Preferential water remediation of cationic dyes using structurally engineered novel organoselenium based self-assembled constructs

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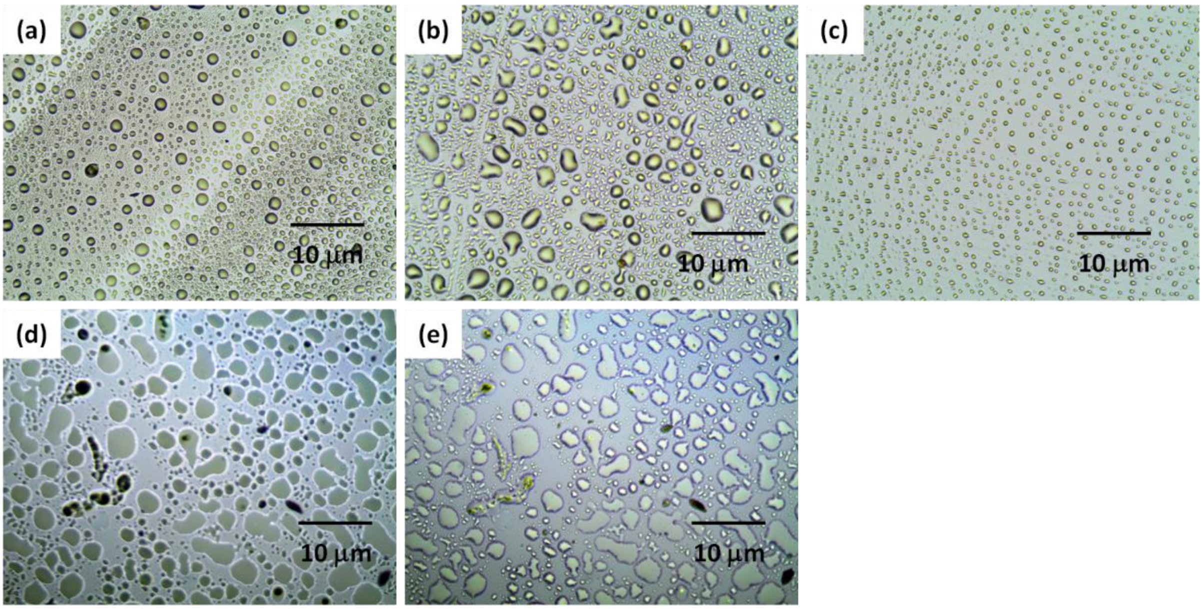

Fig. S1 Optical microscopic images of self-assembled IPSeX1 in (a) Acetone (b) Methanol (c) Dichloromethane (d) Acetonitrile (e) 1,4-dioxane

