Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Information

Preparation of magnetic iron oxide nanoparticles modified with imidazolium-based ionic liquids as a sorbent for extraction of eight phthalate acid esters in water samples followed by UPLC-MS/MS analysis: experimental design methodology

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Instruments

Consort C830 Multi-function meter (Belgium) was utilized for measuring the pH of the solutions. Sonication treatment was performed using an Ultrasonic sonication bath (Elmasonic S60H, Elma Schmidbauer, Germany) at 550 Watt of power and 37 kHz of ultrasonic frequency. Nd-Fe-B magnet coated with Ni–Cu–Ni (2Tesla, 5 cm × 5 cm × 5 cm) was used for separation of magnetic NPs. A Field-Emission Scanning Electron Microscope (FE-SEM, MIRA3, TESCAN, Česká Republika) was used to morphology analysis of the NPs. An IRAffinity-1S Fourier Transform Infrared (FTIR) spectrometer (Shimadzu, Japan) was utilized for achieving IR spectra. The crystalline phases of the nanomaterials were verified using Powder X-ray diffraction (XRD). MNPs' XRD patterns were obtained using X'Pert PRO MPD model of X-ray Diffractometer manufactured by PANalytical B.V. (Netherlands). Using MPMS®3 Vibrating Sample Magnetometer (VSM, Quantum Design, Inc, USA), magnetic properties of MNPs were investigated. MNPs's surface electrical features were analyzed as a function of pH applying electrophoretic measurements through a Malvern Panalytical Zetasizer Nano ZSP (Malvern Panalytical Ltd., UK).

Box-Behnken experimental design

Conventional optimization methods namely one-variable-at-a time have an extensive application. They usually suffer from some disadvantages. These disadvantages are deficiency viz necessity, requiring a large number of experimental runs and chemical waste production, labor effort and being tedious and high cost. Moreover, these methods are incapable of differentiating between the significance of each variable, and as a result of that, the influences of interaction between variables are ignored, and the correct optimum level cannot be achieved. To overcome these impediments, multivariate optimization is an appropriate and valid statistical method capable of eliminating the restrictions of traditional optimization [1]. Response surface methodology is a dominant statistical-based strategy to evaluate the effects of different factors simultaneously which enables the optimum conditions for providing the desirable response [2, 3]. The Box–Behnken design-based response surface methodology enables us to distinguish discrete variables and their interactions on target response empirically polynomial function with minimum time and cost. Thus, appreciated info was achieved for a predetermined procedure using the methodologies of the experimental strategy. Responses are considered as dependent variables, and factors are independent variables [4].

The fitting and analysis of the data resulting from the experiment design comply with the second-order polynomial model and the general form of which for response surface analysis will be described in the following [5].

$$Y = \beta_0 + \sum_{i=1}^{k}\beta_i x_i + \sum_{i=1}^{k}\beta_{ii}{x_i}^2 + \sum_{i=1}^{k-1}\sum_{j=2}^{k}\beta_{ij}x_i x_j \tag{1}$$

Where Y is the predicted response, X_i and X_j are the independent variables that, these are the experimental factors, and β_0, β_i, $\beta_{ii,}$ and β_{ij} are the regression coefficients for the intercept, linear, quadratic, and interaction terms, respectively.

The analysis of variance statistical test is used for the analysis of variances and analyzes significance factors and their mutual interactions and on other factors. By the use of the response surface methodology, the validated model is then designed in three dimensions followed by interpretation for finding optimum condition for the procedure.

Desirability function

To obtain the global optimal conditions based on Derringer's desirability function, desirability function is a common and routine technique since it differentiates and reaches an input variable, makes a function for each individual response and in the end determines a global function that shall be maximized accompanying variety of optimum amount of affective variables, taking into account their interaction [6].

Qualitative and quantitative information can be obtained by desirability functions since it metamorphoses various responses and relates team to measurement. The response (Y) is converted into desirability function (df_i) in the range of 0 to 1 (where values near zero and one recommend non-desirable and very desirable), all of which can be calculated and formulated according to the following equation.

$$df_i = (\frac{Y-\alpha}{\beta-\alpha})^{wi}.\ \alpha \leq Y \leq \beta$$

$$df_i = 1.\ Y > \beta \qquad (2)$$

$$df_i = 0.\ Y < \alpha$$

i and wi are the weight and α, and β are the minimum and maximum gained values of the response in equation 2. The overall desirability function is mixed with each individual desirability score for the predicted values by computing their geometric mean of different df_i values.

$$DF = [df_1^{V1} \times df_2^{V2} \ldots \times df_n^{vn}]^{\left(\frac{1}{n}\right)}.\ 0 \leq vi \leq 1\ (i = 1.\ 2.\ \ldots.\ n) \qquad (3)$$

$$\sum_{i=1}^{n} vi = 1$$

Where df_i indicates the desirability of the response Yi (i = 1, 2, 3,…,n) and vi represents the desirability of each response on the dependent variables [7].

