Electronic Supplementary Information for:

Triplet excited state of diiodoBOPHY derivatives: preparation, study of the photophysical properties and application in triplet-triplet annihilation upconversion

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Index

1. Molecular structural characterization data……..……..……S2

2. Nanosecond time-resolved transient absorption spectra……S8

3. DFT calculation result and selected frontier molecular orbital…..……..…….S14

4. Singlet oxygen quantum yields…..……..……..…….S20

5. X, Y, Z Coordinates of the compound……...……...…S21

1. Molecular structural characterization data

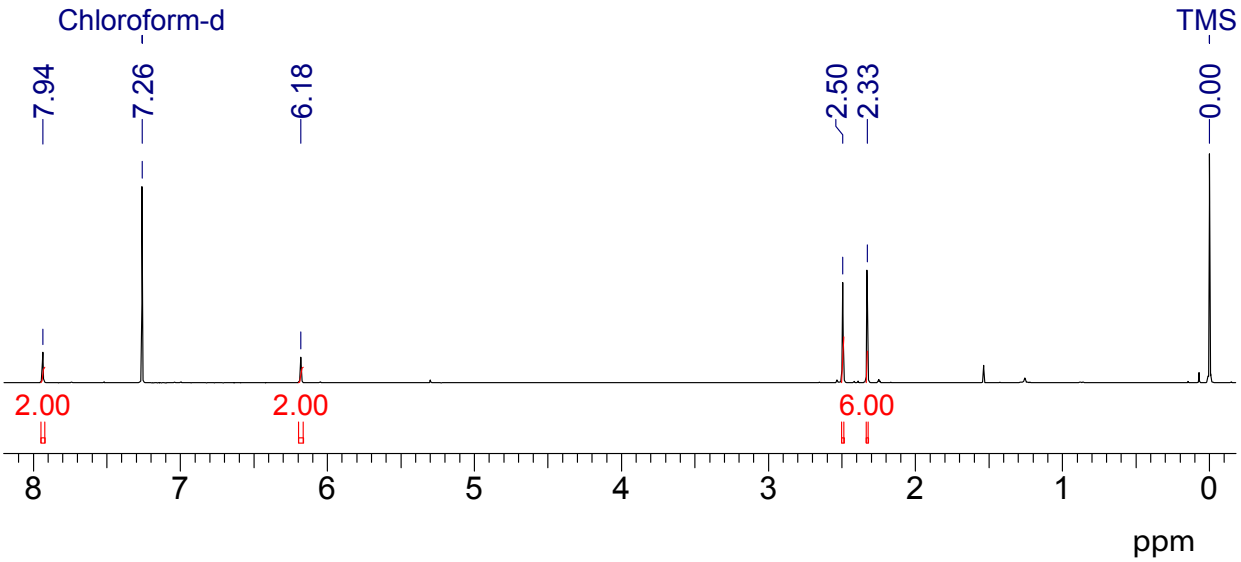

Figure S1. ^{1}H NMR of **C–1** in $CDCl_3$ (400 MHz), 20°C.

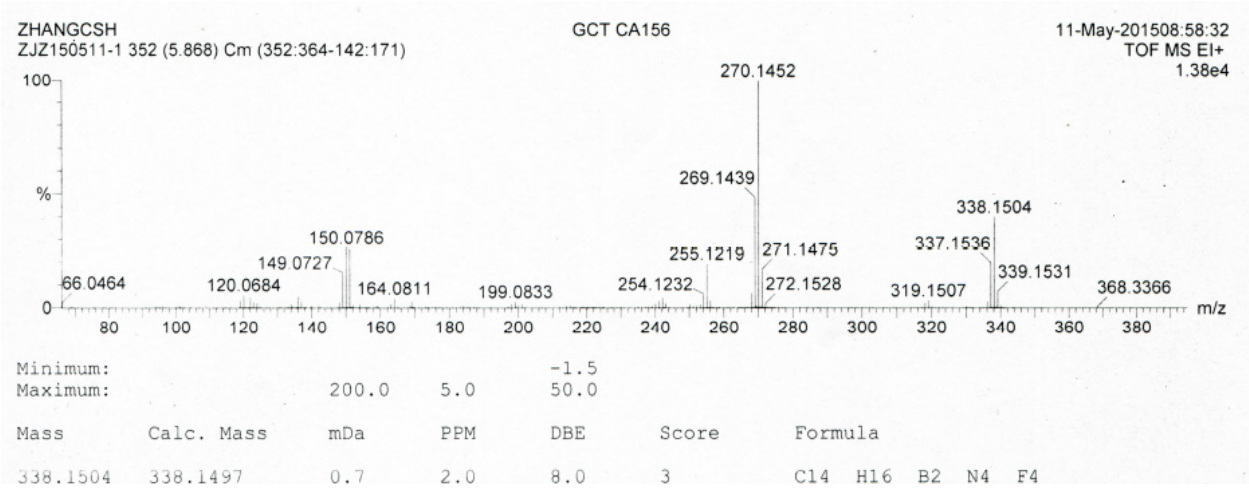

Figure S2. TOF HR MS EI^{+} of **C–1**.

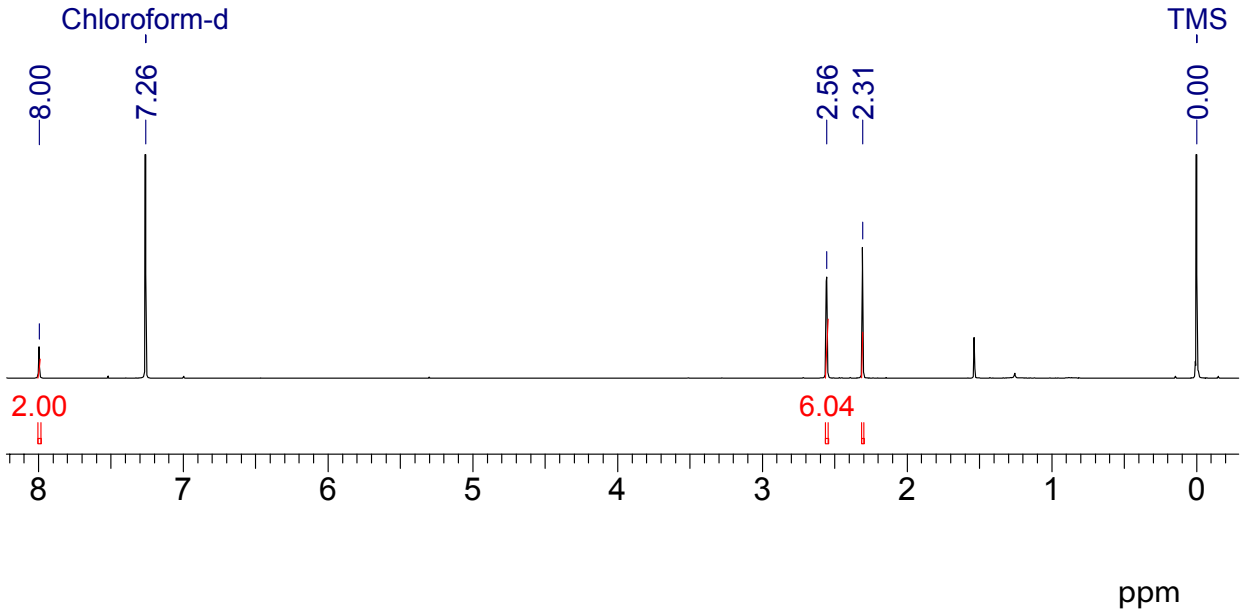

Figure S3. ^{1}H NMR of **C**–**2** in $CDCl_3$ (400 MHz), 20°C.

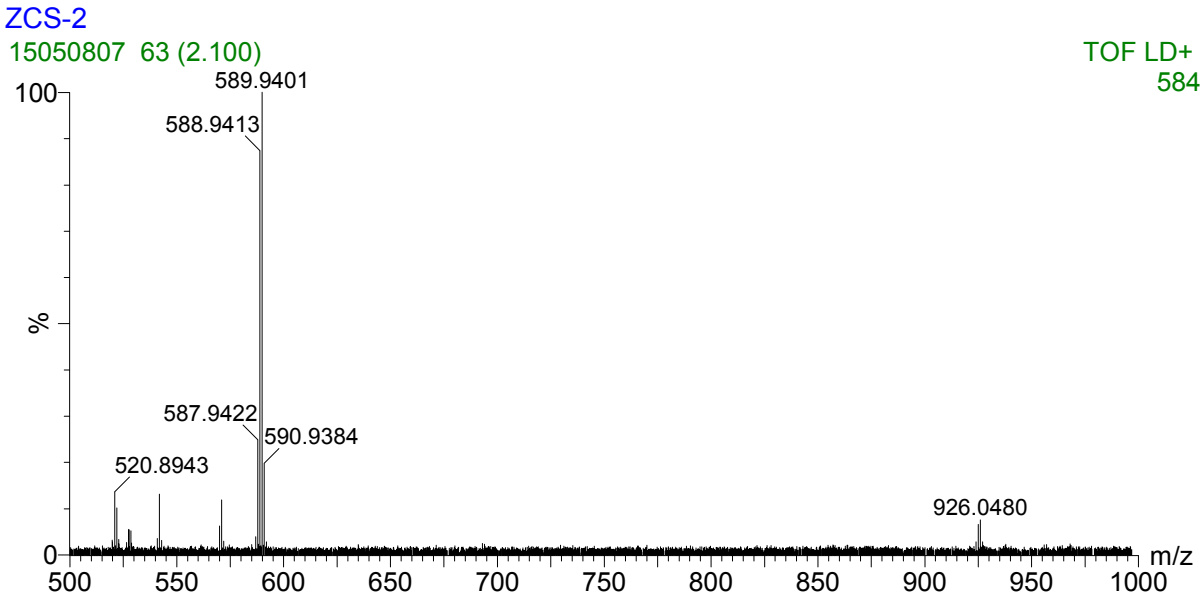

Figure S4. MALDI–HRMS (TOF) of **C**–**2**.

