

Supporting information

Simultaneous enantiomeric analysis of chiral non-steroidal anti-inflammatory drugs in water, river sediment and sludge by chiral liquid chromatography-tandem mass spectrometry

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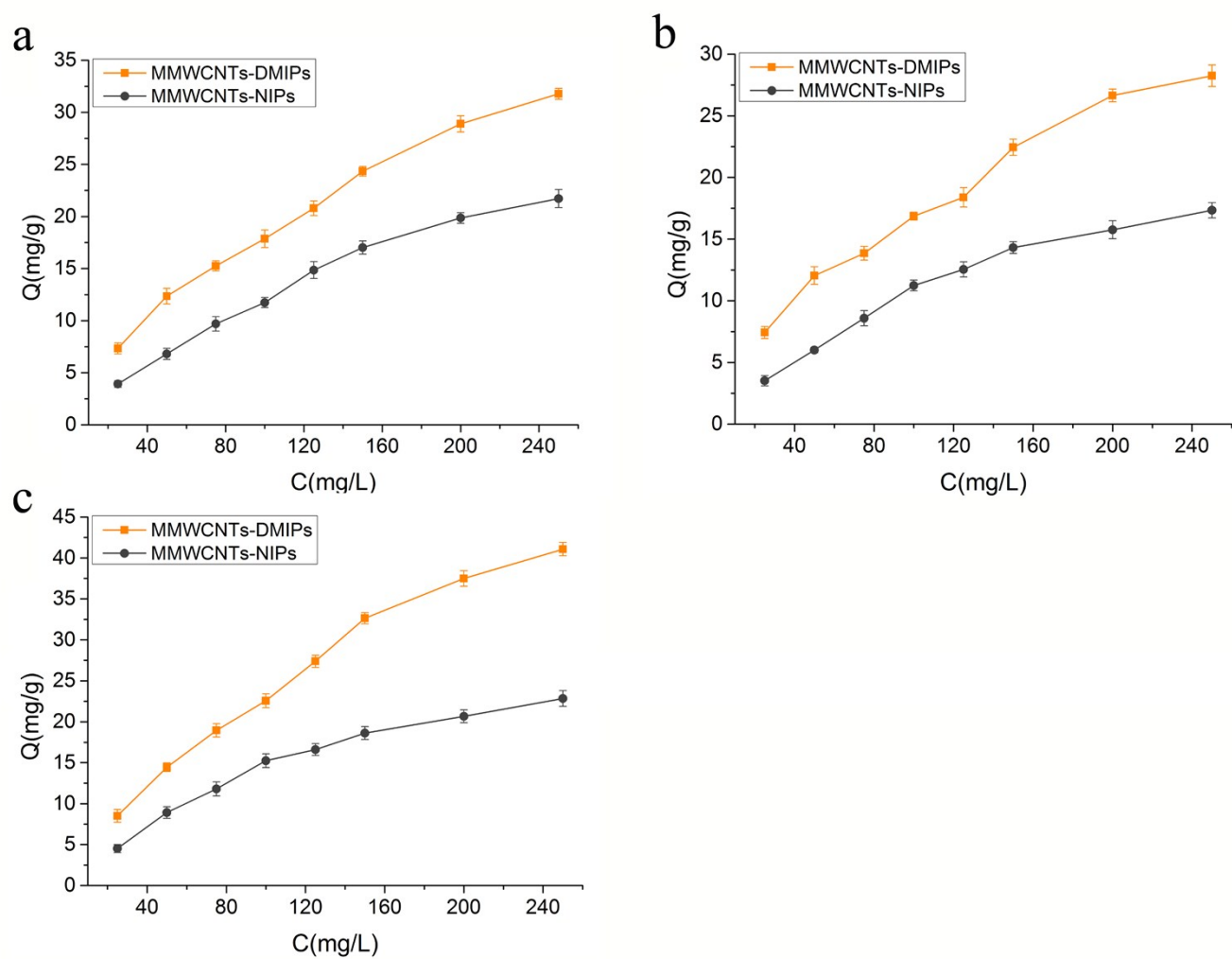


