

Supplementary Supporting Information

White photoluminescence and electroluminescence from a ternary system in solution and polymer matrix

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Sl. No.		Page No.
1	Figure S1 showing the absorption and emission spectra of 1 in methanol	S5
2	Figure S2 showing the absorption and emission spectra of 2 in methanol	S5
3	Figure S3 showing the fluorescence decay profiles of 1 and 2 in methanol	S6
4	Figure S4 showing the changes in the absorption and emission spectra of proflavine hemisulfate (PF) in presence of nile red (NR)	S6
5	Figure S5 showing the spectral overlap between PF emission and NR absorption and excitation spectrum	S6
6	Figure S6 showing the white light emission and CIE coordinates of the white light emission in methanol	S7
7	Figure S7 showing fluorescence decay profiles of PEG film containing 1 , PF and NR under various experimental conditions	S7

1. General experimental techniques

Fluorescence spectra were recorded in 1×1 cm² quartz cuvette. Fluorescence spectra were recorded on a SPEX–Fluorolog F112X spectrofluorimeter. Solid-state photoluminescence was measured using the front face emission scan mode on an SPEX Fluorolog F112X spectrofluorimeter. Measurements of solid-state fluorescence quantum efficiency were carried out using a calibrated integrating sphere in an SPEX Fluorolog spectrofluorimeter. A Xenon-arc lamp was used to excite the film samples placed in the sphere, with 380, 440 and 560 nm as the excitation wavelengths. The quantum yield of solid-state fluorescence was determined by comparing the spectral intensities of the lamp and the sample emission using a reported procedure.¹ Using this experimental setup and the integrating sphere system, the solid-state fluorescence quantum yield of the standard green OLED material, tris-8-hydroxyquinolinolato aluminum (yellowish-green powder) was determined to be 40 ± 2%, which is consistent with previously reported values.² Solvents and reagents were purified and dried by usual methods prior to use.

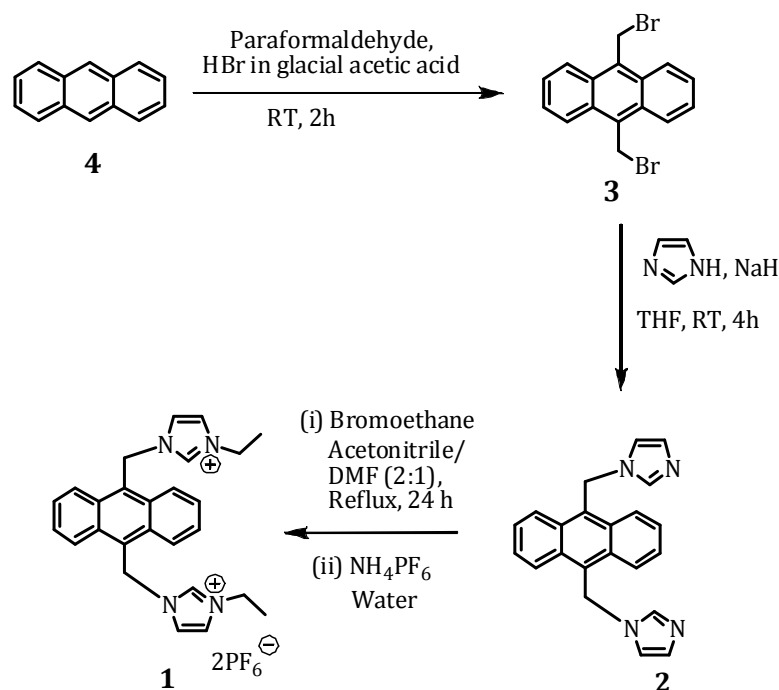
The CIE, Commission Internationale de l'Eclairage (International Commission on Illumination), chromaticity coordinates (1931) (x, y) were calculated using HORIBA Jobin Yvon Color Calculator provided with integrating sphere. Fluorescence lifetimes were measured using IBH (FluoroCube) time-correlated picoseconds single photon counting (TCSPC) system. The films were excited with a pulsed diode laser (<100 ps pulse duration) at a wavelength of 375 nm (NanoLED-11) with a repetition rate of 1 MHz. The detection system consisted of a microchannel plate photomultiplier (5000U-09B, Hamamatsu) with a 38.6 ps response time coupled to a monochromator (5000M) and TCSPC electronics [data station Hub including Hub-NL, NanoLED controller, and preinstalled fluorescence measurement and analysis studio (FMAS) software]. The fluorescence decay profiles were deconvoluted using IBH data station software V2.1 and minimizing the χ^2 values of the fit to 1 ± 0.1 . Film thickness measurements were carried out using a Zeiss EVO 18 Cryo Scanning Electron Microscope (SEM). The operating range was between 100-230 V at 50-60Hz and single phase at 2.5 kVA. The luminescence–voltage (L–V) characteristics of the LEDs were measured using Type PT 168 PMT housing with drawer assembly from Nucleonix systems, India. The LEDs were tested under continuous mode of voltage application and the forward bias threshold voltage and total intensity of the emission were obtained. The current-voltage (I–V) characteristics of the device were measured by using space charge limited current (SCLC) method using Keithley 2400 source meter for ITO/polymer/aluminium layered

