

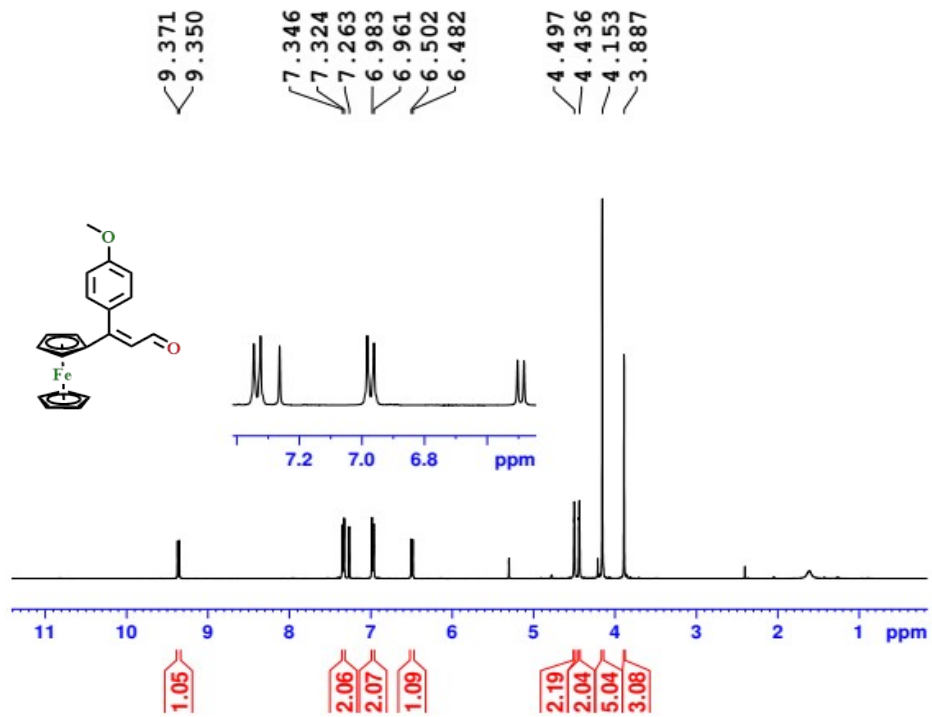
**Enhancement of photovoltaic performance in ferrocenyl  $\pi$ -extended multi donor- $\pi$ -acceptor (D-D'- $\pi$ -A) dyes using chenodeoxycholic acid as a dye co-adsorbent for dye sensitized solar cells**

Selvam Prabu<sup>a</sup>, Thamodharan Viswanathan<sup>a</sup>, Ezhumalai David<sup>a</sup>, Sivanadanam Jagadeeswari<sup>b</sup> and Nallasamy Palanisami<sup>a\*</sup>

<sup>a</sup>Centre for Functional Materials, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India.

<sup>b</sup>Clean Energy Lab, Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India.

