

## SUPPORTING INFORMATION

### Protonable Pyrimidine Derivative for White Light Emission

Sylvain Achelle,<sup>a,b</sup> Julián Rodríguez-López,<sup>b</sup> Nolwenn Cabon,<sup>a</sup> and Françoise Robin-le Guen.<sup>a</sup>

<sup>a</sup> Institut des Sciences Chimiques de Rennes UMR CNRS 6226, IUT de Lannion, rue Edouard Branly, BP 30219, F22302 Lannion Cedex, France. E-mail : [sylvain.achelle@univ-rennes1.fr](mailto:sylvain.achelle@univ-rennes1.fr)  
Tel + 33 296 469 446

<sup>b</sup> Facultad de Ciencias y Tecnologías Químicas, Universidad de Castilla-La Mancha, 13071 Ciudad Real, Spain. E-mail: [julian.rodriguez@uclm.es](mailto:julian.rodriguez@uclm.es) Tel + 34 926 295 300

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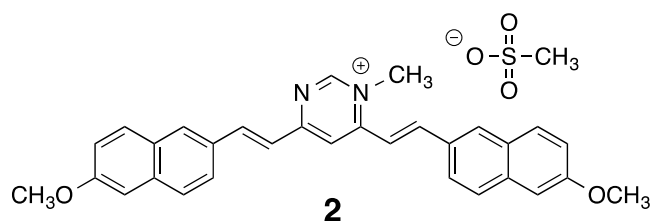
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**General information.**  $^1\text{H}$  NMR and  $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were acquired at room temperature on a Varian Inova-500 instrument. The NMR chemical shifts ( $\delta$ ) are given in ppm and are referenced to the residual protons of the deuterated solvent or carbon nuclei of chloroform ( $^1\text{H}$ ,  $\delta = 7.27$  ppm;  $^{13}\text{C}$ ,  $\delta = 77.0$  ppm) or DMSO ( $^1\text{H}$ ,  $\delta = 2.50$  ppm;  $^{13}\text{C}$ ,  $\delta = 39.5$  ppm). The spectrum of the protonated form of **1** was obtained after adding a few drops of trifluoroacetic acid (large excess) to the NMR tube. UV/vis spectra were recorded on a Jasco V-530 spectrophotometer using standard 1 cm quartz UV cells. Fluorescence spectra were recorded on a Jasco FP-750 spectrofluorimeter. The fluorescence quantum yield ( $\Phi_{\text{F}}$ ) values in solution were calculated by a well-known procedure with two different standards, quinine sulfate in 0.1 M  $\text{H}_2\text{SO}_4$  and 9,10-diphenylanthracene in cyclohexane.<sup>1</sup> The thin film quantum yield measurements were performed using a Horiba Jobin-Yvon Fluorolog III fluorescence spectrometer with a Xe lamp and a Jobin-Yvon integrating sphere ( $\Phi = (E_{\text{c}} - E_{\text{a}})/(L_{\text{a}} - L_{\text{c}})$  with  $E_{\text{c}}$  being the integrated emission spectrum of the sample,  $E_{\text{a}}$  the integrated “blank” emission spectrum,  $L_{\text{a}}$  the “blank” absorption and  $L_{\text{c}}$  the sample absorption at the excitation wavelength). The redox properties were measured by cyclic voltammetry in DMF- $[\text{Bu}_4\text{N}][\text{PF}_6]$ . The working electrode was a glassy carbon disk and the counter electrode was a tungsten wire. A non-aqueous  $\text{Ag}^+/\text{Ag}$  electrode was used as reference. All the potential are quoted against the ferrocenium-ferrocene couple; ferrocene was added as an internal reference at the end of each experiment. Cyclic voltammetry experiments were performed with a  $\mu$ -AUTOLAB III potentiostat monitored by the GPES software (Metrohm). TGA analyses were performed on a TA instruments TGA Q50 under an inert nitrogen atmosphere with a heating rate of  $10\text{ }^\circ\text{C min}^{-1}$ . Compound **1** was obtained as described previously.<sup>2</sup> Films were prepared from 50 mg/10 mL solutions of polystyrene (MW 35000) in  $\text{CH}_2\text{Cl}_2$  doped with 1 wt% of compound **1**. The films were deposited by spraying the volatile solution on glass substrates preheated between 80 and  $120\text{ }^\circ\text{C}$  using an airbrush. The process was carried out in conventional environment (air) under chemical hood.

