Supporting Information

Co-assembly of Charged Complementary Peptides and their Applications as Organic Dye / Heavy Metal Ion (Pb^{2+}, Hg^{2+}) Absorbents and Arsenic (III/V) Detectors

Karabi Roy[1], Monikha Chetia[1], Ankan Kumar Sarkar[1], Sunanda Chatterjee[1*]

1, Department of Chemistry,
Indian Institute of Technology Guwahati
Guwahati, Assam, India 781039.
Email: sunanda.c@iitg.ac.in
Telephone: 0361-2583310

Table of contents

Contents **Page**

Figures

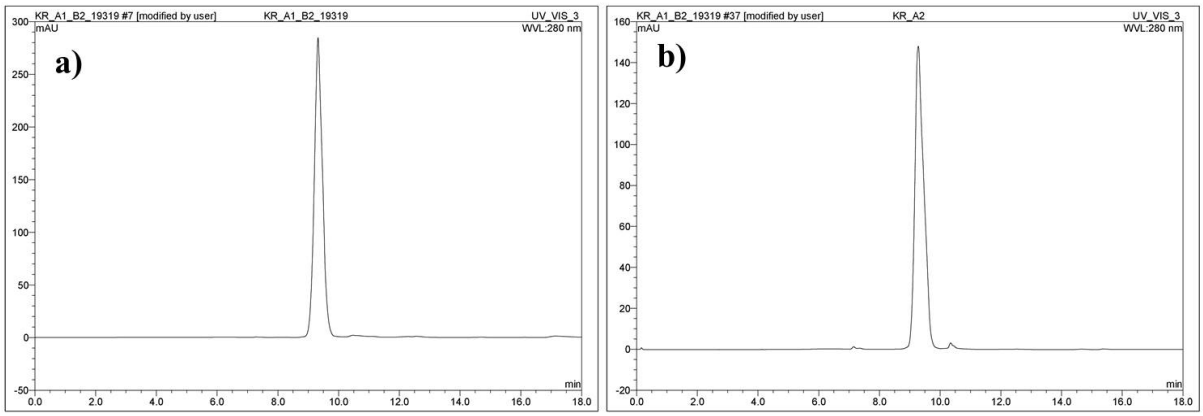

Figure S1: Analytical HPLC trace of the peptides a) A1 and b) A2

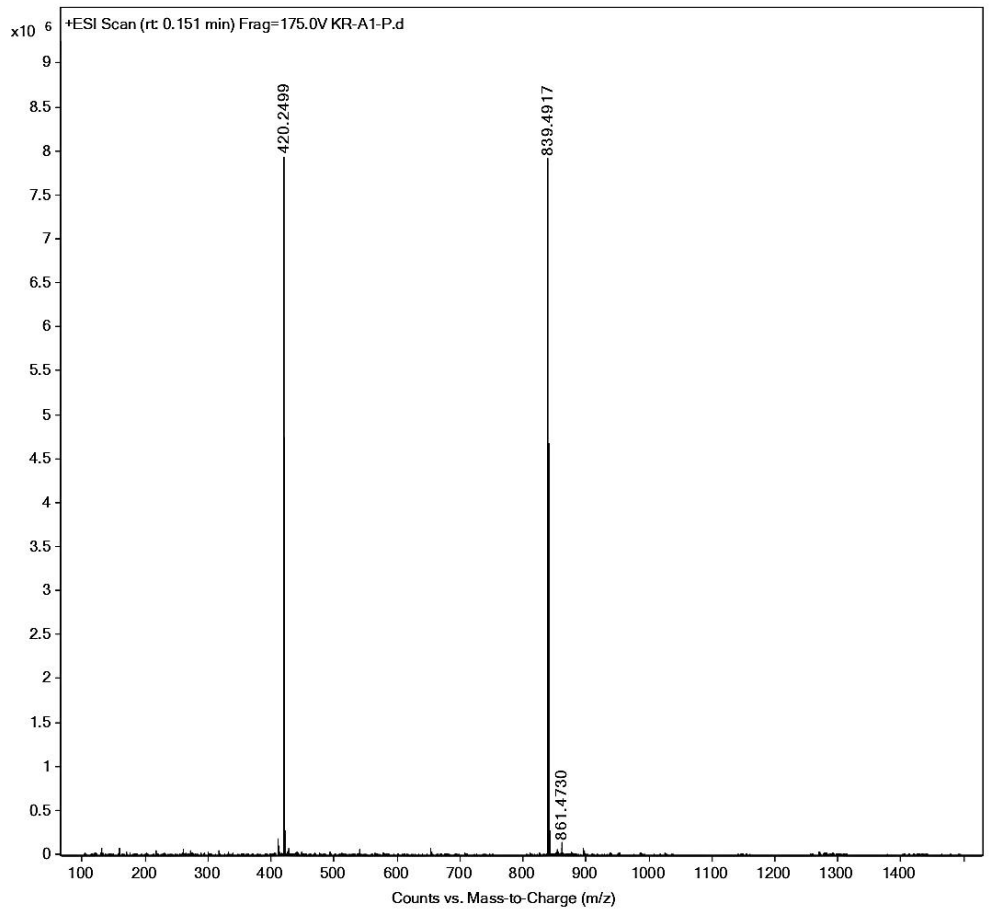

Figure S2: ESI-MS of A1.

