Electronic Supplementary Material (ESI) for Analytical Methods.

Development of a high-throughput device for liquid-phase microextraction coupled with gas chromatography-mass spectrometry for the determination of benzene derivatives in environmental water

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Supporting information

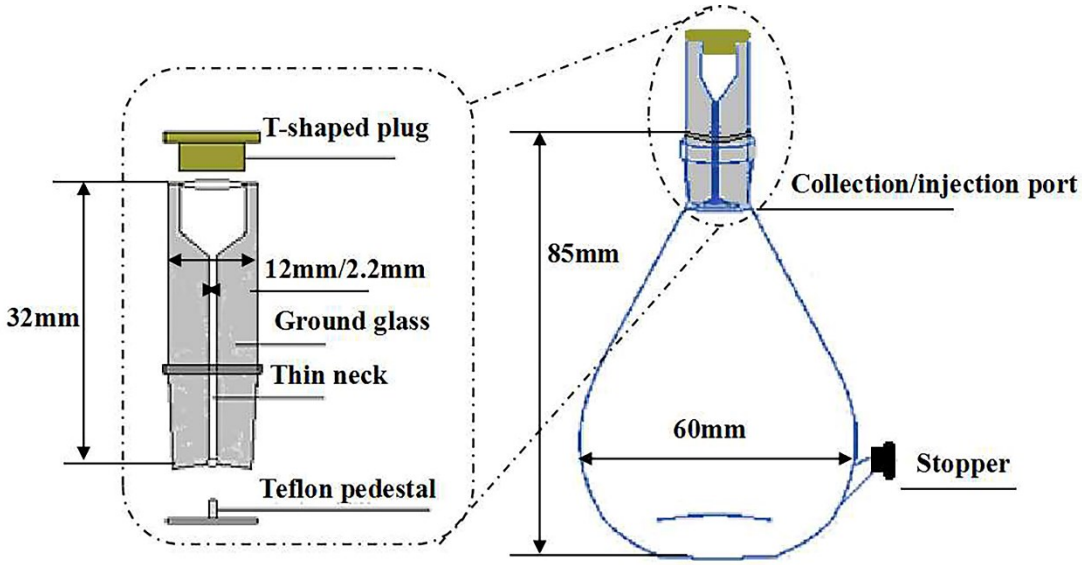


Figure S1. Details of the collection trap vial and extraction bottle.

