Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

for

Blue-emissive two-component supergelator with aggregation induced enhanced emission

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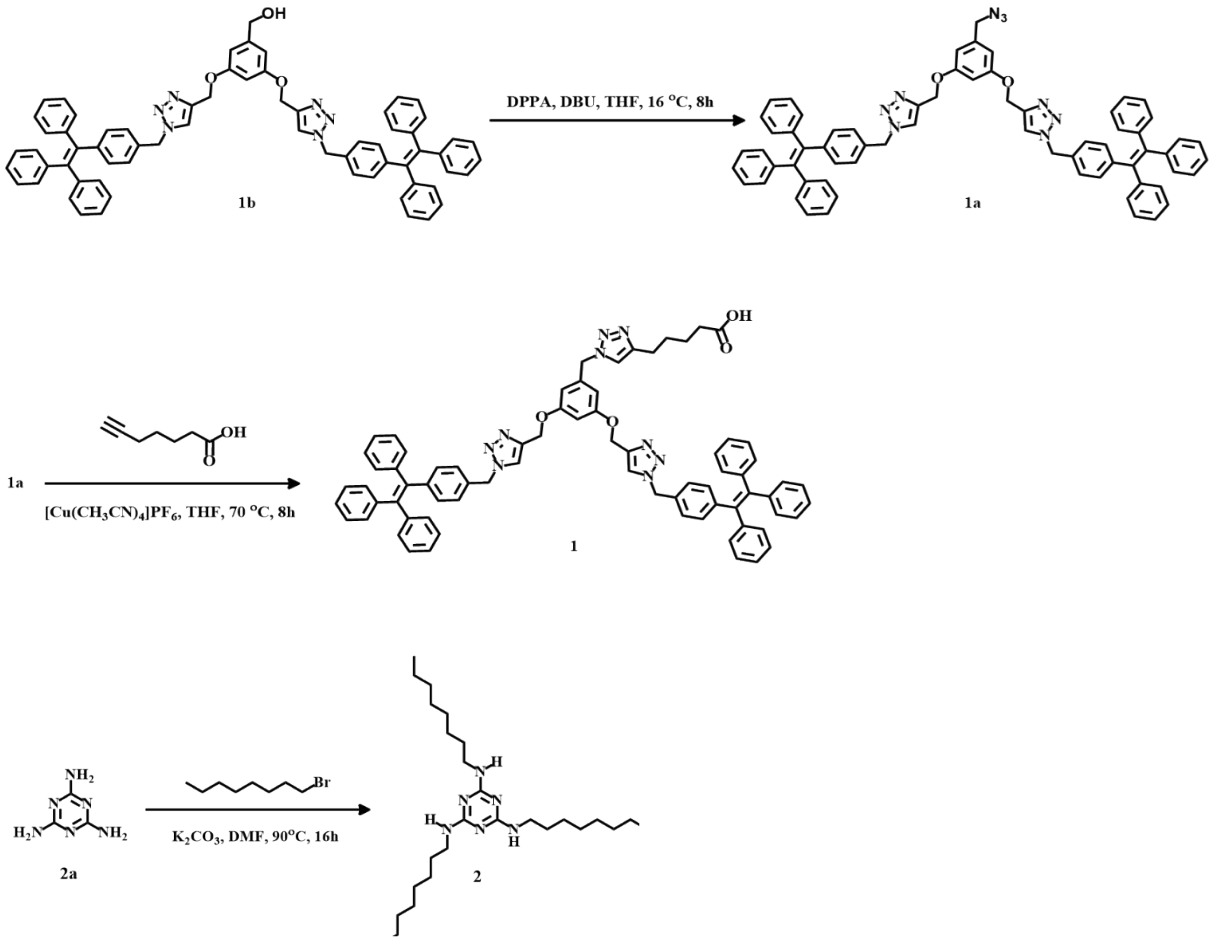
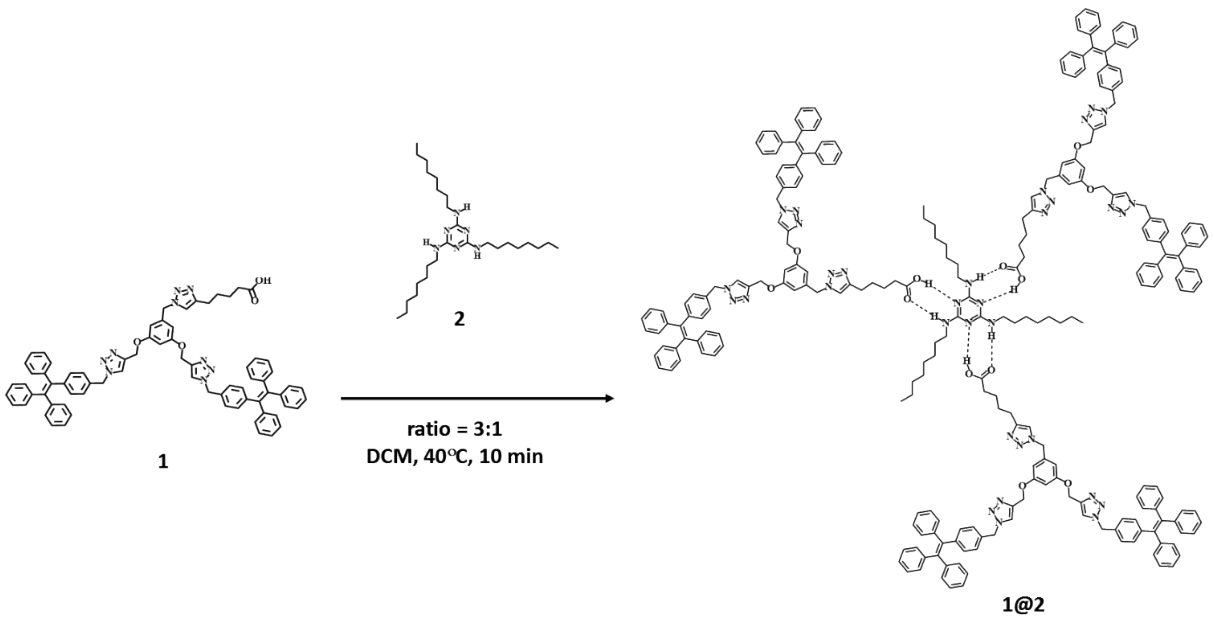
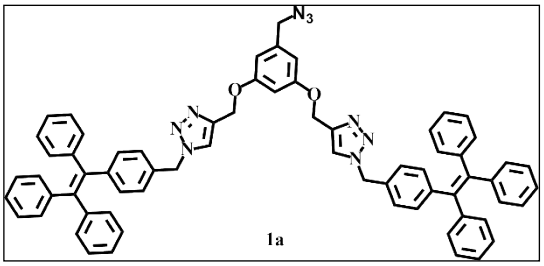


Scheme S1: Scheme for the synthesis of **1** and **2**.



