**One-single extraction procedure for the simultaneous determination of a wide range of polar and non-polar organic contaminants in marine surface water**

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**SUPPLEMENTARY MATERIALS**

**Supplementary Table 1 |** Selected m/z values for the detection and quantification (Q1) of OPEs, PAEs and OCs in GC/MS-SIM mode. Monoisotopic mass and fragments are expressed in g mol-1.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Name** | **Full name** | **Monoisotopic mass** | **Q1** | **Q2** | **Q3** | **Q4** |
| **ORGANOPHOSPHATE ESTERS (OPEs)** |
| TPP | Tripropyl phosphate | 224.1177 | 99 | 141 | 123 | 183 |
| TiBP | Tri-iso-butyl phosphate | 266.1647 | 99 | 155 | 139 |  |
| TnBP | Tri-n-butyl phosphate | 266.1647 | 99 | 155 | 211 |  |
| TCEP | Tris-(2-chloroethyl)phosphate | 283.9539 | 249 | 251 | 143 | 99 |
| TCPP- 1 | Tris- (1-chloro-2-propyl)phosphatea | 326.0008 | 125 | 99 | 157 | 277 |
| TCPP- 2 | Tris- (1-chloro-2-propyl)phosphatea | 326.0008 | 125 | 99 | 157 | 277 |
| TDCP | Tris[2-chloro-1-(chloromethyl)ethyl]phosphate | 427.8839 | 191 | 99 | 381 | 209 |
| TPhP | Triphenyl phosphate | 326.0708 | 326 | 325 | 215 | 170 |
| EHDPP | 2-Ethylhexyl diphenyl phosphate | 362.1647 | 251 | 250 | 362 |  |
| TEHP | Tri(2-ethylhexyl) phosphate | 434.3525 | 99 | 113 | 112 |  |
| TBP-d27 | Tri-n-butyl-d27 phosphate | 293.3341 | 103 | 167 | 231 |  |
| TPhP-d15 | Triphenyl-d15 phosphate | 341.1649 | 341 | 339 | 223 | 180 |
| TCPP-d18 | Tris(2-chloroisopropyl)-d18-phosphate | 344.1138 | 131 | 164 | 193 |  |
| TDCP-d15 | Tris(1,3-dichloro-2-propyl)-d15-phosphate | 442.9781 | 197 | 199 | 217 | 394 |
| TPrP-d21 | Tri-n-propyl-d21 phosphate | 245.2495 | 103 | 131 | 151 | 199 |
| TCEP-d21 | Tris(2-chloroethyl)-d12-phosphate | 296.0292 | 261 | 263 | 148 | 231 |
| MAL-d7 | Malathion-d7 | 337.0800 | 174 | 131 | 128 | 164 |
| **PHTHALATES (PAES)** |
| DMP | Dimethyl phthalate | 194.0579 | 163 |  |  |  |
| DEP | Diethyl phthalate | 222.0892 | 149 | 177 |  |  |
| DiBP | Di-iso-butyl phthalate | 278.1518 | 149 |  |  |  |
| DnBP | Di-n-butyl phthalate | 278.1518 | 149 |  |  |  |
| BBzP | Benzylbutyl phthalate | 390.2770 | 149 | 206 |  |  |
| DEHP | Di-ethylhexyl phthalate | 312.1362 | 149 | 167 | 279 |  |
| DnOP | Di-n-octyl phthalate | 390.2770 | 149 | 279 |  |  |
| DEHP-d4 | Di-ethylhexyl-d4-phthalate | 394.3021 | 153 | 171 | 283 |  |
| DEP-d4 | Dimethyl-d4-phthalate | 226.1143 | 153 | 181 |  |  |
| DnBP-d4 | Di-n-butyl-d4-phthalate | 282.1769 | 153 |  |  |  |
| **ORGANOCHLORINATED (Ocs)** |
| PCB-28 | Polychlorobyphenyl-28 | 255.9613 | 256 | 258 |  |  |
| PCB-52 | Polychlorobyphenyl-52 | 289.9224 | 292 | 290 |  |  |
| PCB-101 | Polychlorobyphenyl-101 | 323.8834 | 326 | 328 |  |  |
| PCB-118 | Polychlorobyphenyl-118 | 323.8834 | 326 | 328 |  |  |
| PCB-138 | Polychlorobyphenyl-138 | 357.8444 | 360 | 362 |  |  |
| PCB-153 | Polychlorobyphenyl-153 | 357.8444 | 360 | 362 |  |  |
| PCB-180 | Polychlorobyphenyl-180 | 391.8054 | 394 | 396 |  |  |
| 4,4-DDT | 4,4-dichlorodiphenyltrichloroethane | 351.9147 | 235 | 237 | 165 |  |
| HCB | Hexachlorobenzene | 281.8131 | 284 | 286 |  |  |
| α-HCH | Alpha-hexachlorocyclohexane | 287.8601 | 219 | 217 | 181 | 183 |
| β-HCH | Beta-hexachlorocyclohexane | 287.8601 | 219 | 217 | 181 | 183 |
| γ-HCH | Gamma-hexachlorocyclohexane | 287.8601 | 219 | 217 | 181 | 183 |
| α-Endosulfan | Alpha-endosulfan | 403.8169 | 241 | 239 | 265 | 195 |
| α-HCH*-d6* | Alpha-hexachlorocyclohexane*-d6* | 293.8977 | 224 | 222 | 185 | 187 |
| 2,4-DDT*-d8* | 2,4-dichlorodiphenyltrichloroethan-*d8* | 359.9649 | 243 | 245 | 173 |  |
| 13C-PCB-28 | Polychlorobyphenyl-28-*13C12* | 268.0016 | 268 | 270 |  |  |
| 13C-PCB-118 | Polychlorobyphenyl-118-*13C12* | 335.9237 | 338 | 336 |  |  |
| α-Endosulfan-d4 | Alpha-endosulfan-d4 | 407.8420 | 237 | 235 | 263 | 343 |
| 4,4-DDT-d8 | 4,4-dichlorodiphenyltrichloroethane-d8 | 359.9649 | 243 | 245 | 173 |  |

