Accurate Mass LC/Q-TOF
A New Direction in Quantitative PFAS Analysis

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A new class of ‘forever chemicals’ is an emerging threat to our health and environment

98% of Canadians have PFAS chemicals in their blood
PFAS Quantitation

• Traditionally preformed with liquid chromatography and triple quadrupole mass spectrometry

• Can it be done by LC/Q-TOF instead?
  • What acquisition mode should I use?
## USEPA Method 533 Target Compounds

<table>
<thead>
<tr>
<th>Analyte</th>
<th>Abbreviation</th>
<th>Compound Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perfluorobutanoic acid</td>
<td>PFBA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluoro-3-methoxypropanoic acid</td>
<td>PFMPA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluoropentanoic acid</td>
<td>PFPeA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluoro-4-methoxybutanoic acid</td>
<td>PFMBMA</td>
<td>acid</td>
</tr>
<tr>
<td>Nonfluoro-3,6-dioxaheptanoic acid</td>
<td>NFDHA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluoroheptanoic acid</td>
<td>PFHeA</td>
<td>acid</td>
</tr>
<tr>
<td>Hexafluoropropylene oxide dimer acid</td>
<td>HFPO-DA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluoroheptanoic acid</td>
<td>PFHpA</td>
<td>acid</td>
</tr>
<tr>
<td>4,8-Dioxa-3H-perfluorononanoic acid</td>
<td>ADONA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluorooctanoic acid</td>
<td>PFOA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluorononanoic acid</td>
<td>PFNA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluorodecanoic acid</td>
<td>PFDA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluoroundecanoic acid</td>
<td>PFUnA</td>
<td>acid</td>
</tr>
<tr>
<td>Perfluorododecanoic acid</td>
<td>PFDoA</td>
<td>acid</td>
</tr>
<tr>
<td>1H,1H,2H,2H-Perfluorohexane sulfonic acid (4:2 Fluorotelomer sulfonate)</td>
<td>4:2FTS</td>
<td>FTS</td>
</tr>
<tr>
<td>1H,1H,2H,2H-Perfluorooctane sulfonic acid (6:2 Fluorotelomer Sulfonate)</td>
<td>6:2FTS</td>
<td>FTS</td>
</tr>
<tr>
<td>1H,1H,2H,2H-Perfluorodecanoic sulfonic acid (8:2 Fluorotelomer sulfonate)</td>
<td>8:2FTS</td>
<td>FTS</td>
</tr>
<tr>
<td>Perfluorobutanesulfonic acid</td>
<td>PFBS</td>
<td>sulfonate</td>
</tr>
<tr>
<td>Perfluoropentanesulfonic acid</td>
<td>PFPeS</td>
<td>sulfonate</td>
</tr>
<tr>
<td>Perfluorohexanesulfonic acid</td>
<td>PFHxS</td>
<td>sulfonate</td>
</tr>
<tr>
<td>Perfluorodecanesulfonic acid</td>
<td>PFHdS</td>
<td>sulfonate</td>
</tr>
<tr>
<td>Perfluorooctanesulfonic acid</td>
<td>PFOS</td>
<td>sulfonate</td>
</tr>
<tr>
<td>Perfluoro (2-ethoxyethane) sulfonic acid</td>
<td>PFEEE A</td>
<td>sulfonate</td>
</tr>
<tr>
<td>9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic acid</td>
<td>9Cl-PF3ONS</td>
<td>sulfonate</td>
</tr>
<tr>
<td>11-Chloroicosfluoro-3-oaundecane-1-sulfonic acid</td>
<td>11Cl-PF3OUnS</td>
<td>sulfonate</td>
</tr>
</tbody>
</table>
## LC Instrument Conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>LC</td>
<td><strong>TQ &amp; All Ions</strong> work: Agilent 1260 series Infinity binary pump, G1367E Infinity ALS, G1316A Infinity thermostated column compartment</td>
</tr>
<tr>
<td></td>
<td><strong>Targeted MS/MS &amp; Q-RAI</strong> work: Agilent 1290 series Infinity II – G7120A High Speed Pump, G7167A Multisampler, G7116B MCT thermostated column compartment</td>
</tr>
<tr>
<td>Analytical Column</td>
<td>Agilent ZORBAX Eclipse Plus C18, 3 × 50 mm; 1.8 μm (p/n 959757-302)</td>
</tr>
<tr>
<td>Delay Column</td>
<td>Agilent ZORBAX SB-C18, 4.6 × 50 mm, 3.5 μm (p/n 835975-902)</td>
</tr>
<tr>
<td>Column Temperature</td>
<td>50°C</td>
</tr>
<tr>
<td>Injection Volume</td>
<td>10 μL</td>
</tr>
<tr>
<td>Mobile Phase</td>
<td>A) 20mM Ammonium Acetate in water (LC Grade)</td>
</tr>
<tr>
<td></td>
<td>B) MeOH (LC Grade)</td>
</tr>
<tr>
<td>Gradient Flow Rate</td>
<td>0.4 mL/min</td>
</tr>
<tr>
<td>Gradient Time</td>
<td>%B</td>
</tr>
<tr>
<td>0.0</td>
<td>5</td>
</tr>
<tr>
<td>0.5</td>
<td>5</td>
</tr>
<tr>
<td>3.0</td>
<td>40</td>
</tr>
<tr>
<td>16.0</td>
<td>80</td>
</tr>
<tr>
<td>18.0</td>
<td>80</td>
</tr>
<tr>
<td>20.0</td>
<td>95</td>
</tr>
<tr>
<td>Stop Time</td>
<td>20.0 minutes</td>
</tr>
<tr>
<td>Post Time</td>
<td>6.0 minutes</td>
</tr>
</tbody>
</table>
# MS – Jet Stream ESI Instrument Source Conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>MS</td>
<td>Agilent 6470 Triple Quadrupole MS/MS with Agilent Jet Stream ESI source</td>
</tr>
<tr>
<td></td>
<td>Agilent 6545 &amp; 6546 LC/Q-TOF with Dual Agilent Jet Stream ESI source</td>
</tr>
<tr>
<td><strong>Source Parameters</strong></td>
<td></td>
</tr>
<tr>
<td>Gas Temperature</td>
<td>230 °C</td>
</tr>
<tr>
<td>Gas Flow</td>
<td>4 L/min</td>
</tr>
<tr>
<td>Nebulizer</td>
<td>20 psi</td>
</tr>
<tr>
<td>Sheath Gas Temperature</td>
<td>375 °C</td>
</tr>
<tr>
<td>Sheath Gas Flow</td>
<td>12 L/min</td>
</tr>
<tr>
<td>Capillary Voltage (Neg)</td>
<td>2,500 / 2,000 V</td>
</tr>
<tr>
<td>Nozzle Voltage (Neg)</td>
<td>0 V</td>
</tr>
</tbody>
</table>
## Additional Method-Specific MS Conditions

