Electronic Supplementary Information

Assembly of Naphthalenediimide Conjugated Peptides: Aggregation Induced Changes in Fluorescence

Shibaji Basak, Jayanta Nanda and Arindam Banerjee[a,] *

[a]Department of Biological Chemistry

Indian Association for the Cultivation of Science

Jadavpur, Kolkata-700032, India.

E-mail: bcab@iacs.res.in

Fax: (+91)332473-2805

Content

Experimental section:

NMR experiments

All NMR studies were carried out on a Brüker DPX 300 MHz and Brüker DPX 400 MHz spectrometer at 300 K. Concentrations were in the range 1–10 mM in $CDCl_3$ or DMSO-d_6.

Mass spectrometry

Mass spectra were recorded on a Q-Tof micro^{TM} (Waters Corporation) mass spectrometer by positive mode electro spray ionization process.

MALDI-TOF MS

MALDI-TOF MS analysis has been performed by using Applied Biosystems MALDI TOF/TOF Analyzer in dithranol as a matrix.

Field emission scanning electron microscopic (FE-SEM) study

FE-SEM experiments were performed by placing a small portion of gel sample on a microscope cover glass. Then, these samples were dried first in air and then in vacuum and coated with platinum for 90 seconds at 10 kV voltages and 10 μA current. The average thickness of the coating layer of platinum was 3 to 4 nm. After that micrographs were taken by using a Jeol Scanning Microscope JSM-6700F.

Transmission electron microscopy (TEM)

TEM images were recorded on a JEM 2010 electron microscope at an accelerating voltage of 200 KV. A drop of dilute solution of the gel-phase material were placed on carbon coated copper grids (300 mesh) and dried by slow evaporation. Each grid was then allowed to dry in a vacuum for two days and then the images were taken.

Rheology

The rheology experiment was performed by using an Anton Paar Modular Compact Rheometer MCR 302 at 25 °C. Gels were prepared in toluene (2.5 mM).

FT-IR spectroscopy

All FT-IR spectra of dried gels were recorded by using the KBr pellet technique and a Nicolet 380 FT-IR spectrophotometer (Thermo Scientific).

X-ray diffraction study

X-ray diffraction study of the xerogel was carried out by placing the sample on a glass plate. Experiments were carried out by using an X-ray diffractometer (Bruker AXS, Model No. D8 Advance). The instrument was operated at a 40 kV voltages and 40 mA current using Ni-filtered CuK_{α} radiation and the instrument was calibrated with a standard Al_2O_3 (corundum) sample before use. For scan 1°-5°, the scintillation counts detector was used with scan speed 2s and step size 0.02°. In another scan 5°-28°, the LynxEye super speed detector was used with scan speed 0.3s and step size 0.02°.

UV/Vis spectroscopy

UV/Vis absorption spectra were recorded on a hewlett-packard (model 8453) UV/Vis spectrophotometer (varian carry 50.bio).

PL spectroscopy

Fluorescence studies of the gel were carried out in a Perkin Elmer LS55 Fluorescence Spectrometer instrument using the front face geometry. The gel sample was excited at 340 nm wavelength and emission scans were recorded from 350 to 750 nm.

Cyclic voltammetry

Cyclic voltammetry measurements were carried out in a potentiostat/galvanostat (model 273A) machine. In the experiment, Pt electrodes as working as well as counter electrode, Ag/AgCl

electrode as reference electrode and tetrabutylamoniumperchlorate (0.1 M) as supporting electrolyte have been used. Solution of the gelators **NF** and **NV** has been made in dichloromethane solvent (1 mM) for the measurements.

Current-voltage (I-V) measurements

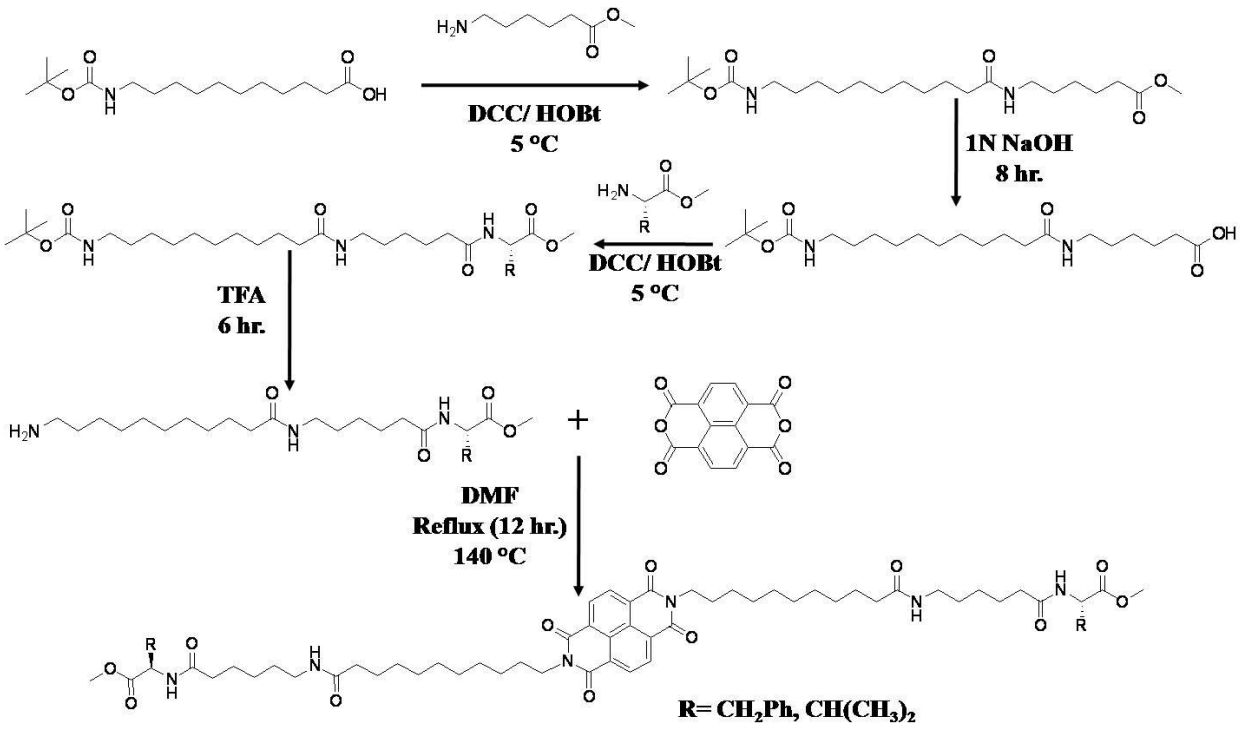
The gels of **NF** and **NV** in toluene were drop-cast on ITO glass, and these samples were allowed to air-dry in a dust free environment. Finally these samples were dried in vacuum for about 12 hr and the I–V characteristics of each film were measured in a two-probe configuration.

Atomic force microscopic (AFM) study

AFM study was carried out by drop casting the gels ITO glass. The material was then allowed to dry in air at room temperature for a few hours then in vacuum. Thickness of the reported films on ITO was examined using tapping-mode atomic force microscope. Images were taken using an Autoprobe CP Base Unit di CP-II instrument (model no. AP-0100).

