Supporting Information for:

Thiol-Activated Triplet-Triplet Annihilation Upconversion: Study of the Different Quenching Effect of Electron Acceptor on the Singlet and Triplet Excited States of Bodipy

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1. Molecular structural characterization data

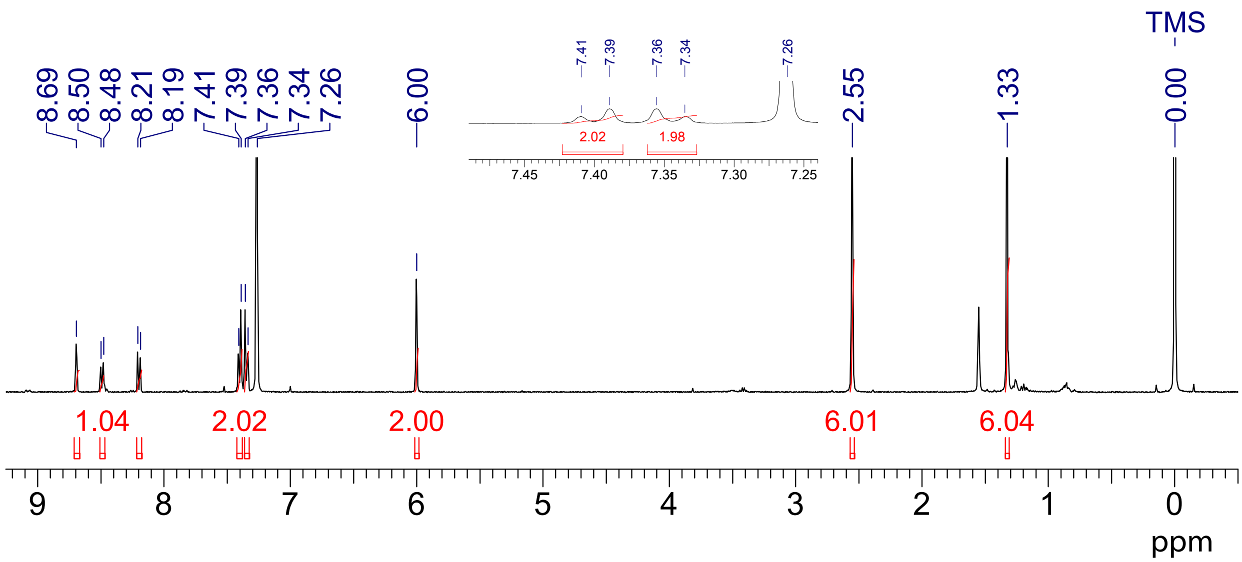


Figure S1. ^{1}H NMR of **2** in $CDCl_3$ (400 MHz), 25°C.

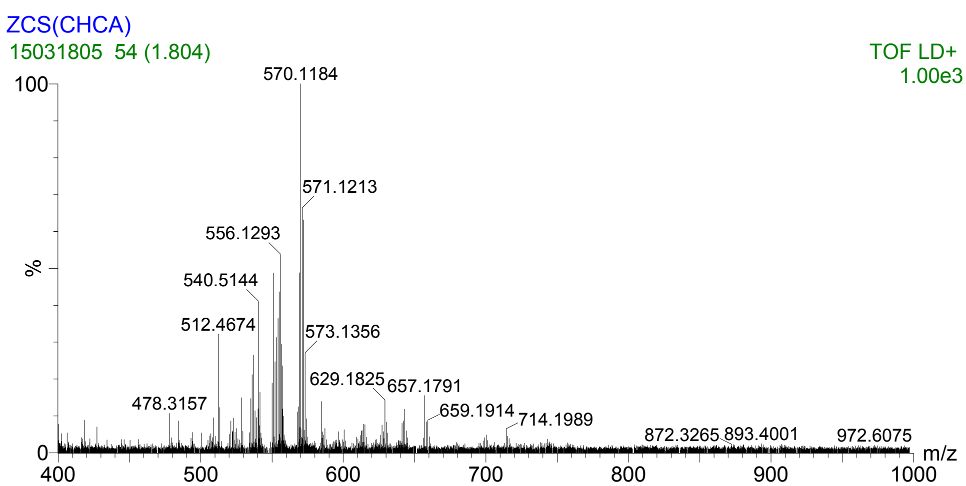


Figure S2. MALDI–HRMS (TOF) of **2**.

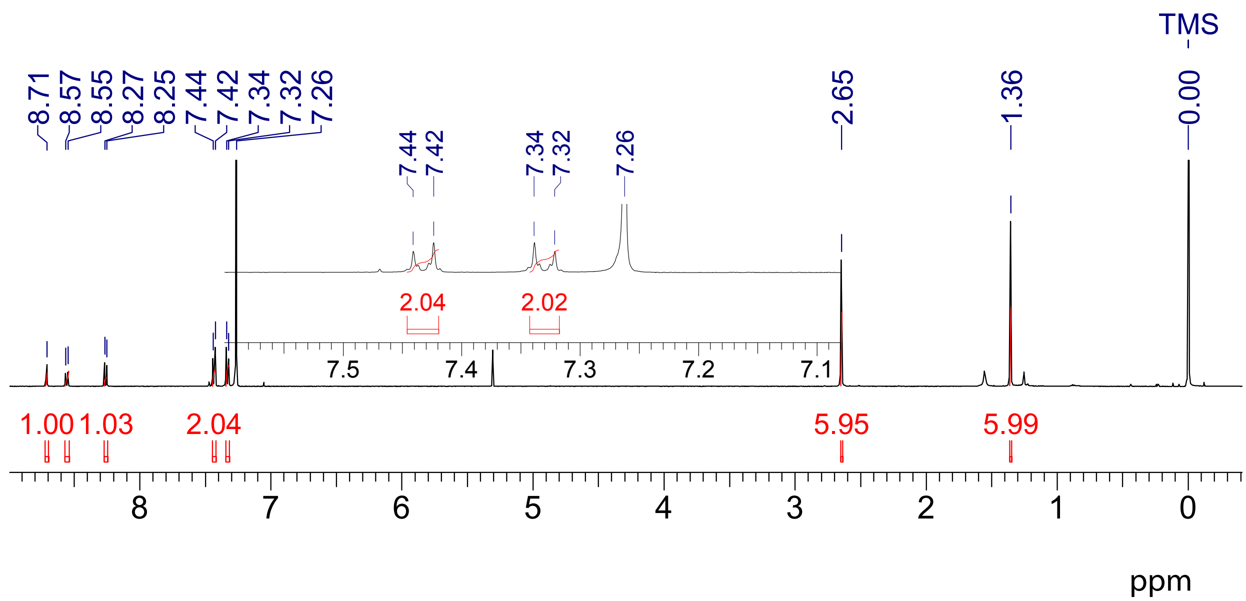


Figure S3. ^{1}H NMR of **C-1** in $CDCl_3$ (500 MHz), 25°C.

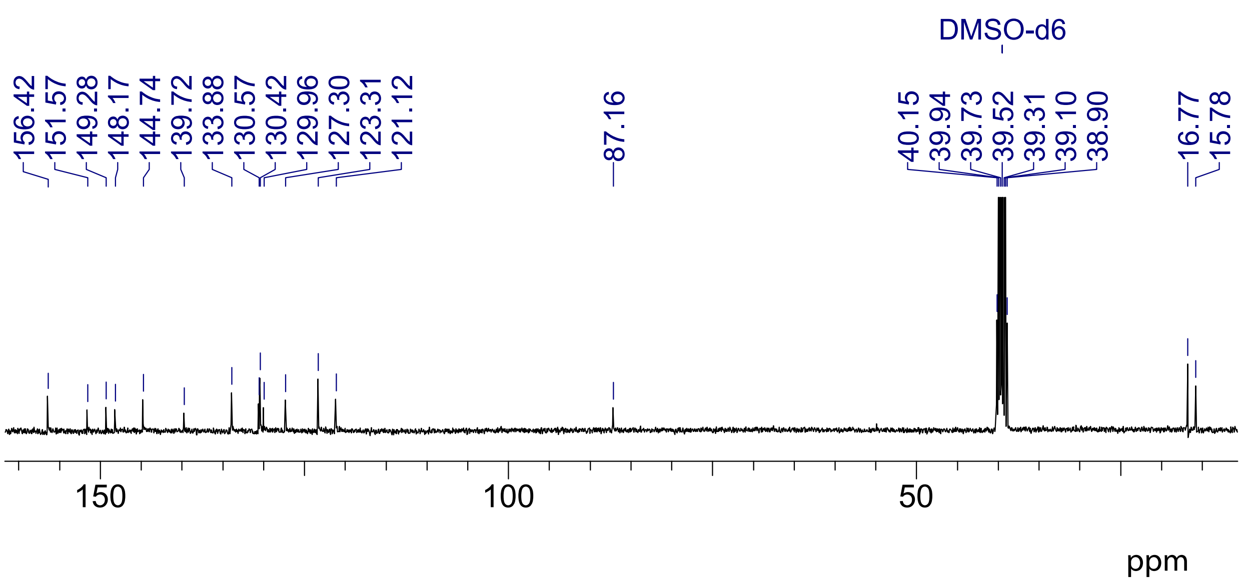


Figure S4. ^{13}C NMR of **C-1** in DMSO-d_6 (100 MHz), 25°C.

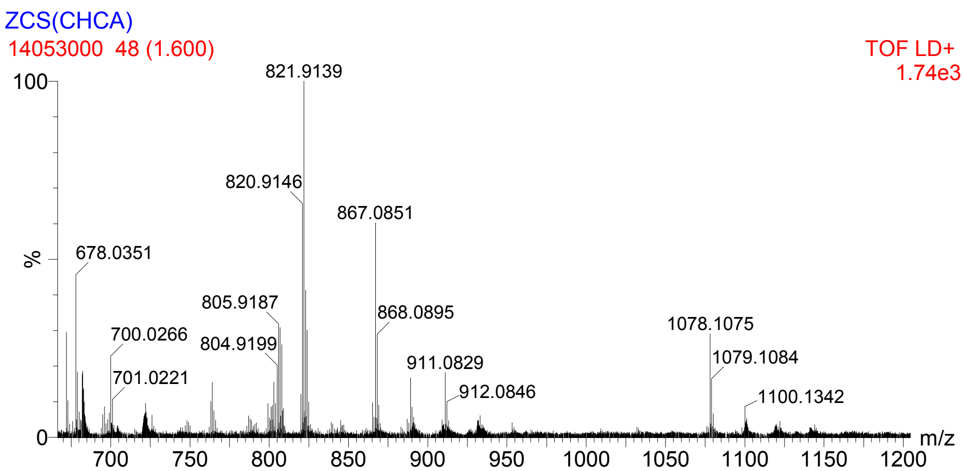


Figure S5. MALDI–HRMS (TOF) of **C-1**.

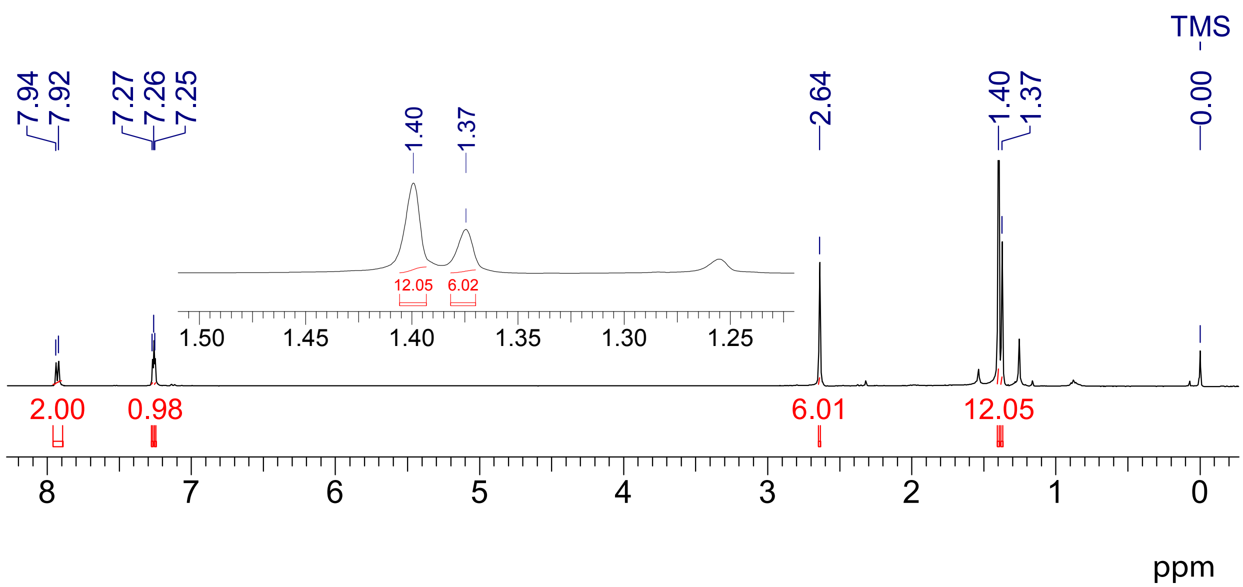


Figure S6. ^{1}H NMR of **4** in $CDCl_3$ (400 MHz), 25°C.

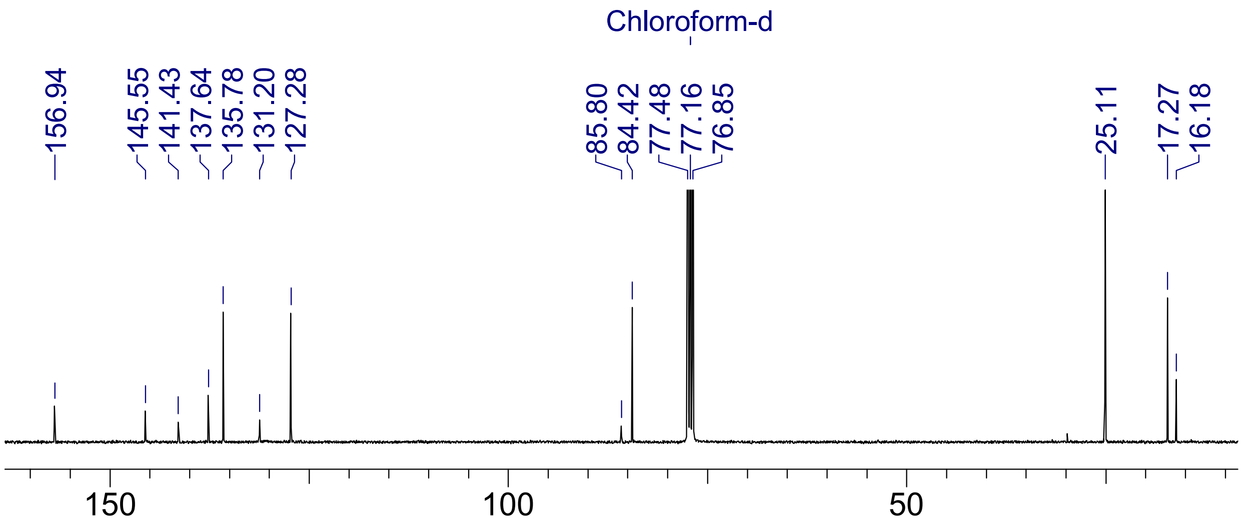


Figure S7. ^{13}C NMR of **4** in $CDCl_3$ (100 MHz), 25°C.

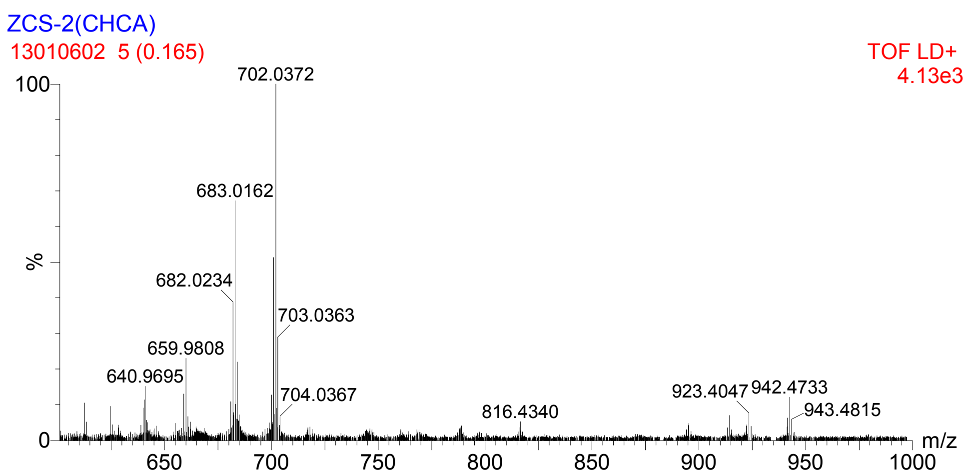


Figure S8. MALDI–HRMS (TOF) of **4**.