<table>
<thead>
<tr>
<th>Method</th>
<th>Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>LC/TQ</td>
<td>d-MRM Transitions</td>
</tr>
<tr>
<td>LC/Q-TOF – TOF Acquisition - All Ions</td>
<td>TOF parameters, Acquisition rates &amp; Collision Energies</td>
</tr>
<tr>
<td>LC/Q-TOF – Targeted MS/MS Acquisition</td>
<td>TOF parameters, Acquisition rates &amp; Targeted transitions</td>
</tr>
<tr>
<td>LC/Q-TOF – Data Independent Acquisition - Q-RAI</td>
<td>TOF parameters, Acquisition rates &amp; Quadrupole Windows</td>
</tr>
</tbody>
</table>
LC/TQ

- Gold standard for quantitation
- Highest sensitivity, excellent selectivity and specificity
- USEPA approved methodology
- Unique fragmentation and collision energy voltages for each product ion
LC/Q-TOF

• Why would you want to quantitate PFAS on a LC/Q-TOF rather than an LC/TQ?

  • One instrument lab
  
  • Able to perform target and non-target analysis
  
  • Accurate mass for assurance of highest quality compound identification
  
  • Suspect screening without standards
**LC/Q-TOF – TOF Acquisition - All Ions**

### Spectral Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>MS TOF</td>
<td></td>
</tr>
<tr>
<td>Fragmentor</td>
<td>100 V</td>
</tr>
<tr>
<td>Skimmer</td>
<td>65 V</td>
</tr>
<tr>
<td>Oct 1 RF Vpp</td>
<td>750 V</td>
</tr>
</tbody>
</table>

### Mass range

- 50 – 1000 m/z

### Acquisition Rate

- 4 spectra/s

### Experiment Table

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Collision Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>20</td>
</tr>
<tr>
<td>4</td>
<td>40</td>
</tr>
</tbody>
</table>
All Ion Acquisition Benefits

✓ All compounds detected
✓ Precursor and fragment ions
✓ Spectral library matching
✓ Simple one-time set up
# LC/Q-TOF – Targeted MS/MS Acquisition

