Supporting Information

Photoinduced Energy Transfer in Carbazole-BODIPY Dyads

Govind Reddy,[a] Naresh Duvva, [a] Sairaman Seetharaman,[b] Francis D'Souza*[b], Lingamallu Giribabu*[a]

[a]Polymers & Functional Materials Division, CSIR-Indian Institute of Chemical Technology, Tarnaka, Hyderabad 500007, TS, India
[b]Department of Chemistry, University of North Texas, 1155 Union Circle, #305070, Denton, TX 76203-5017, USA
giribabu@iict.res.in (ORCID: 0000-0001-5936-7729); francis.dsouza@unt.edu (ORCID: 0000-0003-3815-8949)

Table of Contents		Page No.
Fig. S1	^{1}H NMR spectrum of Compound **(CB1)** in $CDCl_3$	S2
Fig. S2	^{1}H NMR spectrum of Compound **(CB2)**in $CDCl_3$	S2
Fig. S3	^{1}H NMR spectrum of Compound **(CB3)** in $CDCl_3$	S3
Fig. S4	^{13}C NMR spectrum of Compound **(CB1)** in $CDCl_3$	S3
Fig. S5	^{13}C NMR spectrum of Compound **(CB2)** in $CDCl_3$	S4
Fig. S6	^{13}C NMR spectrum of Compound **(CB3)** in $CDCl_3$	S4
Fig. S7	MALDI-MS spectrum of Compound **(CB1)**	S5
Fig. S8	MALDI-MS spectrum of Compound **(CB2)**	S6
Fig. S9	MALDI-MS spectrum ofCompound **(CB3)**	S6
Fig. S10	Differential pulse voltammograms of oxidation of the indicated compounds in CH_2Cl_2 containing 0.1 M $(n\text{-}C_4H_9)_4NClO_4$. The concentra-tions of the dyads were held at 1 mM; scan rate = 100 mVs^{-1}.	
Fig. S11	Theoretical and Experimental UV-Visible spectra of CB1, CB2 and CB3 in dichloromethane solvent.	S7
Fig. S12	Overlay of the absorption (——) and excitation (———) spectra of the dyads.	S8
Fig. S13	Fluorescence decay curves of **C0**, **B0**, **CB1**, **CB2**, and **CB3** (λ_{ex} = 300 and 485 nm) in Toluene, DCM, and acetonitrile solvents.	S10
Fig. S14	Femtosecond transient absorption spectra of **B0** excited at 340nm in toluene.	S10
Fig. S15	Femtosecond transient absorption spectra of **C0** excited at 339nm in Toluene.	S11
Table S1	Comparison of the experimental optical properties with the theoretical data by B3LYP in dichloromethane.	S11

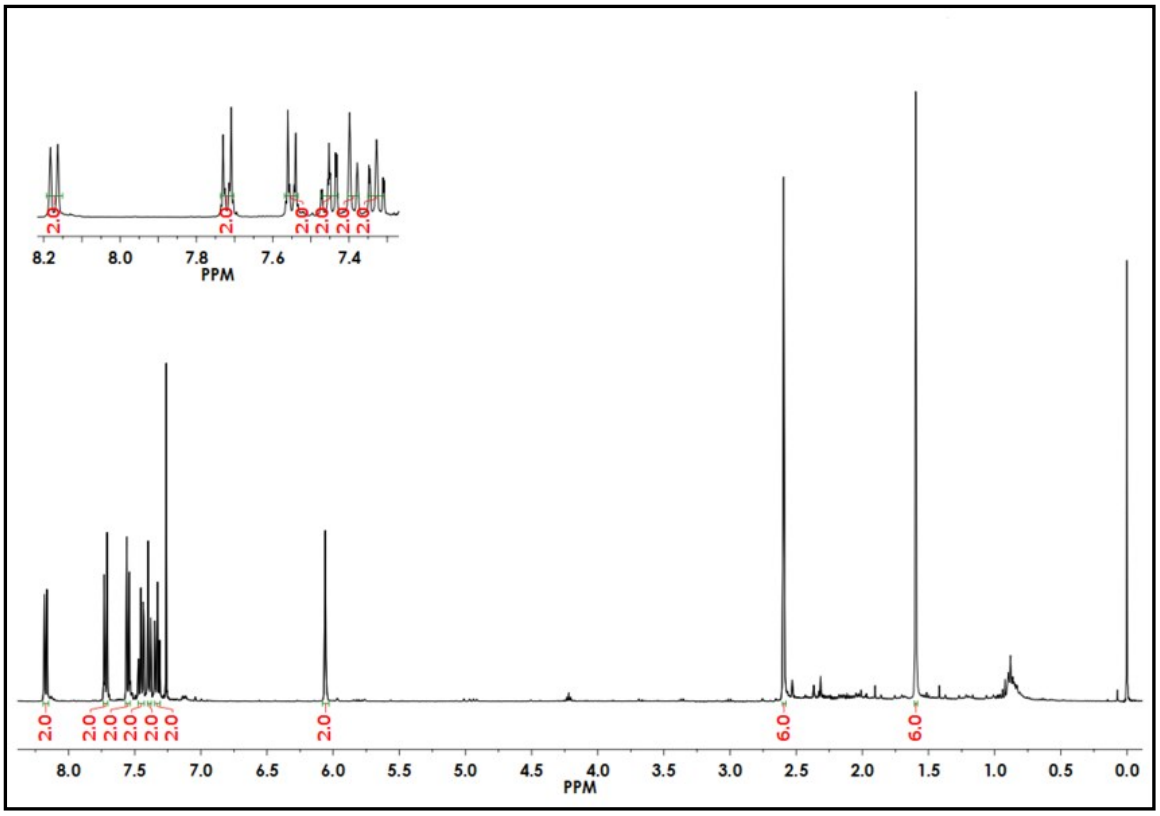

Figure S1. ^{1}H NMR spectrum of Compound **(CB1)** in $CDCl_3$.