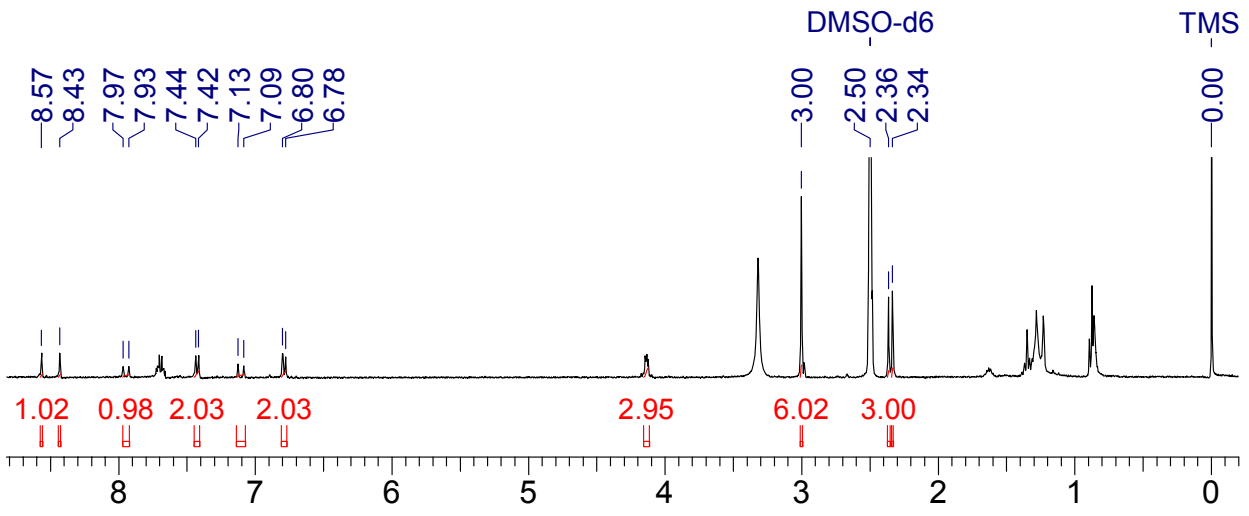

Figure S5. ^{1}H NMR of **C**–**3** in DMSO-d_6 (400 MHz), 20°C.

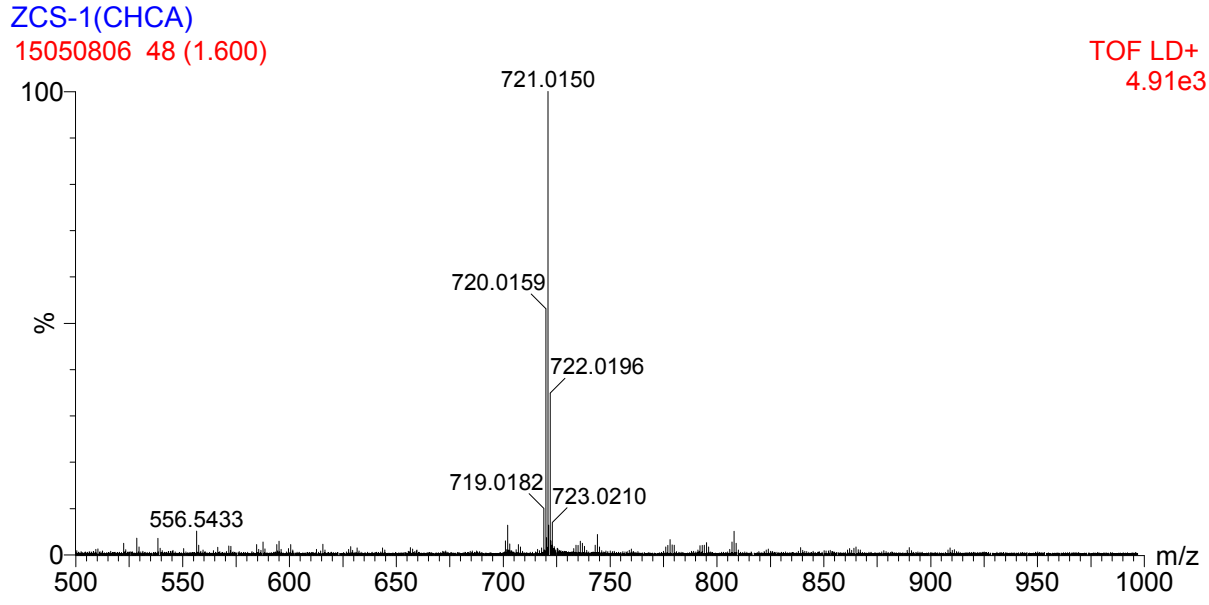

Figure S6. MALDI–HRMS (TOF) of **C**–**3**.

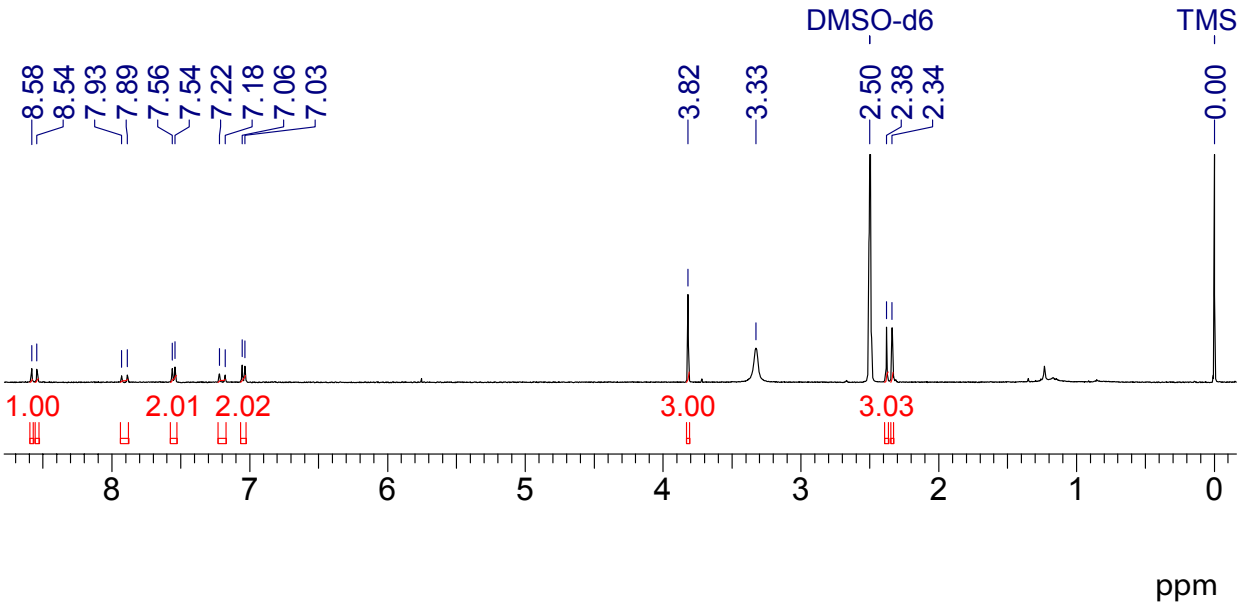

Figure S7. ^{13}C NMR of **C**–**4** in DMSO-d_6 (100 MHz), 25°C.

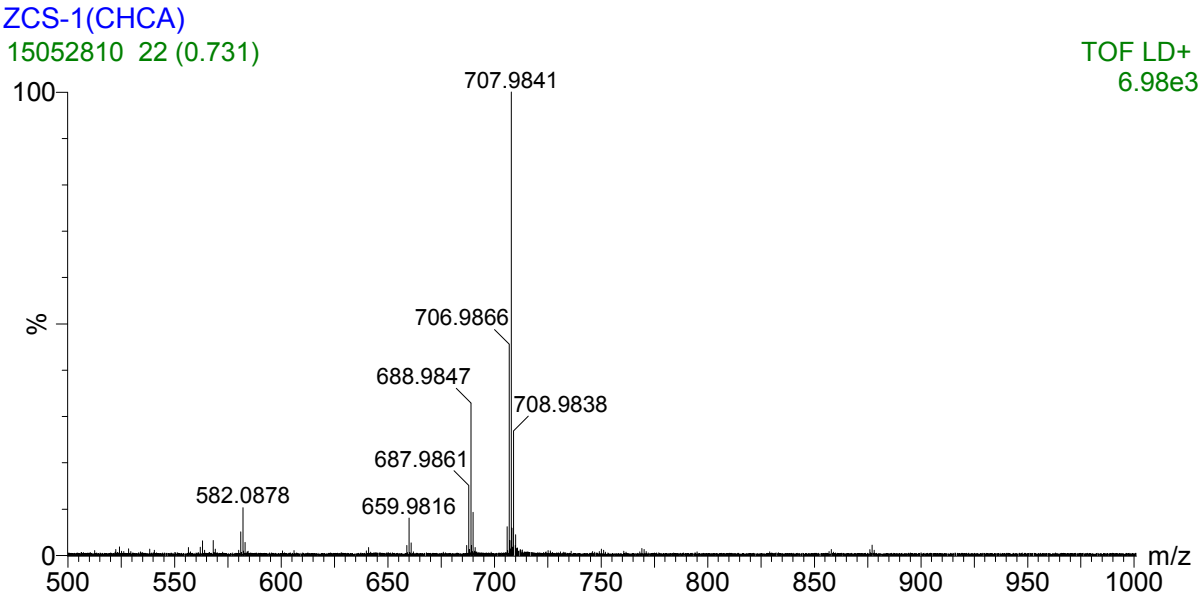

Figure S8. MALDI–HRMS (TOF) of **C**–**4**.