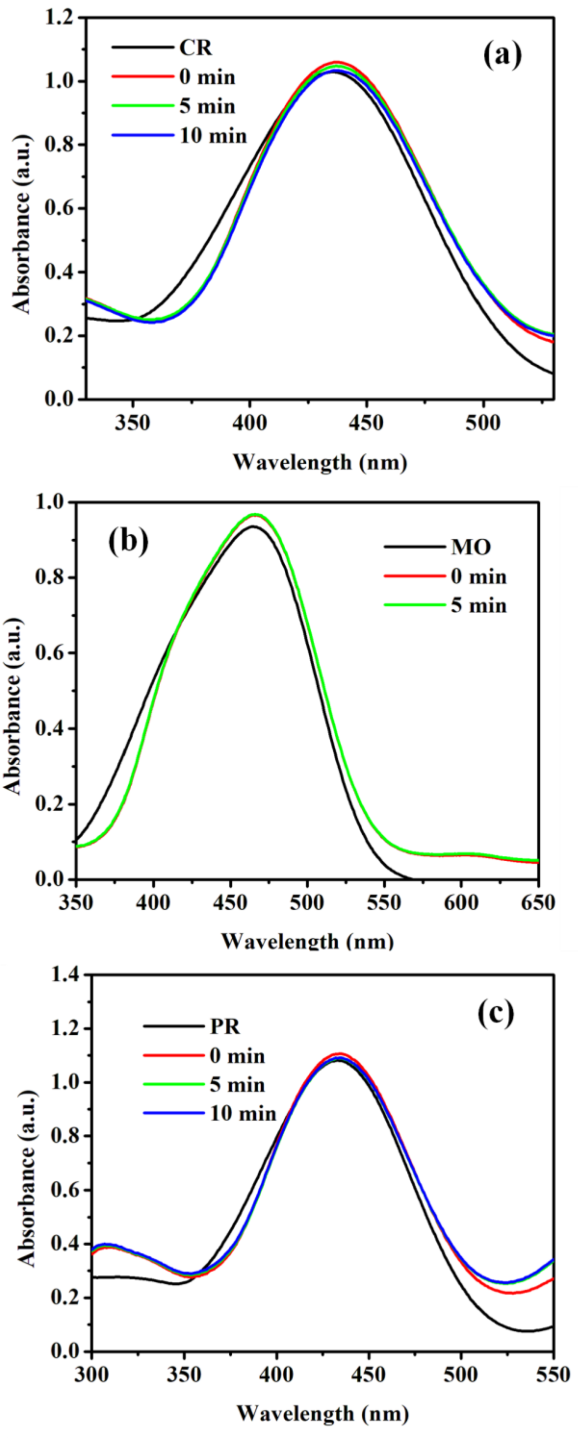

Fig. S2 Absorption spectra of (a) CR (b) MO and (c) PR.

The equilibrium adsorption capacity, $q_e = \dfrac{C_0 - C_e}{W} \times V$

For CV, Dye adsorption capacity at equilibrium: 0.01 mg adsorbent

$$q_e = \frac{(5-2.90)\ \mu g/mL \times (10^{-3}\ mg / 10^{-3}\ L) \times 1\ mL \times 10^{-3}\ L}{0.01 mg \times 10^{-3}\ g}$$

q_e **= 210 mg/g for CV**

For MB, Dye adsorption capacity at equilibrium: 0.01 mg adsorbent

$$q_e = \frac{(5-3.515)\ \mu g/mL \times (10^{-3}\ mg / 10^{-3}\ L) \times 1\ mL \times 10^{-3}\ L}{0.01 mg \times 10^{-3}\ g}$$

