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Supporting Information

Simulation of Phenobarbital Molecularly Imprinted Polymerization Self-assembly System and Its Adsorption Property

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S1 Selection processes of solvents

In the process of preparation the MIPs, the PHN, IA, and crossing-linking should dissolve in the same solvent. Thus, we investigated the solubility of all the components in the six solvents (water, acetonitrile, methyl alcohol, tetrahydrofuran, chloroform, methylbenzene). Moreover, the adsorption capacity of PHN-MIPs to PHN has also been detected. The results are shown in Table S1. As shown in Table S1, all the components are only freely soluble in acetonitrile and methyl alcohol. When the methyl alcohol as the solvent, the adsorption capacity of prepared PHN-MIPs to PHN is the largest. Additionally, the morphology of PHN-MIPs is uniform microspheres. Thus, we choose the methyl alcohol as the solvent to prepare the PHN-MIPs.

Table S1 Solubility of PHN-IA complexes and its adsorption capacities in different solvents

solvent	solubility	status	status after drying	Q (mg/g)
water	insoluble	---	---	---
acetonitrile	freely soluble	gel	microspheres with various shapes	4.85
methyl alcohol	freely soluble	gel	uniform microspheres	5.42
tetrahydrofuran	slight soluble	gel	irregular bulk particles	---
chloroform	slight soluble	gel	irregular bulk particles	---
methylbenzene	insoluble	---	---	---

S2 FT-IR analysis

In the Fig. S1, the peaks are at about 2984 and 1746 cm^{-1}, corresponding to the O—H and C=O from the IA molecule in NIPs. In PHN-MIPs, the peaks of O—H and C=O present blue shift. It reveals that the O—H and C=O from IA may be formed hydrogen bonds with PHN.

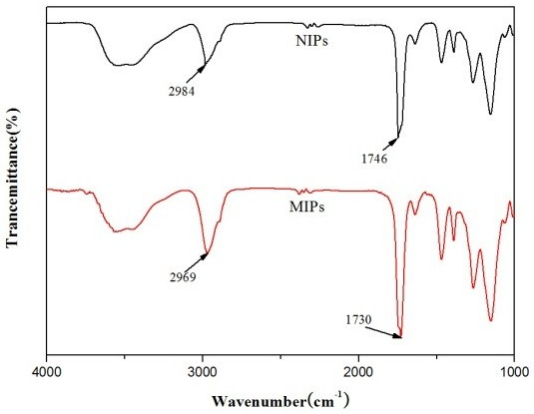

Fig. S1 FT-IR spectra of the PHN-MIPs and NIPs