Fig. S1 Static adsorption curves of the MMWCNTs-DMIPs and MMWCNTs-NIPs for ibuprofen (a), ketoprofen (b) and flurbiprofen (c)

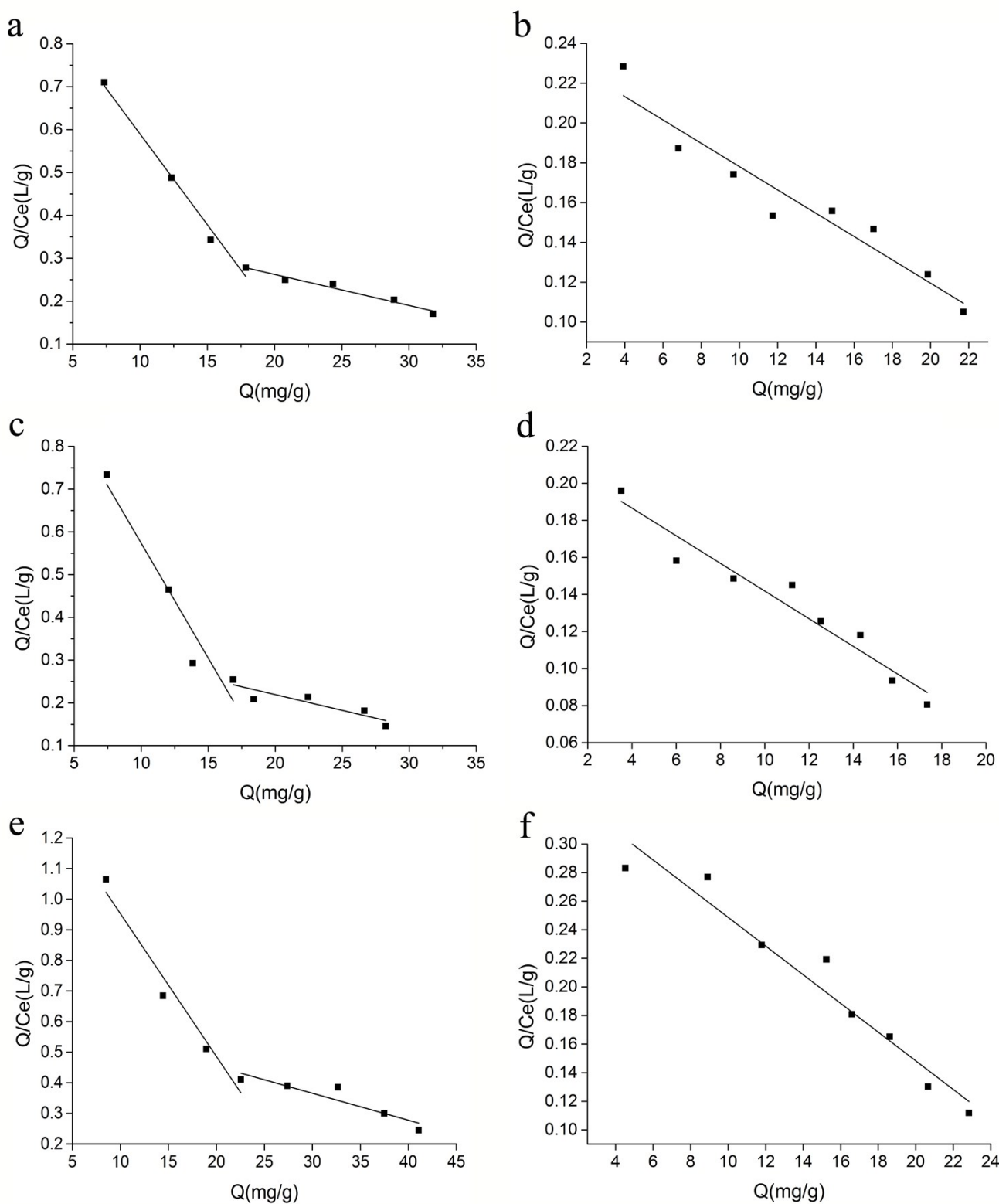


Fig. S2 Scatchard analysis of MMWCNTs-DMIPs for ibuprofen (a), ketoprofen (c) and flurbiprofen (e); scatchard analysis of MMWCNTs-NIPs for ibuprofen (b), ketoprofen (d) and flurbiprofen (f)