Corresponding author: E-mail: palanisami.n@gmail.com; palanisami.n@vit.ac.in



**Figure S1.** <sup>1</sup>H NMR spectrum of 3, 3 (4-

methoxyphenyl) ferrocenyl acrylaldehyde  
in CDCl<sub>3</sub> at 25 °C

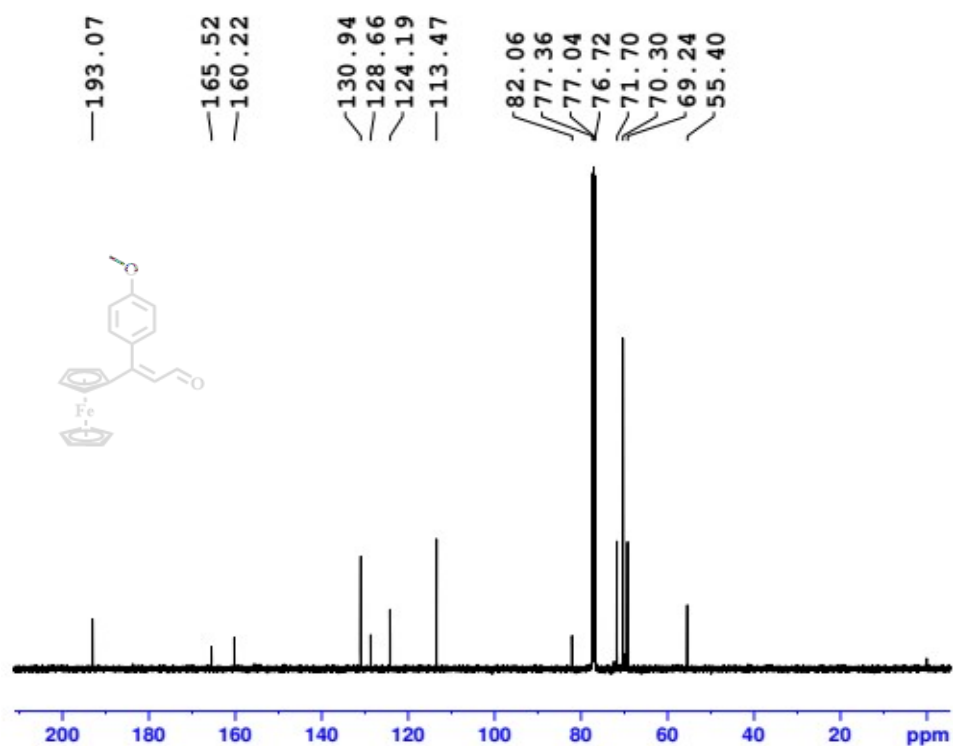


Figure S2. <sup>13</sup>C NMR spectrum of 3,3-(4-methoxyphenyl) ferrocenyl acrylaldehyde in CDCl<sub>3</sub> at 25 °C

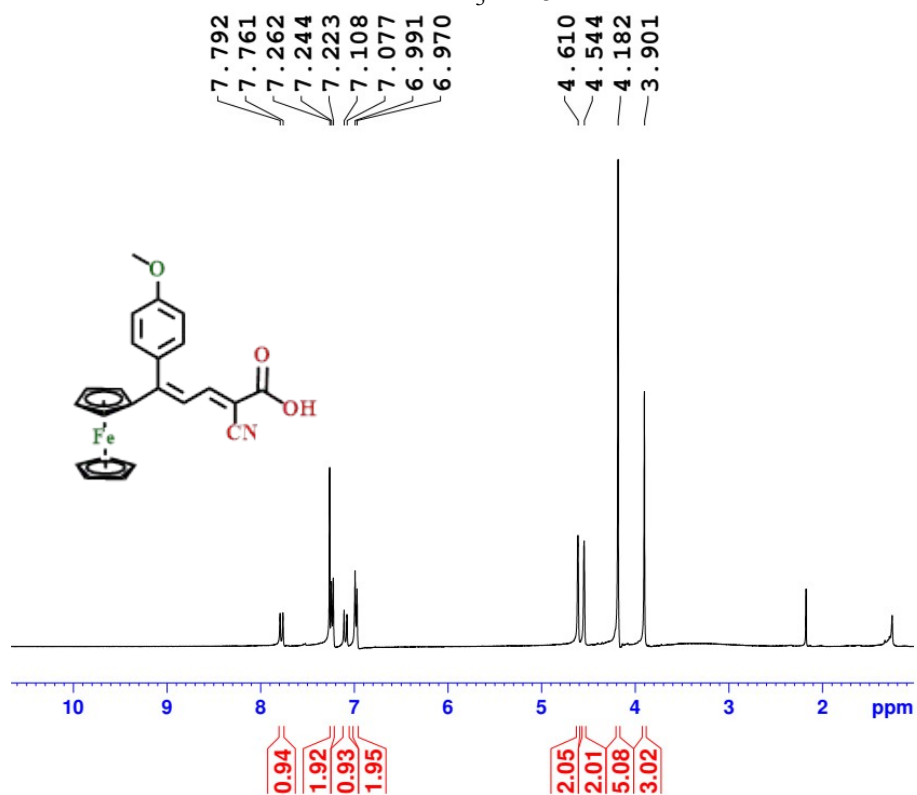


Figure S3.  $^1\text{H}$  NMR spectrum of dye **1** in  $\text{CDCl}_3$  at  $25^\circ\text{C}$