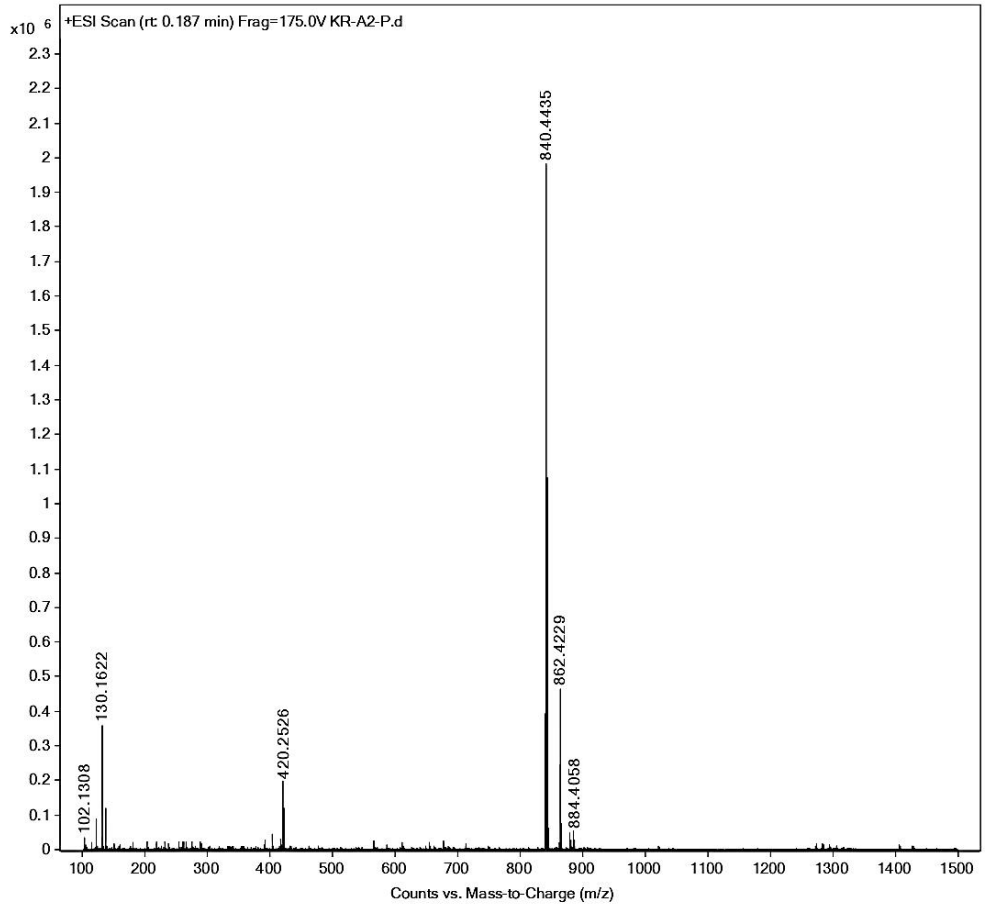

Figure S3: ESI-MS of A2.

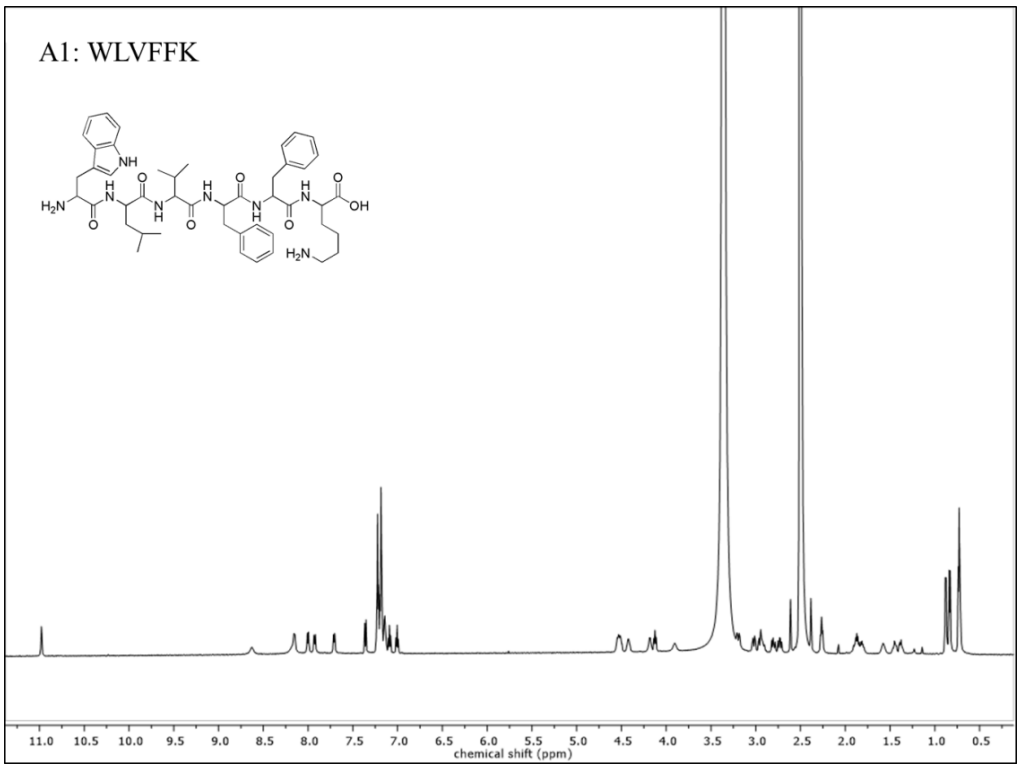

Figure S4: ^{1}H NMR spectra of A1.