q_e **= 148.5 mg/g for MB**

Fig. S3 Dye adsorption capacity at equilibrium for CV and MB

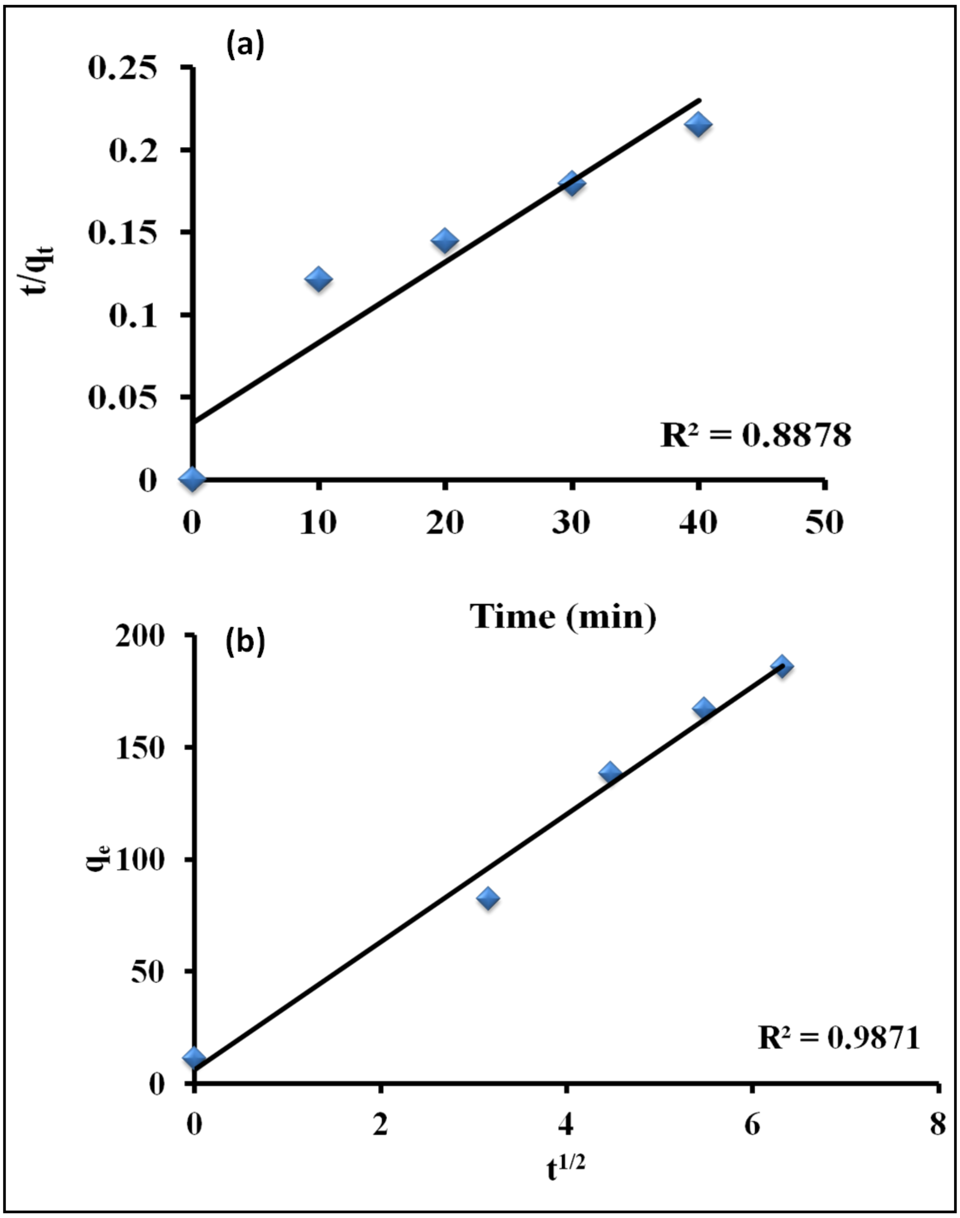

Fig. S4 (a) Pseudo second order (b) Intraparticle diffusion model for adsorption of CV