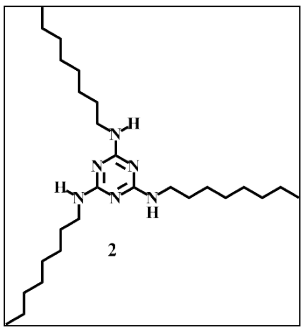
Scheme S2: Scheme for the synthesis of **1@2**.

Synthesis of 1a: To a solution of **1** (4.2 g, 4.23 mmol) in 50 ml anhydrous THF was added 0.89 mL (6.35 mmol) of DBU under N_2 atmosphere and stirred for 30 min at room temperature. To this mixture 1.08 ml (5.90 mmol) of DPPA was added and heated to 65 °C for 16 h. The reaction completion was confirmed by TLC, quenched with saturated NH_4Cl solution, and extracted with DCM. The separated organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude product. The crude was purified by silica column by using DCM containing 0.50 % MeOH as an eluent to afford the expected product **1a** as colourless solid (83.0 %). M.P. = 248.0 °C; TLC [MeOH(2%)/DCM]; R_f = 0.45; ^{1}H NMR (500 MHz, $CDCl_3$), δ (ppm) = 7.494 (s, 2H), 7.122 - 7.117 (m, 18 H), 7.074 - 7.018 (m, 20 H), 6.648 (s, 1H), 6.095 (d, J = 1.5 Hz), 5.456 (s, 4H), 5.198 (s, 4H), 4.283 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_{3)}$, δ (ppm) = 54.01, 54.70, 159.73, 144.51, 144.02, 143.41, 143.34, 143.23, 141.81, 139.99, 137.88, 132.23, 132.01, 131.27, 131.25, 131.23, 127.78, 127.75, 127.68, 127.49, 126.66, 126.63, 126.61, 122.70, 107.51, 101.73, 62.24, 54.70, 54.02. HRMS-ESI m/z for $C_{67}H_{53}N_9O_2$ $[M+H]^+$: 1015.4322 (calcd.); 1016.4406 (expt.).



1a

Synthesis of 2: A 250 mL two-neck round bottom flask equipped with a magnetic bead was charged with 1g of melamine and dried under dynamic vacuum at room temperature using schlenck line followed by which the flask was flushed with inert nitrogen gas. 60mL of dry DMF was added to the flask under inert conditions and was vigorously stirred for 5 minutes followed by the slow addition of NaH under nitrogen gas flow and was stirred for 15 minutes. 4.3mL of 1-Bromooctane was added slowly and the reaction mixture was stirred for 16 hours. The reaction progress was monitored using TLC and upon completion of reaction, NaH was quenched using slow addition of water to the ice-cold reaction mixture. The resultant mixture was then extracted with ethyl acetate and the organic layer was dried over sodium sulfate and the crude mixture obtained was purified using silica gel column chromatography with 10% EtOAc in petroleoum ether to yield the desired product as white solid [yield=40%]. R_f = 0.3[EtOAc: Pet-Ether 10:90]; M.P. = 56 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 0.88-0.90 (m, 9H), 1.28-1.32 (m, 30H), 1.53-1.56 (m, 6H), 3.34 (s, 6H), 4.85 (broad singlet, 3H). ^{13}CNMR *(*125 MHz, CDCl3*), δ (*ppm*)* = 1.01, 14.07, 22.65, 26.96, 29.26, 29.35, 29.90, 31.84, 40.67, 166.20.; LRMS (ESI) m/z value for $C_{27}H_{54}N_6$ = 462.44 (calcd.) 463.5 (expt.)