Reusability of adsorbent

To study the reusability, Fe_3O_4@[Bimi]Cl NPs were recycled by rinsing with UPW and MeOH after use. A couple of continues adsorption-desorption cycles were carried out, and almost 90% of NPs were successfully retrieved from each run. When the experiment of four cycles was done, mean ER of 82% was achieved which showed the recycled Fe_3O_4@[Bimi]Cl NPs were able to be used with no considerable loss of extraction performance. Although, when the fifth run was taken place, severe collapse in the recoveries of extraction was recorded. Since the mass of NPs was lessen after a couple of regenerations as a result of washing them in recycling and reusing procedure and also the modification of Fe_3O_4 NPs with IL got less effective after several times of rinsing, restricted multiple reusabilities of NPs could be ascribed.

Adsorption Kinetics

Several steps can be used to examine the controlling mechanism of adsorption processes such as chemical reaction, diffusion, and mass transfer. In recent years, several kinetic models have been proposed to justify the adsorption mechanism. The kinetic parameters, which are helpful for the prediction of adoption rate, give valuable information for modeling the adsorption processes. In this study, kinetic models are used to test experimental data from the adsorption DMP (as an example) onto Fe_3O_4@[Bimi]Cl NPs. Several kinetic models like Pseudo-first-order [8], Pseudo-second-order [9], and Intraparticle diffusion [10] models were scrutinized to the DMP the adsorption kinetic behavior onto synthesized NPs.

The kinetic parameters of DMP adsorption onto Fe_3O_4@[Bimi]Cl NPs are shown in Table S8. The Pseudo-second-order kinetics are possibly accompanied by adsorption values of DMP due to the fact that values of theoretical equilibrium are compatible with the experimental values. The experimental data is more match with the second-order kinetics than other kinetic models in the whole adsorption procedure based on value of regression coefficients of 0.998 in this study.

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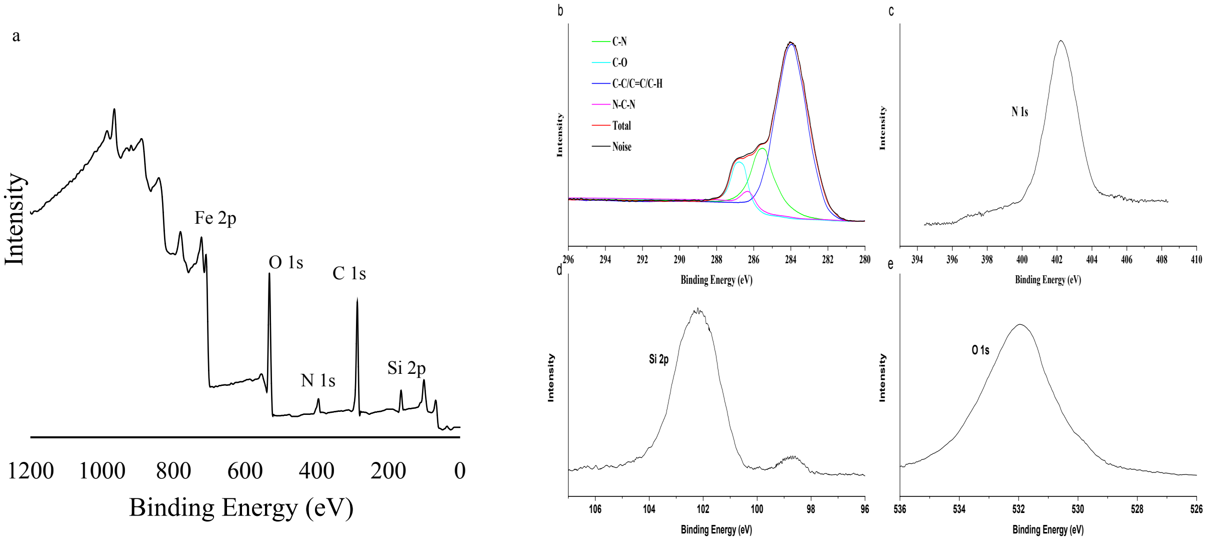


Fig. S1. a) XPS spectrum of Fe_3O_4@[Bimi]Cl NPs, High resolution XPS spectra of Fe_3O_4@[Bimi]Cl NPs, **b)** C1s, **c)** N1s, **d)** Si2p, **e)** O1s.