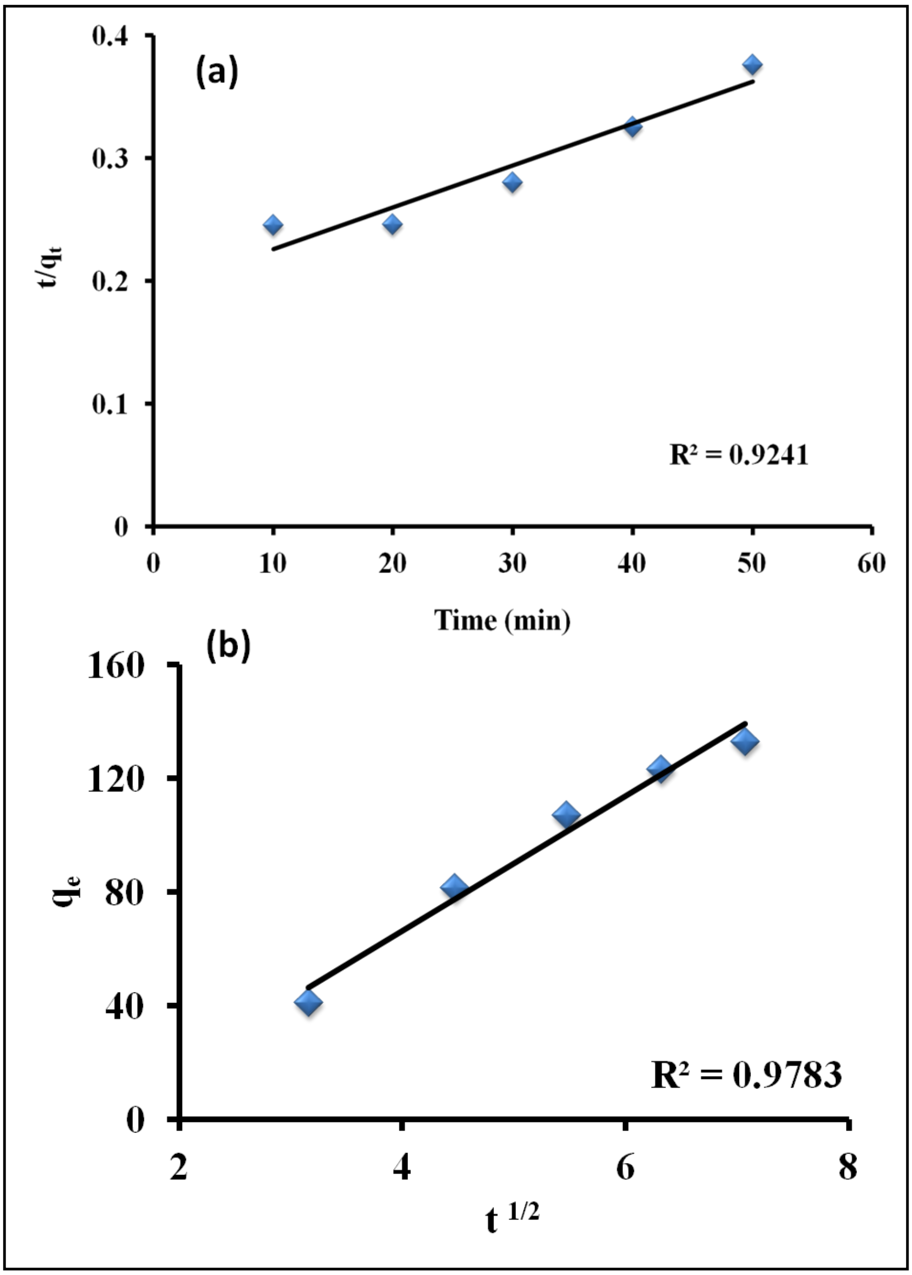

Fig. S5 (a) Pseudo second order (b) Intraparticle diffusion model for adsorption of MB

