Supplementary information

Effective extraction and determination of 9 β-lactams in water and milk samples by a novel magnetic covalent organic framework combined with UPLC-MS/MS

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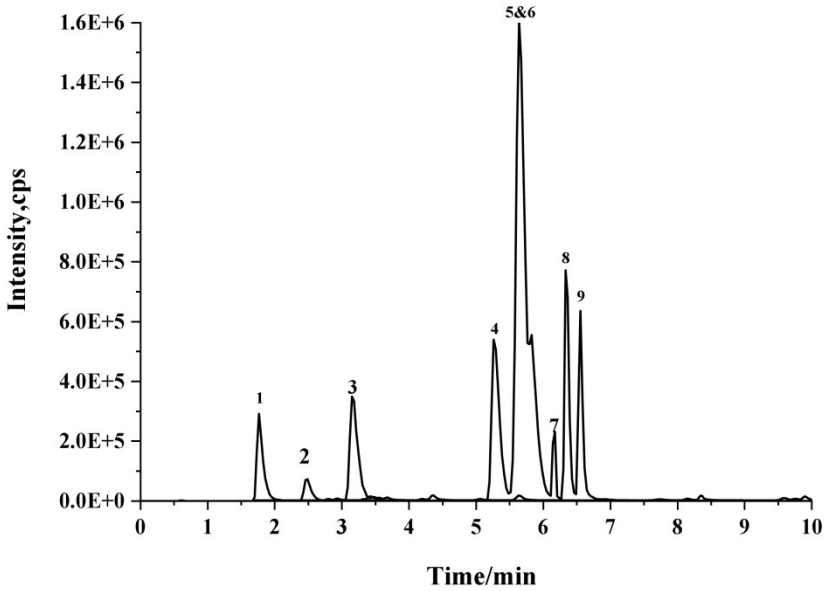

Fig. S1 Total ion chromatograms of 9 β-LAs. 1. CRA, 2. CFP, 3. EFT, 4. CPD, 5. CETP, 6. DIC, 7. CLO, 8. OXA, 9. FLU.

Table S1 The information of 9 β-LAs standard substances

β-LAs	Abbreviation	**CAS**	Molecular formula	Molecular mass	Purity (%)
Cefpiramide acid	CRA	70797-11-4	$C_{25}H_{24}N_8O_7S_2$	612.64	98.0
Cefoperazone	CFP	62893-19-0	$C_{25}H_{27}N_9O_8S_2$	645.67	95.0
Ceftiofur	EFT	80370-57-6	$C_{19}H_{17}N_5O_7S_3$	523.56	97.0
Cefpodoxime proxetil	CPD	87239-81-4	$C_{21}H_{27}N_5O_9S_2$	557.6	99.7
Cefetamet pivoxil hydrochloride	CETP	111696-23-2	$C_{20}H_{26}ClN_5O_7S_2$	548.03	70.2
Dicloxacillin sodium	DIC	13412-64-1	$C_{19}H_{20}Cl_2N_3NaO_6S$	412.33	98.0
Cloxacillin	CLO	61-72-3	$C_{19}H_{18}ClN_3O_5S$	435.88	93.8
Oxacillin sodium	OXA	1173-88-2	$C_{19}H_{18}N_3NaO_5S$	423.42	95.1
Flucloxacillin	FLU	5250-39-5	$C_{19}H_{17}ClFN_3O_5S$	453.87	90.9

Table S2 Mass spectrometry conditions of 9 β-LAs

β-LAs	Retention (min)	Precursor (m/z)	Declustering potential (V)	Product ion (m/z)	Collision (eV)
CRA	1.77	613.1	130.1/129.9	257.3*/285.1	37.7/25.3
CFP	2.48	646.3	136.04/189.9	290.3*/142.9	30.8/43.1
EFT	3.16	524.1	112.0/120.0	241.0*/210.1	24.6/30.3
CPD	5.61	558.2	105.1/77.9	410.1*/428.1	22.8/22.2
CETP	5.65	512.2	95.9/109.9	241.1*/398.1	24.2/27.2
DIC	6.55	470.2	144.9/136.1	159.9*/311.2	17.1/19.2
CLO	6.17	436.2	132.0/140.0	277.2*/159.7	19.0/18.0
OXA	5.28	402.3	101.9/126.1	160.1*/243.1	18.9/19.0
FLU	6.35	454.0	123.0/123.2	160.0*/295.2	16.4/22.8

Table S3 The spiked recoveries and RSDs of 9 β-LAs at three levels in the water and milk samples

Analytes	Water			Milk		
	Spiked concentration ($\mu g \cdot L^{-1}$)	Recovery (%)	RSD (%)	Spiked concentration ($\mu g \cdot L^{-1}$)	Recovery (%)	RSD (%)
CRA	0.4	82.2	7.07	16	74.1	6.49
	1.6	80.2	5.08	40	77.0	4.00
	4	92.3	2.56	200	71. 9	2.76
CFP	0.4	95.3	7.37	16	95.7	8.80
	1.6	78.2	9.18	40	79.9	8.44
	4	79.4	6.29	200	71.7	3.12
EFT	0.4	85.3	7.74	16	82.6	2.60
	1.6	89.9	3.42	40	73.8	2.15
	4	100.5	4.11	200	74.8	2.81
CPD	0.4	82.9	5.35	16	79.4	4.40
	1.6	79.0	1.14	40	82.8	1.57
	4	93.7	2.14	200	72.1	1.54
CETP	0.4	88.8	3.96	16	79.6	3.47
	1.6	84.6	2.02	40	87.9	2.18
	4	95.7	2.41	200	77.1	1.71
DIC	0.4	114.6	2.93	16	113.7	7.39
	1.6	116.6	1.89	40	96.8	4.07
	4	116.1	5.39	200	89.0	5.62
CLO	0.4	99.2	2.88	16	79.2	7.89
	1.6	94.2	7.18	40	95.7	9.46
	4	112.7	6.64	200	96.7	5.92
OXA	0.4	112.9	2.64	16	118.8	2.39
	1.6	118.1	2.80	40	109.9	2.21
	4	117.7	4.32	200	94.9	3.13
FLU	0.4	102.2	4.92	16	105.0	2.14
	1.6	116.9	1.93	40	93.5	1.87
	4	117.4	2.20	200	82.8	3.42

Table S4 Adsorption of different types of antibiotics with Fe_3O_4@SiO_2@Ap-COF

Type	Compounds	Adsorption efficiency (%)
NMZs[a]	Tinidazole	28.39
	4-Nitroimidazole	5.23
	Hydroxymetronidazole	12.09
	2-Methyl-4-nitroimidazole	15.38
	Pymetrozine-hydroxymethyl	8.98
	Metronidazole	8.55
	Ronidazole	25.32
	1,2-Dimethyl-5-nitroimidazole	18.29
	Secnidazole	4.22
	Ornidazole	26.72
	Ipronidazole	6.95
	Hydroxy Ipronidazole	26.88
TCs[b]	4-Epitetracycline	23.05
	Oxytetracycline	15.69
	4-Epioxytetracycline	12.33
	Tetracycline	20.58
	4-Epichlortetracycline	16.83

[a]NMZs: nitroimidazoles. TCs[b]: tetracyclines.