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>MS TOF</strong></td>
<td></td>
</tr>
<tr>
<td>Fragmentor</td>
<td>95 V</td>
</tr>
<tr>
<td>Skimmer</td>
<td>65 V</td>
</tr>
<tr>
<td>Oct 1 RF Vpp</td>
<td>750 V</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Spectral Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>MS</strong></td>
</tr>
<tr>
<td>Mass range</td>
</tr>
<tr>
<td>Acquisition Rate</td>
</tr>
<tr>
<td><strong>MS/MS</strong></td>
</tr>
<tr>
<td>Mass Range</td>
</tr>
<tr>
<td>Acquisition Rate</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compound</th>
<th>Prec. m/z</th>
<th>Ret. Time (min)</th>
<th>Delta Ret. Time (min)</th>
<th>Collision Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>PFBA</td>
<td>212.9813</td>
<td>4.25</td>
<td>0.6</td>
<td>8</td>
</tr>
<tr>
<td>13C3-PFBA</td>
<td>215.9893</td>
<td>4.25</td>
<td>0.6</td>
<td>8</td>
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<tr>
<td>13C4-PFBA</td>
<td>216.9926</td>
<td>4.25</td>
<td>0.6</td>
<td>8</td>
</tr>
<tr>
<td>PFMPA</td>
<td>228.9765</td>
<td>5.16</td>
<td>0.4</td>
<td>12</td>
</tr>
<tr>
<td>PFPeA</td>
<td>262.9788</td>
<td>6.18</td>
<td>0.4</td>
<td>8</td>
</tr>
<tr>
<td>13C5-PFPeA</td>
<td>267.9956</td>
<td>6.18</td>
<td>0.4</td>
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</tr>
<tr>
<td>PFMBa</td>
<td>278.9739</td>
<td>6.85</td>
<td>0.4</td>
<td>12</td>
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<tr>
<td>HFPO-DA-CO2</td>
<td>284.9778</td>
<td>8.95</td>
<td>0.4</td>
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<tr>
<td>13C3-HFPO-DA-13CO2</td>
<td>286.9845</td>
<td>8.95</td>
<td>0.4</td>
<td>4</td>
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<tr>
<td>PFOA</td>
<td>412.9711</td>
<td>12.16</td>
<td>0.4</td>
<td>4</td>
</tr>
<tr>
<td>13C2-PFOA</td>
<td>414.9777</td>
<td>12.16</td>
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<td>4</td>
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<tr>
<td>13C8-PFOA</td>
<td>420.9978</td>
<td>12.16</td>
<td>0.4</td>
<td>4</td>
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<tr>
<td>6:2 FTS</td>
<td>426.9725</td>
<td>12.06</td>
<td>0.4</td>
<td>24</td>
</tr>
<tr>
<td>13C2-6:2 FTS</td>
<td>428.9791</td>
<td>12.06</td>
<td>0.4</td>
<td>24</td>
</tr>
<tr>
<td>PFHpS</td>
<td>448.9384</td>
<td>12.25</td>
<td>0.4</td>
<td>52</td>
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<tr>
<td>PFNA</td>
<td>462.9683</td>
<td>13.64</td>
<td>0.4</td>
<td>4</td>
</tr>
<tr>
<td>13C9-PFNA</td>
<td>471.9985</td>
<td>13.64</td>
<td>0.4</td>
<td>4</td>
</tr>
<tr>
<td>PFOS</td>
<td>498.9357</td>
<td>13.67</td>
<td>0.4</td>
<td>50</td>
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<tr>
<td>13C4-PFOS</td>
<td>502.9492</td>
<td>13.67</td>
<td>0.4</td>
<td>50</td>
</tr>
<tr>
<td>13C8-PFOS</td>
<td>506.9625</td>
<td>13.67</td>
<td>0.4</td>
<td>50</td>
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<tr>
<td>PFDoA</td>
<td>612.9604</td>
<td>16.94</td>
<td>0.4</td>
<td>5</td>
</tr>
<tr>
<td>13C2-PFDoA</td>
<td>614.9604</td>
<td>16.94</td>
<td>0.4</td>
<td>5</td>
</tr>
<tr>
<td>11Cl-PF3OUDs</td>
<td>630.8960</td>
<td>16.53</td>
<td>0.4</td>
<td>32</td>
</tr>
</tbody>
</table>
Targeted MS/MS Acquisition Benefits

✓ Familiar methodology

✓ Decreased background

✓ Specified precursor and fragment ions at unique collision energies

✓ Co-eluting compounds with common fragments are isolated based on precursor mass by the quadrupole
## LC/Q-TOF – Data Independent Acquisition - Q-RAI

### Spectral Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>MS TOF</strong></td>
<td></td>
</tr>
<tr>
<td>Fragmentor</td>
<td>95 V</td>
</tr>
<tr>
<td>Skimmer</td>
<td>65 V</td>
</tr>
<tr>
<td>Oct 1 RF Vpp</td>
<td>750 V</td>
</tr>
</tbody>
</table>