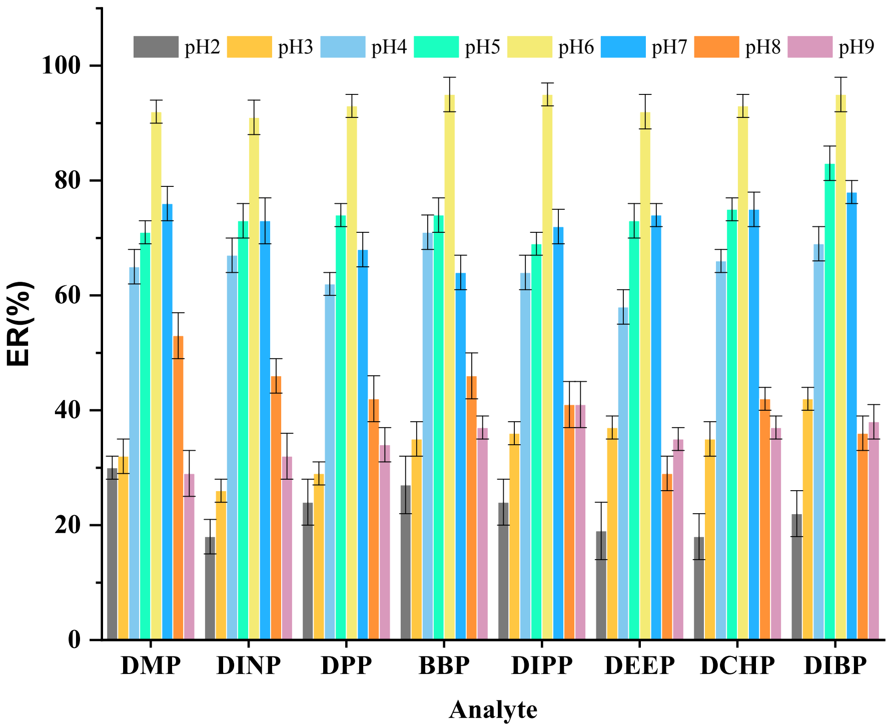


Fig. S2. Effect of pH of sample on the extraction efficiency of the target analytes (Extraction conditions: 50 mL of spiked samples, 47.3 mg of sorbent, 3.1 min of extraction time, 500 µL MeOH:MeCN 75:25 (V/V) as the elution solvent and 2.4 min of deposition time).

