Supporting Information

Stimuli responsive designer supramolecular polymer gel

M. Douzapau,[a] Srayoshi Roy Chowdhury,[a] Surajit Singh,[a] Olamilekan Joseph Ibukun,[a] and Debasish Haldar*[a]

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur -741246, West Bengal, India.

Fax: (+)913325873020; Tel: +913325873119;

Corresponding Author E-mail: deba_h76@yahoo.com; deba_h76@iiserkol.ac.in (D. H.)

Table of contents

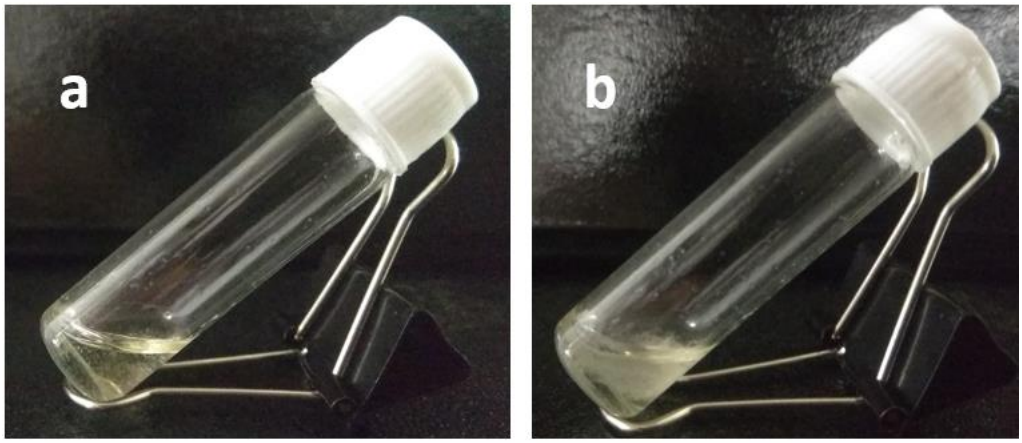

Figure S1: Images of (a) Compound **1** and α-CD in DMSO-H_2O showing no formation of gel; (b) Compound **1** and γ-CD in DMSO-H2O showing no formation of gel.