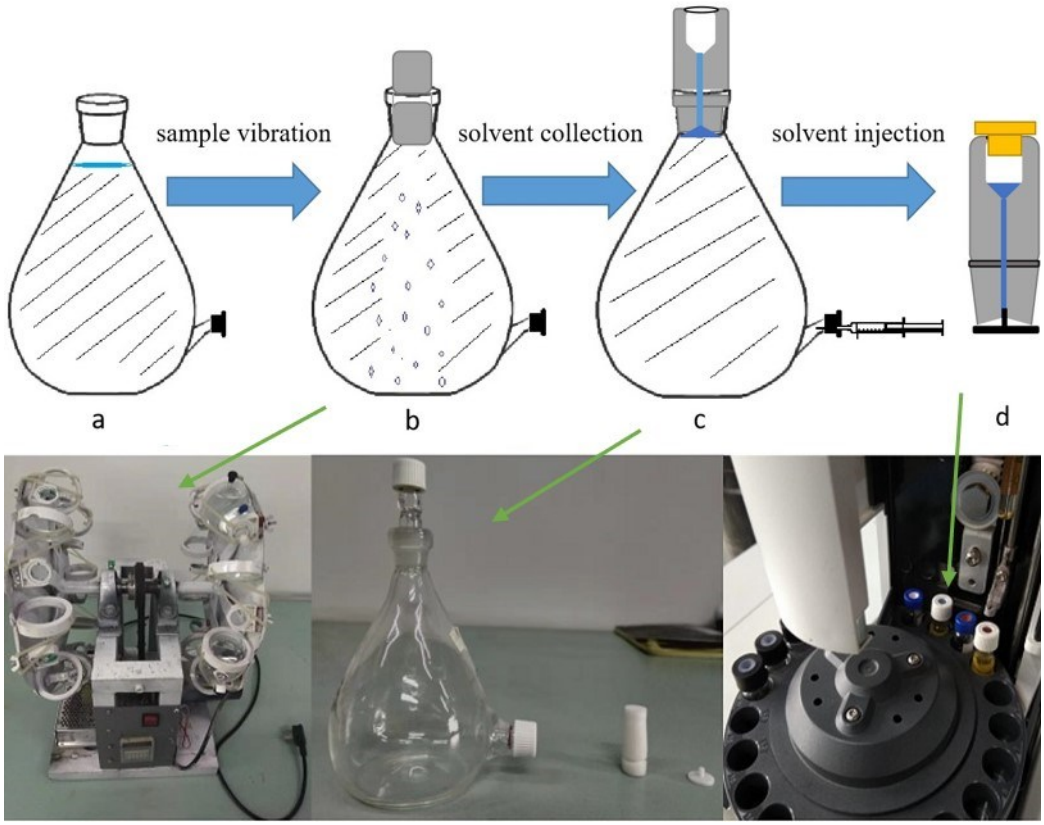


Figure S2. Photography of device.

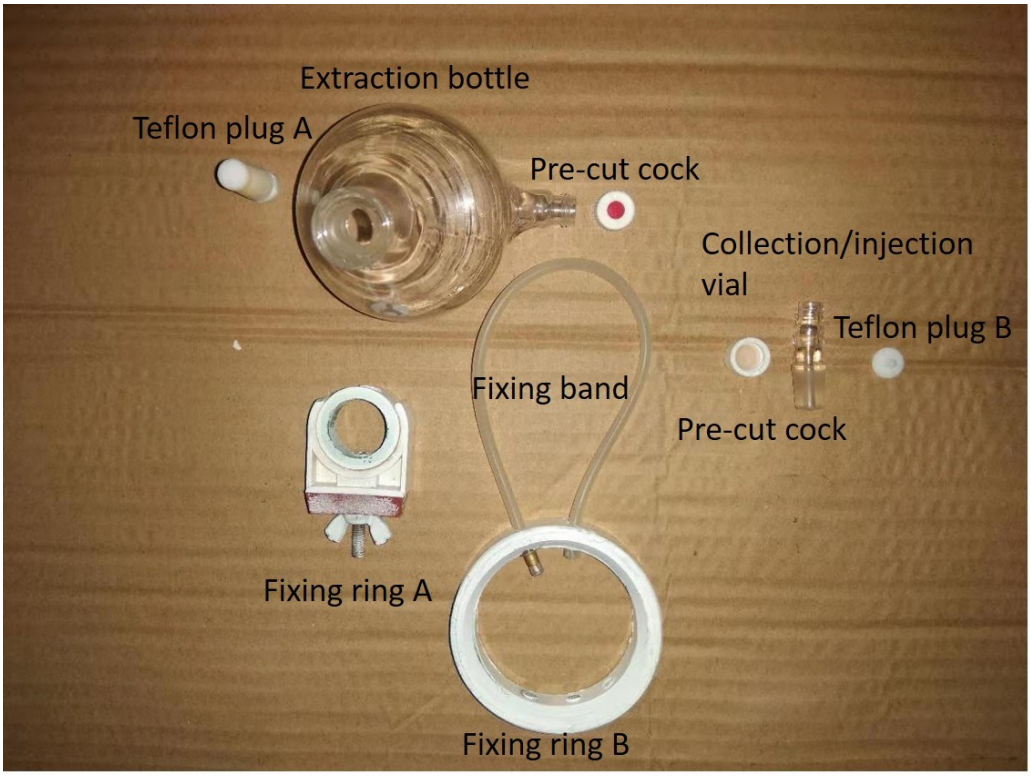


Figure S3. Photography of the disassembly of the device.