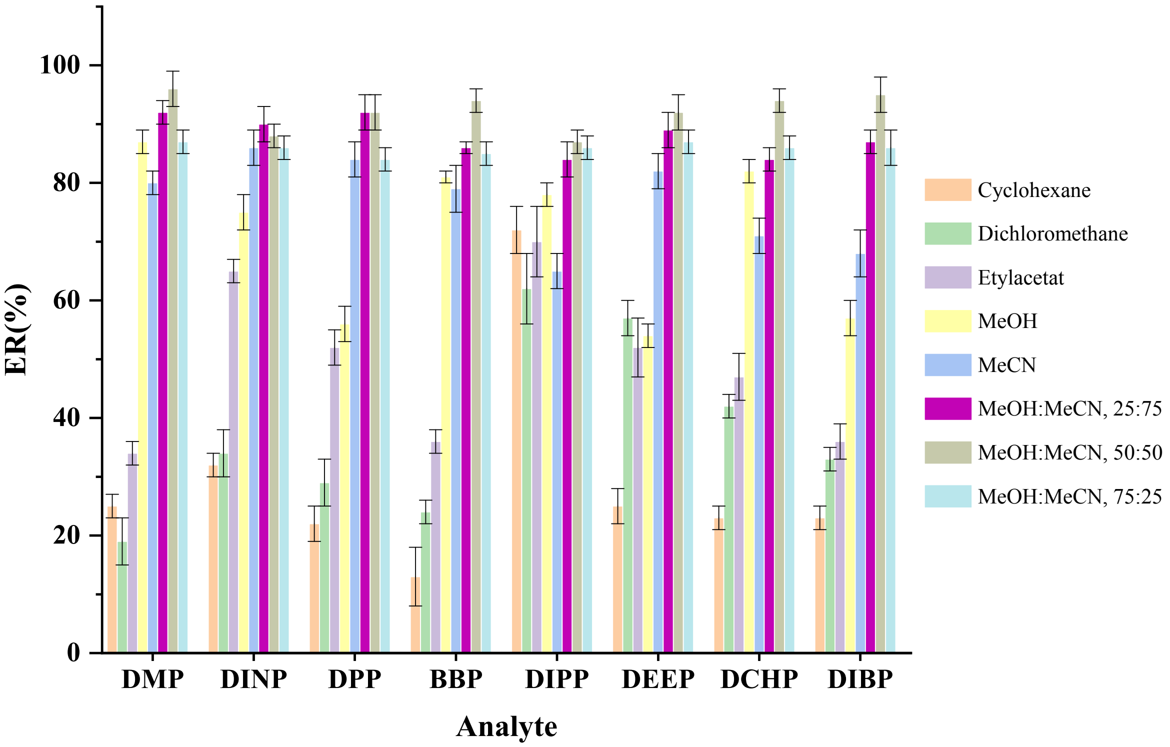


Fig. S3. Influence of the desorption solvent on the ER of the analytes (Extraction conditions: 50 mL of spiked samples, pH value of 6 for sample solutions, 47.3 mg of sorbent, 3.1 min of contact time, and 2.74 min of deposition time).

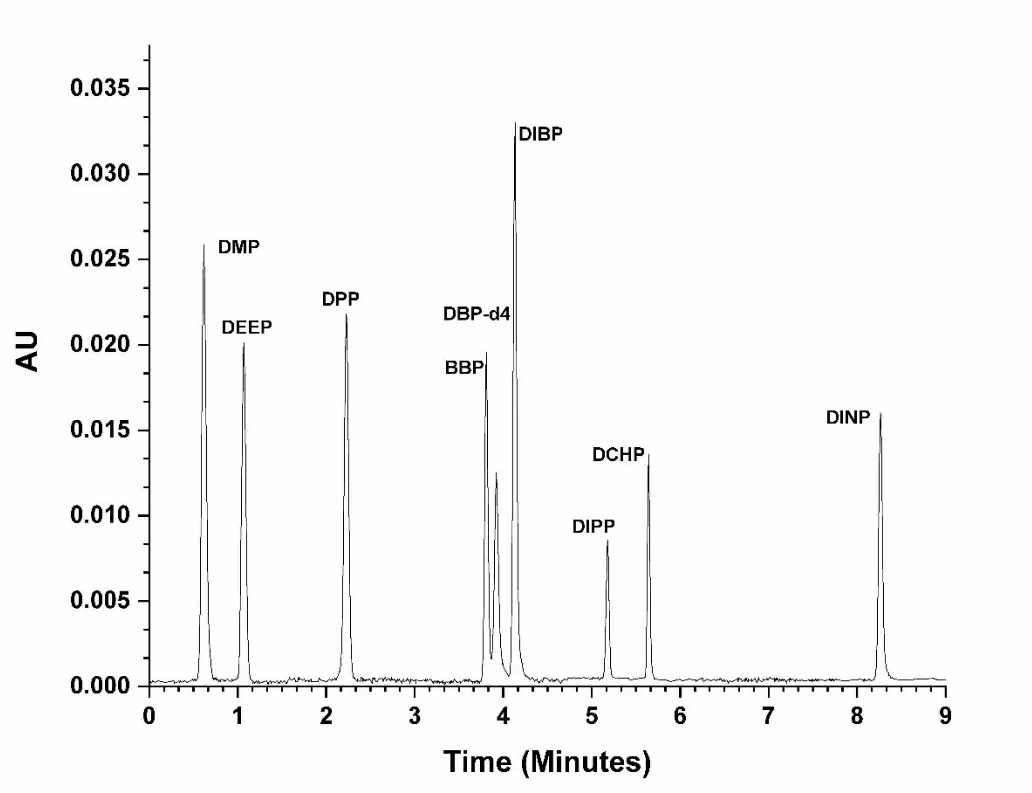


Fig. S4. UPLC-DAD chromatogram of PAEs of a spiked river water sample at concentration of 50 µg.L^{-1} after the D-micro-SPE procedure (wavelength=225 nm).

Tables

Table S1: Structure of PAEs.

