Supplementary data for

Modeling rapid and selective capture nNOS-PSD-95 uncouplers from Sanhuang Xiexin Decoction by novel molecularly imprinted polymers based on metal-organic frameworks

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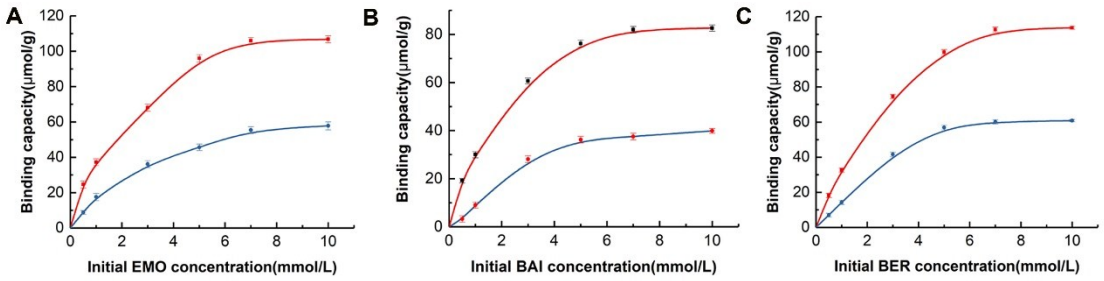

Fig. S1 Static adsorption curve of (A) EMO@MIPs, (B) BAI@MIPs, (C) BER@MIPs.

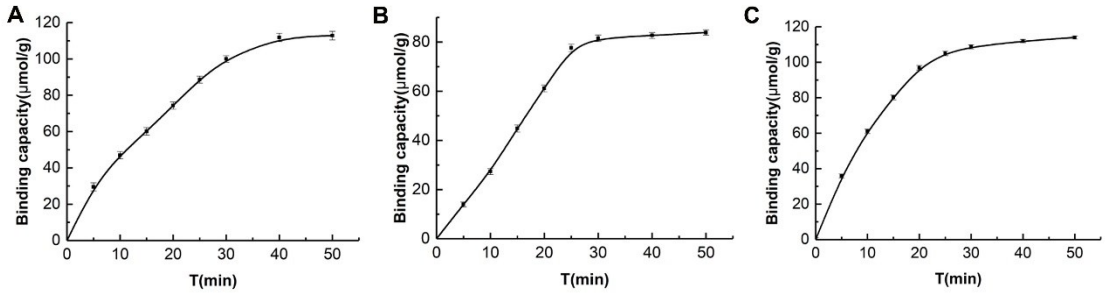

Fig. S2 Kinetic adsorption curve of (A) EMO@MIPs, (B) BAI@MIPs, (C) BER@MIPs.

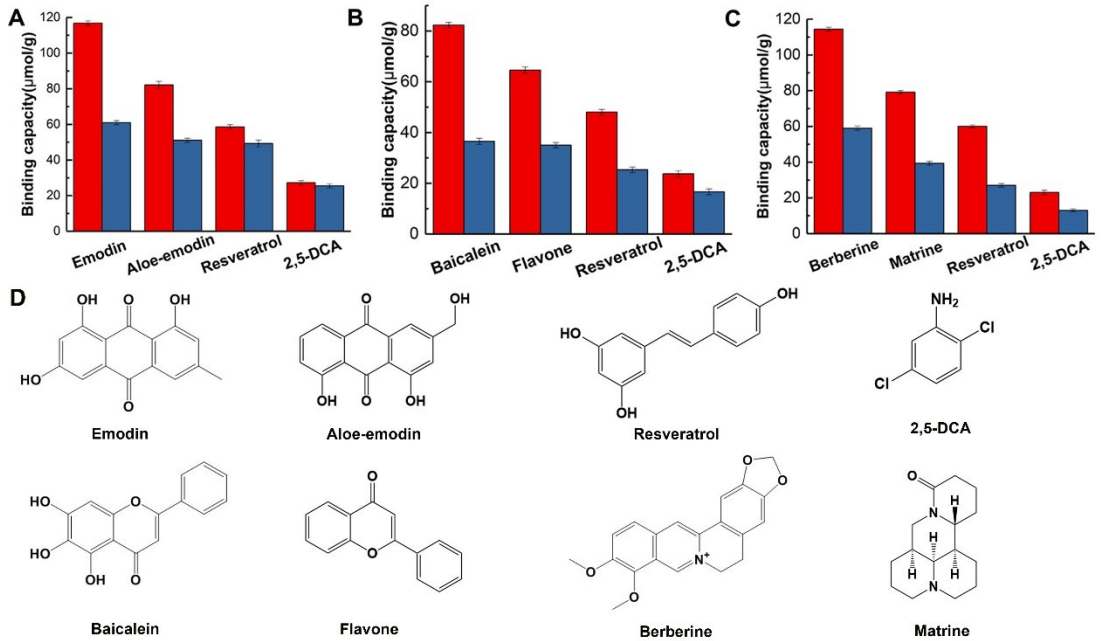

Fig. S3 Selective adsorption ability of (A) EMO@MIPs, (B) BAI@MIPs, (C) BER@MIPs, (D) the structure of the compounds detected.