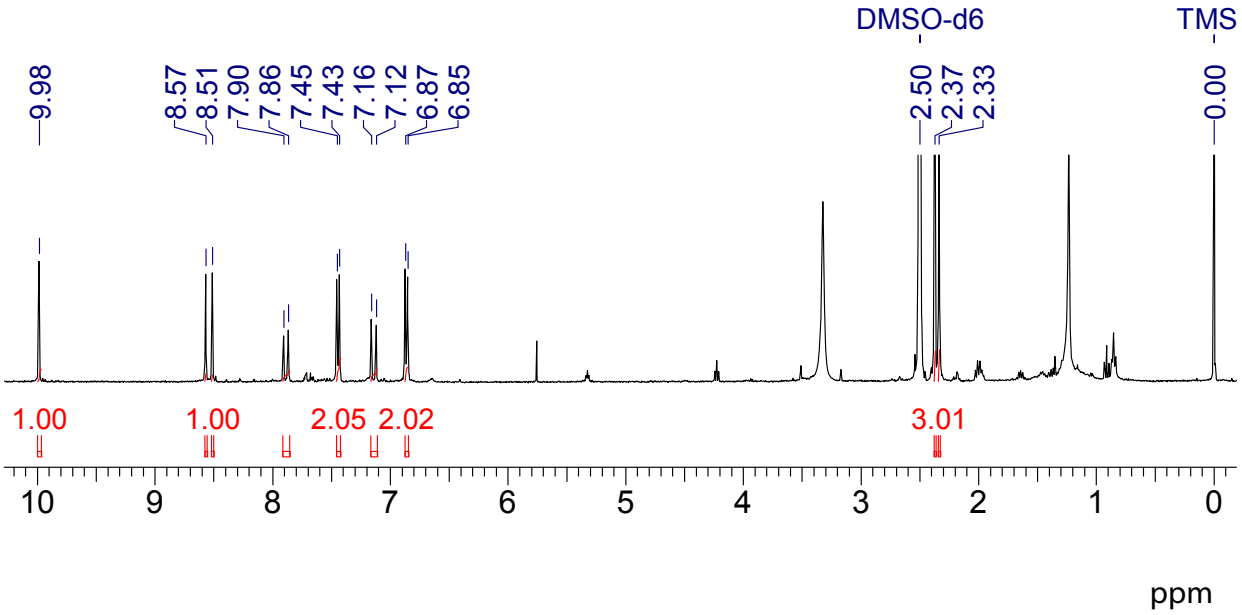

Figure S9. ^{1}H NMR of compound **C**–**5** in DMSO-d_6 (400 MHz), 25°C.

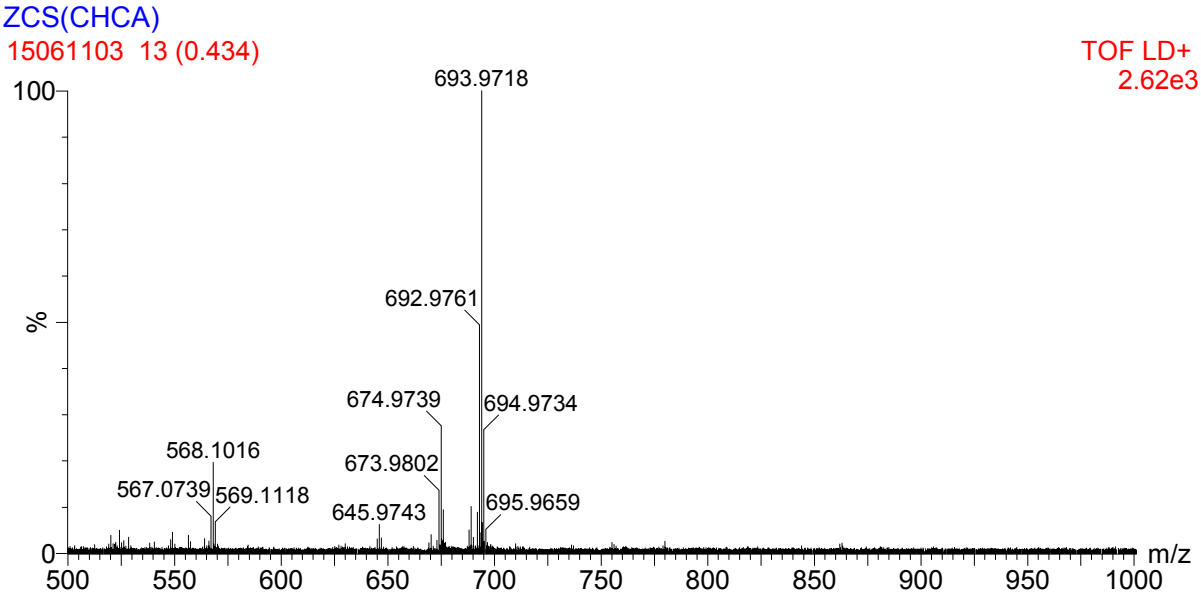

Figure S10. MALDI–HRMS (TOF) of **C**–**5**.

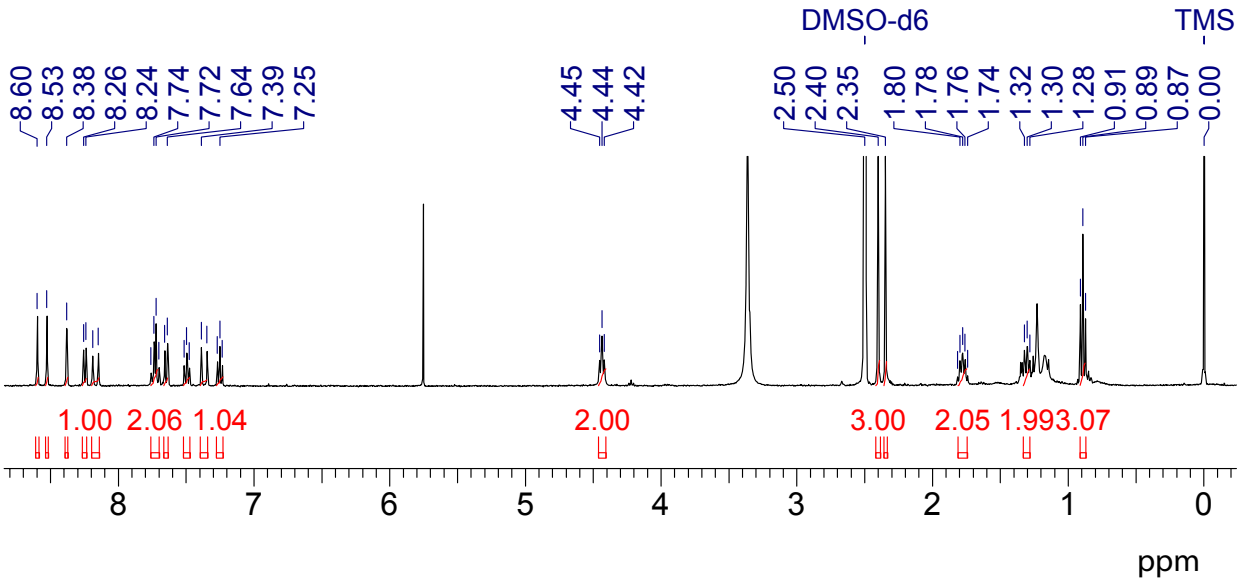

Figure S11. ^{1}H NMR of compound **C**–**6** in DMSO-d_6 (400 MHz), 25°C.

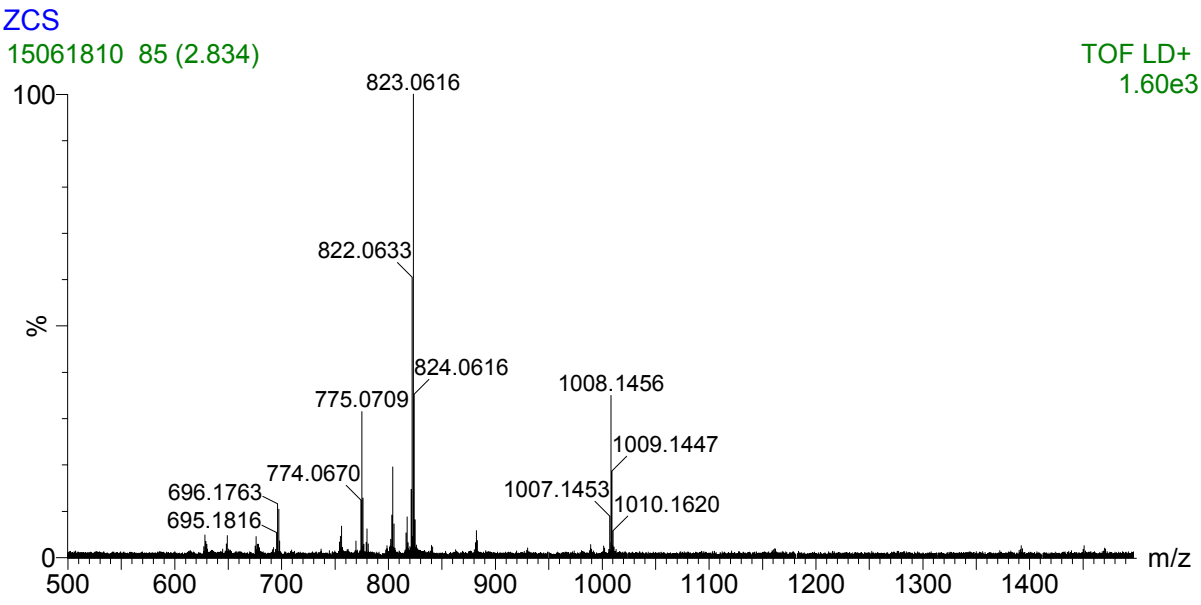

Figure S12. MALDI–HRMS (TOF) of **C**–**6**.