2

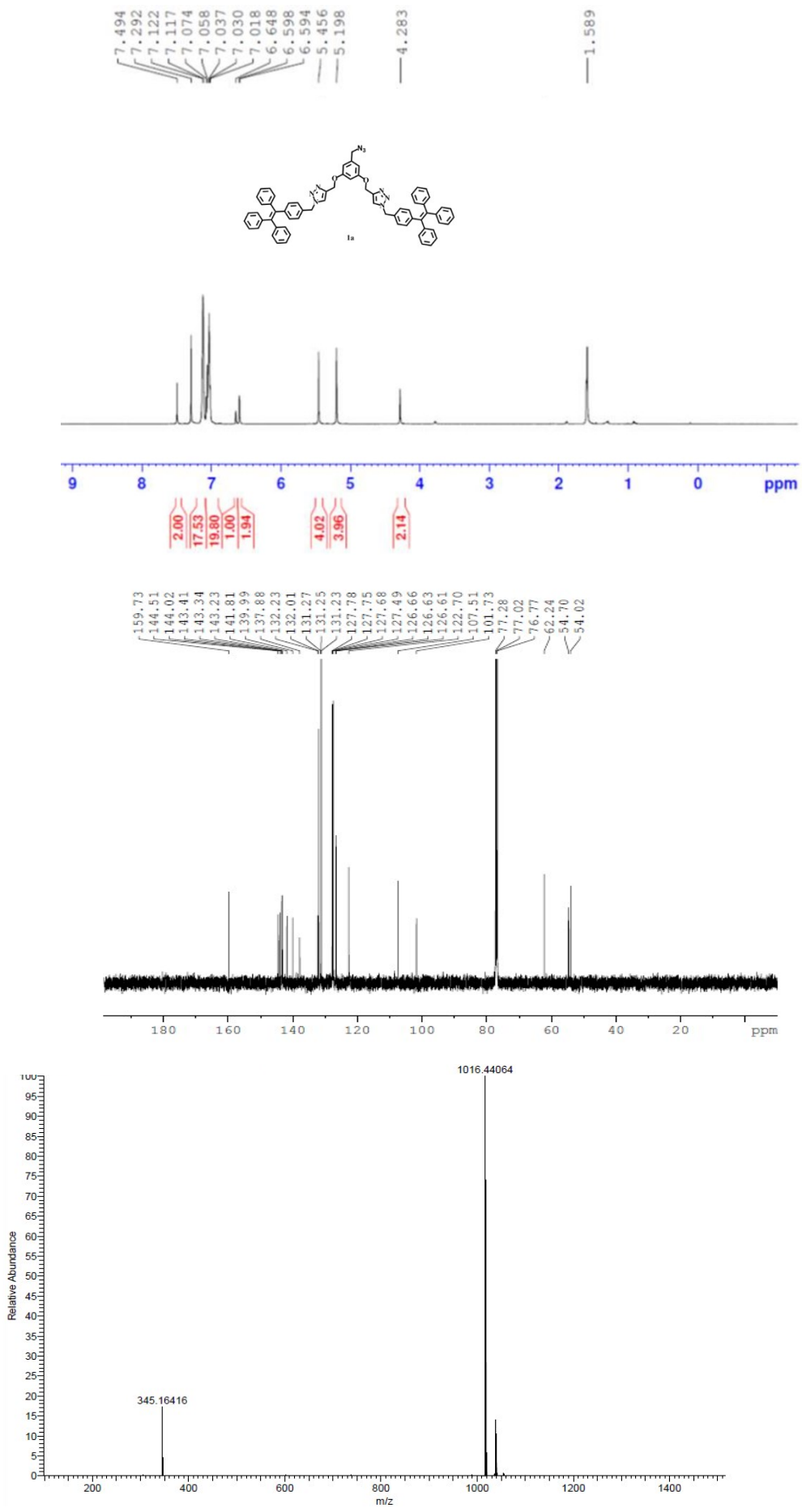


Figure S1: ^{1}H-NMR (above), ^{13}C-NMR (middle) and ESI-MS (bottom) spectra of **1a**.

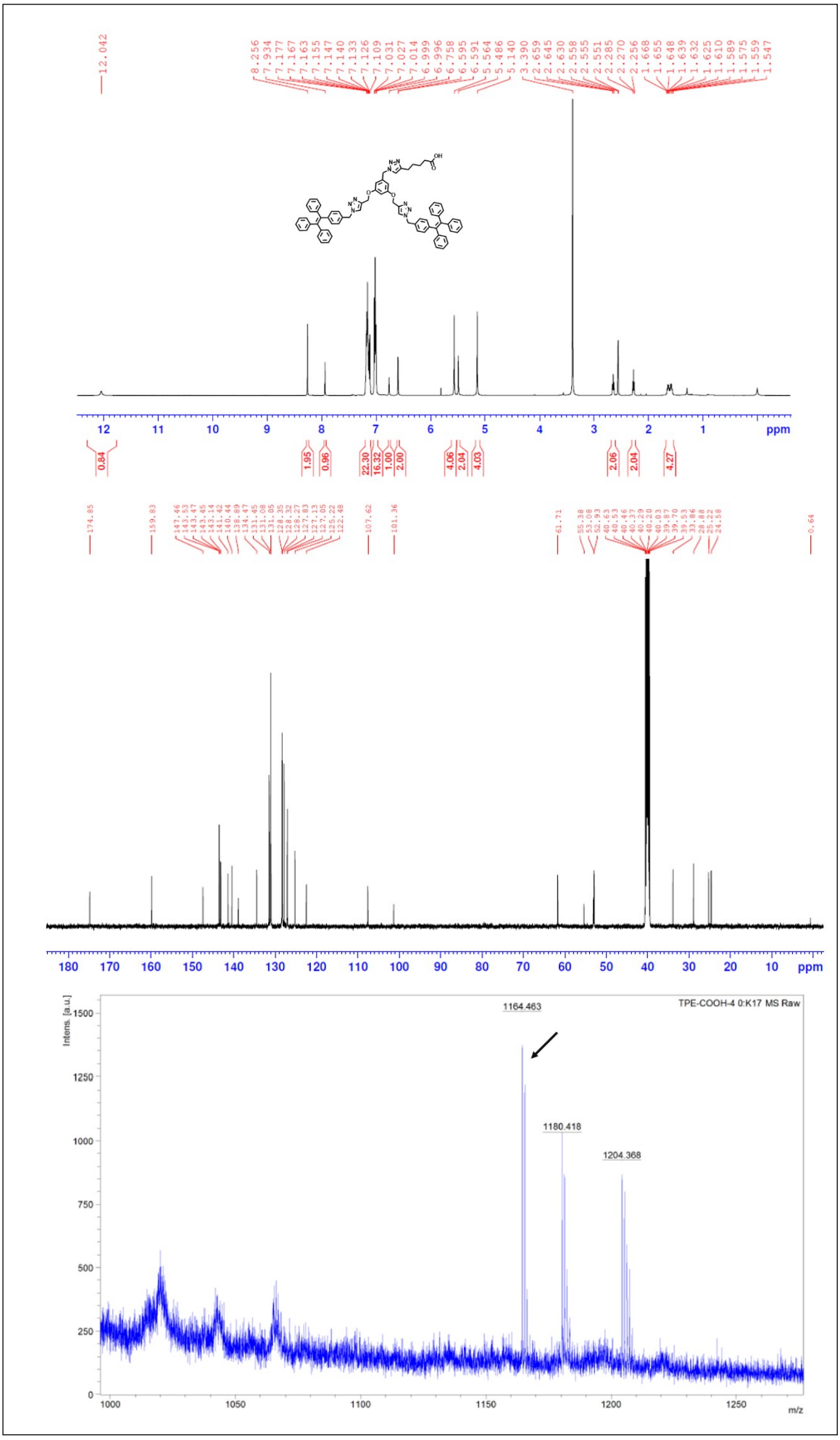


Figure S2: ^{1}H-NMR (above), ^{13}C-NMR (middle) and MALDI-ToF (bottom) spectra of **1**.