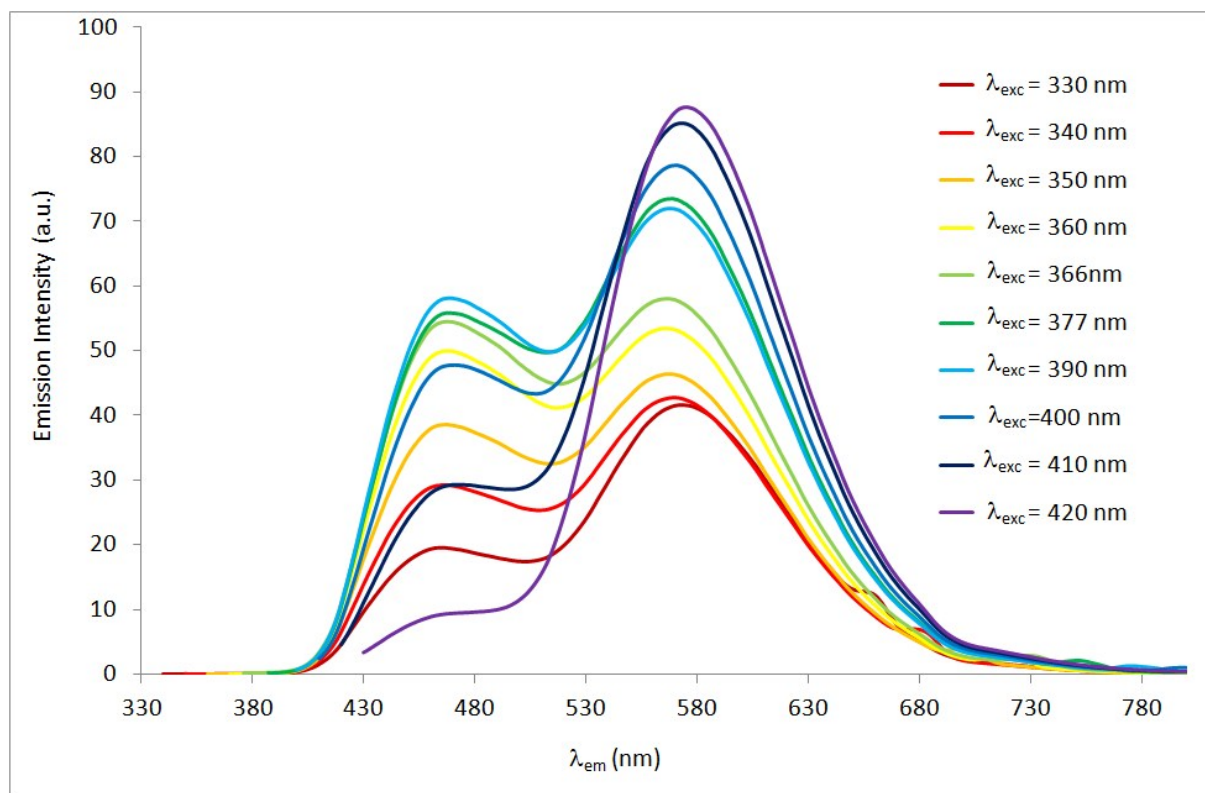
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<sup>1</sup> D. F. Eaton, *Pure Appl. Chem.*, 1988, **60**, 1107–1114.