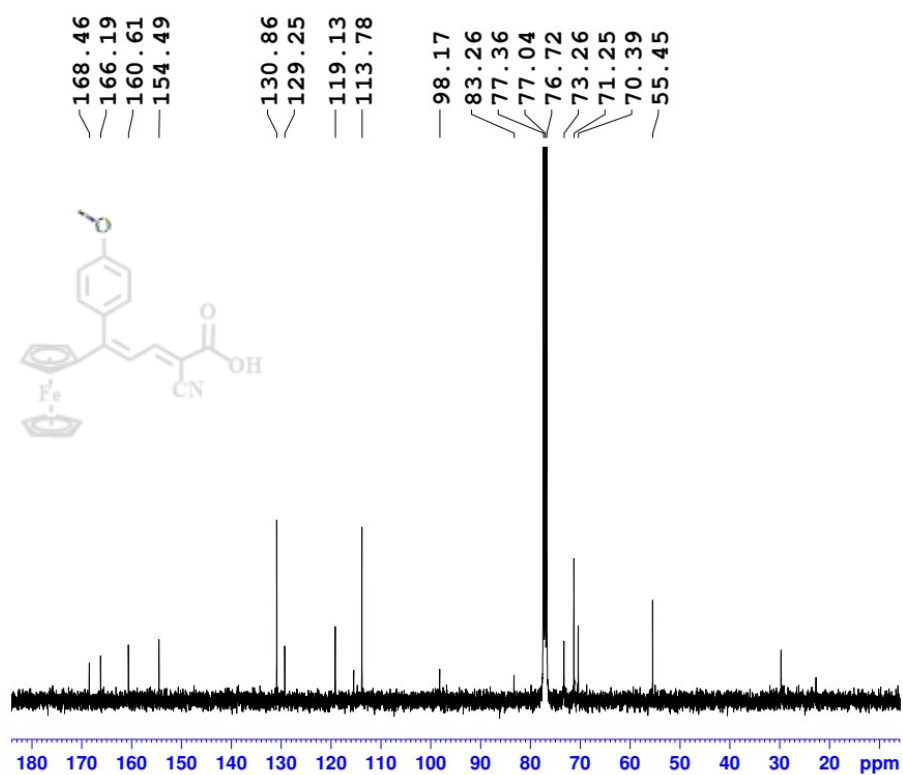
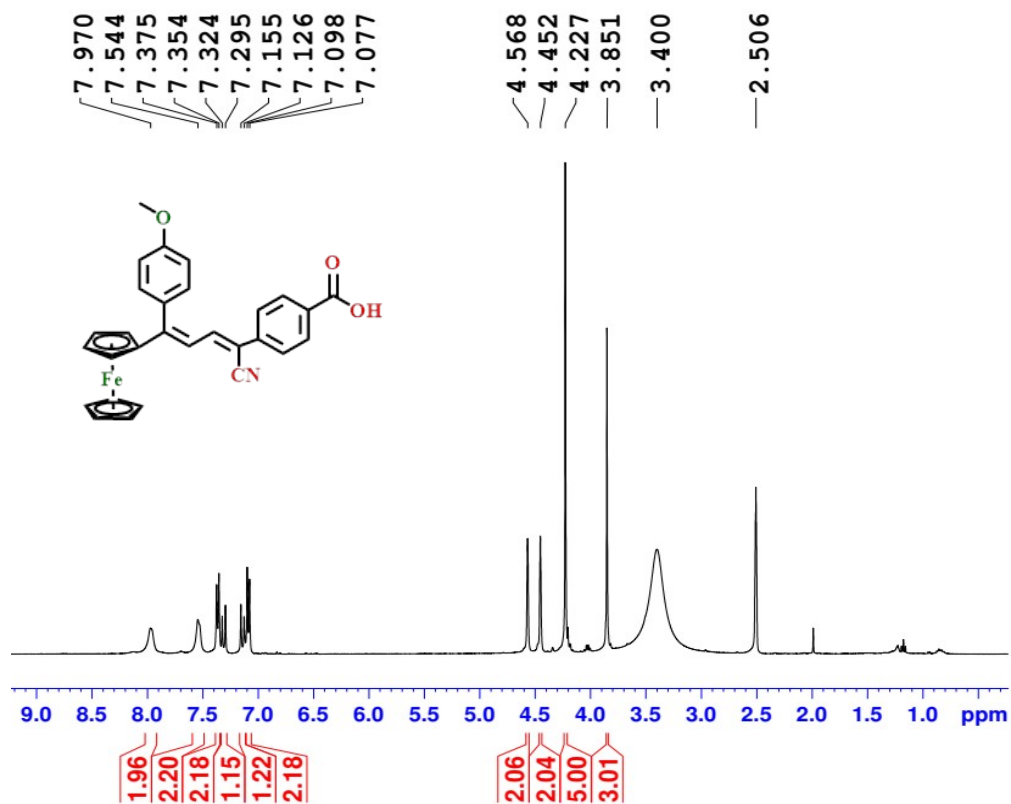
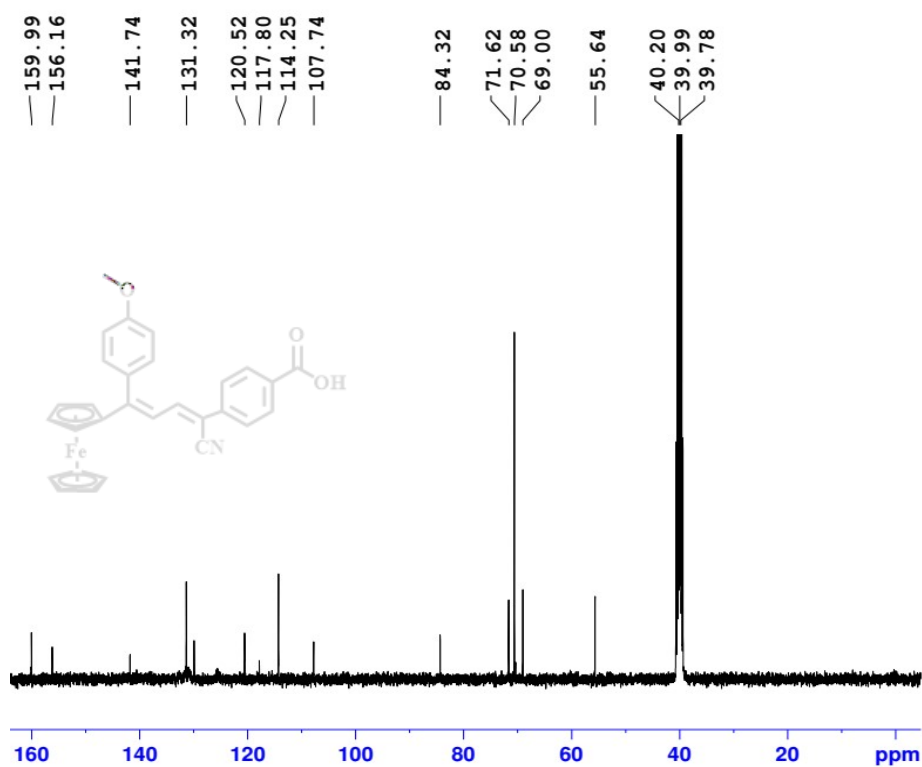


