### Sodium Perfluoroalkyl Phosphinates

| Compound | Molecular Formula                                  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|----------|--|------------------|----------|----------------|---------------------|-------------------|
| 6:6PFPI  | C <sub>12</sub> F <sub>26</sub> PO <sub>2</sub> Na | 724.0528         | 80       | 45             | 701                 | 401               |
| 6:8PFPI  | C <sub>14</sub> F <sub>30</sub> PO <sub>2</sub> Na | 824.0685         | 80       | 45             | 801                 | 501               |
| 8:8PFPI  | C <sub>16</sub> F <sub>34</sub> PO <sub>2</sub> Na | 924.0841         | 80       | 45             | 901                 | 501               |

### Mono-Substituted Polyfluorinated Phosphate Esters

| Compound     | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|--------------|--|------------------|----------|----------------|---------------------|-------------------|
| 6:2PAP       | C <sub>8</sub> H <sub>4</sub> F <sub>13</sub> PO <sub>4</sub> Na <sub>2</sub>  | 488.0500         | 25       | 20             | 443                 | 97                |
| 6:2PAP [M+2] | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>6</sub> H <sub>4</sub> F <sub>13</sub> PO <sub>4</sub> Na <sub>2</sub> | 490.0347         | 25       | 20             | 445                 | 97                |
| 8:2PAP       | C <sub>10</sub> H <sub>4</sub> F <sub>17</sub> PO <sub>4</sub> Na <sub>2</sub>   | 588.0656         | 25       | 20             | 543                 | 97                |
| 8:2PAP [M+2] | <sup>13</sup> C <sub>2</sub> <sup>12</sup> C <sub>8</sub> H <sub>4</sub> F <sub>17</sub> PO <sub>4</sub> Na <sub>2</sub> | 590.0503         | 25       | 20             | 545                 | 97                |

### Di-Substituted Polyfluorinated Phosphate Esters

| Compound       | Molecular Formula  | Molecular Weight | Cone (V) | Collision (eV) | Precursor Ion (m/z) | Product Ion (m/z) |
|----------------|--|------------------|----------|----------------|---------------------|-------------------|
| 6:2diPAP       | C <sub>16</sub> H <sub>8</sub> F <sub>26</sub> PO <sub>4</sub> Na  | 812.1592         | 30       | 20             | 789                 | 443               |
| 6:2diPAP [M+4] | <sup>13</sup> C <sub>4</sub> <sup>12</sup> C <sub>12</sub> H <sub>8</sub> F <sub>26</sub> PO <sub>4</sub> Na | 816.1286         | 30       | 20             | 793                 | 445               |
| 8:2diPAP       | C <sub>20</sub> H <sub>8</sub> F <sub>34</sub> PO <sub>4</sub> Na  | 1012.1904        | 35       | 25             | 989                 | 543               |
| 8:2diPAP [M+4] | <sup>13</sup> C <sub>4</sub> <sup>12</sup> C <sub>16</sub> H <sub>8</sub> F <sub>34</sub> PO <sub>4</sub> Na | 1016.1598        | 35       | 25             | 993                 | 545               |

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

|                             |               |              |
|-----------------------------|---------------|--------------|
| <sup>12</sup> C = 12.011    | N = 14.0067   | P = 30.97376 |
| <sup>13</sup> C = 13.003355 | O = 15.9994   | Na = 22.9898 |
| H = 1.00794                 | F = 18.998403 | K = 39.0983  |
| <sup>2</sup> H = 2.014      | S = 32.064    |              |

Reference = <http://web/utk.edu/~bartmess/massabun.txt>

**The LC/MS/MS parameters presented were determined using a Micromass Quattro micro API MS and are meant as starting points only. *Further optimization is recommended.***