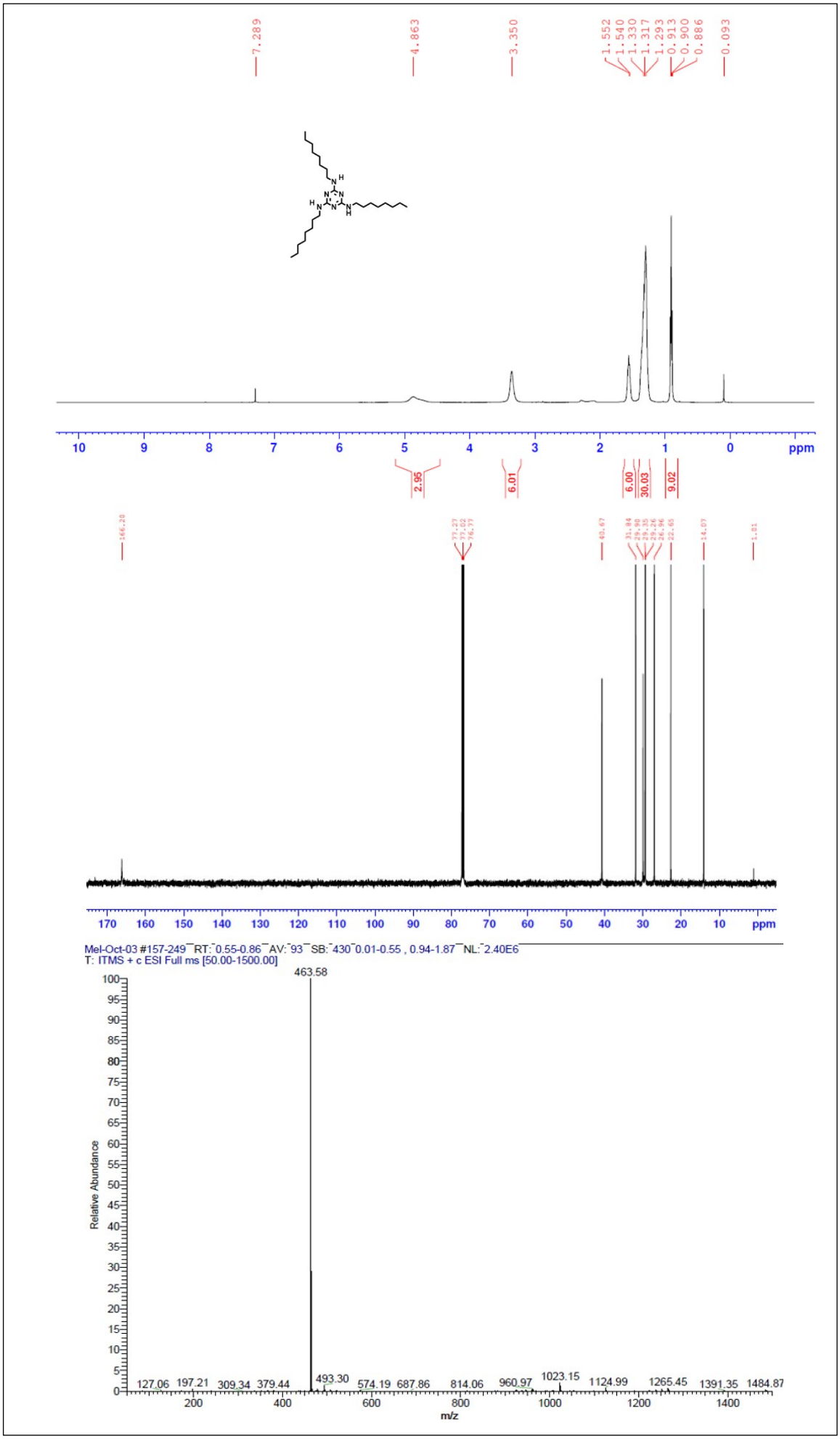


Figure S3: ^{1}H-NMR (above), ^{13}C-NMR (middle) and ESI-MS (bottom) spectra of **2**.

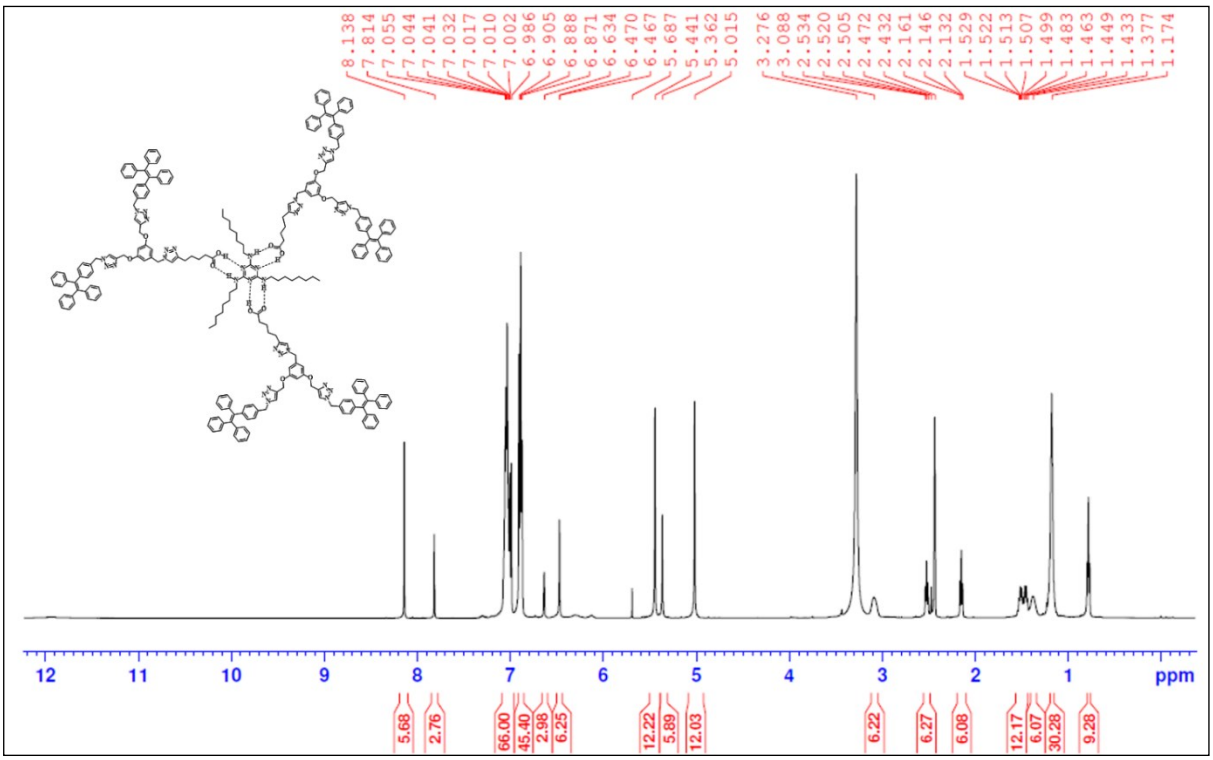


Figure S4: ^{1}H-NMR spectrum of **1@2**.