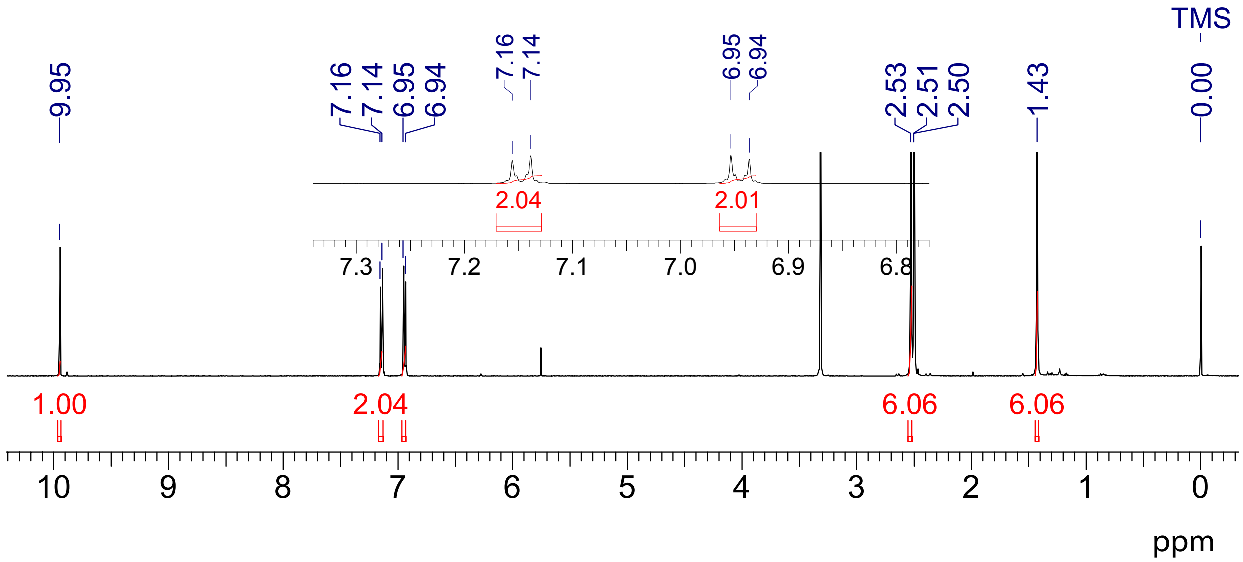


Figure S9. ^{1}H NMR of compound **5** in DMSO-d_6 (500 MHz), 25°C.

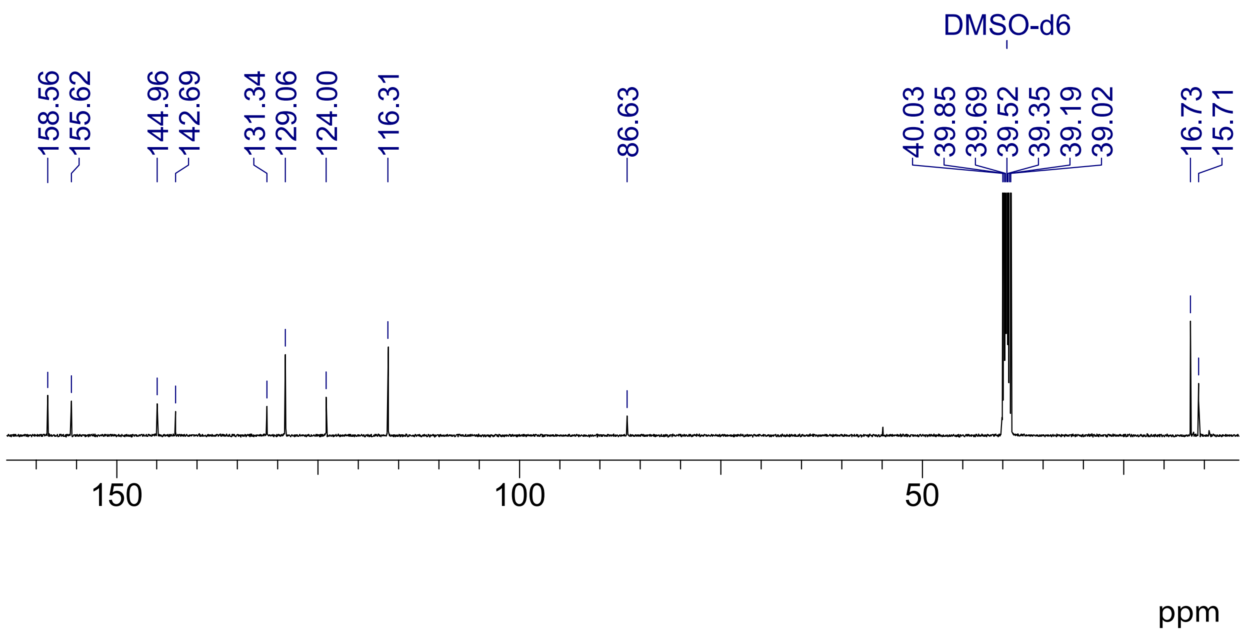


Figure S10. ^{13}C NMR of **5** in DMSO-d_6 (125 MHz), 25°C.

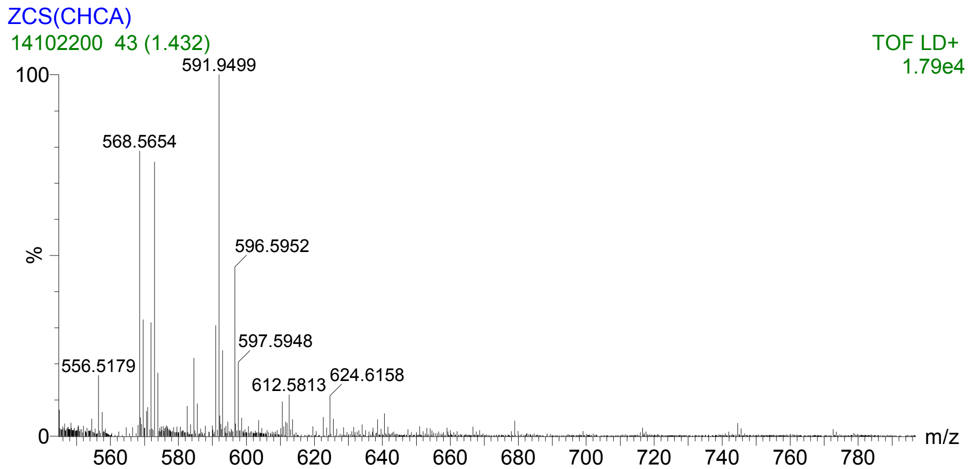


Figure S11. MALDI–HRMS (TOF) of **5**.

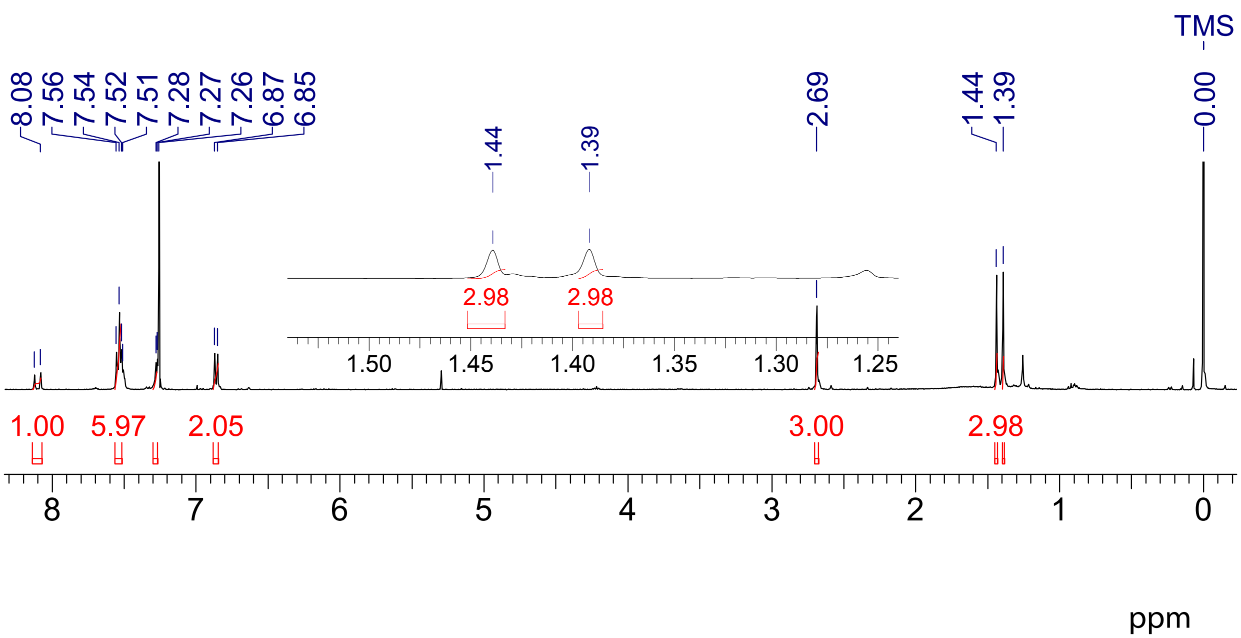


Figure S12. [1]H NMR of compound **7** in $CDCl_3$ (400 MHz), 25°C.

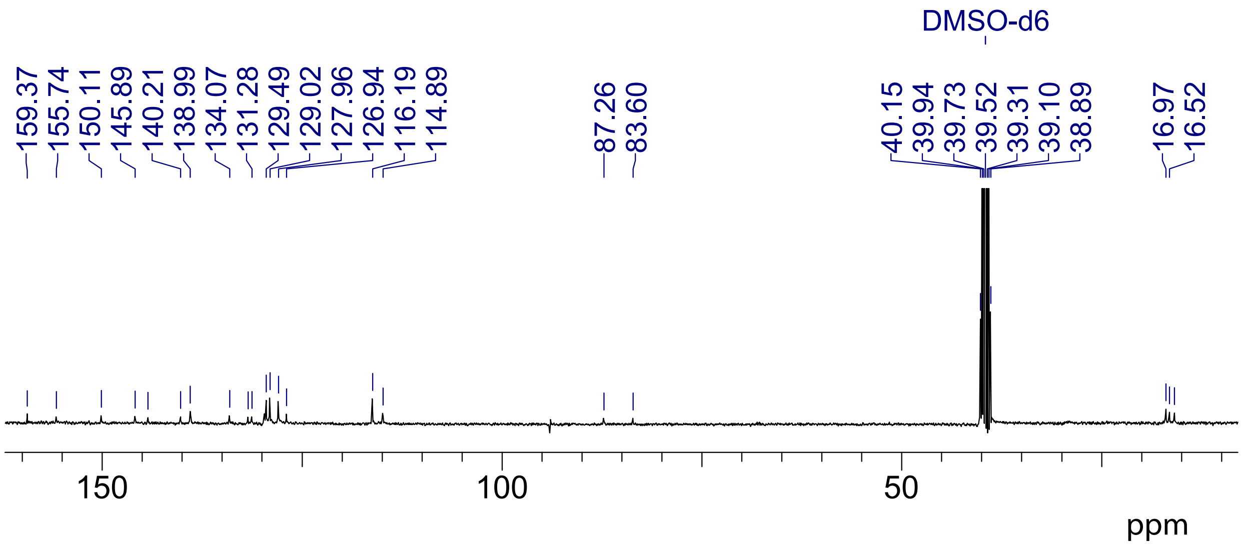


Figure S13. ^{13}C NMR of **7** in DMSO-d_6 (100 MHz), 25°C.

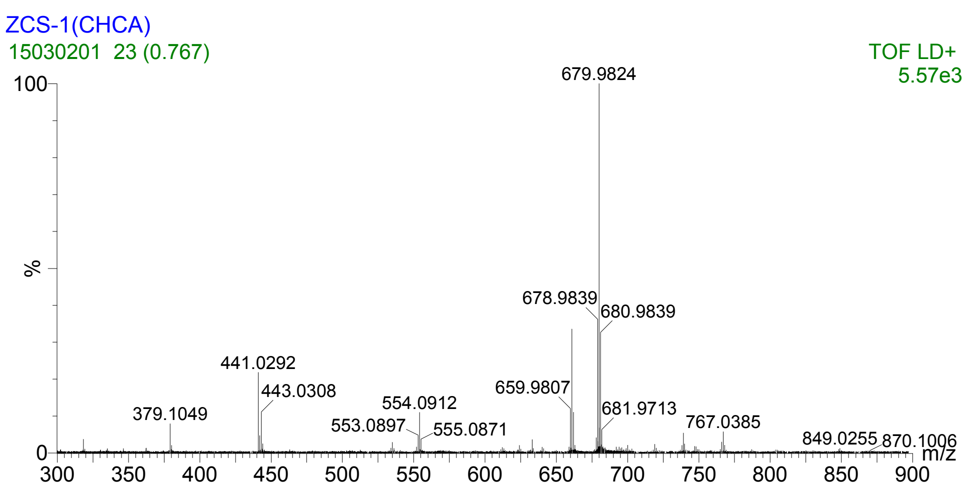


Figure S14. MALDI–HRMS (TOF) of **7**.

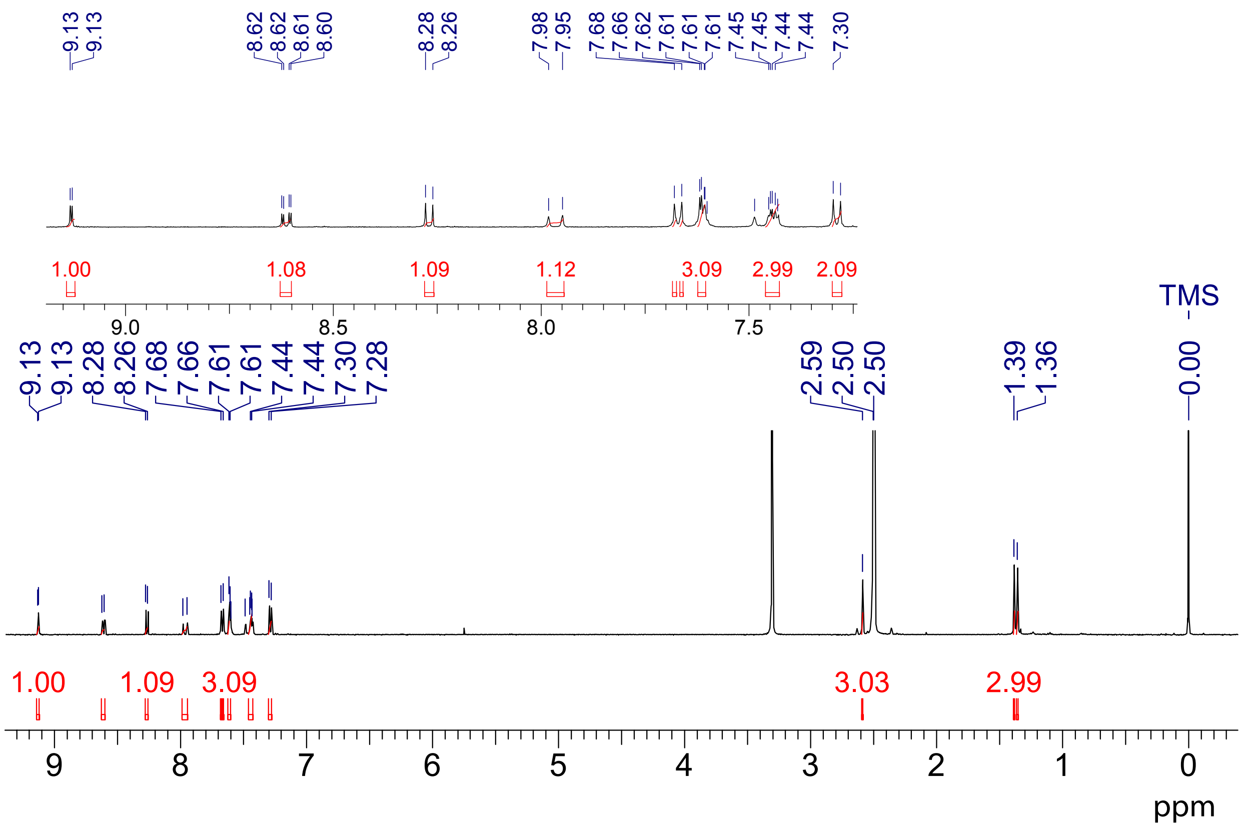


Figure S15. ^{1}H NMR of compound **C-2** in DMSO-d_6 (500 MHz), 25°C.