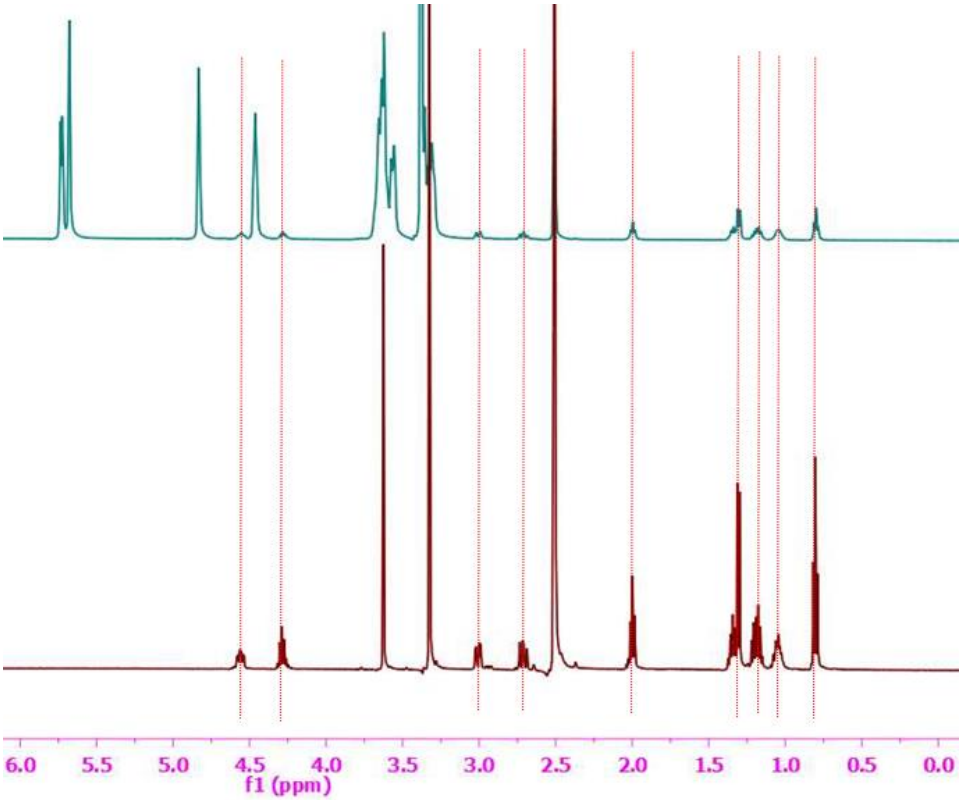

Figure S2: Part of the ^{1}H-NMR spectra of compound **1** and β-CD Gel in DMSO-D_6, showing no change of compound 1 aliphatic peaks with addition of β-CD.

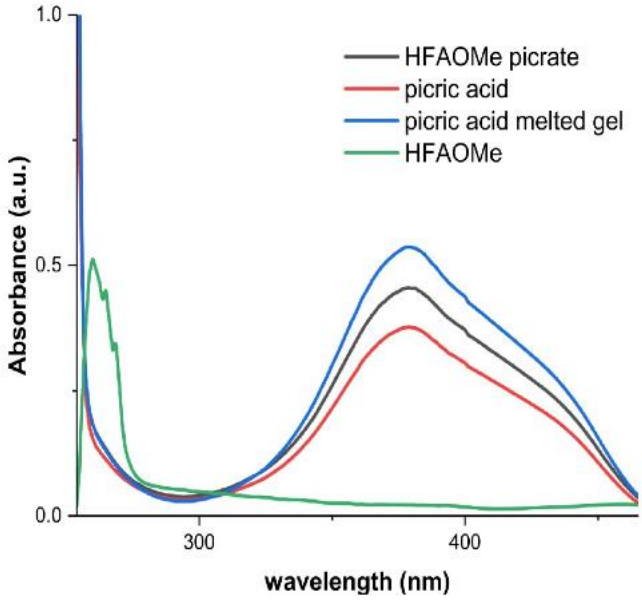

Figure S3: Absorption spectra of compound **1** (green), picric acid (red), compound **1**-picric acid (black), picric acid melted gel of compound **1** and β-CD in DMSO-H_2O.

