

## Supplementary Materials

**Table S1.** SPE conditions employed for each studied family of compounds.

| Family         | Mode     | Cartridge                                                                                   | Sample volume (mL) | pH                                                   | Elution                                         |
|----------------|----------|---------------------------------------------------------------------------------------------|--------------------|------------------------------------------------------|-------------------------------------------------|
| UV stabilizers | On-line  | Oasis HLB Direct Connect HP Column (2.1×30 mm, 20 µm)                                       | 5                  | 3                                                    | MeOH<br>0.1% (v/v) FA                           |
| Cytostatics    | Off-line | <i>Wastewater</i><br>Oasis HLB (6 cc, 500 mg)<br><i>Seawater</i><br>Bond Elut (6 cc, 50 mg) | 250                | <i>Wastewater</i><br>pH=4<br><i>Seawater</i><br>pH=2 | 5 ml MeOH                                       |
| Hormones       | On-line  | Oasis HLB Direct Connect HP Column (2.1×30 mm, 20 µm)                                       | 2                  | 5-6                                                  | H <sub>2</sub> O + 0.1% NH <sub>3</sub><br>MeOH |

**Table S2.** MAE conditions employed for each matrix and family of studied EOCs.

| Family          | Sample amount (g) | Power (W) or temperature (°C) | Time (min) | Solvent | Extractant volume (mL) |
|-----------------|-------------------|-------------------------------|------------|---------|------------------------|
| <b>Sludge</b>   |                   |                               |            |         |                        |
| UV stabilizers  | 1.00              | 300 W                         | 5          | ACN     | 2.0                    |
| Cytostatics     | 0.05              | 60°C                          | 5          | MeOH    | 14                     |
| <b>Sediment</b> |                   |                               |            |         |                        |
| UV stabilizers  | 1.00              | 300 W                         | 5          | ACN     | 2.0                    |
| Cytostatics     | 0.05              | 60°C                          | 5          | MeOH    | 14                     |
| <b>Fish</b>     |                   |                               |            |         |                        |
| UV stabilizers  | 0.10              | 300 W                         | 10         | ACN     | 2.5                    |
| Cytostatics     | 0.05              | 50°C                          | 5          | MeOH    | 7.0                    |
| Hormones        | 0.10              | 450 W                         | 7          | MeOH    | 5.0                    |

**Table S3.** Ionization parameters for the selected families of pollutants.

| Family         | Capillary voltage               | Cone voltage                           | Source temp. | Desolvation temp. | Nitrogen gas flow      |
|----------------|---------------------------------|----------------------------------------|--------------|-------------------|------------------------|
| UV stabilizers | 3.0 kV                          | 50 V                                   | 120 °C       | 450 °C            | 800 L·h <sup>-1</sup>  |
| Cytostatics    | 3.5 kV                          | 40 V                                   | 120 °C       | 400 °C            | 1000 L·h <sup>-1</sup> |
| Hormones       | 3.5 kV (ESI+)<br>-2.5 kV (ESI-) | 20 – 38 V (ESI+)<br>-50 – -65 V (ESI-) | 150 °C       | 500 °C            | 1000 L·h <sup>-1</sup> |

Table S4. Mass spectrometer parameters for the studied compounds.