a. TCPP isomers

 **Supplementary Table 2 |** Retention times of compounds analyzed by LC-HRMS.

|  |  |  |
| --- | --- | --- |
| **Compound** | **Type** | **Retention time (min)** |
| **BISPHENOLS (BPs)** |
| BPA | analyte | 8.4 |
| BPAF | analyte | 8.9 |
| BPAP | analyte | 9.1 |
| BPF | analyte | 7.7 |
| BPP | analyte | 10.1 |
| BPS | analyte | 6.3 |
| BPZ | analyte | 9.4 |
| 4nOP*-d17* | surrogate | 10.7 |
| BPA*-d16* | internal standard | 8.4 |
| **PERFLUORINATED COMPOUNDS (PFCs)** |
| PFHA | analyte | 7.1 |
| PFHS | analyte | 7.8 |
| PFOA | analyte | 8.4 |
| PFOS | analyte | 8.7 |
| PFOSF | analyte | 8.7 |
| PFHA-*13C5* | internal standard | 7.1 |
| PFHepA-*13C4* | internal standard | 7.8 |
| PFNA-*13C9* | internal standard | 8.8 |
| PFBS-*13C3* | internal standard | 6.4 |
| PFHS-*13C3* | internal standard | 7.8 |
| PFOS-*13C8* | internal standard | 8.7 |

**Supplementary Table 3 |** Contaminant concentrations (ng L-1) found in procedural blanks. Validation experiment refers to section 3.3, and real sample refers to section 3.4.

|  |
| --- |
| **ORGANOPHOSPHATE ESTERS (OPEs)** |
| TPP | n.d. |
| TiBP | 0.39 ± 0.55 |
| TnBP | n.d. |
| TCEP | n.d. |
| TCPPs | 2.95 ± 2.58 |
| TDCP | 0.21 ± 0.36 |
| TPhP | 0.16 ± 0.28 |
| EHDPP | 0.05 ± 0.08 |
| TEHP | n.d. |
| **PHTHALATES (PAEs)** |
| DMP | 1.02 ± 0.88 |
| DEP | n.d. |
| DBP | 1.62 ± 0.24 |
| DiBP | 3.4 ± 0.52 |
| DEHP | n.d. |
| BBP | 1.17 ± 2.02 |
| DnOP | n.d. |
| **BISPHENOLS (BPs)** |
| BPA | 0.2 ± 0.35 |
| BPAF | 0.63 ± 1.1 |
| BPAP | 0.6 ± 1.04 |
| BPF | 0.9 ± 1.56 |
| BPP | n.d. |
| BPS | 0.7 ± 1.21 |
| BPZ | n.d. |
| **PERFLUORINATED COMPOUNDS (PFCs)** |
| PFHA | 0.03 ± 0.06 |
| PFHS | n.d. |
| PFOA | 0.07 ± 0.12 |
| PFOS | n.d. |
| PFOSF | 0.03 ± 0.06 |
| **ORGANOCHLORINATED** |
| PCB-28 | 0.02 ± 0.03 |
| PCB-52 | n.d. |
| PCB-101 | n.d. |
| PCB-118 | n.d. |
| PCB-138 | n.d. |
| PCB-153 | n.d. |
| PCB-180 | n.d. |
| 4,4-DDT | n.d. |
| 4,4-DDD | n.d. |
| 4,4-DDE | n.d. |
| HCB | n.d. |
| α-HCH | n.d. |
| β+γ-HCH | n.d. |

n.d. not detected

**Supplementary Table 4 |** Results from the analysis of OCs in real water samples.

|  |  |
| --- | --- |
|  | Concentrations (ng L-1) |
|  | Estaque | Frioul | Cortiou |
| PCB-28 | 0.4 | 0.5 | 0.6 |
| CB-52 | < LQ | < LQ | 0.4 |
| CB-101 | n.d | n.d | < LQ |
| CB-118 | < LQ | < LQ | 0.3 |
| CB-138 | < LQ | < LQ | < LQ |
| CB-153 | < LQ | < LQ | < LQ |
| CB-180 | < LQ | < LQ | < LQ |
| HCB | < LQ | n.d | < LQ |
| α-HCH | n.d | n.d | 5.9 |
| β+γ-HCH | n.d | n.d | n.d |
| 4,4-DDT | < LQ | < LQ | < LQ |
| α-Endosulfan | 29.0 | 29.2 | 67.0 |
| n.d.= not detected; LQ=limit of quantification  |

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**Supplementary Figure 1 |** LC-QTOF chromatogram of selected contaminants. 1 ng injected from a native standard solution mix. 10 ppm mass tolerance extraction from total ion current (TIC).