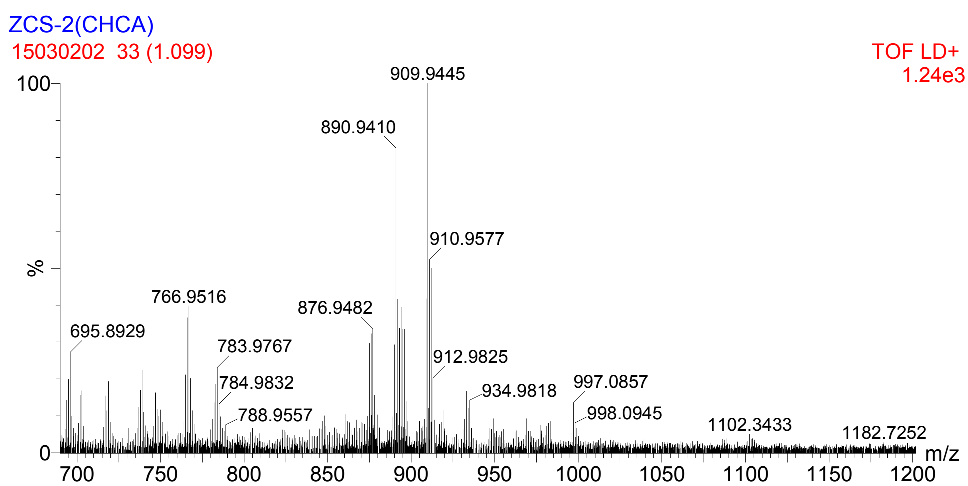


Figure S16. MALDI–HRMS (TOF) of **C-2**.

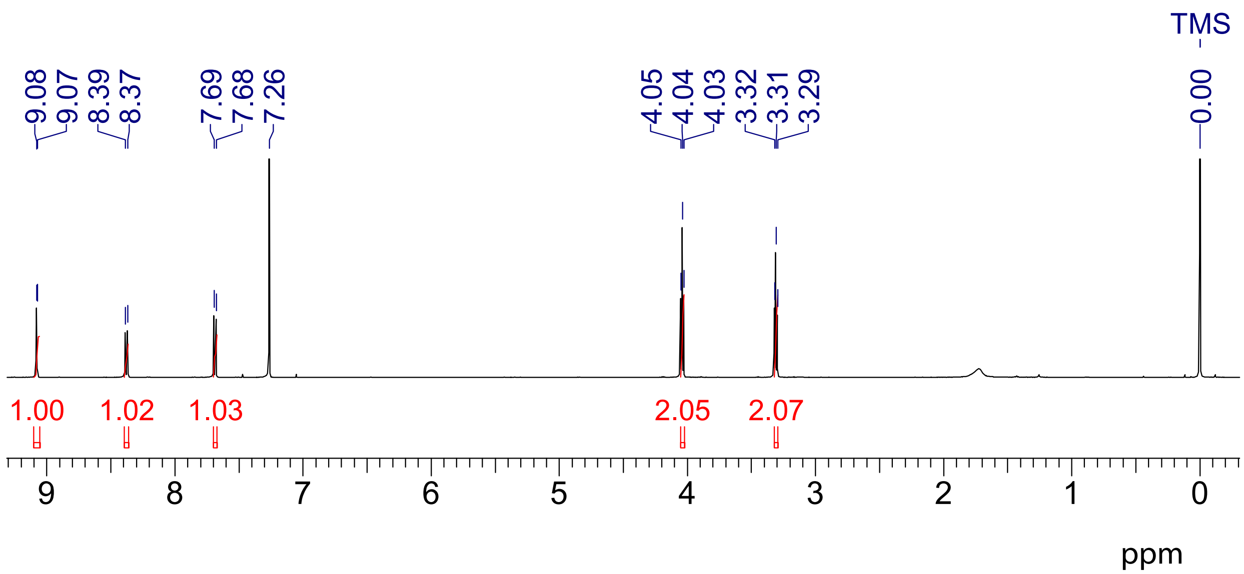
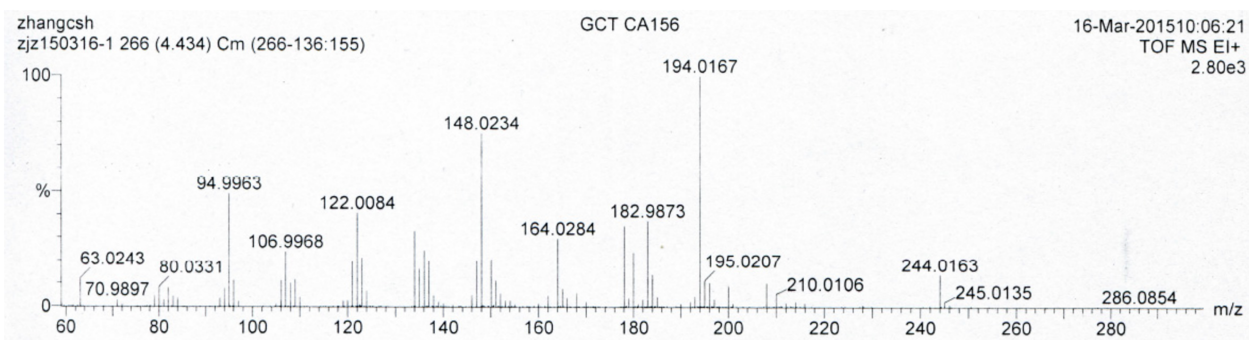


Figure S17. ^{1}H NMR of compound **10** in $CDCl_3$ (500 MHz), 25°C.



Minimum:				-1.5		
Maximum:		200.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
244.0163	244.0154	0.9	3.7	6.0	3	C8 H8 N2 O5 S
	244.0280	-11.7	-47.8	5.5	2	C9 H10 N O5 S
	243.9579	58.4	239.4	12.0	1	C10 N2 O4 S

Figure S18. TOF HRMS EI^+ of **10**.

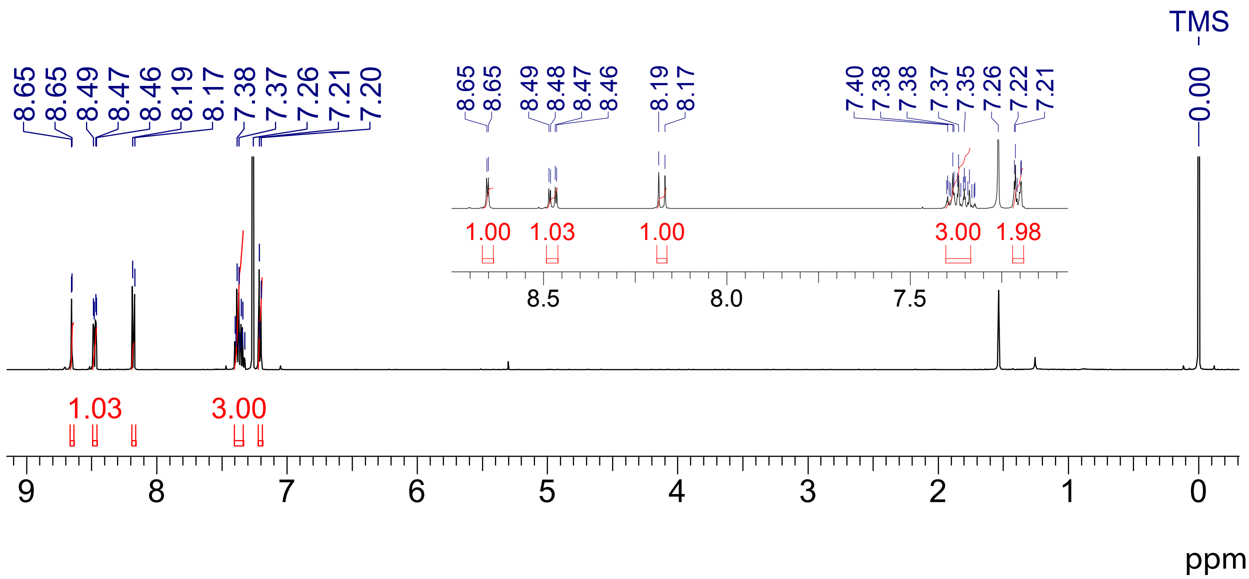
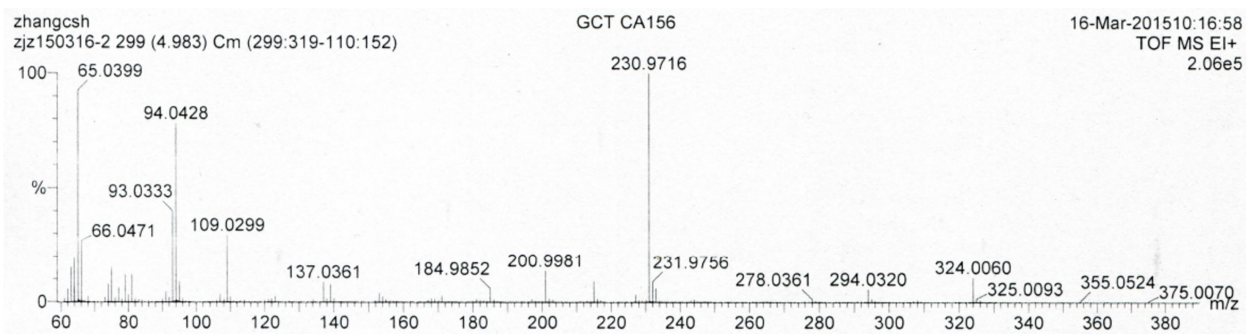


Figure S19. ^{1}H NMR of compound **13** in $CDCl_3$ (500 MHz), 25°C.



Minimum:				-1.5		
Maximum:		200.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
324.0060	324.0052	0.8	2.4	10.0	1	C12 H8 N2 O7 S
	324.0178	-11.8	-36.4	9.5	2	C13 H10 N O7 S
	323.9477	58.3	179.9	16.0	3	C14 N2 O6 S

Figure S20. TOF HRMS EI^{+} of **13**.

2. UV-vis absorption spectra and fluorescence emission.

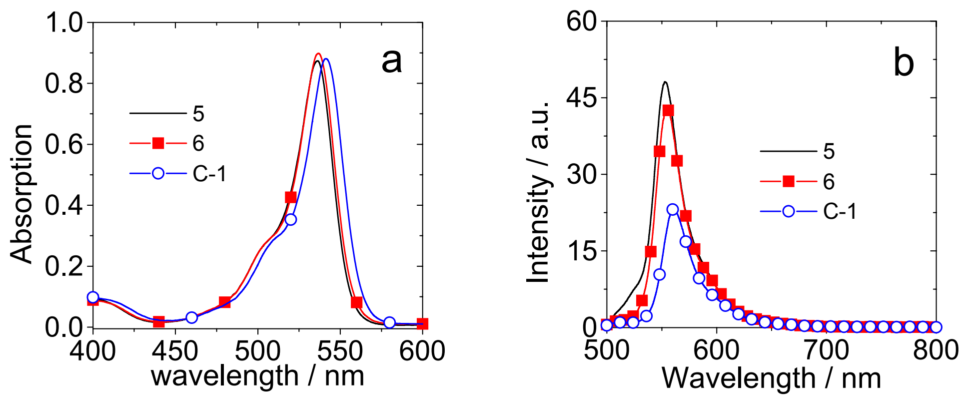
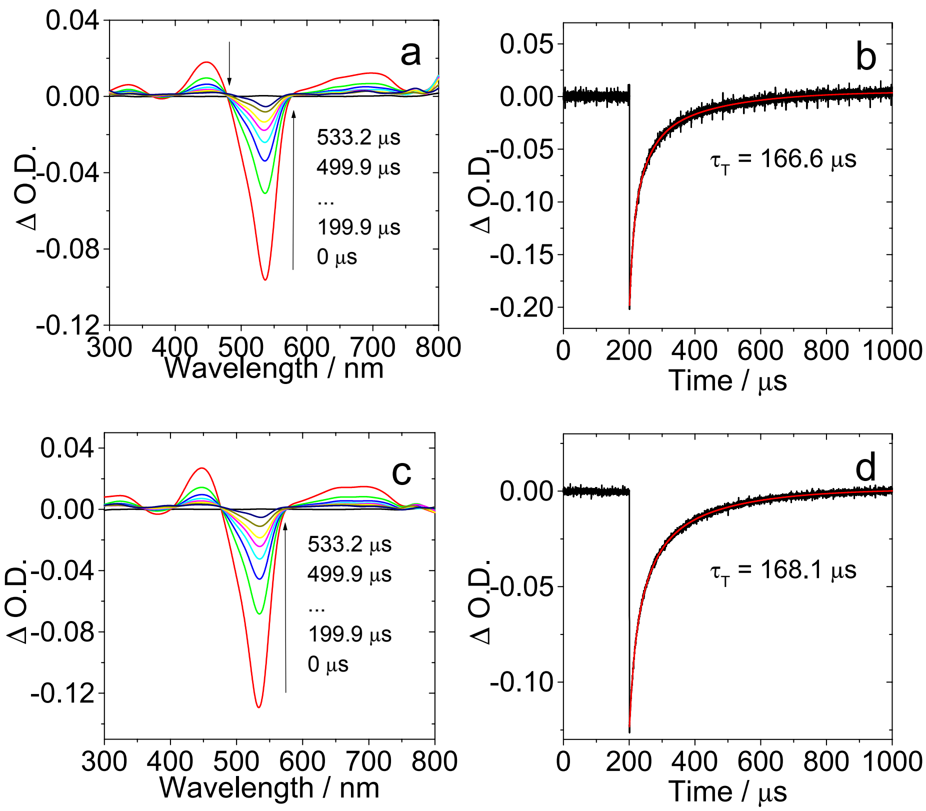
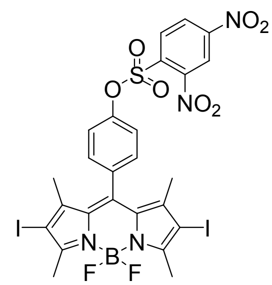


Figure S21. UV–vis absorption spectra (a) and fluorescence emission (b) of **5**, **6**, and **C-1**. in toluene. For (a), c = 1.0×10^{-5} M. For (b), λ_{ex} = 480 nm and optically matched solutions were used. 20 °C.