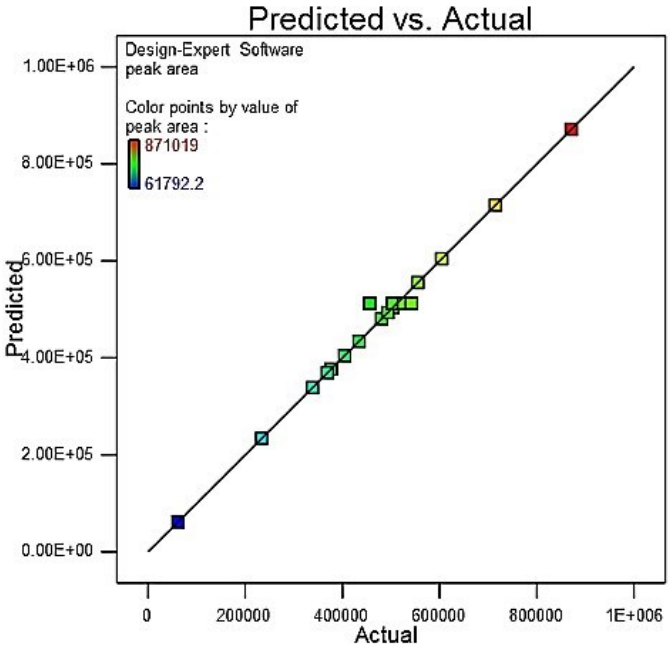


Figure S4. The correlation between predicted and experimental values of optimization.

Table S1 Physical and Chemical Properties of Benzene derivatives.

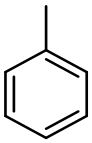
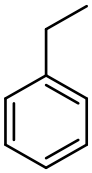
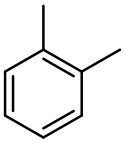
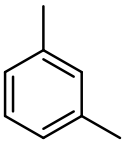
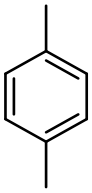
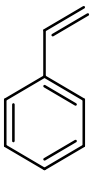
	Structural formula	Boiling point (℃)	Density(g/mL)	Solubility in water (g/100mL)	Log $K_{o/w}$	CAS number
Benzene		80	0.879	0.18	2.13	71-43-2
Toluene		111	0.867	0.05	2.73	108-88-3
Ethylbenzene		136-140	0.865	0.02	3.15	100-41-4
o-Xylene		143-145	0.879	-	3.12	95-47-6
m-Xylene		139	0.868	-	3.2	108-38-3
p-Xylene		138	0.861	-	3.15	106-42-3
Styrene		146	0.909	-	3.2	100-42-5

Table S2 Parameter setting of SIM method.

	Time quantum (min)	Fragment ion	Total residence time (ms)	Resolution ratio
Benzene	3-5	51/77/78		
Toluene	5-8	65/91/92		
Ethylbenzene	8-11	91/105/106		
o-Xylene	8-11	91/105/106	300	Low
m-Xylene	8-11	91/105/106		
p-Xylene	8-11	91/105/106		
Styrene	11-15.5	78/103/104		

Table S3 Experimental parameters and plan of the central composite design.

Variable			Low axial (-1.68)	Low factorial (-1)	Center (0)	High factorial (+1)	High axial (+1.68)
A Volume of solvent(μL)			100	108	120	132	140
B extraction Time (min)			21.5	25	30	35	38.5
C Salt concentration (%)			0	0.8	2	3.2	4
NO.	Volume (μL)	Time (min)	Salt concentration (%,W/V)	No.	Volume (μL)	Time (min)	Salt concentration (%,W/V)
1	132	35	3.2	11	132	35	3.2
2	108	35	3.2	12	108	35	3.2
3	120	30	2	13	120	30	2
4	132	25	0.8	14	132	25	0.8
5	132	35	0.8	15	132	35	0.8
6	140	30	2	16	140	30	2
7	120	30	2	17	120	30	2
8	108	25	0.8	18	108	25	0.8
9	120	30	2	19	120	30	2
10	120	30	2	20	120	30	2

