

Deconjugation characteristics of natural estrogen conjugates by acid-catalyzed solvolysis and its application for wastewater samples

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Supplementary materials

Table S1 Recovery efficiencies of free estrogens by C18

| Estrogens | Recovery efficiencies (%) | | | | RSD (%) |
|-----------|---------------------------|-------|-------|---------|---------|
| | n=1 | n=2 | n=3 | average | |
| E1 | 95.2 | 106.3 | 99.8 | 100.4 | 5.6 |
| E2 | 97.6 | 110.6 | 104.5 | 104.2 | 6.2 |
| E3 | 96.3 | 116.7 | 105.6 | 106.2 | 9.6 |

Table S2 LOD and LOQ of the three target free estrogens by GC-MS

| Natural estrogens | Standard concentration 10 ng/mL | | | | | | | | |
|-------------------|---|---------|------|------------|-------------|------|-------------|------|------|
| | Measured concentration from calibration curve (ng/mL) | | | | | | | | |
| | n=1 | n=2 | n=3 | n=4 | n=5 | n=6 | n=7 | n=8 | n=9 |
| E1 | 9.5 | 10.3 | 9.8 | 9.1 | 10.3 | 9.9 | 11.3 | 10.3 | 10.3 |
| E2 | 9.2 | 11.5 | 11.4 | 9.6 | 11.7 | 10.7 | 11.5 | 12.0 | 11.5 |
| E3 | 8.5 | 9.9 | 9.6 | 8.4 | 10.1 | 9.1 | 9.6 | 9.8 | 10.2 |
| | Mean (ng/mL) | C.V (%) | | SD (ng/mL) | LOD (ng/mL) | | LOQ (ng/mL) | | |
| E1 | 10.1 | 6.2 | | 0.63 | 1.9 | | 6.3 | | |
| E2 | 11.0 | 8.9 | | 0.98 | 2.9 | | 9.8 | | |
| E3 | 9.5 | 6.8 | | 0.65 | 1.9 | | 6.5 | | |

Table S3 Occurrence and fate of natural free estrogens and their conjugates
 in WWTP*

| Target chemicals | Influent | | PE | | Effluent | |
|------------------|----------------------|---------|----------------------|---------|----------------------|---------|
| | Concentration (ng/L) | C.V (%) | Concentration (ng/L) | C.V (%) | Concentration (ng/L) | C.V (%) |
| E1 | 32.7 | 9.7 | 34.8 | 4.0 | 31.7 | 6.7 |
| E2 | 13.0 | 16.3 | 10.8 | 5.0 | -- ^d | -- |
| E3 | 140 | 12.2 | 107 | 1.7 | -- | -- |
| E1-3S | 7.7 | 6.9 | 4.8 | 3.2 | 0.7 ^a | 14.3 |
| E2-3S | n.d | -- | n.d | -- | n.d | -- |
| E3-3S | 36.1 | 13.4 | 32.5 | 9.3 | 2.1 ^b | 7.4 |
| E1-3G | n.d | -- | n.d | -- | n.d ^c | -- |
| E2-3G | n.d | -- | n.d | -- | n.d | -- |
| E3-3G | n.d | -- | n.d | -- | n.d | -- |

*Values on concentrations of estrogen conjugates are concentrations of their corresponding free estrogens; ^abelow LOD; ^babove LOD but below LOQ; ^cnot detected; ^dnot applicable