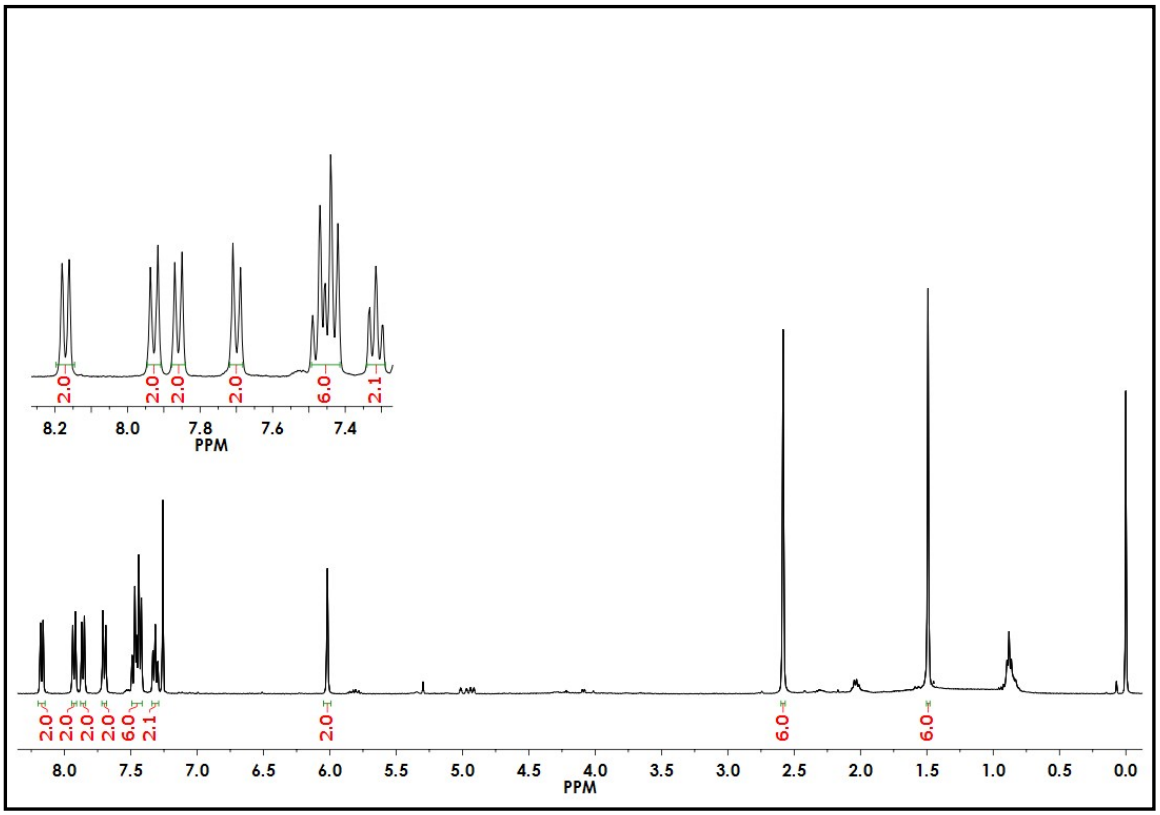

Figure S2. ^{1}H NMR spectrum of Compound **(CB2)** in $CDCl_3$.

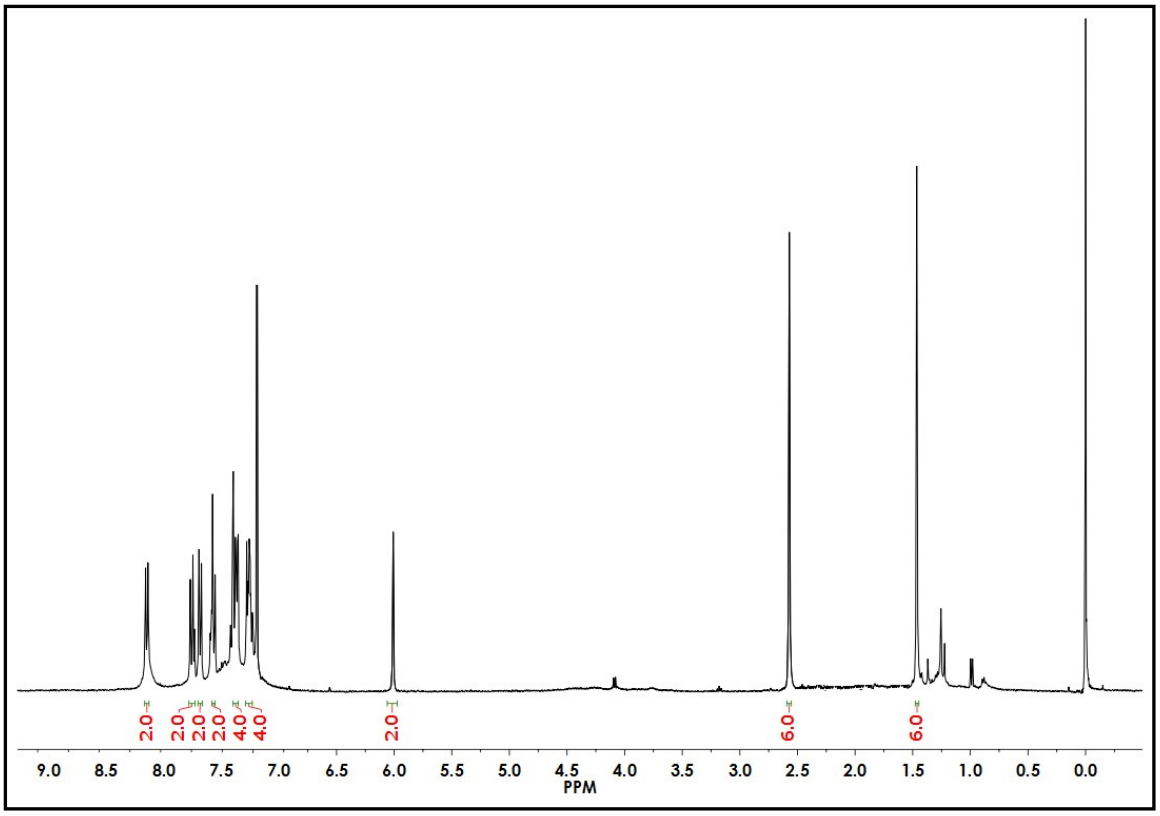

Figure S3. ^{1}H NMR spectrum of Compound **(CB3)** in $CDCl_3$.