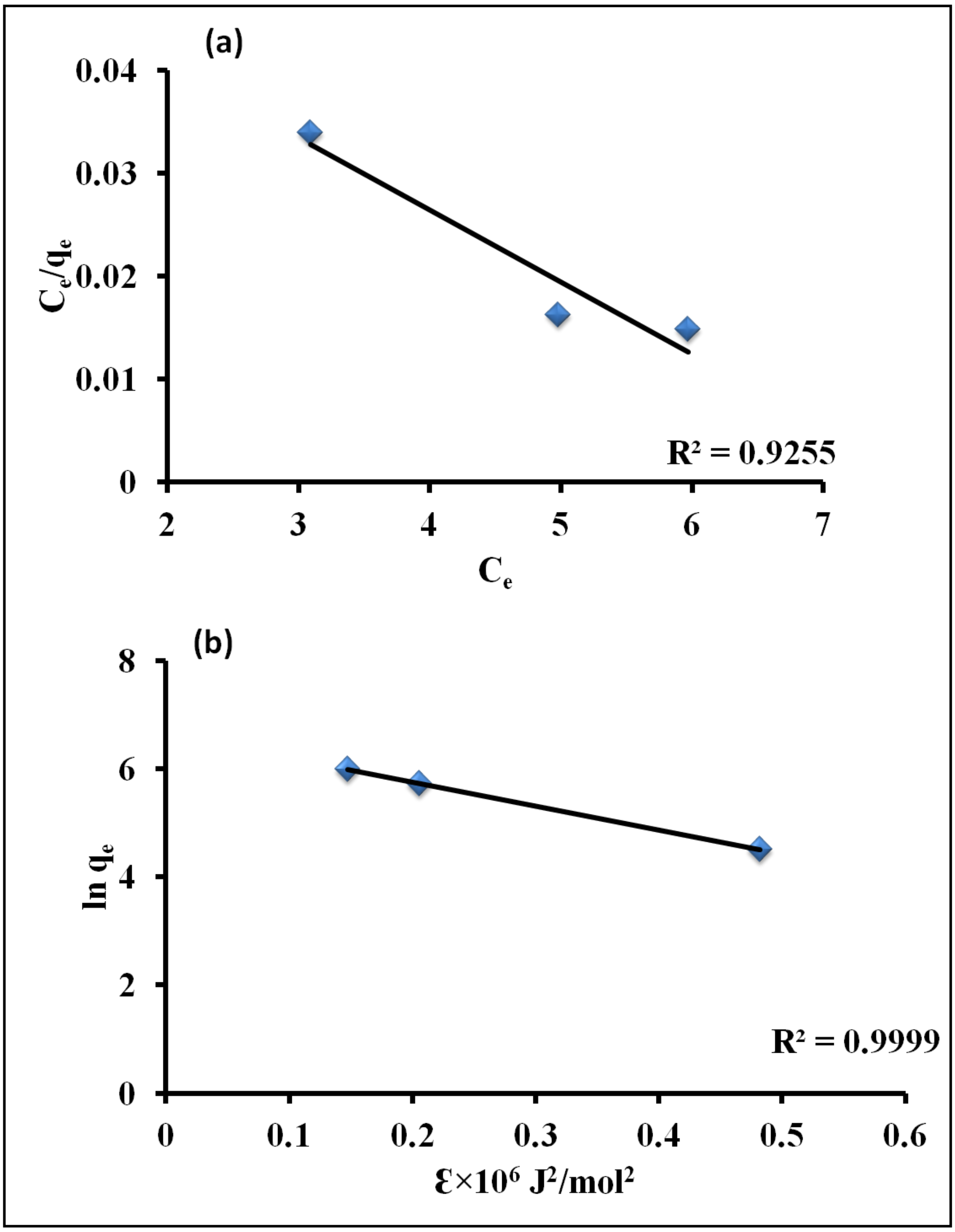

Fig. S6 (a) Langmuir adsorption isotherm (b) D-R adsorption isotherm for CV

Adsorption Isotherms for CV:

Freundlich adsoprtion isotherm:

$$\ln q_e = \frac{1}{n} \ln C_e + \ln K_F$$

$R^2 = 0.991$

From the graph $\ln q_e$ versus $\ln C_e$,

y= 2.3168x+ 1.9202

$\frac{1}{n} = 2.3168$; n =0.431

$K_F = 6.822$

D-R adsorption isotherm:

$$\ln q_e = \ln q_m - \beta \varepsilon^2$$

From the graph $\ln q_m$ versus ε^2

y= -4.4251x+6.6426

$R^2 = 0.9999$

$\beta = 4.4251$, $E = 1/(2\beta)^{1/2}$

Energy of adsorption = 0.475 Kj/ mol

$\ln q_m = 6.6426$

$q_m = 767.08$ mg/g

Fig. S7 Maximum dye adsorption capacity, q_m for CV using Freundlich and D-R adsorption isotherm

