

Electronic Supplementary Information (ESI)

Water-compatible molecularly imprinted polymers prepared using metal-organic gel as porogen

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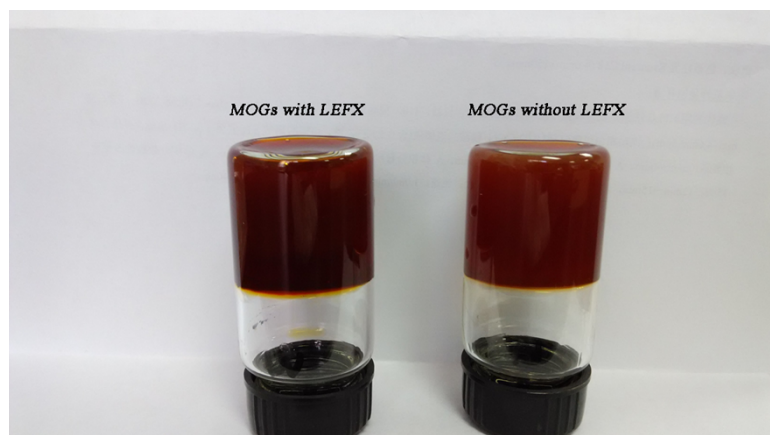


Fig. S1 Image of MOGs containing LEFX and without containing LEFX

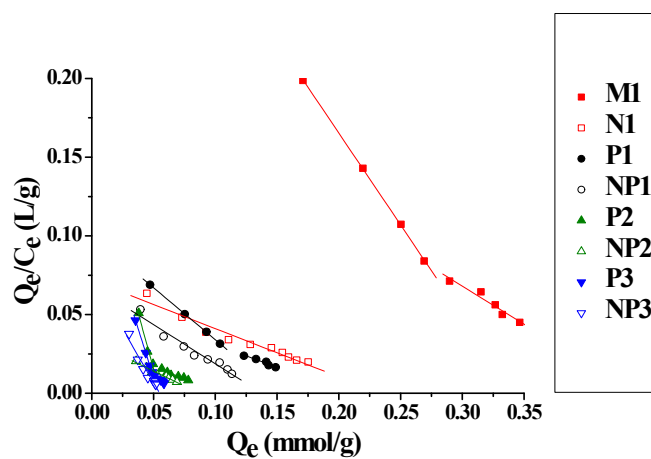


Fig. S2 Scatchard analysis of LEFX on the MIPs and NIPs with different of blank controls. $V=3.0$ mL, $C_0=0-10$ mmol/L, $t=5$ h, 20 mg of the polymers. M1: MIP- Fe^{3+} - H_3BTC ; N1: NIP- Fe^{3+} - H_3BTC ; P1: MIP- Fe^{3+} ; NP1: NIP- Fe^{3+} ; P2: MIP- H_3BTC ; NP2: NIP- H_3BTC . P3: MIP; NP3: NIP.