Table S4 ANOVA for Central composite design model

Source	Sum of squares	df	Mean of Square	F Value	P-Value Prob>F
Model	52.20	14	3.73	37.76	0.0004
A-Volume	20.28	1	20.28	205.37	<0.0001
B-time	6.93	1	6.93	70.23	0.0004
C-Salt	1.73	1	1.73	17.51	0.0086
AB	0.69	1	0.69	7.01	0.0455
BC	0.42	1	0.42	4.28	0.0935
BC	3.62	1	3.62	36.70	0.0018
A^2	0.24	1	0.24	2.46	0.1774
B^2	10.48	1	10.48	106.18	0.0001
C^2	0.37	1	0.37	3.78	0.1094
ABC	0.29	1	0.29	2.93	0.1476
A^2B	4.43	1	4.43	44.83	0.0011
A^2C	0.75	1	0.75	7.57	0.0402
AB^2	3.69	1	3.69	37.42	0.0017
A^2B^2	1.76	1	1.76	17.82	0.0083
Pure Error	0.49	5	0.10		
Cor Total	52.69	19			

Table S5 The quality analytical parameters of the GC-MS without preconcentration step

	Calibration slope (L μg^{-1})	Line range ($\mu g \cdot L^{-1}$)	R^2	RSD (100 $\mu g \cdot L^{-1}$, n=3, %)	LOD (μg L^{-1})
Benzene	5.989	50-12000	0.996	3.0	31.3
Toluene	15.913	20-10000	0.999	5.1	12.9
Ethylbenzene	16.615	20-10000	0.999	2.6	16.6
p-Xylene	16.106	20-10000	0.999	5.7	13.4
m-Xylene	16.832	20-10000	0.998	1.2	11.2
o-Xylene	18.635	20-10000	0.997	1.0	15.9
Styrene	14.534	30-10000	0.997	5.1	27.1

Table S6 The t-test for actual and standard samples at two concentrations.

Sample	Compound	Spiked (5μg L^{-1})		Spiked (50μg L^{-1})	
		t[a]	H_0	t[a]	H_0
River 1	Benzene	-2.04	Accepted	-1.00	Accepted
	Toluene	1.84	Accepted	-1.47	Accepted
	Ethylbenzene	0.30	Accepted	1.37	Accepted
	p-Xylene	-0.20	Accepted	0.52	Accepted
	m-Xylene	-0.38	Accepted	-3.49	Accepted
	o-Xylene	-2.14	Accepted	-1.80	Accepted
	Styrene	2.74	Accepted	-0.22	Accepted
River 2	Benzene	2.85	Accepted	0.98	Accepted
	Toluene	2.81	Accepted	1.29	Accepted
	Ethylbenzene	0.19	Accepted	3.20	Accepted
	p-Xylene	-2.76	Accepted	0.04	Accepted
	m-Xylene	2.39	Accepted	-1.69	Accepted
	o-Xylene	-2.95	Accepted	-1.99	Accepted
	Styrene	-0.05	Accepted	-0.61	Accepted
River 3	Benzene	2.88	Accepted	3.33	Accepted
	Toluene	-2.63	Accepted	1.56	Accepted
	Ethylbenzene	-3.68	Accepted	2.24	Accepted
	p-Xylene	-0.44	Accepted	1.73	Accepted
	m-Xylene	-3.25	Accepted	0.06	Accepted
	o-Xylene	2.45	Accepted	2.46	Accepted
	Styrene	-3.58	Accepted	1.52	Accepted
River 4	Benzene	2.70	Accepted	-3.69	Accepted
	Toluene	0.51	Accepted	-2.45	Accepted
	Ethylbenzene	0.24	Accepted	-7.60	Unaccepted
	p-Xylene	3.33	Accepted	-4.45	Unaccepted
	m-Xylene	-0.87	Accepted	-5.14	Unaccepted
	o-Xylene	-0.81	Accepted	-3.39	Accepted
	Styrene	0.83	Accepted	-8.20	Unaccepted

[a] $t(\alpha=0.02, n=4)=3.75$