Electronic Supplementary Material (ESI) for Analyst.

Electronic supplementary information

A computational exploration of imprinted polymers affinity based on voriconazole metabolites

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Molecular modelling: molecules and methods

Table S1. ESP partial charges for the molecules (**1**), (**1**) in polymer, ethylene glycol dimethacrylate, ethylene glycol dimethacrylate in polymer and **L1**; In square brackets [RMS] values.

(1) [0.00394]		**(1) (in polymer)** [0.00373]		**ethylene glycol dimethacrylate** [0.00246]		**ethylene glycol dimethacrylate (in polymer)|** [0.00194]		**L1** [0.00374]	
Atom	**ESP**	**Atom**	**ESP**	**Atom**	**ESP**	**Atom**	**ESP**	**Atom**	**ESP**
C	0.027	C	0.249	C	-0.310	C	-0.307	F	-0.208
C	-0.404	C	-0.184	C	-0.022	C	0.208	F	-0.192
C	-0.005	C	-0.164	C	-0.092	C	-0.144	O	-0.467
C	0.167	C	0.061	H	0.034	H	0.034	N	-0.615
C	-0.165	C	-0.146	H	0.051	H	0.04	N	-0.588
H	0.102	H	0.092	H	0.040	H	0.037	N	0.269
C	-0.064	C	-0.084	H	0.134	H	0.061	C	0.528
H	0.086	H	0.088	H	0.154	H	0.086	H	0.023
C	-0.116	C	-0.116	C	0.632	C	0.614	C	0.220
H	0.092	H	0.086	O	-0.498	O	-0.496	H	0.083
C	-0.056	C	-0.046	O	-0.365	O	-0.456	C	-0.187
H	0.082	H	0.077	C	0.122	C	0.166	H	0.126
C	-0.191	C	-0.190	H	0.063	H	0.066	H	0.051
H	0.115	H	0.101	H	0.055	H	0.045	C	0.616
H	0.028	H	0.052	C	0.122	C	0.167	C	-0.316
H	0.014	H	0.023	O	-0.365	O	-0.457	C	0.386
H	0.002	H	0.006	C	0.632	C	0.614	C	-0.390
H	0.133	H	0.054	C	-0.022	C	0.208	H	0.197
H	0.153	H	-0.025	C	-0.310	C	-0.307	C	0.444
		H	0.047	H	0.154	H	0.086	C	-0.315
		H	0.022	H	0.134	H	0.061	H	0.167
				C	-0.092	C	-0.144	C	0.064
				H	0.051	H	0.04	H	0.104
				H	0.034	H	0.034		
				H	0.040	H	0.037		
				O	-0.498	O	-0.496		
				H	0.063	H	0.066		
				H	0.055	H	0.044		
				H	0.071				
				H	-0.026				
				H	-0.025				
				H	0.072				

Table S2. ESP partial charges for the molecules **L2 - L6**. In square brackets [RMS] values.

L2 [0.00324]		**L3** [0.00303]		**L4** [0.00369]		**L5** [0.00291]		**L6** [0.00297]	
Atom	**ESP**	**Atom**	**ESP**	**Atom**	**ESP**	**Atom**	**ESP**	**Atom**	**ESP**
C	-0.297	C	-0.266	F	-0.214	O	-0.517	F	-0.212
H	0.151	H	0.143	F	-0.209	O	-0.633	F	-0.204
H	0.044	H	0.033	O	-0.637	O	-0.602	N	-0.637
C	0.343	C	0.380	N	-0.627	O	-0.663	N	-0.601
C	-0.096	C	-0.052	N	-0.577	O	-0.441	N	0.47
H	0.061	H	0.043	N	0.236	O	-0.638	C	0.487
C	-0.030	C	-0.017	C	0.519	O	-0.525	H	0.048
H	0.022	H	0.016	H	0.026	C	0.137	C	0.173
H	-0.017	H	-0.022	C	0.225	C	0.155	H	0.118
H	0.023	H	0.019	H	0.100	C	0.25	C	-0.692
C	0.542	C	0.271	C	-0.185	C	0.137	H	0.212
C	0.672	C	0.178	H	0.057	C	0.577	H	0.144
H	-0.001	H	0.103	H	0.110	C	0.748	C	0.881
C	0.408	C	-0.115	C	0.592	H	0.007	C	-0.215
H	0.062	H	0.181	C	-0.299	H	0.091	C	0.304
C	-0.123	C	0.127	C	0.352	H	0.03	C	-0.342
C	0.184	C	0.181	C	-0.363	H	0.035	H	0.190
H	0.103	H	0.104	H	0.191	H	-0.052	C	0.386
C	0.465	C	0.473	C	0.407	H	0.0423	C	-0.315
H	0.050	H	0.049	C	-0.323	H	0.384	H	0.161
C	0.024	C	-0.006	H	0.163	H	0.441	C	0.006
C	-0.075	C	-0.067	C	0.022	H	0.434	H	0.103
H	0.130	H	0.128	H	0.106	F	-0.198	H	-0.075
C	-0.284	C	-0.290	H	0.362	O	-0.725	O	-0.643
H	0.159	H	0.162	H	-0.034	N	-0.612	O	-0.641
C	0.379	C	0.384			N	-0.564	O	-0.600
C	-0.371	C	-0.381			N	0.304	O	-0.643
H	0.200	H	0.203			C	0.485	O	-0.612
C	0.301	C	0.316			H	0.037	O	-0.634
F	-0.153	F	-0.152			C	0.197	O	-0.534
F	-0.214	F	-0.215			H	0.102	C	0.26
F	-0.209	F	-0.208			C	-0.378	C	0.056
N	0.376	N	0.363			H	0.154	C	0.047
N	-0.610	N	-0.612			H	0.095	C	0.289
N	-0.611	N	-0.611			C	0.623	C	0.666
N	-0.698	N	-0.448			C	-0.183	C	0.729
N	-0.667	N	0.340			C	0.301	H	-0.003
O	-0.635	O	-0.632			C	-0.395	H	0.118
H	0.392	H	0.370			H	0.195	H	0.055
		O	-0.473			C	0.512	H	-0.009
						C	-0.371	H	0.022

