

Electronic Supplementary Information

for

Long-term stability and reusability of molecularly imprinted polymers

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1-(4-vinylphenyl)-3-(3,5-bis(trifluoromethyl)phenyl)urea

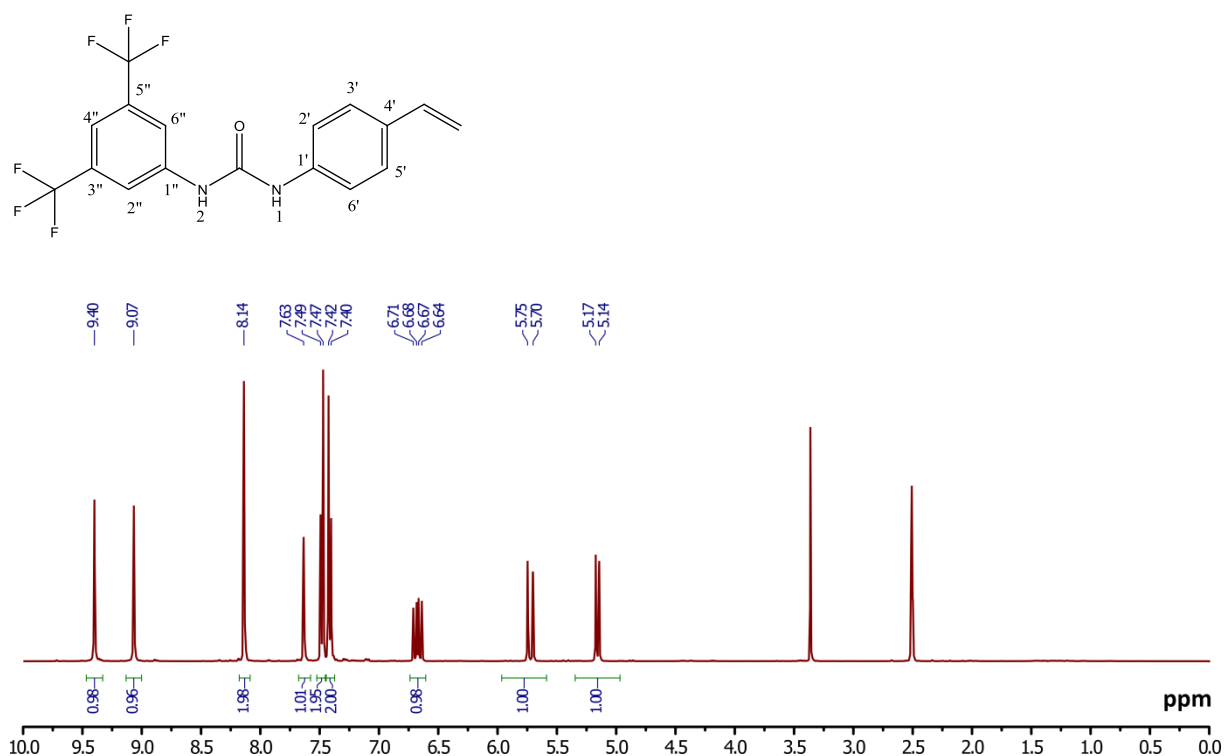


Figure S1. $^1\text{H-NMR}$ spectrum of 1-(4-vinylphenyl)-3-(3,5-bis(trifluoromethyl)phenyl)urea functional monomer. $^1\text{H-NMR}$ (400 MHz, DMSO-d_6) δ : 5.16 (1H, dd, $J=10.8$ Hz, 0.8 Hz, CH=CH_2), 5.73 (1H, dd, $J=17.6$ Hz, 0.8 Hz, CH=CH_2), 6.68 (1H, dd, $J_{AB}=10.8$ Hz, CH=CH_2), 7.41 and 7.48 (2 \times 2H, dd, $J_{AA'BB'}$ =8.6 Hz, Ar-CH-2',6' and Ar-CH-3',5'), 7.63 (1H, s, Ar-CH-4''), 8.14 (2H, s, Ar-CH-2'', 6''), 9.07 (1H, s, urea-NH-3), 9.40 (1H, s, urea-NH-1) ppm.