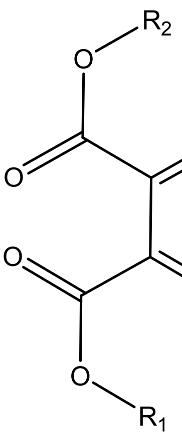
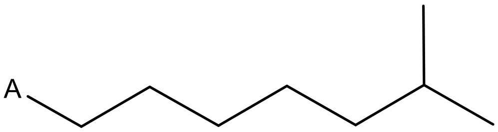
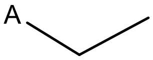
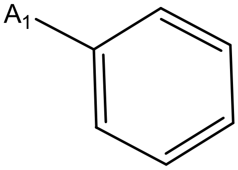
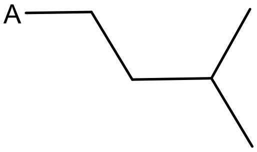
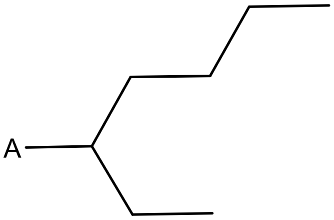
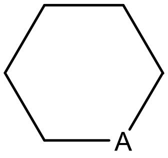
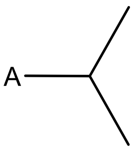
	R_1, R_2: CH_3	Dimethyl phthalate
	R_1, R_2: 	Diisononyl phthalate
	R_1, R_2: 	Dipropyl phthalate
	R_1: 	Benzyl butyl phthalate
	R_2: 	
	R_1, R_2: 	Bis(4-methylpentyl)phthalate
	R_1, R_2: 	Bis(2-ethylhexyl) phthalate
	R_1, R_2: 	Dicyclohexyl phthalate
	R_1, R_2: 	Diisobutyl phthalate

Table S2. MS/MS parameters of the PAEs and IS.

Analyte	**Precursor ion (m/z)**	**Product ion (m/z)**	**Collision energy (eV)**	**Cone voltage (V)**
DMP	195.03	76.93 (Q)	32	16
		162.92 (I)	8	
DINP	419.4	70.95 (Q)	16	28
		127.03 (I)	12	
DPP	251.09	148.89 (Q)	16	18
		190.95 (I)	6	
BBP	313.36	90.90 (Q)	16	22
		204.98 (I)	8	
DIPP	307.22	42.94 (Q)	28	22
		70.95 (I)	14	
DEEP	311.17	72.96 (Q)	12	16
		221.01 (I)	6	
DCHP	331.22	148.94 (Q)	26	22
		166.94 (I)	12	
DIBP	279.12	148.93 (Q)	16	22
		204.95 (I)	6	
DBP-d_4 (IS)	283.15	152.96 (Q)	12	20
		208.98 (I)	8	

Q: Ion for quantification, I: Ion for identification.

Table S3. Experiment results based on the BBD.

	Independent variable[a]			Extraction Recovery (%)							
Run	A	B	C	DMP	DINP	DPP	BBP	DIPP	DEEP	DCHP	DIBP
1	0	1	-1	84.5	87.5	85.4	83.5	81.5	82.5	80.2	81.5
2	1	1	0	88.1	91.2	86	87.4	73.4	87.4	85.4	86.5
3	1	0	1	88.2	90.5	90.1	88.4	89.5	89.2	85.6	87.3
4	0	0	0	89	89.4	91.4	89.2	87.4	87.5	86.4	86.3
5	0	-1	-1	74.2	76.7	76.4	74.2	74.5	72.6	70.2	71.7
6	0	0	0	91.5	91.5	93.2	89.7	89.2	89.4	92.1	89.5
7	-1	0	1	76.4	76.5	77.4	77.6	78.7	74.2	76.5	74.2
8	-1	0	-1	66.7	67.6	68.5	64.2	66.8	68.7	63.4	65.3
9	0	0	0	92.5	93.2	92.4	91.4	90.2	90.5	89.4	91.2
10	0	1	1	88.4	91.2	89.8	89.5	90.1	87.4	86.2	89.4
11	-1	-1	0	57	57.4	61.4	58.4	53.4	57.6	55.1	56.2
12	0	0	0	87.4	90.3	87.6	89.4	85.2	88.3	89.2	87.2
13	1	0	-1	87.2	88.5	90.4	87.1	84.5	86.2	83.5	86.7
14	1	-1	0	79.4	79.6	80.3	76.2	78.6	77.1	76.8	77.2
15	-1	1	0	75.1	75.4	76.4	72.4	72.1	73.9	73.1	71.8
16	0	0	0	90.4	91.2	91.2	89.5	87.2	88.6	87	89.9
17	0	-1	1	76.4	75.8	78.5	74.2	76.3	74.2	72.2	74.6

a: A: Adsorbent quantity (mg), B: Extraction time (min), C: Desorption time (min).

Table S4. ANOVA for the regression models.