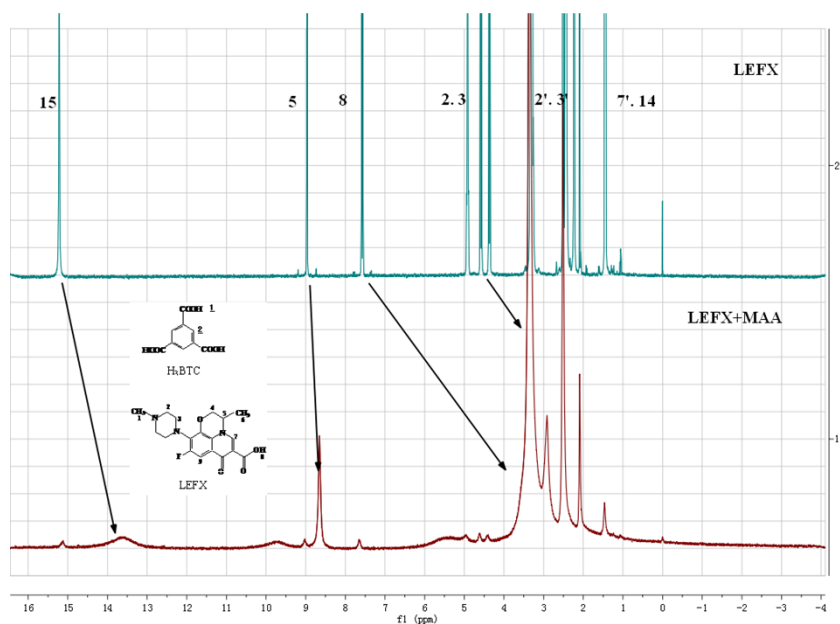


Fig. S3a Comparison of $^1\text{H-NMR}$ spectroscopy of and LEFX+MAA

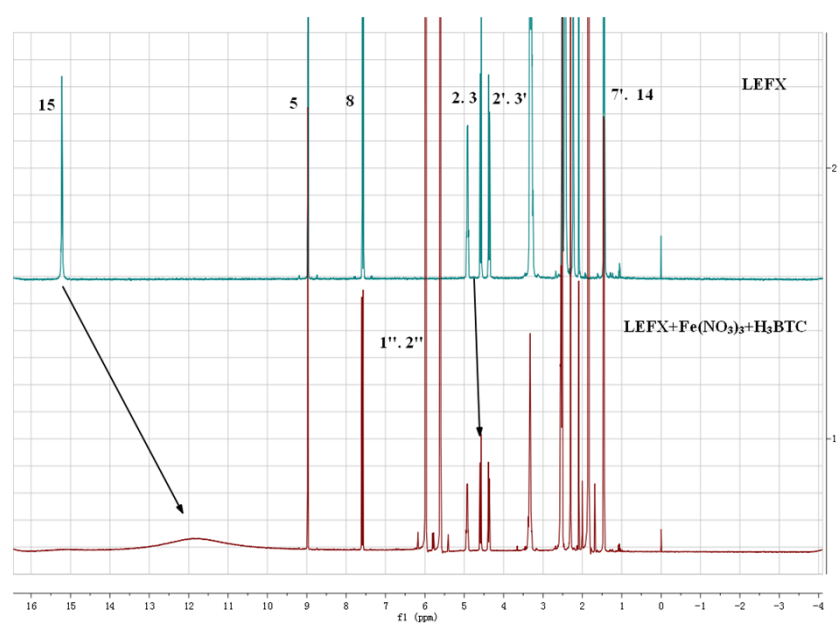


Fig. S3b Comparison of $^1\text{H-NMR}$ spectroscopy of LEFX and LEFX + Fe(NO₃)₃+H₃BTC