device. The Electroluminescence spectra of LEDs were recorded on Varian Cary eclipse fluorescence spectrophotometer in chemiluminescence mode. All experiments were carried out at room temperature (25 ± 1 °C), unless otherwise mentioned.

2. Materials

Proflavine hemisulfate (**PF**), Nile red (**NR**) and ammonium hexafluorophosphate were purchased from Sigma–Aldrich and used as received. Anthracene, paraformaldehyde, HBr in glacial acetic acid, imidazole, sodium hydride and polyethylene glycol were purchased from local suppliers and used as such. 9,10-Bis(bromomethyl)anthracene (**3**) was prepared according to the reported procedure.^{3,4} Dry methanol was used for all the solution state studies.

3. Synthesis of compounds 1 and 2



Scheme S1

Synthesis of 9,10-bis[(1H-imidazol-1-yl)methyl] anthracene (2). To a reaction mixture of imidazole (0.5 g, 7.4 mmol) in dry THF (100 mL) was added NaH (0.33 g, 13.8 mmol) at 0°C. After the reaction mixture was stirred for 30 min at 0°C, 9,10-bis(bromomethyl)anthracene (**3**, 0.5 g, 1.4 mmol) was added. After additional stirring for 4 h at 25°C, the reaction mixture was poured into 100 mL of water and extracted with dichloromethane. The organic layer was then separated, dried over anhydrous sodium sulfate and concentrated to get a residue which was further purified by column chromatography over

silica gel. Elution of the column with ethyl acetate yielded 0.37 g (78%) of **2**, which was then re-crystallized from a mixture of acetonitrile and ethyl acetate (4:1). mp 246-247 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 6.29 (s, 4H), 6.78 (s, 2H), 6.93 (s, 2H), 7.67 – 7.73 (m, 6H), 8.61 – 8.64 (m, 4H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 109.9, 113.6, 119.1, 124.7, 124.9, 128.3, 129.1, 130.1; HRMS (FAB): *m/z* calcd for C₂₂H₁₉N₄: 339.4132, found 339.4508.

Synthesis of 1,1'-[anthracene-9,10-diylbis(methylene)] bis(3-ethyl-1H-imidazol-3-ium) dihexafluorophosphate (1). To a solution of 9,10-bis((1H-imidazol-1-yl)methyl)anthracene (**2**, 0.25 g, 0.74 mmol) in a mixture of acetonitrile (100mL) and DMF (50 mL) was added bromoethane (0.81 g, 0.74 mmol). The reaction mixture was then refluxed for 24 h and after cooling to room temperature the precipitated product was filtered and washed with 30 mL dry acetonitrile. Further, it was dissolved in water and precipitated with ammonium hexafluorophosphate to get compound **1**. Yield 40%. mp 276-277 °C; ¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 1.37 (t, *J*=7 Hz, 6H), 4.04 (q, *J*=7.5 Hz, 4H), 6.39 (s, 4H), 7.32 (d, *J*=7Hz, 2H), 7.38 (s, 2H), 7.75 (q, *J*=3.5 Hz, 4H), 8.24 (s, 2H), 8.39 (q, *J*=3.5 Hz, 4H); ¹³C NMR (125 MHz, Acetonitrile-*d*₃) δ 14.0, 44.7, 45.3, 122.1, 123.9, 125.9, 127.7, 130.7, 134.6; HRMS (FAB): *m/z* calcd for C₂₆H₂₈N₄P₂F₁₂ – PF₆: 541.4915, found 541.7100 (M – PF₆)⁺.