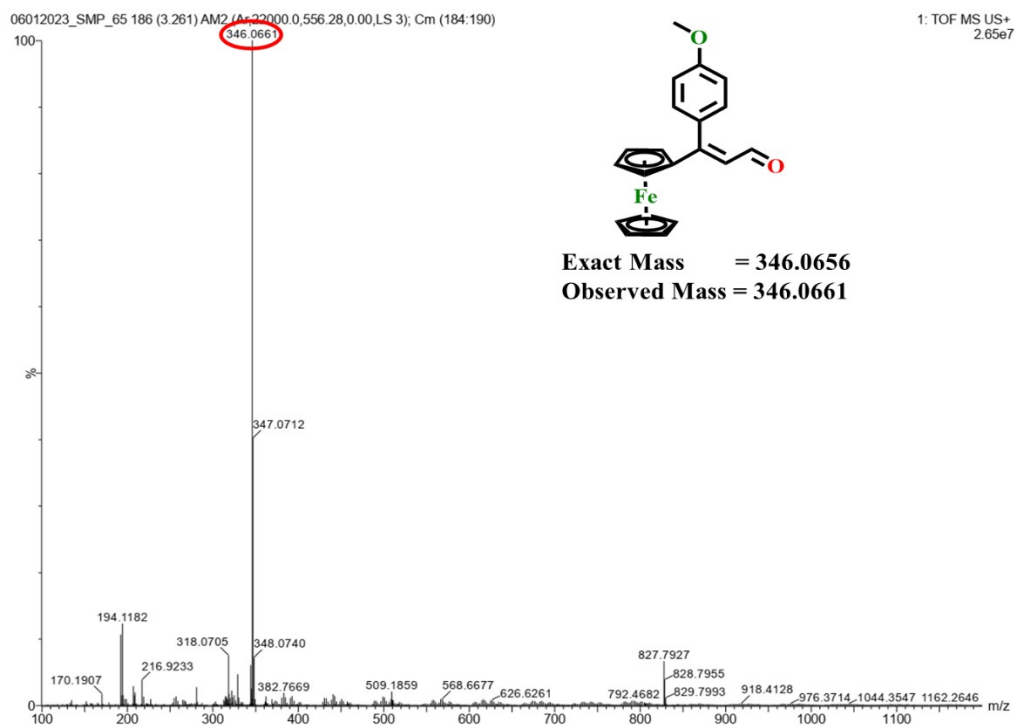
Figure S4.  $^1\text{H}$  NMR spectrum of dye **1** in  $\text{CDCl}_3$  at  $25^\circ\text{C}$