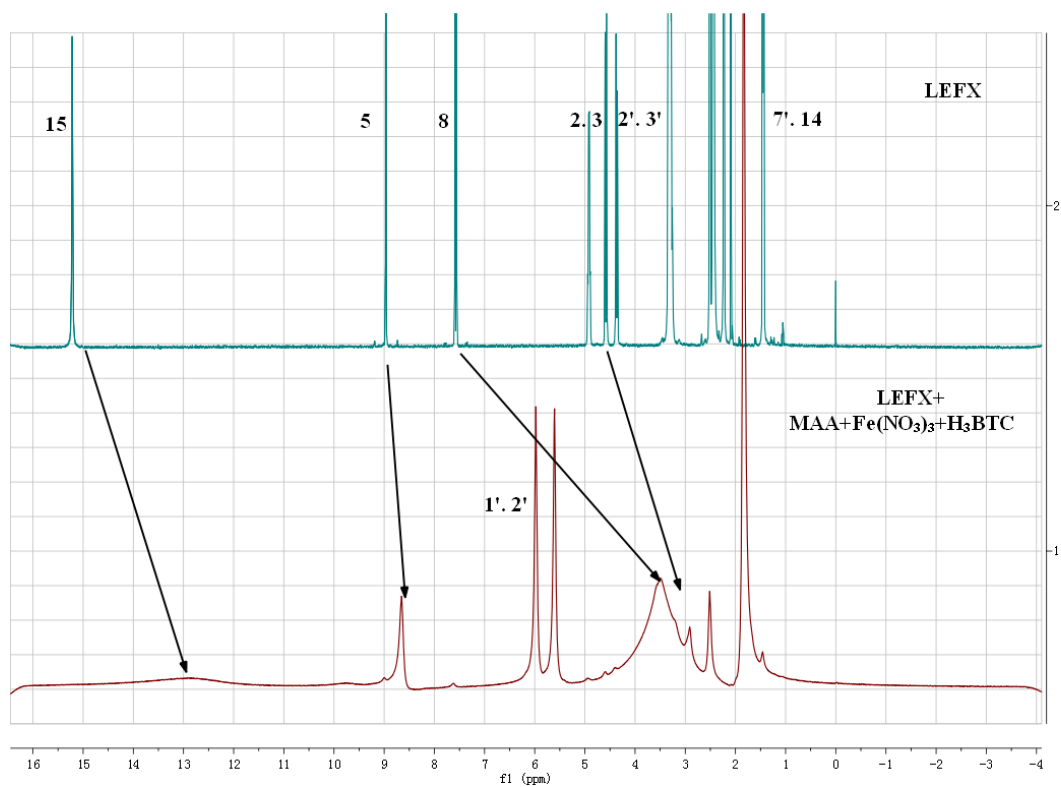


Fig. S3c Comparison of $^1\text{H-NMR}$ spectroscopy of LEFX and LEFX + $\text{Fe}(\text{NO}_3)_3 + \text{H}_3\text{BTC} + \text{MAA}$

