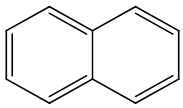
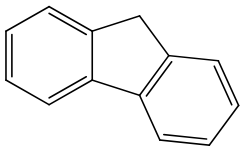
Electronic Supplementary Material (ESI) for Analytical Methods.

Electronic Supplementary Material

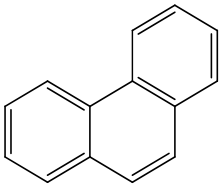
S- Table 1. PAHs and MIP components structures



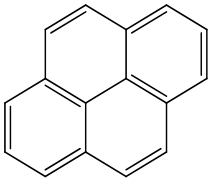
naphthalene



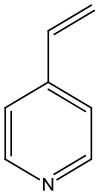
fluorene



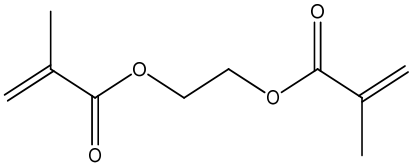
phenanthrene



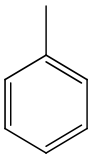
pyrene



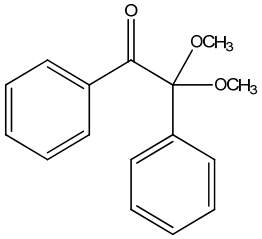
4-vinyl pyridine (4-VP)



ethylene glycol dimethacrylate (EGDMA)



toluene



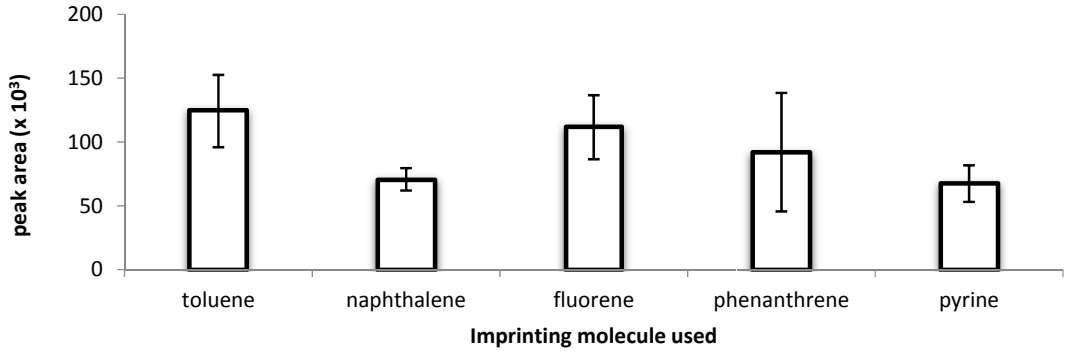
2,2-dimethoxy-2-phenylacetophenone (DMPA)

S-Table 2. MIP and NIP composition

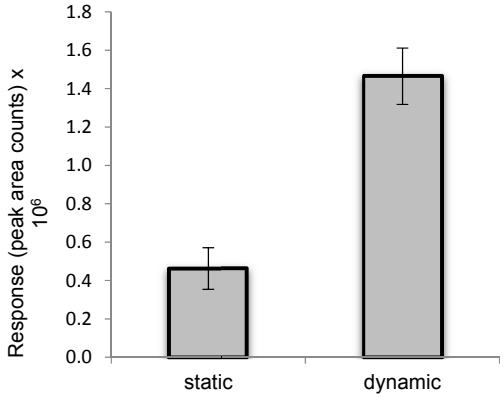
Pre-polymer component	MIP	NIP
toluene	4.25 µL (0.0405 mmol)	_
4-VP	17.0 µL (0.158 mmol)	17.0 µL (0.158 mmol)
EGDMA	151 µL (0.801 mmol)	151 µL (0.801 mmol)
DMPA	3.20 mg (0.0125 mmol)	3.20 mg (0.0125 mmol)
1-octanol	200 µL (1.26 mmol)	204 µL (1.28 mmol)

S-Table 3. GC-MS settings: Quantifier and qualifier ions used to identify the PAHs

	Quantifier (m/z)	Qualifier (m/z)
naphthalene	128	127
fluorene	165	166
phenanthrene	178	176
pyrene	202	200
octane	114	85
octanol	97	84
p- cresol	108	107
acenaphthene d_{10}	162	158



S-Fig. 1 Peak area corresponding to total PAH upload from 0.1 µg L^{-1} for two hours PAHs, for MIPs with different templates; GC-MS in SIM mode