3. Nanosecond time-resolved transient absorption spectra.





C-1

Figure S22. Nanosecond time-resolved transient difference absorption of **C-1** before (a) and after (c) addition of mercaptoethanol. Decay trace of **C-1** before (b) and after (d) addition of mercaptoethanol at 533 nm, λ_{ex} = 529 nm. In DCM. c = 1.0×10^{-5} M. 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

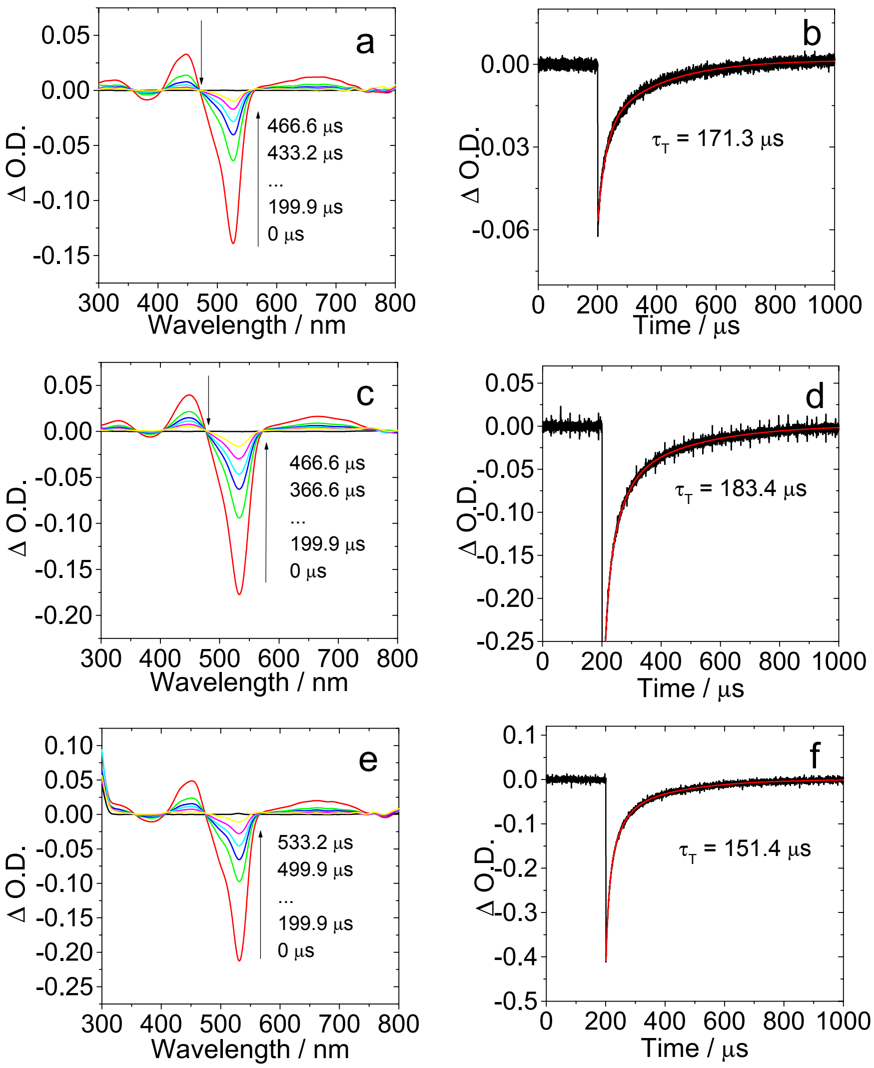


Figure S23. Nanosecond time-resolved transient difference absorption of **5** (a) in CH_3CN, (c) in toluene and (e) in DCM. Decay trace of **5** (b) in CH_3CN, (d) in toluene and (f) in DCM at 533 nm, λ_{ex} = 529 nm. $c = 1.0\times10^{-5}$ M. 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

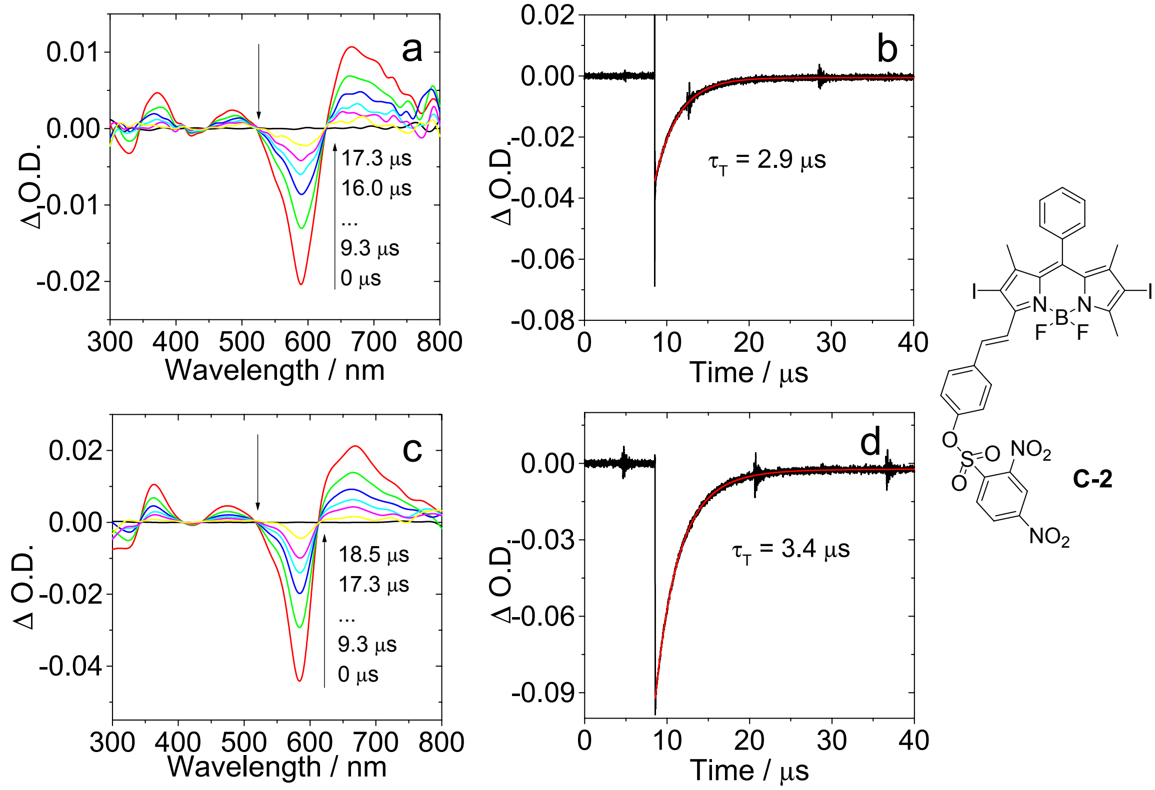


Figure S24. Nanosecond time-resolved transient difference absorption of **C-2** before (a) and after (c) addition of mercaptoethanol. Decay trace of **C-2** before (b) and after (d) addition of mercaptoethanol at 586 nm, λ_{ex} = 589 nm. In toluene. c = 1.0×10^{-5} M. 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

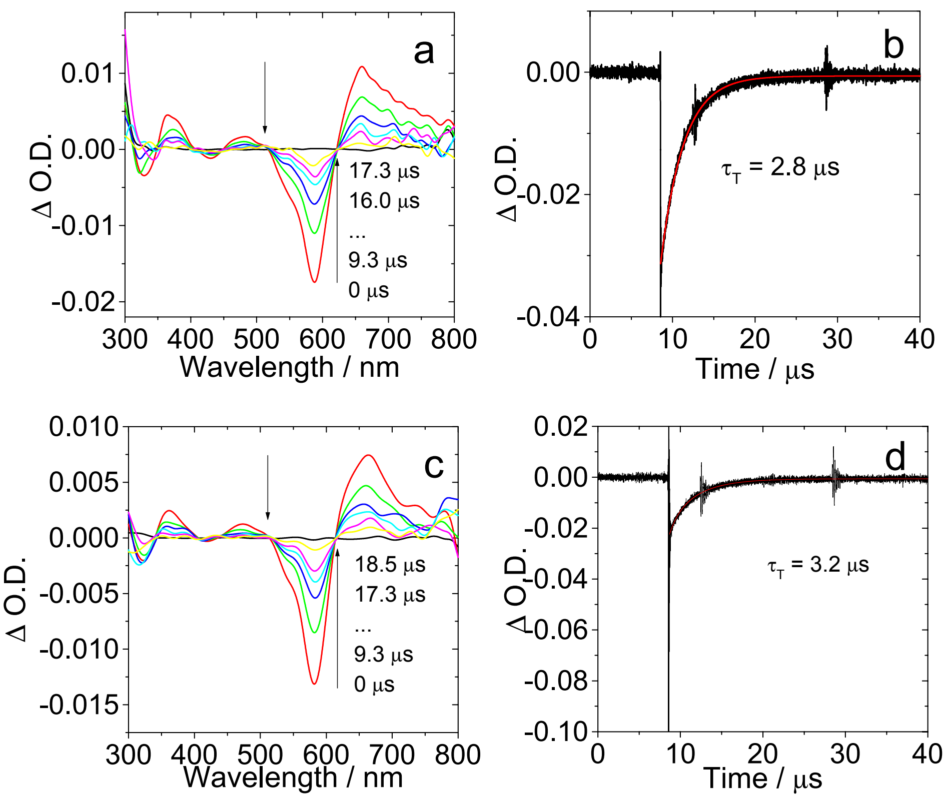


Figure S25. Nanosecond time-resolved transient difference absorption of **C-2** before (a) and after (c) addition of mercaptoethanol. Decay trace of **C-2** before (b) and after (d) addition of mercaptoethanol at 586 nm, λ_{ex} = 589 nm. In DCM. $c = 1.0 \times 10^{-5}$ M. 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

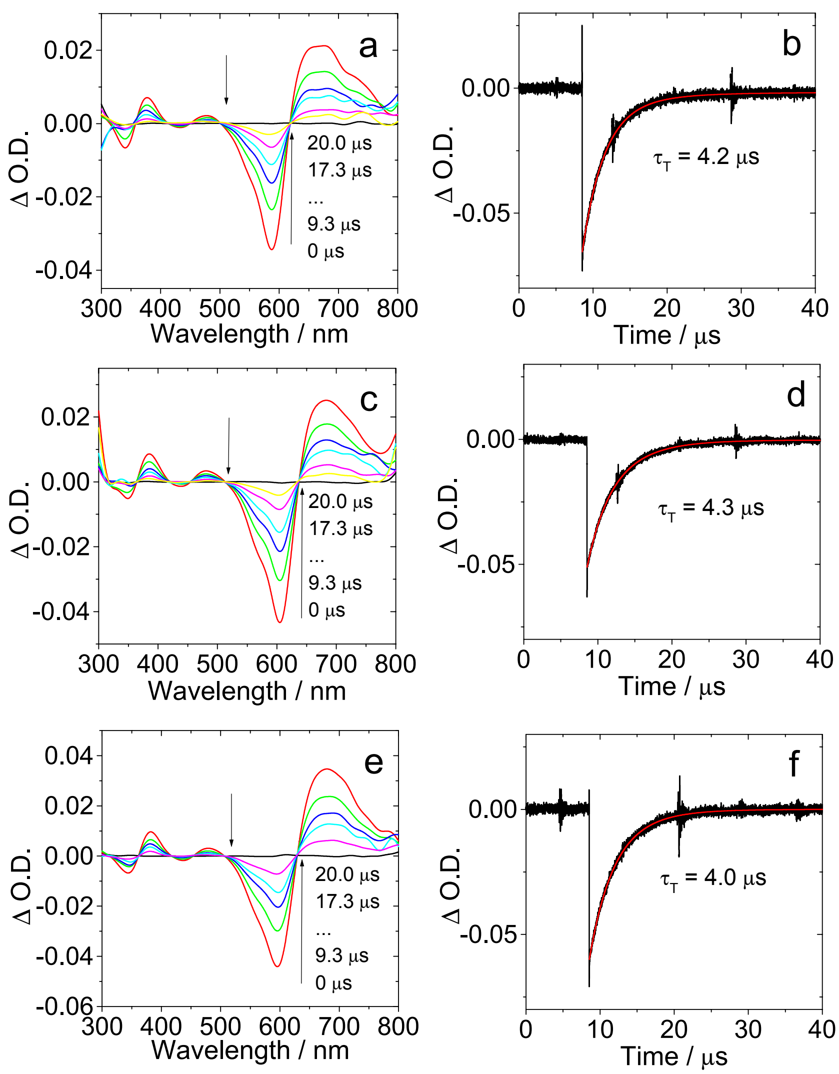


Figure S26. Nanosecond time-resolved transient difference absorption of **7**. (a) in CH_3CN (b) in toluene and (c) in DCM. Decay trace of **7** (b) in CH_3CN (d) in toluene and (e) in DCM at 533 nm, λ_{ex} = 589 nm. $c = 1.0\times10^{-5}$ M. 20 °C Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

4. Selected Frontier Molecular Orbital and Simplified Jablonski Diagram Illustrating.

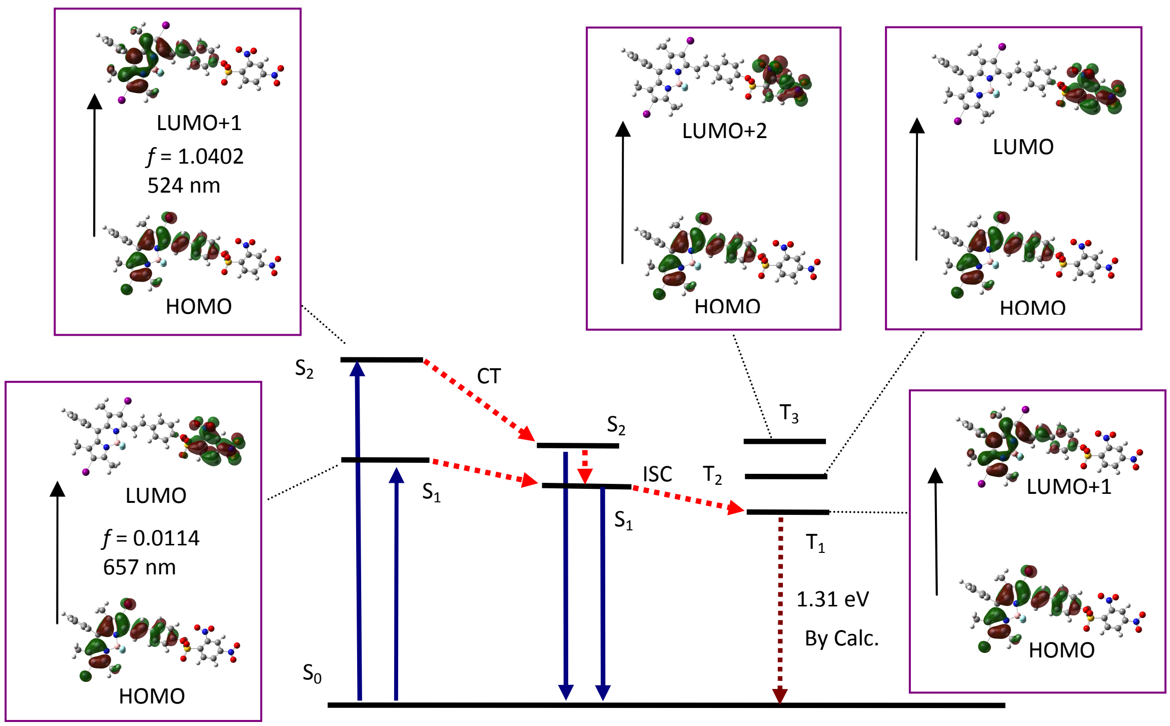


Figure S27. Selected frontier molecular orbitals involved in the excitation and emission of **C-2**. CT stands for conformation transformation. The calculations are at the B3LYP/6–31G(d)/ level using Gaussian 09W. In CH_3CN.

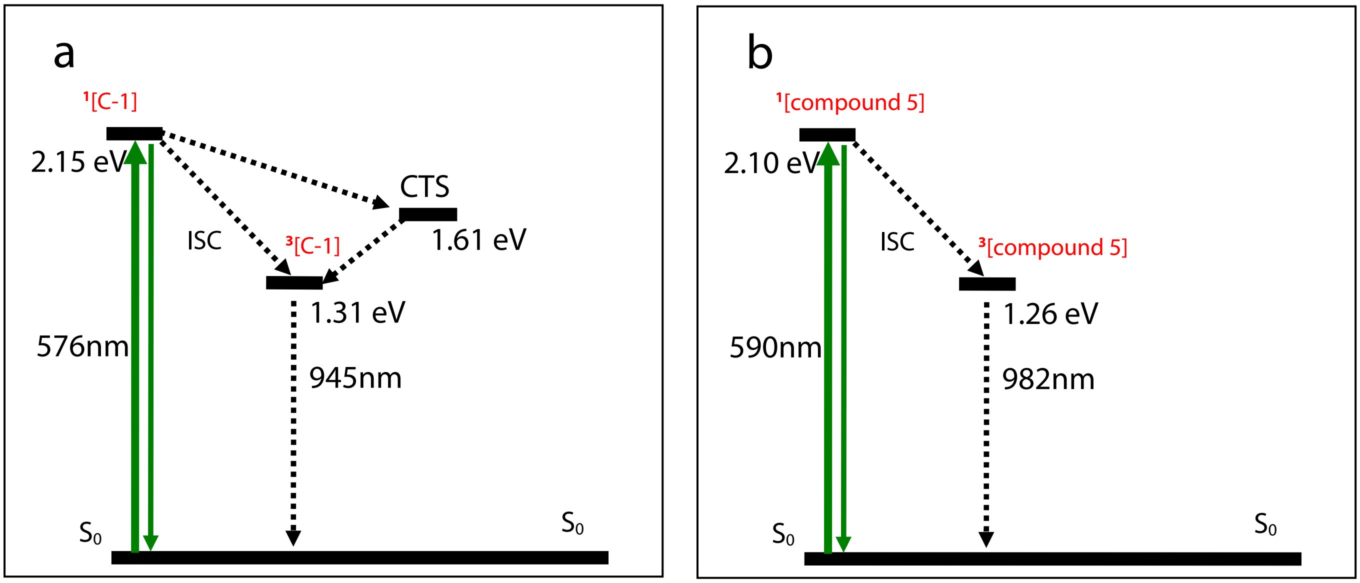
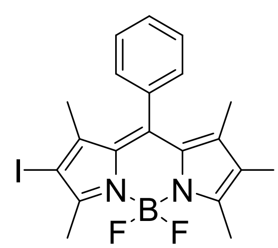


Figure S28. Simplified Jablonski Diagram Illustrating, the Photophysical Processes Involved in (a) **C-2** in the Absence of thiols, (b) Compound 7 (the Cleaved Product of **C-2** in the Presence of thiols).