2. Nanosecond time-resolved transient absorption spectra

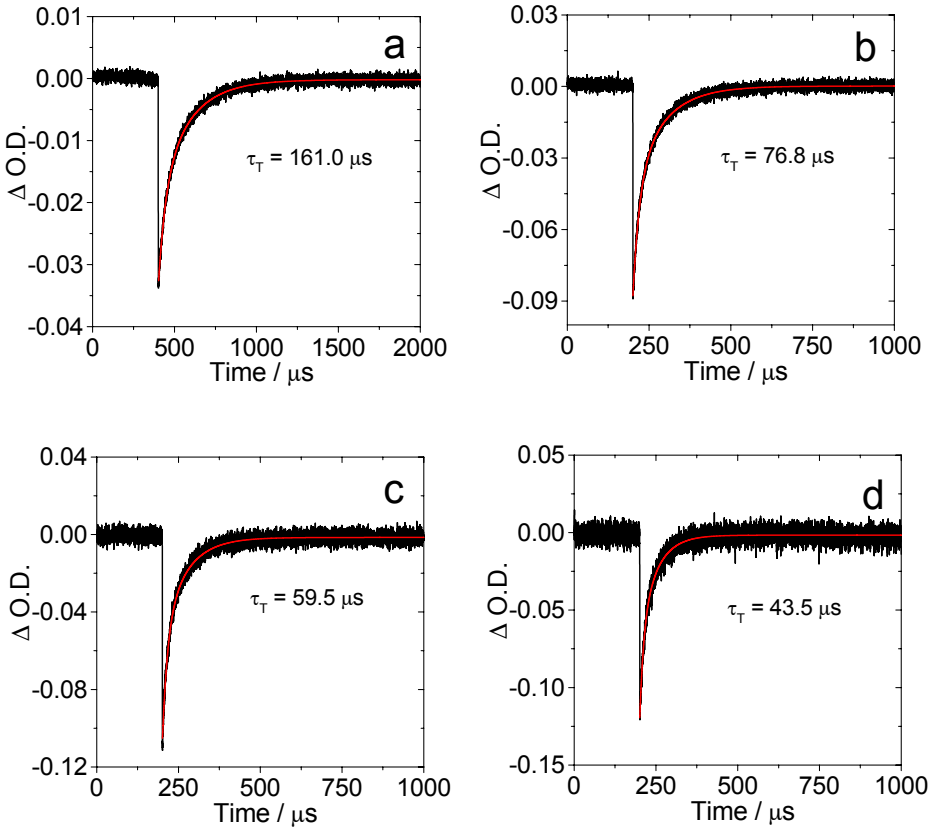

Figure S13. The decay trace of **C–2** at 485 nm (λ_{ex} = 483 nm) with different concentration. In toluene. 20 °C. (a) [**C–2**] = 5.0×10^{-6} M. (b) [**C–2**] = 1.5×10^{-5} M. (c) [**C–2**] = 2.0×10^{-5} M. (d) [**C–2**] = 2.5×10^{-5} M.

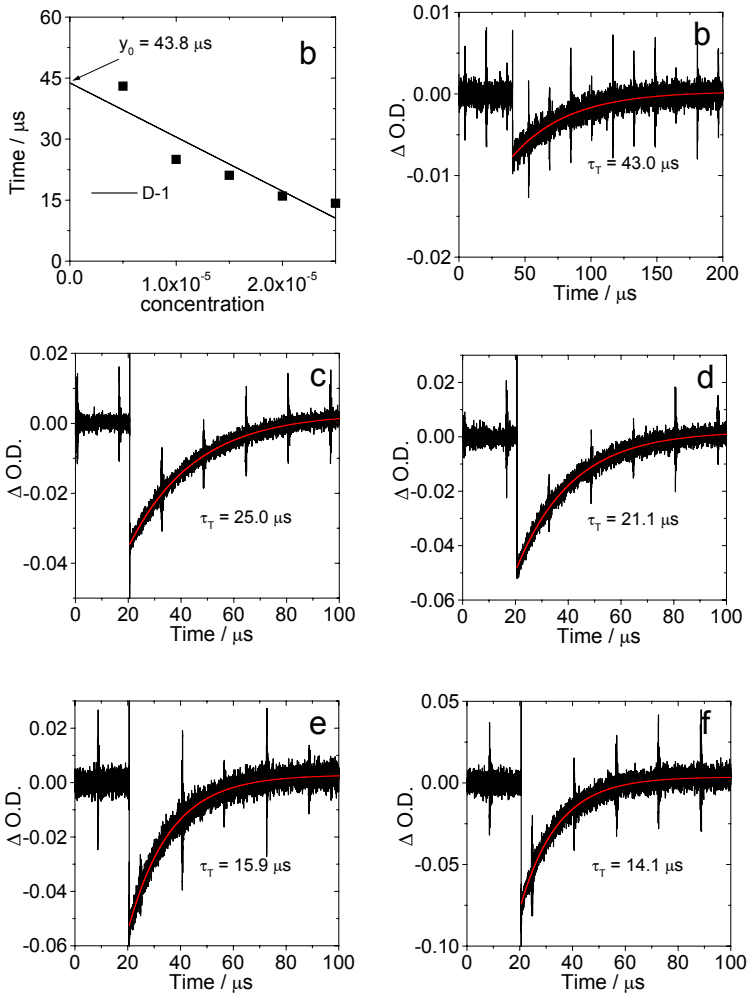

Figure S14. (a) Plotting of the triplet state life time for **C**–**2** at different concentration. The decay trace of **C**–**1** at 485 nm (λ_{ex} = 483 nm) with different concentration. In DMF. 20 °C. (b) [**C**–**2**] = 5.0×10^{-6} M. (c) [**C**–**2**] = 1.0×10^{-5} M. (d) [**C**–**2**] = 1.5×10^{-5} M. (e) [**C**–**2**] = 2.0×10^{-5} M. (f) [**C**–**2**] = 2.5×10^{-5} M.

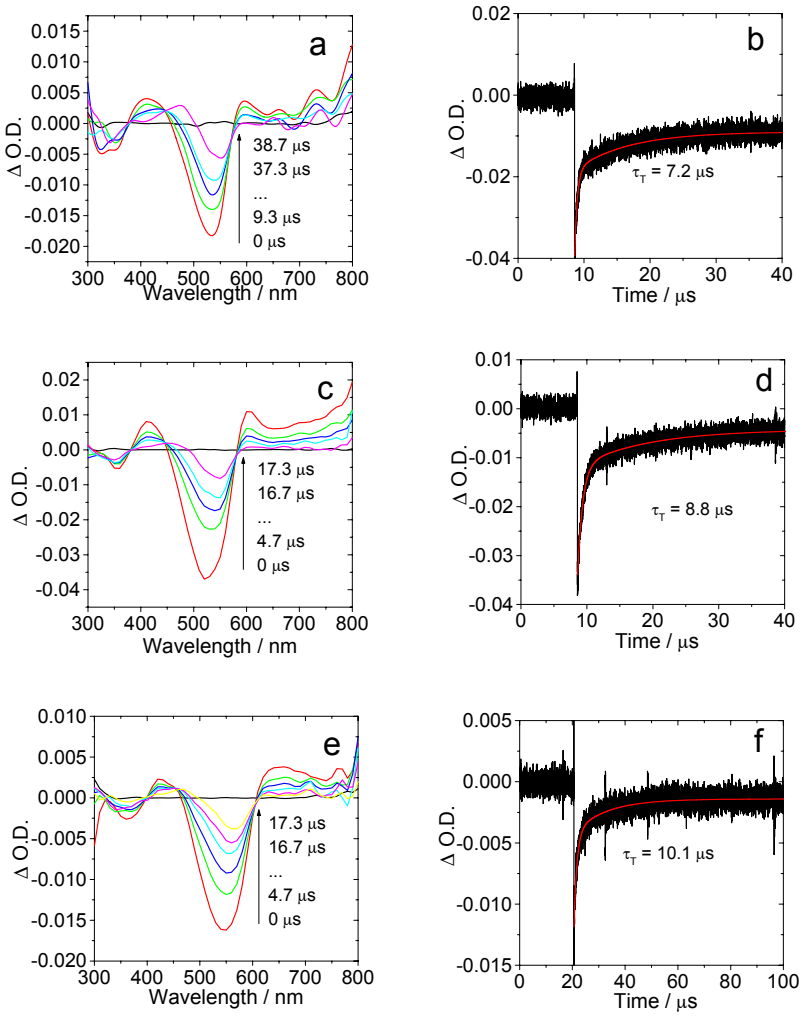

Figure S15. (a) Nanosecond transient absorption spectra of **C–4** ($c_{\text{[C–4]}} = 2.0 \times 10^{-5}$ M) and (d) the corresponding decay trace of **C–4** at 540 nm (λ_{ex} = 535 nm), ($c_{\text{[C–4]}} = 1.0 \times 10^{-5}$ M). (c) Nanosecond transient absorption spectra of **C–5** ($c_{\text{[C–5]}} = 2.0 \times 10^{-5}$ M) and (d) the corresponding decay trace of **C–5** at 543 nm (λ_{ex} = 545 nm), ($c_{\text{[C–5]}} = 1.0 \times 10^{-5}$ M) (e) Nanosecond transient absorption spectra of **C–6** ($c_{\text{[C–6]}} = 2.0 \times 10^{-5}$ M) and (f) the corresponding decay trace of **C–6** at 561 nm (λ_{ex} = 565 nm), ($c_{\text{[C–6]}} = 1.0 \times 10^{-5}$ M). In toluene. 20 °C.

