Electronic Supporting Information for

Uniform Core-Shell Molecularly Imprinted Polymers: A Correlation Study between Shell Thickness and Binding Capacity

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Equation S1

$$Q = \frac{(C_0 - C)V}{m} \qquad (1)$$

where, Q is the binding amount of Sudan I adsorbed by unit mass of MIPs, C_0 is the initial concentration of Sudan I in solutions, C is the free concentration of Sudan I in solutions after adsorption by MIPs, V is the volume of the Sudan I solutions tested, and m is the mass of the MIPs used.

Equation S2

$$\varphi = \frac{(r + x)^3 - r^3}{r^3} \qquad (2)$$

where, φ is the ratio of shell volume to the total volume, r is the radius of core, x is the shell thickness.

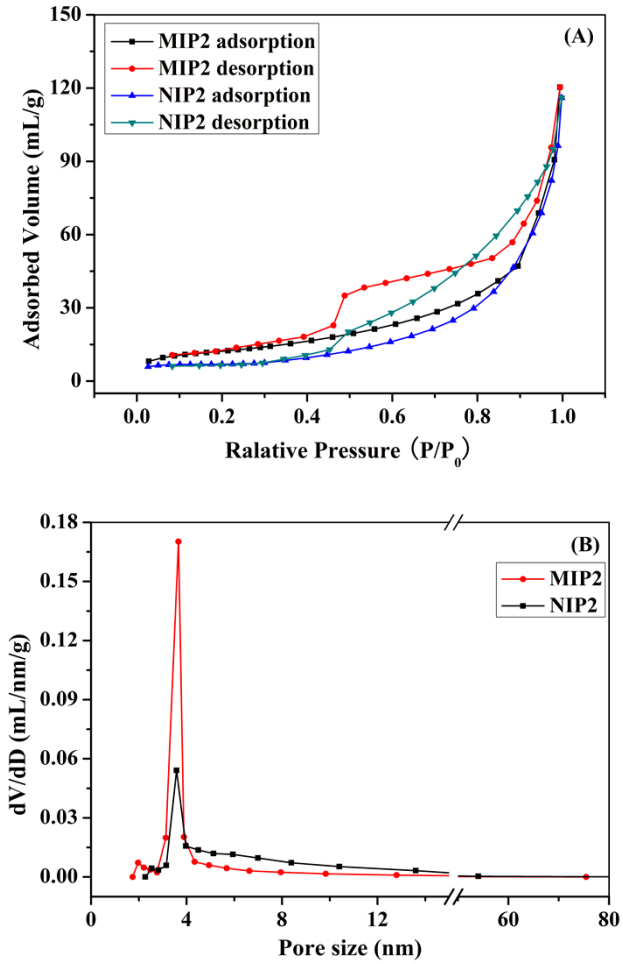

Figure S1. (A) N_2 adsorption-desorption isotherm of MIP2 and NIP2 and (B) pore distribution of MIP2 and NIP2.

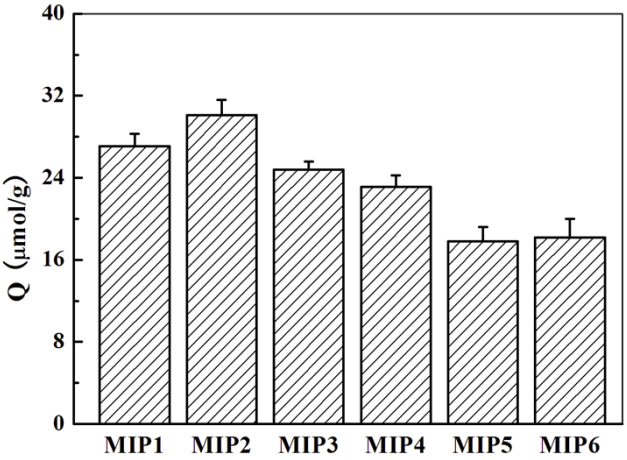

Figure S2. Maximum binding capacity of six different CS-MIPs for Sudan I in acetonitrile. Experimental conditions: V = 2.0 mL; mass of polymer, 20 mg; adsorption time, 12 h.