5. Photooxidation.

Table S1. Singlet oxygen quantum yields (Φ_Δ) for the photooxidations of DPBF using different triplet photosensitizers before and after added thiols.

	Φ_Δ [a]	Φ_Δ [b]	Φ_Δ [c]
C-1 [e]	0.74	0.37	0.59
C-1 [d,e]	0.88	0.34	0.65
C-2 [f]	0.20	0.13	0.20
C-2 [d,f]	0.20	0.13	0.24



6

[a] In CH_3CN. [b] In DCM. [c] In toluene. [d] With thiol added . [e] With compound **6** as standard (Φ_Δ= 0.87 in DCM). [f] With Methylene blue (MB) as standard (Φ_Δ = 0.57 in CH_2Cl_2).

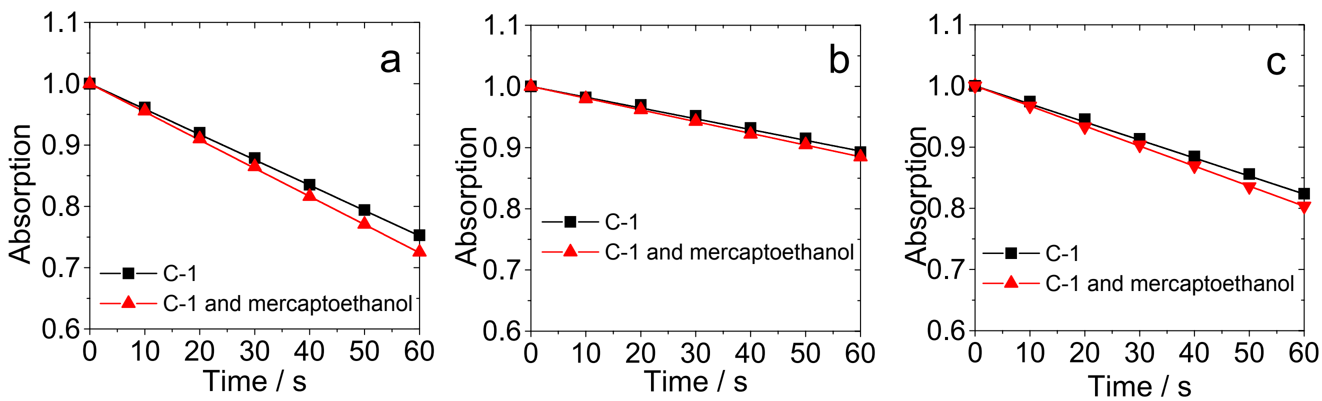


Figure S29. Verification of the light-harvesting effect of **C-1**by plotting of the absorption changes of 1,3-diphenylisobenzofuran (DPBF) at 414 nm vs. photoirradiation time for **C-1** before and after added mercaptoethanol (a) in CH_3CN, (b) in DCM, (c) in toluene. Excited at 526 nm. 20 °C.

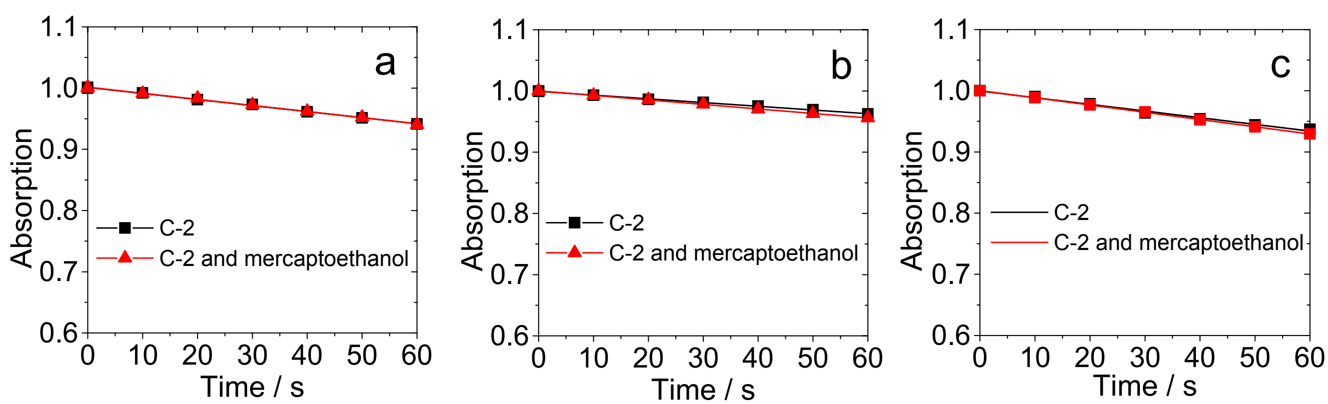


Figure S30. Singlet oxygen photosensitizing of **C-2** by plotting of the absorption changes of 1,3-diphenylisobenzofuran (DPBF) at 414 nm vs. photoirradiation time for **C-2** before and after added mercaptoethanol (a) in CH_3CN, (b) in DCM, (c) in toluene. Excited at 526 nm. 20 °C.

6. TTA Upconversion, Stern-Volmer Plots and Details.

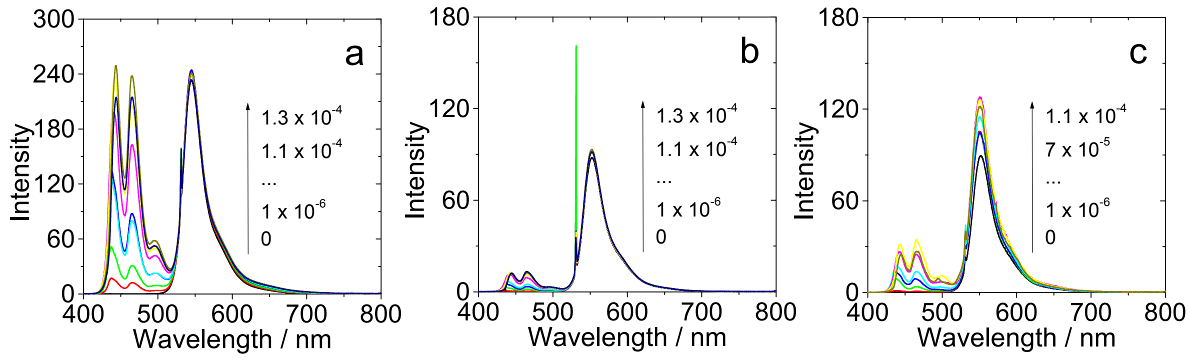


Figure S31. TTA upconversion with different concentration perylene as the triplet acceptor / emitter. For (a) take compound **5** as the triplet photosensitizers. For (b) and (c), take **C-1** before (b) and after (c) additional of mercaptoethanol as the triplet photosensitizers. Excited with 532 nm CW laser (5 mW, power density: 28 mW cm^{-2}). *c*[photosensitizers] = 1.0×10^{-5} M. In CH_3CN. 20 °C. the best concentration of perylene for **5**, **C-1** and **C-1** after additional of mercaptoethanol are 1.1×10^{-4} M, 1.1×10^{-4} M and 9.0×10^{-5} M, respectively. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

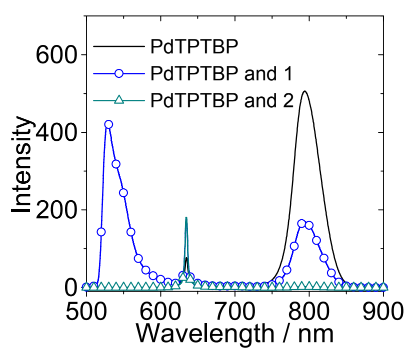
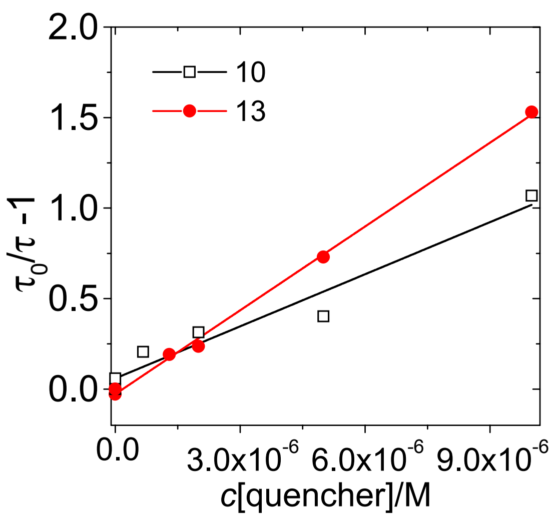
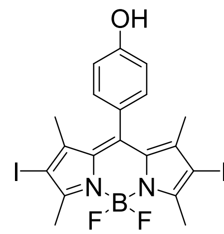


Figure 32. TTA upconversion of compounds **1** and **2** as the triplet acceptor / emitter. Excited with 635 nm CW laser (5 mW, power density: 28 mW cm^{-2}). PdTPTBP as triplet state photosensitizer, *c*[photosensitizers] = 5.0×10^{-6} M, *c*[compound 1] = 8.0×10^{-4} M, *c*[compound 2] = 8.0×10^{-4} M. In toluene. 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.





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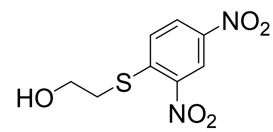

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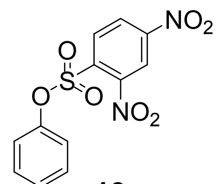

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Figure S33. Stern-Volmer plots for the lifetime quenching of the triplet photosensitizers with increasing the concentration of compound **10** and **13**; *c*[photosensitizers] = 1.0×10^{-5} M. In CH_3CN. The triplet excited-state lifetimes were measured with transient absorption spectrum upon OPO laser excitation; Decay trace of photosensitizer at 533 nm, λ_{ex} = 529 nm; 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

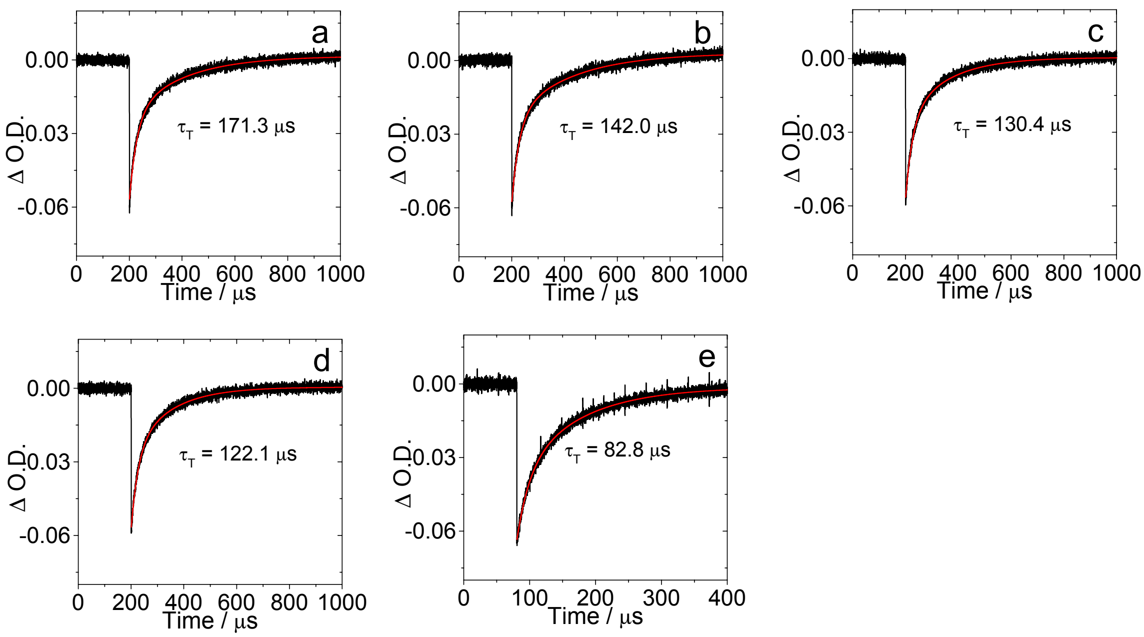


Figure S34. Decay trace of compound **5** at 533 nm with different concentration of compound **10**, λ_{ex} = 529 nm. (a) $c_5 = 0$, (b) $c_5 = 6.7 \times 10^{-7}$ M. (c) $c_5 = 2.0 \times 10^{-6}$ M. (d) $c_5 = 5.0 \times 10^{-6}$ M, (e) $c_5 = 1.0 \times 10^{-5}$ M. In CH_3CN. $c_5 = 1.0 \times 10^{-5}$ M. 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

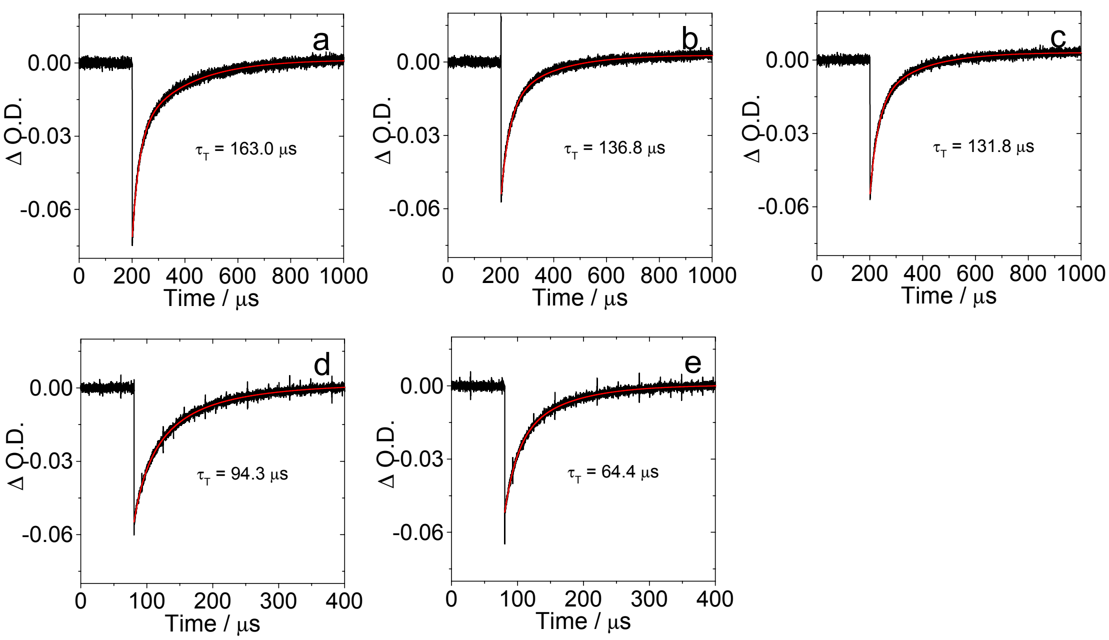


Figure S35. Decay trace of compound **5** at 533 with different concentration of compound **13**, λ_{ex} = 529 nm. (a) $c_5 = 0$, (b) $c_5 = 1.3 \times 10^{-6}$ M. (c) $c_5 = 2.0 \times 10^{-6}$ M. (d) $c_5 = 5.0 \times 10^{-6}$ M, (e) $c_5 = 1.0 \times 10^{-5}$ M. In CH_3CN. c [**5**] = 1.0×10^{-5} M. 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

