

Supplementary information:

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Synthesis and Ligand Recognition of Paracetamol Selective Polymers: Semi-covalent versus Non-covalent Molecular Imprinting

Synthesis and Ligand Recognition of Paracetamol Selective Polymers: Semi-covalent *versus* Non-covalent Molecular Imprinting

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Table of contents

Spectroscopic data for:

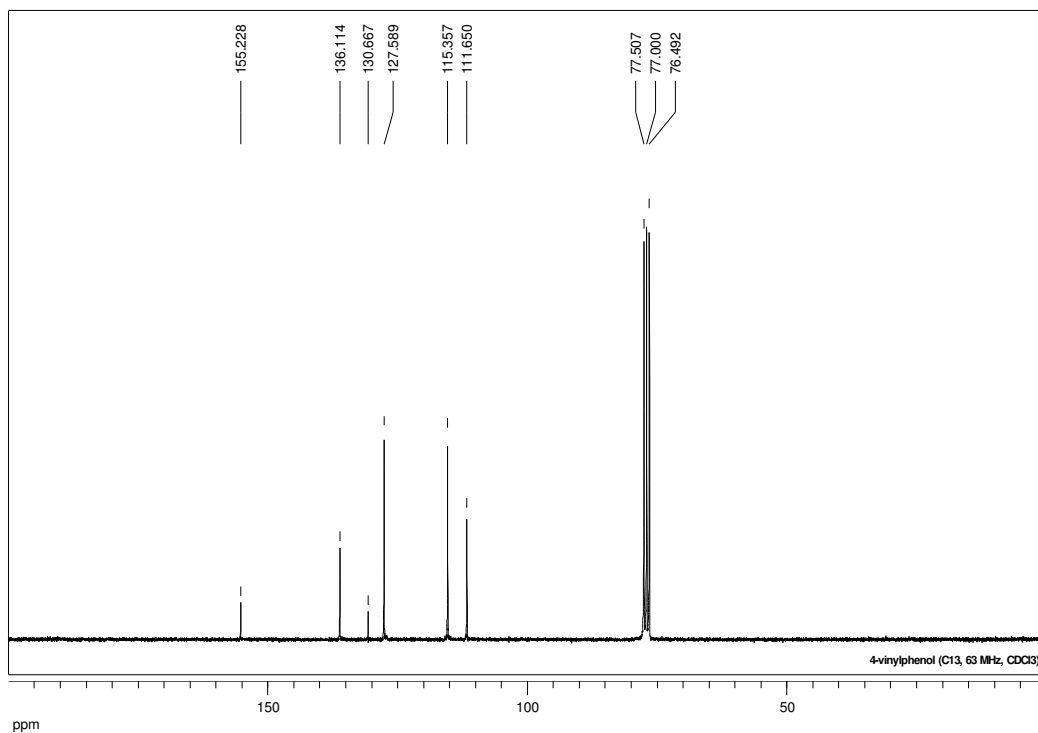
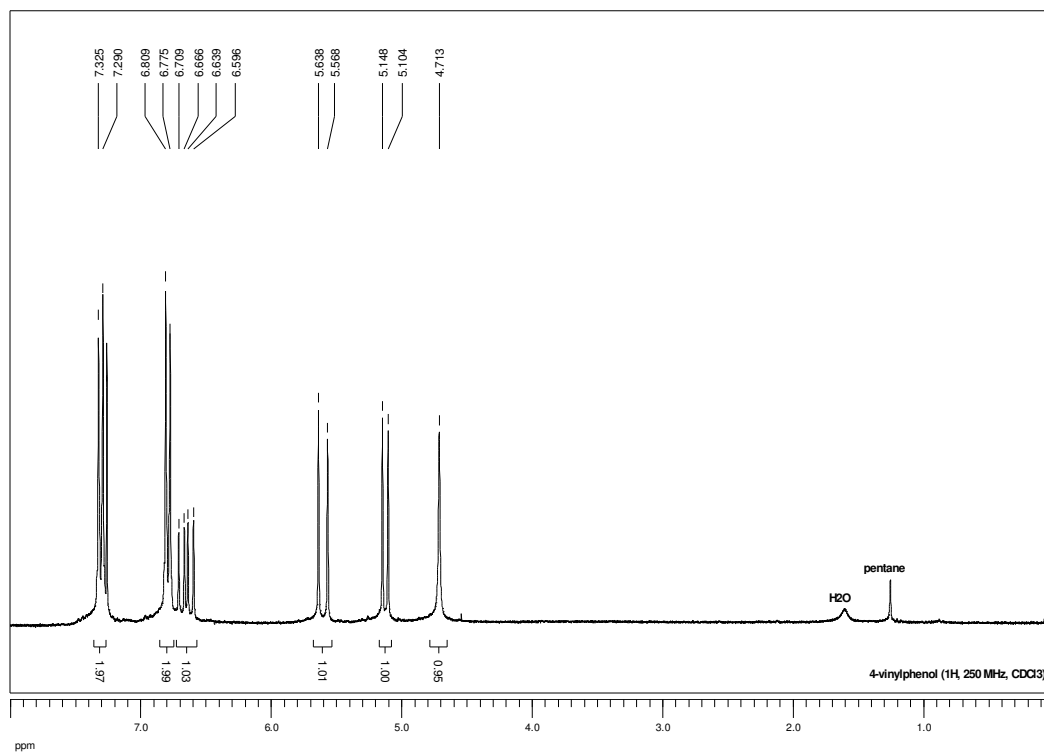
4-vinylphenol (2)	Page 2
Crude 4-acetamidophenyl chloroformate (3)	Page 3
4-acetamidophenyl-(4-vinylphenyl) carbonate (4)	Page 4
Phenyl-(4-vinylphenyl) carbonate (5)	Page 5
Methyl-(4-vinylphenyl) carbonate (6)	Page 6
4-hydroxybenzanilide (7)	Page 7
Acetanilide (8)	Page 8
Physical data for P1-P11	Page 9
Polymer titrations	Page 10
Equilibrium binding experiments	Page 11
Competitive binding experiments	Page 12
NMR titration data	Page 13

Supplementary information:

Rosengren-Holmberg J.P.; Karlsson J.G.; Svenson J.; Andersson H.S.; Nicholls I.A.