Figure S5. Photograph of the gel obtained without pre-forming **1@2** complex.

a) b)

Figure S6. Photographs of the gels of 1:1 and 1:2 molar ratios **1** and **2**, respectively.

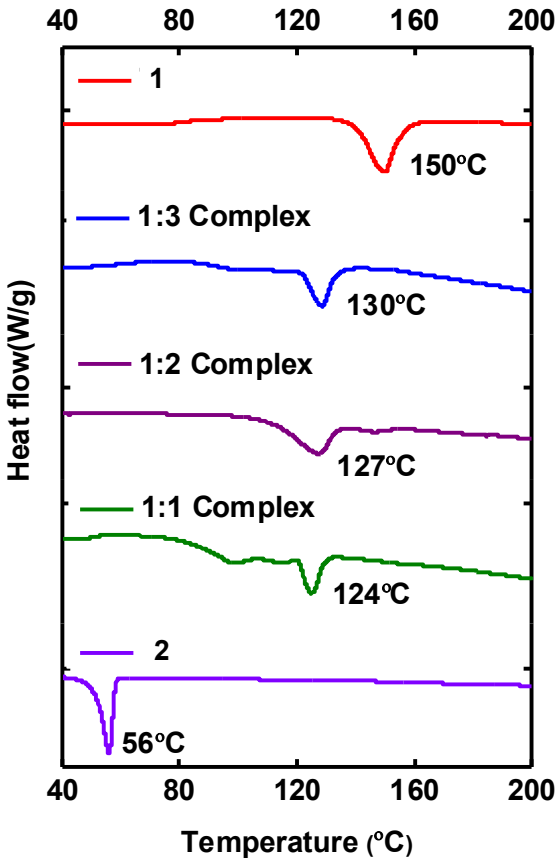


Figure S7. DSC thermograms of 1:3, 1:1 and 1:2 molar ratios of **1@2**.

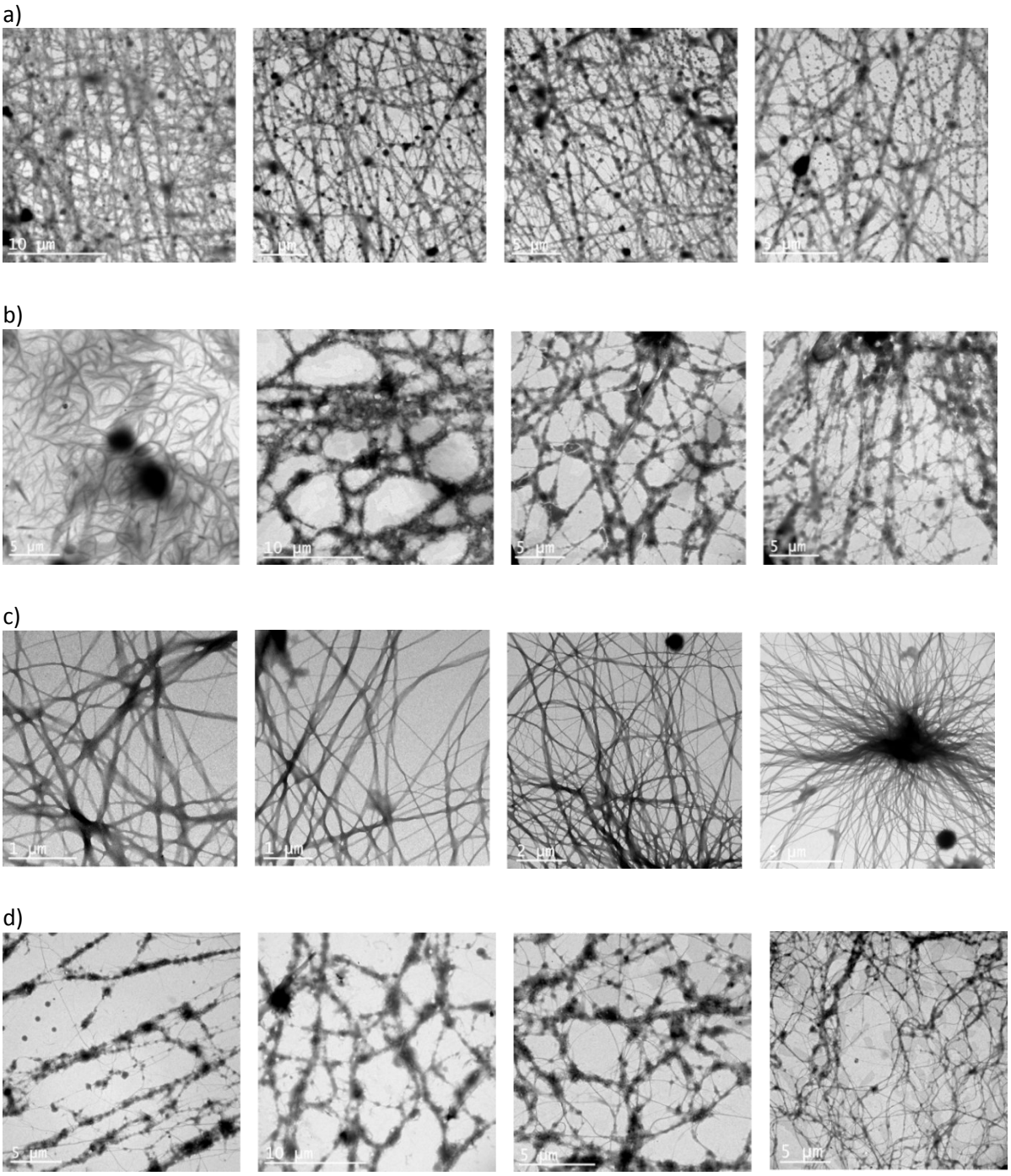


Figure S8: TEM images of the gels of **1@2** in (a) toluene, (b) o-xylene, (c) p-xylene and (d) mesitylene.