### MS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass range</td>
<td>50 – 1100 m/z</td>
</tr>
<tr>
<td>Acquisition Rate</td>
<td>2 spectra/s</td>
</tr>
</tbody>
</table>

### MS/MS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Range</td>
<td>25 – 800 m/z</td>
</tr>
<tr>
<td>Acquisition Rate</td>
<td>11 spectra/s</td>
</tr>
</tbody>
</table>

### Quadrupole Resolved All Ions (Q-RAI) List Table

<table>
<thead>
<tr>
<th>Start m/z</th>
<th>End m/z</th>
<th>Window Width</th>
<th>Collision Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>98</td>
<td>198</td>
<td>100</td>
<td>20</td>
</tr>
<tr>
<td>196</td>
<td>296</td>
<td>100</td>
<td>20</td>
</tr>
<tr>
<td>294</td>
<td>394</td>
<td>100</td>
<td>20</td>
</tr>
<tr>
<td>392</td>
<td>492</td>
<td>100</td>
<td>20</td>
</tr>
<tr>
<td>490</td>
<td>590</td>
<td>100</td>
<td>20</td>
</tr>
<tr>
<td>588</td>
<td>688</td>
<td>100</td>
<td>20</td>
</tr>
<tr>
<td>686</td>
<td>786</td>
<td>100</td>
<td>20</td>
</tr>
<tr>
<td>210</td>
<td>270</td>
<td>60</td>
<td>5</td>
</tr>
<tr>
<td>510</td>
<td>570</td>
<td>60</td>
<td>10</td>
</tr>
<tr>
<td>330</td>
<td>410</td>
<td>80</td>
<td>40</td>
</tr>
<tr>
<td>440</td>
<td>502</td>
<td>62</td>
<td>40</td>
</tr>
</tbody>
</table>
Q-RAI Acquisition Benefits

- Non-targeted method
- Decreased background
- Reduced risk of co-eluting compounds with common fragments
- Generic method is simple to set up
General Chromatography (LC/TQ) – 1.6 ng/mL (6.3 ng/L in Water)
PFOA Chromatography – 0.4 ng/mL (1.6 ng/L in Water) Targets only

**LC/TQ**

**LC/Q-TOF – All Ions**

**LC/Q-TOF – Targeted MS/MS**

**LC/Q-TOF – Q-RAI**
PFOA Chromatography – 0.4 ng/mL (1.6 ng/L in Water) Targets & Qual

**LC/TQ**

- Transition 413.0 -> 369.0 @ CE = 4 V
- Transition 413.0 -> 169.0 @ CE = 12 V

**LC/Q-TOF – Targeted MS/MS**

- Precursor 412.9711 -> all product ions @ CE = 4 V

[Graphs showing chromatograms and mass spectrometry data]
PFOA Chromatography – 0.4 ng/mL (1.6 ng/L in Water) Targets & Qual

LC/Q-TOF - All Ions

All Ions Comments:
- Collision energies collected: 10, 20, 40 V
- Fragment ions 368.9766 & 168.9907 use CE = 10 V

LC/Q-TOF – Q-RAI

Q-RAI Comments:
- Precursor quadrupole window collision energy = 20 V
- Fragment ion 368.9766 is largely lost at this collision energy and would require a lower CE to be detected
PFOS Chromatography – 0.4 ng/mL (1.6 ng/L in Water) Targets only

**LC/TQ**

- Smoothed Data
- Raw Data

**LC/Q-TOF – All Ions**

- Smoothed Data
- Raw Data

**LC/Q-TOF – Targeted MS/MS**

- Smoothed Data
- Raw Data

**LC/Q-TOF – Q-RAI**

- Smoothed Data
- Raw Data
PFOS Chromatography – 0.4 ng/mL (1.6 ng/L in Water) Targets & Qual

LC/TQ

Transition 498.9 -> 80.0 @ CE = 50 V
Transition 498.9 -> 99.0 @ CE = 50 V

LC/Q-TOF – Targeted MS/MS

Precursor 498.9357 -> all product ions @ CE = 50 V
PFOS Chromatography – 0.4 ng/mL (1.6 ng/L in Water) Targets & Qual

**LC/Q-TOF - All Ions**

- **Smoothed Data**
- **Raw Data**

**All Ions Comments:**
- Collision energies collected: 10, 20, 40 V
- Fragment ions 79.9574 & 98.9558 use CE = 40 V
- ISTD/IDA contribution to both fragment ions

