SUPPORTING INFORMATION

Insights into the formation, structural properties and performance of RAFT polymerized L-phenylalanine anilide molecularly imprinted polymers

Mahadeo R. Halhalli¹ and Börje Sellergren^{1,2}

- Department of Chemistry, TU-Dortmund, Otto Hahn Str. 6, 44221 Dortmund, Germany
- Department of Biomedical Sciences, Faculty of Health and Society, Malmö University, 20506 Malmö, Sweden. Tel: +46+703-620062, Email: borje.sellergren@mah.se

Polymer	Enthalpy	Enthalpy	Double bond conversion
	$(J/g)/^{o}C$	(J/mol)	%
MIPA	131	32095	58,5
MIPB	141	34545	63,0
MIPC	142	34790	63,4
MIPD	178	43610	79,5
MIPE	144	35280	64,3
MIPF	178	43610	79,5
NIPA	136	33320	60,7
NIPB	162	39690	72,4
NIPC	178	43610	79,5
NIPD	205	50225	91,6
NIPE	207	50715	92,5
NIPF	192	47040	85,8

Table S1. Heat generation and vinyl conversions during dynamic temperature scans of prepolymerization mixtures corresponding to the polymers in Table 1.

Table S2. Temperature at x % weight loss of imprinted and non imprinted polymers.

	Onset (^O C)	Temperature	Temperature at 'x'% mass loss			
Polymer code		$T_{25}(^{0}C)$	$T_{50}(^{0}C)$	T ₇₅ (⁰ C)		
MIPA	248	279	320	395		
MIPB	263	294	336	399		
MIPC	309	311	360	409		
MIPD	339	345	384	416		
MIPE	343	356	387	416		
MIPF	347	357	396	420		
NIPA	240	274	313	390		
NIPB	261	294	336	395		
NIPC	315	320	370	408		
NIPD	325	345	378	412		
NIPE	336	354	385	414		
NIPF	345	354	390	416		

Table S3. Pore analysis parameters of the imprinted polymers determined by nitrogen sorption porosimetry

	Pore	Pore	Surface
Polymer	diameter	volume	area
Code	(nm)	(mL/g)	(m^2/g)
NIPA	32	0.67	356
NIPB	24	0.82	386
NIPC	16	0.76	381
NIPD	7.6	0.51	354
NIPE	4.4	0.34	318
NIPF	3.7	0.20	274

The parameters were calculated from the nitrogen adsorption isotherms as described in the experimental part.



Figure S1. Heat generation during a dynamic temperature scan (10°C/min) of the NIP prepolymerisation mixtures corresponding to the compositions in Table 1.





Figure S2. Physical appearance of the imprinted (A) and nonimprinted (B) polymers prepared at the indicated CTA/ABDV ratios.



Figure S3. Transmission FTIR spectra (KBr) of the imprinted polymers prepared using different CTA/ABDV ratios.



Figure S4. SEM images of the the imprinted (upper two rows) and nonimprinted (lower two rows) polymers prepared using different CTA/ABDV ratios.



Figure S5. DSC curves for the melting of acetonitrile in the L-PA imprinted polymers. The sample was frozen by rapidly quenching to -60 $^{\circ}$ C. The heating curves shows the pore melt and excess melt.