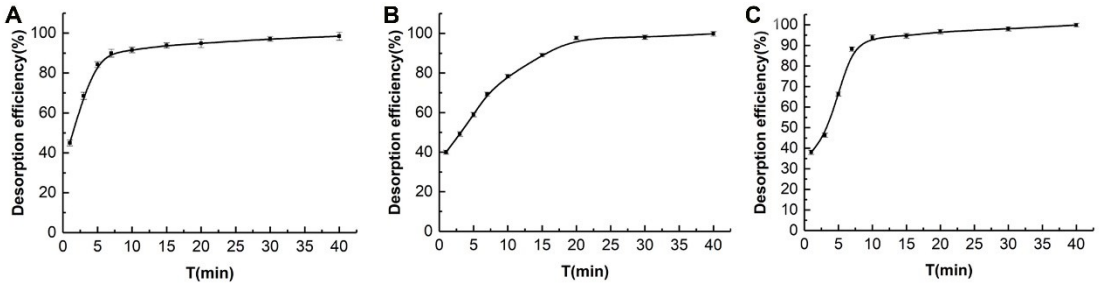

Fig. S4 Desorption efficiency of (A) EMO@MIPs, (B) BAI@MIPs, (C) BER@MIPs.

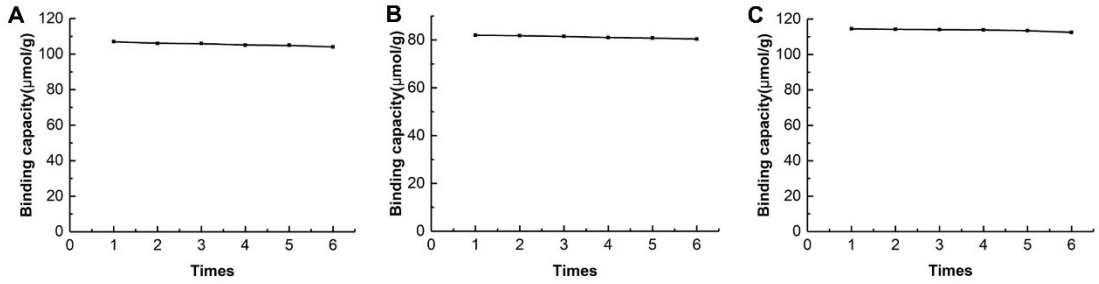

Fig. S5 Reusability of (A) EMO@MIPs, (B) BAI@MIPs, (C) BER@MIPs.

Table S1

The chromatographic condition of Sanhuang Xiexin Decoction

	Sanhuang Xiexin Decoction	
Mobile phase	A: 1% formic acid; B: ACN	
Gradient	0-7 min	2% B
	10 min	20% B
	30-40 min	25% B
	45 min	50% B
	55 min	60% B
	70 min	75% B
	85 min	100% B
Detection	280nm	

Table S2

The adsorption capacity of different EMO@MIPs under different conditions

Polymer	Emodin (mmol)	Solvent	Functional Monomer	Molar ratio[a]	$Q_{EMO@MIPs}$ (μmol/g)	IF[b]
EMO@MIPs-1	0.4	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	19.08	1.04
EMO@MIPs-2	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	108.54	1.95
EMO@MIPs-3	0.6	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	50.01	1.29
EMO@MIPs-4	0.5	Tetrahydrofuran/ethanol (1:2,v/v)	MAA	1:6:30	58.40	1.52
EMO@MIPs-5	0.5	Acetonitrile/ethanol (2:1,v/v)	MAA	1:6:30	100.50	1.94
EMO@MIPs-6	0.5	Acetonitrile/ethanol (1:2,v/v)	MMA	1:6:30	79.74	1.08
EMO@MIPs-7	0.5	Acetonitrile/ethanol (1:2,v/v)	4-VP	1:6:30	76.61	1.20
EMO@MIPs-8	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:5:25	100.70	1.36
EMO@MIPs-9	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:7:35	57.22	1.44

[a] Molar ratio refers to the ratio of template, functional monomer and cross-linker.

[b] IF represents the value of $Q_{EMO@MIPs}/Q_{EMO@NIPs}$, where $Q_{EMO@MIPs}$ and $Q_{EMO@NIPs}$ refer to the binding capacity of EMO@MIPs and EMO@NIPs, respectively.