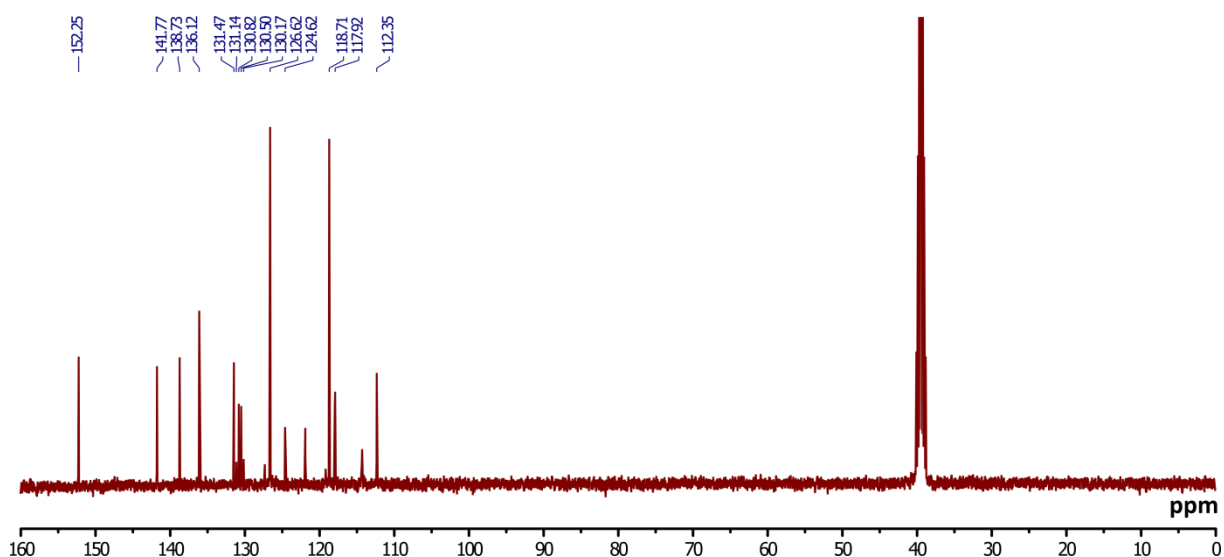


Figure S2. $^{13}\text{C-NMR}$ spectrum of 1-(4-vinylphenyl)-3-(3,5-bis(trifluoromethyl)phenyl)urea functional monomer. $^{13}\text{C-NMR}$ (100 MHz, DMSO-d_6) δ : 112.35 (CH=CH_2), 117.92 (Ar-CH-4''), 118.71 (Ar-CH-2'', 6''), 124.62 (CF_3), 126.62 (Ar-CH-3',5'), 127.33 (Ar-CH-4'), 130.66 (q, Ar-CH-3'',5''), 131.47 (Ar-CH-2', 6'), 136.12 (CH=CH_2), 138.73 (Ar-CH-1'), 141.77 (Ar-CH-1''), 152.25 (urea C) ppm.

Methylene diamine dihydrochloride

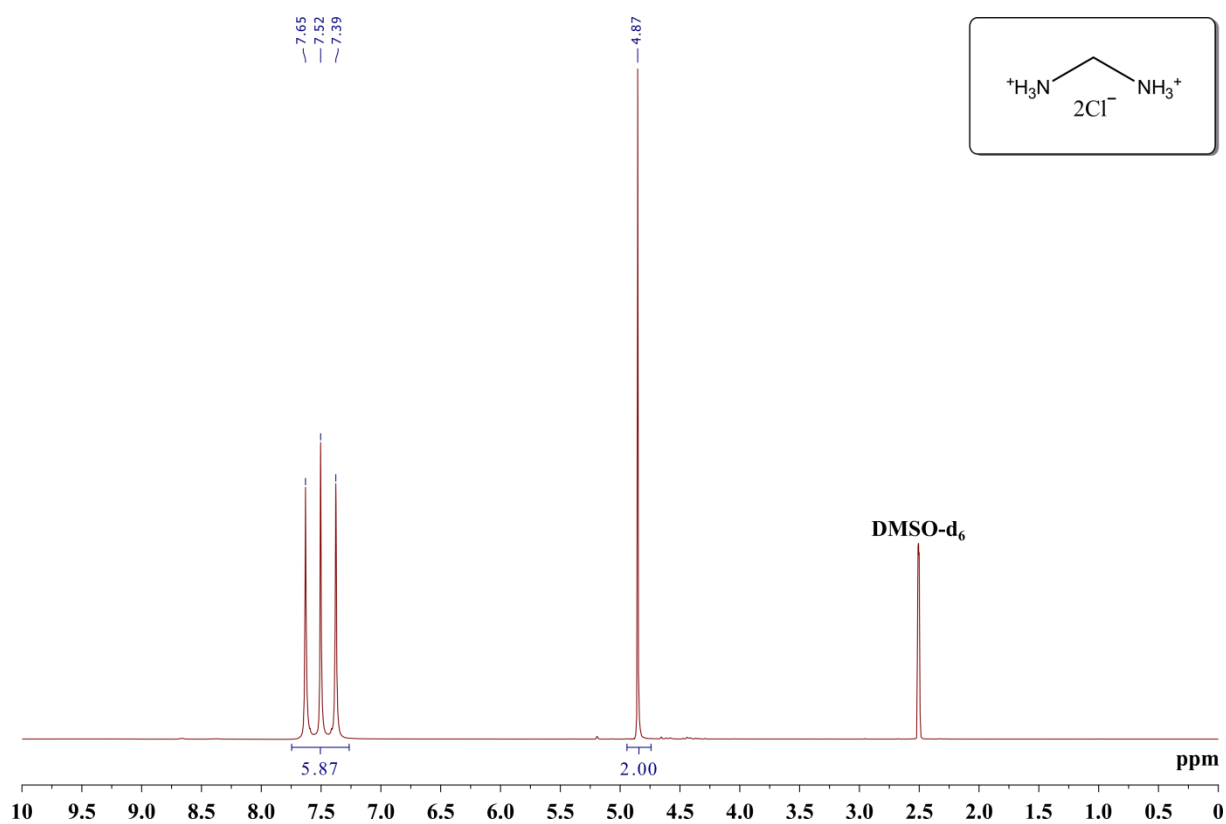


Figure S3. $^1\text{H-NMR}$ spectrum of methylenediamine dihydrochloride. $^1\text{H-NMR}$ (400 MHz, DMSO-d_6) δ : 4.87 (2H, s, CH_2), 7.52 (6H, t, $J=50.8$ Hz, NH_3^+) ppm.

