Evaluation of 4-substituted phenyl styrenes as functional monomers for the synthesis of theophylline-specific molecularly imprinted polymers

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Electronic Supporting Information

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Table 1 Calculated ΔE^o (kcal/mol) values for template-monomer clusters from molecular modelling experiments for theophylline and monomers **M1-M6**.

Number of Monomer Units	$\Delta E°_{(cluster)}$ (kcal/mol) for Theophylline-Monomer Cluster					
	M1	**M2**	**M3**	**M4**	**M5**	**M6**
1	-6.3	-9.2	-4.2	-9.6	-11.9	-6.8
2	-4.4	-15.1	-4.9	-4.8	-12.0	-9.8
3	-7.9	-9.3	-4.2	-9.7	-10.8	-8.1
4	-6.8	-13.1	-4.9	-10.8	-17.7	-5.0
5	-3.1	-4.6	-17.1	-13.7	+1.3	-0.6

Table 2. Swelling factor of thermal MIPs and NIPs of based on functional monomers **M1-M6**.

Polymer	Swelling factor[a]	
	MIP	NIP
M1	2.2	2.2
M2	3.5	3.5
M3	2.2	2.0
M4	2.0	2.0
M5	5.0	4.3
M6	3.2	3.3

[a] ratio of the volume of the wet polymer to its dry volume

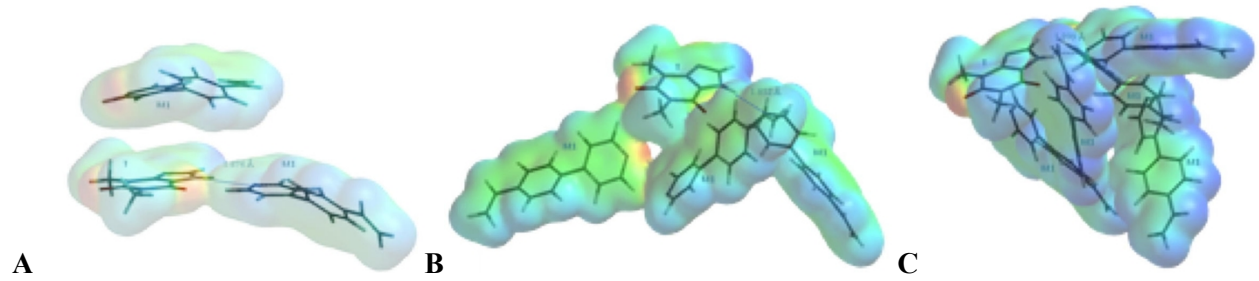


Figure 1. Molecular modelling images of theophylline-**M1** (**A**) 1:2, (**B**) 1:3 and (**C**) 1:5 clusters. Labels **T** and **M1** stand for theophylline and monomer-**M1**, respectively. The $\Delta E°_{(cluster)}$ values for these T-M clusters are -4.4 and -7.9 and -3.1 kcal/mol, respectively.

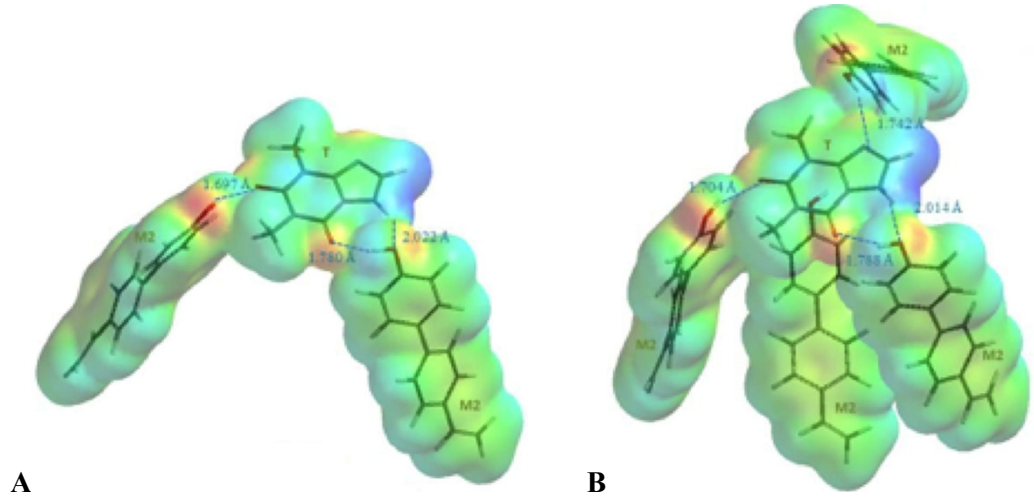


Figure 2. Molecular modelling images of theophylline-**M2** (**A**) 1:2 and (**B**) 1:4 clusters. Labels **T** and **M2** represent theophylline and monomer-**M2**, respectively**.** The $\Delta E°_{(cluster)}$ values for these T:M clusters are -15.1and -13.1 kcal/mol, respectively.

