The calculated reference masses are based on the following values for isotopic masses:

- $^1$H 1.0078250321 u
- $^{12}$C 12.0000000000 u
- $^{13}$C 13.0033548378 u
- $^{16}$O 15.9949146221 u
- $^{35}$Cl 34.9688527100 u
- $^{37}$Cl 36.9659026000 u
- $^{79}$Br 78.9183376 u
- $^{81}$Br 80.9162910 u

All listed masses refer to singly positively charged ions. The mass of the electron (0.000548579911 u) was taken into account for the calculation of the ionic masses. Reference: Nuclear Phys. A 1995, 595, 409-480; J. Phys. Chem. Ref. Data 1999, 28 (6), 1713-1852 and references cited therein.
Polybrominated Diphenyl Ethers

Reference Mass Table

Calibration Solutions

<table>
<thead>
<tr>
<th>Native PBDEs</th>
<th>CS1</th>
<th>CS2</th>
<th>CS3</th>
<th>CS4</th>
<th>CS5</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[mg/mL]</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4-Bromodiphenyl ether (3)</td>
<td>1</td>
<td>5</td>
<td>20</td>
<td>100</td>
<td>400</td>
</tr>
<tr>
<td>2,4-Dibromodiphenyl ether (7)</td>
<td>1</td>
<td>5</td>
<td>20</td>
<td>100</td>
<td>400</td>
</tr>
<tr>
<td>4,4’-Dibromodiphenyl ether (15)</td>
<td>1</td>
<td>5</td>
<td>20</td>
<td>100</td>
<td>400</td>
</tr>
<tr>
<td>2,2’-Aryl-hexabromodiphenyl ether (47L)</td>
<td>1</td>
<td>5</td>
<td>20</td>
<td>100</td>
<td>400</td>
</tr>
<tr>
<td>2,2’,4,4’-Tetrabromodiphenyl ether (99L)</td>
<td>1</td>
<td>5</td>
<td>20</td>
<td>100</td>
<td>400</td>
</tr>
<tr>
<td>2,2’,4,4’,5,5’-Hexabromodiphenyl ether (13L)</td>
<td>1</td>
<td>5</td>
<td>20</td>
<td>100</td>
<td>400</td>
</tr>
</tbody>
</table>

All concentrations are given for calibration solutions BDE-CVS-A as available from Wellington Laboratories Inc., Ontario, Canada.

13C Labeled PBDE Standards

<table>
<thead>
<tr>
<th>Native PBDEs</th>
<th>CS1</th>
<th>CS2</th>
<th>CS3</th>
<th>CS4</th>
<th>CS5</th>
</tr>
</thead>
<tbody>
<tr>
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<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
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<tr>
<td>4-Bromodiphenyl ether (3)</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>2,4-Dibromodiphenyl ether (7)</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>4,4’-Dibromodiphenyl ether (15L)</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>2,2’,4,4’-Tetrabromodiphenyl ether (28L)</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
</tbody>
</table>

Spectra acquired @ 40eV (source temperature 280 °C). With bromination degree higher than 4, the [M-2Br]+ ion is more abundant than the M+ ion. The fragmentation pattern is dependent on the ion source temperature.

Experimental conditions: EI, 40 eV, ion source temp. 280 °C, R = 10,000 (10 % valley), Ref.: PFK, GC: Trace GC Ultra, DB5ms (15/0.25/0.1), constant flow 1 mL/min, splitless injection (1 min), inj. Temp. 280 °C, oven program 120 °C/2 min – 230 °C/15 – 270 °C/5 – 330 °C/10, transfer line temp. 280 °C.