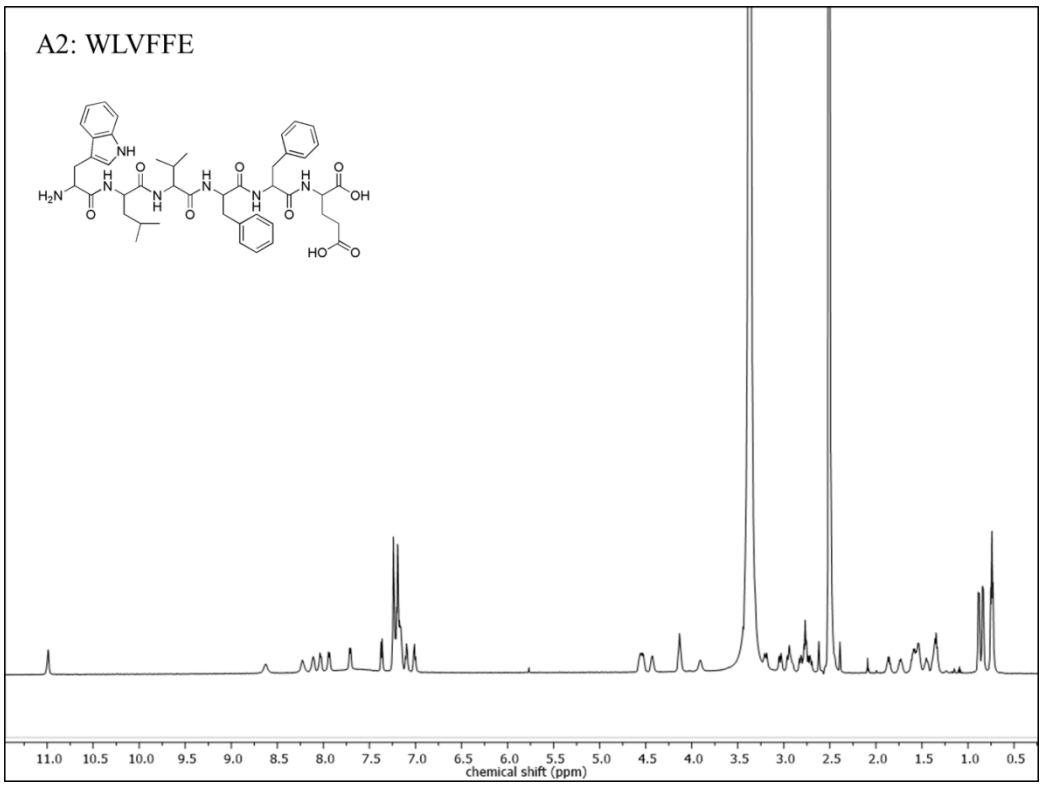

Figure S5: ^{1}H NMR spectra of A2.

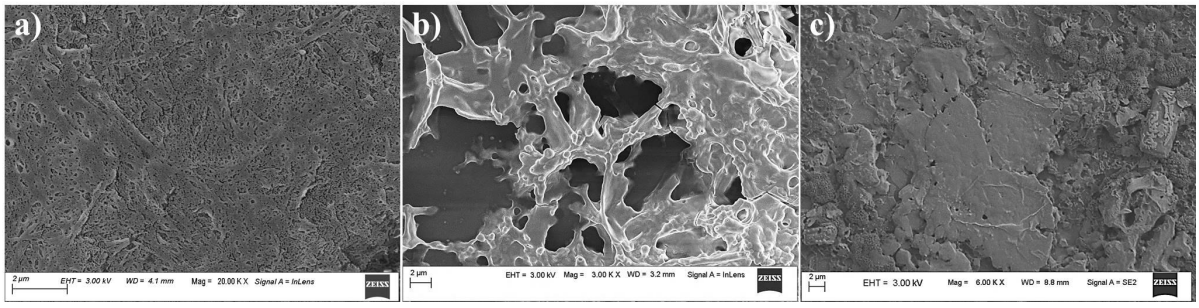

Figure S6: FESEM images in sodium phosphate buffer (pH=7.0) of a) hydrogel of A1, b) hydrogel of A1 in EtOH/phosphate buffer system at MGC and c) viscous solution of A2 at 5 mM.