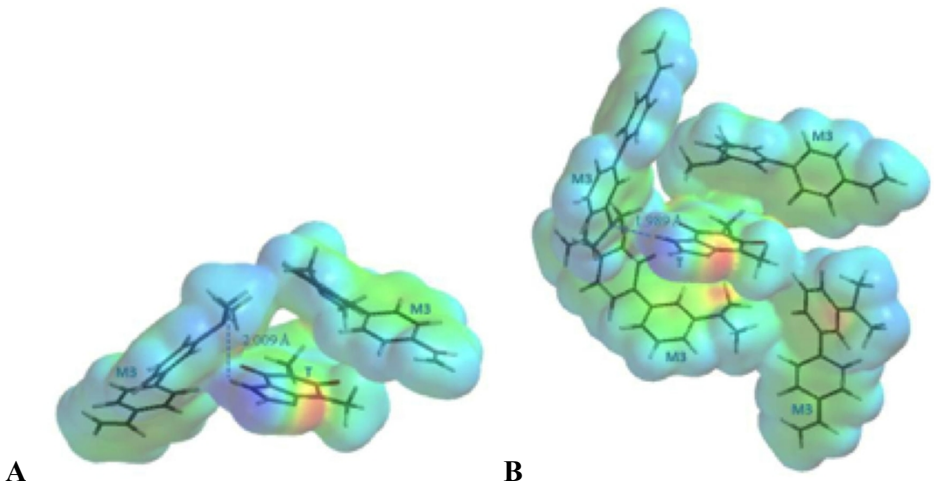
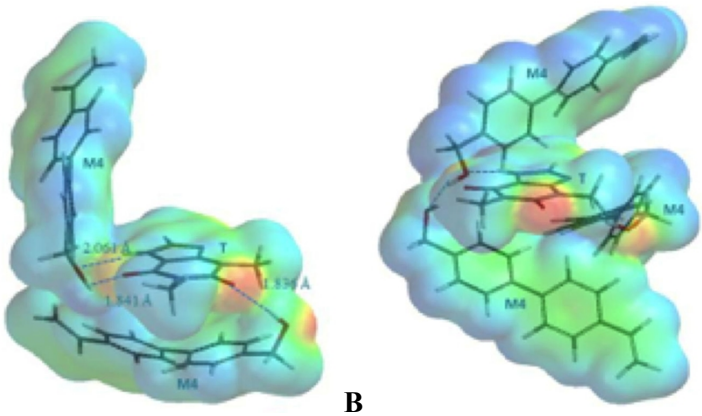
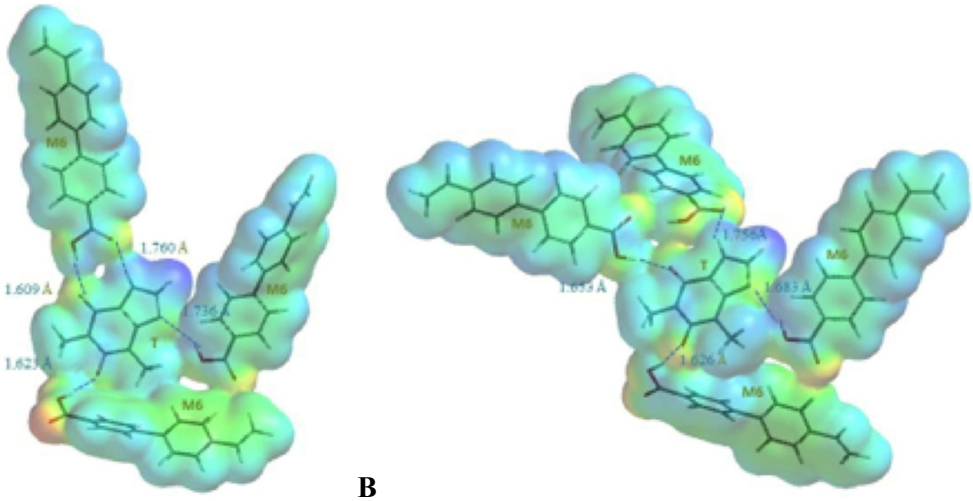


Figure 3. Molecular modelling images of theophylline-**M3** (**A**) 1:2 and (**B**) 1:4 clusters. Labels **T** and **M3** stand for theophylline and monomer-**M3**, respectively. The $\Delta E°_{(cluster)}$ value for both T:M clusters is -4.9 kcal/mol.