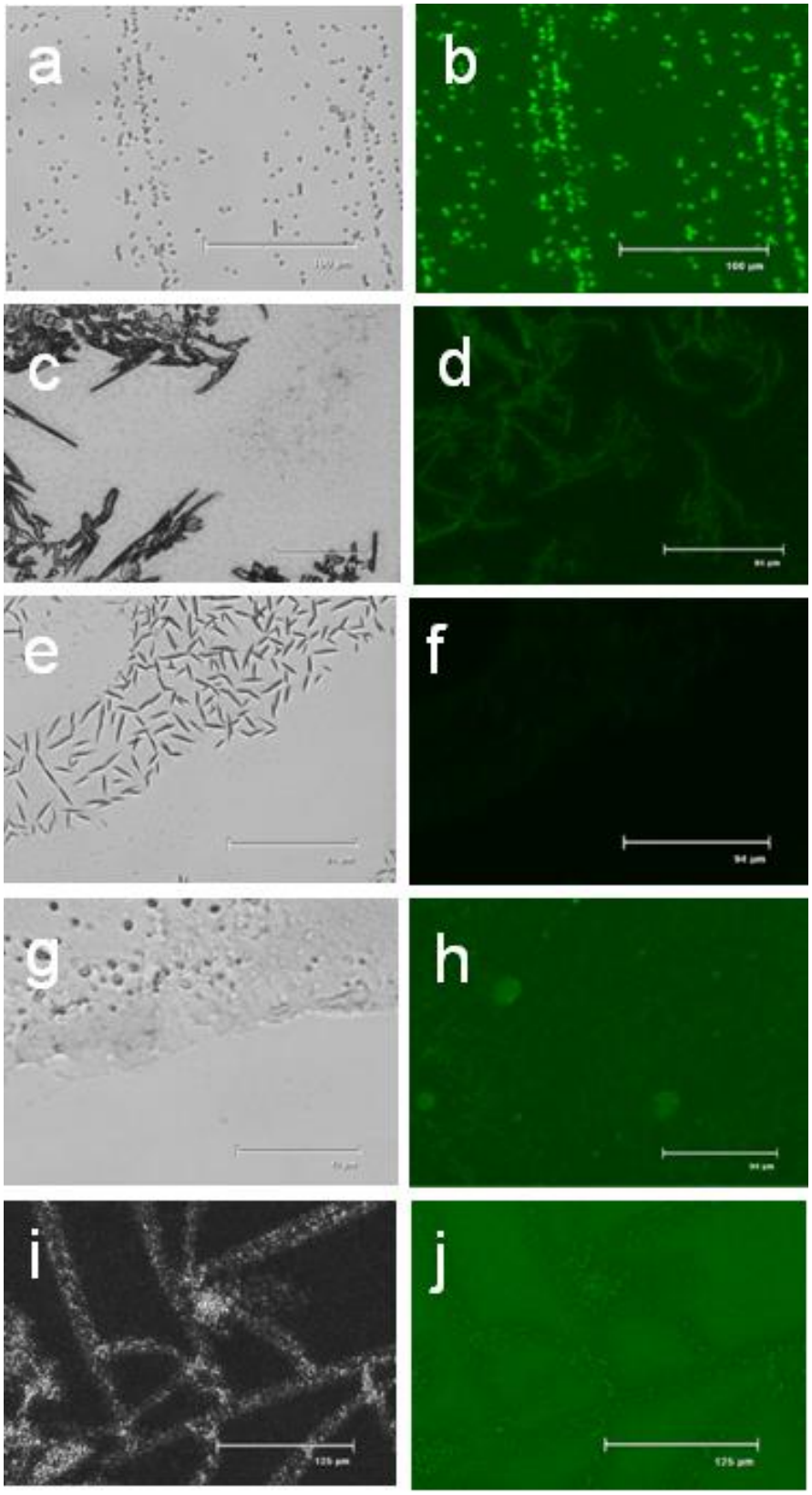

Figure S4: Fluorescence microscopy images of Compound **1** under (a) white light (b) greenlight, Picric acid under (c) white light (d) green light, Compound **1** + Picric acid under (e) white light (f) green light, Compound **1** + β-CD under (g) white light (h) green light, Picric acid melted Compound **1** + β-CD gel under (i) white light (j) green light.

Empirical formula	C_{19} H_{28} N_2 O_4
Formula weight	348.44
Temperature/K	100
Crystal system	monoclinic
Space group	*P 21*
a/Å	11.1442(6)
b/Å	4.8587(3)
c/Å	17.6234(10)
α/°	90
β/°	96.473(6)
γ/°	90
Volume/Å^3	974.99(10)
Z	2
ρ_{calc}g/cm^3	1.221
μ/mm^{-1}	0.085
F(000)	376
Crystal size/mm^3	0.01 × 0.02 × 0.03
Radiation	CuKα (λ = 0.71073)
2Θ range for data collection/°	41.8 to 25.0
Flack parameter	-1.2(7)

Table S1: Crystal data and structure refinement for compound 1.

Experimental Section:

The reported peptides were synthesized by conventional solution-phase methods using racemisation free fragment condensation strategy. For N-terminal protection, caproic acid used and the C- terminal was protected as a methyl ester. Coupling was mediated by dicyclohexylcarbodiimide /1-hydroxybenzotriazole (DCC/HOBt). The product was purified by column chromatography using the silica (100-200-mesh size) gel as a stationary phase and n-hexane-ethylacetate mixture as eluent. The final compounds were fully characterized by 400MHz ^{1}H NMR spectroscopy, ^{13}C NMR spectroscopy, mass spectrometry and IR Spectroscopy.

