Electronic Supplementary Information

Adsorption behavior of computer-aid designed magnetic molecularly imprinted polymer via response surface methodology

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S1 Minimized energies of template and functional monomers

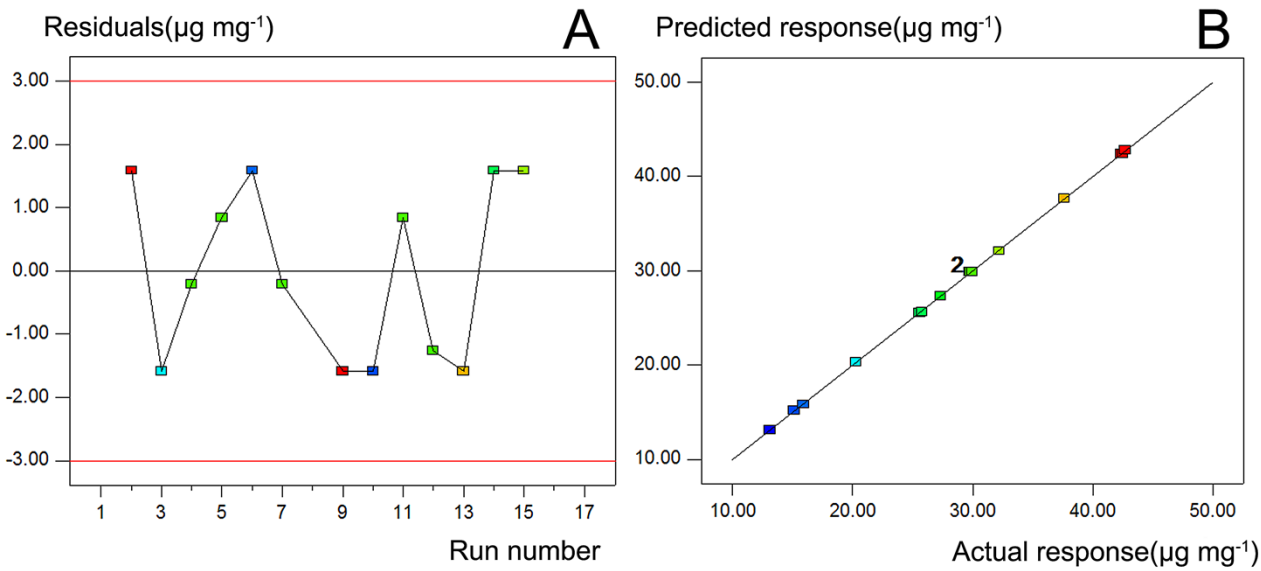
Structures	E(kcal mol^{-1})
AML	-7.79
MAA	-14.91
AA	-29.20
MAM	-29.84
AM	-32.76
2-VP	-2.10
4-VP	-2.63

S2 Docking energies of AML with 6 functional monomers in different ratio

Ratio of AML to functional monomer	Docking energy (kcal mol^{-1})					
	MAA	AA	MAM	AM	2-VP	4-VP
1:1	17.59	12.29	2.49	7.79	1.44	2.54
1:2	15.51	16.51	7.44	11.71	16.25	7.22
1:3	16.84	6.37	18.36	14.65	2.03	10.83
1:4	24.95	2.81	15.86	18.97	15.60	14.58
1:5	6.08	3.15	10.33	16.37	5.14	15.03
1:6	9.86	15.18	18.78	11.00	11.47	12.48

S3 Combinations of experimental conditions according to Box-Behnken Design

No.	Amount of material (mg)	Concentration of solution (μg mL^{-1})	Temperature (K)
1	5	25	310.5
2	5	50	298
3	5	50	323
4	5	75	310.5
5	10	25	298
6	10	25	323
7	10	50	310.5
8	10	50	310.5
9	10	50	310.5
10	10	50	310.5
11	10	50	310.5
12	10	75	298
13	10	75	323
14	15	25	310.5
15	15	50	298
16	15	50	323
17	15	75	310.5



S4 (A) Residuals of 17 combinations; (B) comparison of actual and predicted responses