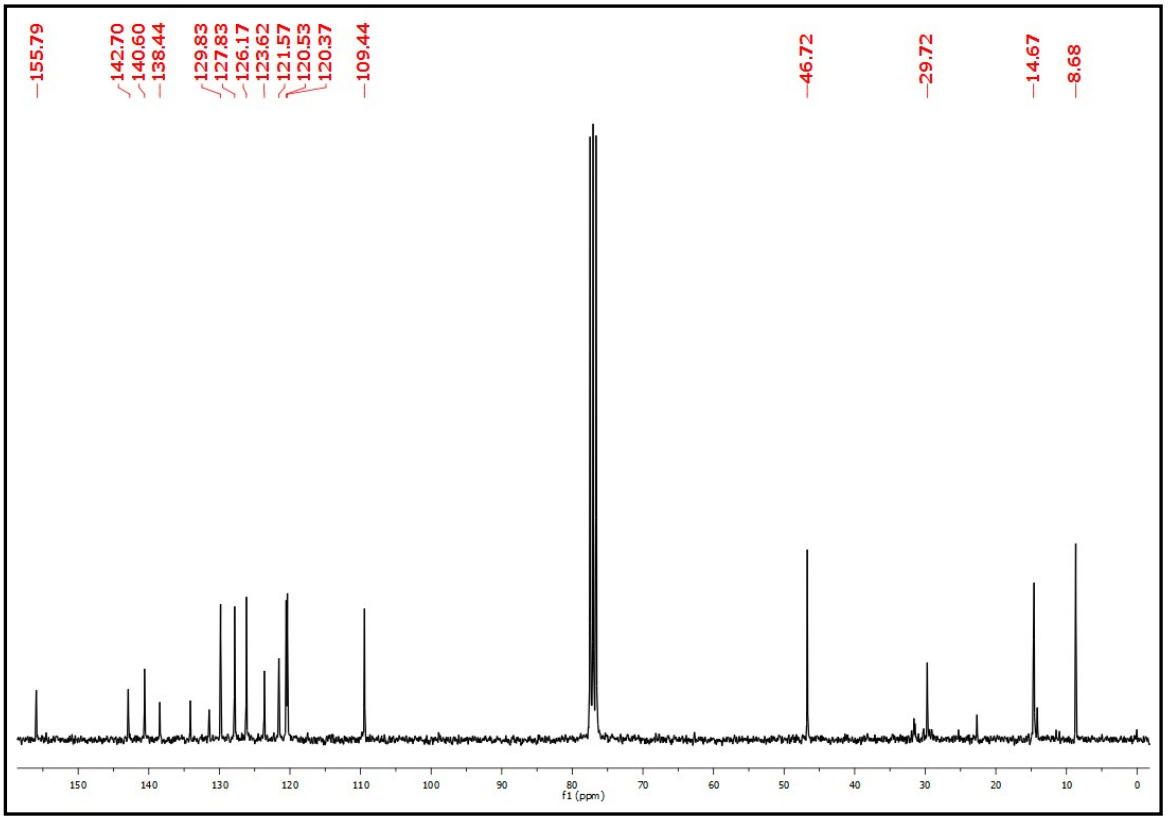

Figure S4. ^{13}C NMR spectrum of Compound **(CB1)** in $CDCl_3$.

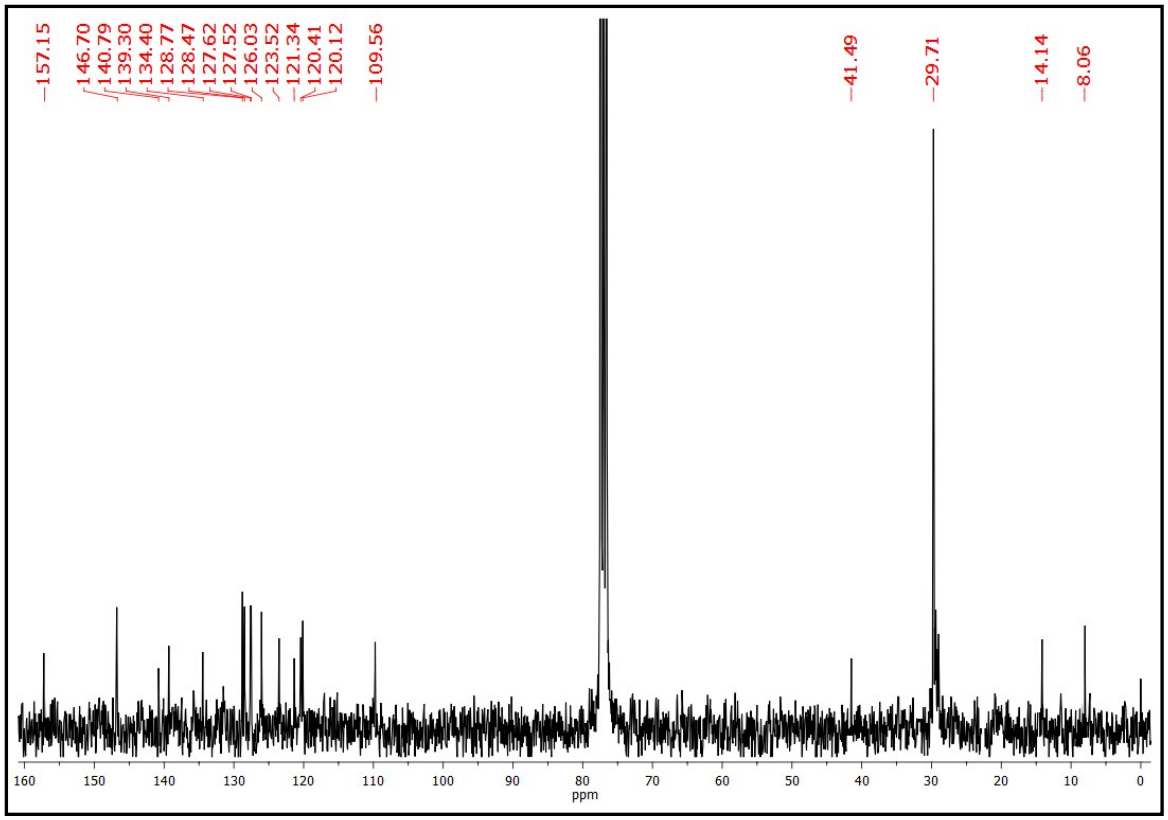

Figure S5. ^{13}C NMR spectrum of Compound **(CB2)** in $CDCl_3$.

