

SUPPLEMENTARY MATERIAL TO  
**Highly selective water-compatible molecularly imprinted  
polymers for benzophenone-4**

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Table S-I. NIP2 adsorption isotherm data

$c_0 / \text{mmol dm}^{-3}$	0.10	0.25	0.50	1.00	2.00	4.00	6.00	7.00	8.00	9.00	10.00
$c_f / \text{mmol dm}^{-3}$	0.03	0.02	0.02	0.03	0.63	2.41	4.41	5.43	6.51	7.39	8.44
$Q / \mu\text{mol g}^{-1}$	13.93	45.58	96.12	193.29	274.39	318.78	318.60	314.03	297.59	321.21	311.38

Table S-II. MIP2 NIP2 adsorption isotherm data

$c_0 / \text{mmol dm}^{-3}$	0.10	0.25	0.50	1.00	2.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00
$c_f / \text{mmol dm}^{-3}$	0.03	0.02	0.02	0.04	0.03	0.98	1.80	2.82	3.68	4.85	5.65	6.81
$Q / \mu\text{mol g}^{-1}$	14.86	45.73	96.51	192.9	393.8	604.9	639.8	635.3	664.6	629.8	669.7	638.8
				8	7	0	0	0	5	3	6	9

Table S-III. NIP4 adsorption isotherm data.

$c_0 / \text{mmol dm}^{-3}$	0.10	0.25	0.50	1.00	2.00	4.00	6.00	7.00	8.00	9.00	10.00
$c_f / \text{mmol dm}^{-3}$	0.01	0.02	0.03	0.04	0.06	1.23	2.94	3.94	4.83	5.77	6.77
$Q / \mu\text{mol g}^{-1}$	17.09	45.55	94.65	191.36	387.67	554.28	612.31	611.27	633.01	646.06	645.06

Table S-IV. MIP4 adsorption isotherm data

$c_0 / \text{mmol dm}^{-3}$	0.10	0.25	0.50	1.00	2.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00
$c_f / \text{mmol dm}^{-3}$	0.02	0.03	0.03	0.04	0.03	0.09	0.51	1.06	1.80	2.85	3.65	4.46
$Q / \mu\text{mol g}^{-1}$	15.11	44.66	94.65	192.72	394.69	781.84	897.53	987.70	1039.7	1029.1	1069.4	1108.1
									9	4	6	4

Table S-V. NIP5 adsorption isotherm data

$c_0 / \text{mmol dm}^{-3}$	0.10	0.25	0.50	1.00	2.00	4.00	6.00	7.00	8.00	9.00	10.00
$c_f / \text{mmol dm}^{-3}$	0.02	0.02	0.02	0.05	0.41	2.19	4.16	5.14	6.26	7.14	8.31
$Q / \mu\text{mol g}^{-1}$	15.55	46.42	96.29	190.11	317.22	361.49	367.37	372.58	347.90	371.22	337.98

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Table S-VI. MIP5 adsorption isotherm data

$c_0 / \text{mmol dm}^{-3}$	0.10	0.25	0.50	1.00	2.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00
$c_f / \text{mmol dm}^{-3}$	0.02	0.02	0.01	0.03	0.02	1.04	1.88	2.80	3.83	4.79	5.67	7.05
$Q / \mu\text{mol g}^{-1}$	15.88	46.85	97.16	194.6	395.8	591.7	624.1	639.7	634.6	641.8	666.0	590.7
				7	5	6	8	9	4	2	8	3

$c_0$  – total concentration of BP4,  $c_f$  – free concentration of BP4 after binding,  $Q$  – adsorption capacity

Table S-VII. Elemental analysis data for polymer pairs NIP/MIP2, NIP4/MIP4 and NIP5/MIP5

Element	Content, %		
	C	H	N
NIP2	84.05	8.47	2.04
MIP2	83.11	8.59	1.96
NIP4	88.14	8.13	1.96
MIP4	79.26	7.26	1.64
NIP5	85.78	7.80	1.00
MIP5	89.74	8.01	1.00

Table S-VIII. Capacity data for polymer pairs NIP/MIP2, NIP4/MIP4 and NIP5/MIP5.

Polymer	$c_N / \text{mmol g}^{-1}$		Adsorption capacity, $\text{mmol g}^{-1}$	Content of N (cond), $\text{mmol g}^{-1}$	Specific surface area (BET), $\text{m}^2 \text{g}^{-1}$
	Calculated	Determined			
NIP2	1.236	1.454	0.311	0.830	290
MIP2	1.236	1.400	0.639	0.996	339
NIP4	1.321	1.400	0.645	1.317	539
MIP4	1.321	1.145	1.108	0.952	663
NIP5	0.710	0.714	0.338	0.601	551
MIP5	0.710	0.714	0.591	0.590	634

Calculated content of N – based on monomer composition, determined content of N – N determined by EA, adsorption capacity – determined from adsorption isotherms, N content determined by conductometric titration – based on HCl consumption