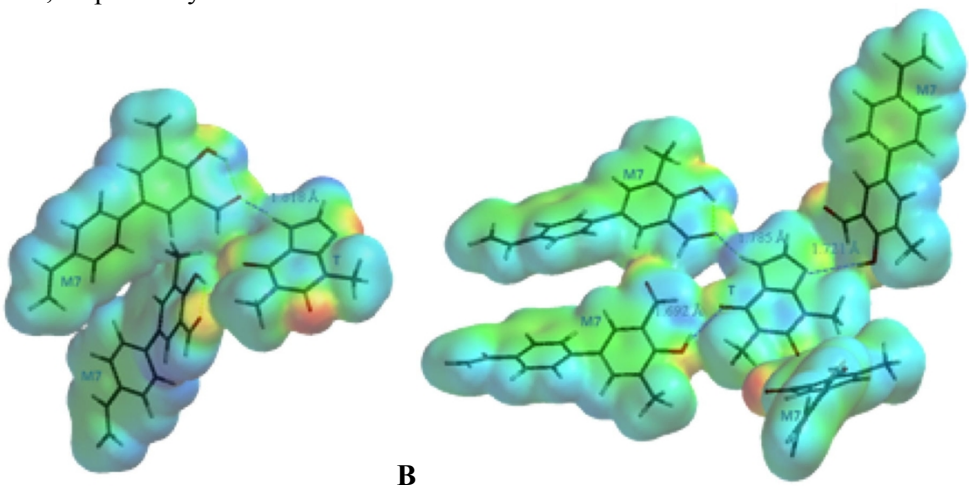
A **B**

Figure 4. Molecular modelling images of theophylline-**M4** (**A**) 1:2 and (**B**) 1:3 clusters. Labels **T** and **M4** stand for theophylline and monomer-**M4**, respectively. The $\Delta E°_{(cluster)}$ values for these T-M clusters are -4.8 and -9.7 kcal/mol, respectively.



A **B**

Figure 5. Molecular modelling images of theophylline-**M5** (**A**) 1:3 and (**B**) 1:4 clusters. Labels **T** and **M5** stand for theophylline and monomer-**M5**, respectively. The $\Delta E°_{(cluster)}$ values for these T-M clusters are -10.8 and -17.7 kcal/mol, respectively.



A **B**

Figure 6. Molecular modelling images of theophylline-M**6** (A) 1:2 and (B) 1:4 clusters. Labels T and **M6** stand for theophylline and monomer-**M6**, respectively. The $\Delta E°_{(cluster)}$ values for these T:M clusters are -9.8 and -5.0 kcal/mol, respectively.

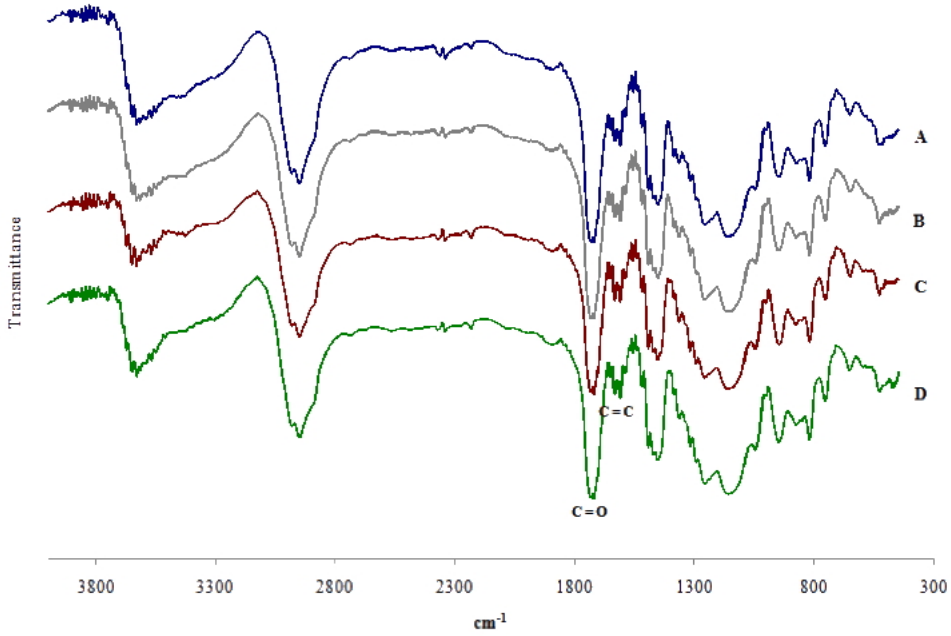


Figure 7. Infrared spectra of (A) **MIP$_{M2}$**, (B) **NIP$_{M2}$**, (C) MW-**MIP$_{M2}$** and (D) MW-**NIP$_{M2}$**.