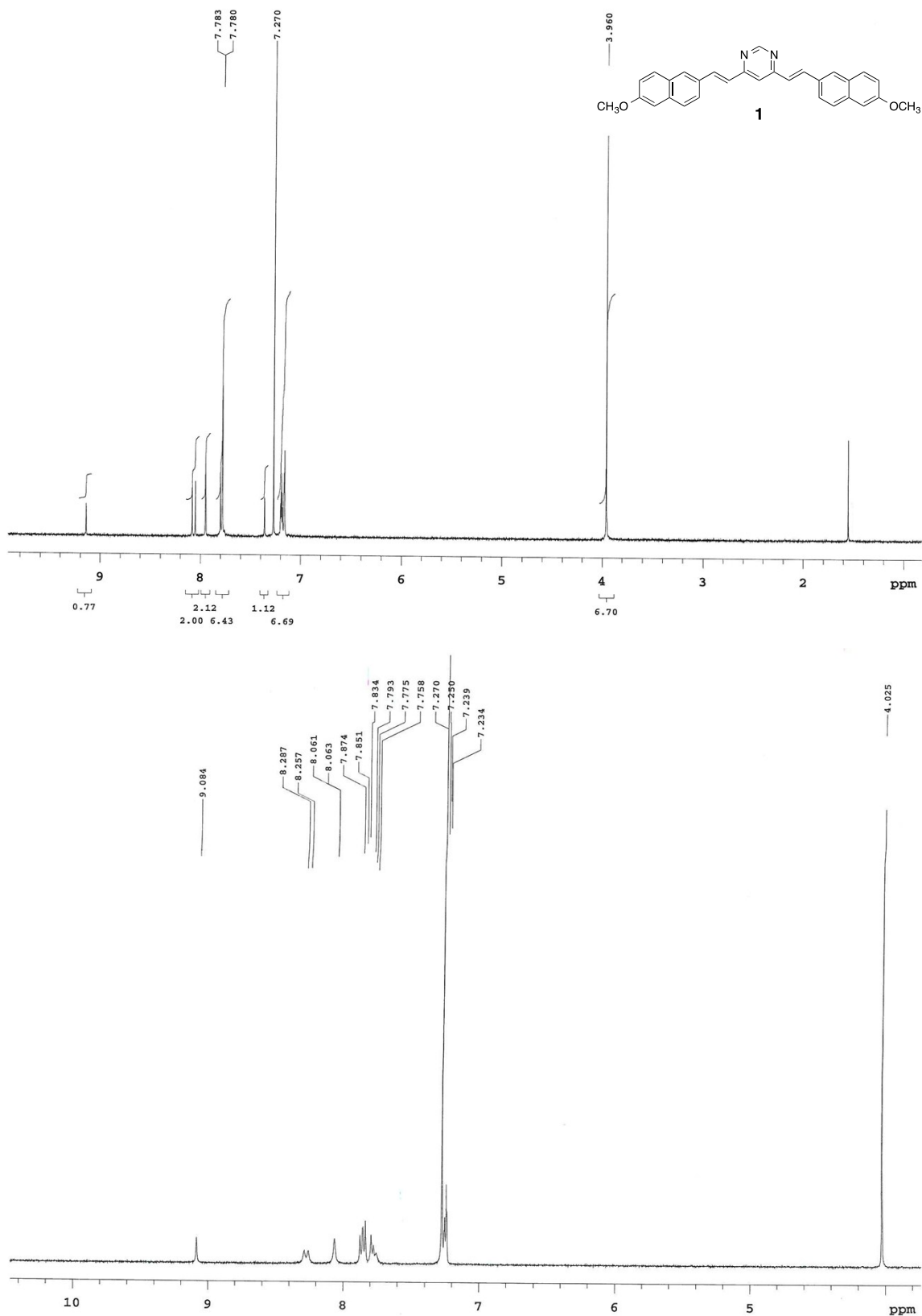
<sup>2</sup> S. Achelle, I. Nouira, B. Pfaffinger, Y. Ramondenc, N. Plé and J. Rodríguez-López, *J. Org. Chem.*, 2009, **74**, 3711-3717.