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4-vinylphenol (2)

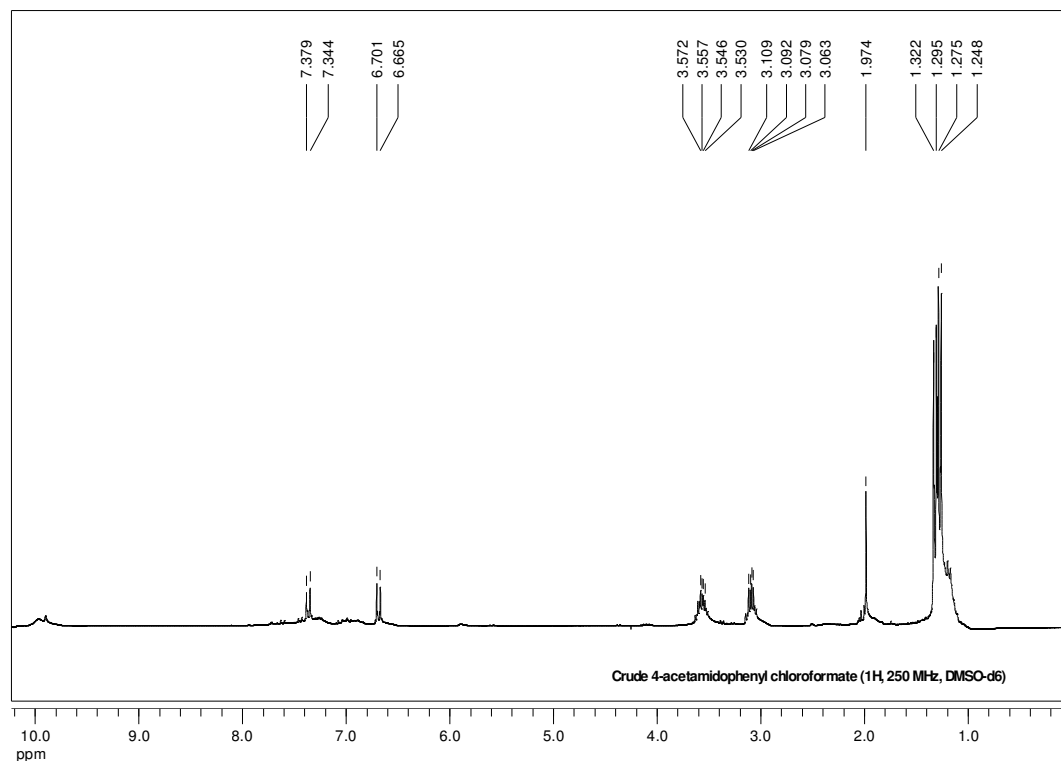


Supplementary information:

Rosengren-Holmberg J.P.; Karlsson J.G.; Svenson J.; Andersson H.S.; Nicholls I.A.

Synthesis and Ligand Recognition of Paracetamol Selective Polymers: Semi-covalent versus Non-covalent Molecular Imprinting

Crude 4-acetamidophenyl chloroformate (3)