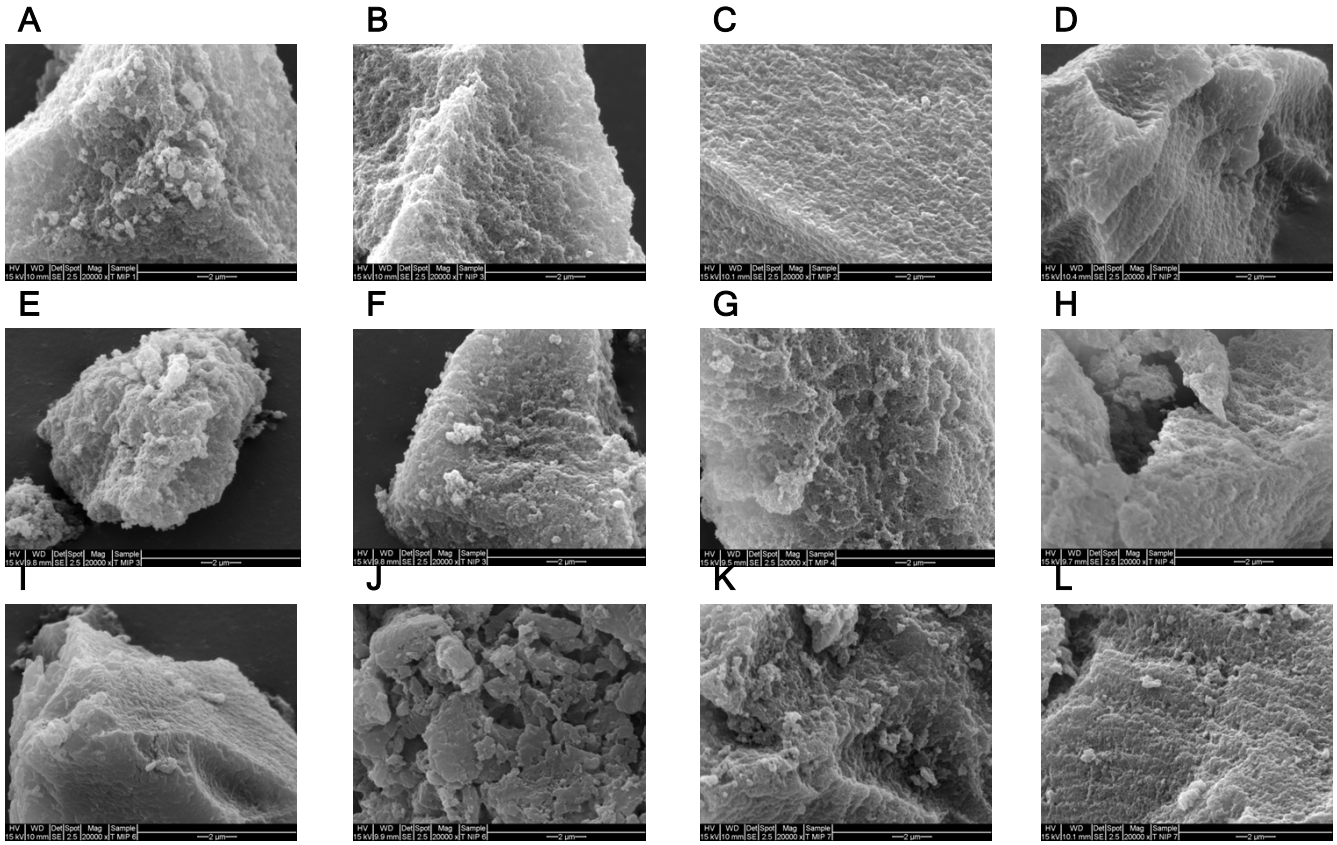


Figure 8. Scanning electron micrographs of (A) $MIP_{M1\text{-}1}$; (B) $NIP_{M1\text{-}1}$; (C) $MIP_{M2\text{-}1}$; (D) $NIP_{M2\text{-}1}$; (E) $MIP_{M3\text{-}1}$; (F) $NIP_{M3\text{-}1}$; (G) $MIP_{M4\text{-}1}$; (H) $NIP_{M4\text{-}1}$; (I) $NIP_{M5\text{-}1}$; (J) $NIP_{M5\text{-}1}$; (K) $MIP_{M6\text{-}1}$; and (L) $NIP_{M6\text{-}1}$; at 20000x magnification.