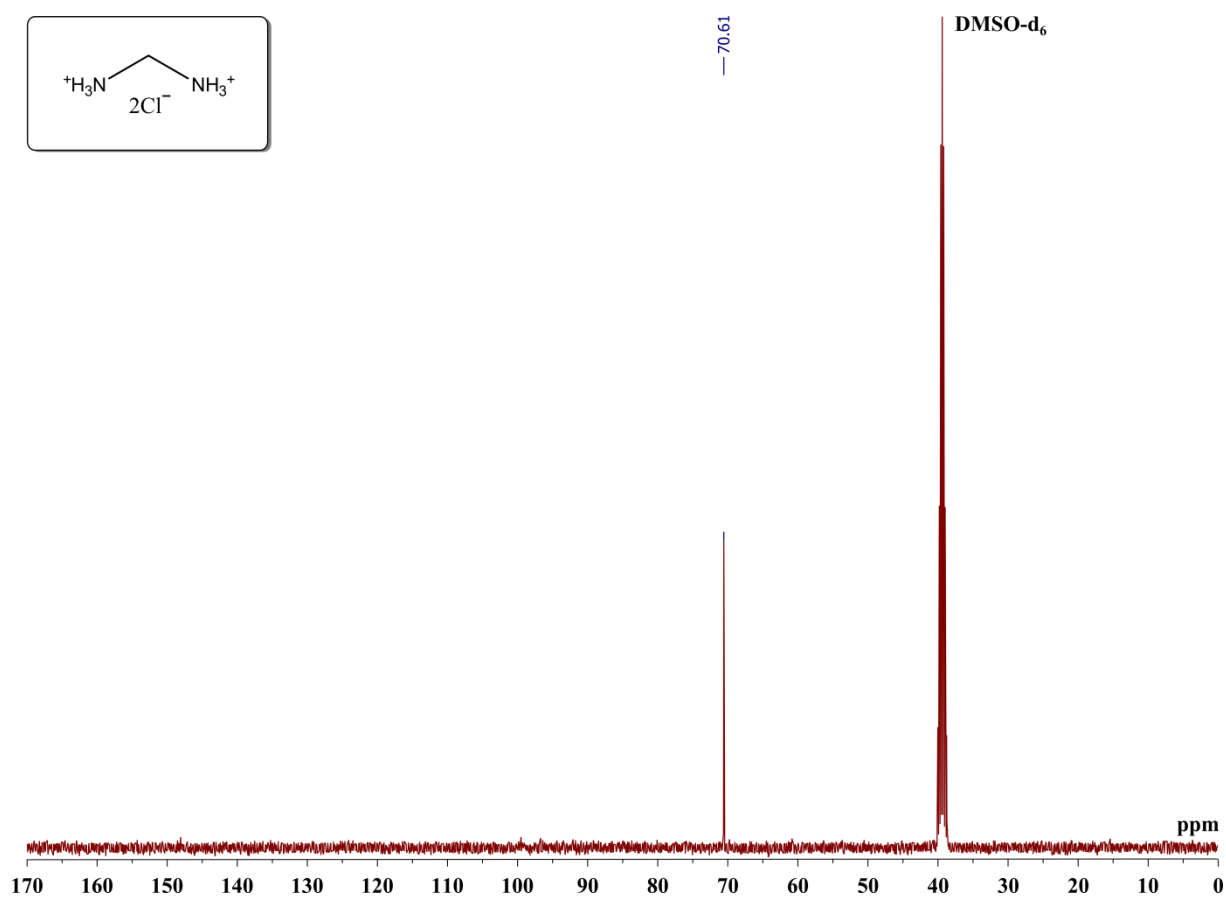
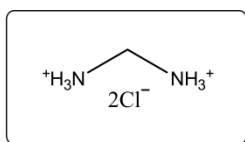


Figure S4. ¹³C-NMR spectrum of methylenediamine dihydrochloride. ¹³C-NMR (100 MHz, DMSO-d₆)
δ: 70.61 (CH₂) ppm.