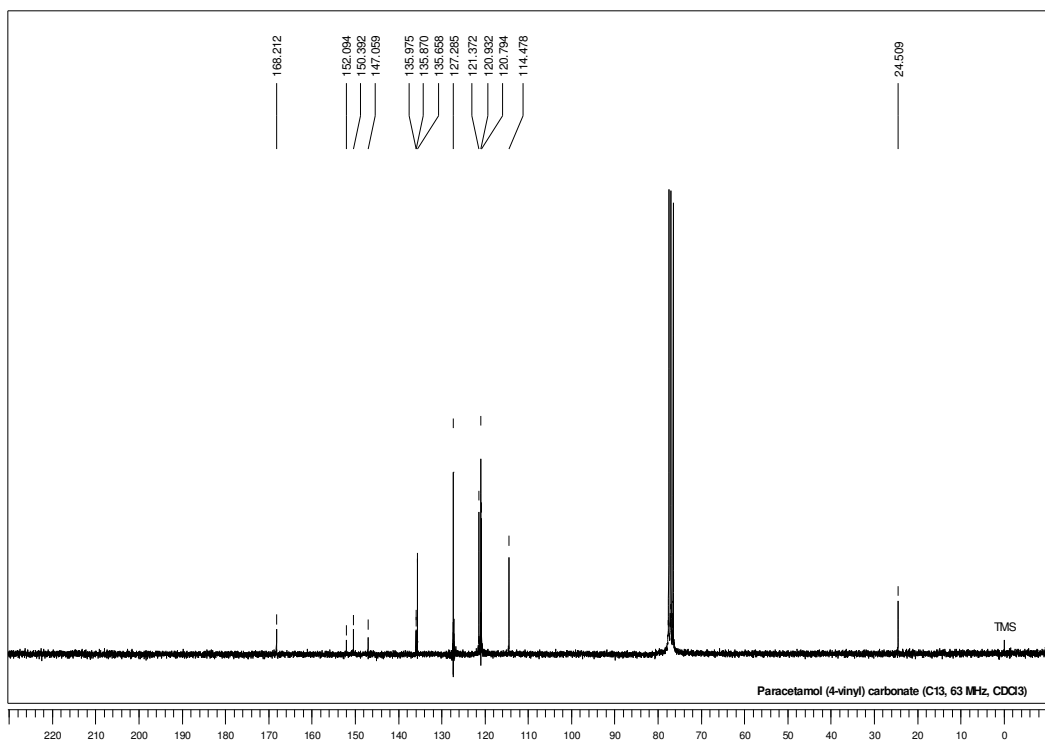
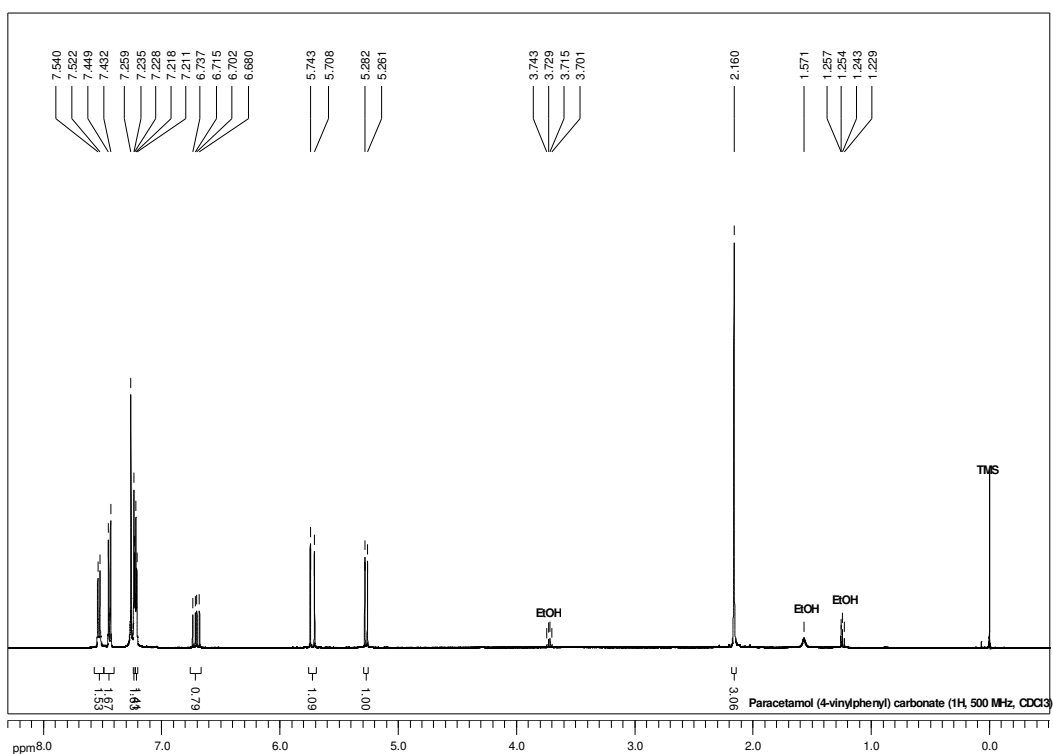


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4-acetamidophenyl-(4-vinylphenyl) carbonate (4)

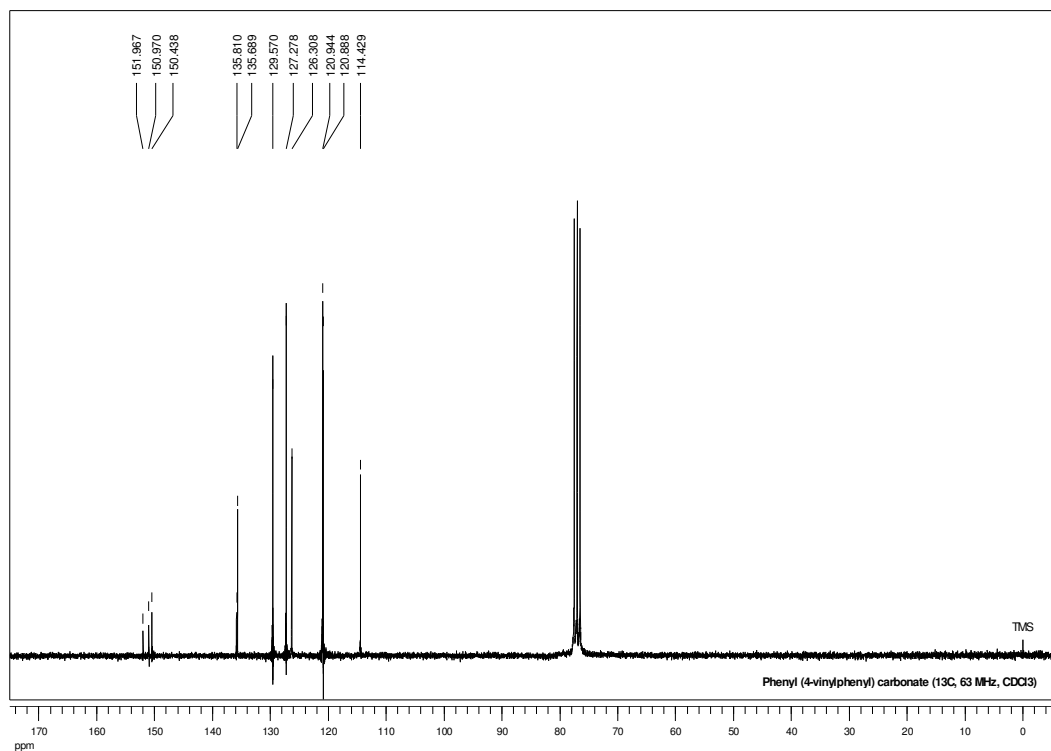
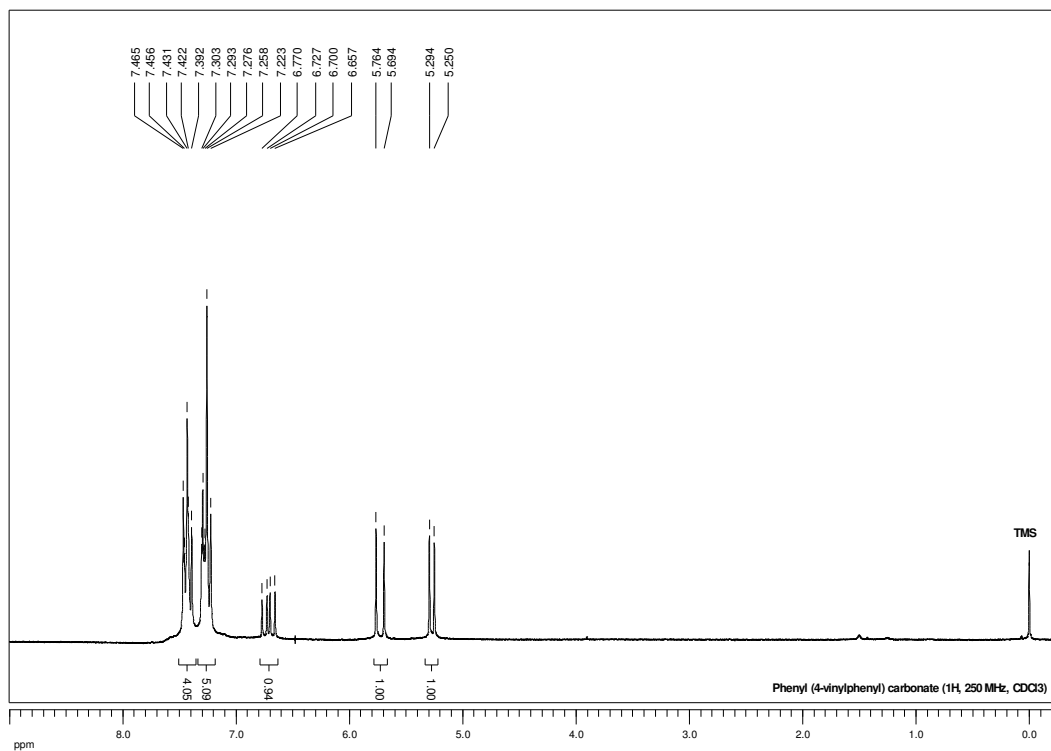