4. Preparation of polyethylene glycol films

An approximately 10% (w/w) solution of polyethylene glycol (molecular weight ~4000) in methanol was prepared by dissolving 8 g of PEG in 100 mL methanol. Stock solutions (1mM) of compound **1**, **PF** and **NR** in methanol were prepared separately.

Preparation of films of individual fluorophores. To 5 mL of PEG (10%, w/w) solution add 5 mL of **1** or **PF** or **NR** (1mM) are mixed together to get a uniform solution. The above solution is drop-casted on a glass substrate and allowed the solvent to evaporate (25°C) to get a good quality film.

Preparation of film containing 1-PF-NR. The above individual solutions were mixed together in the molar ratio 1:0.5:0.2 and stirred well to get a uniform solution. Then the solution is drop-casted on a glass substrate and allowed the solvent to evaporate (25°C) to get good quality film.

4. Fabrication of LEDs

Light emitting diodes were fabricated by spin coating the emissive polymer layer over the indium tin oxide (ITO) coated (100 nm thickness) glass plates. The thin film was formed by spin coating the methanol solution of compound **1**, **PF** and **NR** in PEG in the ratio of (1:

0.5: 0.2) at 3000 rpm. Aluminum was coated over the electro emissive layer, which serves as cathode and ITO acts as anode in the diode.

5. References

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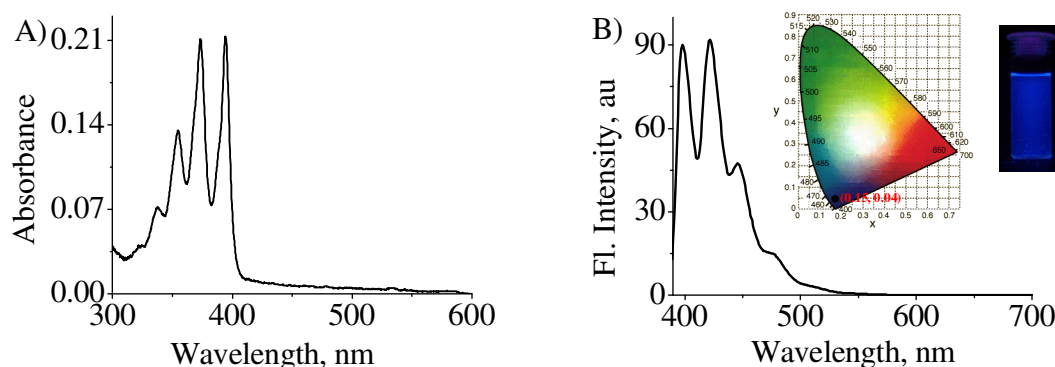


Figure S1. (A) Absorption and (B) emission spectra of compound **1** (15 μ M) in methanol (λ_{ex} = 380 nm). Insets of (B) show the 1931 CIE coordinates and photograph of fluorescence of **1** in methanol under 365 nm UV lamp.