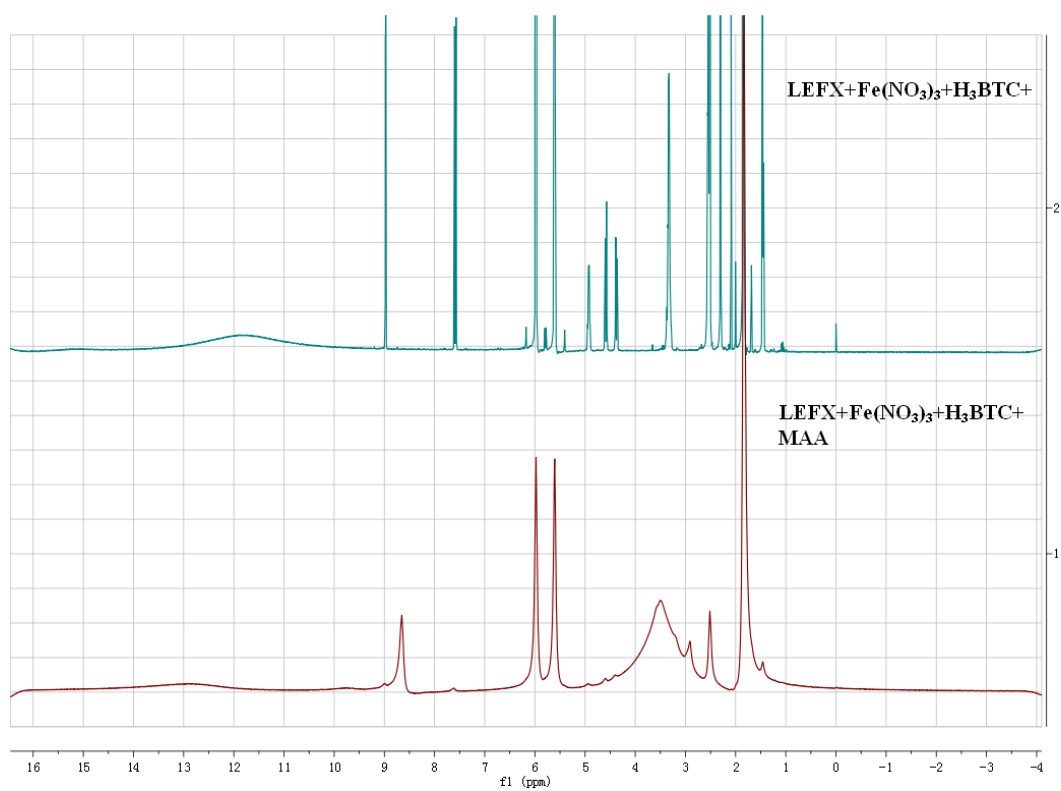


Fig. S3d Comparison of $^1\text{H-NMR}$ spectroscopy of LEFX + $\text{Fe}(\text{NO}_3)_3 + \text{H}_3\text{BTC}$ and LEFX + $\text{Fe}(\text{NO}_3)_3 + \text{H}_3\text{BTC} + \text{MAA}$