Materials:

L-Phenylalanine, L-Valine, 11-Aminoundecanoic acid (Und) and 1,4,5,8-Naphthalenetetracarboxylic dianhydride were purchased from Aldrich. 6-aminocaproic acid (Acp), 1-Hydroxybenzotriazole (HOBt), N, N'-Dicyclohexylcarbodiimide (DCC) and all gelling solvents were purchased from SRL, India.



Scheme S1. Chemical structure and the synthesis of compounds**.**

Synthesis Procedures:

Boc-11-aminoundecanoic acid (Boc-Und-COOH): A solution of 11-aminoundecanoic acid (2.01 g, 10 mmol) in a mixture of dioxane (20 ml), water (10 ml) and 1N NaOH (10 ml) was stirred and cooled in an ice-water bath. Ditertbutylpyrocarbonate (2.39 g, 11 mmol) was added and stirring was continued at room temperature for 6h. Then the solution was concentrated in *vacuum* to about 20 ml to 30 ml, cooled in an ice water bath, covered with a layer of ethyl acetate (about 50 ml) and acidified with a dilute solution of $KHSO_4$ to pH 2-3 (Congo red). The aqueous phase was extracted with ethyl acetate and this operation was done repeatedly. The ethyl acetate extracts were pooled, washed with water and dried over anhydrous Na_2SO_4 and evaporated in *vacuum*. A white material was obtained.

Yield: 2.7 g, (9 mmol, 90%).

Boc-Und-Acp-OMe: 2.7 g (9 mmol) of Boc-Und-COOH was dissolved in 10 ml of DMF in an ice water bath. H-Acp-OMe was isolated from 3.63 g (20 mmol) of the corresponding methyl ester hydrochloride by neutralization and subsequent extraction with ethyl acetate and ethyl acetate extract was concentrated to 10 ml. It was then added to the reaction mixture, followed immediately by 1.85 g (9 mmol) DCC and 1.37 g (9 mmol) of HOBt. The reaction mixture was allowed to come to room temperature and stirred for 3 days. The residue was taken up in ethyl acetate (40 ml) and dicyclohexylurea (DCU) was filtered off. The organic layer was washed with 1N HCl (3 × 30 ml), brine (1 × 30 ml), 1M sodium carbonate (3 × 30 ml) and brine (2 × 30 ml) and dried over anhydrous Na_2SO_4 and evaporated in *vacuum.* A white material was obtained.

Yield: 2.56 g (6 mmol, 66.6 %).

^{1}H NMR (300 MHz, $CDCl_3$, TMS, 25 °C): δ 5.63 (NH, 1H, br), 4.54 (NH, 1H, br), 3.65 (OCH_3, 3H, s), 3.24-3.20 ($^{\alpha}CH_2$, 2H, q), 3.08-3.07 ($^{\alpha}CH_2$, 2H, m), 2.31-2.28 ($^{\alpha}CH_2$, 2H, t, *J* = 7.5), 2.15-2.12 ($^{\alpha}CH_2$, 2H, t, *J* = 7.5), 1.69-1.56 ($^{\beta}CH_2$, 6H, m), 1.52-1.47 ($^{\beta}CH_2$, 2H, m), 1.42 (Boc, 9H, s), 1.36-1.25 ($6CH_2$, 12H, m), 1.16-1.05 (CH_2, 2H, m). ^{13}C NMR (75 MHz, $CDCl_3$, TMS, 25 °C): δ 174.13, 173.36, 156.13, 79.05, 51.61, 51.53, 40.68, 39.24, 36.84, 33.91, 30.10, 29.50, 29.34, 28.48, 26.82, 26.42, 25.88, 24.53. HRMS (m/z): 429.2771 $(M+ H)^+$, 451.2523 $(M+ Na)^+$.

Boc-Und-Acp-OH: To 2.56 g (6 mmol) Boc-Und-Acp-OMe, 35 ml MeOH and 25 ml 1N NaOH were added and the progress of saponification was monitored by thin layer chromatography (TLC). The reaction mixture was stirred. After 10 h, methanol was removed under *vacuum*, the residue was taken in 50 ml of water, washed with diethylether (2 × 50 ml). Then the pH of the aqueous layer was adjusted to 2 using 1N HCl and it was extracted with ethyl acetate (3 × 50 ml). The extracts were pooled, dried over anhydrous Na_2SO_4 and evaporated in *vacuum*. A white solid material was obtained.

Yield: 2.27 g (5.5 mmol, 91.6 %).

^{1}H NMR (300 MHz, DMSO-D_6, 25 °C): δ 11.96 (-COOH, 1H, br), 7.70 (NH, 1H, br), 6.72 (NH, 1H, br), 3.02-2.96 ($^{\alpha}CH_2$, 2H, q), 2.90-2.84 ($^{\alpha}CH_2$, 2H, q), 2.19-2.14 ($^{\alpha}CH_2$, 2H, t, *J* = 7.3), 2.03-1.98 ($^{\alpha}CH_2$, 2H, t, *J* = 7.3), 1.50-1.35 ($^{\beta}CH_2$, 4H, m), 1.31-1.27 ($^{\beta}CH_2$ and Boc Hs, 13H, m), 1.21 ($7CH_2$, 14H, s). ^{13}C NMR (75 MHz, DMSO-D_6, 25 °C): δ 174.39, 171.87, 155.55, 77.23, 38.18, 35.42, 33.60, 29.47, 28.90, 28.70, 28.23, 26.28, 25.95, 25.32, 24.21. HRMS (m/z): 437.4409 $(M+ Na)^+$, 453.4262 $(M+ K)^+$.

Boc-Und-Acp-Phe-OMe: 2.27 g (5.5 mmol) of Boc-Und-Acp-OH was dissolved in 10 ml of DMF in an ice water bath. H-Phe-OMe was isolated from 2.15 g (10 mmol) of the corresponding methyl ester hydrochloride by neutralization and subsequent extraction with ethyl acetate and ethyl acetate extract was concentrated to 10 ml. It was then added to the reaction mixture, followed immediately by 1.13 g (5.5 mmol) of DCC and 0.84 g (5.5 mmol) of HOBt. The reaction mixture was allowed to come to room temperature and stirred for 3 days. The residue was taken up in ethyl acetate (40 ml) and DCU was filtered off. The organic layer was washed with 1N HCl (3 × 30 ml), brine (1 × 30 ml), 1M sodium carbonate (3 × 30 ml) and brine (2 × 30 ml) and dried over anhydrous Na_2SO_4 and evaporated in *vacuum.* A white material was obtained.

Yield: 2.3g (4 mmol, 72.7 %).

^{1}H NMR (300 MHz, $CDCl_3$, TMS, 25 °C): δ 7.27-7.06 (Phe Hs, 5H, m), 6.11-6.09 (NH, 1H, d, *J* = 7.5), 5.88 (NH, 1H, br), 4.86-4.82 ($C^{\alpha}H$, 1H, q), 4.59 (NH, 1H, br) 3.69 (OCH_3, 3H, s), 3.20-3.17 ($^{\alpha}CH_2$, 4H, m), 3.11-3.02 ($C^{\beta}H$, 2H, m), 2.16-2.11 ($^{\alpha}CH_2$, 4H, m), 1.60-1.54 ($^{\beta}CH_2$, 4H, m), 1.48-1.41 ($^{\beta}CH_2$ and Boc Hs, 13H, m), 1.30-1.24 ($7CH_2$, 14H, m). ^{13}C NMR (75 MHz, $CDCl_3$, TMS, 25 °C): δ 173.34, 172.61, 172.29, 136.02, 129.25, 128.63, 127.17, 53.10, 52.35, 39.16,

37.91, 36.83, 36.12, 30.10, 29.39, 29.41, 29.34, 29.28, 28.50, 26.82, 26.30, 25.87, 24.96. HRMS (m/z): 576.1545 $(M+ H)^+$, 598.1310 $(M+ Na)^+$, 614.1167 $(M+ K)^+$.