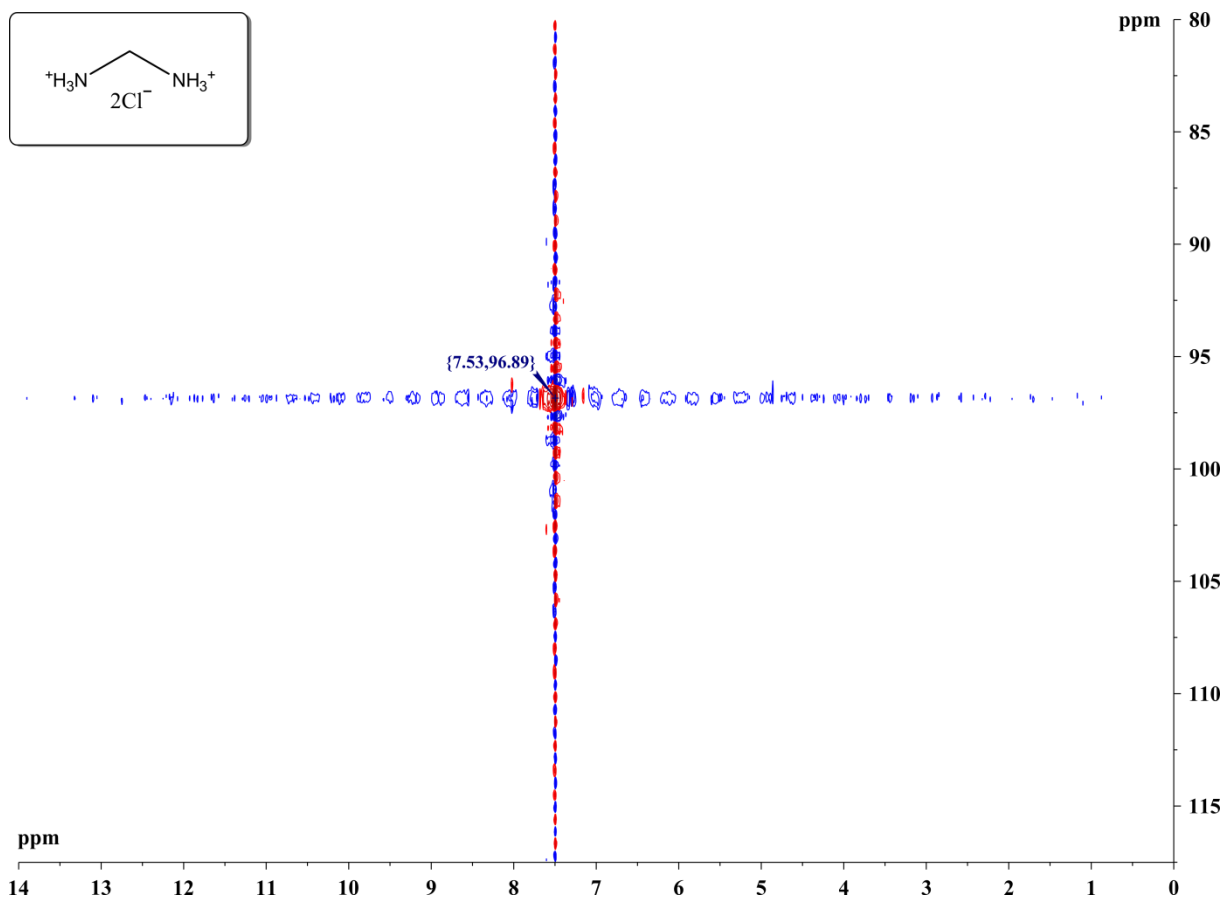


Figure S5. ^{15}N -NMR spectrum of methylenediamine dihydrochloride. ^{15}N -NMR (50.8 MHz, DMSO-d_6) δ : 96.85 (NH_3^+) ppm.