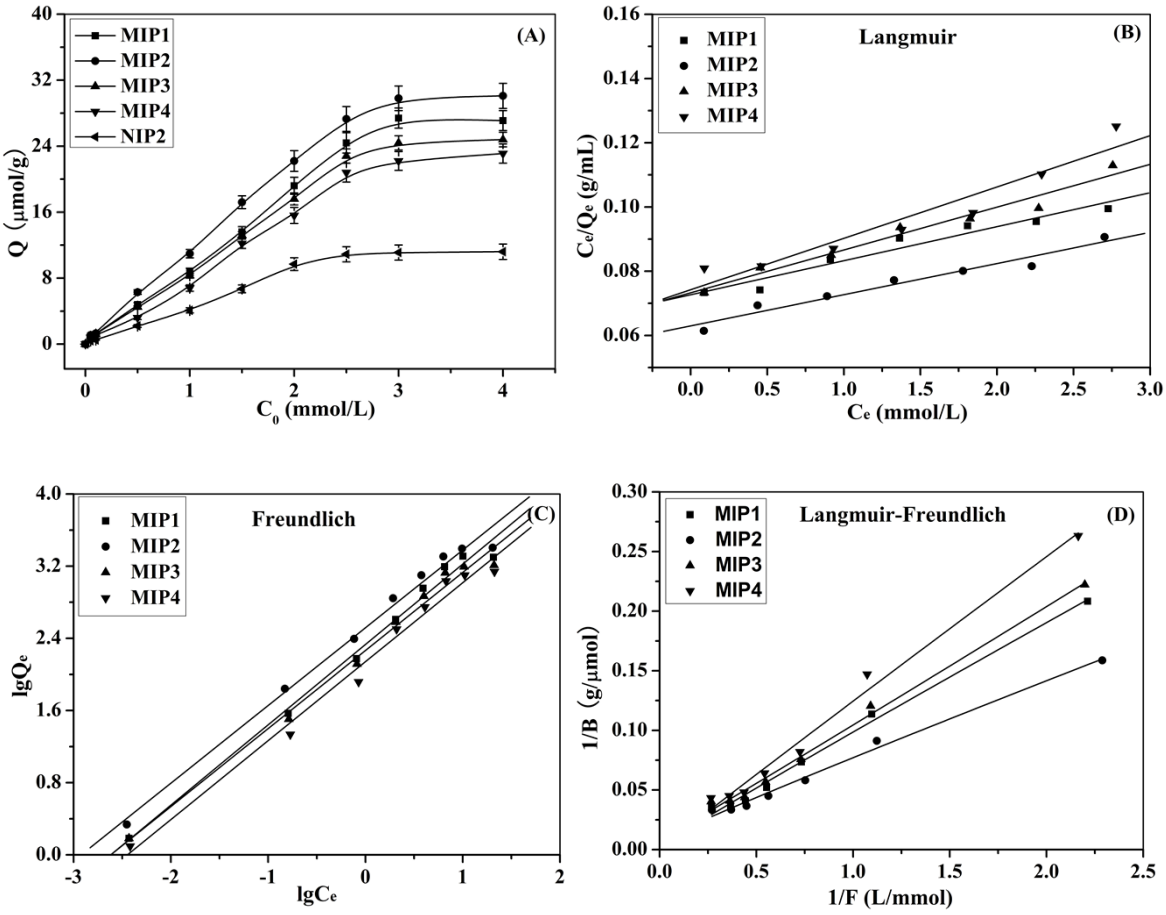

Figure S3. (A) Binding isotherms of four CS-MIPs and NIP2. (B) Langmuir, (C) Freundlich and (D) Langmuir-Freundlich isotherm models of four CS-MIPs adsorption process. Experimental conditions: V = 2.0 mL; mass of polymer, 20 mg; adsorption time, 12 h.