H_2N-Und-Acp-Phe-OMe: To 2.3 g (4 mmol) of Boc-Und-Acp-Phe-OMe, 4 ml of trifluoroacetic acid (TFA) was added and removal of Boc group was monitored by TLC. After 8 h, TFA was removed under *vacuum*. The residue was taken in water (20 ml) and covered with ethyl acetate (about 50 ml) and basified with a solution of $NaHCO_3$. The aqueous phase was extracted with ethyl acetate and this operation was done repeatedly. The ethyl acetate extracts were pooled, washed with water and dried over anhydrous Na_2SO_4 and evaporated in *vacuum*. A white material was obtained.

Yield: 1.18 g (2.5 mmol, 62.5 %).

^{1}H NMR (300 MHz, DMSO-D_6, 25 °C): δ 7.31-7.10 (Phe Hs, 5H, m), 6.09-6.07 (NH, 1H, d, *J* = 7.0), 5.73 (NH, 1H, br), 4.91-4.87 ($C^{\alpha}H$, 1H, q), 3.74 (OCH_3, 3H, s), 3.25-3.21 ($^{\alpha}CH_2$, 2H, m), 3.18-3.07 ($C^{\beta}H$, 2H, m), 2.69-2.66 ($^{\alpha}CH_2$, 2H, t, *J* = 7.0), 2.20-2.14 ($^{\alpha}CH_2$, 4H, m), 1.69 (NH_2, 2H, br), 1.65-1.60 ($^{\beta}CH_2$, 4H, m), 1.52-1.41 ($^{\beta}CH_2$, 4H, m), 1.34-1.29 ($7CH_2$, 14H, m). ^{13}C NMR (75 MHz, DMSO-D_6, 25 °C): δ 173.29, 172.59, 172.34, 136.04, 129.32, 128.70, 127.25, 53.10, 52.42, 42.32, 39.19, 37.99, 36.96, 36.19, 33.83, 29.62, 29.54, 29.51, 29.42, 29.30, 26.96, 26.34, 25.91, 25.00. HRMS (m/z): 476.2970 $(M+ H)^+$.

OMe-Phe-Acp-Und-NDI-Und-Acp-Phe-OMe (NF): H_2N-Und-Acp-Phe-OMe (0.50 g, 1.05 mmol) and 1,4,5,8-napthalenetetracarboxylicbisanhydride (0.130 g, 0.5 mmol) were placed in a round-bottomed flask along with dry DMF (15 ml) and the reaction mixture was stirred for 12 h at 140 °C under N_2 atmosphere. The heating was stopped and the solution was allowed to cool to room temperature and placed in the refrigerator for 30 min while the product came out as precipitate, which was filtered, and the obtained solid was washed with MeOH several times.

The product was further purified by column chromatography by using silica gel as stationary phase and 3 % MeOH in $CHCl_3$ as eluent.

Yield: 0.4 g (0.338 mmol, 32.5%).

^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C): δ 8.75 (Aromatic Hs of NDI, 4H, s), 7.31-7.08 (Aromatic Hs of Phe, 10H, m), 5.93-5.91 (NH, 2H, d, *J* = 8.0), 5.67 (NH, 2H, br), 4.90-4.85 ($C^{\alpha}H$, 2H, m), 4.20-4.16 ($^{\alpha}CH_2$, 4H, t, *J* = 7.6), 3.73 (OCH_3, 6H, s), 3.25-3.20 ($^{\alpha}CH_2$, 4H, m), 3.17-3.05 ($C^{\beta}H$, 4H, m), 2.20-2.13 ($^{\alpha}CH_2$, 8H, m), 1.77-1.69 ($^{\beta}CH_2$, 4H, s), 1.64-1.57 ($^{\beta}CH_2$, 8H, s), 1.52-1.28 ($^{\beta}CH_2$ and $14CH_2$, 32H, m). ^{13}C NMR (100 MHz, $CDCl_3$, TMS, 25 °C): δ 173.44, 172.58, 172.33, 162.99, 136.01, 131.08, 129.35, 128.73, 127.30, 126.87, 126.82, 53.12, 52.47, 41.12, 39.29, 38.04, 36.92, 36.22, 29.55, 29.50, 29.43, 29.26, 28.21, 27.19, 26.34, 25.95, 24.96. MALDITOF MS: calculated 1182.6617, found 1182.4879$[M]^+$.

Boc-Und-Acp-Val-OMe: 2.0 g (5 mmol) of Boc-Und-Acp-OH was dissolved in 10 ml of DMF in an ice water bath. H-Val-OMe was isolated from 1.67 g (10 mmol) of the corresponding methyl ester hydrochloride by neutralization and subsequent extraction with ethyl acetate and ethyl acetate extract was concentrated to 10 ml. It was then added to the reaction mixture, followed immediately by 1.0 g (5 mmol) of DCC and 0.76 g (5 mmol) of HOBt. The reaction mixture was allowed to come to room temperature and stirred for 3 days. The residue was taken up in ethyl acetate (40 ml) and DCU was filtered off. The organic layer was washed with 1N HCl (3 × 30 ml), brine (1 × 30 ml), 1M sodium carbonate (3 × 30 ml) and brine (2 × 30 ml) and dried over anhydrous Na_2SO_4 and evaporated in *vacuum.* A white material was obtained.

Yield: 1.9 g (3.6 mmol, 72.0 %).

^{1}H NMR (300 MHz, $CDCl_3$, TMS, 25 °C): δ 6.13-6.10 (NH, 1H, d, *J* = 8.7), 5.92 (NH, 1H, br), 4.54-4.50 ($C^{\alpha}H$ and NH, 2H, m), 3.71 (OCH_3, 3H, s), 3.25-3.18 ($^{\alpha}CH_2$, 2H, m), 3.05 ($^{\alpha}CH_2$, 2H,

br), 2.25-2.20 ($^{\alpha}CH_2$, 2H, t, *J* = 7.35), 2.18-2.07 ($^{\alpha}CH_2$ and $C^{\beta}H$ of Val, 3H, m), 1.69-1.55 ($^{\beta}CH_2$, 4H, m), 1.52-1.38 ($^{\beta}CH_2$ and Boc Hs, 13H, m), 1.36-1.28 ($7CH_2$, 14H, m), 0.92-0.87 ($2CH_3$, 6H, m). ^{13}C NMR (75 MHz, $CDCl_3$, TMS, 25 °C): δ 173.53, 173.11, 172.82, 156.17, 79.10, 57.10, 52.19, 40.70, 39.21, 36.81, 36.27, 31.23, 30.11, 29.50, 29.42, 29.34, 29.29, 29.17, 28.51, 26.82, 26.34, 25.89, 25.09, 19.05, 17.97. HRMS (m/z): 528.2437 $(M+ H)^+$, 550.1994 $(M+ Na)^+$.