Trimethyl borate

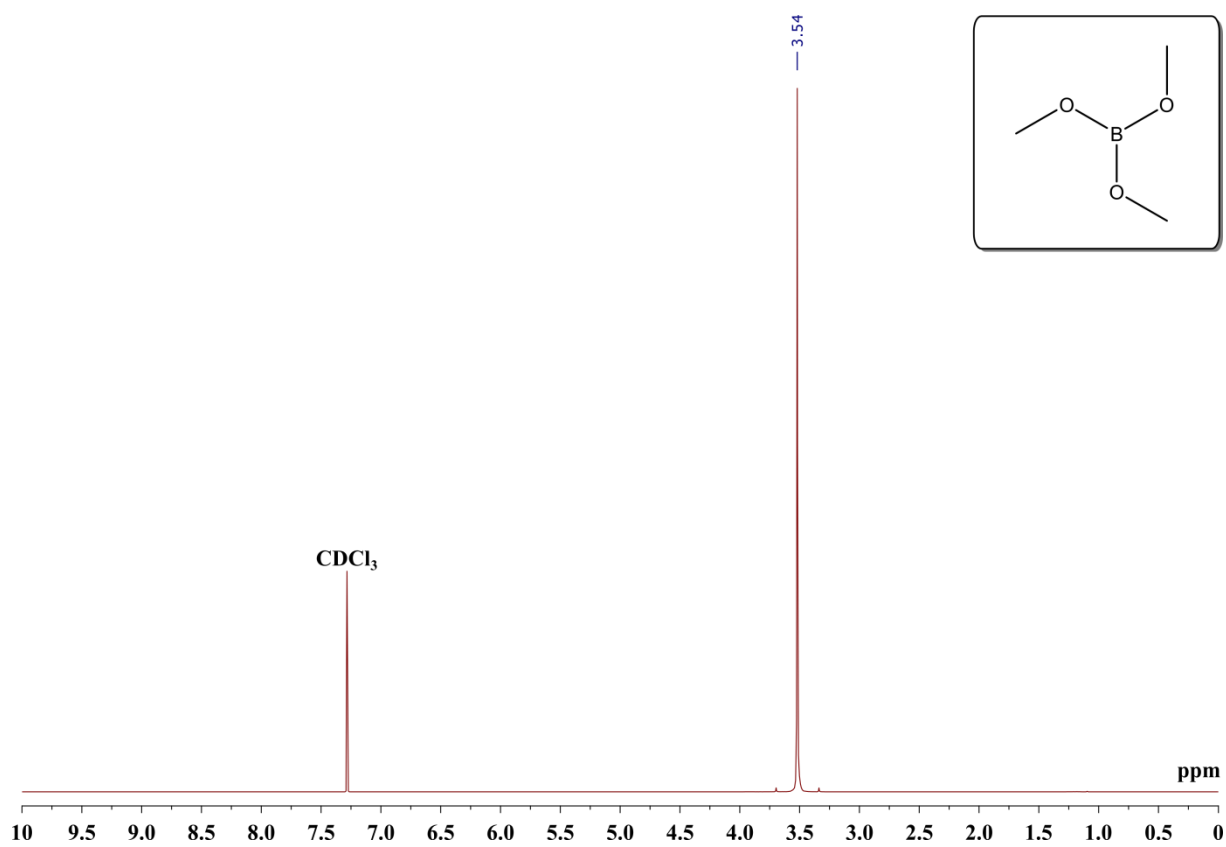


Figure S6. $^1\text{H-NMR}$ spectrum of trimethyl borate. $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ : 3.52 (9H, s, OCH_3) ppm.

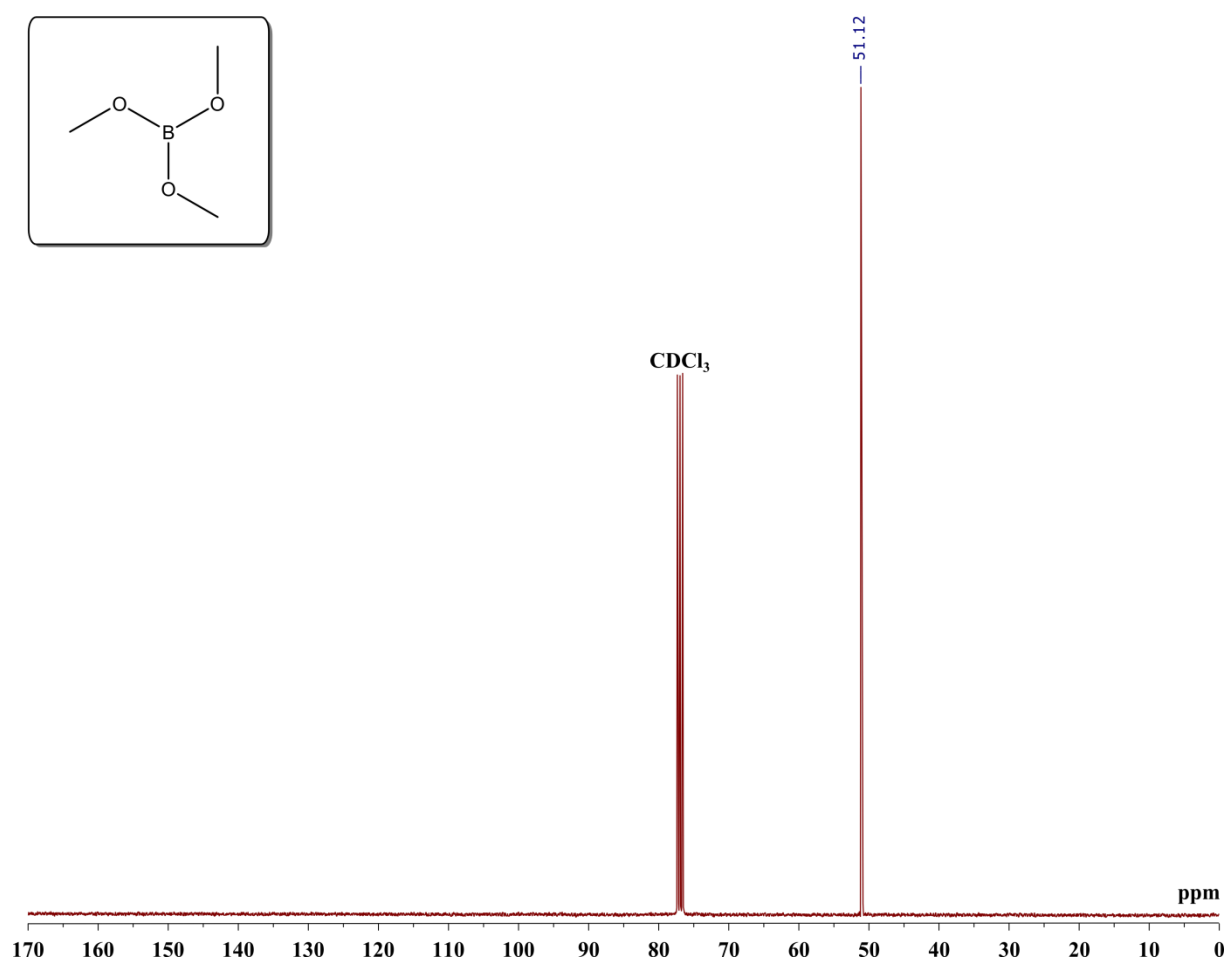
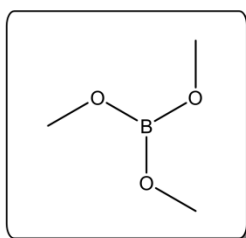