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Phenyl-(4-vinylphenyl) carbonate (5)

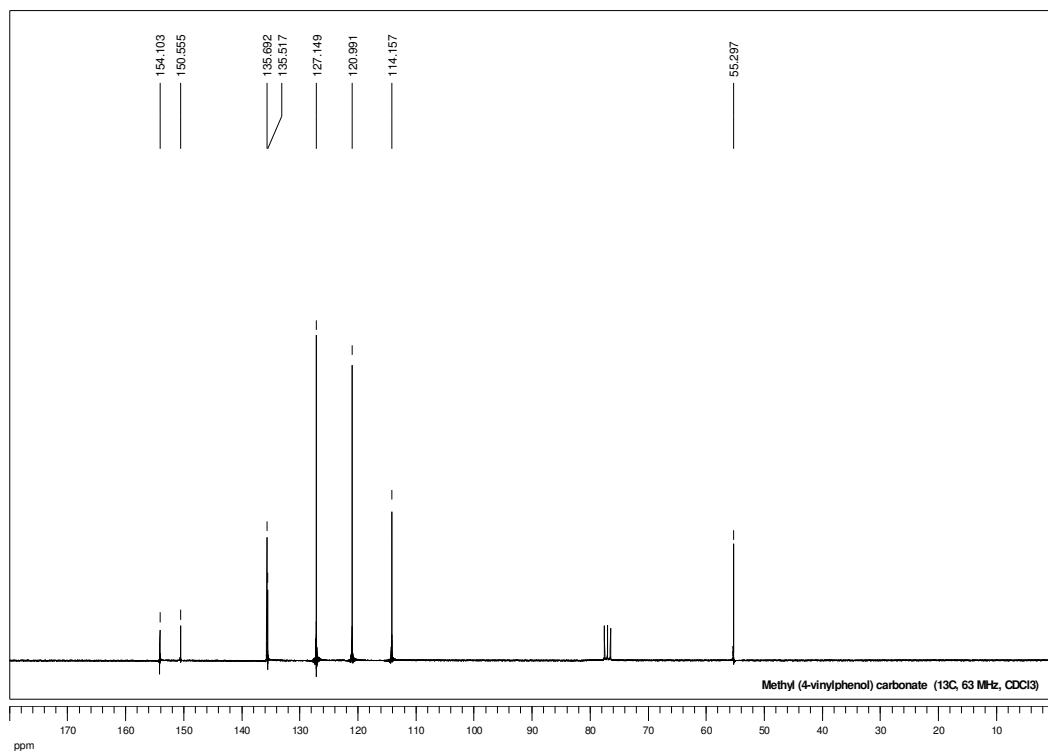
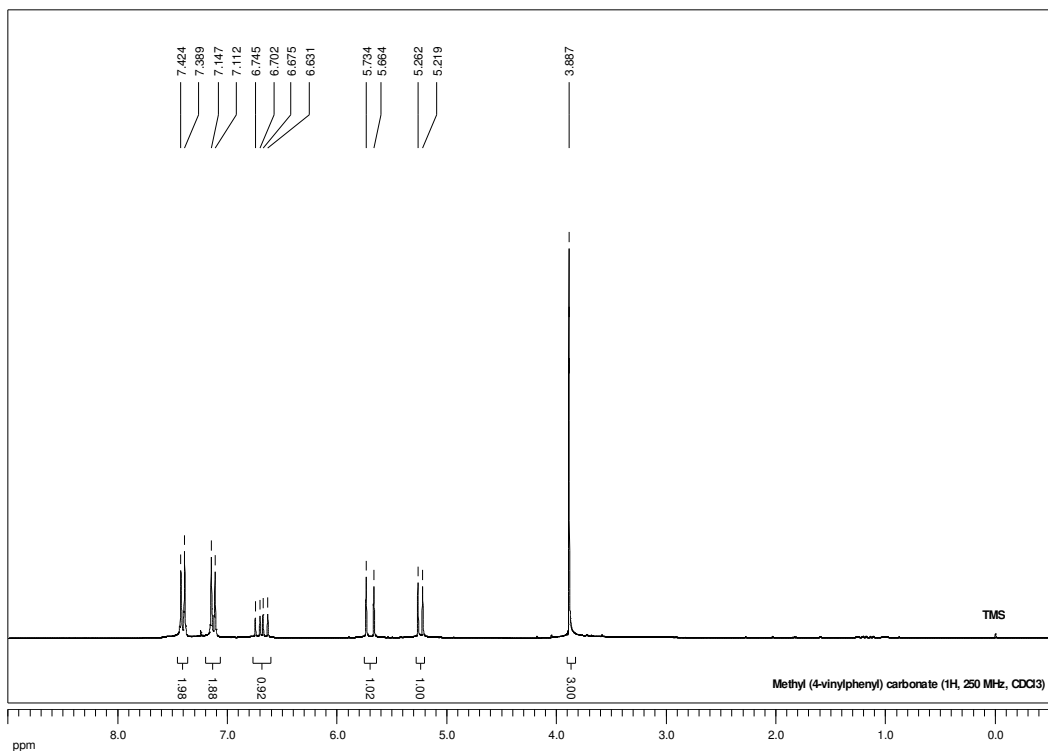