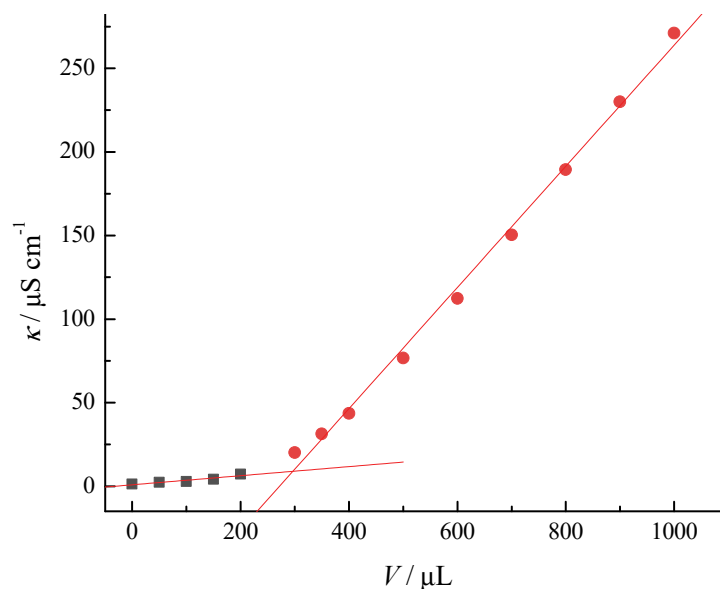


Figure S-1. Example of titration graph for conductometric titration of MIP5 with HCl. 52.6 mg of polymer was placed in a titration cell, 20.0 mL of ACN added, suspension was stirred using a magnetic stirrer and titrated with  $0.1024 \text{ mol dm}^{-3}$  HCl solution at  $25.0 \pm 0.5 \text{ }^\circ\text{C}$

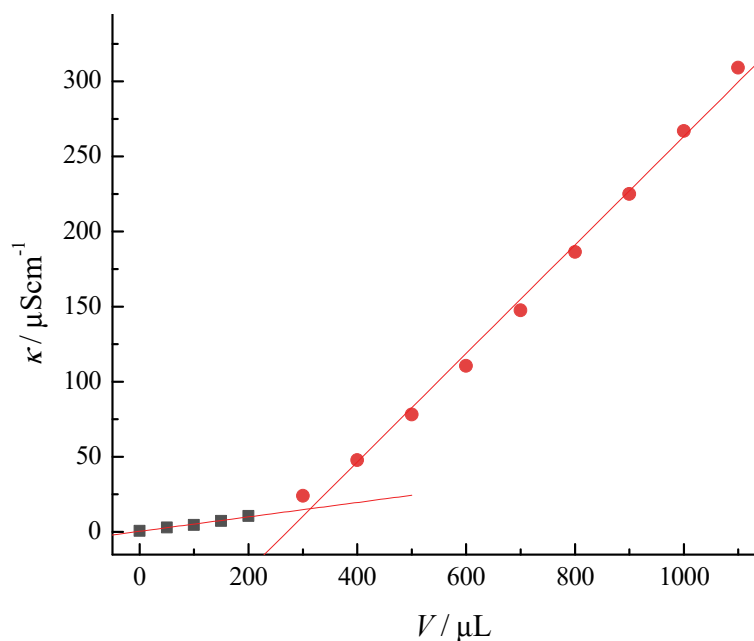


Figure S-2. Example of titration graph for conductometric titration of NIP5 with HCl. 50.2 mg of polymer was placed in a titration cell, 20.0 mL of ACN added, suspension was stirred using a magnetic stirrer and titrated with  $0.1024 \text{ mol dm}^{-3}$  HCl solution at  $25.0 \pm 0.5 \text{ }^\circ\text{C}$

Table S-IX. Selectivity data for binding of UV filters to MIP2

Compound	BP3	OCT	AVB	OS	HMS	PABA-O	BP8	BP4
$c_0 / \text{mmol dm}^{-3}$	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
$c_f / \text{mmol dm}^{-3}$	4.92	4.86	4.80	4.96	0.00	4.88	4.91	1.80
$Q / \mu\text{mol g}^{-1}$	15.90	27.51	40.14	8.40	0.00	23.80	18.19	639.80

Table S-X. Selectivity data for binding of UV filters to MIP4

Compound	BP3	OCT	AVB	OS	HMS	PABA-O	BP8	BP4
$c_0 / \text{mmol dm}^{-3}$	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
$c_f / \text{mmol dm}^{-3}$	4.88	4.82	4.76	4.91	4.94	4.89	4.81	0.51
$Q / \mu\text{mol g}^{-1}$	24.41	35.31	47.82	18.04	11.82	22.64	38.86	897.53

Table S-XI. Selectivity data for binding of UV filters to MIP5

Compound	BP3	OCT	AVB	OS	HMS	PABA-O	BP8	BP4
$C_0 / \text{mmol dm}^{-3}$	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
$C_f / \text{mmol dm}^{-3}$	4.91	4.79	4.73	4.95	4.89	4.89	4.87	1.88
$Q / \mu\text{mol g}^{-1}$	17.60	41.72	54.54	9.22	21.84	21.24	26.35	624.16

$c_0$  – total concentration of BP4,  $c_f$  – free concentration of BP4 after binding,  $Q$  – adsorption capacity