## General Structure of Various Fluorinated Compounds

|                     |  |                                    |               |  |
|---------------------|--|------------------------------------|---------------|--|
| <b>PFCA</b>         | $R_f\text{-CO}_2\text{H}$  | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 20 |  |
| <b>PFAS</b>         | $R_f\text{-SO}_3^-$  | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 20 |  |
| <b>PFASI</b>        | $R_f\text{-SO}_2^-$  | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 20 |  |
| <b>FOSA</b>         | $R_f\text{-SO}_2\text{NH}_2$   | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 7$       |  |
| <b>N-alkylFOSA</b>  | $R_f\text{-SO}_2\text{NRR}'$   | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 7$       | R = Me or Et<br>R' = H                                     |
| <b>N-alkylFOSAA</b> | $R_f\text{-SO}_2\text{NRR}'$   | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 7$       | R = $\text{CH}_2\text{CO}_2\text{H}$<br>R' = H or Me or Et |
| <b>N-alkylFOSE</b>  | $R_f\text{-SO}_2\text{NRR}'$   | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 7$       | R = $\text{CH}_2\text{CH}_2\text{OH}$<br>R' = Me or Et     |
| <b>FTOH</b>         | $R_f\text{-CH}_2\text{CH}_2\text{OH}$<br>$R_f\text{-CH}(\text{OH})\text{CH}_3$ | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 15 |  |
| <b>FTA</b>          | $R_f\text{-CH}_2\text{CO}_2\text{H}$   | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 15 |  |
| <b>FTUA</b>         | $R_f\text{-CF}=\text{CHCO}_2\text{H}$  | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 15 |  |
| <b>PFAPA</b>        | $R_f\text{-PO}_3\text{H}_2$  | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 15 |  |
| <b>PFPI</b>         | $(R_f)_2\text{P}(\text{O})\text{OH}$   | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 10 |  |
| <b>PAP</b>          | $R_f\text{CH}_2\text{CH}_2\text{OP}(\text{O})(\text{OH})_2$                    | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 10 |  |
| <b>diPAP</b>        | $(R_f\text{CH}_2\text{CH}_2\text{O})_2\text{P}(\text{O})\text{OH}$             | $R_f = \text{CF}_3(\text{CF}_2)_n$ | $n = 0$ to 10 |  |

## Commonly Used Units of Measure

| wt/wt basis |                  |                 |       | wt/vol basis |                 |                  |                   |
|-------------|------------------|-----------------|-------|--------------|-----------------|------------------|-------------------|
| <b>ppm</b>  | mg/kg            | $\mu\text{g/g}$ | ng/mg | <b>ppm</b>   | mg/l            | $\mu\text{g/ml}$ | ng/ $\mu\text{l}$ |
| <b>ppb</b>  | $\mu\text{g/kg}$ | ng/g            | pg/mg | <b>ppb</b>   | $\mu\text{g/l}$ | ng/ml            | pg/ $\mu\text{l}$ |
| <b>ppt</b>  | ng/kg            | pg/g            | fg/mg | <b>ppt</b>   | ng/l            | pg/ml            | fg/ $\mu\text{l}$ |
| <b>ppq</b>  | pg/kg            | fg/g            | ag/mg | <b>ppq</b>   | pg/l            | fg/ml            | ag/ $\mu\text{l}$ |



## Common Acronyms

|              |  |
|--------------|--|
| <b>PFA</b>   | <b>P</b> er <b>f</b> luoro <b>a</b> lky <b>l</b> carboxy <b>l</b> ic <b>a</b> cid                            |
| <b>PFOA</b>  | <b>P</b> er <b>f</b> luoro <b>o</b> ctanecarboxy <b>l</b> ic <b>a</b> cid                                    |
| <b>PFAS</b>  | <b>P</b> er <b>f</b> luoro <b>a</b> lky <b>l</b> sulfon <b>a</b> te  |
| <b>PFOS</b>  | <b>P</b> er <b>f</b> luoro <b>o</b> ctan <b>e</b> sulfon <b>a</b> te   |
| <b>PFASi</b> | <b>P</b> er <b>f</b> luoro <b>a</b> lky <b>l</b> sulfon <b>i</b> ate   |
| <b>FOSA</b>  | Per <b>f</b> luoro <b>o</b> ctan <b>e</b> sulfon <b>a</b> mid <b>e</b>                                       |
| <b>FOSAA</b> | Per <b>f</b> luoro <b>o</b> ctan <b>e</b> sulfon <b>a</b> mid <b>o</b> ac <b>e</b> t <b>i</b> c <b>a</b> cid |
| <b>FOSE</b>  | Per <b>f</b> luoro <b>o</b> ctan <b>e</b> sulfon <b>a</b> mid <b>o</b> eth <b>a</b> no <b>l</b>              |
| <b>FTOH</b>  | <b>F</b> luorinated <b>t</b> elomer <b>a</b> lcohol ( <b>-OH</b> functional group)                           |
| <b>FTA</b>   | <b>F</b> luorinated <b>t</b> elomer <b>a</b> cid   |
| <b>FTUA</b>  | <b>F</b> luorinated <b>t</b> elomer <b>u</b> nsaturated <b>a</b> cid   |
| <b>FTS</b>   | <b>F</b> luorinated <b>t</b> elomer <b>s</b> ulfon <b>a</b> te   |
| <b>PFAPA</b> | <b>P</b> er <b>f</b> luoro <b>a</b> lky <b>l</b> phosphon <b>i</b> c <b>a</b> cid                            |
| <b>PFPi</b>  | <b>P</b> er <b>f</b> luoro <b>a</b> lky <b>l</b> phosphin <b>a</b> te  |
| <b>PAP</b>   | Mono-substituted <b>p</b> oly <b>f</b> luoro <b>a</b> lky <b>l</b> phosph <b>a</b> te ester                  |
| <b>diPAP</b> | <b>D</b> i-substituted <b>p</b> oly <b>f</b> luoro <b>a</b> lky <b>l</b> phosph <b>a</b> te ester            |
| <b>PFAI</b>  | <b>P</b> er <b>f</b> luoro <b>a</b> lky <b>l</b> <b>i</b> odid <b>e</b>                                      |
| <b>SFA</b>   | <b>S</b> em <b>i</b> fluorinated <b>a</b> lkane  |
| <b>FTI</b>   | <b>F</b> luorinated <b>t</b> elomer <b>i</b> odid <b>e</b>   |
| <b>FTO</b>   | <b>F</b> luorinated <b>t</b> elomer <b>o</b> lefin   |
| <b>FTAC</b>  | <b>F</b> luorinated <b>t</b> elomer <b>a</b> crylate   |

