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|---|--|----------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| <b>Method name</b>  | <b>LC-MS/MS-ESI(-)-5<br/>(corresponds to QuPpe M1.6)</b> |                      |                     |                     |                     |                     |                     |                     |
| <b>Instrument</b>   | LC-MS/MS   |                      |                     |                     |                     |                     |                     |                     |
| <b>Chromatographic method</b>                             | LC   |                      |                     |                     |                     |                     |                     |                     |
| <b>Extraction method</b>                                  | QuPpe  |                      |                     |                     |                     |                     |                     |                     |
| Clean-up  | no   |                      |                     |                     |                     |                     |                     |                     |
| Use of AP (analyte protectant)                            | no   |                      |                     |                     |                     |                     |                     |                     |
| Internal standard   | respective IL-IS   |                      |                     |                     |                     |                     |                     |                     |
| <b>Instrument parameters</b>                              |  |                      |                     |                     |                     |                     |                     |                     |
| Ionisation mode   | ESI(-)   |                      |                     |                     |                     |                     |                     |                     |
| Column  | Waters APPC, 130Å, 5 µm, 2.1 mm x 100 mm                 |                      |                     |                     |                     |                     |                     |                     |
| Pre-column  | Waters APPC VanGuard Cartridge, 130Å, 5µm, 2.1 mm X 5 mm |                      |                     |                     |                     |                     |                     |                     |
| Column temperature (°C)                                   | 50   |                      |                     |                     |                     |                     |                     |                     |
| Eluent <b>A1</b>  | 1.2% formic acid in water                                |                      |                     |                     |                     |                     |                     |                     |
| Eluent <b>B1</b>  | 0.5% formic acid in ACN                                  |                      |                     |                     |                     |                     |                     |                     |
| <b>Gradient</b>   | <b>%A</b>  | <b>Flow [mL/min]</b> |                     | <b>Time [ min]</b>  |                     |                     |                     |                     |
|   | 10   | 0.5                  |                     | 0                   |                     |                     |                     |                     |
|   | 10   | 0.5                  |                     | 0.5                 |                     |                     |                     |                     |
|   | 80   | 0.5                  |                     | 1.5                 |                     |                     |                     |                     |
|   | 90   | 0.5                  |                     | 4.5                 |                     |                     |                     |                     |
|   | 90   | 0.5                  |                     | 17.5                |                     |                     |                     |                     |
|   | 10   | 0.5                  |                     | 17.6                |                     |                     |                     |                     |
|   | 10   | 0.5                  |                     | 23                  |                     |                     |                     |                     |
| Injection volume (µL)                                     | <b>10</b>  |                      |                     |                     |                     |                     |                     |                     |
| <b>Acquired mass transitions</b>                          | <b>Target</b>  |                      | <b>Qualifier 1</b>  |                     | <b>Qualifier 2</b>  |                     | <b>Qualifier 3</b>  |                     |
|   | <b>Q1<br/>(m/z)</b>                                      | <b>Q3<br/>(m/z)</b>  | <b>Q1<br/>(m/z)</b> | <b>Q3<br/>(m/z)</b> | <b>Q1<br/>(m/z)</b> | <b>Q3<br/>(m/z)</b> | <b>Q1<br/>(m/z)</b> | <b>Q3<br/>(m/z)</b> |
| Phosphonic acid   | 81   | 79                   | 81                  | 63                  |                     |                     |                     |                     |
| Phosphonic acid <sup>18</sup> O <sub>3</sub> (IL-IS)      | 87   | 85                   | 87                  | 67                  |                     |                     |                     |                     |
| Bromide   | 81   | 81                   | 79                  | 79                  |                     |                     |                     |                     |
| Chlorate  | 83   | 67                   | 85                  | 69                  |                     |                     |                     |                     |
| Chlorate <sup>18</sup> O <sub>3</sub> (IL-IS)             | 89   | 71                   | 91                  | 73                  |                     |                     |                     |                     |
| Trifluoroacetic acid                                      | 113  | 69                   | 113                 | 113                 | 69                  | 19                  |                     |                     |
| Trifluoroacetic acid <sup>13</sup> C <sub>2</sub> (IL-IS) | 115  | 70                   |                     |                     |                     |                     |                     |                     |