Analyte	**DMP**		**DINP**		**DPP**		**BBP**	
Source[a]	**F-value**	**p-value**	**F-value**	**p-value**	**F-value**	**p-value**	**F-value**	**p-value**
Model	51.92	< 0.0001	67.92	< 0.0001	43.24	< 0.0001	96.46	< 0.0001
A	176.91	< 0.0001	245.32	< 0.0001	147.28	< 0.0001	302.79	< 0.0001
B	93.05	< 0.0001	143.73	< 0.0001	62.18	< 0.0001	169.81	< 0.0001
C	10.89	0.0131	8.66	0.0216	8.43	0.0228	29.34	0.0010
AB	6.82	0.0348	3.78	0.0929	6.40	0.0393	1.07	0.3346
AC	5.84	0.0463	4.40	0.0743	6.26	0.0409	20.05	0.0029
BC	0.2231	0.6511	1.95	0.2049	0.3914	0.5514	4.93	0.0618
A^2	88.60	< 0.0001	115.60	< 0.0001	80.34	< 0.0001	171.87	< 0.0001
B^2	63.80	< 0.0001	67.68	< 0.0001	62.90	< 0.0001	133.48	< 0.0001
C^2	6.76	0.0354	4.61	0.0688	2.92	0.1314	8.17	0.0244
Lack of Fit	0.5219	0.6899	1.78	0.2893	0.3778	0.7750	4.04	0.1055
Std. Dev.	1.80		1.65		1.84		1.35	
Mean	81.91		83.15		83.32		81.31	
C.V. %	2.20		1.98		2.21		1.66	
R^2	0.9852		0.9887		0.9823		0.9920	
Adjusted R^2	0.9663		0.9741		0.9596		0.9817	
Predicted R^2	0.9170		0.8888		0.9161		0.9007	
Adeq Precision	23.3369		27.2759		21.6135		31.1687	

a: A: Adsorbent quantity (mg), B: Extraction time (min), C: Desorption time (min).

Continued Table S4.

Analyte	**DIPP**		**DEEP**		**DCHP**		**DIBP**	
Source	**F-value**	**p-value**	**F-value**	**p-value**	**F-value**	**p-value**	**F-value**	**p-value**
Model	43.80	< 0.0001	151.04	< 0.0001	40.88	< 0.0001	74.95	< 0.0001
A	96.48	< 0.0001	516.04	< 0.0001	114.17	< 0.0001	258.66	< 0.0001
B	37.52	0.0005	297.11	< 0.0001	73.18	< 0.0001	128.61	< 0.0001
C	23.77	0.0018	27.06	0.0012	15.38	0.0057	21.63	0.0023
AB	36.44	0.0005	8.66	0.0216	5.05	0.0594	4.17	0.0806
AC	3.04	0.1249	1.50	0.2598	6.92	0.0339	7.23	0.0311
BC	2.95	0.1296	2.62	0.1496	0.9146	0.3707	2.62	0.1493
A^2	98.91	< 0.0001	211.79	< 0.0001	62.93	< 0.0001	125.05	< 0.0001
B^2	84.52	< 0.0001	235.87	< 0.0001	63.72	< 0.0001	99.05	< 0.0001
C^2	2.85	0.1350	17.11	0.0044	11.69	0.0111	7.32	0.0304
Lack of Fit	1.11	0.4442	0.5276	0.6868	0.6667	0.6151	0.0330	0.9908
Std. Dev.		1.98	1.02		2.09		1.54	
Mean		79.92	80.90		79.55		80.38	
C.V. %		2.48	1.26		2.63		1.92	
R^2		0.9826	0.9949		0.9813		0.9897	
Adjusted R^2		0.9601	0.9883		0.9573		0.9765	
Predicted R^2		0.8585	0.9710		0.8810		0.9804	
Adeq Precision		24.8706	39.5372		20.4469		27.7863	

Table S5. The regression equation of responses for 8 PAEs.

Analyte	Equation[a]
DMP	$Y_1=90.16+8.46A+6.14B+2.10C-2.23AB-2.18AC+0.4250BC-8.26A^2-7.01B^2-2.28C^2$
DINP	$Y_2=91.12+9.11A+6.98B+1.71C-1.60AB-1.73AC+1.15BC-8.62A^2-6.60B^2-1.72C^2$
DPP	$Y_3=91.16+7.89A+5.13B+1.89C-2.33AB-2.30AC+0.5750BC-8.03A^2-7.11B^2-1.53C^2$
BBP	$Y_4=89.84+8.31A+6.23B+2.59C-0.7000AB-3.02AC+1.50BC-8.63A^2-7.61B^2-1.88C^2$
DIPP	$Y_5=87.84+6.88A+4.29B+3.41C-5.98AB-1.73AC+1.70BC-9.60A^2-8.87B^2+1.63C^2$
DEEP	$Y_6=88.86+8.19A+6.21B+1.88C-1.50AB-0.6250AC+0.8250BC-7.23A^2-7.63B^2-2.05C^2$
DCHP	$Y_7=88.82+7.90A+6.33B+2.90C-0.35AB-2.75AC+1.0000BC-8.09A^2-8.14B^2-3.49C^2$
DIBP	$Y_8=88.82+8.78A+6.19B+2.54C-1.58AB-2.08AC+1.25BC-8.41A^2-7.49B^2-2.04C^2$

a: A: Adsorbent quantity (mg), B: Extraction time (min), C: Desorption time (min).