## Conversion Factors and Units of Measure

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

## Typical HPLC/UPLC Flow Rates

| Column ID (mm) | Particle Size 5 $\mu$ m | Particle Size 3 $\mu$ m | Particle Size 2 $\mu$ m | Particle Size sub 2 $\mu$ m* |
|----------------|-------------------------|-------------------------|-------------------------|------------------------------|
| 1.0            | 0.05 ml/min             | 0.07 ml/min             | 0.1 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

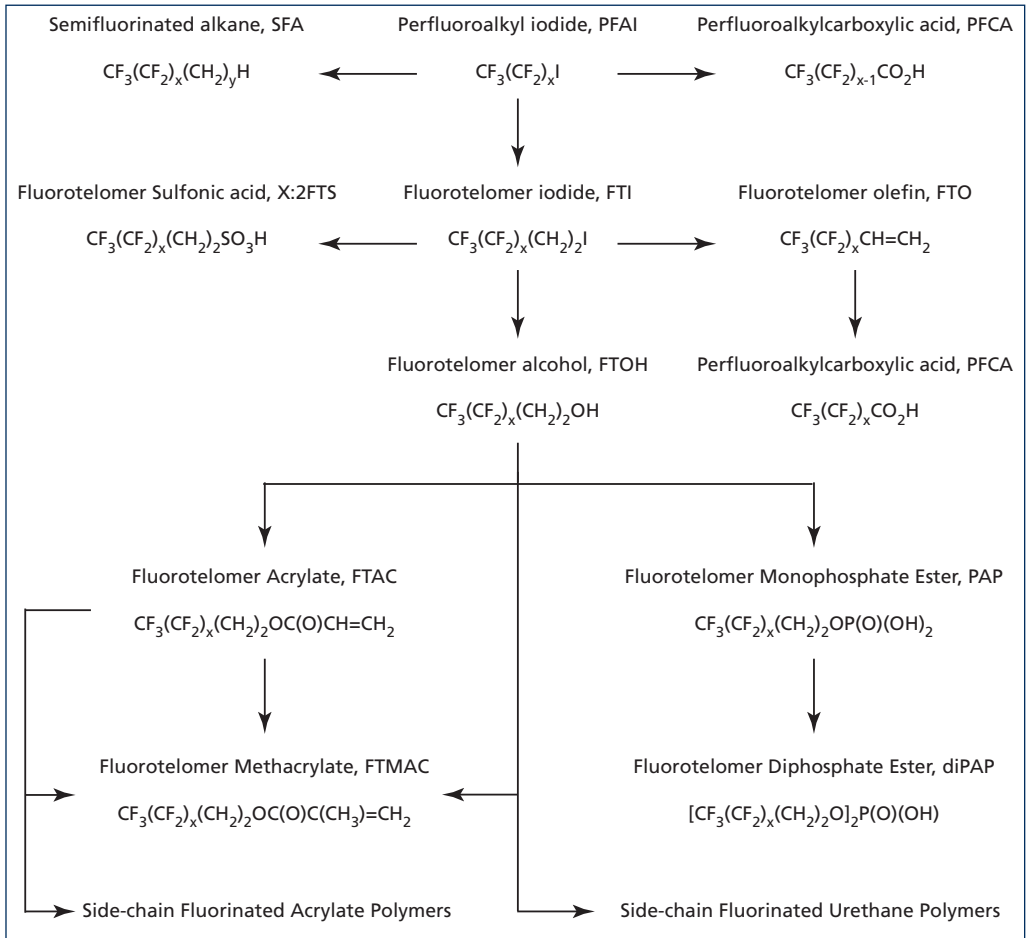
| Buffer Type | pKa                | Buffer pH Range                       | Examples  |
|-------------|--------------------|---------------------------------------|---|
| Acetate     | 4.8                | 3.8 - 5.8                             | Ammonium Acetate<br>Acetic Acid<br>Sodium Acetate   |
| Ammonia     | 9.2                | 8.2 - 10.2                            | Ammonium Hydroxide<br>Ammonium Phosphate (mono- and di-basic)<br>Ammonium Carbonate                             |
| Borate      | 9.2                | 8.2 - 10.0                            | Sodium Borate<br>Boric Acid   |
| Carbonate   | 10.2               | 9.2 - 11.2                            | Ammonium Carbonate<br>Ammonium Bicarbonate  |
| Citrate     | 3.1<br>4.7<br>5.4  | 2.1 - 4.1<br>3.7 - 5.7<br>4.4 - 6.4   | Trisodium Citrate<br>Diammonium Citrate<br>Triammonium Citrate<br>Citric Acid                                   |
| Formate     | 3.8                | 2.8 - 4.8                             | Ammonium Formate<br>Formic Acid   |
| Phosphate   | 2.1<br>7.2<br>12.3 | 1.1 - 3.1<br>6.2 - 8.2<br>11.3 - 13.3 | Potassium Phosphate Monobasic<br>Potassium Phosphate Dibasic<br>Potassium Phosphate Tribasic<br>Phosphoric acid |