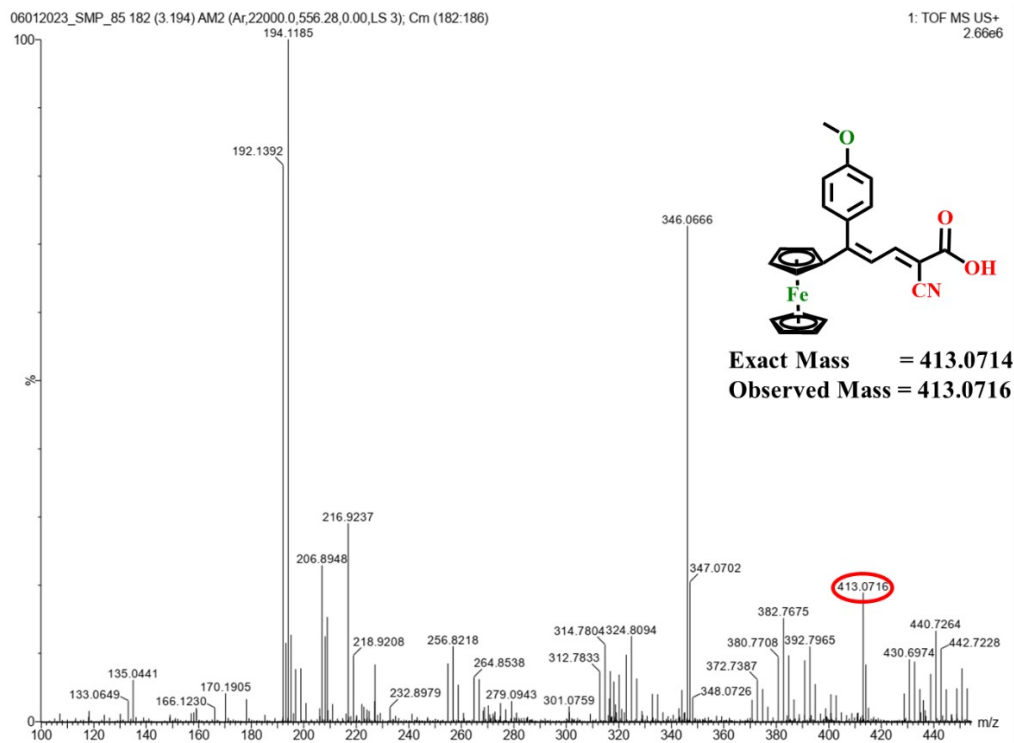
**Figure S5.**  $^1\text{H}$  NMR spectrum of dye **2** in  $\text{DMSO-d}_6$  at  $25^\circ\text{C}$