| Family         | Compound                      | Precursor ion (m/z)      | Cone voltage (ion mode) | Quantification ion, m/z (collision potential, V) | Confirmation ion, m/z (collision potential, V) |
|----------------|-------------------------------|--------------------------|-------------------------|--------------------------------------------------|------------------------------------------------|
| UV stabilizers | UV P                          | 226.2 [M-H] <sup>+</sup> | 40 (ESI+)               | 107.1 (20)                                       | 120.1 (20)                                     |
|                | UV 326                        | 316.3 [M-H] <sup>+</sup> | 40 (ESI+)               | 260.2 (20)                                       | 107.1 (25)                                     |
|                | UV 327                        | 358.3 [M-H] <sup>+</sup> | 60 (ESI+)               | 302.3 (20)                                       | 246.1 (30)                                     |
|                | UV 328                        | 352.3 [M-H] <sup>+</sup> | 50 (ESI+)               | 71.00 (30)                                       | 282.2 (20)                                     |
|                | UV 329                        | 324.2 [M-H] <sup>+</sup> | 50 (ESI+)               | 57.00 (25)                                       | 212.2 (25)                                     |
|                | UV 360                        | 658.6 [M-H] <sup>+</sup> | 40 (ESI+)               | 336.3 (25)                                       | 224.2 (35)                                     |
| Cytostatic     | Etoposide                     | 589.5 [M-H] <sup>+</sup> | 40 V (ESI+)             | 229.2 (15)                                       | 185.3 (20)                                     |
|                | Vinblastine                   | 812.8 [M-H] <sup>+</sup> | 40 V (ESI+)             | 224.1 (45)                                       | 124.4 (43)                                     |
|                | Gemcitabine                   | 264.2 [M-H] <sup>+</sup> | 35 V (ESI+)             | 112.1 (20)                                       | 87.00 (20)                                     |
|                | 5-Fluorouracil                | 129.1 [M-H] <sup>-</sup> | 30 V (ESI-)             | 58.19 (19)                                       | 85.90 (19)                                     |
|                | Methotrexate                  | 455.1 [M-H] <sup>+</sup> | 30 V (ESI+)             | 308.1 (15)                                       | 175.0 (17)                                     |
|                | Tamoxifen                     | 372.3 [M-H] <sup>+</sup> | 40 V (ESI+)             | 72.12 (20)                                       | 129.2 (20)                                     |
|                | Cyclophosphamide              | 261.2 [M] <sup>+</sup>   | 30 V (ESI+)             | 140.0 (20)                                       | 106.1 (18)                                     |
|                | Vincristine                   | 825.8 [M-H] <sup>+</sup> | 40 V (ESI+)             | 140.2 (55)                                       | 122.2 (60)                                     |
| Hormones       | Estriol                       | 287.2 [M-H] <sup>-</sup> | -65 V (ESI -)           | 171.0 (37)                                       | 145.2 (39)                                     |
|                | 17-oestradiol                 | 271.2 [M-H] <sup>-</sup> | -65 V (ESI -)           | 183.1 (40)                                       | 145.1 (45)                                     |
|                | 17 $\alpha$ -ethynylestradiol | 295.2 [M-H] <sup>-</sup> | -65 V (ESI -)           | 145.1 (38)                                       | 143.1 (45)                                     |
|                | Estrone                       | 269.2 [M-H] <sup>-</sup> | -65 V (ESI -)           | 145.0 (36)                                       | 143.0 (48)                                     |
|                | Diethylstilboestrol           | 267.1 [M-H] <sup>-</sup> | -50 V (ESI -)           | 237.1 (29)                                       | 251.1 (25)                                     |
|                | Norethisterone                | 299.2 [M-H] <sup>+</sup> | 30 V (ESI +)            | 109.1 (25)                                       | 91.00 (40)                                     |
|                | Norgestrel                    | 313.2 [M-H] <sup>+</sup> | 38 V (ESI +)            | 109.0 (26)                                       | 245.1 (18)                                     |
|                | Megestrol acetate             | 385.5 [M-H] <sup>+</sup> | 30 V (ESI +)            | 267.3 (15)                                       | 224.2 (30)                                     |
|                | Progesterone                  | 315.3 [M-H] <sup>+</sup> | 30 V (ESI +)            | 97.00 (18)                                       | 109.1 (25)                                     |
|                | Boldenone                     | 287.2 [M-H] <sup>+</sup> | 30 V (ESI +)            | 121.0 (28)                                       | 135.1 (15)                                     |
|                | Nandrolone                    | 275.2 [M-H] <sup>+</sup> | 35 V (ESI +)            | 109.1 (20)                                       | 83.00 (30)                                     |
|                | Testosterone                  | 289.2 [M-H] <sup>+</sup> | 38 V (ESI +)            | 97.00 (22)                                       | 104.0 (21)                                     |
|                | Prednisone                    | 359.3 [M-H] <sup>+</sup> | 30 V (ESI +)            | 147.0 (15)                                       | 237.0 (20)                                     |
|                | Cortisone                     | 361.3 [M-H] <sup>+</sup> | 30 V (ESI +)            | 163.0 (25)                                       | 121.0 (45)                                     |
|                | Prednisolone                  | 361.3 [M-H] <sup>+</sup> | 20 V (ESI +)            | 147.1 (20)                                       | 173.1 (25)                                     |

Table S5. Chromatographic conditions for selected families of compounds.

| Family                   | Column                                                    | Mobile phase                                                         | Flow                     | Gradient mode                                                                                  |
|--------------------------|-----------------------------------------------------------|----------------------------------------------------------------------|--------------------------|------------------------------------------------------------------------------------------------|
| UV stabilizers           | ACQUITY BEH C18 (Waters)<br>50 x 2.1 mm, 1.7 $\mu$ m      | MeOH + 0.1% Formic Acid                                              | 0.6 mL·min <sup>-1</sup> | Isocratic                                                                                      |
| Cytostatic               | Luna Omega Polar (Phenomenex)<br>50 x 2.1 mm, 1.6 $\mu$ m | A: H <sub>2</sub> O + 0.1% Formic Acid<br>B: MeOH + 0.1% Formic Acid | 0.4 mL·min <sup>-1</sup> | 0 min: 40% A, 0.5 min: 90% A, 1 min: 0% A, 2 min: 0% A, 3 min: 40% A, 5 min: 40% A             |
| Hormones (water samples) | ACQUITY BEH C18 (Waters)<br>50 x 2.1 mm, 1.7 $\mu$ m      | A: H <sub>2</sub> O + 0.1% NH <sub>3</sub> .<br>B: MeOH.             | 0.3 mL·min <sup>-1</sup> | 0 min: 80% A, 4.1 min: 80% A, 7.0 min: 0% A, 8.0 min: 0% A, 10.5 min: 80% A.                   |
| Hormones (solid samples) |                                                           |                                                                      |                          | 0 min: 80% A, 1.5 min: 40% A, 2.75 min: 25% A, 3.75 min: 0% A, 6.0 min: 80% A, 6.5 min: 80% A. |