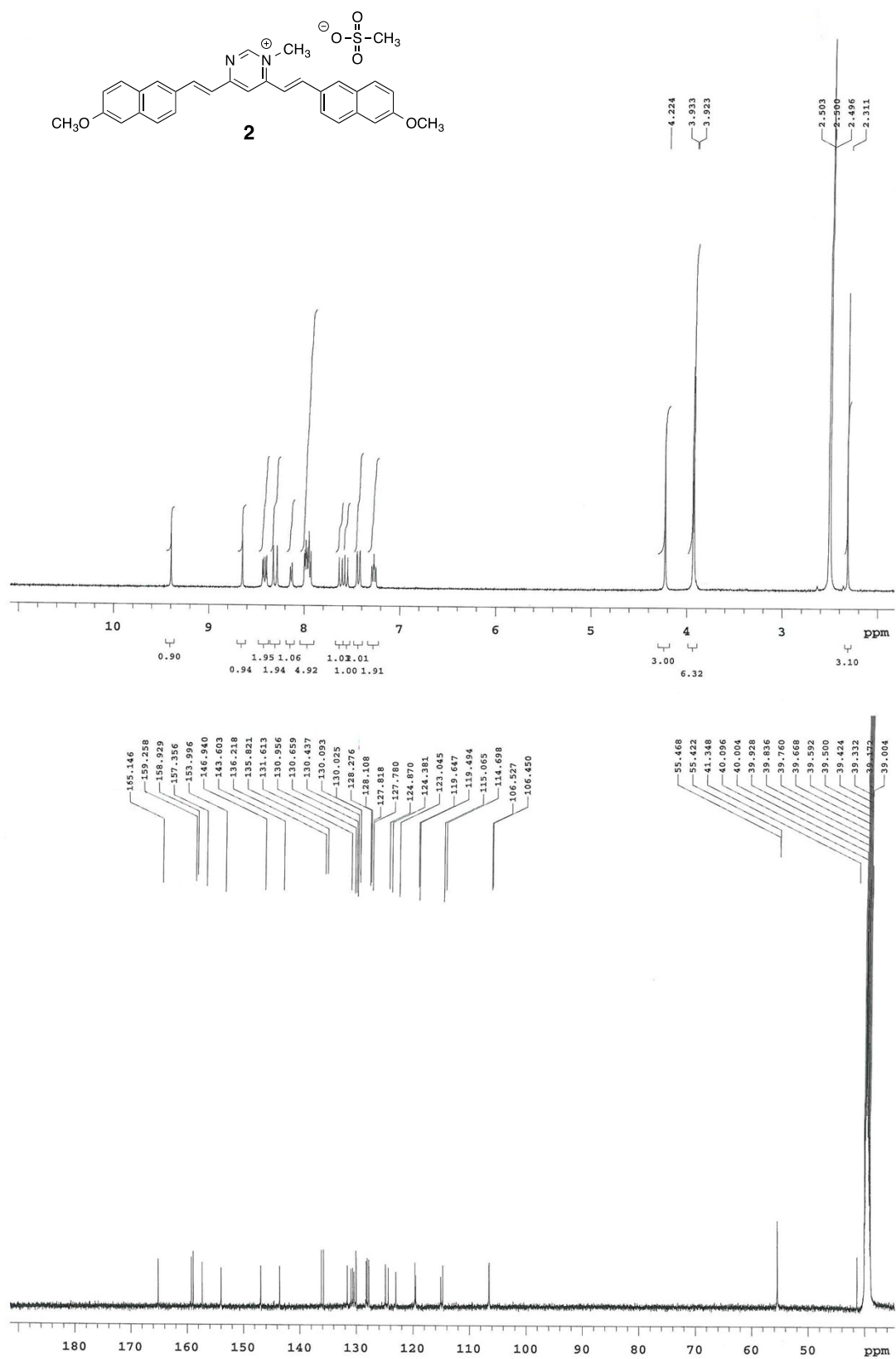
**Preparation of (*E,E*)-*N*-methyl-4,6-bis[2-(6-methoxynaphthalen-2-yl)vinyl]pyrimidinium methanesulfonate (**2**).** A mixture of 80 mg (0.18 mmol) of the pyrimidine derivative **1** and 1 mL of methyl methanesulfonate was heated at 90 °C and stirred for 30 h. After cooling, diethyl ether was added and the insoluble solid was filtered off and washed several times with more diethyl ether to remove the excess of reagent. After drying under vacuum, 95 mg (96%) of the title compound was obtained as a deep red solid. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ: 2.31 (s, 3H, CH<sub>3</sub>SO<sub>3</sub><sup>-</sup>), 3.92 (s, 3H, OCH<sub>3</sub>), 3.93 (s, 3H, OCH<sub>3</sub>), 4.22 (s, 3H, NCH<sub>3</sub>), 7.27 (m, 2H, ArH), 7.42 (d, 1H, *J* = 2.5 Hz, ArH), 7.45 (d, 1H, *J* = 2.5 Hz, ArH), 7.56 (A of AB<sub>q</sub>, 1H, *J* = 16.0 Hz, CH=), 7.62 (A of AB<sub>q</sub>, 1H, *J* = 16.0 Hz, CH=), 7.93-8.00 (m, 5H, ArH), 8.13 (dd, 1H, *J* = 8.5 Hz, *J* = 1.5 Hz, ArH), 8.28 (s, 1H, ArH), 8.32 (s, 1H, ArH), 8.41 (B of AB<sub>q</sub>, 1H, *J* = 16.0 Hz, CH=), 8.42 (B of AB<sub>q</sub>, 1H, *J* = 16.0 Hz, CH=), 8.65 (s, 1H, ArH), 9.40 (s, 1H, ArH). <sup>13</sup>C NMR and DEPT (DMSO-*d*<sub>6</sub>, 125 MHz) δ: 39.8 (CH<sub>3</sub>SO<sub>3</sub><sup>-</sup>), 41.3 (NCH<sub>3</sub>), 55.4 (OCH<sub>3</sub>), 55.5 (OCH<sub>3</sub>), 106.4 (CH), 106.5 (CH), 114.7 (CH), 115.1 (CH), 119.5 (CH), 119.6 (CH), 123.0 (CH), 124.4 (CH), 124.9 (CH), 127.8 (CH), 127.8 (CH), 128.1 (C), 128.3 (C), 130.0 (C), 130.1 (C), 130.4 (CH), 130.7 (CH), 131.0 (CH), 131.6 (CH), 135.8 (C), 136.2 (C), 143.6 (CH), 146.9 (CH), 154.0 (CH), 157.4 (C), 158.9 (C), 159.3 (C), 165.1 (C).