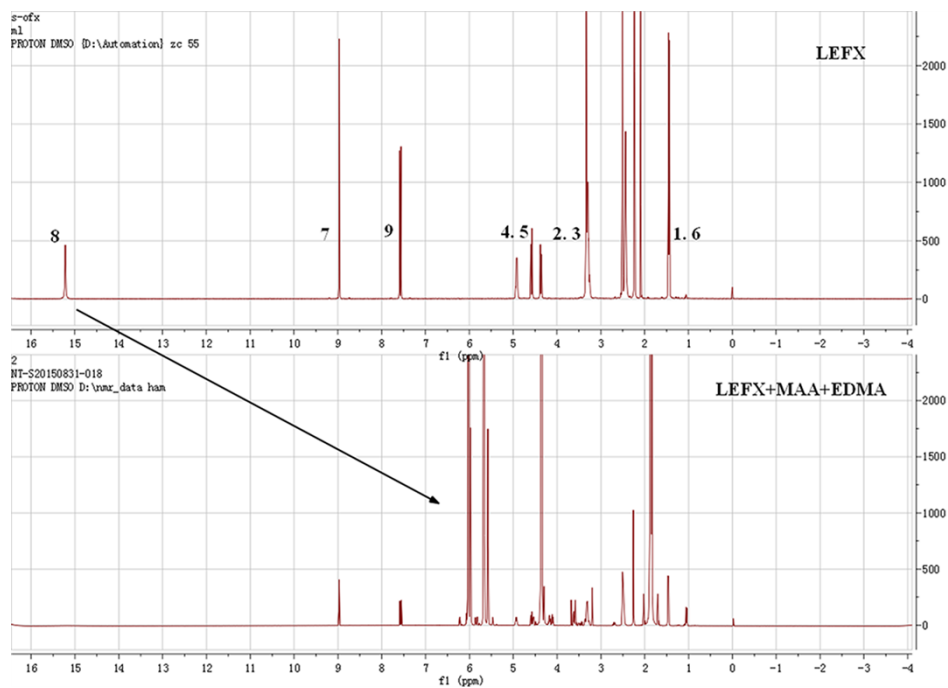


Fig. S3e Comparison of H^1 -NMR spectroscopy of LEFX and LEFX +MAA+EDMA

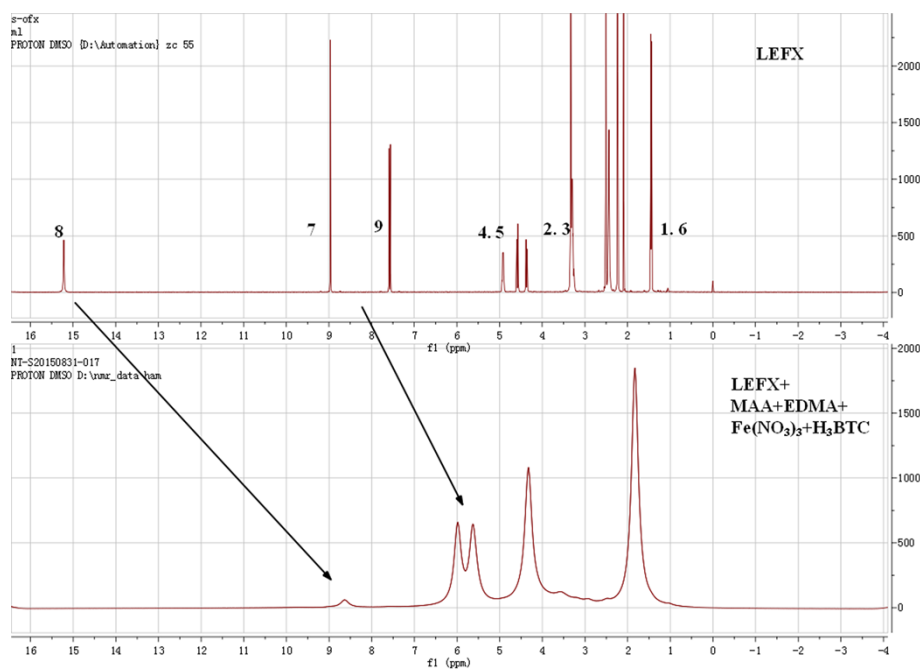


Fig. S3f Comparison of H^1 -NMR spectroscopy of LEFX and LEFX + $Fe(NO_3)_3+H_3BTC$ +MAA+EDMA

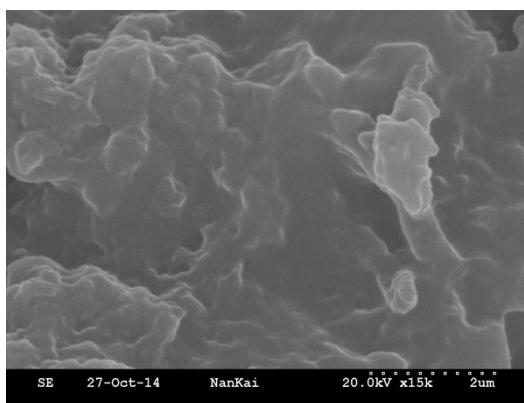


Fig. S4 Scanning electron micrographs of Fe^{3+} - H_3BTC hydrogel.

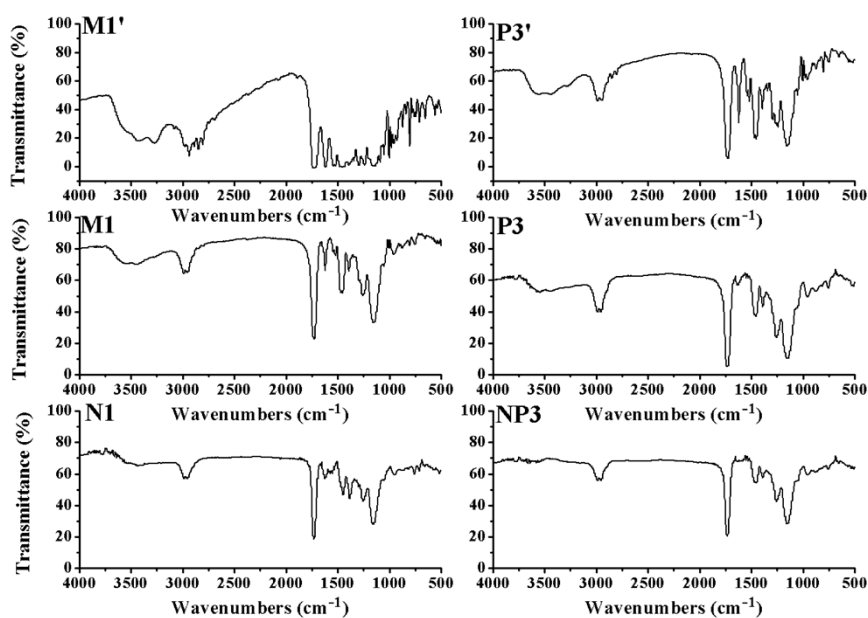


Fig. S5 The infrared spectroscopy of different polymers. M1': MIP- Fe^{3+} - H_3BTC before remove template; M1: MIP- Fe^{3+} - H_3BTC ; N1: NIP- Fe^{3+} - H_3BTC ; P3': MIP before remove template; P3: MIP; NP3: NIP