Figure S7. ¹³C-NMR spectrum of trimethyl borate. ¹³C-NMR (100 MHz, CDCl₃) δ= 51.17 (OCH₃) ppm.

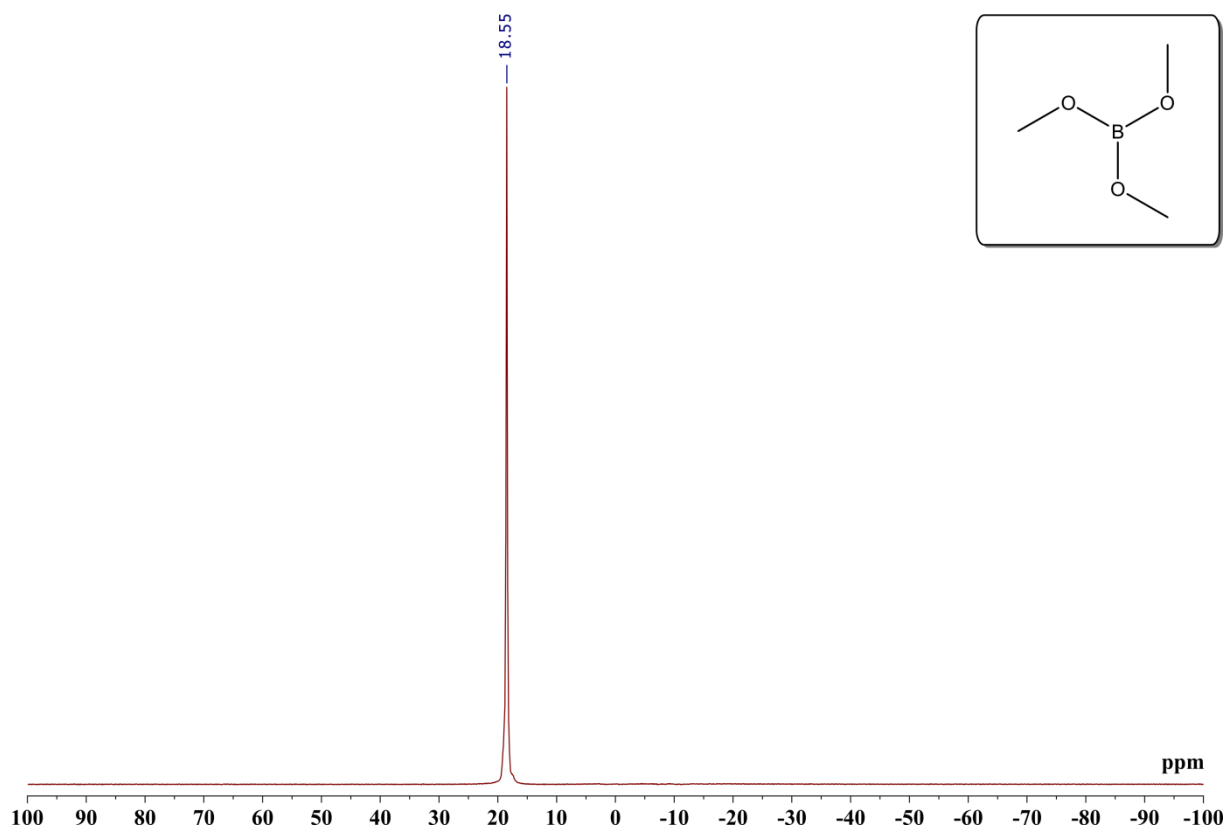


Figure S8. ^{11}B -NMR spectrum of trimethyl borate. ^{11}B -NMR (160.5 MHz, CDCl_3) $\delta = 18.49$ [$\text{B}(\text{OCH}_3)_3$] ppm.