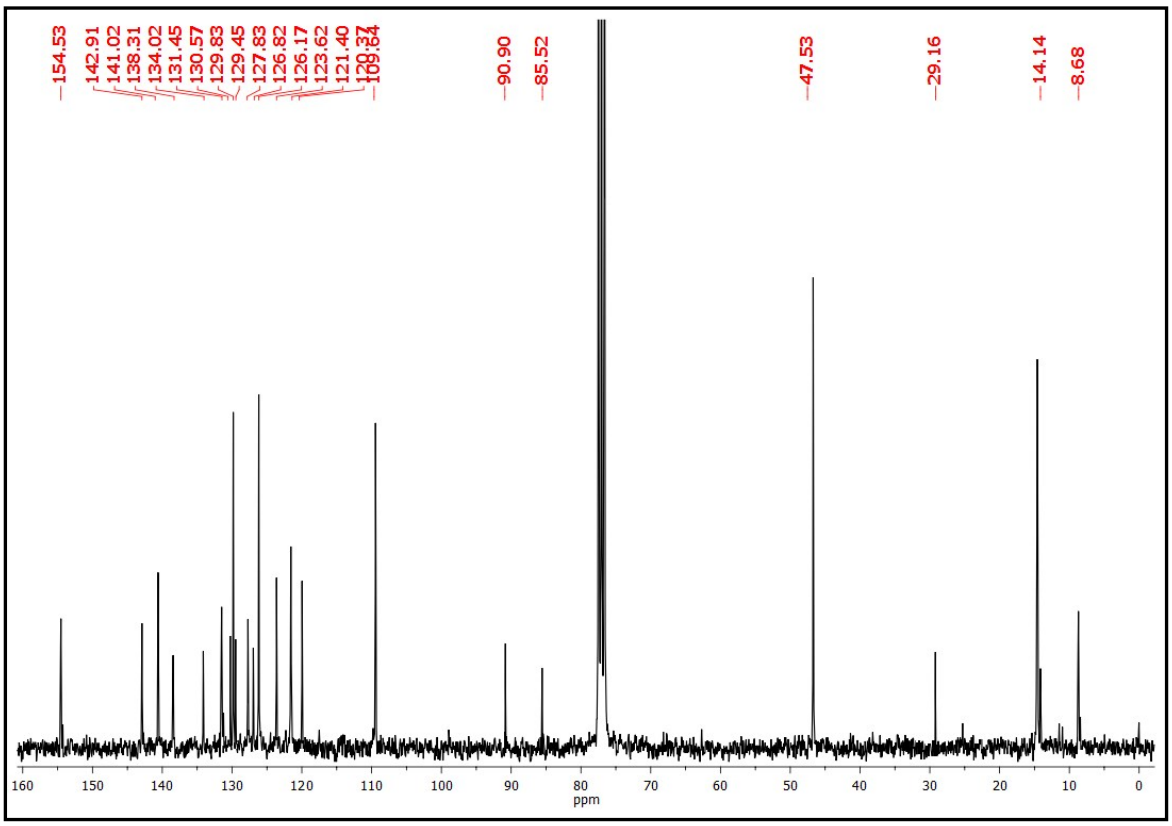

Figure S6. ^{13}C NMR spectrum of Compound **(CB3)** in $CDCl_3$.

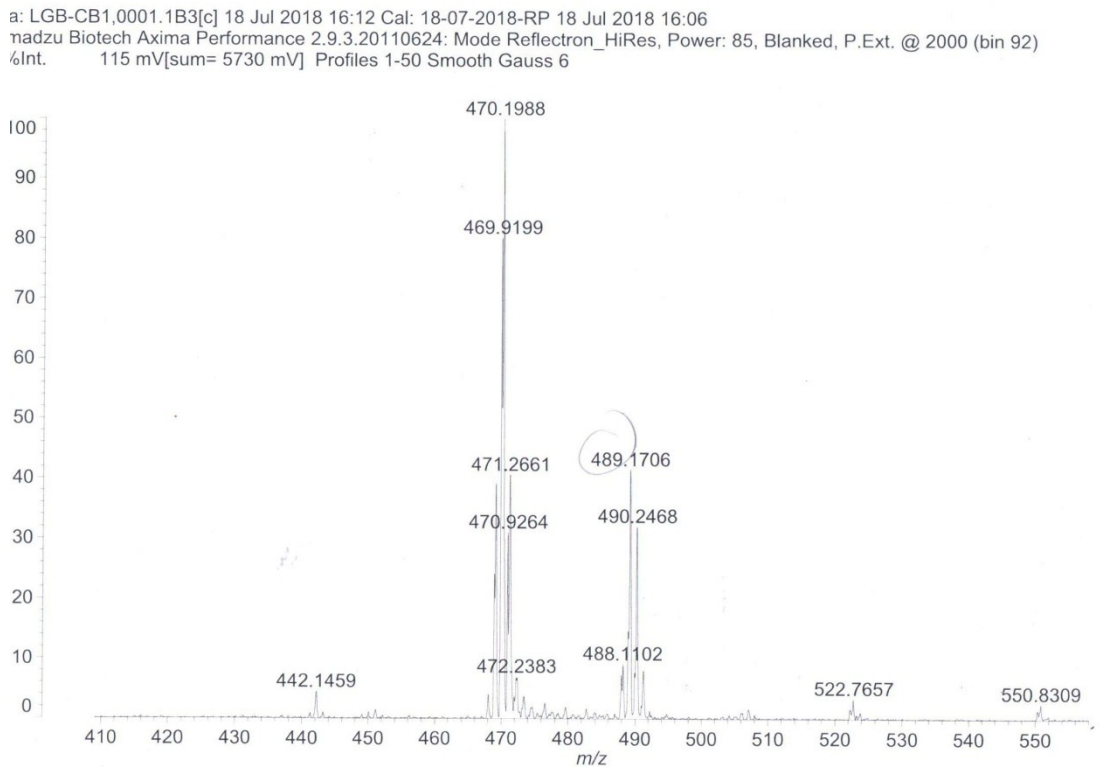

Figure S7.MALDI-MS spectrum of Compound **(CB1)**.