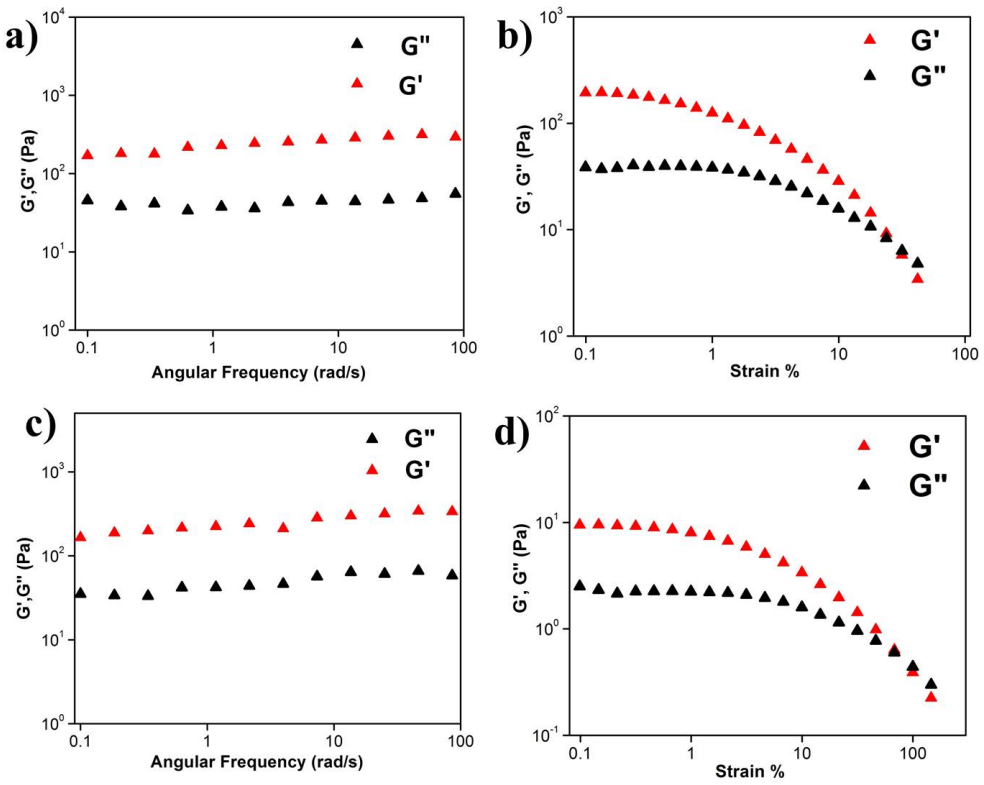

Figure S7: Angular frequency and strain dependence of the dynamic storage moduli (G′) and the loss moduli (G″) of hydrogel A1 at 0.45 % wt/v in a, b) sodium phosphate buffer; c, d) 20% EtOH/phosphate buffer system respectively.

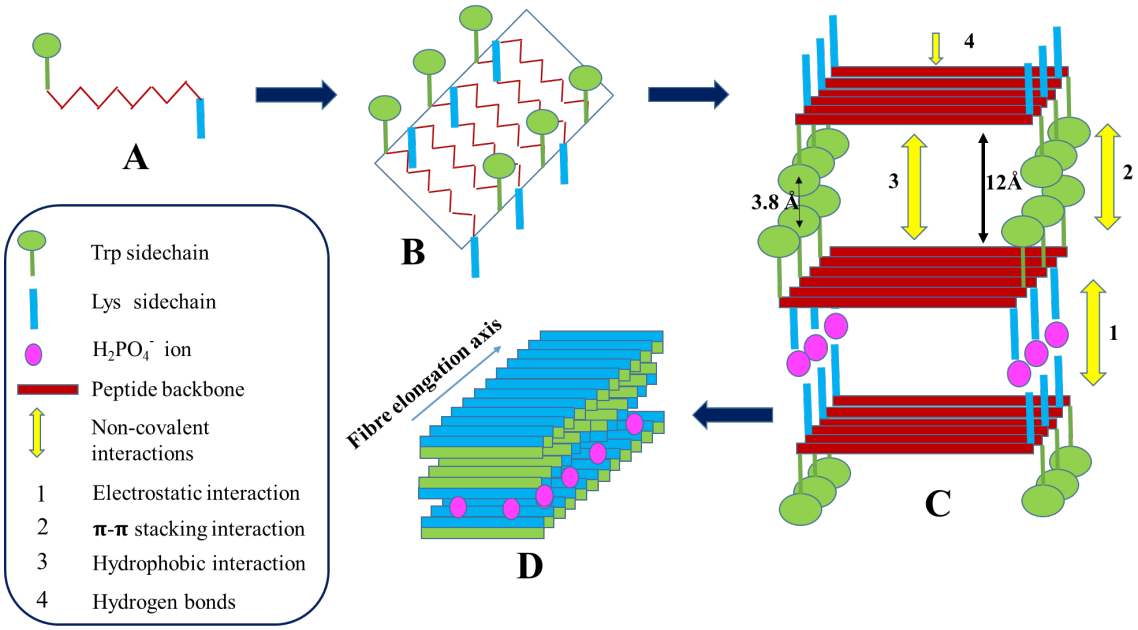

Figure S8: Schematic representation of the molecular arrangement involved in the self-assembly of A1.