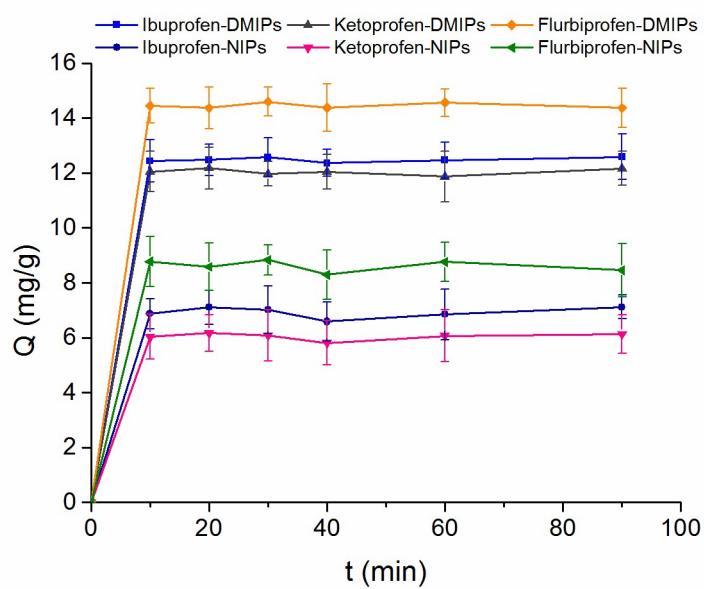


Fig. S3 Dynamic adsorption curves of the MMWCNTs-DMIPs and MMWCNTs-NIPs for ibuprofen, ketoprofen and flurbiprofen