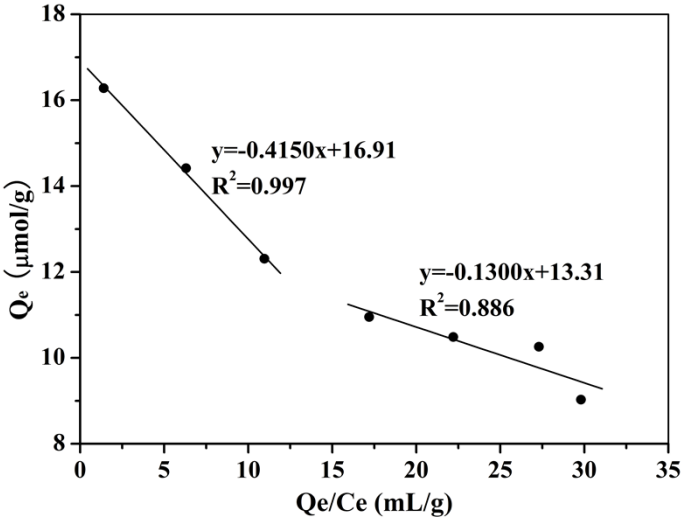

Figure S4. Scatchard plots of the MIP2.

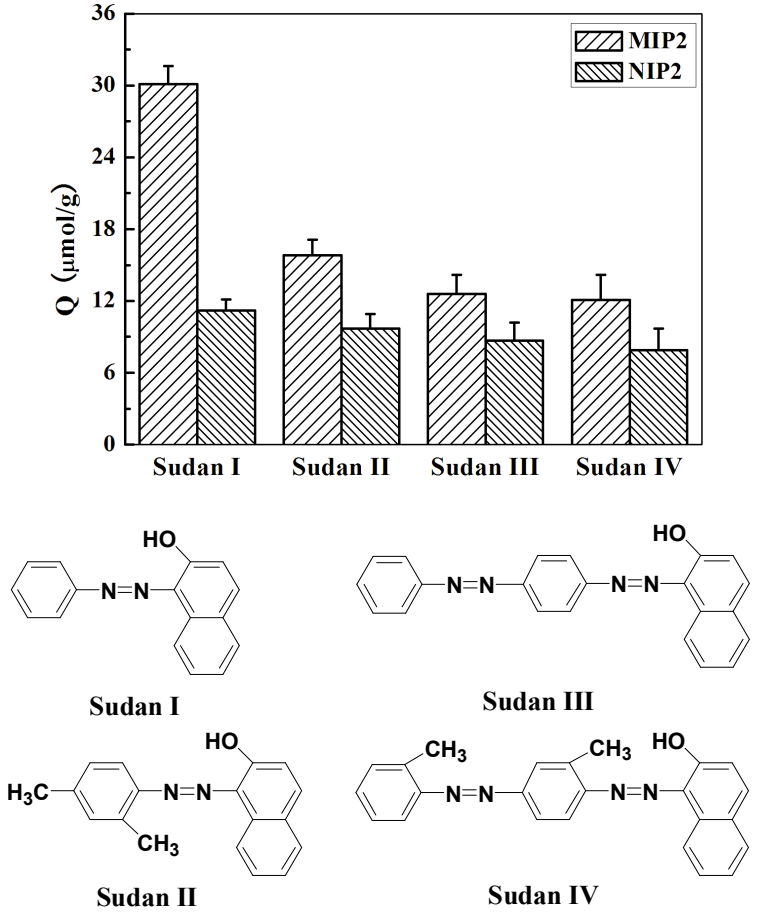

Figure S5. (Upper) Binding capacities of MIP2 and NIP2 for Sudan I, II, III, and IV, (below) chemical structures of the four Sudan dyes.

Table S1. Specific surface area and other related data of MIP2 and NIP2 obtained by BET analysis.

Polymers	Specific surface area (m^2/g)	Pore volume (mL/g)	Pore diameter (nm)
MIP2	43.27	0.205	9.42
NIP2	22.92	0.128	5.62

Table S2. Effect of SDS amount on the particle size for the MIP2.

Polymers	SDS(mg)	*d*(0.5)	*D*[3,2]	Residual	PDI
MIP-30	30	4.220	4.264	1.363%	2.75
MIP-60	60	3.287	3.760	1.384%	3.6
MIP-90	90	2.823	3.319	1.532%	7.2

Table S3. Adsorption isothern constants for four MIPs.