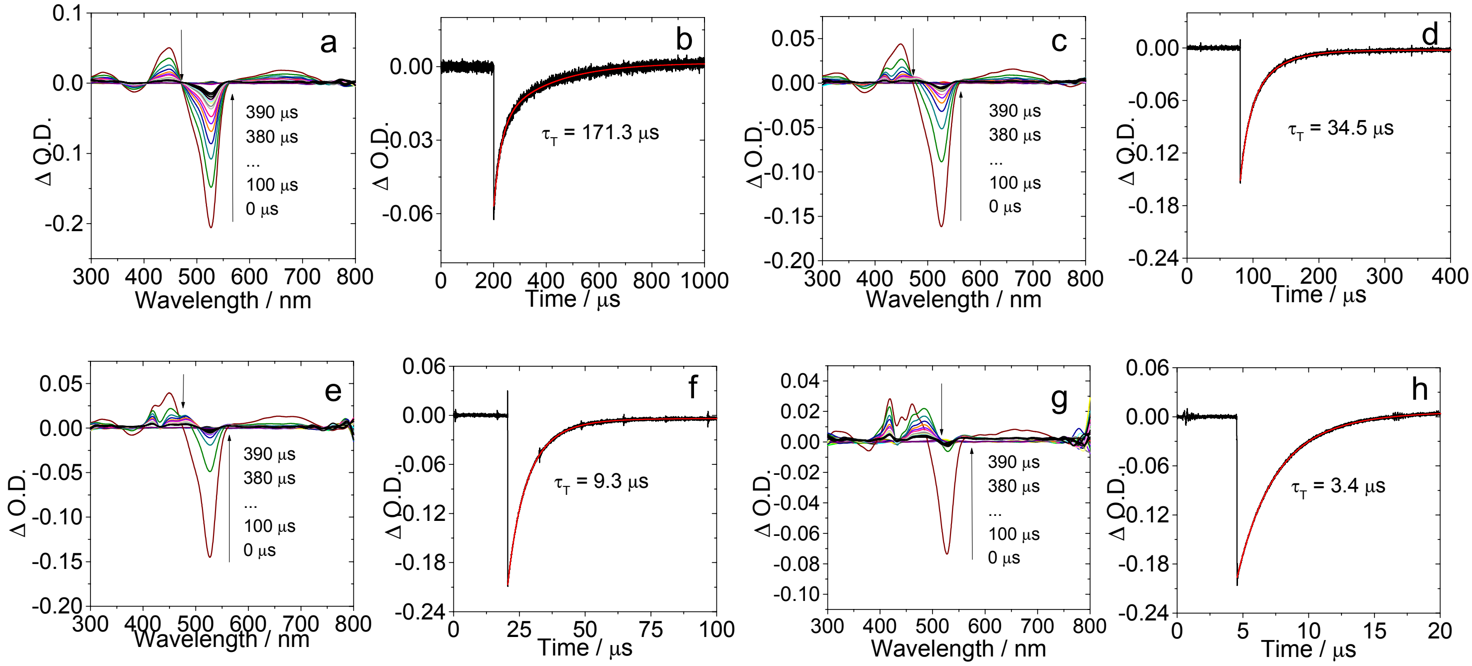


Figure S36. Nanosecond time-resolved transient difference absorption and decay trace of compound **5** at 533 with different concentration of perylene, λ_{ex} = 529 nm. In CH_3CN. c_5 = 1.0×10^{-5} M. 20 °C. (a and b) $c_{perylene}$ = 0, (c and d) $c_{perylene}$ = 2.0×10^{-6}. (e and f) $c_{perylene}$ = 1.0×10^{-5}. (g and h) $c_{perylene}$ = 3.0×10^{-5}. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

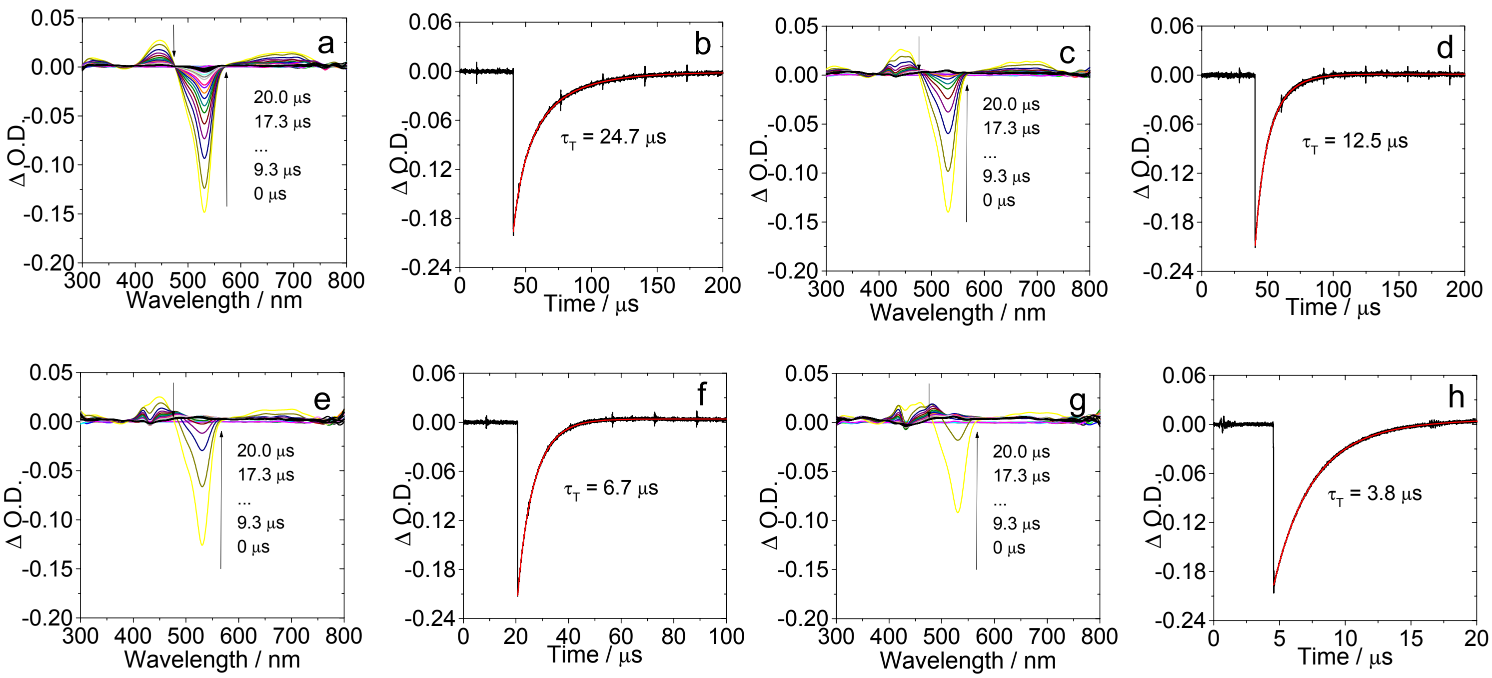


Figure S37. Nanosecond time-resolved transient difference absorption and decay trace of **C-1** at 533 with different concentration of perylene, λ_{ex} = 529 nm. In CH_3CN. $c_5 = 1.0\times10^{-5}$ M. 20 °C. (a and b) $c_{perylene}$ = 0, (c and d) $c_{perylene} = 4.0 \times 10^{-6}$. (e and f) $c_{perylene} = 1.0 \times 10^{-5}$. (g and h) $c_{perylene} = 3.0 \times 10^{-5}$. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

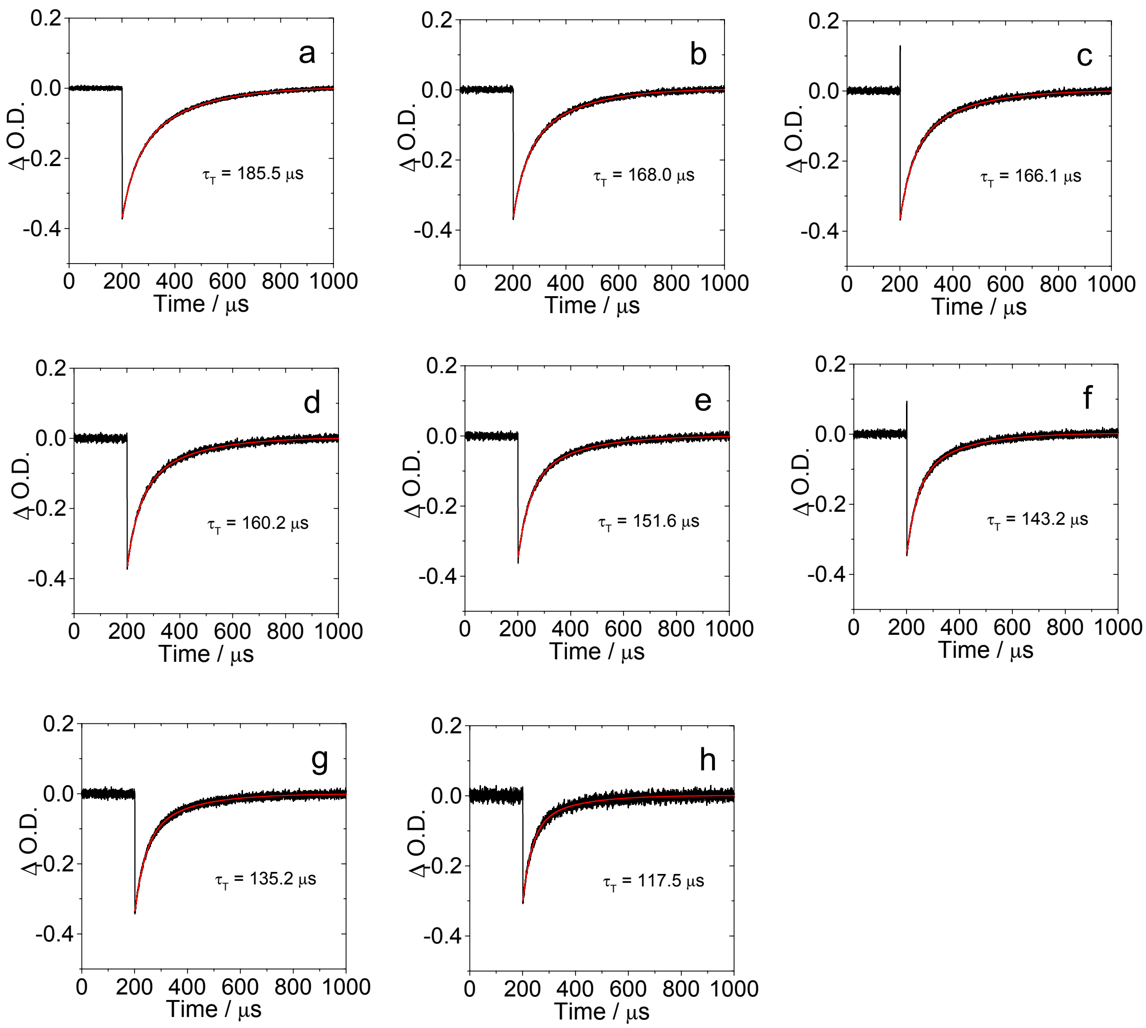


Figure S38. Decay trace of **PdTPTBP** at 440 nm with different concentration of compound **1**, λ_{ex} = 445 nm. In toluene. $c_{\text{PdTPTBP}} = 5.0\times10^{-6}$ M. 20 °C. (a) $c_1 = 0$, (b) $c_1 = 1.0 \times 10^{-5}$, (c) $c_1 = 2.0 \times 10^{-5}$, (d) $c_1 = 3.0 \times 10^{-5}$, (e) $c_1 = 4.0 \times 10^{-5}$, (f) $c_1 = 5.0 \times 10^{-5}$, (g) $c_1 = 6.0 \times 10^{-5}$, (h) $c_1 = 1.0 \times 10^{-4}$. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

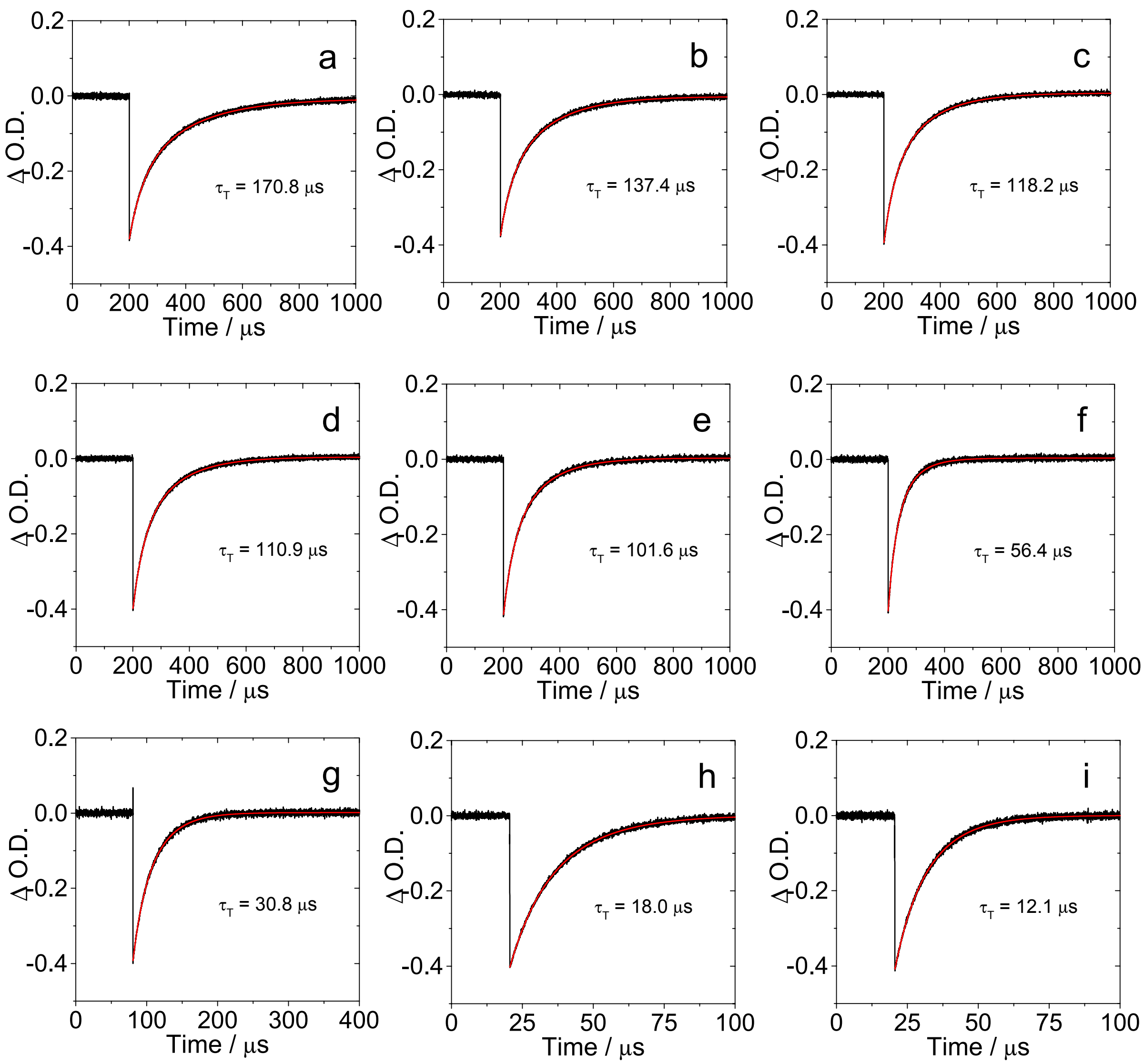


Figure S39. Decay trace of **PdTPTBP** at 440 nm with different concentration of compound **2**, λ_{ex} = 445 nm. In toluene. $c_{\text{PdTPTBP}} = 5.0\times10^{-6}$ M. 20 °C. (a) $c_2 = 0$, (b) $c_2 = 3.3\times10^{-7}$, (c) $c_2 = 1.0\times10^{-6}$, (d) $c_2 = 1.7\times10^{-6}$, (e) $c_2 = 2.0\times10^{-6}$, (f) $c_2 = 5.0\times10^{-6}$, (g) $c_2 = 1.0\times10^{-5}$, (h) $c_2 = 2.0\times10^{-5}$, (i) $c_2 = 3.0\times10^{-5}$. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