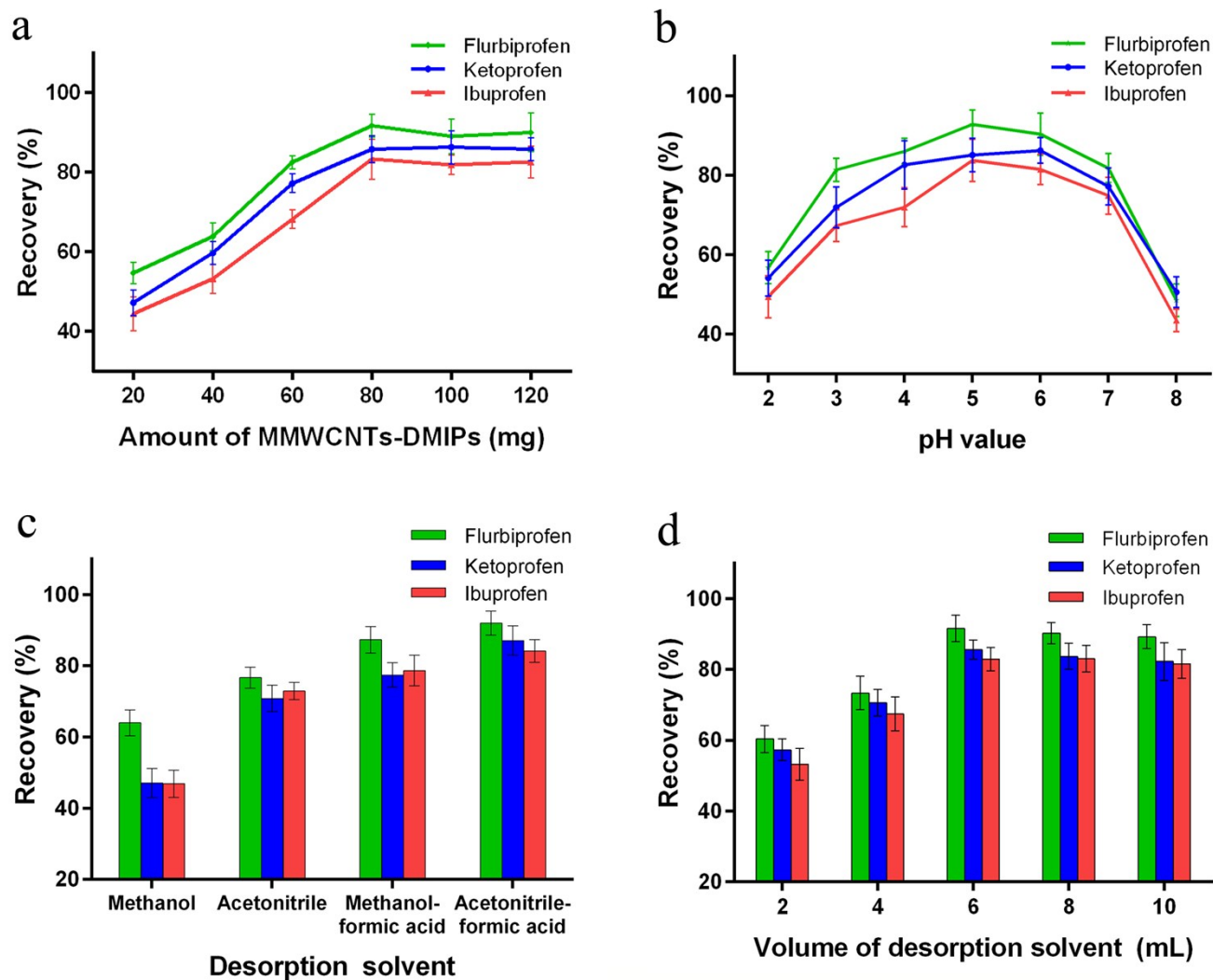


Fig. S4 Effect of the amount of sorbent (a), pH of sample solution (b), the type of desorption solvent (c), the volume of desorption solvent (d) on the extraction efficiency of the analytes for MSPE