The synthetic procedure of compound 1

The synthetic procedures are in the manuscript.

Characterization of Compound 1.

^{1} H NMR (500 MHz, DMSO-d^{6} , δ ppm): 8.45-8.44 [1H, d, NH], 7.98-7.97 [1H, d, NH], 7.26-7.18 [5H, m, ArH], 4,59-4.53 [1H,m, Phe CαH], 4.32-4.24 [1H, m, Ala CαH], 3.63 [3H, s, OMe-H], 3.03-2.99 [1H, m, Phe-CβH], 2.74-2.69 [1H, m, Phe-CβH], 2.01-1.98 [2H, t, Aliphatic-H], 1.37-1.30 [4H, m, Aliphatic-H].1.22-1.16 [3H, m, Ala-CβH], 1.08-1.03 [2H, m, Aliphatic-H], 0.82-0.79 [3H, t, Aliphatic-H]. ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm): 170.04, 170.3, 170.1, 130.7, 120.9, 120.8, 120.7, 50.4, 50.3, 40.8, 30.9, 30.1, 20.6, 20.2, 10.8, 10.4 ESI-MS (MeOH): m/z (Calc): C19H28N2O4Na [M+Na]+ 371.44; found: 371.08. Yield: 70%. White colour solid.

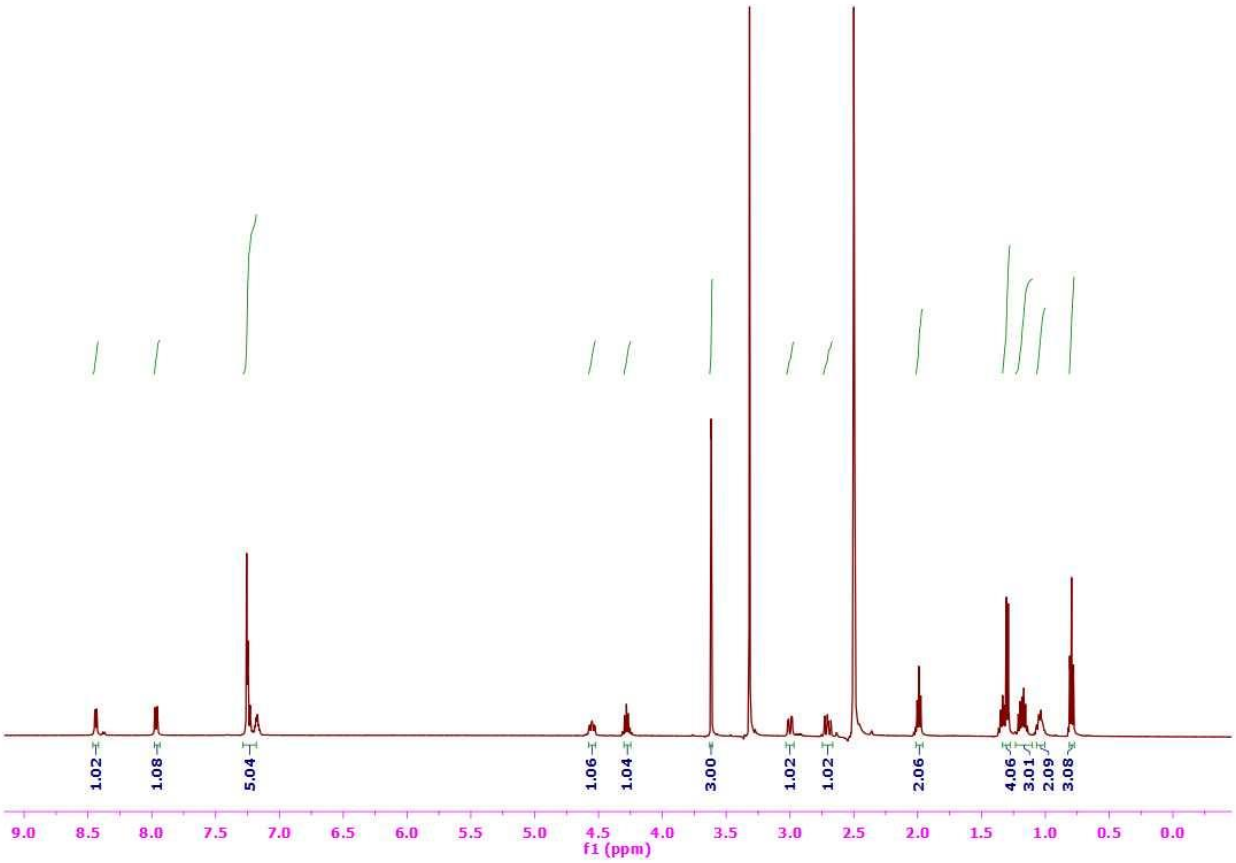

Figure S5: [1]H NMR (500MHz, DMSO-d_6, δ in ppm, 298K) spectra of compound **1**.

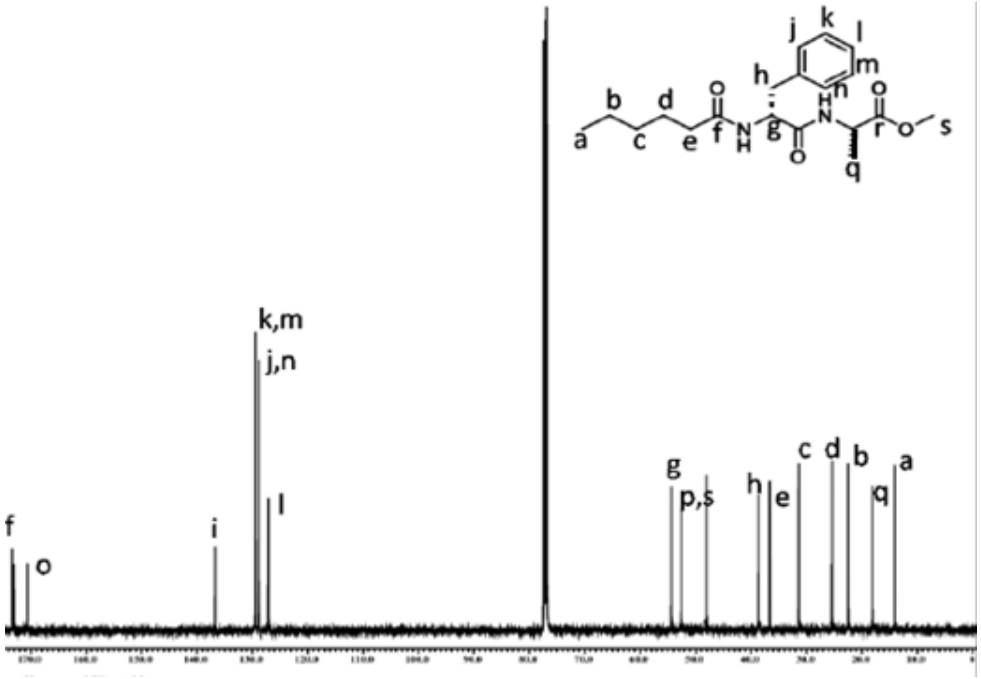

Figure S6: **[13]C** NMR (125 MHz, DMSO-d_6, δ in ppm, 298K) spectra of compound **1**.