Table S6. Results of the ME study of the D-micro-SPE method for the target analytes in the different water matrices at two levels of concentration.

Analyte	Type of water									
	River Water		Tap Water		Mineral bottled water		Pound Water		Wastewater	
	ME[a] (%)	RSD (%)	ME (%)	RSD (%)	ME (%)	RSD (%)	ME (%)	RSD (%)	ME (%)	RSD (%)
DMP	94	2.3	99	2.6	94	2.1	102	2.3	85	3.4
DINP	91	2.7	101	2.2	92	1.6	102	1.9	122	3.0
DPP	98	2.2	102	1.9	88	2.2	104	2.6	92	2.9
BBP	101	1.8	89	2.0	95	2.5	86	2.4	118	3.3
DIPP	96	2.4	98	2.2	101	2.1	91	2.6	97	3.1
DEEP	103	2.6	105	1.8	102	1.9	92	2.1	107	2.8
DCHP	102	2.2	96	2.2	101	1.6	95	2.5	103	2.9
DIBP	95	1.9	95	2.7	101	1.7	103	2.4	94	2.9

a: Matrix effect results obtained as an average of each analyte at two levels of concentration (10 $\mu g.L^{-1}$ and 100 $\mu g.L^{-1}$).

Table S7: Results of the accuracy study of the developed method.