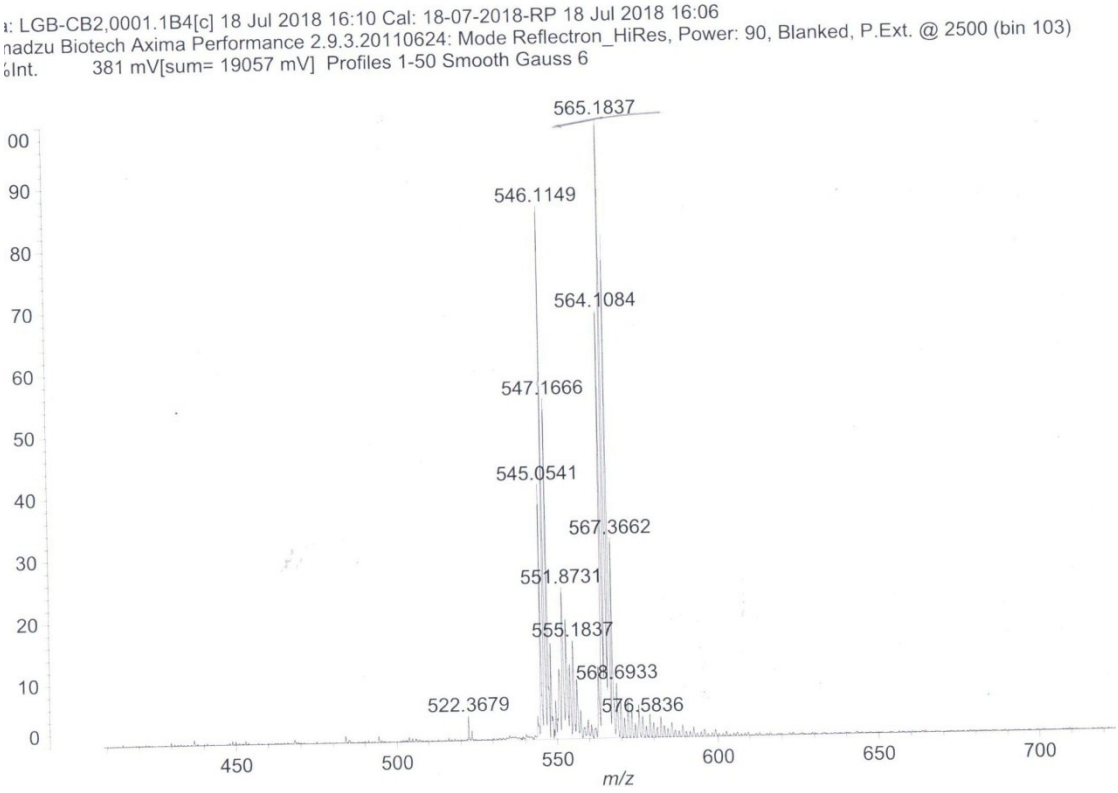

Figure S8. MALDI-MS spectrum of Compound **(CB2)**.

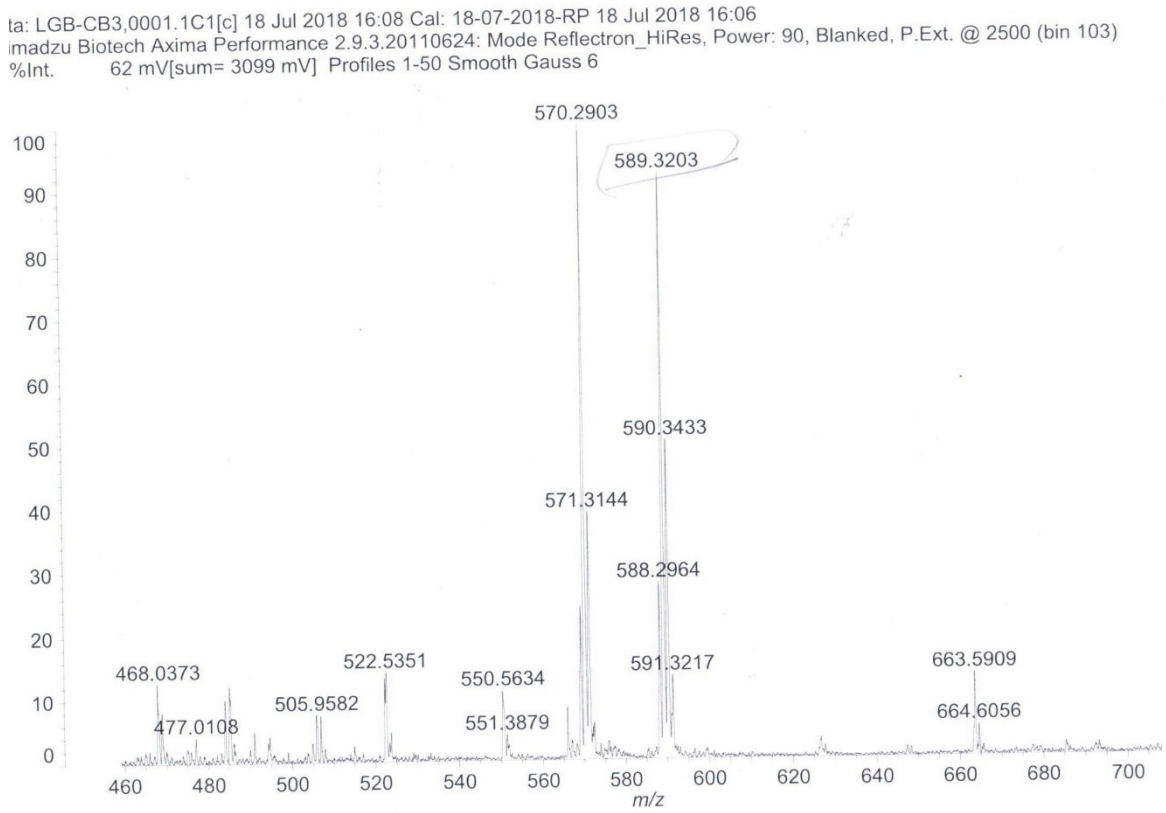

Figure S9. MALDI-MS spectrum of Compound **(CB3)**.

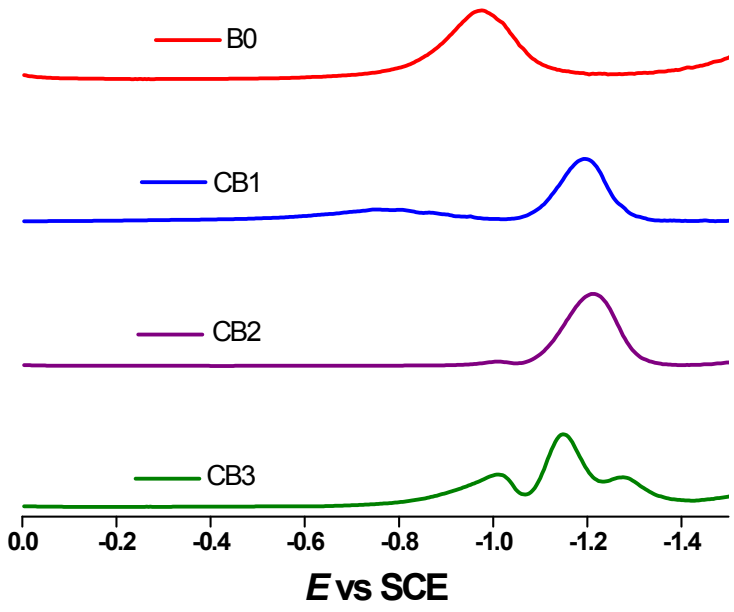

Figure S10. Differential pulse voltammograms of oxidation of the indicated compounds in CH_2Cl_2 containing 0.1 M $(n\text{-}C_4H_9)_4NClO_4$. The concentra-tions of the dyads were held at 1 mM; scan rate = 100 mVs^{-1}.