H_2N-Und-Acp-Val-OMe: To 1.9 g (3.6 mmol) of Boc-Und-Acp-Val-OMe, 4 ml of trifluoroacetic acid (TFA) was added and removal of Boc group was monitored by TLC. After 8 h, TFA was removed under *vacuum*. The residue was taken in water (20 ml) and covered with ethyl acetate (about 50 ml) and basified with a solution of $NaHCO_3$. The aqueous phase was extracted with ethyl acetate and this operation was done repeatedly. The ethyl acetate extracts were pooled, washed with water and dried over anhydrous Na_2SO_4 and evaporated in *vacuum*. A white material was obtained.

Yield: 1.2 g (2.8 mmol, 77.7 %).

^1H NMR (300 MHz, DMSO-D_6, 25 °C): δ 8.07-8.04 (NH, 1H, d, *J* = 8.1), 7.70 (NH, 1H, br), 4.16-4.11 ($^{\alpha}CH_2$, 2H, t, *J* = 7.35), 3.81 ($C^{\alpha}H$ of Val, 1H, br), 3.60 (OCH_3, 3H, s), 2.98-2.96 ($^{\alpha}CH_2$, 2H, m), 2.58-2.53 (NH_2, 2H, m), 2.13-2.10 ($^{\alpha}CH_2$, 2H, m), 2.02-1.97 ($^{\alpha}CH_2$ and $C^{\beta}H$ of Val, 3H, m), 1.45-1.43 ($^{\beta}CH_2$, 4H, m), 1.35 ($^{\beta}CH_2$, 4H, m), 1.21 (7CH2, 14H, s), 0.86-0.76 ($2CH_3$, 6H, m). ^{13}C NMR (75 MHz, DMSO-D_6, 25 °C): δ 173.15, 172.86, 172.46, 171.71, 57.91, 52.14, 36.35, 36.03, 35.39, 31.88, 31.53, 30.38, 29.58, 29.53, 29.50, 29.45, 29.38, 29.28, 29.17, 28.98, 26.87, 26.63, 25.92. HRMS (m/z): 428.2601 $(M+ H)^+$.

OMe-Val-Acp-Und-NDI-Und-Acp-Val-OMe (NV): H_2N-Und-Acp-OMe (0.98 g, 3 mmol) and 1,4,5,8-napthalenetetracarboxylicbisanhydride (0.402 g, 1.5 mmol) were placed in a round-bottomed flask along with dry DMF (15 ml) and the reaction mixture was stirred for 12 h at 140

°C under N_2 atmosphere. The heating was stopped and the solution was allowed to cool to room temperature and placed in the refrigerator for 30 min while the product came out as precipitate, which was filtered, and the obtained solid was washed with MeOH several times. The product was further purified by column chromatography by using silica gel as stationary phase and 3 % MeOH in $CHCl_3$ as eluent.

Yield: 0.5 g (0.563 mmol, 18.76%).

^{1}H NMR (300 MHz, $CDCl_3$, TMS, 25 °C): δ 8.75 (Aromatic Hs of NDI, 4H, s), 5.98-5.95 (NH, 2H, d, *J* = 8.1), 5.74 (NH, 2H, s), 4.58-4.53 ($C^{\alpha}H$, 2H, m), 4.21-4.16 ($^{\alpha}CH_2$, 4H, t, *J* = 7.5), 3.74 (OCH_3, 6H, s), 3.26-3.24 ($^{\alpha}CH_2$, 4H, m), 2.28-2.23 ($^{\alpha}CH_2$, 4H, t, *J* = 7.2), 2.18-2.12 ($^{\alpha}CH_2$ and $C^{\beta}H$ of Val, 6H, m), 1.76-1.50 ($^{\beta}CH_2$, 16H, m), 1.47-1.27 ($14CH_2$, 32H, m), 0.94-0.88 ($4CH_3$, 12H, m). ^{13}C NMR (75 MHz, $CDCl_3$, TMS, 25 °C): δ 173.03, 172.84, 163.00, 131.10, 126.88, 126.82, 57.14, 52.34, 41.12, 39.44, 36.47, 31.39, 29.83, 29.57, 29.54, 29.47, 29.41, 29.30, 28.23, 27.21, 26.47, 26.06, 25.13, 19.16, 18.10. MALDITOF MS: calculated 1086.6617, found 1086.4139 $[M]^+$.

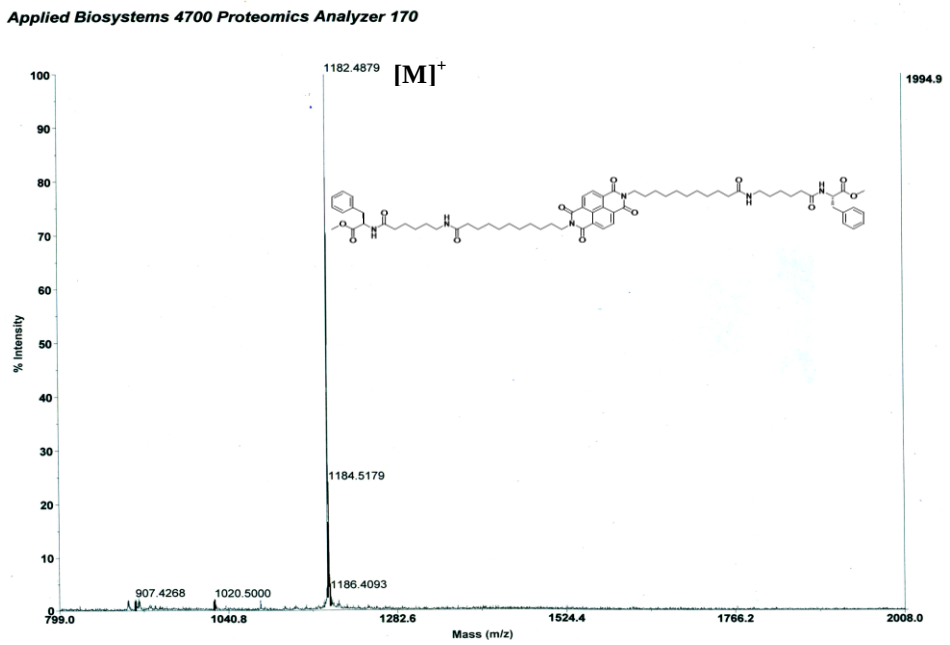


Fig. S1 MALDITOF MS spectra of **NF**.