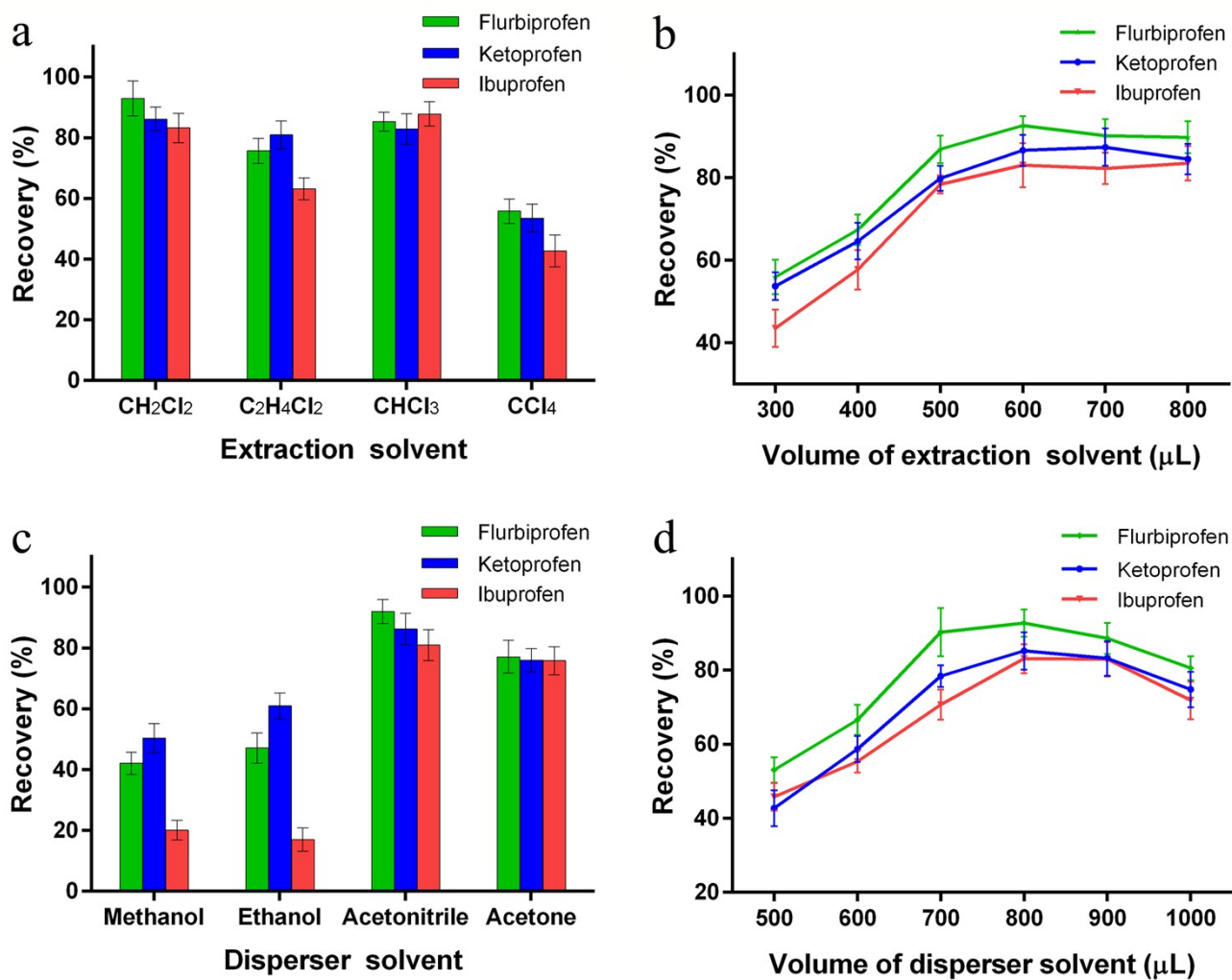


Fig. S5 Effect of the type of extraction solvent (a), the volume of extraction solvent (b), the type of disperser solvent (c), the volume of disperser solvent (d) on the extraction efficiency of the analytes for DLLME

Table S1 Dissociation constant (K_d) and maximum adsorption quantity ($Q_{\max}$) of MMWCNTs-DMIPs and MMWCNTs-NIPs

Analyte	MMWCNTs-DMIPs				MMWCNTs-NIPs	
	Left part		Right part		K_d (mg L ⁻¹)	$Q_{\max}$ (mg g ⁻¹)
	K_d (mg L ⁻¹)	$Q_{\max}$ (mg g ⁻¹)	K_d (mg L ⁻¹)	$Q_{\max}$ (mg g ⁻¹)		
Ibuprofen	23.66	23.95	138.12	56.25	170.65	40.39
Ketoprofen	18.62	20.68	135.87	49.81	134.05	29.01
Flurbiprofen	21.43	30.42	113.51	71.53	99.60	34.77

Table S2 Imprinting factor (α) of MMWCNTs-DMIPs

Analyte	$Q_{\text{MMWCNTs-DMIPs}} (\text{mg g}^{-1})$	$Q_{\text{MMWCNTs-NIPs}} (\text{mg g}^{-1})$	α
Ibuprofen	12.34	6.85	1.80
Ketoprofen	12.05	5.97	2.02
Flurbiprofen	14.41	8.92	1.62

Table S3 Accuracy and precision of the proposed method in different water samples