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Synthesis and Ligand Recognition of Paracetamol Selective Polymers: Semi-covalent versus Non-covalent Molecular Imprinting

Methyl-(4-vinylphenyl) carbonate (6)

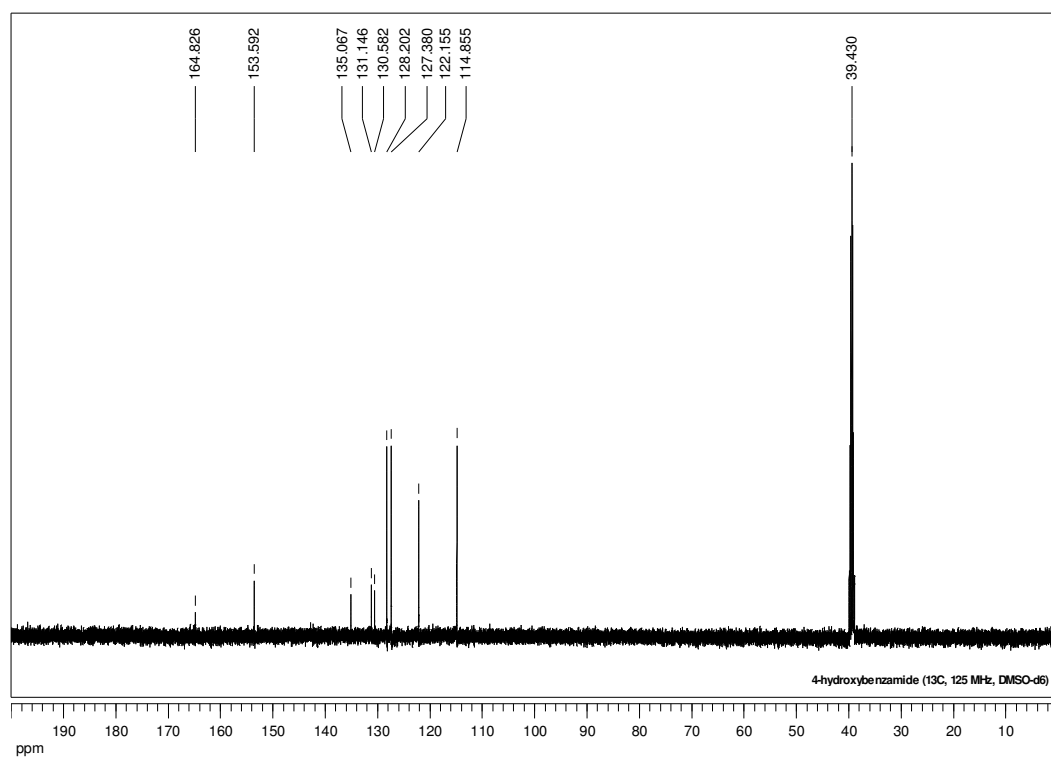
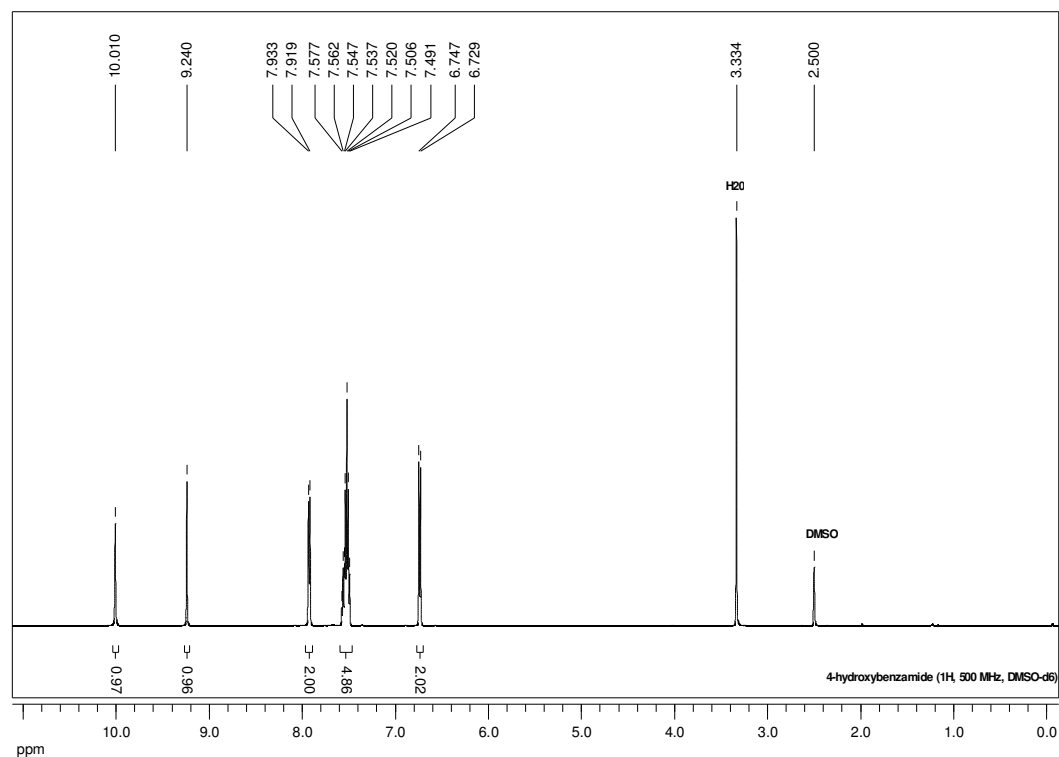