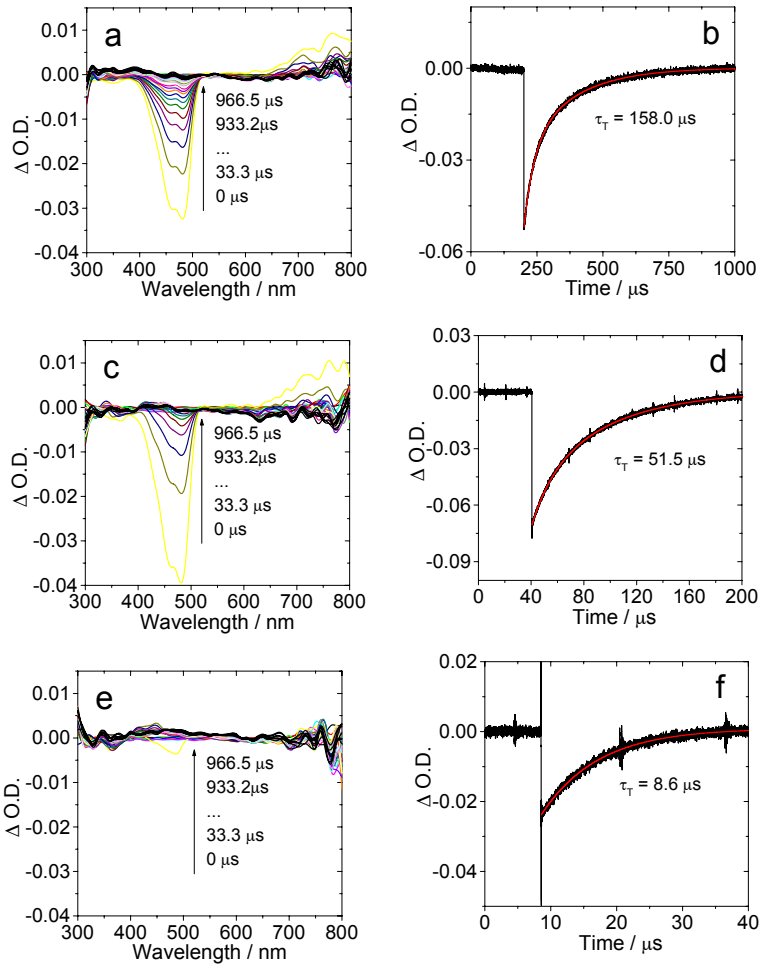

Figure S16. Nanosecond time-resolved transient difference absorption and decay trace of compound **C–2** at 485 with different concentration of DPA, λ_{ex} = 483 nm. In toluene. $c_{c\text{-}2}$ = 5.0×10^{-6} M. 20 °C. (a and b) $c_{DPA} = 0$, (c and d) $c_{DPA} = 3.0 \times 10^{-6}$. (e and f) $c_{DPA} = 3.0 \times 10^{-5}$. 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.

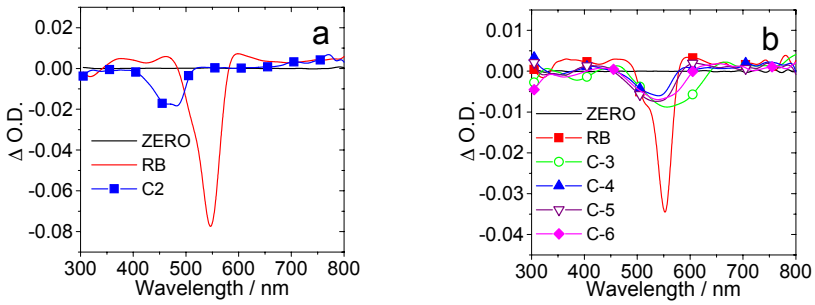

Figure S17. Nanosecond transient absorption spectra of RB (Rose bengal) and **C–2-C–6**. Optically matched solutions were used. In toluene. 20 °C. (a) λ_{ex} = 500 nm. (b) λ_{ex} = 550 nm.

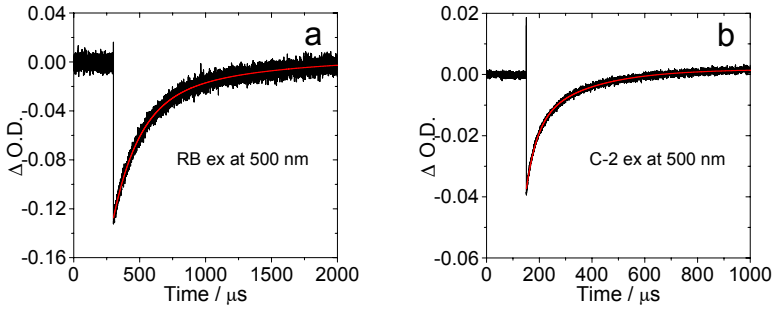

Figure S18. The decay trace of (a) RB (Rose bengal) in methanol and (b) **C–2** in toluene. λ_{ex} = 500 nm, 20 °C. In toluene. Optically matched solutions were used.

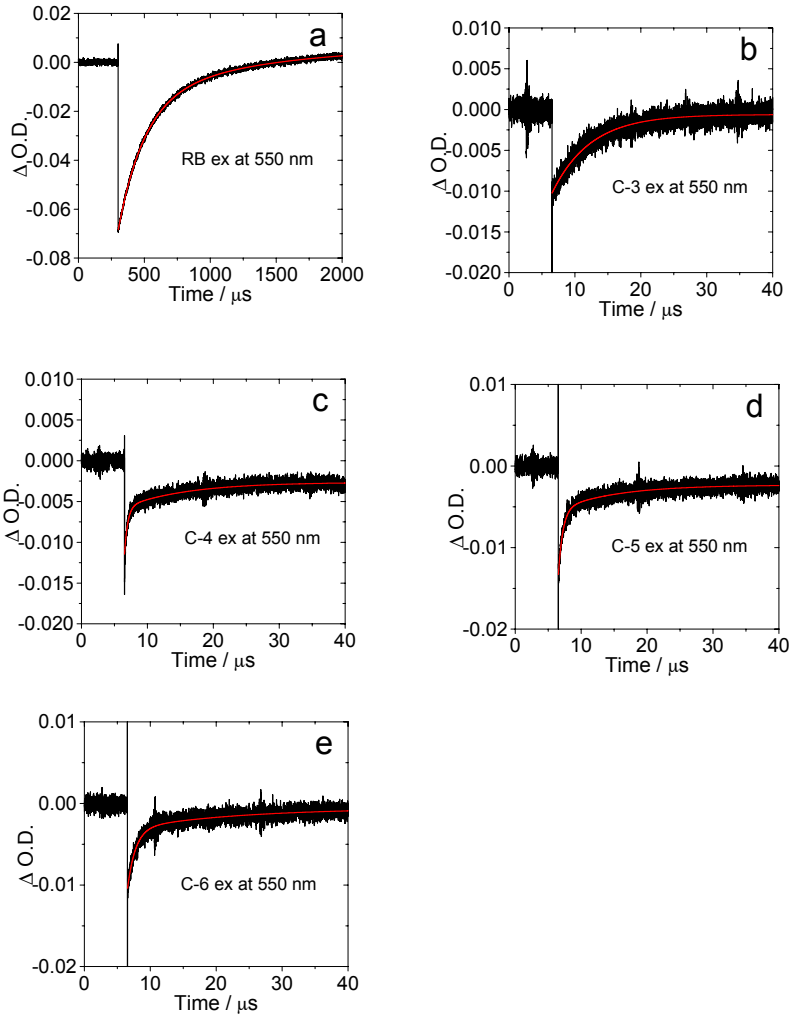

Figure S19. The decay trace of (a) RB in methanol, (b) **C–3**, (c) **C–4**, (d) **C–5**, (e) **C–6.** In toluene. λ_{ex} = 550 nm. 20 °C. Optically matched solutions were used.

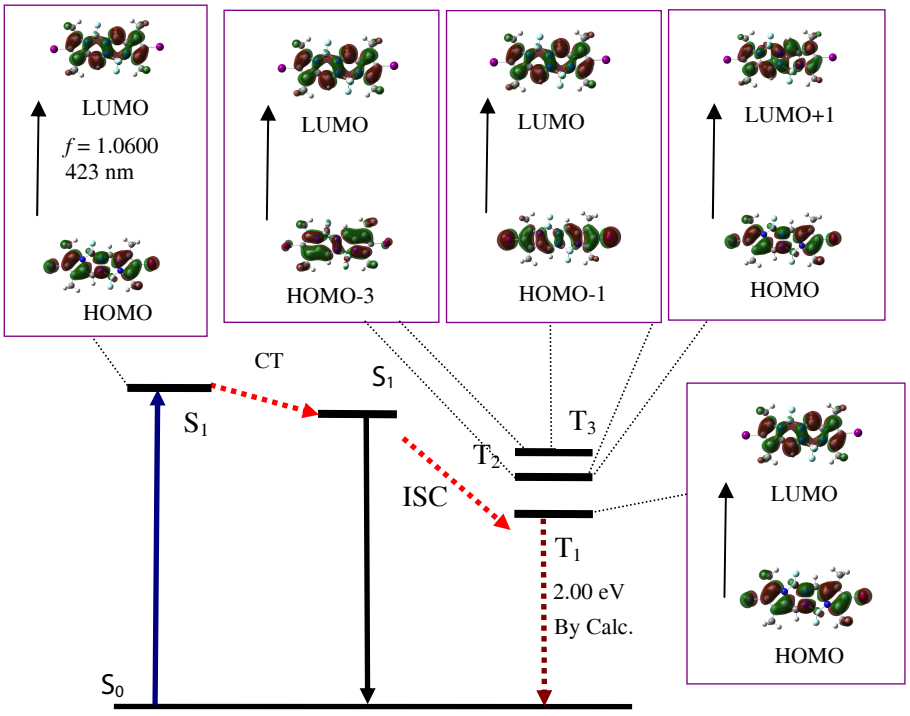

Figure S20. Selected frontier molecular orbitals involved in the excitation and emission of **C–2**. CT stands for conformation transformation. The calculations are at the B3LYP/6–31G(d)/ level using Gaussian 09W. In toluene.