Analyte	Spiked (ng L ⁻¹)	River water			Lake water			Waste water		
		Accuracy	Precision (RSD%)		Accuracy	Precision (RSD%)		Accuracy	Precision (RSD%)	
			Intra-day	Inter-day		Intra-day	Inter-day		Intra-day	Inter-day
Ibuprofen-E1	20	83.5	5.4	7.5	84.0	9.3	7.5	82.7	3.7	6.4
	100	85.2	6.3	5.6	85.8	5.6	4.6	84.8	8.6	9.1
	500	86.3	4.8	7.1	88.2	7.5	5.3	85.7	7.4	5.8
Ibuprofen-E2	20	82.8	3.6	5.8	84.6	4.7	8.3	83.5	5.3	6.5
	100	85.1	7.5	10.2	84.9	2.1	6.4	85.2	9.5	11.7
	500	87.0	5.4	6.7	87.3	3.9	7.6	87.4	4.8	5.6
Ketoprofen-E1	20	76.6	4.7	6.3	76.4	7.2	5.8	77.8	5.2	7.8
	100	78.4	3.5	5.7	77.9	3.3	6.4	80.3	2.9	6.2
	500	79.2	4.3	3.9	81.6	2.6	5.3	79.1	6.5	8.3
Ketoprofen-E2	20	78.1	5.6	7.3	76.8	4.7	8.5	76.4	4.2	4.9
	100	77.9	5.1	6.8	79.3	4.2	6.1	78.0	4.6	7.8
	500	80.4	7.2	6.5	80.2	6.4	4.8	81.5	5.3	10.8
Flurbiprofen-E1	20	87.1	7.2	8.6	85.8	5.5	11.3	84.3	5.5	8.4
	100	90.6	2.8	5.3	86.4	5.3	7.6	92.1	7.0	7.8
	500	90.2	4.7	5.6	89.5	8.4	6.9	88.9	3.6	5.3
Flurbiprofen-E2	20	85.7	8.2	10.5	87.3	4.7	6.0	86.0	4.7	6.2
	100	89.5	4.6	6.8	85.3	3.7	5.2	90.4	6.4	10.7
	500	91.4	6.0	8.4	90.8	6.5	9.3	89.6	3.6	4.5

Table S4 Accuracy and precision of the proposed method in river sediment and sludge samples

Analyte	Spiked (ng g ⁻¹)	River sediment			Sludge		
		Accuracy	Precision (RSD%)		Accuracy	Precision (RSD%)	
			Intra-day	Inter-day		Intra-day	Inter-day
Ibuprofen-E1	4	83.8	4.7	7.4	82.6	5.6	7.7
	20	86.4	6.5	7.1	85.3	5.2	6.4
	100	85.8	8.3	6.5	84.2	2.5	4.7
Ibuprofen-E2	4	82.5	4.8	7.3	83.9	9.5	12.4
	20	84.5	5.1	4.9	86.4	6.4	6.8
	100	84.0	3.6	5.2	84.8	4.3	6.2
Ketoprofen-E1	4	77.6	3.2	5.8	76.2	5.4	4.7
	20	80.4	5.6	5.2	78.7	3.6	4.2
	100	78.7	4.5	6.2	78.1	6.5	6.3
Ketoprofen-E2	4	78.9	4.3	5.6	75.8	4.6	7.4
	20	79.3	7.8	11.2	79.8	4.3	8.2
	100	81.0	6.3	5.6	76.5	7.3	10.8
Flurbiprofen-E1	4	88.6	3.1	4.4	87.3	5.7	7.6
	20	90.2	7.2	9.5	87.0	8.3	6.9
	100	91.1	5.6	3.6	90.2	4.5	5.2
Flurbiprofen-E2	4	87.8	5.7	7.4	88.4	2.7	4.1
	20	88.5	4.5	8.3	86.7	7.4	6.5
	100	90.8	3.7	5.2	91.6	3.2	5.6

Table S5 Comparison with other methods

Matrix	Analytes	Extraction method	Analytical method	MQL	Recovery (%)	References
Waste water	Ibuprofen Naproxen	SPE	Chiral-GC-MS	100 ng/L	52-80	[44]
Waste water Surface water Sediment	Ibuprofen	SPE	Chiral-LC-UV	2400 ng/L (water samples) 120 ng/g (Sediment)	16-62	[45]
Waste water	Ibuprofen Ketoprofen Naproxen	Micro-extraction	Chiral-LC-MS/MS	2-5 ng/L	58-102	[46]
River water Lake water	Ibuprofen	MSPE-DLLME	Chiral-LC-MS/MS	7-12 ng/L (water samples)	75-92	Present work
Waste water	Ketoprofen			2-3 ng/g (river sediment and Sludge)		
River sediment Sludge	Flurbiprofen					