**Figure S6.**  $^{13}\text{C}$  NMR spectrum of dye **2** in  $\text{DMSO-d}_6$  at  $25^\circ\text{C}$



**Figure S7.** HR-Mass spectrum of 3, 3 (4-methoxyphenyl) ferrocenyl acrylaldehyde.



**Figure S8.** HR-Mass spectrum of dye 1.

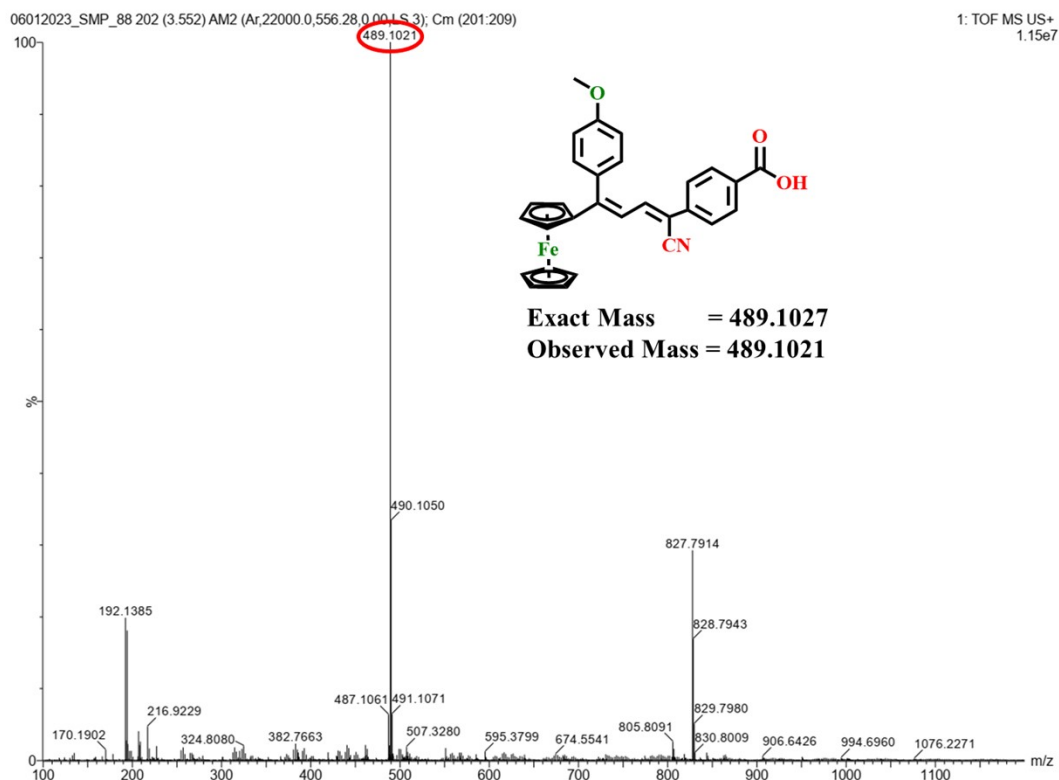


Figure S9. HR-Mass spectrum of dye 2.

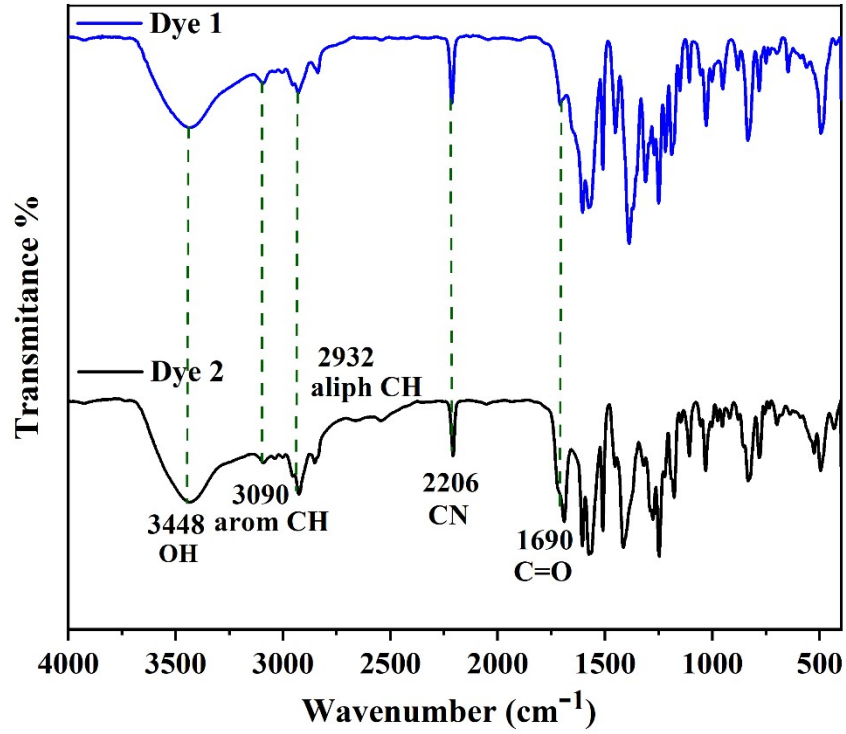


Figure S10. FT-IR spectra of dyes 1 and 2.

