Supplementary information

Universal carbon nanotubes-polybenzimidazole SPME coating and its application for both gas and liquid chromatography

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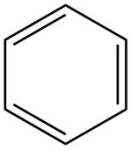
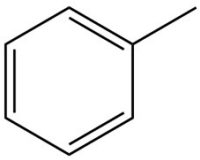
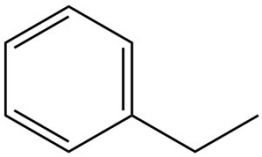
Table S1. Quantification ion transitions and mass spectrometry parameters for the analyzed drugs of abuse

Analyte	Precursor ion (*m/z*)	Product ion (*m/z*)	Collision energy (V)	S-Lens (V)
Atenolol	267.1	145.1	17	89
Acetaminophen	152.1	110.1	17	86
Morphine	286.1	165.1	42	137
Codeine	300.1	215.1	42	122
Oxazepam	287	241	33	120
Cocaine	304.1	182.1	32	101
Carbamazepine	237.1	194.1	31	101
Diazepam	285	193.1	26	113
Nordiazepam	271	140	28	133
Propranolol	260.1	183.1	24	99
Fentanyl	337.2	188.1	35	121

Table S2. Chemical structures and physical-chemical properties of GC-amenable analytes

Analyte	Chemical structure	Molecular mass (g mol^{-1})	LogP
Benzene		78.11	2.13
Toluene		92.14	2.73
Ethylbenzene		106.16	3.15

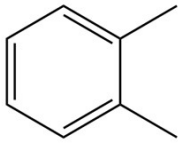
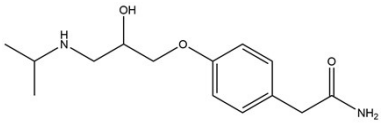
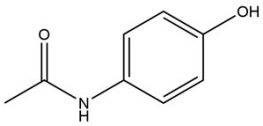
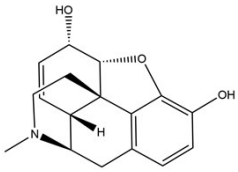
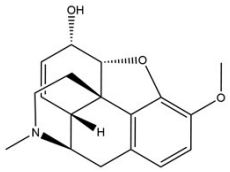
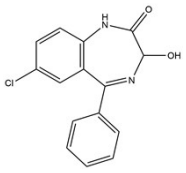
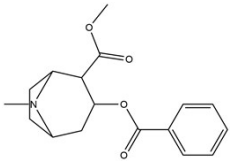
o-Xylene		106.16	3.12

Table S3. Chemical structures and physical-chemical properties of LC-amenable analytes

Analyte	Chemical structure	Molecular mass (g mol^{-1})	LogP
Atenolol		266.34	0.20
Acetaminophen		151.16	0.50
Morphine		285.34	0.85
Codeine		299.4	1.19
Oxazepam		286.71	2.24
Cocaine		303.35	2.30

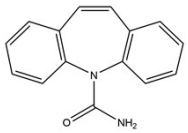
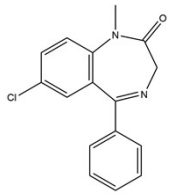
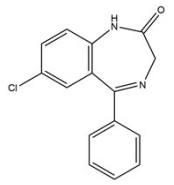
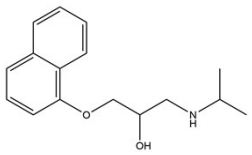
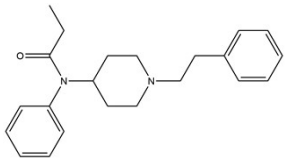
Carbamazepine		236.26	2.51
Diazepam		284.74	2.82
Nordiazepam		270.71	2.93
Propranolol		259.34	3.48
Fentanyl		336.5	4.05

Figure S1. Extraction time profiles for benzene, toluene, ethylbenzene and xylene using CNT-PBI arrow (10 mm length, 30 µm thickness). Particle to binder ratio equal 1%. Extractions performed from standard gas generating vials at 30 °C under static condition.

