

Table S1 Physico-chemical properties of selected estrogens

compound	molecular formula	CAS no.	pK _a [*]	Log K _{ow} [*]
E1	C ₁₈ H ₂₂ O ₂	53-16-7	10.33	4.31
E2	C ₁₈ H ₂₄ O ₂	50-28-2	10.38	3.75
EE2	C ₂₀ H ₂₄ O ₂	57-63-6	10.33	3.90
E3	C ₁₈ H ₂₄ O ₃	50-27-1	10.33	2.67

* DrugBank - ChemAxon

Table S2 Selected physical characteristics of tested materials

Compound	Precursor ion (m/z)	Quantitation/qualification ion (m/z)	Collision energy (V)	Fragmentor voltage (V)
E1	504	171/156	140	38
E2	506	171/156	140	42
EE2	530	171/156	140	40
E3	522	171/156	140	42

Table S3 Method validation parameters

compound	MDL [ng/L]	ML [ng/L]	CV ^a [%] inter-day	CV ^a [%] intra-day	CV ^b [%] inter-day	CV ^b [%] intra-day	CV ^c [%] inter-day	CV ^c [%] intra-day
E1	0.2	0.5	7.54	10.41	12.22	11.59	11.18	9.97
E2	0.2	0.5	4.47	7.33	13.03	13.08	5.29	4.51
EE2	0.1	0.4	3.69	7.65	8.88	8.76	5.62	4.50
E3	0.2	0.6	6.43	3.84	13.25	13.28	13.94	15.09

^a 100 ng/L - deionized water; ^b 300 ng/L – tap water; ^c 500 ng/L – tap water; MDL = limit of detection, ML