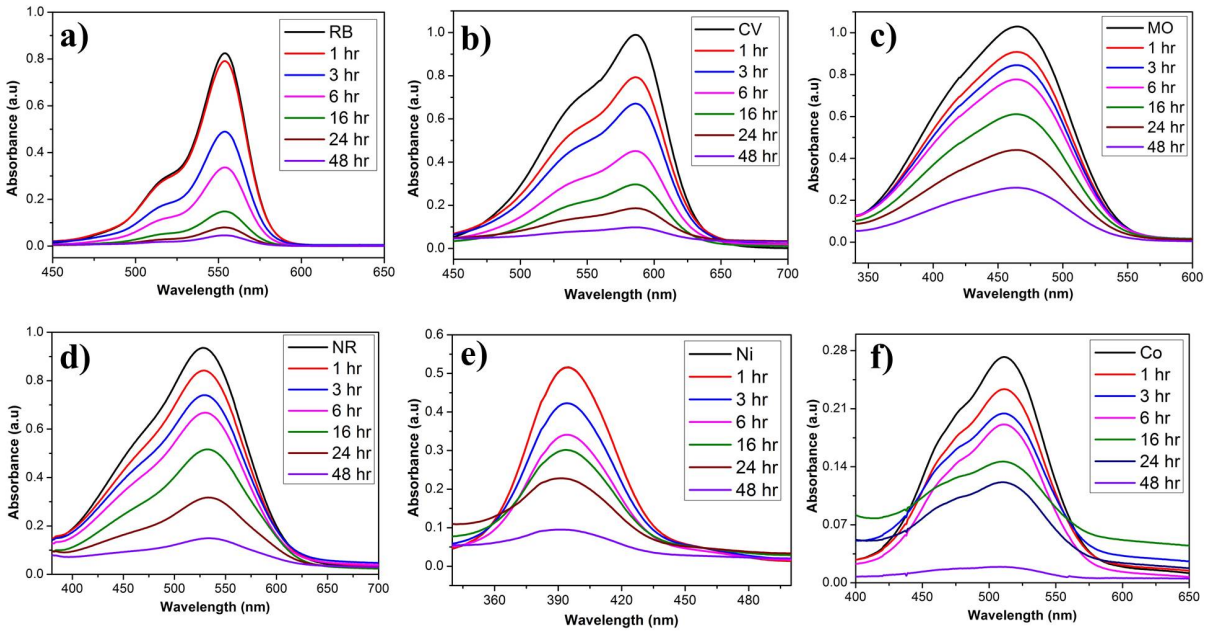

Figure S9: Dye/Metal ion absorption by A1 hydrogel a) RB b) CV c) MO d) NR e) Nickel Chloride and f) Cobalt Chloride by UV-Vis spectroscopy.

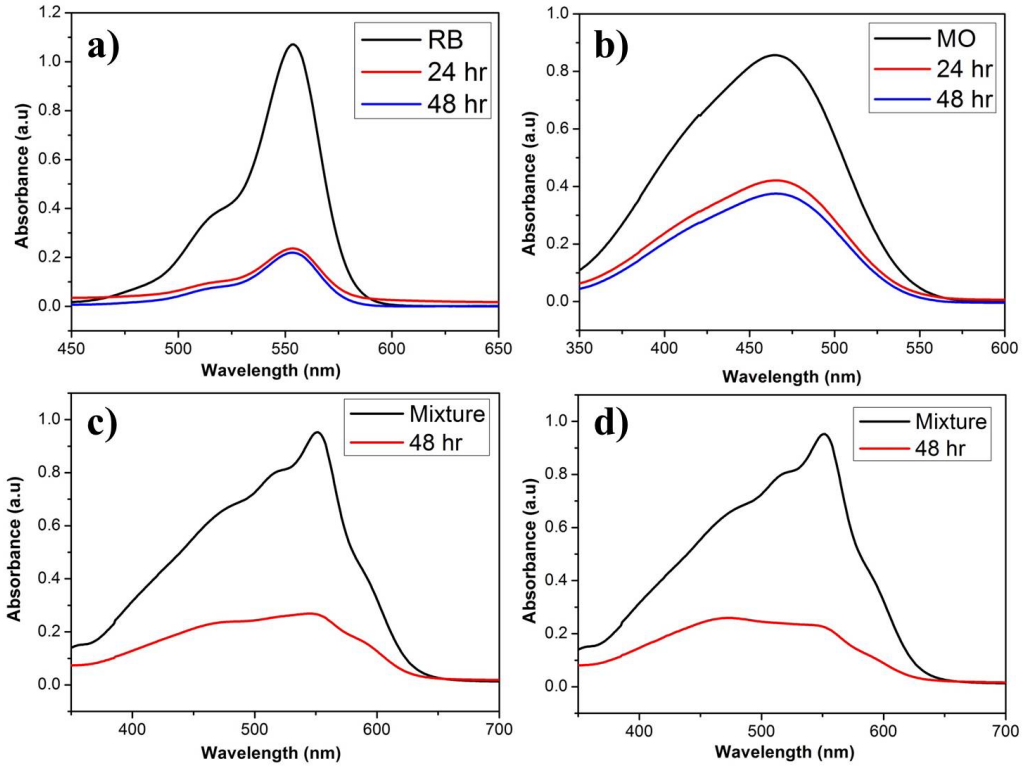

Figure S10: UV-Vis studies to show a) RB and b) MO absorbed by co-assembled A1+A2 (1:1) hydrogel. UV-Vis studies to show an all component mixture absorption by hydrogels c) A1 and d) A1+A2.