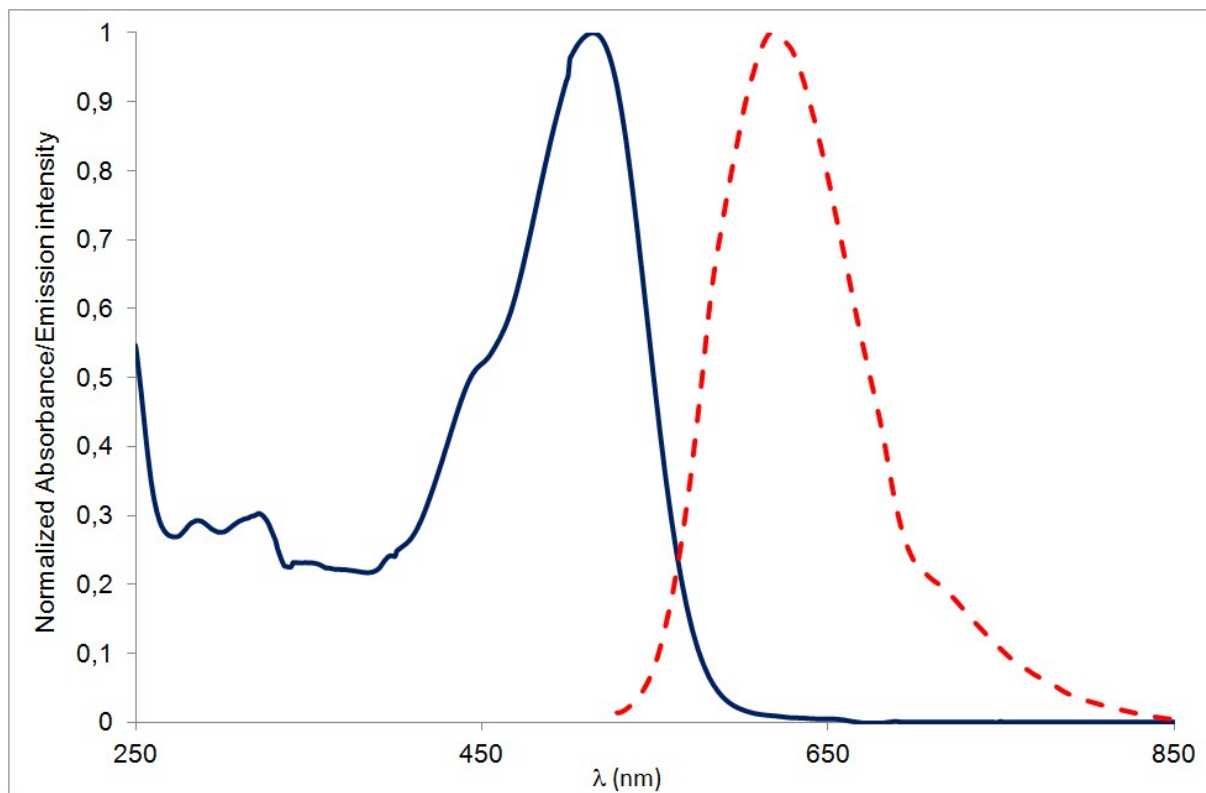
**Figure S1.** Emission spectra of **1** in  $\text{CH}_2\text{Cl}_2$  ( $c = 8.8 \cdot 10^{-3} \text{ M}$ ) with 100 equivalents of TFA by changing excitation wavelength.