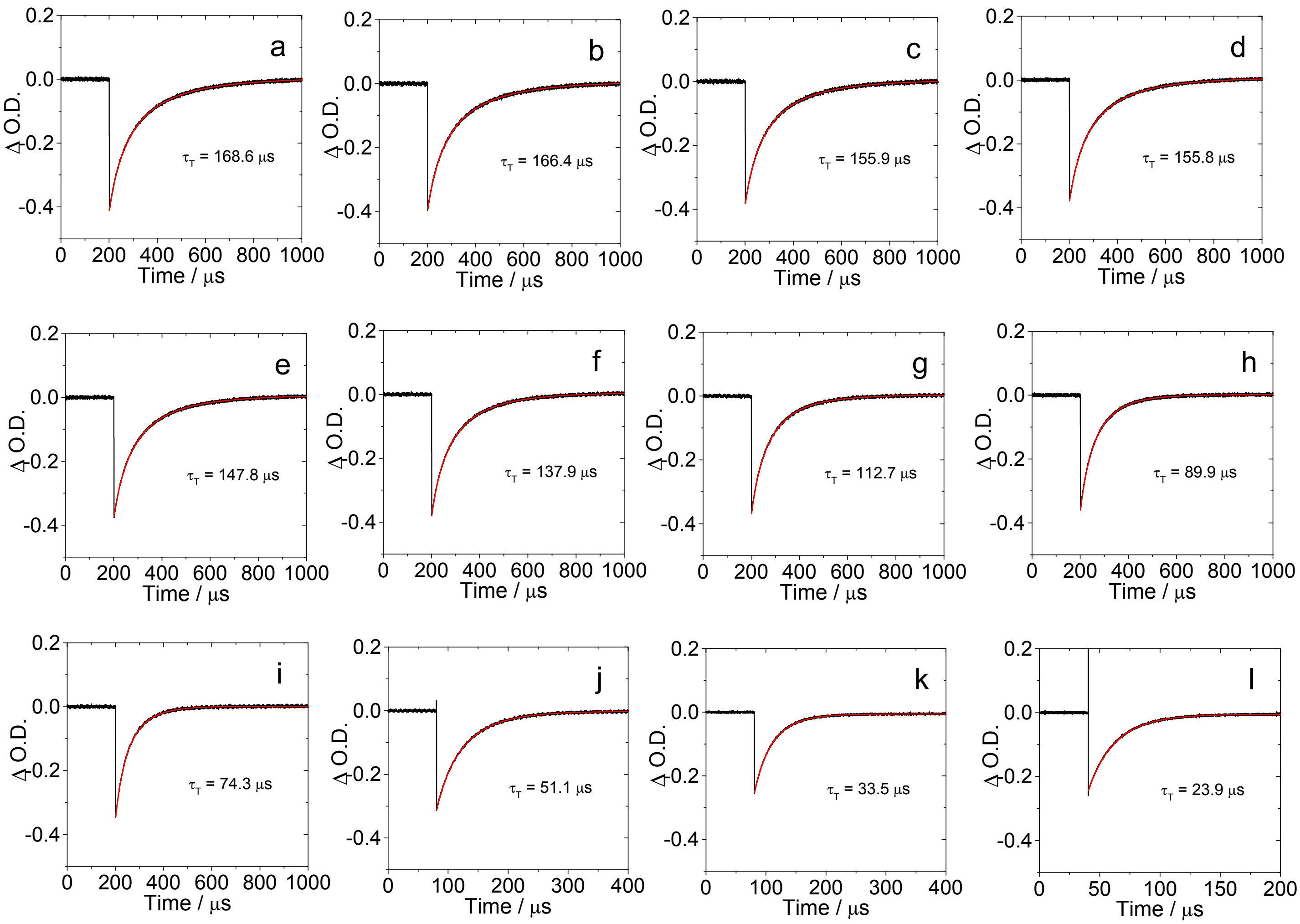


Figure S40. Decay trace of **PdTPTBP** at 440 nm with different concentration of compound **10**, λ_{ex} = 445 nm. In toluene. $c_{\text{PdTPTBP}} = 5.0\times10^{-6}$ M. 20 °C. (a) $c_{10} = 0$, (b) $c_{10} = 3.3 \times 10^{-7}$, (c) $c_{10} = 1.0 \times 10^{-5}$, (d) $c_{10} = 2.0 \times 10^{-5}$, (e) $c_{10} = 3.0 \times 10^{-5}$, (f) $c_{10} = 5.0 \times 10^{-5}$, (g) $c_{10} = 1.0 \times 10^{-4}$, (h) $c_{10} = 1.5 \times 10^{-4}$, (i) $c_{10} = 2.0 \times 10^{-4}$, (j) $c_{2} = 3.0 \times 10^{-4}$, (k) $c_{2} = 4.0 \times 10^{-4}$, (l) $c_{10} = 5.0 \times 10^{-4}$. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

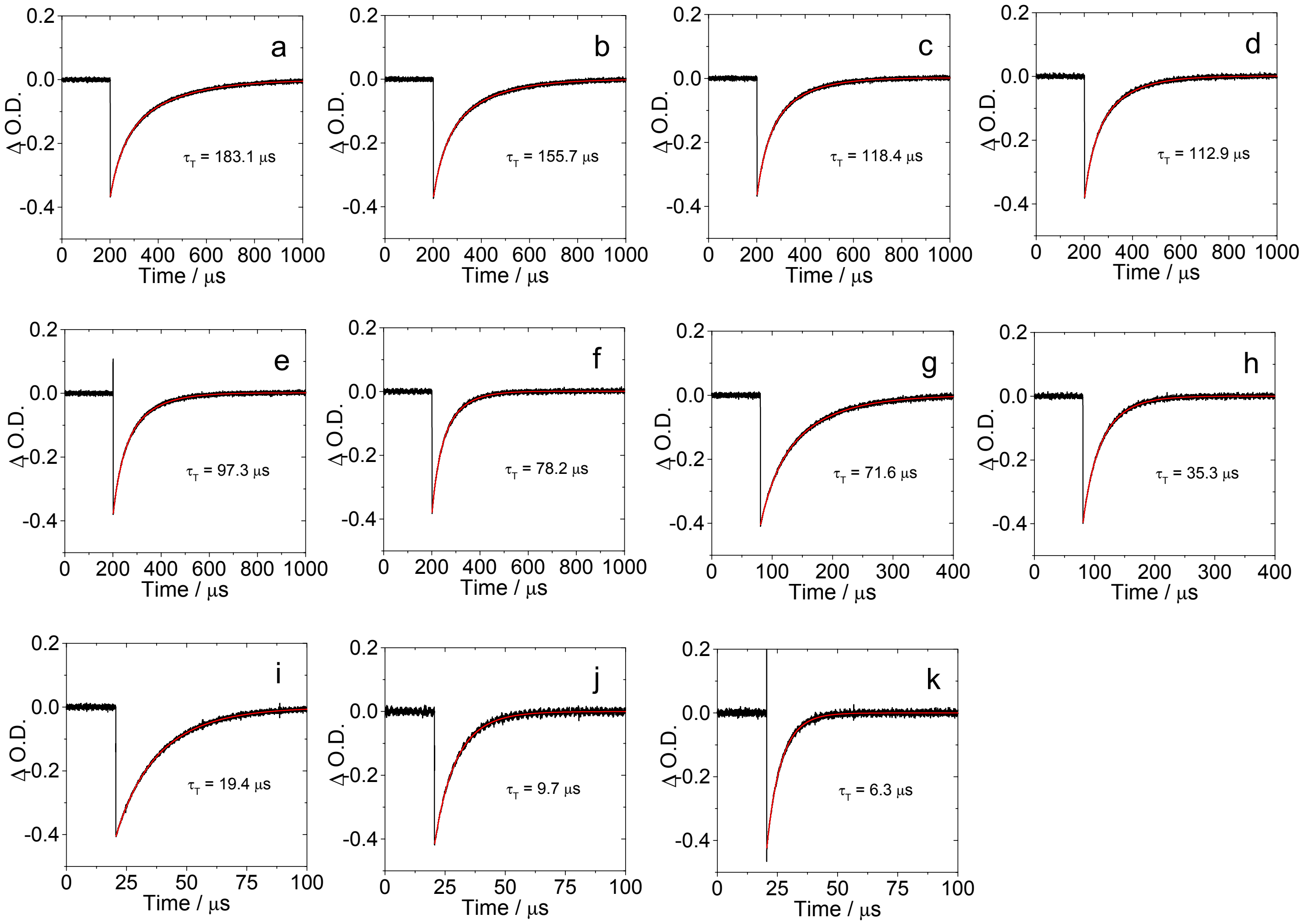


Figure S41. Decay trace of **PdTPTBP** at 440 nm with different concentration of compound **13**, λ_{ex} = 445 nm. In toluene. $c_{\text{PdTPTBP}} = 5.0\times10^{-6}$ M. 20 °C. (a) $c_{13} = 0$, (b) $c_{13} = 3.3 \times 10^{-7}$, (c) $c_{13} = 6.7 \times 10^{-7}$, (d) $c_{13} = 1.0 \times 10^{-6}$, (e) $c_{13} = 1.3 \times 10^{-6}$, (f) $c_{13} = 1.7 \times 10^{-6}$, (g) $c_{13} = 2.0 \times 10^{-6}$, (h) $c_{13} = 5.0 \times 10^{-6}$, (i) $c_{13} = 1.0 \times 10^{-5}$, (j) $c_{13} = 2.0 \times 10^{-5}$, (k) $c_{13} = 3.0 \times 10^{-5}$. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

7. Spectra for Measurement of Triplet state quantum yield.

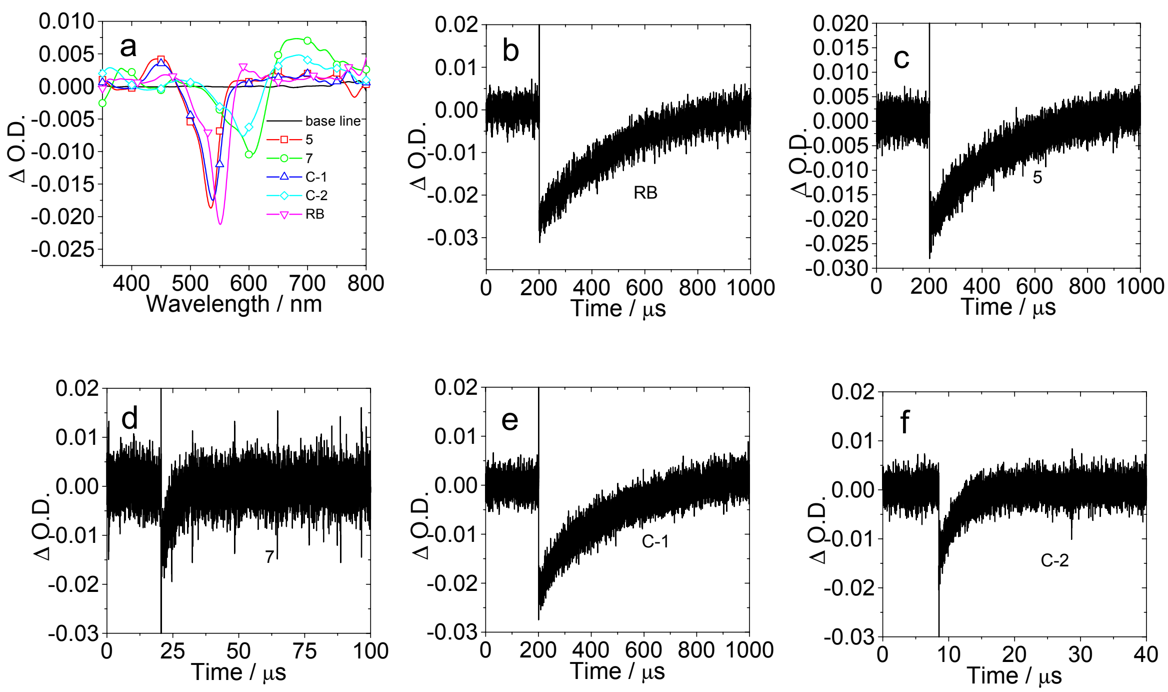
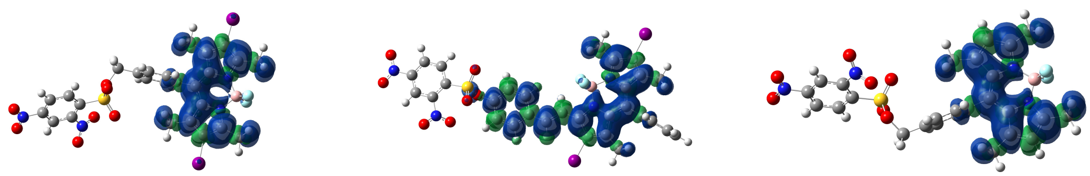


Figure S42. Nanosecond transient absorption of **RB**, **5**, **7**, **C-1** and **C-2** (a). For (c) **5** and (e) **C-1**, decay trace at 540 nm, for (d) **7**, decay trace at 610 nm, for (f) **C-2**, decay trace at 600 nm, for (b) RB, decay trace at 550 nm. In toluene. λ_{ex} = 537 nm and the absorbance at 537 nm are less than 0.2. 20 °C. Note, all the samples in flash photolysis experiments were deaerated with N_2 for 15 min before measurement and the gas flow was maintained during the measurement.

8. DFT Computation results of the Compounds



C-1 C-2 2

Figure S43. Isosurfaces of spin density of **C–1**, **C–2** and **2** at the optimized triplet state geometries. CH_3CN was used as the solvent in the calculations. Calculation was performed at B3LYP/6-31G(d)/LANL2DZ level with Gaussian 09W.

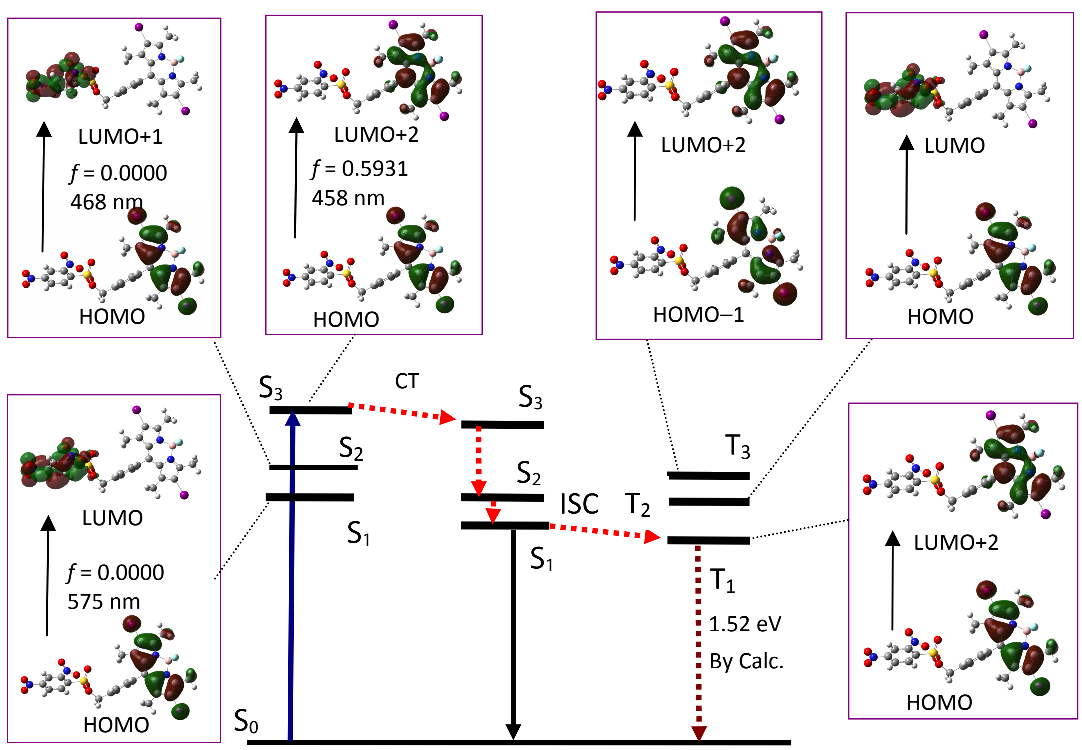


Figure S44. Selected frontier molecular orbitals involved in the excitation and emission of **C–1**. CT stands for conformation transformation. The calculations are at the B3LYP/6–31G(d)/ level using Gaussian 09W. In CH_3CN.