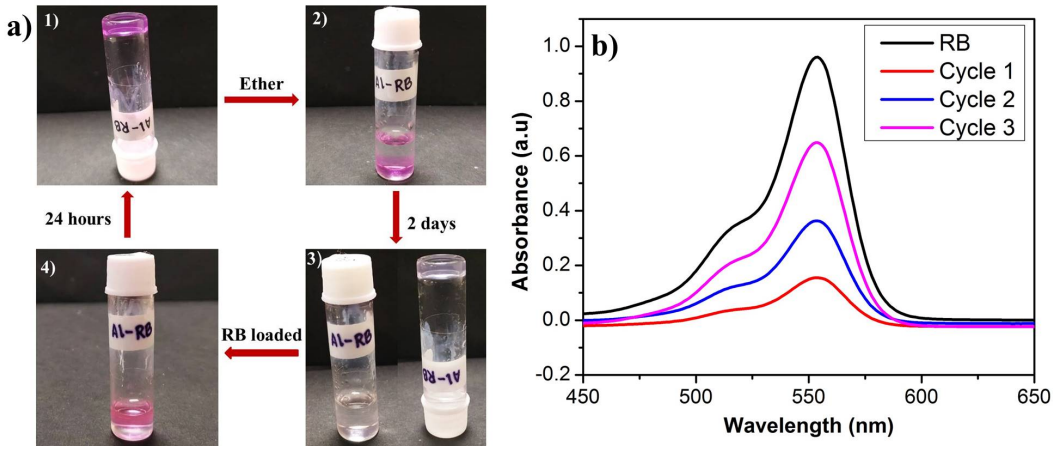

Figure S11: Reusability of hydrogel A1: a) Reusing hydrogel A1 for dye absorption and b) UV-Vis study for reusability of the hydrogel A1 with RB.

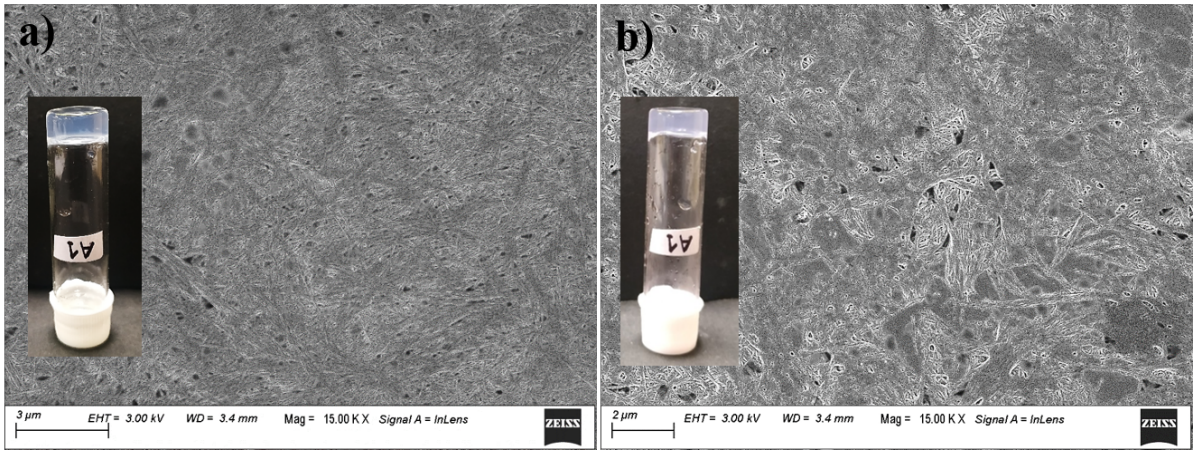

Figure S12: Morphology of hydrogel A1 a) before absorption and b) after release of the dye Rhodamine B.

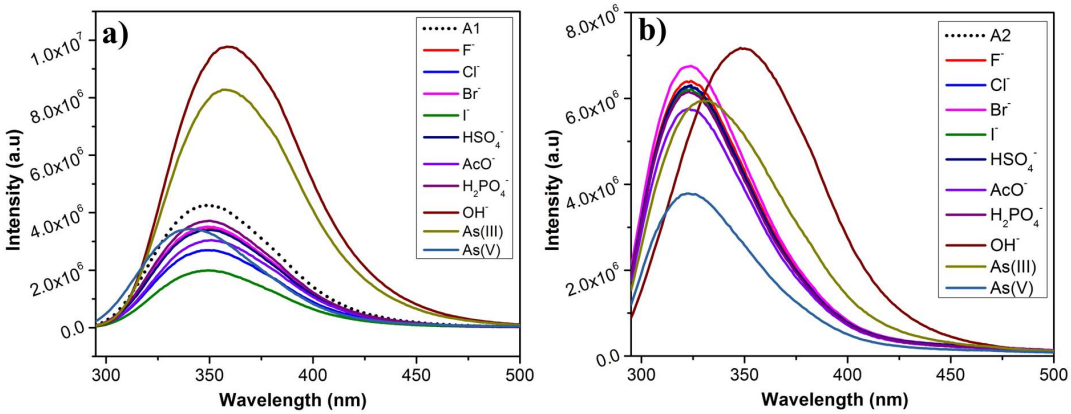

Figure S13: Sensing of anions by a) A1 and b) A2 (Anions=0.1mM, A1=0.1 mM and A2=0.1 mM).