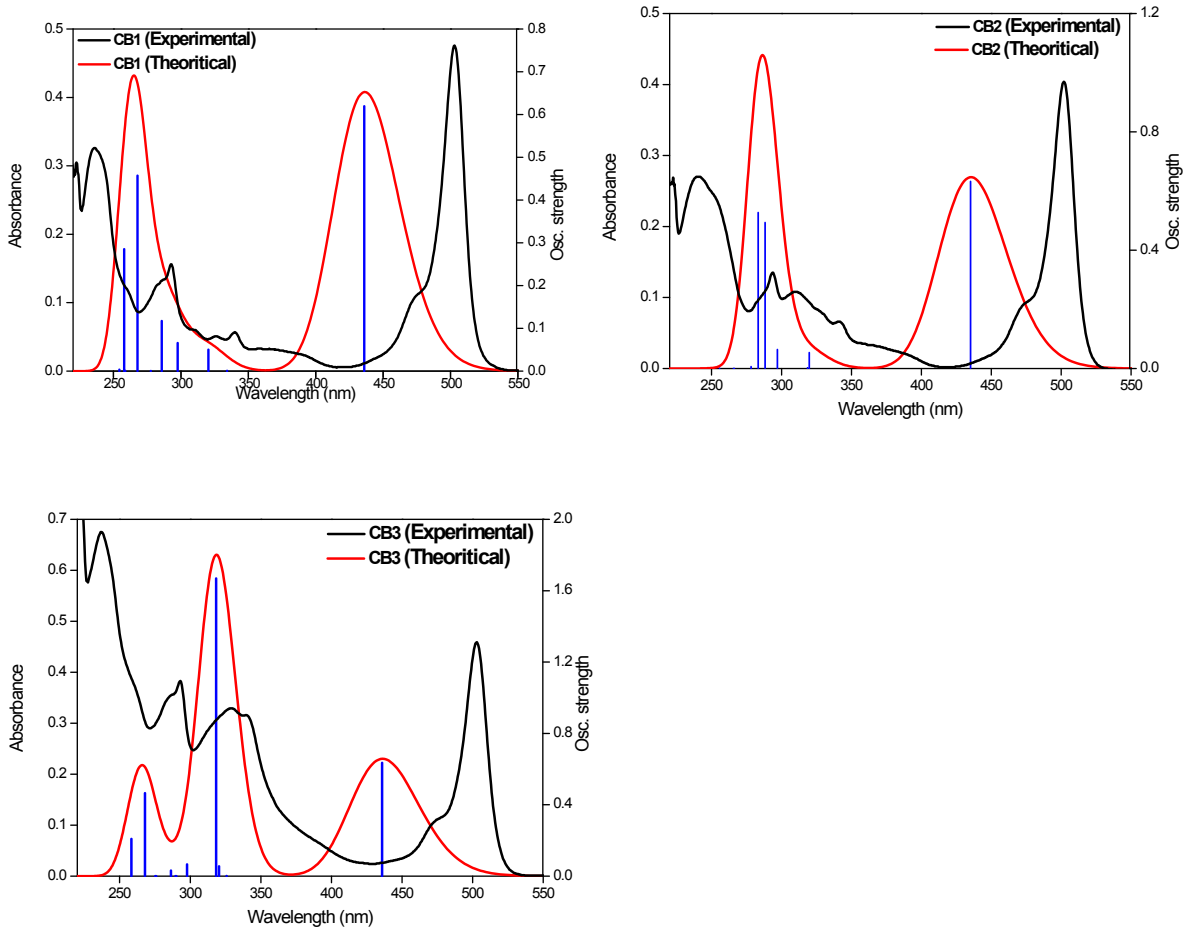

Figure11. Theoretical and Experimental UV-Visible spectra of CB1, CB2 and CB3 in dichloromethane solvent.

