Supporting Information for Analytical Methods

A visible-light-responsive molecularly imprinted polyurethane for specific detection of dibenzothiophene in gasoline

Yamin Si, Feng Jiang, Liang Qiang, Xiaotong Teng, Chengbin Gong* and Qian Tang*

The Key Laboratory of Applied Chemistry of Chongqing Municipality, College of Chemistry and Chemical Engineering, Southwest University, Chongqing, 400715, P. R. China.

S1. Synthesis of HPB	.2
S2. FT-IR spectra	.3
S3. Gas chromatography analysis	.3
S4. Reversibility of photoisomerization for HPB	.4
S5. Selective adsorption of DBT, biphenyl and fluorene by VMIPU and VNIPU	.4
References	.5



Scheme S1. Synthetic route for HPB.



Fig. S1. ¹H NMR (top) and ¹³C NMR (bottom) spectra of HPB.

S2. FT-IR spectra



Fig. S2. FT-IR spectra of MDI, VMIPU, VNIPU and HPB.

S3. Gas chromatography analysis



Fig. S3. Variation of the peak area of DBT (A), biphenyl (b) and fluorine (c) with concentration in DMSO. The peak area was measured by an Agilent 6890A gas chromatogram.

S4. Reversibility of photoisomerization for HPB



Fig. S4. Reversibility of the photoisomerization processes of azobenzene chromophores in the HPB in DMSO upon alternate irradiation at 440 and 650 nm.

S5. Selective adsorption of DBT, biphenyl and fluorene by VMIPU and VNIPU

Materials	Adsorbents _	K _D (L g ⁻¹)		k	k'
		K _{D(DBT)}	K _{D(Analogue)}	A	ĸ
DBT/Biphenyl	VMIPU	0.1629	0.0280	5.8179	5 5068
	VNIPU	0.0368	0.0354	1.0395	5.5908
DBT/Fluorene	VMIPU	0.1519	0.0164	9.2622	
	VNIPU	0.0392	0.0202	1.9406	4.7729

 Table S1 The selectivity parameters of VMIPU and VNIPU.

 K_D , distribution coefficient; $K_D = \{(C_0 - C_e)/C_e\} \times (V/W)$, where C_0 is the initial concentration, C_e is the final concentration solution, V is the volume of the solution, and W is the mass of the adsorbent; k, selectivity coefficient, $k = K_{D(template)}/K_{D(analogue)}$; k', relative selectivity coefficient, $k' = k_{imprinted}/k_{nonimprinted}$.¹

References

[1] D.M. Han, G.Z. Fang, X.P. Yan. Preparation and evaluation of a molecularly imprinted sol – gel material for on-line solid-phase extraction coupled with high performance liquid chromatography for the determination of trace pentachlorophenol in water samples. *J. Chromatogr. A* 1100 (2005) 131 – 136.