	H	0.171	H	0.419
	C	-0.033	H	0.382
	H	0.143	H	0.451
	H	0.421	H	0.435
	H	-0.059		

Evaluation of the theoretical systems P_M and P_{MC}

Figs. S1 and S2 shows the binding capacity versus the complexation energies in two systems, P_{MC} and P_M.

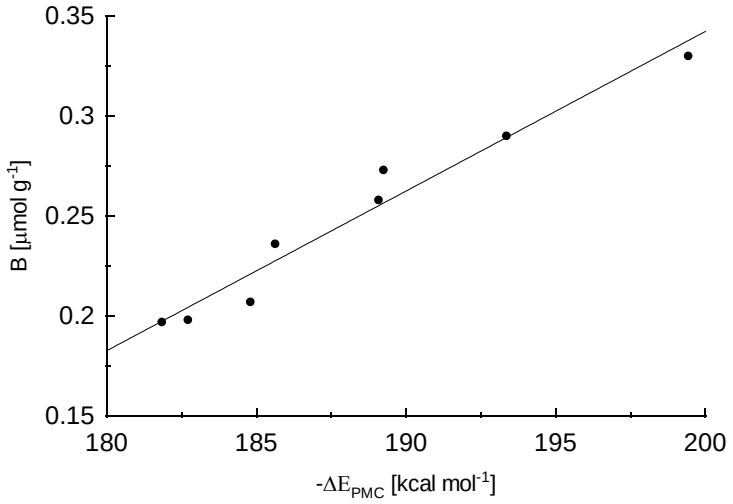

Fig. S1. The plot of experimental binding capacities B *versus* $\Delta E_{PMC.}$

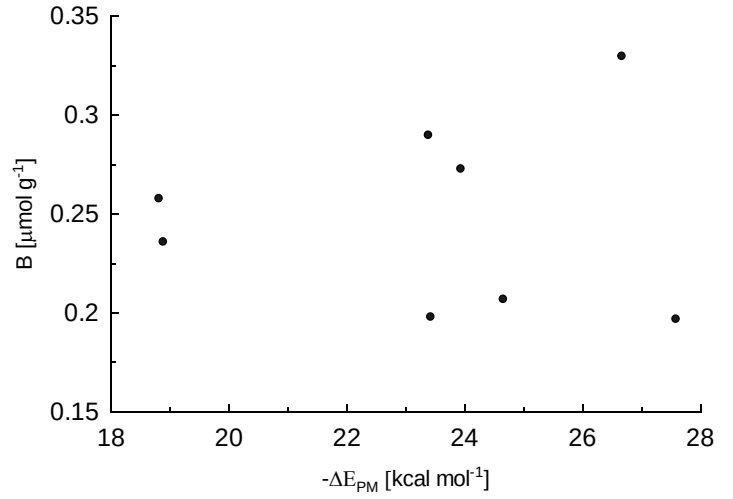

Fig. S2. The plot of experimental binding capacities B *versus* ΔE_{PM}.

As can be seen, the correlation exists only for P_{MC} system.

The presented correlations together with the intermolecular interactions analysis in P_{MC} system showed that the intermolecular interactions with the cross-linker are crucial for the selectivity studies of polymer matrix.