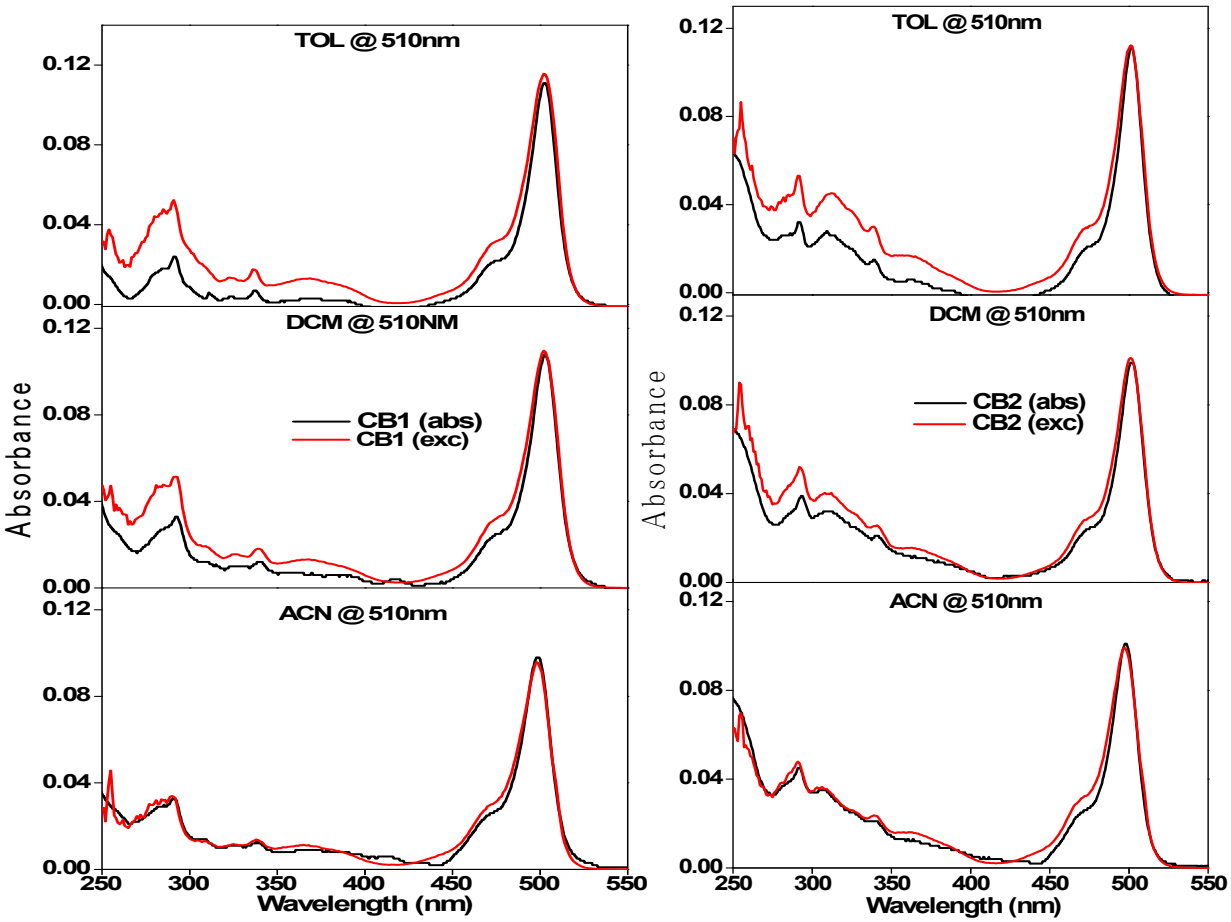

Figure S12. Overlay of the absorption (——) and excitation (———) spectra of the dyads.

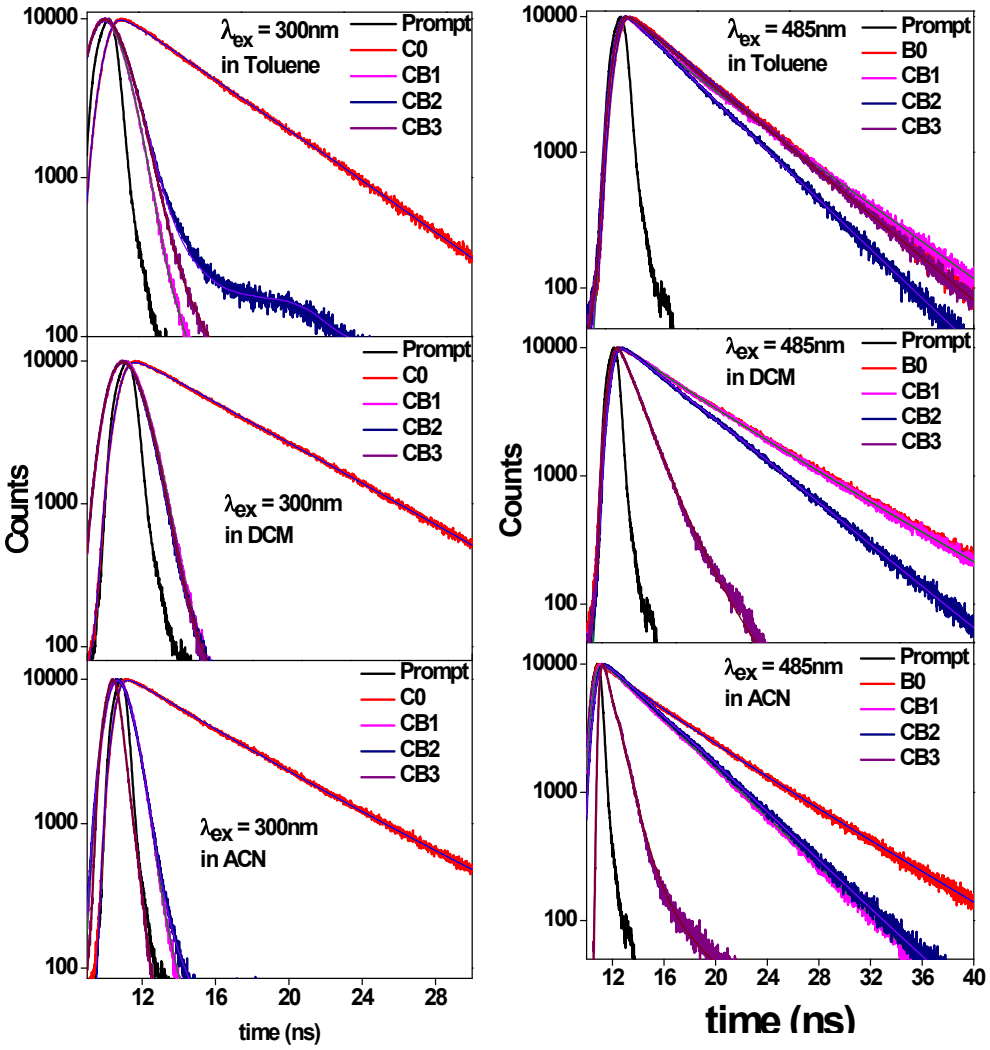

Figure S12. Fluorescence decay curves of **C0**, **B0**, **CB1**, **CB2**, and **CB3** (λ_{ex} = 300 and 485 nm) in Toluene, DCM, and acetonitrile solvents.

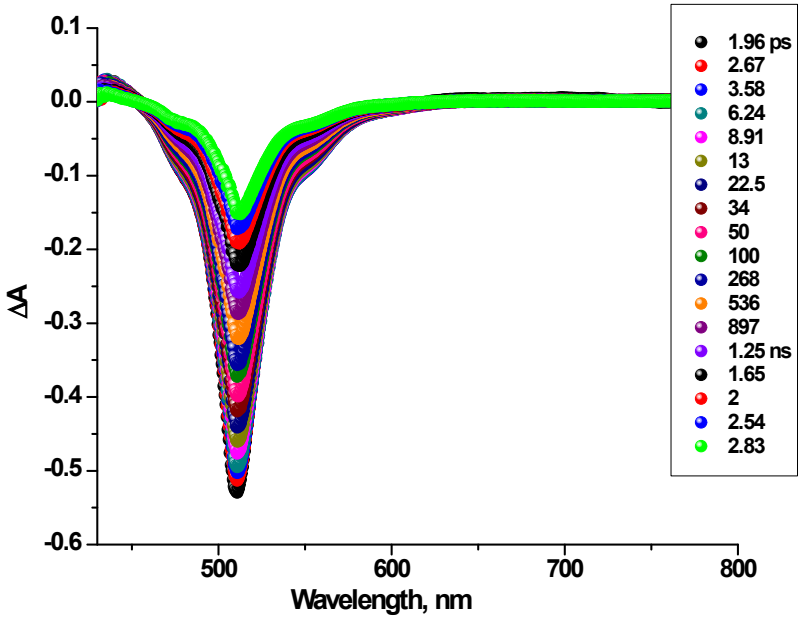

Figure S13. Femtosecond transient absorption spectra of B0 excited at 502nm in toluene.