Supplementary information:

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Synthesis and Ligand Recognition of Paracetamol Selective Polymers: Semi-covalent versus Non-covalent Molecular Imprinting

(4-hydroxyphenyl)benzamide (7)

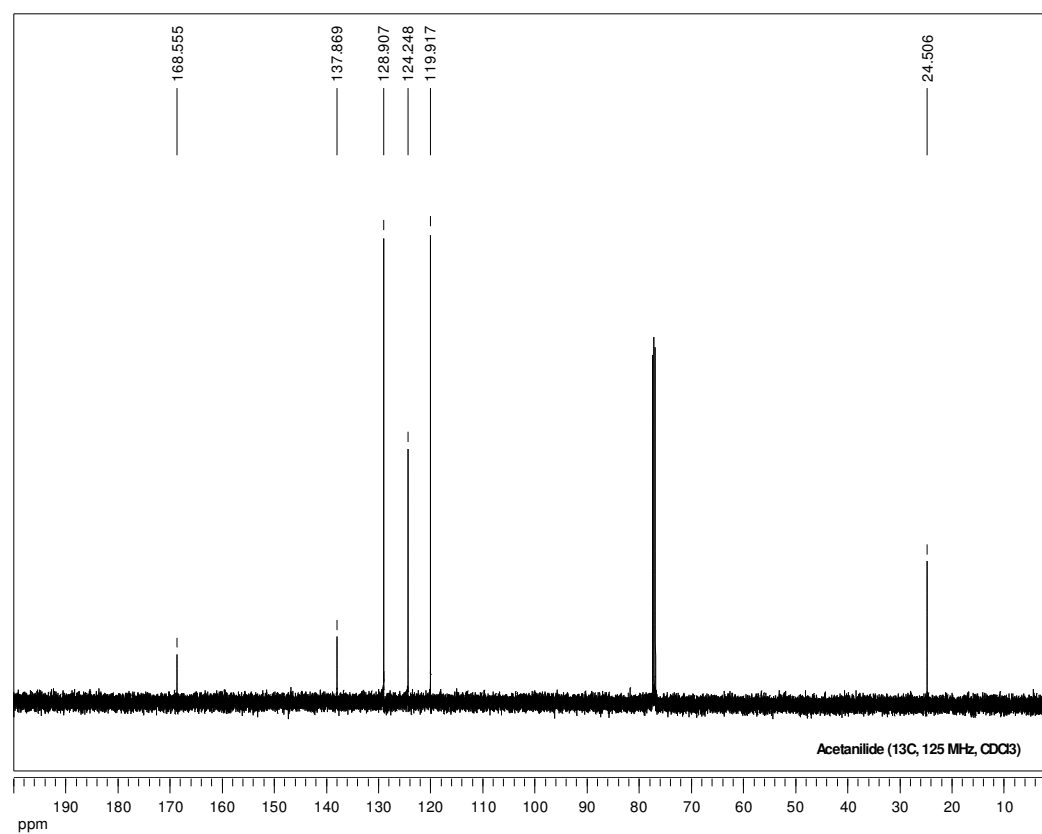
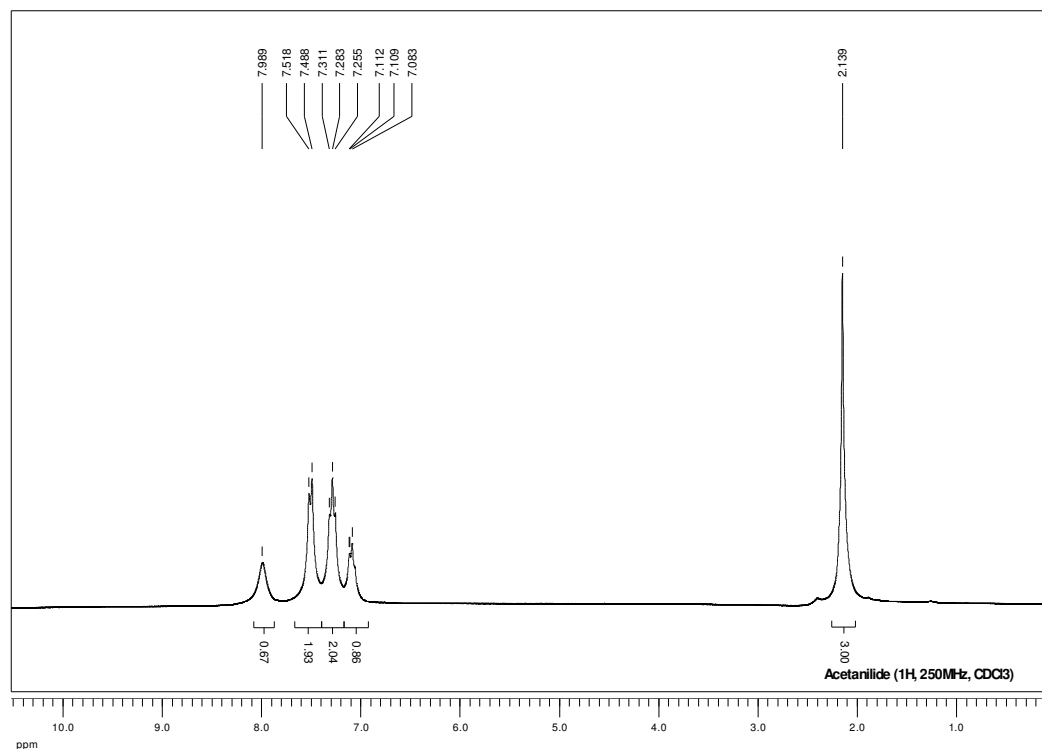


