Supporting Information

Novel surface imprinted magnetic mesoporous silica as artificial antibodies for efficient discovery and catch of candidate nNOS－PSD-95 uncouplers for stroke treatment

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Table S1 The chromatographic conditions of Corydalis rhizoma, Macleaya cordata and Zanthoxylum nitidum.

	Corydalis rhizoma	Macleaya cordata	Zanthoxylum nitidum
Aqueous phase (A)	0.2% H_3PO_4; pH 5.0	0.1% H_3PO_4	0.2% H_3PO_4; pH 2.0
Organic phase (B)	ACN	ACN	ACN
Gradient	0 min, 20% B 15 min,36% B 20 min, 49% B 30 min, 80% B 31 min, 95% B 40 min, 95% B	0 min, 27% B 5 min, 27% B 17 min, 54% B 28 min, 90% B 33 min, 27% B 43 min, 27% B	0 min, 15% B 5 min, 21% B 10 min, 25% B 15 min, 36% B 25 min, 44% B 30 min, 70% B 45 min, 85% B 55 min, 100% B
Detection	280 nm	284 nm	273 nm

Table S2 The synthesis of MMS@MIPs with different quantities of ZL006.

	ZL006 (mmol)	S_{BET} (m^2/g)	$Q_{MMS@MIPs}$[a] (μmol/g)	IF[b]
MMS@MIP-1	0.3	75.1	83.5	1.74
MMS@MIP-2	0.4	64.4	106.41	1.92
MMS@MIP-3	0.5	59.2	72.4	1.48

[a]The binding capacity were determined by adding polymers (20 mg) in ZL006 acetonitrile/ethyl alcohol (9:1, v/v) solution (2.5 mmol/L, 5 mL) for 30 min (n=3).[b]IF=$Q_{MMS@MIPs}/Q_{MMS@NIPs}$, where $Q_{MMS@MIPs}$ and $Q_{MMS@NIPs}$ were defined as the binding capacity of ZL006 on MMS@MIPs and MMS@NIPs, respectively.

Table S3 Compositions and adsorbing performance of Different MMS@MIPs.

Polymer[a]	FM (mmol)	CL (mmol)	solvent	$Q_{MMS@MIPs}$ (μmol/g)	IF
MMS@MIP-1	2 (MMA)	10	DMF	45.45	1.22
MMS@MIP-2	2 (MMA)	10	toluene/ethanol (9:1，v/v)	52.15	2.00
MMS@MIP-3	2 (MMA)	10	acetonitrile/ethanol (9:1，v/v)	63.90	3.04
MMS@MIP-4	2 (AM)	10	acetonitrile/ethanol (9:1，v/v)	106.41	1.92
MMS@MIP-5	2 (MBA)	10	acetonitrile/ethanol (9:1，v/v)	77.94	2.30
MMS@MIP-6	1.6 (AM)	8	acetonitrile/ethanol (9:1，v/v)	99.13	1.70
MMS@MIP-7	2.4 (AM)	12	acetonitrile/ethanol (9:1，v/v)	90.38	1.29
MMS@MIP-8	2 (AM)	8	acetonitrile/ethanol (9:1，v/v)	93.25	1.46
MMS@MIP-9	2 (AM)	12	acetonitrile/ethanol (9:1，v/v)	83.62	1.59

[a]The polymers were prepared using ZL006 (0.4 mmol) as the template，EGDMA as the cross-linker, AIBN as the initiator.

Table S4 Porosities of polymers determined by N_2 adsorption/desorption analysis**.**

	S_{BET} (m^2/g)	V_t (cm^3/g)
MMS	329.5	0.34
MMS-MPS	252.7	0.15
MMS@MIPs	64.4	0.08

64 **Table S5** The performance characteristics of the proposed method (n=3).