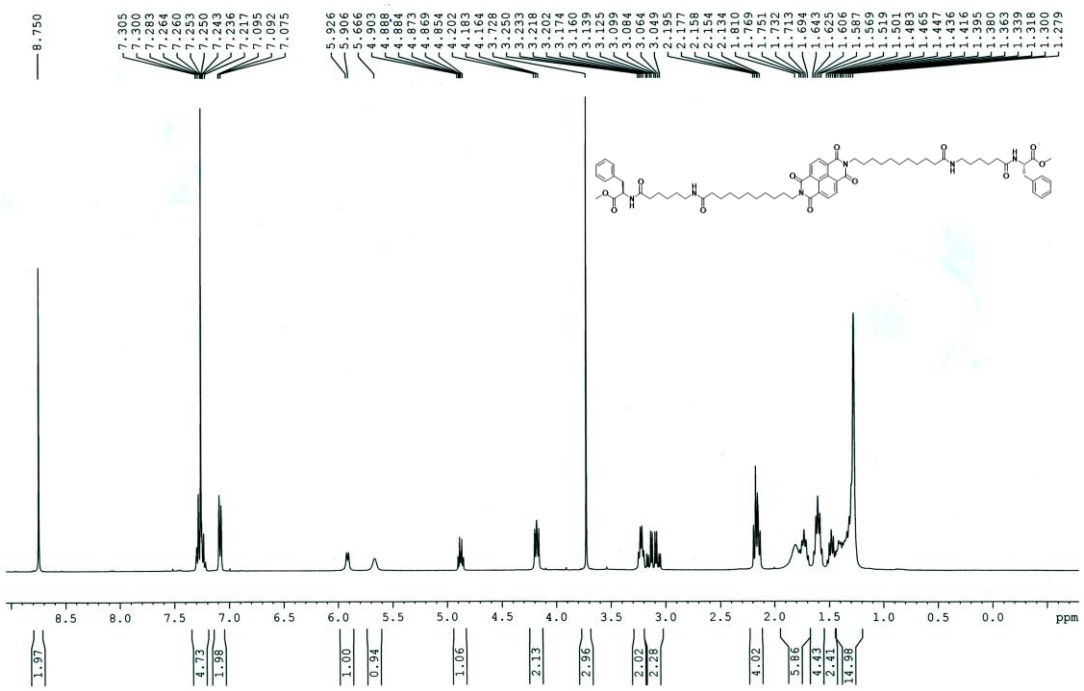


Fig. S2 ^{1}H NMR spectrum in $CDCl_3$ of **NF** recorded in 400 MHz.

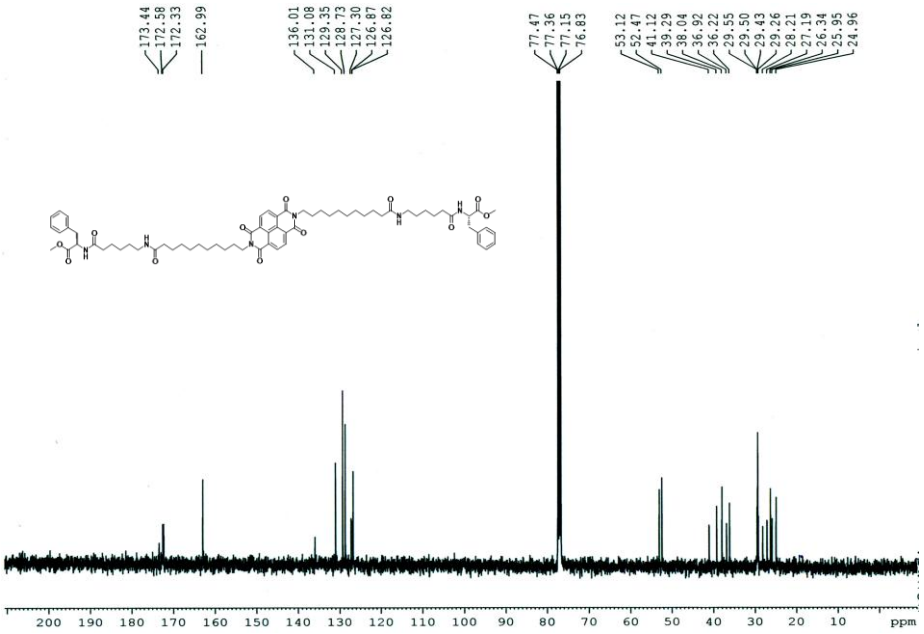


Fig. S3 ^{13}C NMR spectrum in $CDCl_3$ of **NF** recorded in 75 MHz.

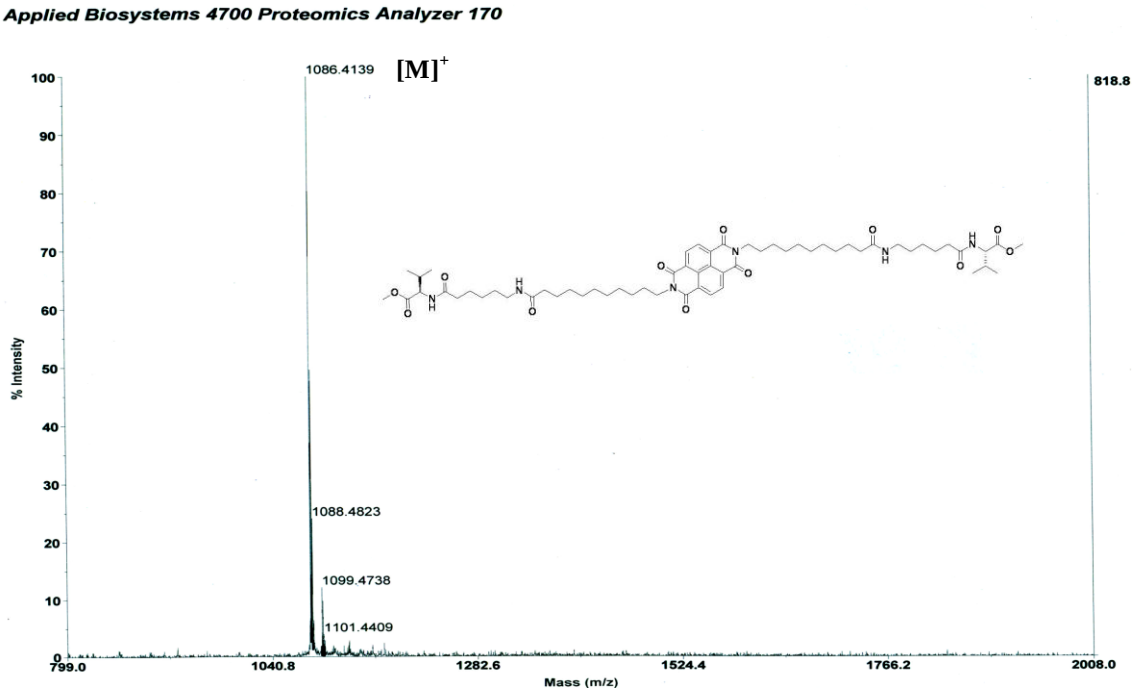


Fig. S4 MALDITOF MS spectra of **NV**.