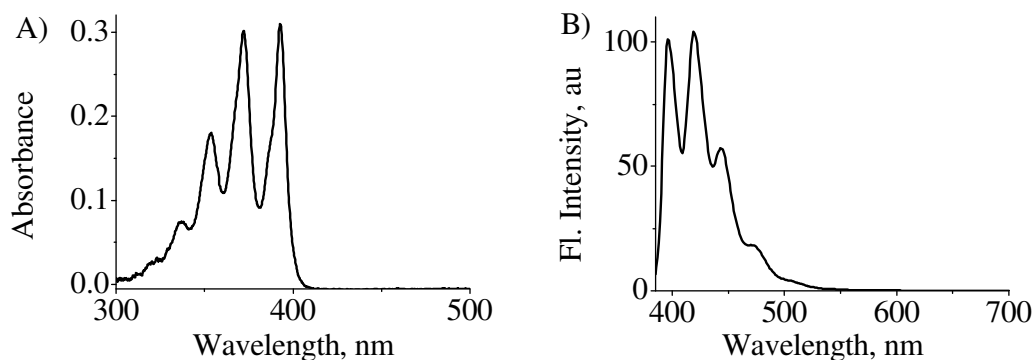


Figure S2. (A) Absorption and (B) emission spectra of compound **2** (10 μ M) in methanol (λ_{ex} = 380 nm).

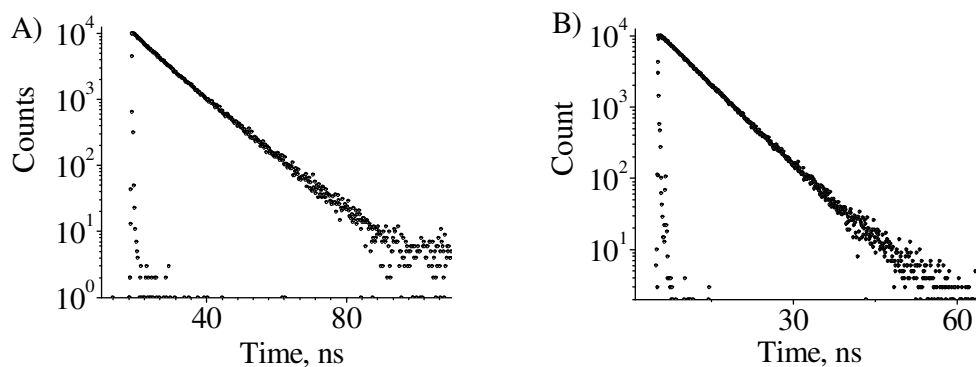


Figure S3. Fluorescence decay profile of compound (A) **1** and (B) **2** in methanol when emission monitored at 430 nm ($\lambda_{\text{ex}} = 375$ nm).

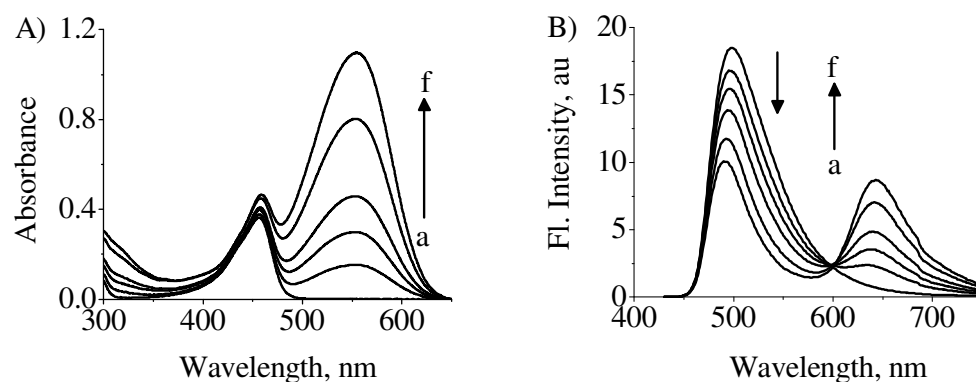


Figure S4. Changes in the (A) Absorption and (B) fluorescence spectra of **PF** (5.7 μM) by the addition of **NR** in methanol ($\lambda_{\text{ex}} = 420$ nm). [**NR**], (a) 0 and (f) 27.5 μM .