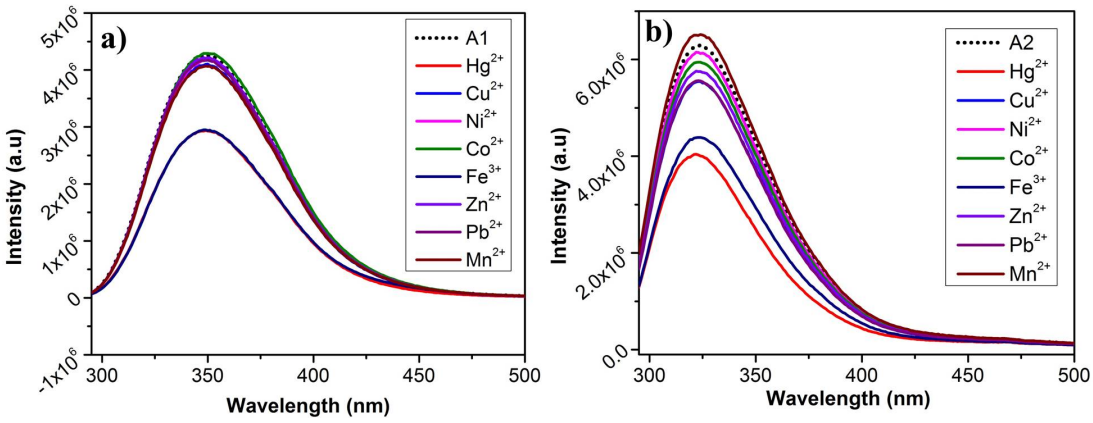

Figure S14: Sensing of metal ions by a) A1 and b) A2 (Metal ions=0.1mM, A1=0.1 mM and A2=0.1 mM).

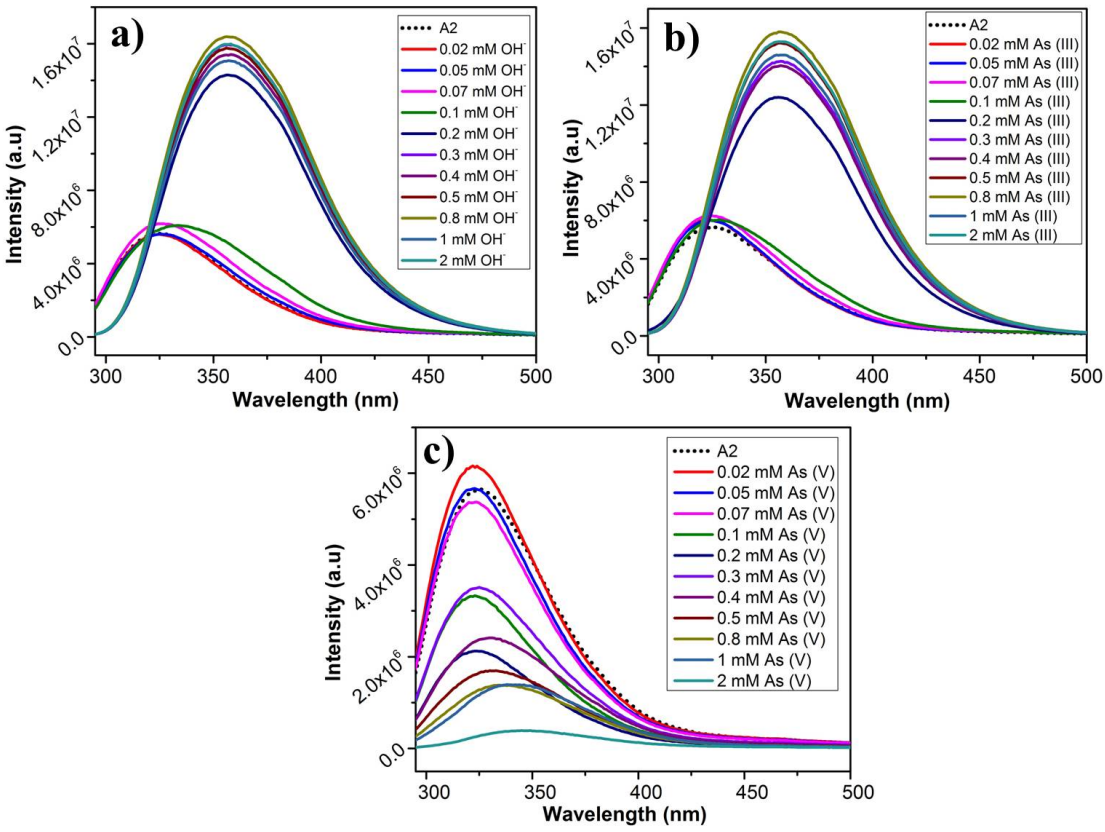

Figure S15: Anion sensing by A2: Titration of A2 with a) OH^-, b) As (III), and c) As (V).