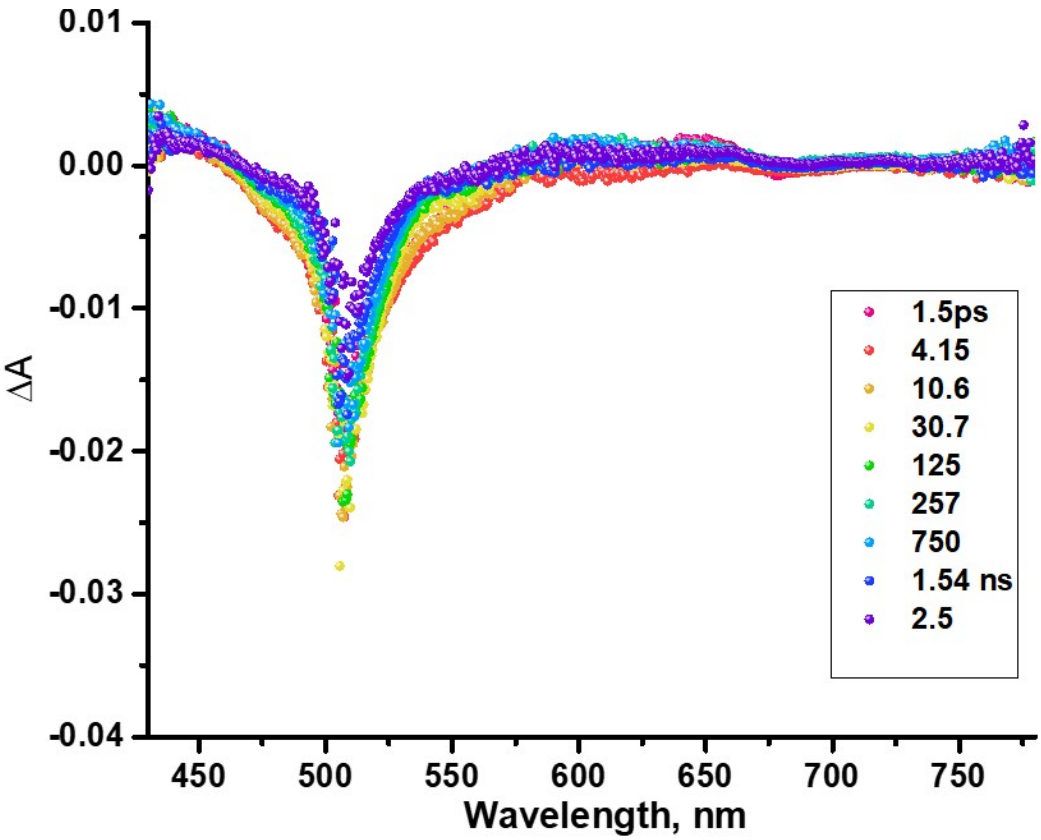

Figure S14. Femtosecond transient absorption spectra of B0 excited at 340nm in toluene.

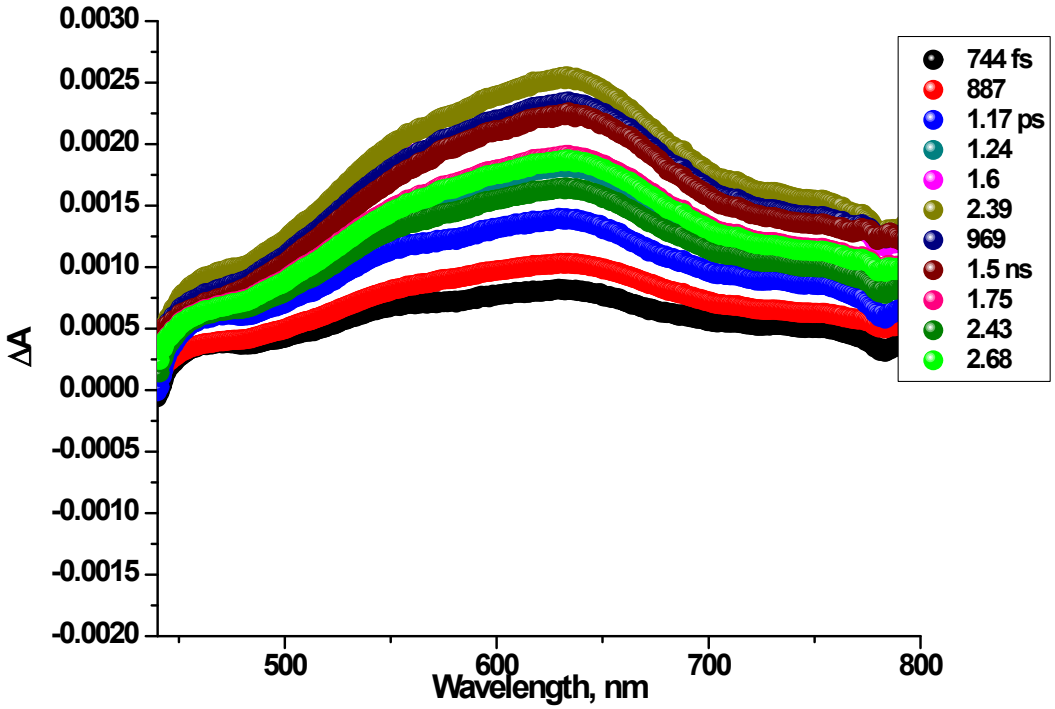

Figure S15. Femtosecond transient absorption spectra of C0 excited at 339nm in Toluene.

Table S1. Comparison of the experimental optical properties with the theoretical data by B3LYP in dichloromethane.

Dye	[a]λ_{max}	[b]λ_{max}	[c]f	[d] **E (eV)**	**% of Molecular Orbital Composition**
CB1	503	436	0.6193	2.843	HOMO->LUMO (98%)
CB2	502	435	0.6324	2.849	HOMO->LUMO (98%)
CB3	503	436	0.6353	2.844	HOMO->LUMO (98%)

[a]Recorded absorbance in nm, [b] theoretical absorbance in nm, [c] Oscillation strength, and [d] excited state energy in eV.