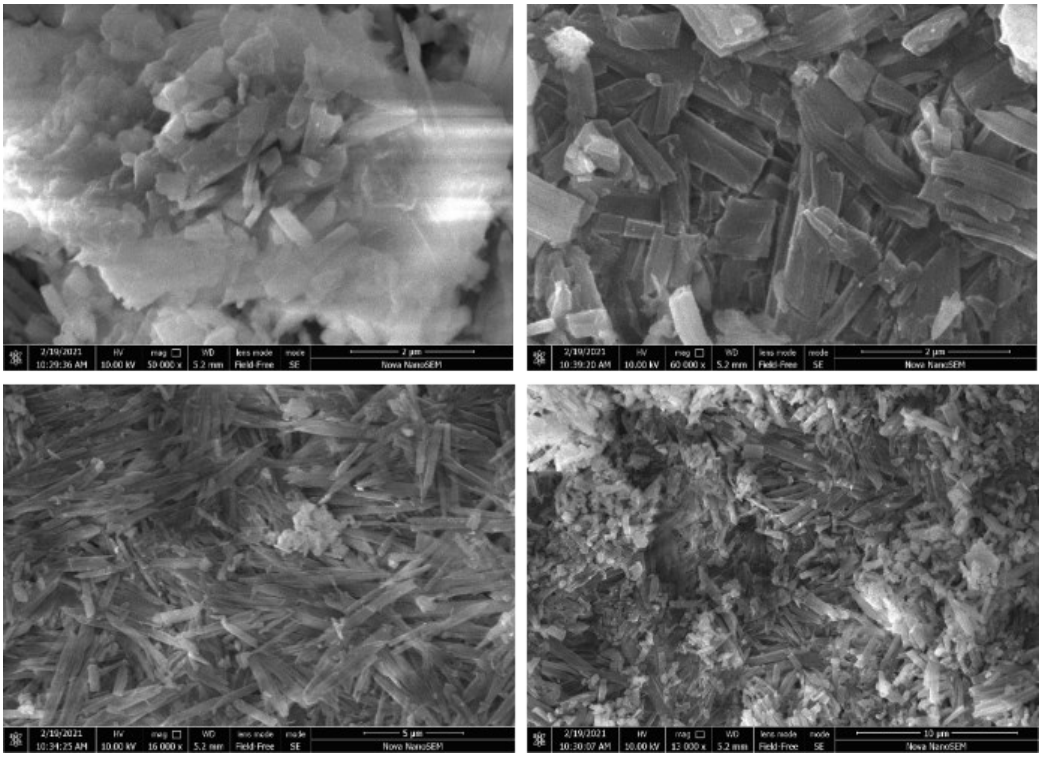


Figure S9: SEM images of the gels of **1@2** in toluene.

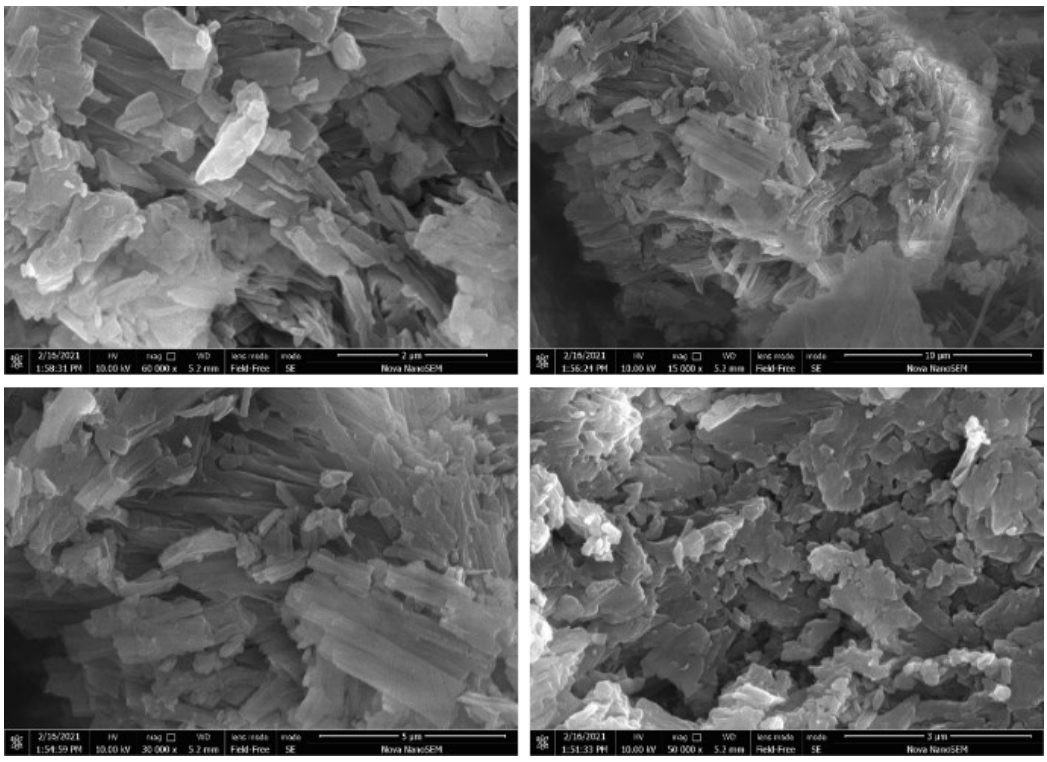


Figure S10: SEM images of the gels of **1@2** in o-xylene.