Ethylene glycol

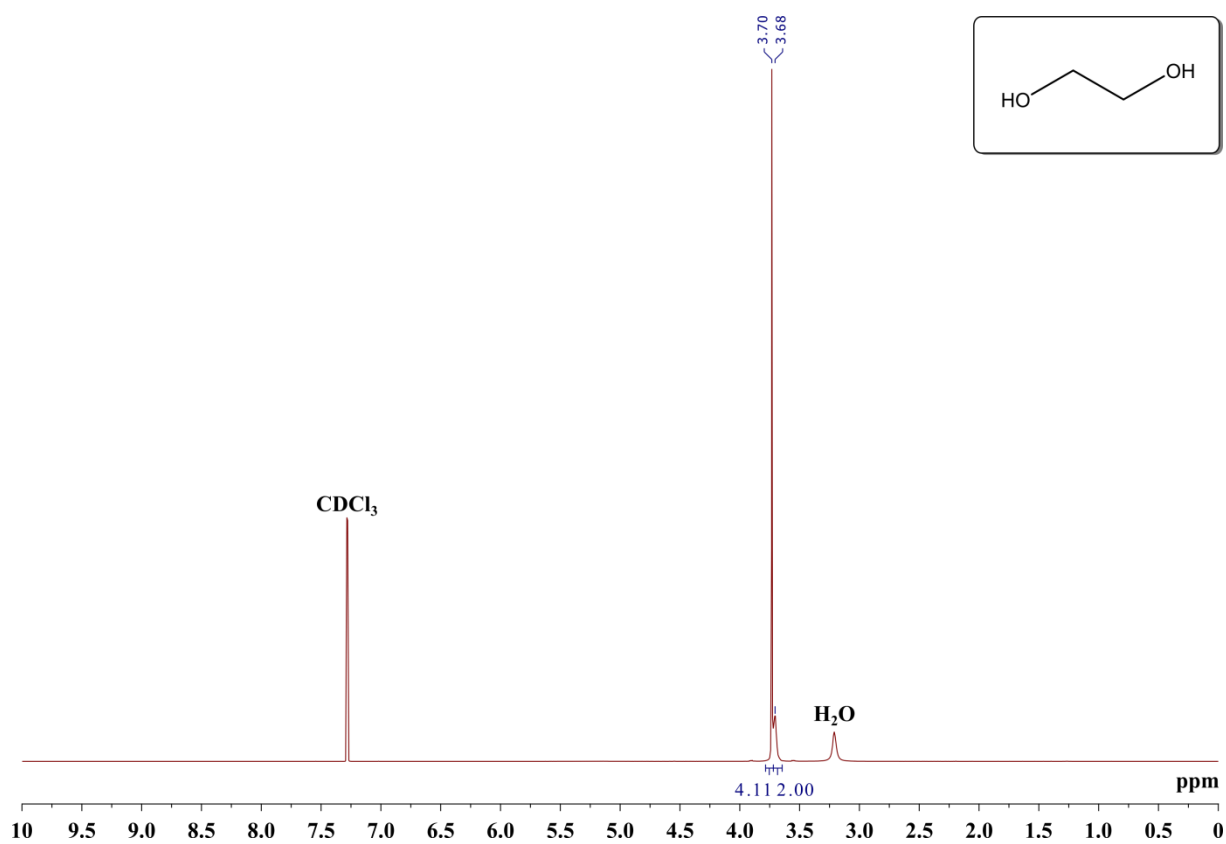


Figure S9. ¹H-NMR spectrum of ethylene glycol. ¹H-NMR (400 MHz, CDCl₃) δ: 3.68 (2H, br. s, OH), 3.70 (4H, s, CH₂) ppm.