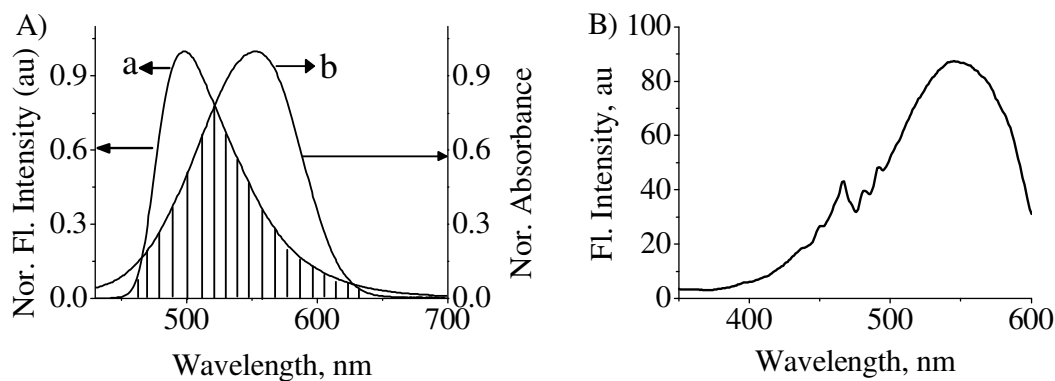


Figure S5. (A) Spectral overlap between (a) **PF** emission and (b) **NR** absorption ($\lambda_{\text{ex}} = 420$ nm) spectra and (B) Excitation spectrum of a solution containing **PF** and **NR** when emission monitored at 640 nm.

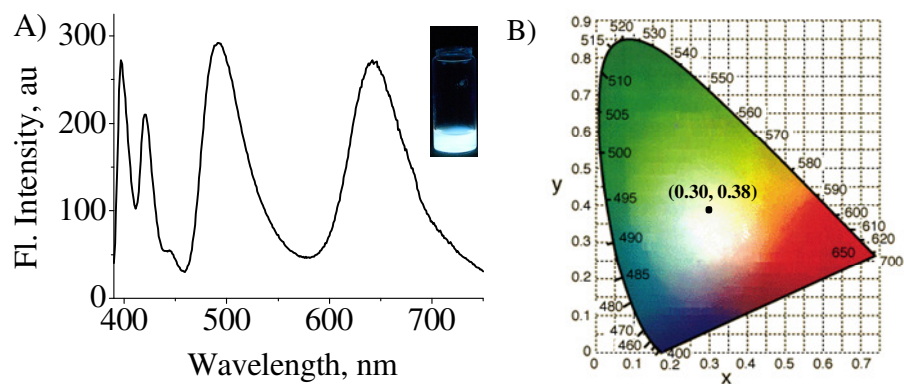


Figure S6. (A) Emission spectrum of solution containing compound **1**, **PF** and **NR** in the molar ratio 1.0: 4.5: 5.0 in methanol (λ_{ex} = 380 nm). Inset of (A) shows photograph of the visual fluorescence of the corresponding solution under UV lamp (365 nm) and (B) shows the CIE coordinates of the emission spectrum.

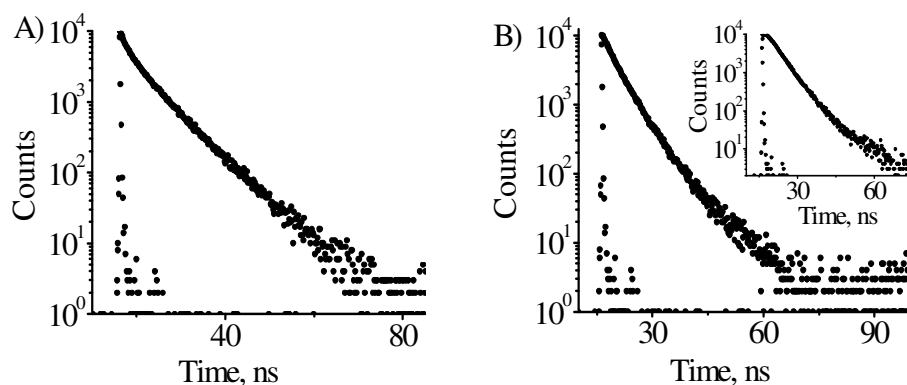


Figure S7. Fluorescence decay profiles of PEG film containing compound **1**, **PF** and **NR** monitored at (A) 430 nm and (B) 510 nm. Inset of (B) shows the fluorescence decay corresponding to the emission monitored at 640 nm (λ_{ex} = 375 nm).