Analyte	Type of water	LOD (µg.L^{-1})	Intra-day accuracy (n=5)						Inter-day accuracy					
			Level I[a]		Level II[b]		Level III[c]		Level I		Level II		Level III	
			Recovery	RSD	Recovery	RSD	Recovery	RSD	Recovery	RSD	Recovery	RSD	Recovery	RSD
DMP	River	0.005	90.2	4.2	91.3	3.8	92.0	3.9	90.8	5.6	91.5	5.2	91.8	5.4
	Tap	0.003	92.5	3.8	91.2	3.2	94.2	3.2	92.1	4.9	93.4	4.2	94.3	4.7
	Mineral[d]	0.003	91.4	3.4	92.1	2.8	89.4	2.9	91.7	5.2	90.8	4.8	90.2	4.2
	Pound	0.009	98.2	4.9	95.6	4.9	94.3	4.4	97.8	5.8	96.6	5.7	95.3	5.5
	Wastewater	0.011	105.3	5.4	99.4	4.4	109.2	5.2	104.0	6.9	98.5	5.9	108.5	6.4
DINP	River	0.008	88.4	3.2	86.7	2.6	88.2	2.8	88.7	4.4	88.1	4.0	85.9	3.5
	Tap	0.007	88.9	2.5	88.2	1.9	89.7	2.0	89.2	3.4	89.0	2.9	85.3	2.8
	Mineral	0.009	90.7	3.1	92.1	2.8	92.5	2.7	91.1	4.9	92.3	4.7	93.4	4.4
	Pound	0.009	95.2	3.5	94.5	3.5	95.5	3.4	94.8	5.2	94.8	5.4	95.1	4.8
	Wastewater	0.010	94.5	4.5	93.1	4.2	92.3	4.3	89.4	6.8	92.1	6.2	97.3	6.5
DPP	River	0.002	88.6	2.8	89.0	2.6	89.1	2.6	89.6	4.0	88.4	3.8	89.5	3.9
	Tap	0.002	90.2	3.2	90.2	2.8	91.6	2.9	91.0	5.1	91.7	4.8	92.1	4.4
	Mineral	0.002	88.4	4.7	88.4	4.0	89.2	3.5	89.2	5.6	88.2	5.3	88.3	5.1
	Pound	0.003	92.7	4.8	91.2	4.3	91.1	4.3	91.4	6.2	91.1	5.9	90.9	5.8
	Wastewater	0.003	105.1	5.8	103.8	5.4	104.1	5.4	103.8	7.1	104.8	6.8	105.1	6.7
BBP	River	0.003	92.4	2.6	93.5	2.2	93.5	2.5	92.8	3.5	93.6	3.6	93.4	3.5
	Tap	0.002	93.2	2.4	92.1	2.0	91.7	1.9	92.6	3.2	91.4	3.0	92.6	3.0
	Mineral	0.002	92.5	3.0	92.3	2.7	92.5	2.4	92.7	3.8	91.8	3.7	91.4	3.4
	Pound	0.003	95.4	3.5	94.4	3.2	94.2	3.3	93.3	5.3	94.1	4.8	95.2	4.9
	Wastewater	0.004	91.6	4.4	92.7	4.2	92.8	4.2	92.4	5.9	91.7	5.8	92.8	5.7
DIPP	River	0.002	90.6	3.5	90.8	3.1	91.1	3.1	91.2	4.4	91.5	4.2	91.7	4.5
	Tap	0.003	90.8	3.7	91.1	3.4	91.5	3.2	91.2	4.8	91.7	4.6	92.3	4.7
	Mineral	0.002	89.2	3.9	89.3	3.5	88.6	3.7	88.8	4.8	89.5	4.7	89.1	4.9
	Pound	0.002	90.4	4.0	91.0	3.8	90.4	3.8	91.1	5.2	91.5	4.9	92.3	4.7
	Wastewater	0.004	103.4	5.3	102.5	5.1	104.5	5.1	103.2	6.1	103.1	6.2	104.7	6.1
DEEP	River	0.004	89.3	3.6	89.1	3.2	88.9	3.3	90.2	4.6	89.8	4.3	89.5	4.2
	Tap	0.004	90.5	3.3	91.1	3.2	90.9	3.2	91.2	4.5	91.8	4.4	92.1	4.4
	Mineral	0.004	89.8	3.5	90.3	3.4	90.1	3.3	91.0	4.4	89.7	4.6	90.0	4.1
	Pound	0.005	90.4	3.5	91.6	3.5	90.3	3.2	91.3	4.5	92.3	4.4	91.2	4.3
	Wastewater	0.006	82.7	4.5	82.2	4.4	83.1	4.2	83.5	5.7	84.2	5.6	83.2	5.2
DCHP	River	0.005	94.2	2.5	93.8	2.3	93.5	2.4	93.8	3.4	92.9	3.6	93.1	3.4
	Tap	0.005	93.8	2.2	93.9	1.9	93.9	1.9	93.9	3.0	93.6	2.7	94.2	2.7
	Mineral	0.006	92.6	2.6	92.3	2.5	92.3	2.5	93.0	3.7	92.7	3.5	92.9	3.5
	Pound	0.006	98.5	3.5	98.2	3.4	98.7	3.4	100.2	4.8	99.7	4.6	100.9	4.6
	Wastewater	0.005	103.8	4.7	103.2	4.5	103.5	4.5	103.9	5.8	103.6	5.8	103.5	5.7
DIBP	River	0.006	95.2	3.4	94.4	3.2	95.1	3.2	95.7	4.5	95.2	4.4	95.6	4.6
	Tap	0.006	94.5	2.9	93.8	2.8	93.7	2.8	94.6	3.8	93.8	3.9	94.3	3.9
	Mineral	0.004	95.5	2.8	95.2	2.7	95.0	2.9	96.0	4.1	95.5	3.8	95.1	4.3
	Pound	0.008	93.1	3.4	96.8	3.2	95.8	3.2	94.5	4.6	95.2	4.4	95.6	4.4
	Wastewater	0.012	109.2	5.9	109.5	5.5	108.8	5.6	110.7	7.2	111.2	7.0	109.8	6.9

a: Concentration of PAEs in the samples: 0.1 µg.L^{-1}.

b: Concentration of PAEs in the samples: 5 µg.L^{-1}.

c: Concentration of PAEs in the samples: 50 µg.L^{-1}.

d: Mineral bottled plastic water.

Table S8: Kinetic parameteres of DMP onto Fe_3O_4@[Bimi]Cl: 20 mg.L^{-1} concentration, 47.3 mg sorbent at ambient temperature.

Kinetic model	**Parameters**^{a}	
Pseudo-first-order	q_e (mg.g^{-1})	3.13
	K_1 (min-^{1})	2.68
	R^2	0.868
Pseudo-second-order	q_e (mg.g^{-1})	150.75
	K_2 (g(mg.min)$^{-1}$)	4.75
	R^2	0.998
Intraparticle Diffusion	C (mg.g^{-1})	32.91
	K_{dif} (mg^{-1}.min$^{-1/2}$)	5.74
	R^2	0.901

a: q_e: adsorption capacity at equilibrium, K rate constant.