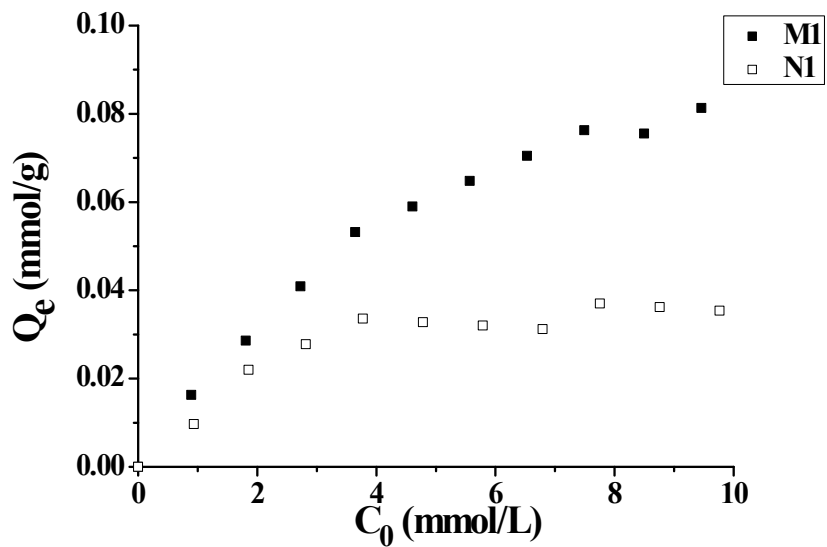


Fig. S6 Adsorption isotherms of LEFX on the MIPs and NIPs in water containing Fe(III). M1: MIP; N1: NIP.

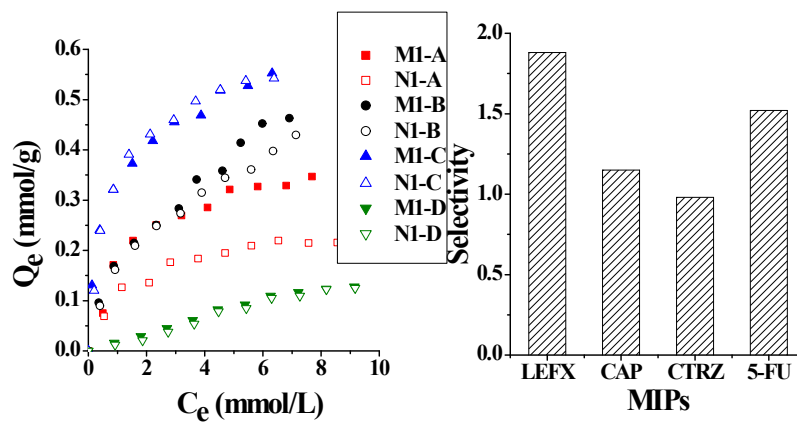


Fig. S7 Adsorption isotherms of LEFX and nonanalogues on the MIPs and NIPs. $V=3.0$ mL, $C_0=0-10$ mmol/L, $t=5$ h, 20 mg of the polymers. A: LEFX is the template; B: CAP; C: CTRZ; D: 5-FU. CAP, CTRZ and 5-FU are nonanalogues.