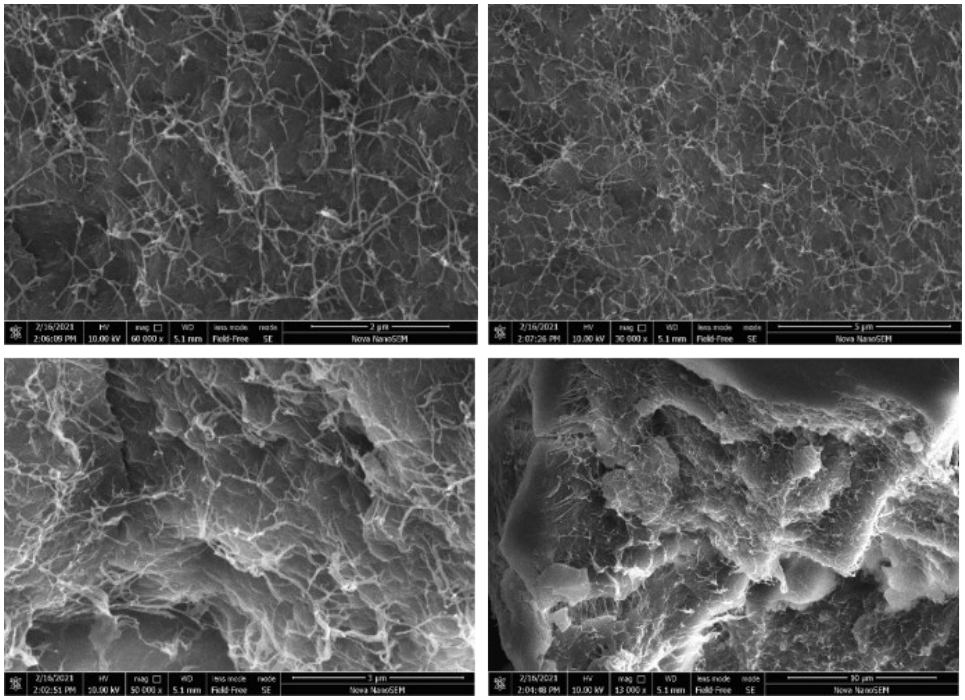


Figure S11: SEM images of the gels of **1@2** in p-xylene.

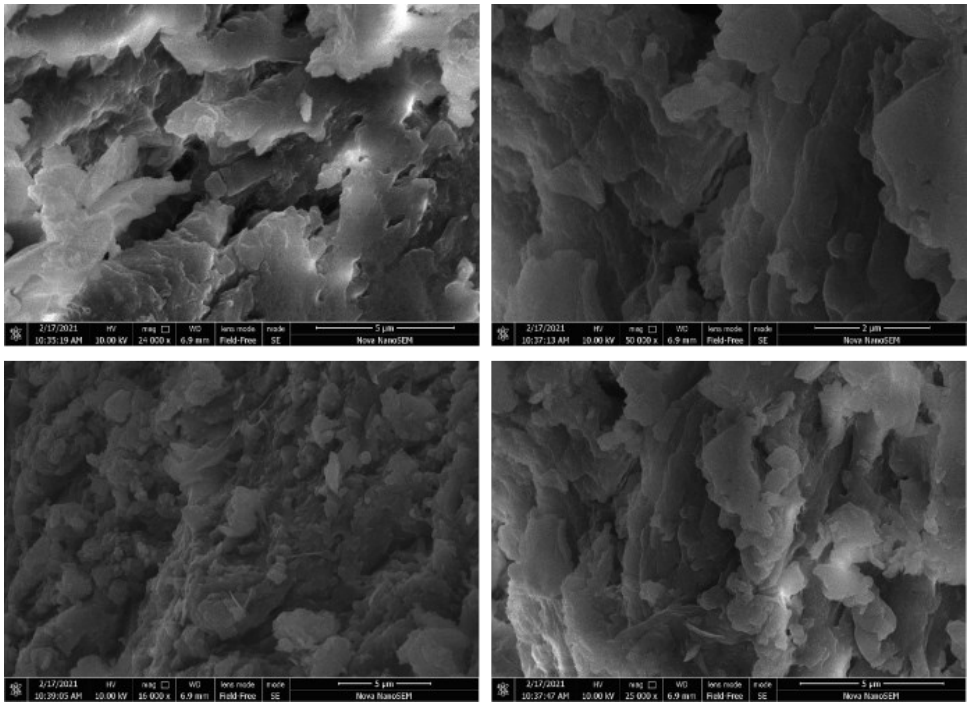


Figure S12: SEM images of the gels of **1@2** in mesitylene.

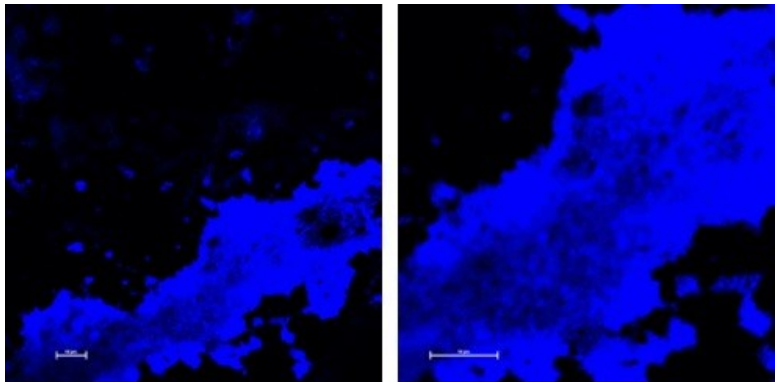


Figure S13. Confocal microscopic images of **1@2** gel.