Supplementary information:

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Synthesis and Ligand Recognition of Paracetamol Selective Polymers: Semi-covalent versus Non-covalent Molecular Imprinting

Acetanilide (8)



Supplementary information:

Rosengren-Holmberg J.P.; Karlsson J.G.; Svenson J.; Andersson H.S.; Nicholls I.A.

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Physical data for P1-P11

Table 1. Physical data obtained for P1-P11.

	BET surface area (m²/g)		Pore diameter (Å)		Elemental analysis* (%)		
	Unhydrolysed	Hydrolysed	Unhydrolysed	Hydrolysed	C (calc.)	H (calc.)	N (calc)
P1	373.3 ± 2.49	422.9 ± 4.34	71.8	40.5	59.70 (61.32)	7.05 (7.13)	< 0.3 (0.28)
P2	369.8 ± 3.01	410.8 ± 5.51	55.2	40.9	60.00 (61.32)	7.10 (7.13)	< 0.3 (0.28)
P3	442.6 ± 5.86	435.6 ± 5.13	69.3	48.3	59.95 (61.32)	7.15 (7.13)	< 0.3 (0.28)
P4	406.0 ± 3.98	465.9 ± 5.43	57.3	50.6	60.30 (61.57)	7.20 (7.16)	< 0.3 (0.28)
P5	412.5 ± 2.70	506.4 ± 6.58	61.3	63.3	59.15 (60.86)	7.10 (7.14)	< 0.3 (0.28)
P6	502.4 ± 4.40	530.5 ± 6.74	54.5	64.7	59.20 (60.94)	7.05 (7.15)	< 0.3 (0.28)
P7	474.6 ± 2.98	509.7 ± 5.40	105.5	93.6	59.00 (60.86)	7.15 (7.14)	< 0.3 (0.28)
P8	481.7 ± 4.61	492.8 ± 5.40	88.7	84.5	58.90 (60.62)	7.15 (7.14)	< 0.3 (0.28)
P9	476.8 ± 5.27	477.4 ± 5.31	84.0	99.3	58.63 (60.62)	7.13 (7.14)	< 0.3 (0.28)
P10	374.9 ± 4.34	350.0 ± 4.29	95.2	89.1	57.05 (60.29)	7.00 (7.12)	< 0.3 (0.16)
P11	400.7 ± 3.78	364.1 ± 3.90	81.0	76.2	56.85 (60.29)	7.00 (7.12)	< 0.3 (0.16)

*Of hydrolysed polymers

Supplementary information:

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Polymer titrations

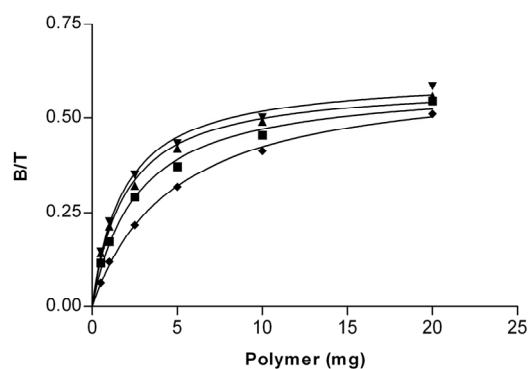


Figure 1. Titration of polymers prepared by semi-covalent molecular imprinting (P1-P4).

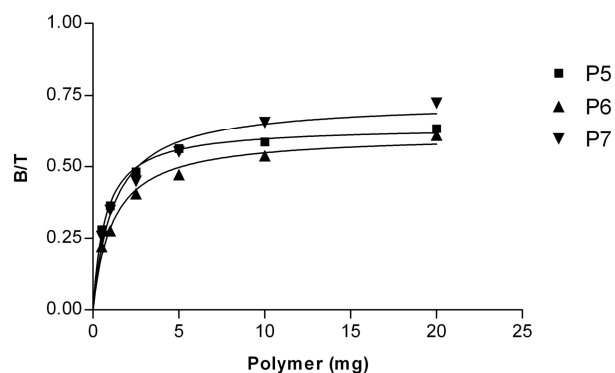


Figure 2. Titration of polymers (P5-P7) prepared by a mixture of semi-covalent and non-covalent imprinting.