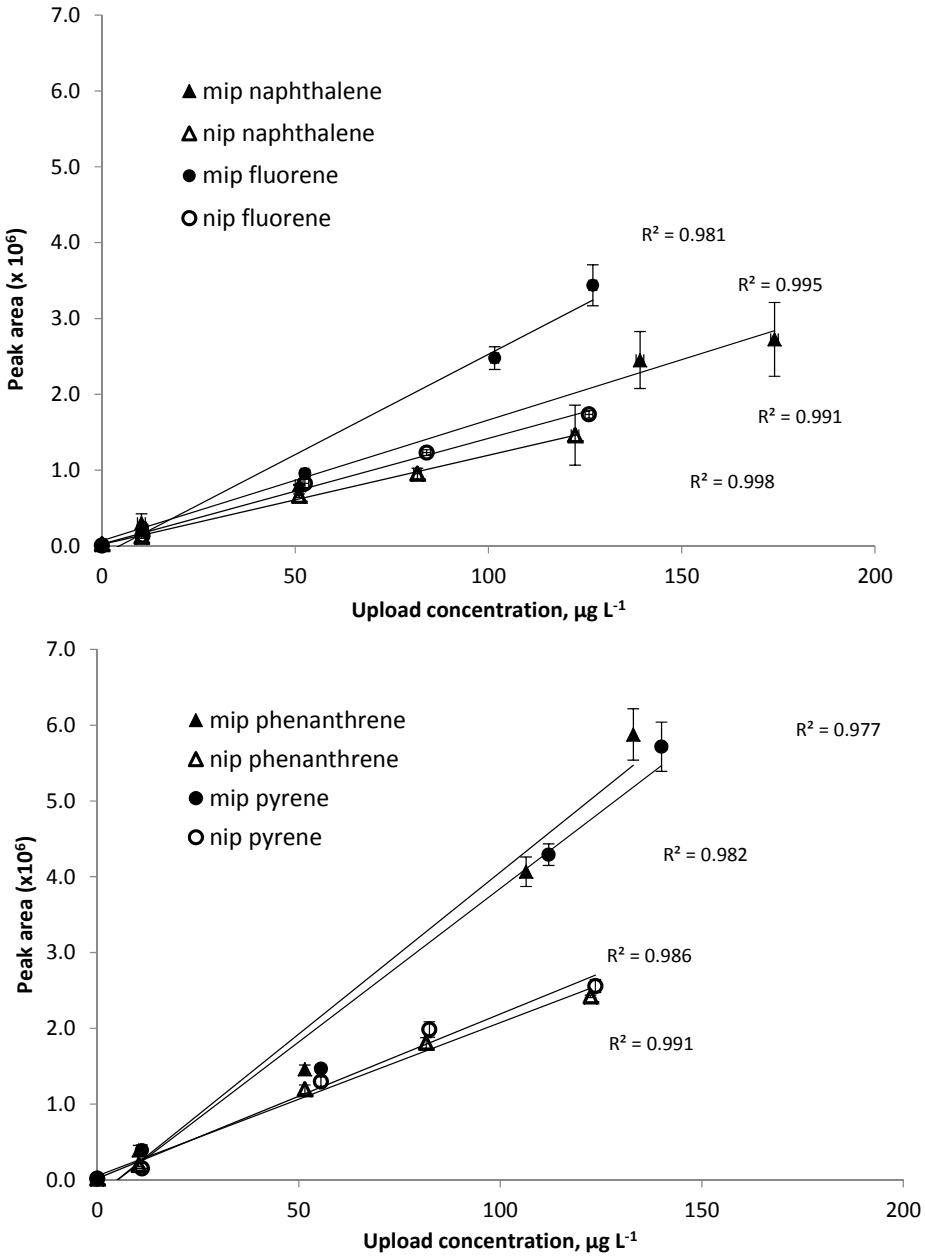


S-Fig. 2. Effect of stirring over the total PAH uptake of the MIP over 18 h, expressed in terms of the detector signal

S-Table 4. Physicochemical properties and carcinogenic potency of the PAHs studied

Compound	MW	Log K_{ow}	Water solubility at 25°C (mg L^{-1})	Melting point (°C)	Vapour pressure at 25 °C (mPa)	Carcinogenic potency (IARC/US EPA classification)	Concentration in produced water (µg L^{-1}), [29]
naphthalene	128.16	3.5	31.7	80.5	11960		5.3-394
fluorine	166	4.18	1.98	116.5	94.7		0.06- 21.7
phenanthrene	178.24	4.5	1.29	101	90.7	3	0.11- 32.0
pyrene	202.26	4.9	0.135	156	$91.3x10^{-6}$	3	0.01- 1.9
toluene	92	2.69					_
1-octanol		2.8-3.15					_

3-possibly carcinogenic to human



S-Fig. 3. Increase in detector response with the concentration in the upload solution: (a) for naphthalene and fluorene (b) for phenanthrene and pyrene; experimental conditions of 80.0 mL sample for two hours, GC-MS in SIM mode. Bars represent standard deviation.