Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Enrichment-free analysis of anionic micropollutants in the sub-ppb range in drinking water by capillary electrophoresis-high resolution mass spectrometry

Oliver Höcker, Tobias Bader, Torsten C. Schmidt, Wolfgang Schulz, Christian Neusüß
Fig. S1 Presentation of data from Table S1 of intensities in logarithmic scale of additional analytes found in the water samples
Table S1 Organic and inorganic suspects that were screened in water samples. Only compounds found in all three replicates are listed. Sum formulas were deviated from exact mass on MS1 level

| Group          | Compound                        | Sum formula | Ion            | Theoretical suspect m/z | Experimental m/z | m/z deviation [ppm] | Sample name and measured intensity [counts] |
|----------------|----------------------------------|-------------|----------------|-------------------------|-----------------|---------------------|--------------------------------------------|
|                |                                  |             |                |                         |                 |                     | WS-1 | WS-1-T | WS-2 | WS-2-T | WS-4 | WS-4-C |
| Organic suspects | Methyl bisulfate                 | CH₄O₄S     | [M-H]-         | 110.9758                | 110.9755        | 2.1                 | 6.E+05 | 8.E+06 | -    | 3.E+06 | 1.E+05 | 1.E+05 |
|                | Methanesulfonic acid             | CH₂SO₃     | [M-H]-         | 94.9808                 | 94.9806         | 2.4                 | 1.E+06 | 1.E+06 | 5.E+05 | 2.E+06 | 2.E+06 | 4.E+05 |
|                | Sulfamic acid                    | H₃NSO₃     | [M-H]-         | 95.9761                 | 95.9759         | 2.4                 | -     | 2.E+06 | 2.E+06 | 1.E+06 | 5.E+05 | 6.E+05 |
|                | Ethyl sulfate                    | C₂H₆O₄S    | [M-H]-         | 124.9914                | 124.9911        | 2.2                 | 1.E+05 | 2.E+05 | 8.E+04 | -     | 4.E+05 | 1.E+05 |
|                | Vinyl sulfate                    | C₂H₄O₄S    | [M-H]-         | 122.9758                | 122.9755        | 2.2                 | 2.E+04 | 6.E+04 | -     | -     | 6.E+04 | 4.E+04 |
|                | Acesulfam                        | C₃H₅NO₃S   | [M-H]-         | 161.9867                | 161.9864        | 1.4                 | -     | -     | -     | -     | 4.E+05 | 2.E+05 |
|                | p-Toulenesulfonic acid           | C₄H₆O₃S    | [M-H]-         | 171.0121                | 171.0121        | 0.6                 | 1.E+05 | 1.E+05 | 3.E+05 | 2.E+05 | 3.E+05 | 1.E+06 |
|                | Dimethylbenzenesulfonic acid     | C₉H₁₀O₃S   | [M-H]-         | 185.0278                | 185.0277        | 0.4                 | 8.E+03 | -     | -     | -     | 3.E+04 | 3.E+04 |
|                | Naphthalene-2-sulfonic acid      | C₁₀H₈O₃S   | [M-H]-         | 207.0121                | 207.0118        | 1.7                 | 1.E+06 | -     | -     | -     | 6.E+05 | 2.E+06 |
|                | Cyclamate                        | C₆H₅NO₃S   | [M-H]-         | 178.0543                | 178.0541        | 1.2                 | -     | -     | -     | -     | 1.E+04 | 1.E+04 |
| Inorganic suspects | Bromide                          | Br          | [M]-           | 78.9189                 | 78.9187         | 2.4                 | 2.E+05 | 2.E+04 | 2.E+05 | 4.E+05 | 1.E+06 | 8.E+05 |
|                | Bromate                          | BrO₃        | [M]-           | 126.9036                | 126.9041        | 4.1                 | 4.E+04 | -     | 6.E+04 | 8.E+04 | 2.E+04 | 2.E+04 |
|                | Iodide                           | I           | [M]-           | 126.9050                | 126.9045        | 3.9                 | -     | 4.E+04 | -     | -     | 7.E+04 | 2.E+05 |
|                | Sulfate                          | SO₄         | [M]-           | 82.9541                 | 82.9540         | 2.4                 | 2.E+05 | 3.E+05 | 2.E+05 | 2.E+05 | 3.E+05 | 2.E+05 |
|                | Chlorate                         | ClO₃        | [M]-           | 95.9523                 | 95.9525         | 2.0                 | 8.E+04 | 1.E+05 | 1.E+05 | -     | 1.E+07 | 1.E+07 |
|                | Iodade                           | IO₃         | [M]-           | 174.8898                | 174.8896        | 0.7                 | 3.E+04 | -     | 1.E+05 | -     | 4.E+06 | 3.E+06 |
|                | Phosphate                        | PO₃         | [M]-           | 78.9591                 | 78.9588         | 2.6                 | 4.E+06 | 5.E+06 | 1.E+06 | 9.E+05 | 4.E+06 | 5.E+06 |
| Screened suspects | Pentfluoroethanesulfonic acid    | C₅H₅F₅O₅S | [M-H]-         | 198.9494                | not found       |                     |                   |                   |                   |                   |                   |                   |
|                | Pentfluoroproionic acid          | C₅H₅F₅O₂   | [M-H]-         | 162.9824                | not found       |                     |                   |                   |                   |                   |                   |                   |
|                | Heptfluoropropanesulfonic acid   | C₅H₇F₇O₅S  | [M-H]-         | 248.9462                | not found       |                     |                   |                   |                   |                   |                   |                   |
|                | Perfluorobutanesulfonic acid     | C₅H₈F₈O₅S  | [M-H]-         | 298.9430                | not found       |                     |                   |                   |                   |                   |                   |                   |
|                | Salicylic acid                   | C₇H₆O₃     | [M-H]-         | 138.0322                | not found       |                     |                   |                   |                   |                   |                   |                   |