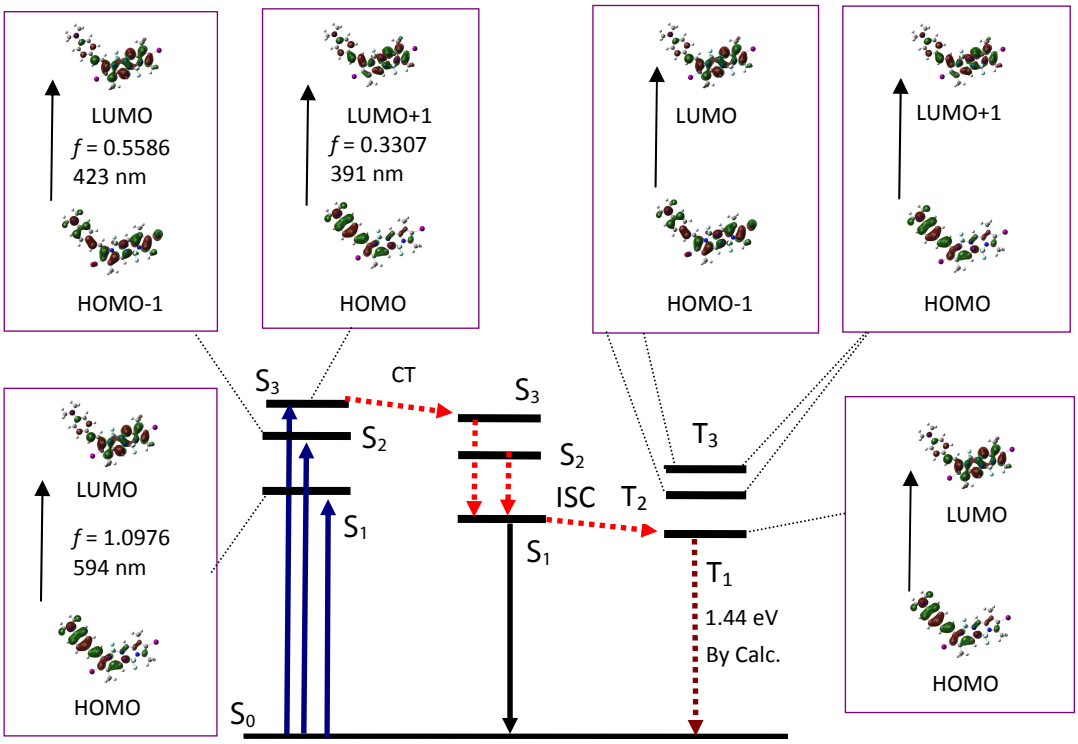

Figure S21. Selected frontier molecular orbitals involved in the excitation and emission of **C–3**. CT stands for conformation transformation. The calculations are at the B3LYP/6–31G(d)/ level using Gaussian 09W. In toluene.

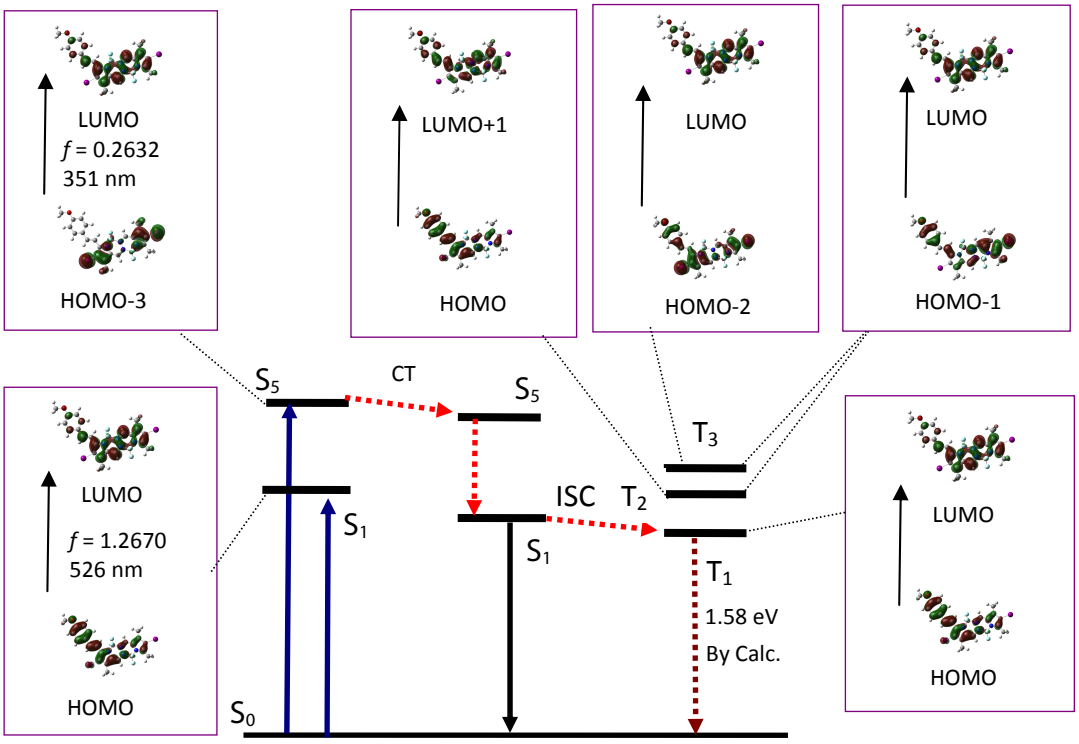

Figure S22. Selected frontier molecular orbitals involved in the excitation and emission of **C–4**. CT stands for conformation transformation. The calculations are at the B3LYP/6–31G(d)/ level using Gaussian 09W. In toluene.

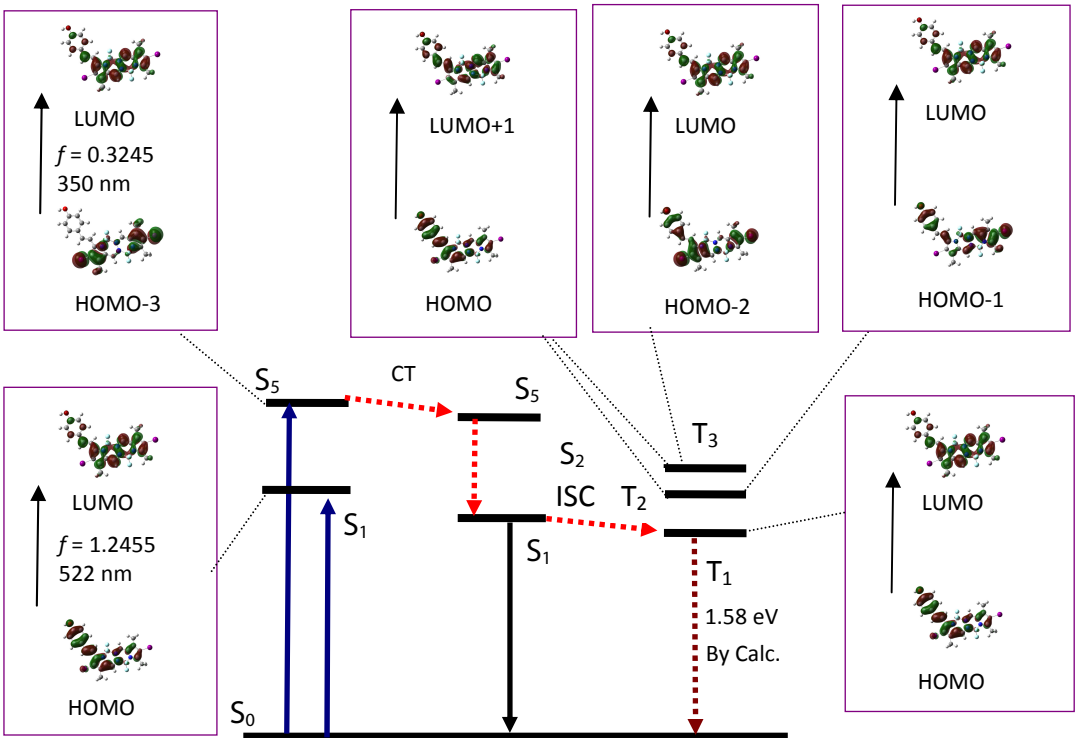

Figure S23. Selected frontier molecular orbitals involved in the excitation and emission of **C–5**. CT stands for conformation transformation. The calculations are at the B3LYP/6–31G(d)/ level using Gaussian 09W. In toluene.