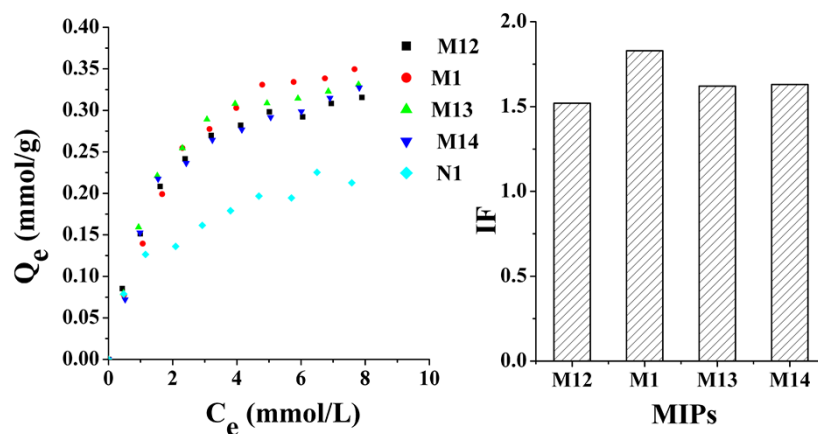


Fig. S8 Adsorption isotherms of LEFX on the MIPs and NIPs with different molar ratio of template to functional monomer. $V = 3.0$ mL, $C_0 = 0-10$ mmol/L, $t = 5$ h, 20 mg of the polymers. M7: T/M=1/6; M1: T/M=1/8; M8: T/M=1/10; M9: T/M=1/12.

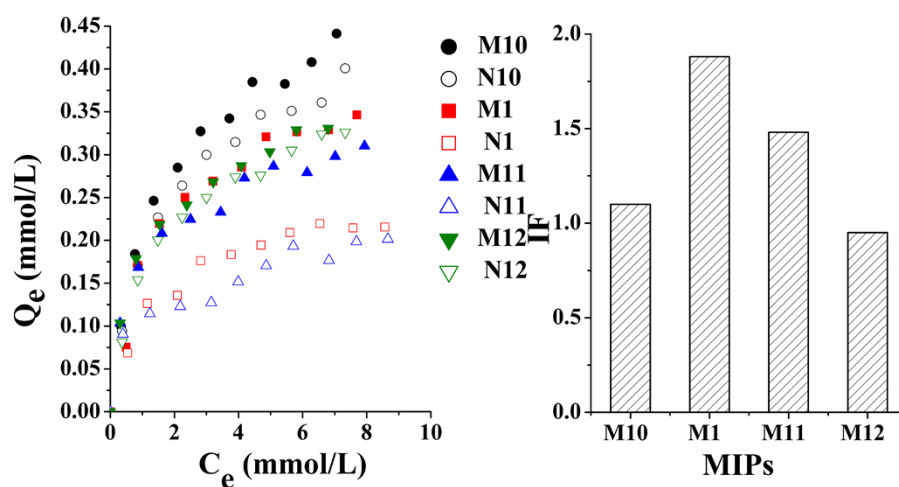


Fig. S9 Adsorption isotherms of LEFX on the MIPs and NIPs with different degree of cross linking. $V=3.0$ mL, $C_0=0-10$ mmol/L, $t=5$ h, 20 mg of the polymers. M10, N10: 75%; M1, N1:80%; M11, N11: 83%; M12, N12:85%.

Table S1 Adsorption parameters of polymers

Model	Fited parameters	M1	N1
Langmuir	Q_{\max} (mmol/g)	0.138	0.040
	b (L/mmol)	0.154	0.750
	R^2	0.992	0.992
Freundlich	K_F (L/g)	0.0229	0.0173
	$1/n$	0.58	0.35
	R^2	0.983	0.917

Table S2 The swelling rate of the polymers in different solvent

Polymers	Water	PBS (pH 7.40)	Ethanol
M1	4.17 %	6.67 %	11.93 %
N1	9.00 %	9.28 %	14.60 %
P3	3.27 %	3.99 %	3.62 %
NP3	2.41 %	3.79 %	2.91 %

Table S3. Fitting data of kinetic binding on M1 and N1.

	Pseudo-first-order			Pseudo-second-order		
	k_1 (min ⁻¹)	Q_e (mmol/g)	R ²	k_2 (g/mmol/min)	Q_e (mmol/g)	R ²
M1	0.0252	0.6181	0.988	111.00	0.7892	0.996
N1	0.0327	0.5101	0.978	128.61	0.2795	0.989