**LC/Q-TOF – Q-RAI**

- **Smoothed Data**
- **Raw Data**

**Q-RAI Comments:**
- Precursor quadrupole window collision energy = 40 V
- No ISTD/IDA fragment ion contribution
## Calibration

<table>
<thead>
<tr>
<th>Method</th>
<th>Quantitation</th>
<th>Calibration Curve Fit</th>
</tr>
</thead>
<tbody>
<tr>
<td>LC/TQ</td>
<td>Quantitation and qualification is done on transitions from quadrupole isolated precursors to product ions</td>
<td>All target compounds have $R^2$ values &gt; 0.999</td>
</tr>
<tr>
<td>LC/Q-TOF – All Ions</td>
<td>Quantitation is done on zero energy (collision cell) accurate mass precursor ions. Coeluting higher energy fragment ions are used to qualify target identification</td>
<td>All target compounds have $R^2$ values &gt; 0.99</td>
</tr>
<tr>
<td>LC/Q-TOF – Targeted MS/MS</td>
<td>Quantitation is done on transitions from precursor ions to accurate mass product ions. Additional transitions are used to qualify target identification</td>
<td>All target compounds have $R^2$ values &gt; 0.98 with the majority &gt; 0.995</td>
</tr>
<tr>
<td>LC/Q-TOF – Q-RAI</td>
<td>Quantitation is done on zero energy (collision cell) accurate mass precursor ions. Coeluting higher energy fragment ions are used to qualify target identification</td>
<td>All target compounds have $R^2$ values &gt; 0.997</td>
</tr>
</tbody>
</table>
Performance – Low System Background

- All instruments (6470 LC/TQ, 6545 LC/Q-TOF and 6546 LC/Q-TOF) were assessed for system background PFAS contamination.

- Evidence of low system background is demonstrated by injecting a laboratory reagent blank (LRB) immediately following the high calibrator and evaluating the concentration of each analyte in the LRB. The LRB is an aliquot of reagent water fortified with the isotope dilution analogues and processed as a field sample. LRBs are used to determine if method analytes are introduced from the lab equipment, reagents, glassware, or extraction apparatus.

- While low trace levels of PFAS were seen in some of the LRBs, which could be due to contamination from sample preparation, etc. unextracted instrument blanks that were 80% MeOH did not contain any significant PFAS contamination, indicating that all the LC-MS systems were PFAS-free.
Performance - %RSD (Graphic)

%RSD

EPA limit

6470 dMRM  6545 All Ions  6546 Targeted MS/MS  6546 QRAI  EPA Limit

Vegon Laboratory Services Ltd.
LCMRL (ng/L)
(or Lowest Calibrator where LCMRL was not determined)
# PFAS Acquisition Mode Review

<table>
<thead>
<tr>
<th>Feature</th>
<th>LC/TQ</th>
<th>Targeted MS/MS</th>
<th>All Ions</th>
<th>Q-RAI</th>
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<tbody>
<tr>
<td>EPA level sensitivity</td>
<td>✔ ✔ ✔</td>
<td>✔ ✔ ✔</td>
<td>✔ ✔ ✔</td>
<td>✔ ✔ ✔</td>
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<tr>
<td>Lowest detection limits</td>
<td>✔ ✔ ✔</td>
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<td>Accurate mass</td>
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<td>✔ ✔ ✔</td>
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<tr>
<td>Fragment ions for confirmation</td>
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<td>✔</td>
<td>✔ ✔ ✔</td>
<td>✔</td>
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<td>Method Setup &amp; ease of adding additional compounds</td>
<td>✔</td>
<td>✔</td>
<td>✔ ✔ ✔</td>
<td>✔</td>
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<tr>
<td>Background/Noise reduction</td>
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<td>Labeled ISTD/IDAs</td>
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<tr>
<td>Simultaneous Unknowns Analysis</td>
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<td>✔</td>
<td>✔ ✔ ✔</td>
<td>✔</td>
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</tbody>
</table>
Summary

• The instrument conditions are presented for quantitation of USEPA 533 PFAS compounds for LC/TQ (dMRM), and LC/Q-TOF (All Ions, Targeted MS/MS and Q-RAI)

• Agilent 6545 and 6546 LC/Q-TOFs have adequate sensitivity, linearity and reproducibility, relative to EPA Method 533 performance criteria, to quantitate PFAS compounds in multiple acquisition modes
Acknowledgements

• Agilent Technologies
  • Tarun Anumol
    • Director, Global Environment & Food Applied Markets
  • James Pyke
    • Senior Application Scientist
  • Chris Klein
    • LC/Q-TOF and IM-QTOF Product Manager