## Conversion Factors for Units of Pressure Measurement

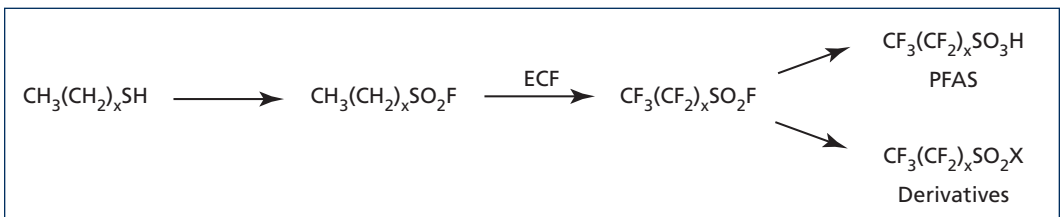
|                      | PSI     | bar     | torr   | kPa    | atm     | inches Hg | kg/cm <sup>2</sup> |
|----------------------|---------|---------|--------|--------|---------|-----------|--------------------|
| PSI=                 | 1       | 0.06895 | 51.713 | 6.8948 | 0.068   | 2.0359    | 0.0703             |
| 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/cm <sup>2</sup> = | 14.223  | 0.9806  | 735.5  | 98.06  | 0.967   | 28.958    | 1                  |

# The Telomerization and ECF Processes

Although perfluorinated products were historically produced using electrochemical fluorination, today the majority of industrially manufactured perfluorinated compounds are obtained through the telomerization process. This process generates a perfluoroalkyl iodide intermediate which can be utilized to produce a variety of fully and partially fluorinated compounds. The flow-chart below illustrates the synthesis of common perfluorinated products from a perfluoroalkyl iodide (*Integr Environ Assess Manag*, **2011**, 7, 513-541).



Perfluoroalkanesulfonates (PFAS) and perfluoroalkanesulfonyl fluorides are still being produced using electrochemical fluorination (ECF). This method commonly results in a mixture of linear and branched perfluorinated isomers and homologues.





The popularity of our Reference and Handling Guide for Halogenated Aromatic Compounds has prompted us to introduce this *Quick Reference Guide for Perfluoroalkyl Compounds*. A full *Reference and Handling Guide for Perfluoroalkyl Compounds* containing information on stability, analytical challenges, and recommended storage is available on our web-site.

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.

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