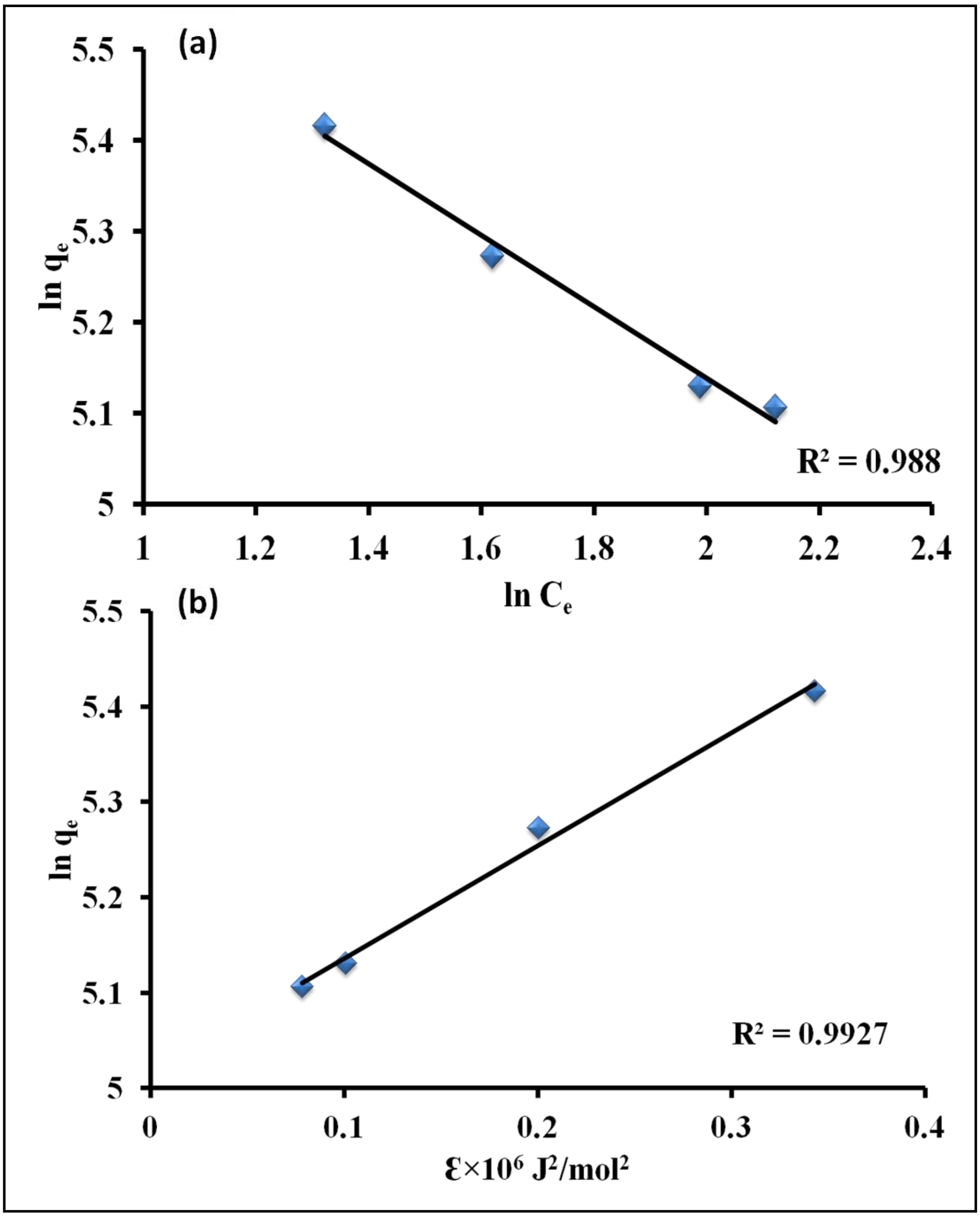

Fig. S8 (a) Freundlich adsorption isotherm (b) D-R adsorption isotherm for MB

Adsorption Isotherms for MB:

Langmuir adsorption isotherm:

$$\frac{C_e}{q_e} = \frac{1}{K_L q_m} + \frac{C_e}{q_m}$$

From the graph C_e / q_e versus q_e

$y = 0.0074x - 0.0114$

$$\text{Slope} = \frac{1}{q_m} = 0.0074$$

Maximum adsorption capacity for MB, q_m = 135.13mg/g

Fig. S9 Maximum dye adsorption capacity, q_m for MB using Langmuir adsorption isotherm

pH Value	**Dye adsorption capacity (mg/g)**	
	CV	**MB**
2	17.5	15.2
5	20.8	19.9
7	195.4	180.78
9	350.8	302.6
12	389.6	323.3

Table S1. Dye adsorption capacity of CV and MB at different pH values (2-12).