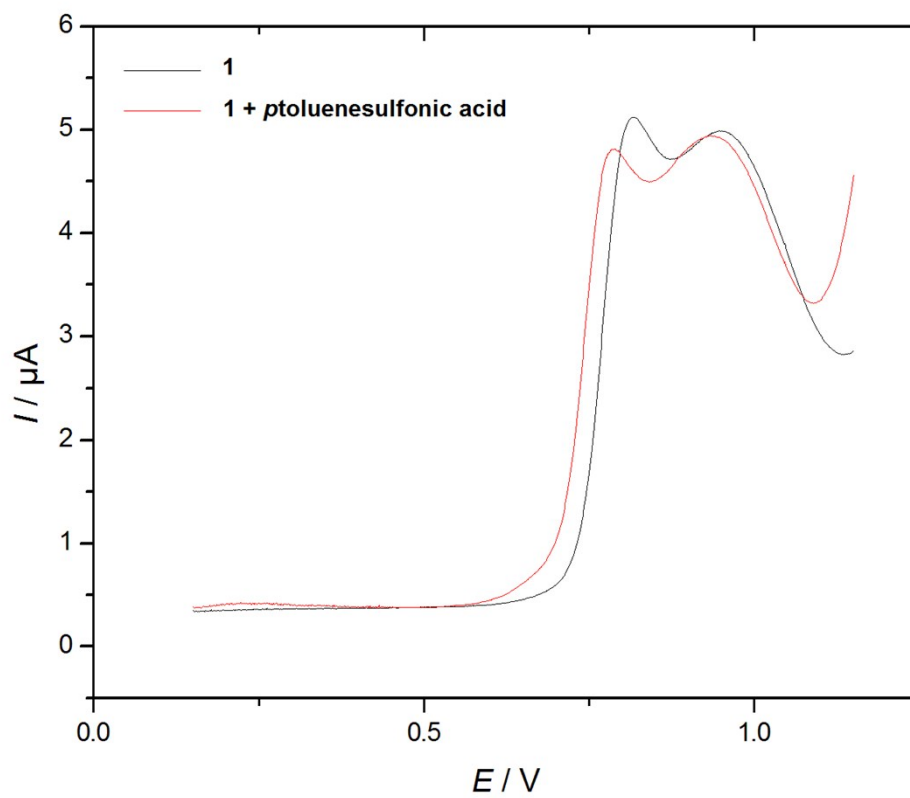
**Figure S2.** <sup>1</sup>H NMR spectra of compound **1** before (top) and after (bottom) adding a few drops (large excess) of TFA (CDCl<sub>3</sub>, 500 MHz).