Polymers	$I^{(a)}$	R^2_1	$K_{d1}{}^{(b)}$	$Q_{max1}{}^{(c)}$	R^2_2	K_{d2}	Q_{max2}
MIP1	2.42	0.964	1.93	26.75	0.866	4.29	64.56
MIP2	2.69	0.997	2.41	40.75	0.886	7.69	117.77
MIP3	2.21	0.947	1.57	21.70	0.823	5.78	69.19
MIP4	2.12	0.939	1.22	15.02	0.909	3.85	47.05

(a) Imprinting factor; (b) Dissociation; (c) Maximum binding capacity, μmol/g.

Table S4. Isotherm model parameters for four CS-MIP.

Isotherm Model	Parameter	MIP1	MIP2	MIP3	MIP4
Langmuir $(\frac{C_e}{Q_e}=\frac{1}{Q_{max}}C_e+\frac{1}{K_l Q_{max}})$	$R^{2(a)}$	0.974	0.978	0.983	0.962
	$Q_{max}^{(b)}$	94.43	102.99	75.02	62.50
	$K_l^{(c)}$	0.146	0.154	0.182	0.216
Freundlich $(\lg Q_e=\frac{1}{n}\lg C_e+\lg K_f)$	R^2	0.990	0.989	0.989	0.985
	$K_f^{(d)}$	10.299	12.391	9.631	8.507
	$1/n^{(e)}$	0.891	0.861	0.865	0.875
Langmuir-Freundlich $(\frac{1}{B}=\frac{1}{N_t}\frac{1}{\alpha}\frac{1}{F^m}+\frac{1}{N_t})$	R^2	0.993	0.9924	0.9940	0.9891
	$N_t^{(f)}$	119.62	126.16	123.92	92.59
	$\alpha^{(g)}$	0.0870	0.115	0.0837	0.0867
	$m^{(h)}$	0.967	0.951	1.021	0.981

(a) Correlation coefficient; (b) Maximum binding capacity, μmol/g; (c) Langmuir constant; (d) Indicative constant for adsorption capacity of the adsorbent; (e) Reflect the adsorption intensity or surface heterogeneity, ranging from 0 to 1; (f) Total number of binding sites, μmol /g; (g) Equal to the median binding affinity constant, g/μmol; (h) Heterogeneity index, which will be equal to 1 for a homogeneous material, or will take values within 0 and 1 if the material is heterogeneous.

Table S5. Parameters obtained of MIP2 adsorption from four Kinetic Models.

Kinetic Models	Parameters		
Pseudo-first-order	k_1 (min^{-1}) [a]	Q_e(μmol/g) [b]	R^2
$\ln(Q_e - Q_t) = \ln Q_e - k_1 t$	0.1091	29.12	0.9480
Pseudo-second-order	k_2(g/(μmol·min)) [c]	Q_e(μmol/g)	R^2
$\frac{t}{Q_t} = \frac{1}{k_2 Q_e^2} + \frac{t}{Q_e}$	0.007062	31.00	0.9997
Elovich	α (μmol/g) [d]	β (min·g/μmol)	R^2
$Q_t = \frac{1}{\beta}\ln(a\beta) + \frac{1}{\beta}\ln(t)$	2.753	0.04038	0.9358
Intraparticle diffusion	k_p(μmol/(g $min^{0.5}$)) [e]	C(μmol/g) [f]	R^2
$Q_t = k_p t^{1/2} + C$	2.634	12.45	0.9740
	0.3341	26.13	0.9050

(a) k_1 is the rate constant of adsorption in pseudo-first-order model; (b) Q_e is the final adsorption amount at equilibrium; Q_t is the instantaneous adsorption amount at time t; (c) k_2 is the rate constant of adsorption in pseudo-second-order model; (d) α and β represent the initial adsorption rate and desorption constant in Elovich model, respectively; (e) k_p indicates the intraparticle diffusion rate constant and relates to the particle size R with the equation $k_p = \frac{6Q_e}{R}(\frac{D}{\pi})^{\frac{1}{2}}$; (f) C provides information about the thickness of the boundary layer.