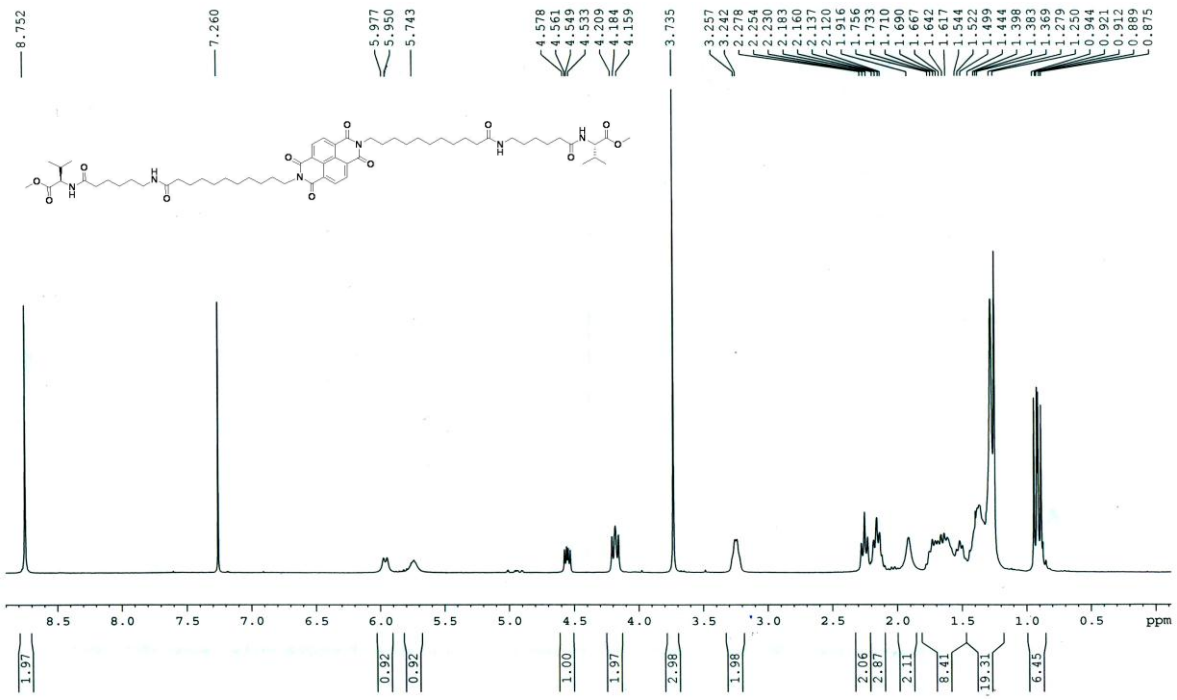


Fig. S5 ^{1}H NMR spectrum in $CDCl_3$ of **NV** recorded in 400 MHz.

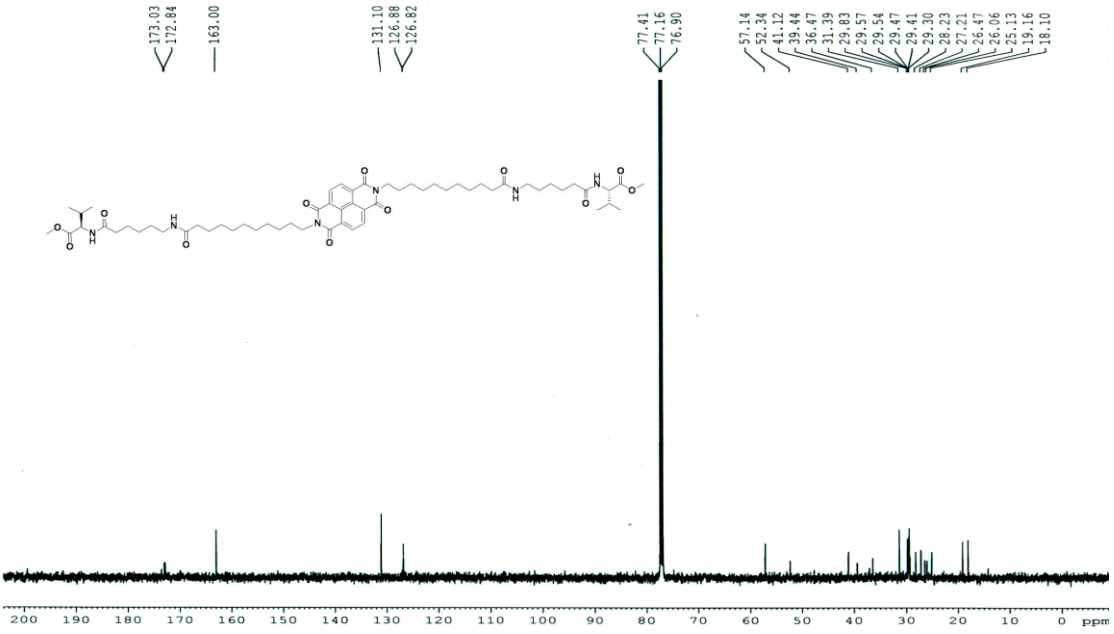


Fig. S6 ^{13}C NMR spectrum in $CDCl_3$ of **NV** recorded in 400 MHz.

Table S1. Gelation property of gelators in pure solvents.

Solvents	**NF (MGC in mM)**	**NV (MGC in mM)**
Toluene	2.11 (G)	1.03 (G)
o-Xylene	2.5 (G)	1.1 (G)
m-Xylene	2.55 (G)	1.11 (G)
p-Xylene	2.3 (G)	1.09 (G)
Chlorobenzene	2.6 (G)	1.15 (G)
1,2-Dichlorobenzene	1.9 (G)	0.95 (G)
Hexane	I	I
Methanol	S	S
Methylcyclohexane	I	I
Cyclohexane	I	I
Dioxane	2.79 (G)	1.17 (G)
Chloroform	16.9 (G)	10.15 (G)
Ethyl acetate	I	I
THF	4.2 (G)	2.5 (G)

Note G = Gel, I = Insoluble and S = Solution.

Table S2 Gelation property of gelator **NF** in mixed solvents.

Solvents	**Composition**	**State**	**NF (MGC in mM)**
Chloroform and Methylcyclohexane	25:75	G	1.6
Chloroform and Hexane	25:75	G	1.8
Chloroform and Ethyl acetate	25:75	G	4.2
Chloroform and Methanol	25:75	G	4.2

Note G = Gel

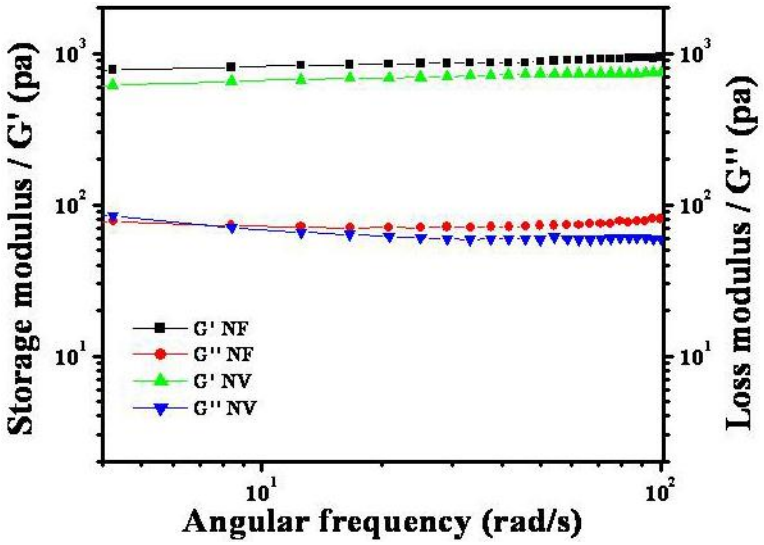


Fig. S7 Plot of storage modulus (G') and loss modulus (G") versus angular frequency of **NF** and **NV** gels at 2.5 mM at 25 °C.