**Figure S3.** <sup>1</sup>H (top) and <sup>13</sup>C NMR (bottom) spectra of compound **2** (DMSO-d<sub>6</sub>, 500 MHz).

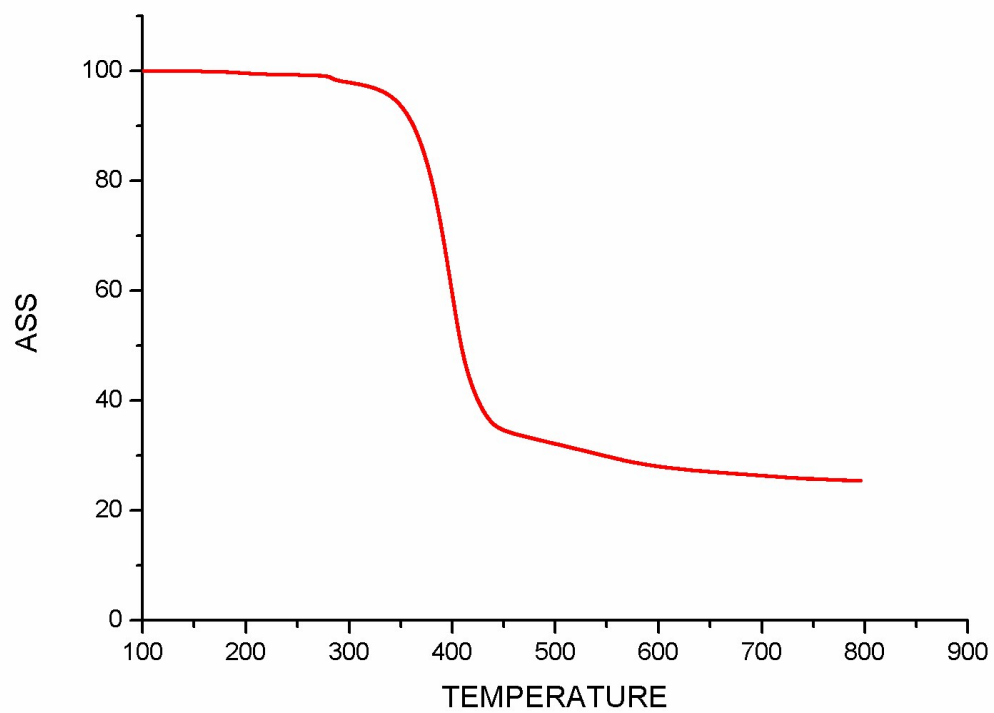


**Figure S4.** Normalized absorption and emission spectra of compound **2** in CH<sub>2</sub>Cl<sub>2</sub>.  $\lambda_{\text{abs}} = 286$ , 321 and 515 nm;  $\lambda_{\text{em}} = 618$  nm.



**Figure S5.** Differential pulse voltammetry for compound **1** ( $c = 1.5 \text{ mM}$ ).  $\nu = 0.1 \text{ V s}^{-1}$ .  $E \text{ (V)}$  vs  $\text{Fc}^+/\text{Fc}$ .





**Figure S6.** TGA plot for compound **1** under an inert nitrogen atmosphere (heating rate: 10 °C min<sup>-1</sup>).