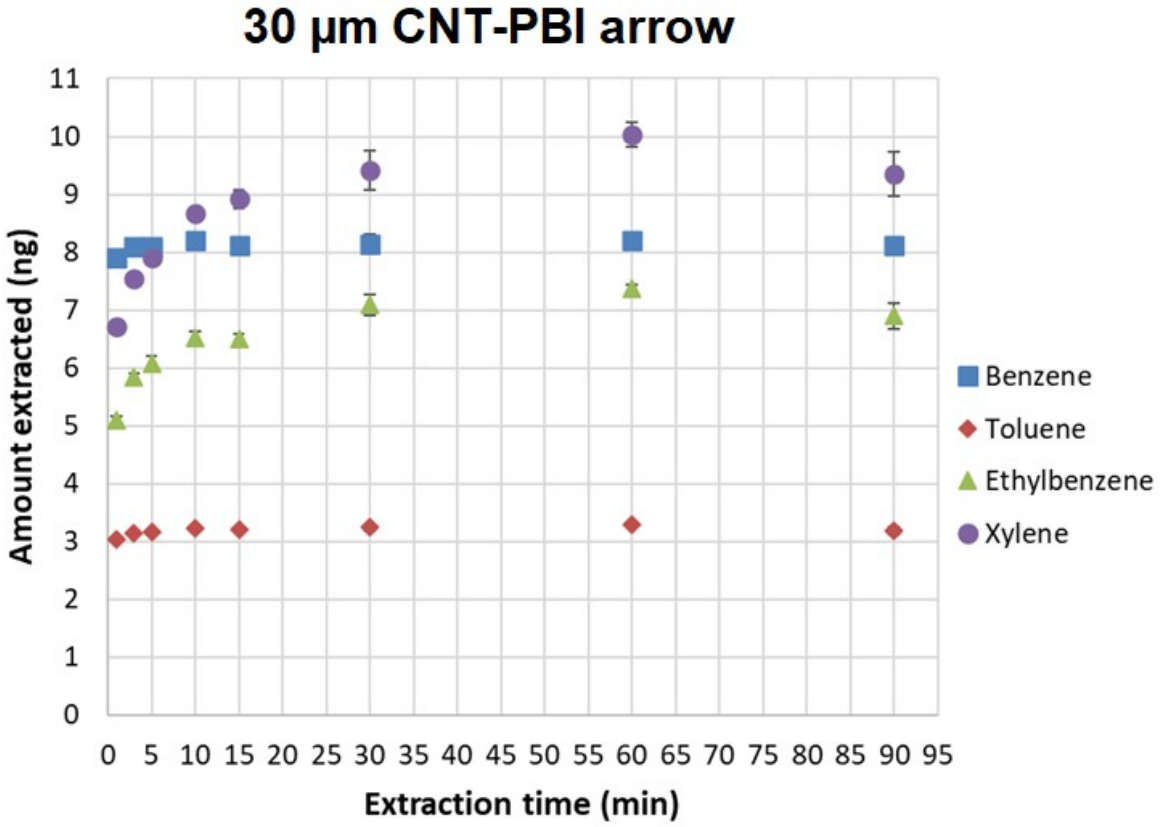


Figure S2. Evaluation of CNT-PBI arrow (10 mm length, 15 µm thickness) robustness. Particle to binder ratio equal 1%. 99 sequential extractions performed from standard gas generating vials at 30 °C under static condition. Amount extracted RSDs: benzene: 0.075 %; toluene: 0.3 %, ethylbenzene: 1.85% and xylene: 1.04%