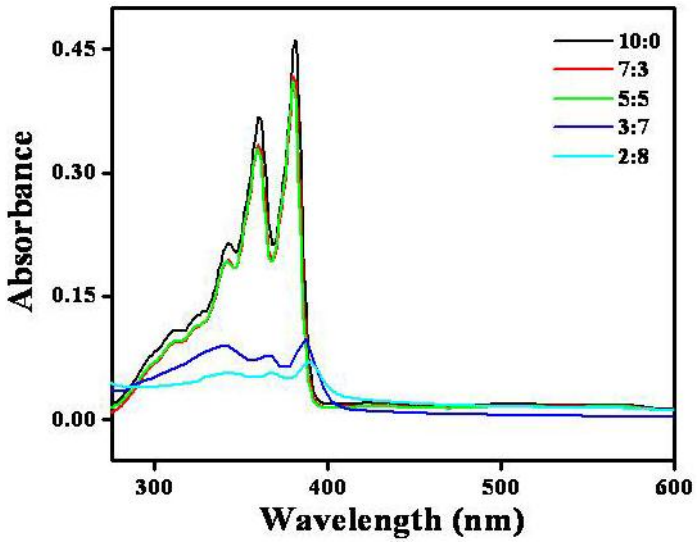


Fig. S8 Solvent dependent UV-visible study of **NV** in different mixtures (chloroform and MCH). Temperature and concentration maintained at 25 °C and 0.05 mM respectively.

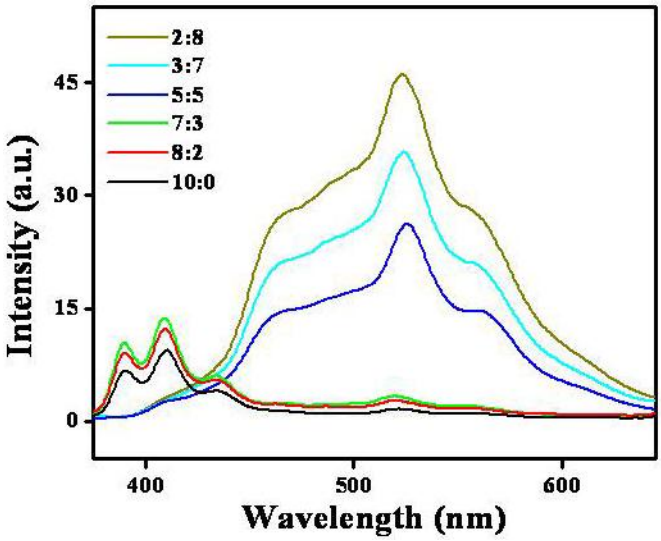


Fig. S9 Solvent dependent photo-luminescent study of **NV** in different chloroform and methylcyclohexane mixtures. Temperature and concentration maintained at 25 °C and 1.6 mM respectively.

Fig. S10 The solution of **NF** at 2:8 composition of chloroform and MCH mixture. The photograph was taken immediately after strong heating.

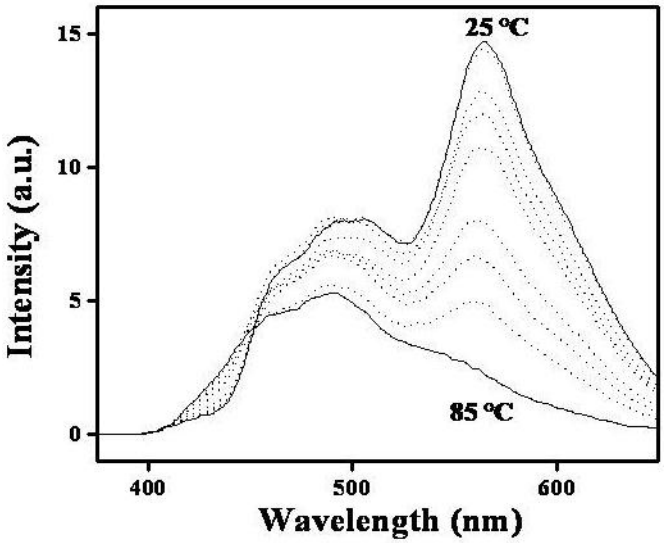


Fig. S11 The temperature dependent fluorescent spectra of **NF** gel in chloroform: toluene (2:8).

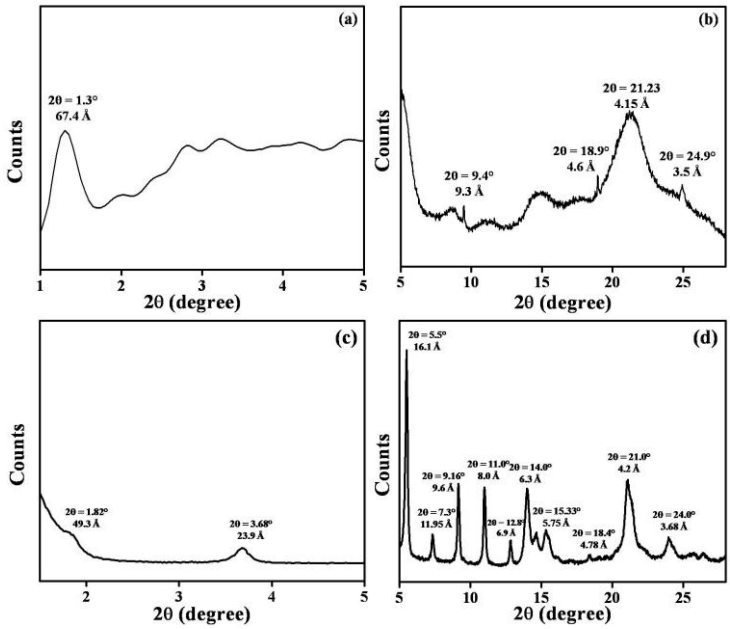


Fig. S12 (a) Small angle and (b) wide angle XRD pattern of **NF** in xerogel state. (c) Small angle and (b) wide angle XRD pattern of **NV** in xerogel state.

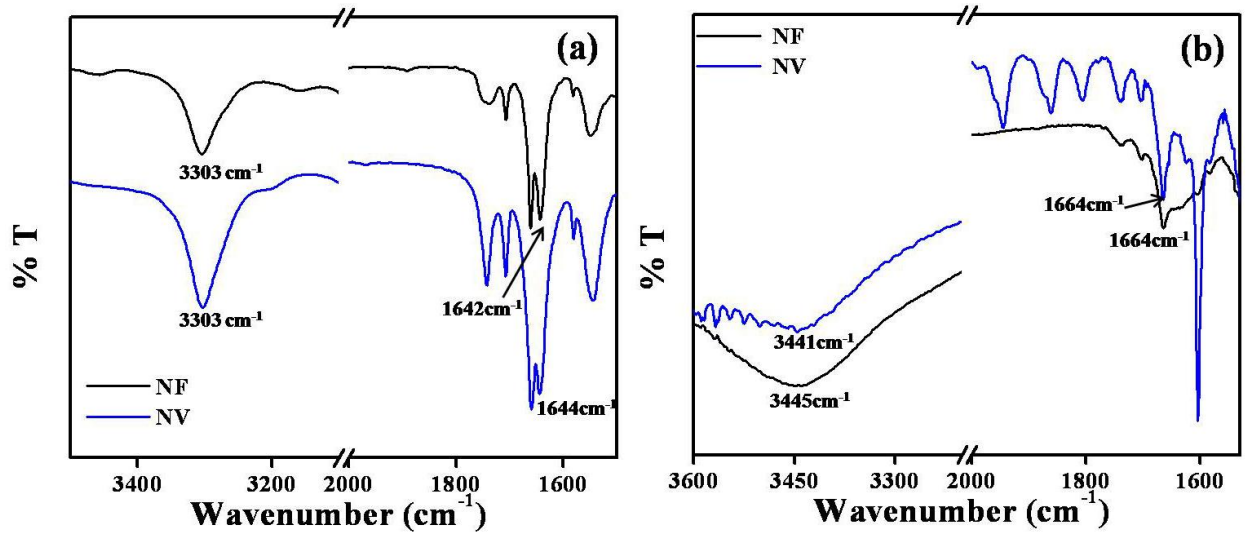


Fig. S13 FT-IR study of **NF** and **NV** at gel (a) and solution (b) state respectively. Temperature and concentration maintained at 25 °C and 4.2 mM respectively.