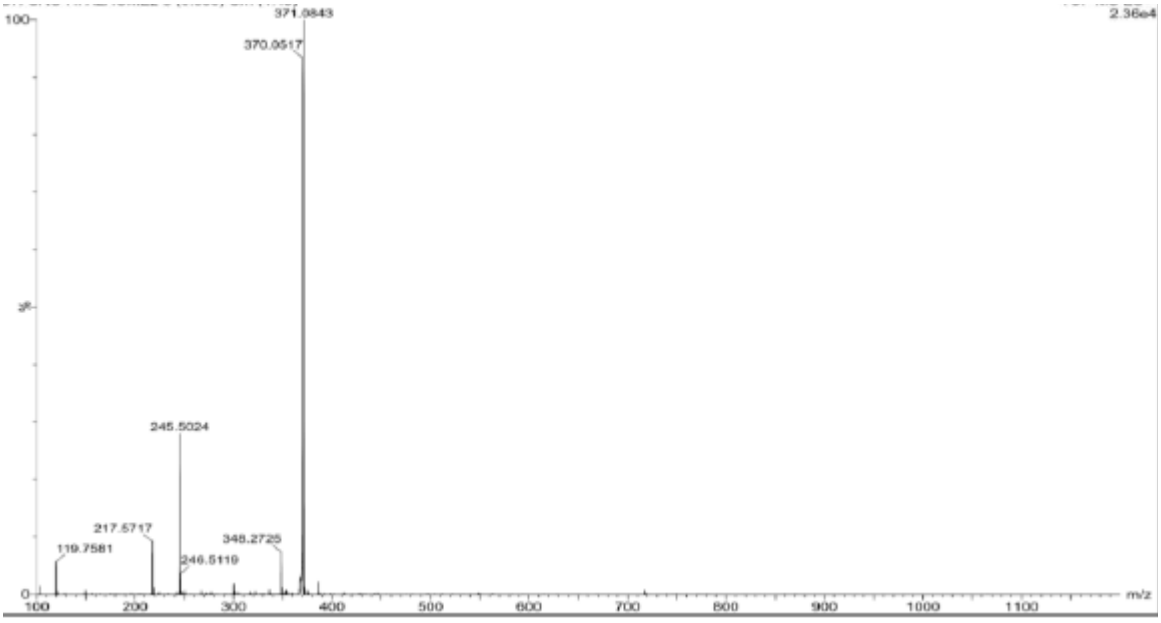

Figure S7: Mass spectra of Compound **1**.

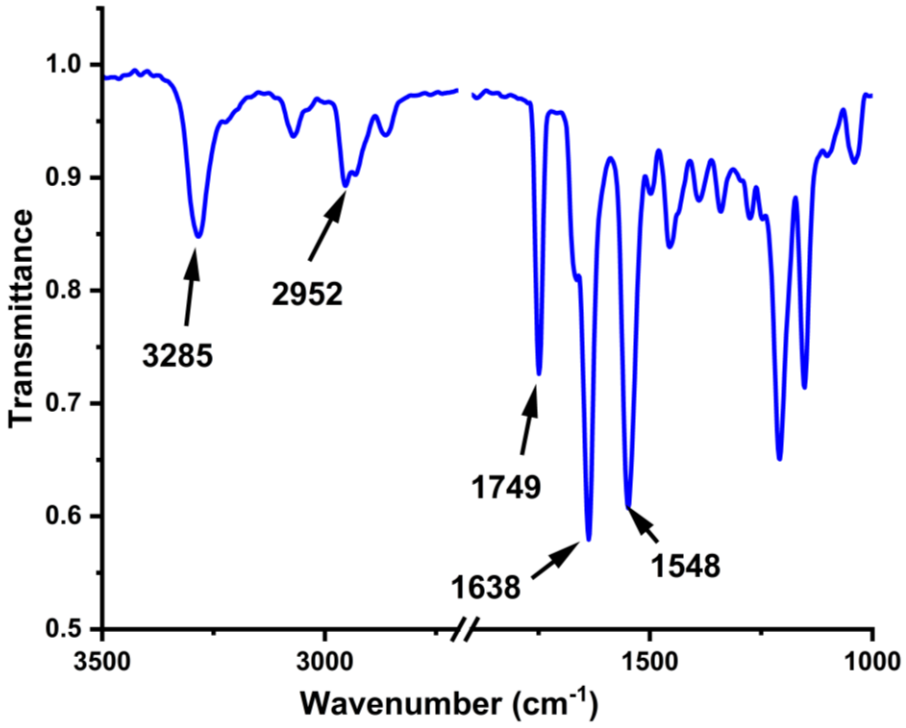

Figure S8: FT-IR spectra of compound **1**.