Table S3

The adsorption capacity of different BAI@MIPs under different conditions

Polymer	Baicalein (mmol)	Solvent	Functional Monomer	Molar ratio[a]	$Q_{BAI@MIPs}$ (μmol/g)	IF[b]
BAI@MIPs-1	0.4	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	58.66	1.08
BAI@MIPs-2	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	81.52	2.06
BAI@MIPs-3	0.6	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	49.46	1.01
BAI@MIPs-4	0.5	Tetrahydrofuran/ethanol (1:2,v/v)	MAA	1:6:30	57.65	1.44
BAI@MIPs-5	0.5	Acetonitrile/ethanol (2:1,v/v)	MAA	1:6:30	76.54	1.60
BAI@MIPs-6	0.5	Acetonitrile/ethanol (1:2,v/v)	MMA	1:6:30	68.27	1.32
BAI@MIPs-7	0.5	Acetonitrile/ethanol (1:2,v/v)	4-VP	1:6:30	79.65	1.28
BAI@MIPs-8	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:5:25	73.31	2.31
BAI@MIPs-9	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:7:35	77.38	2.34

[a] Molar ratio refers to the ratio of template, functional monomer and cross-linker.

[b] IF represents the value of $Q_{BAI@MIPs}/Q_{BAI@NIPs}$, where $Q_{BAI@MIPs}$ and $Q_{BAI@NIPs}$ refer to the binding capacity of BAI@MIPs and BAI@NIPs, respectively.

Table S4

The adsorption capacity of different BER@MIPs under different conditions

Polymer	Berberine (mmol)	Solvent	Functional Monomer	Molar ratio[a]	$Q_{BER@MIPs}$ (μmol/g)	IF[b]
BER@MIPs-1	0.4	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	86.05	1.81
BER@MIPs-2	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	114.46	1.96
BER@MIPs-3	0.6	Acetonitrile/ethanol (1:2,v/v)	MAA	1:6:30	63.40	1.38
BER@MIPs-4	0.5	Tetrahydrofuran/ethanol (1:2,v/v)	MAA	1:6:30	82.46	1.02
BER@MIPs-5	0.5	Acetonitrile/ethanol (2:1,v/v)	MAA	1:6:30	88.72	1.67
BER@MIPs-6	0.5	Acetonitrile/ethanol (1:2,v/v)	MMA	1:6:30	104.76	1.70
BER@MIPs-7	0.5	Acetonitrile/ethanol (1:2,v/v)	4-VP	1:6:30	87.17	1.25
BER@MIPs-8	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:5:25	100.49	1.23
BER@MIPs-9	0.5	Acetonitrile/ethanol (1:2,v/v)	MAA	1:7:35	100.32	1.08

[a] Molar ratio refers to the ratio of template, functional monomer and cross-linker.

[b] IF represents the value of $Q_{BER@MIPs}/Q_{BER@NIPs}$, where $Q_{BER@MIPs}$ and $Q_{BER@NIPs}$ refer to the binding capacity of BER@MIPs and BER@NIPs, respectively.

Table S5

The mass characteristics of the compounds

Peak	Name	Formula	Retention time (min)	$[M+H]^+$	Reference
1	Coptisine	$C_{19}H_{14}NO_4$	27.4	321	[1]
2	Baicalin	$C_{21}H_{18}O_{11}$	30.3	447	[1]
3	Berberine	$C_{20}H_{18}NO_4$	35.3	337	[1]
4	Emodin-8-O-β-D-glucoside	$C_{21}H_{20}O_{10}$	38.4	433	[2]
5	Wogonoside	$C_{22}H_{20}O_{11}$	42.0	461	[1]
6	Baicalein	$C_{15}H_{10}O_5$	49.1	271	[1]
7	Emodin	$C_{15}H_{10}O_5$	56.6	269	[1]
8	Chrysophanol	$C_{15}H_{10}O_4$	61.2	255	[2]
9	Physcion	$C_{16}H_{12}O_5$	64.7	285	[2]

Table S6

EC_{50} values of the compounds on glutamate-injured PC12 cells

Substance	EC_{50} value (μM)
ZL006	26.674±2.886
Emodin	76.205±3.668
Baicalein	25.879±3.076
Berberine	11.940±3.038
SXD extracts	15.470±3.853
Active components	20.548±3.155

References

[1] Q. Zhang, C. H. Wang, Y. M. Ma, E. Y. Zhu and Z. T. Wang, Biomed. Chromatogr., 2013, **27**, 1079-1088.

[2] T. Y. Wu, F. R. Chang, J. R. Liou, I. W. Lo, T. C. Chung, L. Y. Lee, C. C. Chi, Y. C. Du, M. H. Wong, S. H. H Juo, C. C. Lee and Y. C. Wu, Front. Pharmacol., 2016, **7**, 374.