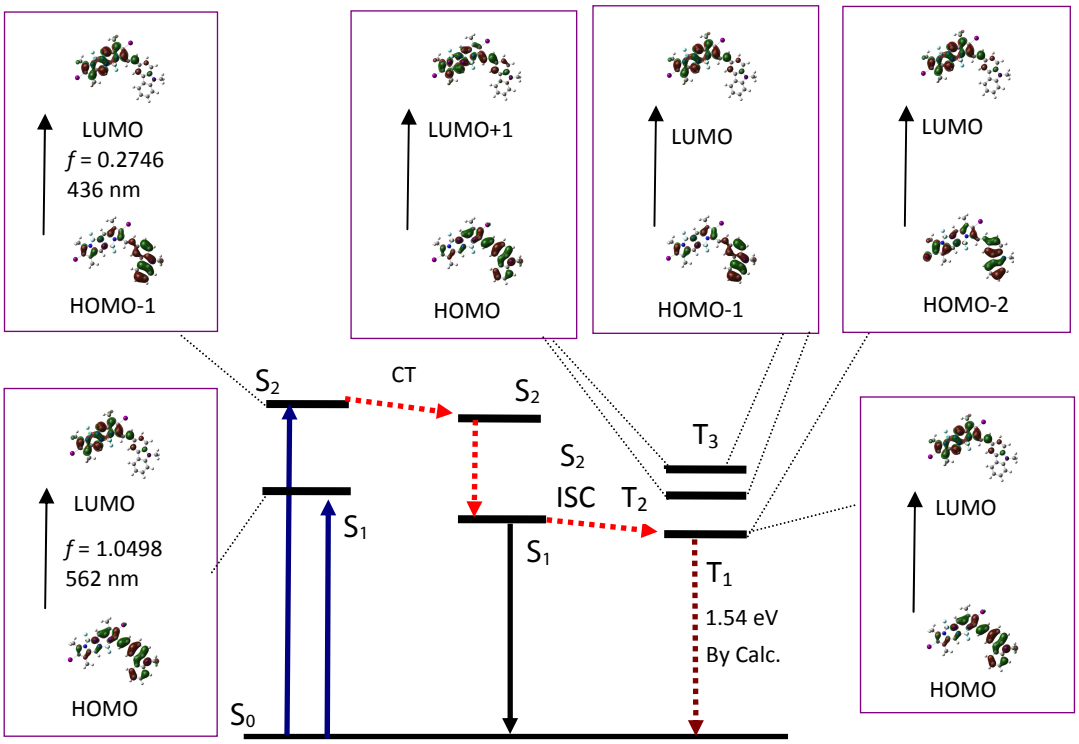

Figure S24. Selected frontier molecular orbitals involved in the excitation and emission of **C–6**. CT stands for conformation transformation. The calculations are at the B3LYP/6–31G(d)/ level using Gaussian 09W. In toluene.

3. DFT calculation result and selected frontier molecular orbital

Table S1. 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-4 and C-5. 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–4	$S_0 \rightarrow S_1$	2.36 eV (526 nm)	1.2670	H→ L	0.7045
	$S_0 \rightarrow S_5$	3.53 eV (351 nm)	0.2632	H–3→ L	0.6038
C–4	$S_0 \rightarrow T_1$	1.58 eV (786 nm)	0.0000	H → L	0.6937
	$S_0 \rightarrow T_2$	2.29 eV (542 nm)	0.0000	H–1→ L	0.5306
				H →L+1	0.3539
	$S_0 \rightarrow T_3$	2.76 eV (450 nm)	0.0000	H–2→ L	0.3494
				H →L+1	0.3889
C–5	$S_0 \rightarrow S_1$	2.37 eV (522 nm)	1.2455	H → L	0.7044
	$S_0 \rightarrow S_5$	3.55 eV (350 nm)	0.3245	H–3→ L	0.5382
				H →L+1	0.3344
C–5	$S_0 \rightarrow T_1$	1.58 eV (787 nm)	0.0000	H →L	0.6676
	$S_0 \rightarrow T_2$	2.29 eV (542 nm)	0.0000	H–1→ L	0.5307
				H →L+1	0.3588
	$S_0 \rightarrow T_3$	2.76 eV (450 nm)	0.0000	H–2→ L	0.3427
				H →L+1	0.3812

[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.

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-6. 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–6	$S_0 \rightarrow S_1$	2.21 eV (562 nm)	1.0498	H → L	0.7043
	$S_0 \rightarrow S_2$	2.85 eV (436 nm)	0.2746	H–1→ L	0.6993
C–6	$S_0 \rightarrow T_1$	1.54 eV (806 nm)	0.0000	H →L	0.6390
	$S_0 \rightarrow T_2$	2.26 eV (548 nm)	0.0000	H–2→ L	0.3779
				H–1→ L	0.3049
				H→ L+1	0.3110
	$S_0 \rightarrow T_3$	2.62 eV (473 nm)	0.0000	H–1→ L	0.4436
				H →L+1	0.3573

[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.

Table S3. Singlet oxygen quantum yields (Φ_Δ) for the photooxidations of DPBF using different triplet photosensitizers.[a]

	Φ_Δ	Φ_Δ	Φ_Δ	average
C–2 [b]	0.5822	0.5822	0.5836	0.5827
C–3 [c]	0.3423	0.3468	0.3553	0.3481
C–4 [c]	0.4136	0.4282	0.4358	0.4258
C–5 [c]	0.3970	0.4116	0.4231	0.4106
C–6 [c]	0.4778	0.4939	0.5030	0.4916

[a] In toluene. [b] Take compound **4** as standard (Φ_Δ = 0.87 in CH_2Cl_2). [c] Take Rose Bengal (RB) as standard (Φ_Δ = 0.80 in CH_3OH).

4. X, Y, Z coordinates of the compound

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

0 3

C	-3.76917800	1.08371000	0.06117700
C	-3.70286900	-1.21190400	-0.02648900
C	-4.52014400	-0.09393700	-0.16534900
C	-2.40328600	-0.67621200	0.28403100
N	-2.47545300	0.70147300	0.32404500
N	0.00994300	0.66405000	0.61557400
B	-1.31942000	1.55496300	0.85086100
F	-1.16613400	2.72896300	0.13862700
F	-1.42118000	1.78885500	2.21026900
C	-4.02555200	-2.66013100	-0.19424500
H	-3.78261800	-3.01076700	-1.20688000
H	-3.45901800	-3.27905100	0.50988200
H	-5.09057700	-2.84552600	-0.02941700
C	-4.18375800	2.51223600	0.06476600
H	-3.60678900	3.08696700	-0.66801500
H	-5.24663800	2.60825500	-0.16290700
H	-3.99405200	2.96693800	1.04532700
C	2.40328400	0.67622000	0.28401900
C	3.70286900	1.21190500	-0.02651200
C	4.52014400	0.09393400	-0.16533700
C	3.76917700	-1.08370700	0.06121900
N	-0.00994600	-0.66402800	0.61559500
N	2.47545000	-0.70146200	0.32407200
B	1.31941600	-1.55493300	0.85091800
F	1.42117400	-1.78877400	2.21033500
F	1.16613100	-2.72896000	0.13872800
C	4.18375900	-2.51223200	0.06485700
H	5.24662400	-2.60826400	-0.16287700
H	3.99411700	-2.96688100	1.04545600
H	3.60674100	-3.08700200	-0.66785300
C	4.02554300	2.66013000	-0.19430000
H	3.45913300	3.27904400	0.50993300
H	5.09059700	2.84550900	-0.02964700
H	3.78243900	3.01078600	-1.20688700
C	1.19627900	1.33240600	0.48176300
H	1.10827400	2.40709200	0.48029400
C	-1.19628000	-1.33238800	0.48179900
H	-1.10827200	-2.40707400	0.48036300
I	6.57355600	0.12974200	-0.65990000
I	-6.57355100	-0.12976800	-0.65992500

Optimized triplet state geometry of **C–3**

0 3

C	5.54288200	−0.33577500	0.09026000
C	4.57019800	1.73779800	−0.10463800
C	5.77026900	1.02153300	−0.20336100
C	3.60288800	0.76467800	0.24738000
N	4.21614300	−0.47797500	0.35178400
N	1.92014100	−1.40883200	0.65481500
B	3.47007400	−1.69303500	0.92573800
F	3.80246400	−2.86697900	0.26753600
F	3.66860300	−1.81017400	2.29401200
C	−0.29990400	−2.29029100	0.28352200
C	−1.27684300	−3.30110900	−0.04457000
C	−2.47224900	−2.62809900	−0.15521400
C	−2.27999900	−1.21947700	0.09450900
N	1.40356300	−0.14574200	0.64689200
N	−0.89619200	−1.06966400	0.35213300
B	−0.13963900	0.12217700	0.96730200
F	−0.30725800	0.17451800	2.34126300
F	−0.47566300	1.33494800	0.37320600
C	1.07569800	−2.45260500	0.49080100
H	1.54413500	−3.42454600	0.48992800
C	2.22719500	0.88985900	0.45014700
H	1.73899700	1.85368000	0.44091300
I	−4.28370300	−3.58860700	−0.68930800
I	7.64229900	1.86544100	−0.72112700
C	−5.23256900	1.21629300	−0.02235800
C	−6.64858700	1.17330000	−0.17906300
C	−4.65919200	2.51167800	0.14422200
C	−7.42898000	2.30778100	−0.17296000
H	−7.12754800	0.20614500	−0.30895200
C	−5.42829400	3.65378400	0.15297500
H	−3.58638400	2.61707800	0.26820300
C	−6.84424000	3.59660700	−0.00668400
H	−8.50007400	2.20641900	−0.29769100
H	−4.93552300	4.60938300	0.28417100
C	−3.10629600	−0.09590900	0.11216500
H	−2.56485900	0.82865600	0.27384600
C	−4.49387900	−0.00031100	−0.04316800
H	−5.07642700	−0.90252100	−0.18493400
N	−7.60877300	4.73174300	−0.00149300
C	−6.98689100	6.04132300	0.16456600
H	−7.75960600	6.80931900	0.13377300
H	−6.46512400	6.11857900	1.12660600
H	−6.26687400	6.24763400	−0.63713300
C	−9.05555500	4.64622000	−0.16874500