Analyte	Linear regression date			RSD(%)		LOD (μg/mL)	LOQ (μg/mL)
	Regression equatoion	R^2	Test range (mg/mL)	Intra-day	Inter-day		
Allocryptopine	y = 12585067 x + 108323	0.9997	0.010 - 1.000	1.9	2.4	0.20	1.53
Coptisine	y = 42801930 x +99484	0.9994	0.001 - 0.200	2.7	1.6	0.18	0.45
Palmatine	y = 66246379 x + 208376	0.9994	0.001 - 0.200	1.9	0.9	0.46	1.24
Dehydrocorydaline	y = 49780595 x + 847187	0.9996	0.001 - 0.800	3.1	1.8	0.32	1.22
Sanguinarine	y = 89354768 x + 740693	0.9993	0.010 - 0.400	3.6	2.5	0.09	1.13
Chelerythrine	y = 88518961 x +410412	0.9994	0.010 - 0.400	0.9	1.3	0.12	0.40
Hesperidin	y = 15231533 x + 355332	0.9996	0.010 – 2.000	2.8	1.7	0.17	0.59
Nitidine chloride	y = 87152361 x + 145910	0.9999	0.010 - 0.200	2.9	3.3	0.24	1.02

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66 **Table S6** The detected chromatographic data of the separated compounds.

Peak	Name	Formula	Retention time (min)	Precursr Ion (m/z)	Reference
1	Allocryptopine	$C_{21}H_{23}NO_5$	13.7	370 $[M^+H]^+$	1
2	Coptisine	$C_{19}H_{14}NO_4$	14.9	320 M^+	1
3	Palmatine	$C_{21}H_{22}NO_4$	17.5	352 M^+	1
4	Dehydrocorydaline	$C_{22}H_{24}NO_4$	19.1	366 M^+	1
5	Sanguinarine	$C_{20}H_{14}NO_4$	14.3	332 M^+	2
6	Chelerythrine	$C_{21}H_{18}NO_4$	17.1	348 M^+	2
7	Hesperidin	$C_{28}H_{34}O_{15}$	16.8	611 $[M^+H]^+$	3
8	Nitidine chloride	$C_{21}H_{18}ClNO_4$	21.7	348 M^+	4

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Table S7 Neuroprotective evaluation about EC_{50} values of the compounds on glutamate-induced PC12 cells injury.

Substance	EC_{50} value (μmol/L)
ZL006	23.541 ± 2.152
Allocryptopine	33.453 ± 3.523
Coptisine	18.248 ± 1.451
Palmatine	26.833 ± 1.718
Dehydrocorydaline	7.706 ± 0.499
Sanguinarine	1.674 ± 0.046
Chelerythrine	3.109 ± 0.070
Hesperidin	21.329 ± 3.560
Nitidine chloride	5.500 ± 0.276

Data is presented as mean±S.D (n=3)

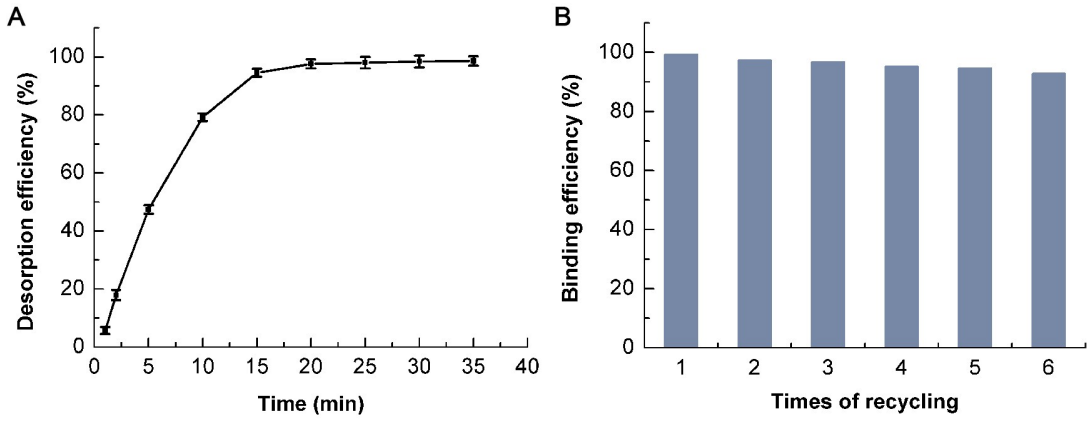

Figure S1 Desorption and regeneration of the artificial antibodies. (A) the desorption dynamics of MMS@MIPs, (B) the reusability of MMS@MIPs.

References

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