Table S3 FT-IR frequency obtained from solution and gel state of **NF** and **NV**.

NF in solution state (Chloroform)	3445 cm^{-1}, 1703 cm^{-1}, 1664 cm^{-1}, 1582 cm^{-1}
NF in gel state (Toluene)	3303 cm^{-1}, 1707 cm^{-1}, 1660 cm^{-1}, 1642 cm^{-1}, 1549 cm^{-1}
NV in solution state (Chloroform)	3441 cm^{-1}, 1703 cm^{-1}, 1664 cm^{-1}, 1584 cm^{-1}
NV in gel state (Toluene)	3303 cm^{-1}, 1707 cm^{-1}, 1660 cm^{-1}, 1644 cm^{-1}, 1545 cm^{-1}

Table S4 Redox Potentials and LUMO energy levels of **NF** and **NV** obtained from Cyclic Voltametry Measurements.

Gelators	E_0-E_{-1} (V)[a]	E_{-1}-E_{-2} (V)[b]	$E_{average}$ (V)[c]	LUMO[d] (eV)
NF	-0.54	-0.95	-0.75	-3.66
NV	-0.59	-1.06	-0.82	-3.58

[a]First reduction potential. [b]Second reduction potential. [c]Average of the first and second reduction potentials. [d]$E_{LUMO} = -e(E_{1/2(redox)} - E_{Fc} + 4.8)$; $E_{Fc} = 0.39$ V (versus Ag/AgCl).

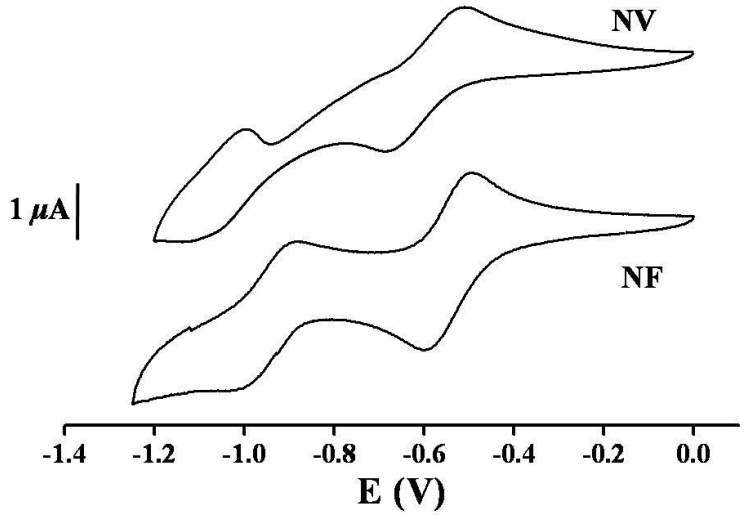


Fig. S14 Cyclic voltammogram of **NF** and **NV**.

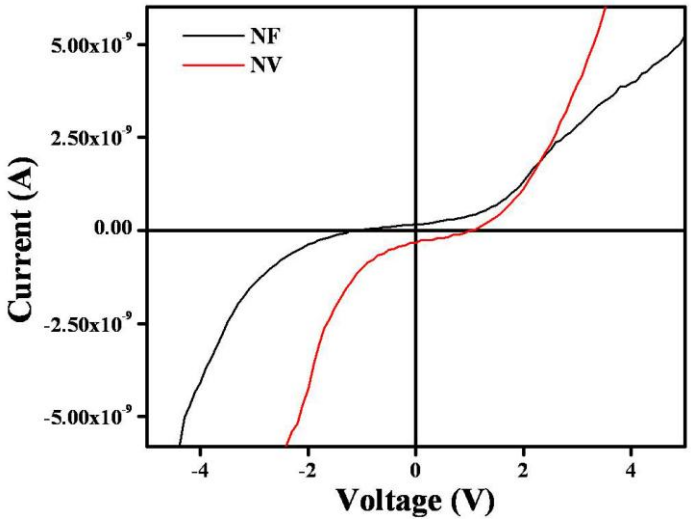


Fig. S15 I–**V** characteristics obtained from **NF** and **NV**.

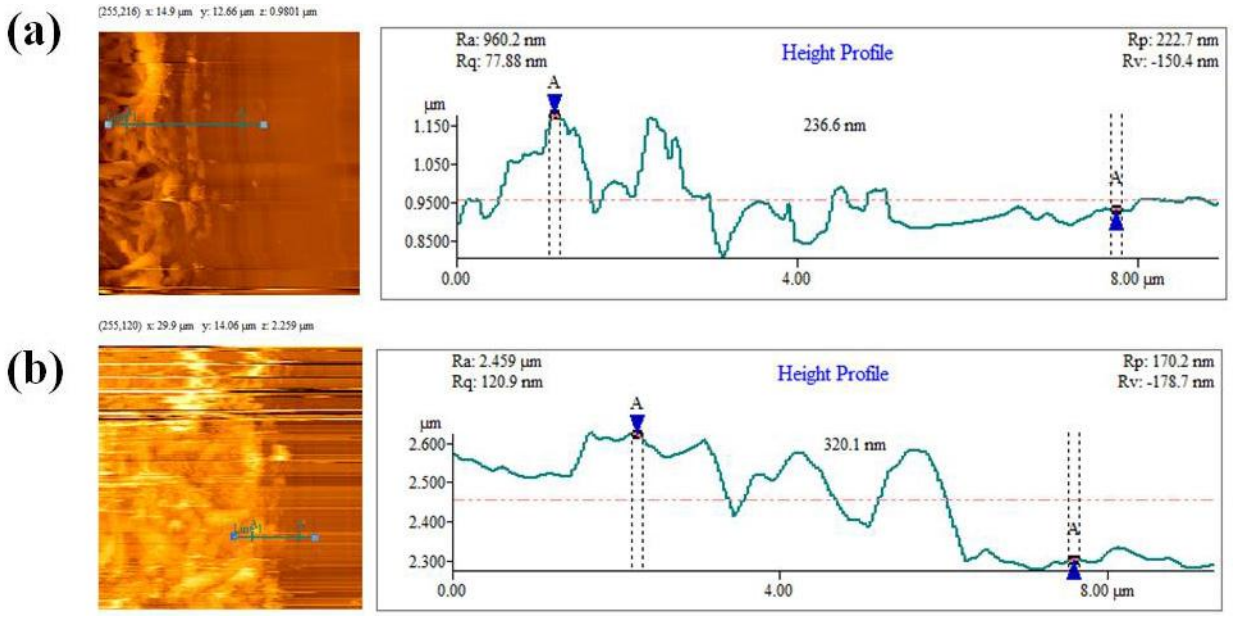


Fig. S16 The AFM height profile diagram of films on ITO glass obtained from **NF** (a) and **NV** (b).