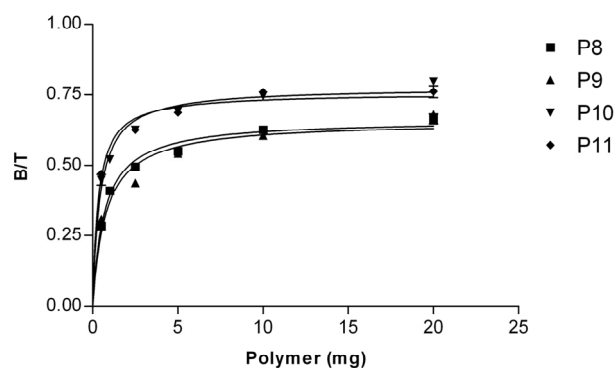


Figure 3. Titration of polymers prepared by non-covalent molecular imprinting (P8-P11).

Supplementary information:

Rosengren-Holmberg J.P.; Karlsson J.G.; Svenson J.; Andersson H.S.; Nicholls I.A.

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Equilibrium binding experiments (P1-P11)

Table 3. Binding of [³H]-4-acetamidophenol to 5 mg polymer P1-P11 in toluene and acetonitrile expressed as B/T ± SEM. B/T denotes the amount of bound radioligand (B) relative to the total amount added (T).

	Toluene	MeCN
P1	0.48 ± 0.03	0.12 ± 0.01
P2	0.48 ± 0.02	0.13 ± 0.01
P3	0.47 ± 0.01	0.15 ± 0.02
P4	0.36 ± 0.01	0.08 ± 0.01
P5	0.55 ± 0.01	0.05 ± 0.01
P6	0.47 ± 0.01	0.06 ± 0.02
P7	0.55 ± 0.01	0.07 ± 0.01
P8	0.58 ± 0.01	0.08 ± 0.01
P9	0.56 ± 0.01	0.07 ± 0.01
P10	0.69 ± 0.01	0.18 ± 0.01
P11	0.70 ± 0.01	0.17 ± 0.01

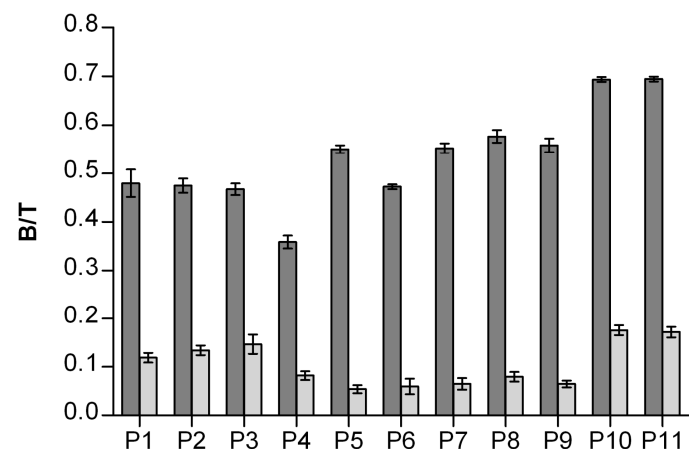


Figure 4. Binding of [³H]-4-acetamidophenol to 5 mg polymer (P1-P11) in toluene (dark grey bar) or acetonitrile (light grey bar) expressed as B/T ± SEM. B/T denotes the amount of bound radioligand (B) relative to the total amount added (T).

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Competitive binding experiments (P1-P11)

Table 4. Binding of [³H]-4-acetamidophenol to 2.5 mg polymer (P1-P11) in toluene containing 0.1% dimethyl formamide in the presence of various concentration unlabelled 4-acetamidophenol. B/T denotes the amount of bound radioligand (B) relative to the total amount added (T). Error bars reflect SEM.

	0 μ M cold ligand	10 μ M cold ligand	100 μ M cold ligand
P1	0.33 $\pm$ 0.02	0.35 $\pm$ 0.01	0.31 $\pm$ 0.01
P2	0.35 $\pm$ 0.01	0.32 $\pm$ 0.03	0.29 $\pm$ 0.03
P3	0.28 $\pm$ 0.01	0.28 $\pm$ 0.01	0.26 $\pm$ 0.01
P4	0.14 $\pm$ 0.01	0.15 $\pm$ 0.01	0.12 $\pm$ 0.02
P5	0.37 $\pm$ 0.01	0.36 $\pm$ 0.01	0.34 $\pm$ 0.01
P6	0.38 $\pm$ 0.01	0.30 $\pm$ 0.01	0.29 $\pm$ 0.01
P7	0.45 $\pm$ 0.01	0.41 $\pm$ 0.01	0.36 $\pm$ 0.02
P8	0.47 $\pm$ 0.01	0.46 $\pm$ 0.01	0.40 $\pm$ 0.01
P9	0.45 $\pm$ 0.01	0.41 $\pm$ 0.02	0.39 $\pm$ 0.01
P10	0.61 $\pm$ 0.01	0.57 $\pm$ 0.01	0.58 $\pm$ 0.02
P11	0.57 $\pm$ 0.01	0.55 $\pm$ 0.02	0.54 $\pm$ 0.01

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NMR titration data

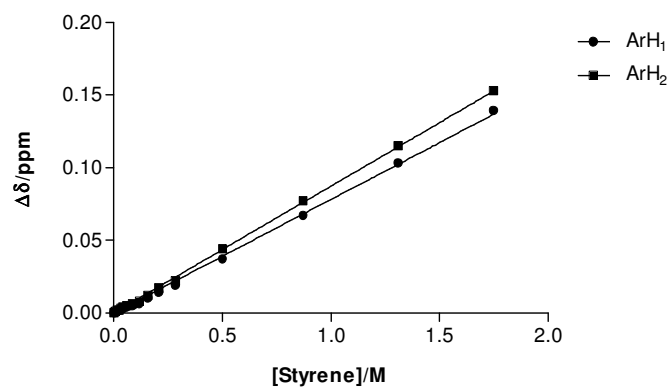


Figure 5. Titration of 29 mM acetanilide with (0-1.75 M) styrene in CDCl₃.