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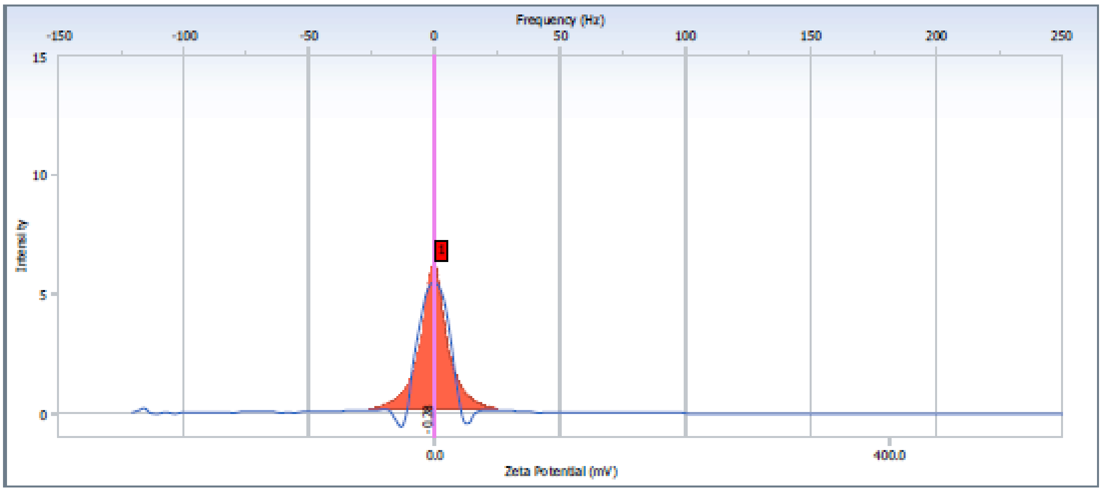
Mobility Distribution



Measurement Results

Zeta Potential	: -0.28	(mV)	Doppler shift	: -0.12	(Hz)
Mobility	: -1.575e-006	(cm^2/Vs)	Base Frequency	: 120.6	(Hz)
Conductivity	: 0.0490	(mS/cm)	Conversion Equation	: Smoluchowski	

Fig. S10 Zeta potential analysis of surface of self-assembled fibrils of IPSeX1

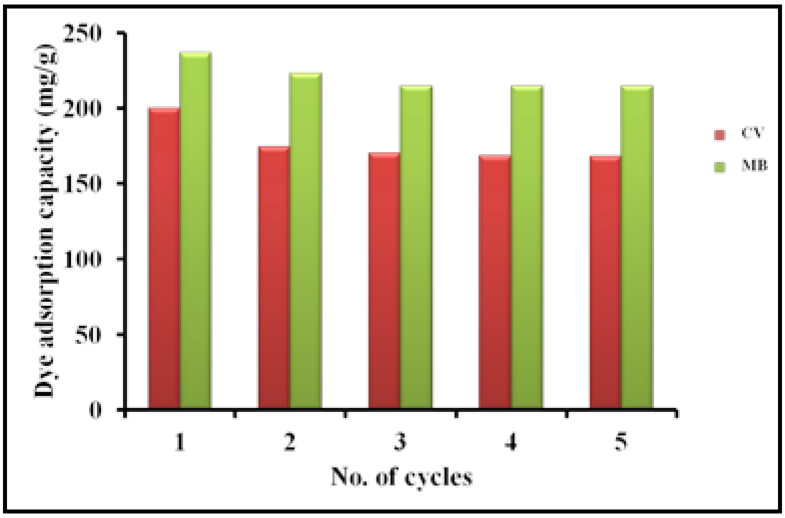


Fig. S11 Recyclability of peptide fibrils for the adsorption of CV and MB