Table S2. Selected Parameters for the UV−vis Absorption and Triplet State Energy of the Compounds. Electronic Excitation Energies (eV) and Oscillator Strengths (*f*), Configurations of the Low-lying Excited States of C−1 and C−2. Calculated by TDDFT//B3LYP/6-31G(d), based on the Optimized Ground State Geometries (Acetonitrile Was Used as Solvent in the Calculation)

	Electronic transition [a]	TDDFT/B3LYP/6-31G(d)			
		Excitation energy	f [b]	Composition [c]	CI [d]
C−1	$S_0 \rightarrow S_1$	2.16 eV (575 nm)	0.0000	H → L	0.7059
	$S_0 \rightarrow S_2$	2.65 eV (468 nm)	0.0000	H→ L+1	0.7059
	$S_0 \rightarrow S_3$	2.71 eV (458 nm)	0.5931	H−1 → L+2	0.2034
				H→ L+2	0.6790
C−2	$S_1 \rightarrow S_0$	1.89 eV (657 nm)	0.0114	H →L	0.7046
	$S_2 \rightarrow S_0$	2.26 eV (524 nm)	1.0402	H → L+1	0.7028
C−1	$T_0 \rightarrow T_1$	1.52 eV (815 nm)	0.0000	H−1 → L+2	0.1557
				H → L+2	0.6965
	$T_0 \rightarrow T_2$	2.16 eV (575 nm)	0.0000	H → L	0.7059
	$T_0 \rightarrow T_3$	2.52 eV (491 nm)	0.0000	H−1 → L+2	0.6736
				H → L+2	0.1498
C−2	$T_0 \rightarrow T_1$	1.31 eV (945 nm)	0.0000	H → L+1	0.6937
	$T_0 \rightarrow T_2$	1.89 eV (657 nm)	0.0000	H → L	0.7024
	$T_0 \rightarrow T_3$	2.42 eV (513 nm)	0.0000	H → L+2	0.6990

[a] Only selected excited states were considered. Numbers in parentheses are the excitation energy in wavelength. [b] Oscillator strength. [c] H stands for HOMO and stands for LUMO. Only the main configurations are presented. [d] Coefficient of the wave function for each excitations. CI coefficients are in absolute values.

9. x,y,z coordinates of the compounds (optimized geometry)

Optimized singlet state geometry of **C-1**

0 1

C	3.34018800	3.39784600	-0.08062500
C	1.30692100	2.33189900	-0.07522200
C	1.93809100	3.57467300	-0.11243900
C	2.37678400	1.37650300	-0.01983400
C	2.36611400	-0.02943800	0.02229400
C	3.56609800	-0.76303300	0.04608000
C	3.81158900	-2.17608000	0.07895600
C	5.20040300	-2.29940100	0.07411700
C	5.79203300	-1.01602000	0.04390900
N	3.59013000	2.07427900	-0.02585400
N	4.79994100	-0.10290900	0.02851900
B	5.00821700	1.43793200	0.02119600
F	5.74345400	1.81908900	-1.10139400
F	5.67351400	1.83522200	1.18636800
C	-0.17071700	2.08506100	-0.09098300
H	-0.46746900	1.44682800	-0.92859300
H	-0.50747300	1.58821300	0.82453300
H	-0.70818800	3.03180500	-0.17844400
C	7.23471800	-0.63437700	0.01626600
H	7.86937700	-1.49861600	0.21826700
H	7.50404500	-0.22487100	-0.96416100
H	7.43656500	0.14273100	0.75857900
C	2.82098900	-3.29902900	0.11213200
H	2.21454800	-3.33008900	-0.79898900
H	3.34189800	-4.25455100	0.20365700
H	2.12920000	-3.20538900	0.95439300
C	1.05909900	-0.75363900	0.03048300
C	0.40843200	-1.02710700	1.24286700
C	0.47154100	-1.16266900	-1.17277300
C	-0.81224500	-1.69830200	1.24710200
H	0.86131400	-0.71796500	2.18020300
C	-0.75606500	-1.82638900	-1.16449500
H	0.97049300	-0.95729000	-2.11517500
H	-1.30666900	-1.90813300	2.19169900
H	-1.20935100	-2.13007700	-2.10350700
S	-4.37875000	-0.82433500	-0.61401900
O	-3.95708500	0.52024900	-0.23366000
O	-4.09033000	-1.30655500	-1.96629800
C	-6.16849500	-0.97767000	-0.36096300
C	-6.89889600	-0.37821500	0.67933900
C	-6.85735400	-1.64763000	-1.37306200
C	-8.28592900	-0.43924400	0.70772700
C	-8.24818600	-1.74744800	-1.34418100
H	-6.30077900	-2.08171000	-2.19413500
C	-8.93611200	-1.13762800	-0.30321100
H	-8.84180400	0.03501500	1.50483800

H	-8.78564100	-2.27663500	-2.12034500
N	-6.26460600	0.31812400	1.81356600
O	-6.86190200	1.28590100	2.27762600
O	-5.20868300	-0.13569100	2.23986200
N	-10.40752100	-1.22209400	-0.26474500
O	-10.96395600	-1.83751100	-1.17066200
O	-10.98499400	-0.67187500	0.67000900
C	-1.40906900	-2.09925700	0.04325000
O	-3.84515700	-1.91482400	0.45895200
C	4.42699700	4.42020400	-0.11583000
H	5.18416000	4.19780200	0.64072500
H	4.92846900	4.41400700	-1.09070300
H	4.02472900	5.41883900	0.06080700
C	-2.73703300	-2.80677400	0.05142300
H	-2.78689400	-3.58095800	0.81812700
H	-2.97970900	-3.23881000	-0.91996200
I	0.98514100	5.46478700	-0.21268400
I	6.29650500	-4.11289300	0.09666100

Optimized singlet state geometry of **C-2**

0 1

C	-1.88876900	1.55802100	-0.21486800
C	-3.82878100	2.78610100	-0.07519600
C	-2.44234300	2.86881000	-0.17495800
C	-4.12635100	1.38247600	-0.06162000
C	-5.36093200	0.70166000	0.01883200
C	-5.40727200	-0.70222200	0.03580700
C	-6.51439400	-1.61850200	0.04905500
C	-5.93161800	-2.88414500	0.04463800
C	-4.52271100	-2.76048300	0.02825600
N	-2.92825100	0.67853500	-0.15167600
N	-4.22301700	-1.44686300	0.01778200
B	-2.78401000	-0.86560400	-0.01096000
F	-2.09399400	-1.39408700	-1.10855400
F	-2.10978900	-1.17929700	1.17050200
C	-4.78149100	3.94064100	-0.00735200
H	-5.34611300	4.05265400	-0.93948200
H	-5.51060500	3.81635900	0.79668700
H	-4.23469300	4.86967600	0.16654000
C	-3.47868700	-3.82646600	0.00985400
H	-3.90590000	-4.78825900	0.29810300
H	-3.04641000	-3.92614500	-0.99270400
H	-2.66375800	-3.57519700	0.69360700
C	-7.98102800	-1.31539500	0.05611700
H	-8.25574800	-0.62737600	-0.74831300
H	-8.55601700	-2.23593300	-0.06808400
H	-8.29125400	-0.84774800	0.99659600
C	-6.63618500	1.47771900	0.07880800
C	-7.24632300	1.73794300	1.31415100

C	-7.23598200	1.94527400	-1.09897900
C	-8.43878400	2.46246700	1.36914300
H	-6.78444900	1.37733800	2.22888200
C	-8.43309900	2.66195200	-1.04073700
H	-6.76727800	1.74370700	-2.05806400
H	-8.90157900	2.66351500	2.33109200
H	-8.89247600	3.01649200	-1.95898100
S	6.54258100	-1.14856300	0.69927200
O	6.42885500	-0.55991500	2.02970700
O	6.00130800	-2.48566500	0.46515800
C	8.26595000	-1.14726200	0.14967100
C	9.21925300	-0.17244100	0.49022800
C	8.67213500	-2.28264300	-0.55175500
C	10.55441000	-0.33014500	0.14442100
C	10.00300200	-2.43975600	-0.93992200
H	7.94527300	-3.05083100	-0.78450800
C	10.91839600	-1.45986900	-0.58023500
H	11.28752300	0.41540800	0.42063200
H	10.32253600	-3.31037800	-1.49774700
N	8.88409100	1.07894500	1.19647000
O	9.70338500	1.49194000	2.01173000
O	7.83738300	1.64017800	0.89239900
N	12.33297200	-1.61847900	-0.96871900
O	12.63480300	-2.62106500	-1.61046000
O	13.11851800	-0.73840300	-0.62567000
C	-9.03513800	2.92376200	0.19265800
H	-9.96436800	3.48451200	0.23700200
C	-0.53238800	1.06453200	-0.33888700
H	-0.46936400	0.05583100	-0.73103800
C	0.60206800	1.71004300	0.01764000
H	0.53804300	2.69497500	0.46789600
H	2.81216600	2.88148600	0.92151100
C	3.02564700	1.93760300	0.42792100
C	1.96267900	1.18536500	-0.11211000
C	4.34406000	1.49649600	0.34625300
C	2.26900800	-0.03296700	-0.75462000
C	4.60142800	0.28704000	-0.29251900
H	5.16185400	2.07525300	0.76017100
C	3.58020300	-0.48597400	-0.84578900
H	1.48072500	-0.63255400	-1.19726300
H	3.81765000	-1.41765000	-1.34735100
O	5.94182600	-0.13121900	-0.44870400
I	-6.95324200	-4.73992000	0.05017400
I	-1.38011500	4.69276400	-0.39281500

Optimized triplet state geometry of **C-1**

0 3

C	3.34069500	3.41747400	-0.09687800
C	1.30651900	2.35482500	-0.08822400
C	1.93784800	3.59074100	-0.11413300
C	2.39441200	1.37644600	-0.05305200

C	2.35218700	-0.04411000	-0.01793800
C	3.58369100	-0.75265600	0.01480000
C	3.84459900	-2.19122500	0.05816200
C	5.22766200	-2.30426400	0.07856200
C	5.81805600	-1.01999300	0.05036400
N	3.59077000	2.06094000	-0.05928700
N	4.79495100	-0.09451500	0.01118400
B	5.00564100	1.43694300	-0.03143200
F	5.72163800	1.79992100	-1.18062900
F	5.70541900	1.86501400	1.10434800
C	-0.16442700	2.08841000	-0.09298500
H	-0.46661600	1.48380400	-0.95472900
H	-0.48171300	1.54298400	0.80241200
H	-0.71602000	3.03067500	-0.12916600
C	7.24755000	-0.61382800	0.06408700
H	7.90317800	-1.48556800	0.05006100
H	7.47061900	0.02096100	-0.80079400
H	7.46592200	-0.01580400	0.95700000
C	2.84479700	-3.30192900	0.07697000
H	2.20619900	-3.28929100	-0.81293100
H	3.35725000	-4.26591500	0.11395800
H	2.17959900	-3.23593400	0.94473700
C	1.04617000	-0.77084700	-0.01774100
C	0.39879200	-1.08359600	1.18933900
C	0.43883000	-1.15155300	-1.22295900
C	-0.82241300	-1.75440700	1.18953500
H	0.86018000	-0.80064000	2.13122800
C	-0.78799900	-1.81747700	-1.22419000
H	0.92827100	-0.92034600	-2.16478200
H	-1.30835900	-1.99009800	2.13274200
H	-1.24968600	-2.09674000	-2.16701200
S	-4.40559100	-0.83976200	-0.64244300
O	-3.96981700	0.49795200	-0.25310400
O	-4.14018400	-1.30703900	-2.00476600
C	-6.19284900	-0.98273600	-0.36584200
C	-6.90375700	-0.38865900	0.69092000
C	-6.90128200	-1.63617500	-1.37521500
C	-8.29072900	-0.43847000	0.73809200
C	-8.29237800	-1.72458600	-1.32810400
H	-6.35972800	-2.06578700	-2.20859900
C	-8.96069500	-1.12024400	-0.27123700
H	-8.83156100	0.03166100	1.54787500
H	-8.84506600	-2.24071900	-2.10235500
N	-6.24804500	0.29046500	1.82345700
O	-6.82977300	1.25953400	2.30440900
O	-5.19140200	-0.17782500	2.23186300
N	-10.43209400	-1.19228500	-0.21349600
O	-11.00641800	-1.79143200	-1.11917700
O	-10.99187400	-0.64862700	0.73577700
C	-1.43099000	-2.12340600	-0.01875000
O	-3.86734700	-1.94688900	0.40913600
C	4.43716600	4.42018300	-0.11425300
H	5.06809800	4.31124900	0.77552600

H	5.08765300	4.25832100	-0.98154600
H	4.03845400	5.43469600	-0.14912000
C	-2.75791300	-2.83139600	-0.01757300
H	-2.80631000	-3.61796700	0.73653800
H	-3.00549300	-3.24688100	-0.99498500
I	0.98760100	5.47914800	-0.17061600
I	6.33083400	-4.10730600	0.14495700

Optimized triplet state geometry of **C-2**

0 3

C	1.86930500	-1.59747400	-0.07868800
C	3.85029000	-2.78447600	-0.08334700
C	2.48257400	-2.90376300	-0.08857100
C	4.12338600	-1.34170300	-0.05597500
C	5.37457300	-0.66035500	-0.03538800
C	5.37193700	0.75367400	-0.01113800
C	6.46644800	1.70626800	-0.04770800
C	5.85519900	2.95612400	0.00156200
C	4.45312300	2.80560600	0.06621400
N	2.93538600	-0.67383400	-0.05742700
N	4.18267900	1.46354800	0.04904000
B	2.77015700	0.85481000	0.15806700
F	1.94019100	1.40540300	-0.83153300
F	2.21437000	1.11159900	1.41772600
C	4.85755500	-3.89015600	-0.10645100
H	5.46335400	-3.86387000	-1.01817700
H	5.55060000	-3.81909200	0.73705300
H	4.35783800	-4.85940200	-0.05787900
C	3.37942000	3.83501600	0.13908000
H	3.80376900	4.82283600	0.32523100
H	2.80715900	3.86903500	-0.79562700
H	2.67212900	3.59204900	0.93846100
C	7.93369200	1.42442900	-0.13088200
H	8.18467700	0.83919900	-1.02159800
H	8.49472700	2.36119500	-0.17013300
H	8.28769200	0.85213200	0.73311700
C	6.66786500	-1.41078100	-0.04754700
C	7.31852300	-1.72800900	1.15495100
C	7.26165300	-1.79710300	-1.25907800
C	8.53262900	-2.41895300	1.14673400
H	6.86824100	-1.43244000	2.09881400
C	8.47620200	-2.48706600	-1.26870500
H	6.76795900	-1.55356500	-2.19610600
H	9.02291400	-2.65882400	2.08621800
H	8.92298300	-2.77909500	-2.21509000
S	-6.60966400	0.81316100	0.98671300
O	-6.64799100	-0.20162800	2.03441700
O	-6.03921700	2.12448200	1.28680500
C	-8.25937800	1.07248800	0.29313100
C	-9.24588300	0.07919300	0.16758800
C	-8.58280900	2.39703200	-0.00192400

C	-10.53326800	0.40193300	-0.23943500
C	-9.86206000	2.73380600	-0.44524200
H	-7.83349100	3.16801300	0.12766700
C	-10.81264100	1.72767000	-0.55277200
H	-11.29365800	-0.36265600	-0.32193100
H	-10.11655200	3.75706500	-0.68910300
N	-8.99423400	-1.35210500	0.42305400
O	-9.90279000	-1.98916300	0.94756300
O	-7.91857900	-1.81443000	0.05913700
N	-12.17437600	2.06948200	-1.00645700
O	-12.40771300	3.24840200	-1.25907100
O	-12.98781600	1.15385600	-1.10228500
C	9.11419300	-2.79966700	-0.06549100
H	10.05858800	-3.33672800	-0.07239700
C	0.54929900	-1.13170600	-0.12275400
H	0.47248000	-0.06028600	-0.25802900
C	-0.63953700	-1.84262500	-0.01086900
H	-0.61386400	-2.90953800	0.17278100
H	-2.91705700	-3.16334300	0.30232800
C	-3.08017800	-2.10914800	0.09794400
C	-1.95849100	-1.26319100	-0.09621500
C	-4.37871000	-1.62158200	0.03274600
C	-2.20250000	0.10776900	-0.36887800
C	-4.57006600	-0.26558800	-0.23429900
H	-5.23554000	-2.26949000	0.17802500
C	-3.49623800	0.60510600	-0.43547200
H	-1.37663700	0.79018300	-0.53664300
H	-3.68365500	1.65143800	-0.65018900
O	-5.88348100	0.22600800	-0.37455400
I	6.83733000	4.83204700	-0.03155400
I	1.47599100	-4.76447900	-0.19528700