H	-9.51632600	4.05047300	0.62907700
H	-9.47924400	5.64965500	-0.13217700
H	-9.32141400	4.19660800	-1.13374900
C	-0.94992500	-4.74792300	-0.22766400
H	-1.83593000	-5.32575100	-0.49891300
H	-0.19957900	-4.88659900	-1.01642200
H	-0.53446700	-5.17859600	0.69247400
C	4.33657200	3.19615800	-0.34070100
H	4.98313600	3.80731600	0.30028700
H	4.56042300	3.47357500	-1.37839700
H	3.29982200	3.47816900	-0.13676500
C	6.49400800	-1.48407400	0.15816200
H	6.50742200	-1.91804900	1.16530900
H	6.19636600	-2.28093800	-0.53075900
H	7.50598300	-1.15975100	-0.09138600

Optimized triplet state geometry of **C–4**

0 3

C	5.35812700	-0.48818600	0.08629600
C	4.50367200	1.63729200	-0.09696100
C	5.66128700	0.85810200	-0.19942700
C	3.48260300	0.71552000	0.24923500
N	4.02638900	-0.55966500	0.34549200
N	1.67970000	-1.36042900	0.64548700
B	3.21442400	-1.73761400	0.90819200
F	3.47501000	-2.91942500	0.23483400
F	3.40554400	-1.87954400	2.27357200
C	-0.58607100	-2.11069600	0.27685600
C	-1.62382200	-3.06751500	-0.05329800
C	-2.77739400	-2.33202600	-0.15908800
C	-2.50562500	-0.93152700	0.09500300
N	1.23697800	-0.07180900	0.64612500
N	-1.11156400	-0.86046400	0.35000500
B	-0.28993700	0.28422600	0.97093500
F	-0.44981600	0.33617700	2.34442100
F	-0.55521700	1.51530200	0.38266800
C	0.77580200	-2.35481600	0.47943500
H	1.18798700	-3.35173500	0.46982000
C	2.11831800	0.91663800	0.45339600
H	1.68482900	1.90638000	0.44791400
I	-4.63911800	-3.18938500	-0.68797500
I	7.57550600	1.59971800	-0.71219000
C	-5.32113800	1.66511000	-0.01155500
C	-6.73218400	1.69234400	-0.17463700
C	-4.66935800	2.92100500	0.17058800
C	-7.45690500	2.87438200	-0.16039800
H	-7.25931600	0.75241400	-0.31562200

C	-5.38175100	4.10055700	0.18675500
H	-3.59311500	2.96305900	0.29972800
H	-8.53240200	2.84340600	-0.28932500
H	-4.88318300	5.05459300	0.32588300
C	-3.26496800	0.23334900	0.11801100
H	-2.67494000	1.12616800	0.28700500
C	-4.64717200	0.40548400	-0.04038100
H	-5.27749700	-0.46244100	-0.19092700
C	-1.37394500	-4.52838000	-0.23853300
H	-2.28618500	-5.05647200	-0.52295400
H	-0.62166500	-4.70258500	-1.01821600
H	-0.99306600	-4.98282400	0.68511500
C	4.35069900	3.10744100	-0.32354500
H	5.00876900	3.67840400	0.34235800
H	4.62015900	3.38032700	-1.35125300
H	3.32416500	3.44022000	-0.14748900
C	6.24487500	-1.68687100	0.14661100
H	6.22209700	-2.13479800	1.14730800
H	5.91102400	-2.45593600	-0.55729900
H	7.27590200	-1.41556300	-0.08757800
C	-6.78437900	4.09644600	0.02130700
O	-7.38080400	5.31013600	0.05256600
C	-8.79627000	5.38709900	-0.11070500
H	-9.31727100	4.84498500	0.68699700
H	-9.04297500	6.44767500	-0.05204400
H	-9.10448300	4.99240900	-1.08585400

Optimized triplet state geometry of **C–5**

0 3

C	5.11050700	-0.68584100	0.10085800
C	4.39652900	1.48870400	-0.10653300
C	5.50086400	0.63480000	-0.19926100
C	3.31733500	0.63896600	0.24829000
N	3.77696200	-0.66781900	0.35908700
N	1.38288300	-1.31145700	0.65979300
B	2.88911800	-1.78404300	0.93287100
F	3.07423700	-2.98818000	0.27432300
F	3.06648700	-1.92125100	2.30041300
C	-0.92450200	-1.91809000	0.28628100
C	-2.02127900	-2.80845200	-0.04111400
C	-3.12372800	-2.00049200	-0.15935200
C	-2.76263200	-0.61832700	0.08598600
N	1.02453000	0.00302000	0.64673400
N	-1.36798600	-0.63576500	0.34636800
B	-0.47743100	0.45933500	0.96162900
F	-0.63952500	0.53365300	2.33375100
F	-0.66115500	1.69968800	0.36165300

C	0.41775800	-2.24739700	0.49773700
H	0.76635600	-3.26835400	0.49872300
C	1.96868100	0.93033900	0.44684300
H	1.59975700	1.94583900	0.43021900
I	-5.03369600	-2.73829600	-0.69706900
I	7.45923400	1.24371400	-0.71905300
C	-5.41638500	2.14310200	-0.03273000
C	-6.82527500	2.24810400	-0.19777800
C	-4.69470900	3.35836800	0.15203600
C	-7.47387300	3.47041400	-0.18009400
H	-7.40503000	1.34028600	-0.34102200
C	-5.33630700	4.58112900	0.17111000
H	-3.61799300	3.33679200	0.28228000
C	-6.73261800	4.65017300	0.00557300
H	-8.55280200	3.52098900	-0.30822400
H	-4.78149600	5.50299300	0.31328300
C	-3.44636700	0.59230500	0.10118900
H	-2.80236300	1.44757500	0.26758000
C	-4.81551300	0.84668300	-0.06024400
H	-5.49454100	0.01642000	-0.21052900
C	-1.86667000	-4.28394700	-0.21433100
H	-2.82077300	-4.76110400	-0.44699900
H	-1.16407200	-4.51336600	-1.02565300
H	-1.46935300	-4.74707700	0.69775800
C	4.33902300	2.96287900	-0.35097700
H	5.04805700	3.49624700	0.29335000
H	4.60490600	3.20333300	-1.38776500
H	3.34125000	3.36682100	-0.15921200
C	5.91828600	-1.93833700	0.17510100
H	6.96458300	-1.73629500	-0.06122700
H	5.86679500	-2.37290100	1.18061300
H	5.53575800	-2.69200300	-0.52067000
O	-7.30221900	5.88093600	0.03471500
H	-8.26315200	5.80116300	-0.08491300

Optimized triplet state geometry of **C–6**

0 3

C	5.98256200	0.02630000	0.10967700
C	4.71622500	1.92669500	-0.15159800
C	6.00899700	1.39438100	-0.22413200
C	3.90008800	0.82998400	0.22529500
N	4.69029500	-0.30409800	0.36977700
N	2.55389700	-1.55589600	0.68672200
B	4.12766700	-1.59963900	0.97585300
F	4.63481000	-2.72964700	0.35464700
F	4.32372400	-1.64564100	2.34765900
C	0.49682500	-2.76978500	0.32578700

C	-0.31566100	-3.92763800	0.01877600
C	-1.59425900	-3.44634600	-0.12619100
C	-1.61878200	-2.01502400	0.08345900
N	1.85643900	-0.38590900	0.63650600
N	-0.27488700	-1.65156000	0.34960900
B	0.28466500	-0.34145500	0.93463000
F	0.09406400	-0.27507700	2.30405700
F	-0.21988500	0.78830800	0.29951900
C	1.87698800	-2.71990300	0.55015700
H	2.48593600	-3.60984500	0.58176200
C	2.52001300	0.75505400	0.41441200
H	1.89375400	1.63449800	0.37115400
I	-3.23125700	-4.68010500	-0.65885000
I	7.74093800	2.48561900	-0.76305100
C	-2.60386300	-1.03092400	0.06415100
H	-2.21277500	-0.03028100	0.20418700
C	-3.98852800	-1.15808300	-0.10025800
H	-4.41734300	-2.14532000	-0.21953500
C	0.22956000	-5.31224200	-0.11485600
H	-0.55945400	-6.03253800	-0.34080900
H	0.97864900	-5.36526700	-0.91527400
H	0.72415100	-5.63101700	0.81151200
C	4.26926100	3.32504000	-0.43730000
H	4.86725600	4.05077200	0.12595500
H	4.38463900	3.57135900	-1.50048600
H	3.21918600	3.47638900	-0.17208800
C	7.09468300	-0.96279800	0.21863700
H	8.04344700	-0.50727100	-0.07061000
H	7.18692600	-1.33066900	1.24797400
H	6.90761900	-1.83300200	-0.41801700
C	-4.75319100	6.01261100	0.36376400
C	-6.08698700	6.44453300	0.27056700
C	-7.13443700	5.53838700	0.09732700
C	-6.80740800	4.18333900	0.01585900
C	-5.46739400	3.72929300	0.11360000
C	-4.43552500	4.65649600	0.28698900
H	-3.96186200	6.74381000	0.49954400
H	-6.31127700	7.50533300	0.33730100
H	-8.16181600	5.88271800	0.03397200
H	-3.40299100	4.32696700	0.36326100
C	-6.89072700	1.93558100	-0.16302000
C	-7.28936100	0.59313100	-0.29282200
C	-6.30813900	-0.37804800	-0.26824000
C	-4.91738600	-0.07218000	-0.11326200
C	-4.54294400	1.29347100	0.02116300
C	-5.51367600	2.28228300	-0.00086400
H	-8.33281300	0.31699900	-0.40415700
H	-6.59492900	-1.42137900	-0.36636400
H	-3.50042800	1.56835200	0.14347700

N	-7.65041600	3.08371700	-0.16404500
C	-9.09628900	3.15976800	-0.26863300
H	-9.56409100	3.27882500	0.71595900
H	-9.37510700	4.00846300	-0.89922200
H	-9.47700600	2.24977400	-0.73475900