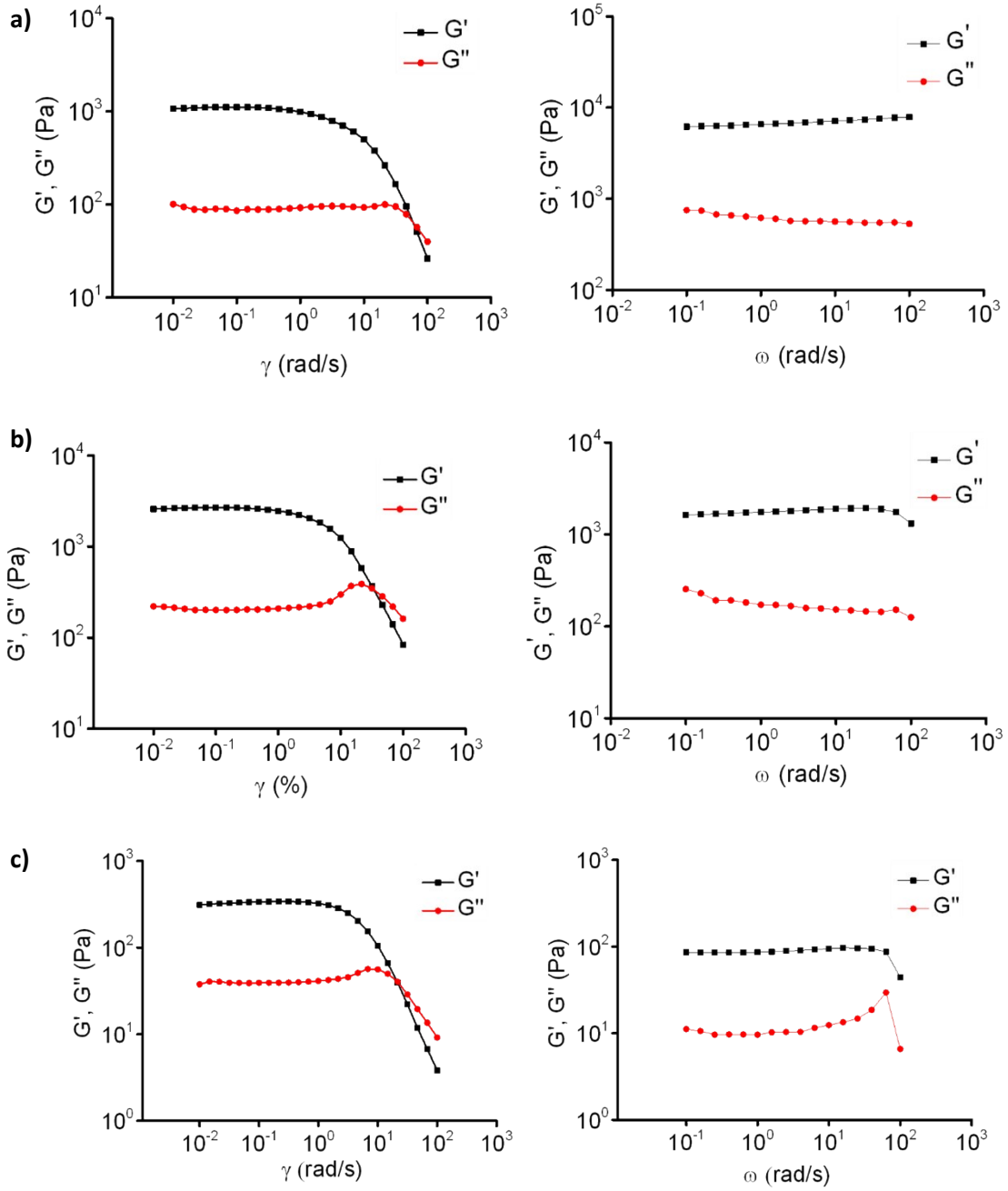


Figure S14: Amplitude (left) and frequency sweep (right) plots of the gels of **1@2** in a) o-xylene, b) p-xylene and d) mesitylene.

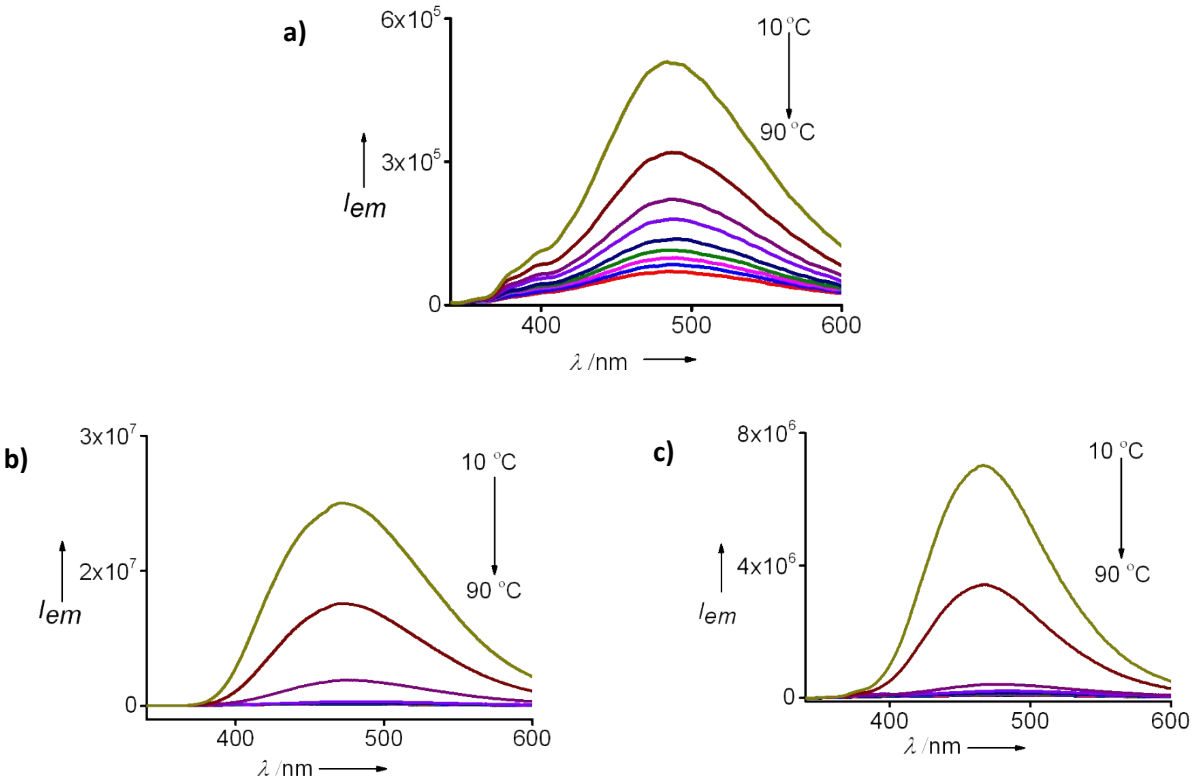


Figure S15: Temperature dependent emission spectra of the gels of **1@2** in a) o-xylene, b) p-xylene and c) mesitylene.