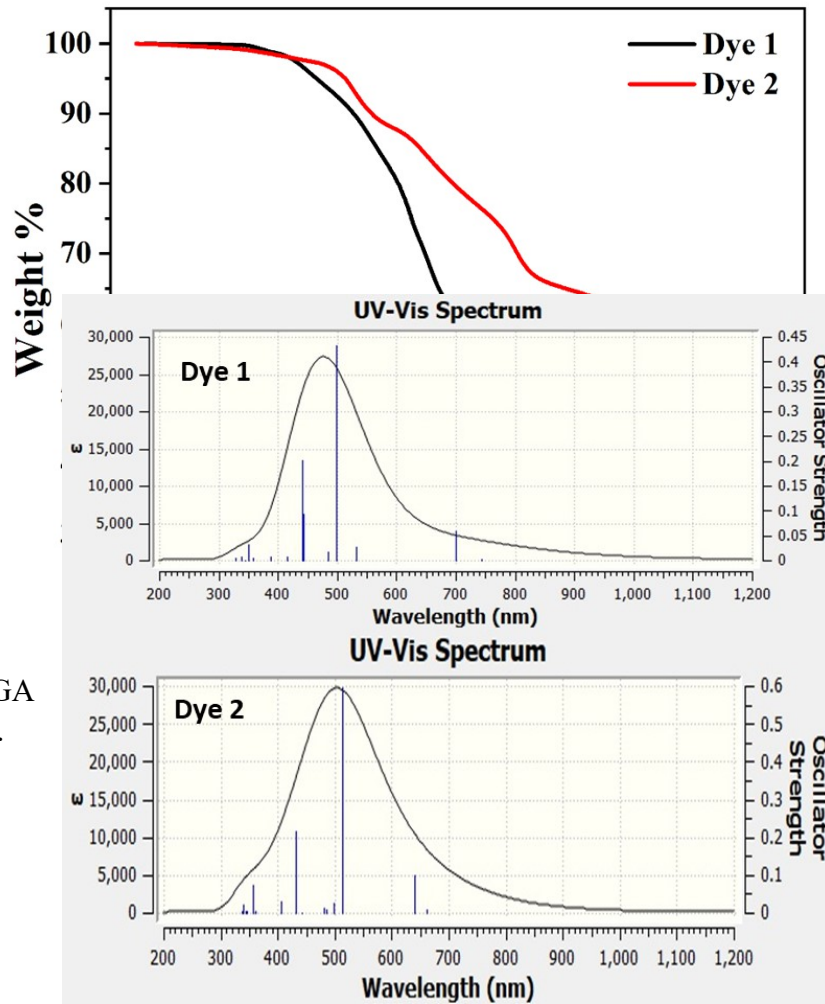


Figure S11. TGA dyes 1 and 2.

curve of the

**Figure S12.** Theoretically calculated absorption spectra for dyes **1** and **2**. The absorption spectra were obtained by TD-DFT calculation with B3LYP/6-31+G(d,p)/LanL2TZf level of theory. The spectra were visualized in Gauss View 6.1.

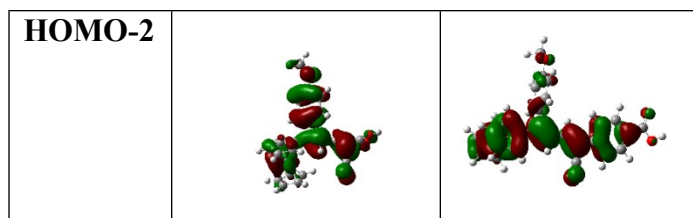
**Table S1.** Selected transitions obtained from TD-DFT calculation with B3LYP/6-31+G(d,p)/LanL2TZf level of theory.