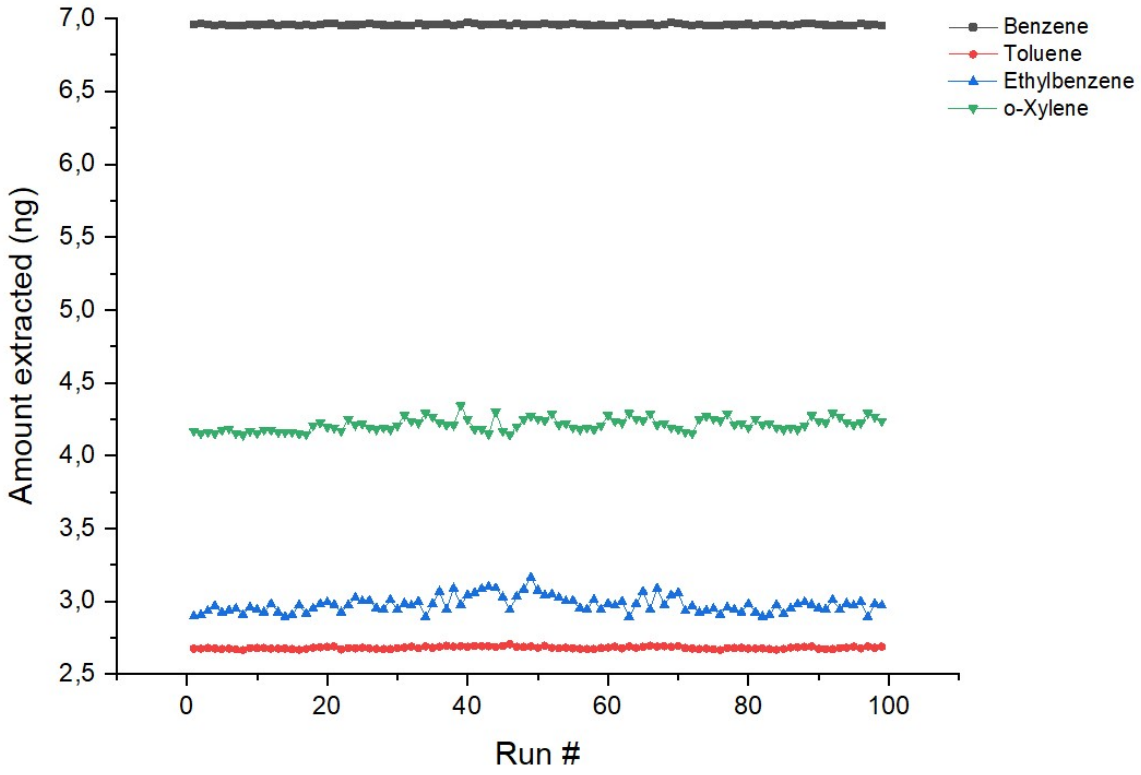


Figure S3. Number of detected features obtained from each group in LC-HRMS analysis of water samples. Used threshold values: signal-to-noise (s/n) of 10, *m/z* error of 10 ppm, 5 s allowance for retention time correction and 5 *m/z* step-size. RV = river samples; WW = wastewater samples; WWTF = wastewater samples after treatment.

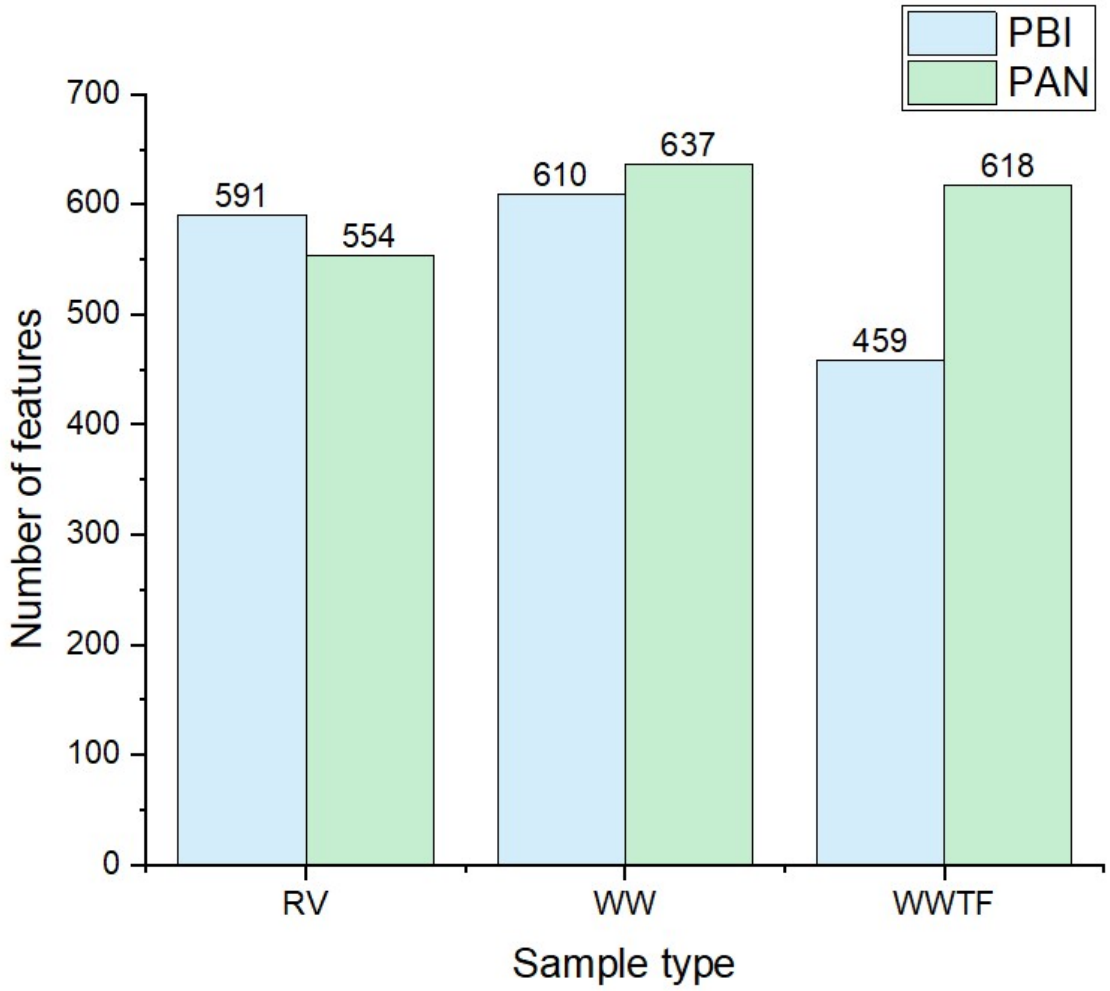


Figure S4. Volcano plots comparing the features obtained using CNT-PBI and CNT-PAN blades in the extraction of river (A), wastewater (B) and wastewater after treatment (C) samples. The volcano plots show the log 2 of fold change (log2 FC) on the x-axis and – log 10 of p-value on the y-axis. The cut-off values of fold change = 2.0 and p-value = 0.05 are shown by the vertical and horizontal dotted lines, respectively. The blue and red dots represent the features that suffered a negative and positive fold-change in the CNT-PBI extracts in relation to the CNT-PAN extracts, respectively.