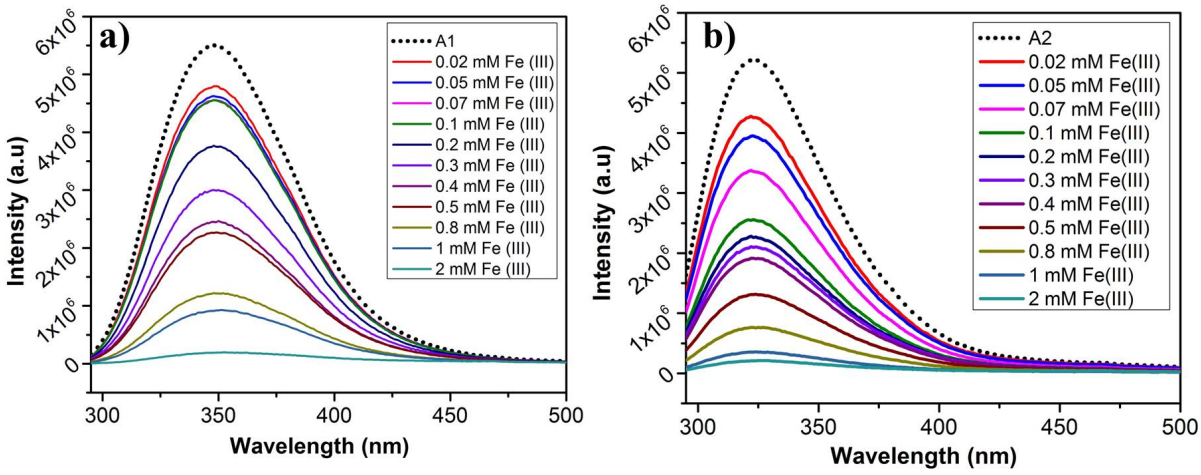

Figure S16: Fe^{3+} sensing by A1 and A2: Titration of a) A1 and b) A2 with different concentrations of Fe^{3+}.

Tables

Table S1: Table summarizing gelation properties, physical state, Minimum Gelation Concentration (MGC) and sol-gel conversion temperature (T_{gel}) of A1, A2 and various ratios of A1+A2 mixtures. (PB: sodium phosphate buffer)

Peptides	**Solvent system**	**MGC**	**T_{gel} (°C)**	**State**
A1	PB (pH=7.0)	0.20 %w/v	60	Transparent
A1	PB (pH=7.0)+ Ethanol	0.20 %w/v	54	Translucent
A2	PB (pH=7.0)	-	-	Viscous solution
A1+A2	PB (pH=7.0)	1 mg each in 0.5 ml (0.40%w/v)	56	Translucent
A1+A2	PB (pH=7.0)	1+ 0.5 mg in 0.5 ml (0.30%w/v)	52	Translucent
A1+A2	PB (pH=7.0)	1+ 2 mg in 0.5 ml (0.60%w/v)	-	Viscous solution
A1+A2	PB (pH=7.0)	1+ 3 mg in 0.5 ml (0.80%w/v)	-	Solution

Table S2: Interplanar distances observed from the PXRD in A1, A2, A1 xerogel, 1:0.5 and 1:1 co-assembled xerogels of A1+A2.

	Peak 1	Peak 2	Peak 3	Peak 4
A1	2θ=7.64°, d=11.56 Å	2θ=23.16°, d=3.84 Å	-	-
A2	2θ=7.82°, d=11.29 Å	2θ=22.86°, d=3.88 Å	-	-
A1 (xerogel)	-	-	2θ=7.20°, d=12.27 Å	2θ=23.12°, d=3.84 Å
A1+A2 (1:0.5) (xerogel)	-	-	2θ=7.02°, d=12.58Å	2θ=22.92°, d=3.87 Å
A1+A2 (1:1) (xerogel)	-	-	2θ=7.12°, d=12.40 Å	2θ=25.02°, d=3.55 Å

Table S3: Percentage of RB absorbed by hydrogel in three cycles

No. of Cycles	RB absorbed (%)
Cycle 1	88.95
Cycle 2	73.80
Cycle 2	52.90

Table S4: Dependence of absorption of Hg^{2+} and Pb^{2+} by A1 hydrogel on the counter anions

Salts	**Loaded (mg/L)**	**Conc. of Pb^{2+} /Hg^{2+} in supernatant (mg/L)**	**Conc. of Pb^{2+} /Hg^{2+} absorbed (mg/L)**	**% absorbed**
Lead chloride	20	2.48	17.52	87.60
Lead acetate	20	2.93	17.07	85.35
Lead nitrate	20	2.61	17.39	86.95
Mercury acetate	100	37.7	62.30	62.30
Mercury chloride	100	29.9	70.10	70.10