Entry	$\lambda$ (nm)	Oscillator strength, $f$	Energy (eV)	Selected Major Transitions <sup>a</sup>
<b>Dye 1</b>	497	0.4317	2.49	H-2 $\rightarrow$ L (79%)
	441	0.2014	2.81	H-4 $\rightarrow$ L (32%)
	699	0.0580	1.77	H $\rightarrow$ L (86%)
	350	0.0314	3.54	H-6 $\rightarrow$ L (39%)
	531	0.0261	2.33	H-3 $\rightarrow$ L (56%)
	484	0.0175	2.55	H $\rightarrow$ L+3 (32%)
<b>Dye 2</b>	513	0.5953	2.41	H-2 $\rightarrow$ L (65%)
	431	0.2158	2.87	H-3 $\rightarrow$ L (63%)
	640	0.1014	1.93	H $\rightarrow$ L (58%)
	356	0.0745	3.47	H $\rightarrow$ L+1 (84%)
	406	0.0290	3.06	H-4 $\rightarrow$ L (54%)
	339	0.0198	3.65	H-6 $\rightarrow$ L (43%)
	485	0.0100	2.55	H-1 $\rightarrow$ L+6 (32%)
661	0.0068	1.87	H-1 $\rightarrow$ L (71%)	

<sup>a</sup> H = HOMO; L = LUMO; only contributions above 10% are included.

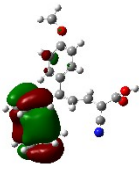
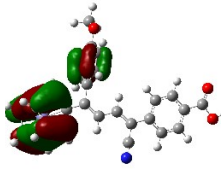
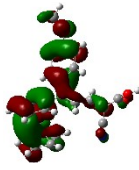
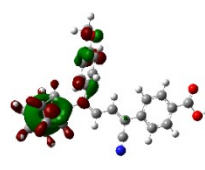
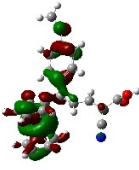
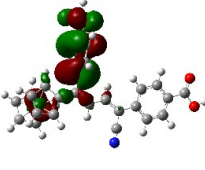


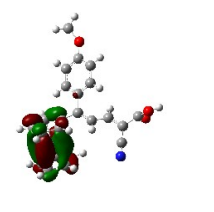
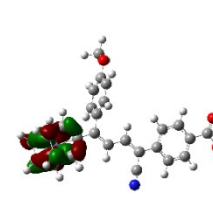
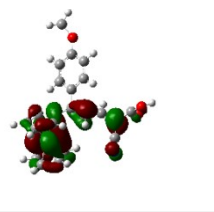
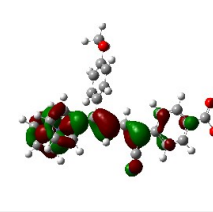
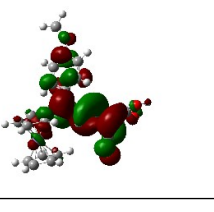
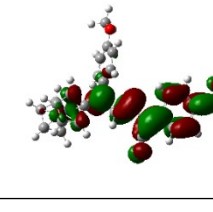
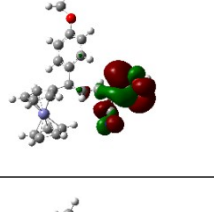
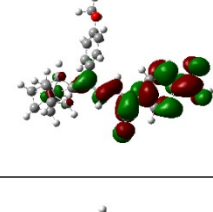
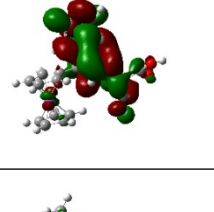
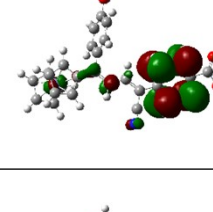
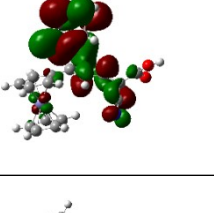
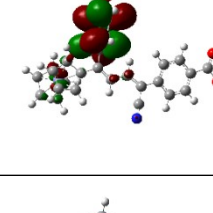
**Table S2.** Density frontier orbitals electronic chromophores **1** derived from



surfaces of the involved in transitions of **2** which is B3LYP/6-

31+G(d,p)/LanL2TZf level of theory using isosurface value of 0.02 au.

<b>Orbitals</b>	<b>Dye 1</b>	<b>Dye 2</b>
<b>HOMO-5</b>		
<b>HOMO-4</b>		
<b>HOMO-3</b>		

<b>HOMO-1</b>		
<b>HOMO</b>		
<b>LUMO</b>		
<b>LUMO+1</b>		
<b>LUMO+2</b>		
<b>LUMO+3</b>		
<b>LUMO+4</b>	