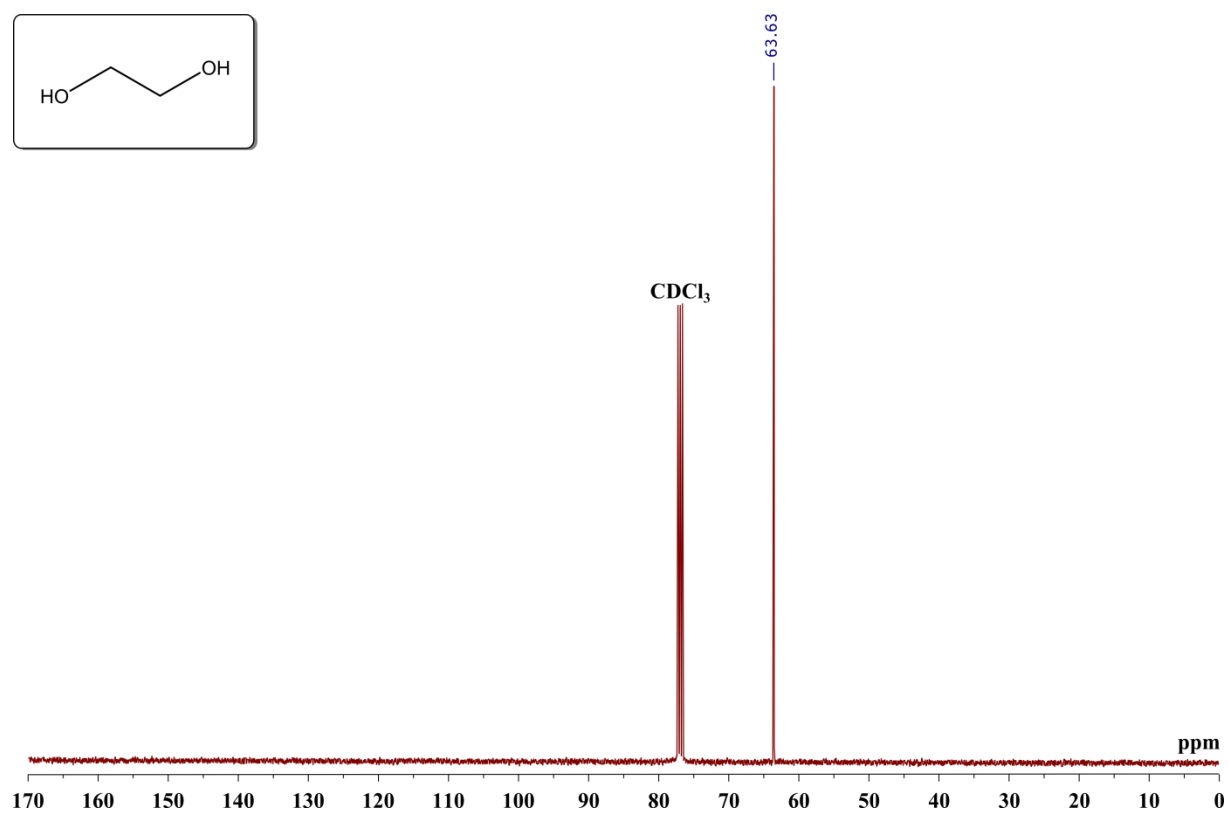
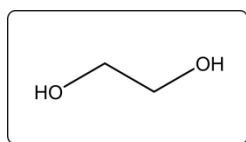


Figure S10. ^{13}C -NMR spectrum of ethylene glycol. ^{13}C -NMR (100 MHz, CDCl_3) δ : 63.67 (CH_2) ppm.

Table S1. Elemental analysis of the imprinted and control polymers after template extraction. Anal. Calcd/Found. See Table 1 in the main manuscript for the conditions of polymer preparation.

Polymers	Carbon (%)	Hydrogen (%)	Nitrogen (%)
IP1	60.87/60.83	7.24/7.25	0.43/0.41
IP2	60.59/60.52	7.17/7.19	0.23/0.26
IP3	61.04/60.96	7.22/7.22	0.02/0.05
IP4	60.74/60.78	7.14/7.16	0.24/0.22
IP5	61.27/61.25	7.19/7.23	0.02/0.04
IP6	60.95/60.86	7.16/7.18	0.01/0.05
IP7	60.87/60.82	7.24/7.21	0.43/0.45
IP8	60.58/60.63	7.21/7.25	0.43/0.39
IP9	61.04/60.11	7.22/7.24	0.02/0.05
IP10	60.88/60.92	7.16/7.12	0.46/0.51
IP11	61.27/61.34	7.19/7.20	0.02/0.03
CP1	60.87/60.89	7.24/7.28	0.43/0.45
CP2	60.59/60.48	7.17/7.15	0.23/0.19
CP3	61.04/60.96	7.22/7.25	0.02/0.05
CP4	60.74/60.78	7.14/7.11	0.24/0.22
CP5	61.27/61.35	7.19/7.18	0.02/0.04
CP6	60.95/61.21	7.16/7.13	0.01/0.00
CP7	60.87/60.59	7.24/7.27	0.43/0.45
CP8	60.58/60.51	7.21/7.18	0.43/0.41
CP9	61.04/60.87	7.22/7.20	0.02/0.05
CP10	60.88/60.96	7.16/7.16	0.46/0.42
CP11	61.27/61.34	7.19/7.22	0.02/0.04

Table S2. Change in BET surface area of the polymers given in $\text{m}^2 \cdot \text{g}^{-1}$ unit. The template extraction method is given after the forward slash. See Table 1 and 2 in the main manuscript for the polymer compositions and the conditions of the template extratcion methods, respectively.

# of adsorption-regeneration cycle	# of adsorption-regeneration cycle						
	IP1/#6	IP3/#6	IP5/#6	IP10/#6	IP10/#5	IP11/#6	IP11/#5
1	62±2	64±3	60±1	50±2	51±1	48±2	49±1
10	58±2	64±2	58±1	50±2	52±1	48±2	49±2
20	54±2	64±3	56±1	50±2	53±1	48±2	51±2
30	52±2	65±2	55±1	50±2	54±1	48±2	52±1
40	50±2	64±2	54±1	49±2	55±1	48±2	53±1
50	47±2	64±2	52±2	49±2	56±1	48±1	55±2
60	43±2	63±2	51±2	50±2	-	48±1	55±1
70	39±3	65±2	50±3	50±2	-	48±2	56±1
80	36±4	64±2	48±3	50±2	-	48±1	57±1
90	34±4	65±2	46±3	50±2	-	47±2	57±1
100	29±4	64±2	44±4	49±2	-	47±2	58±1