Electronic Supplementary Information for:

Bodipy triads triplet photosensitizers enhanced with intramolecular resonance energy transfer (RET): broadband visible light absorption and application in photooxidation

Song Guo,[a] Lihua Ma,[a] Jianzhang Zhao,*[a] Betül Küçüköz,[b] Ahmet Karatay,[b] Mustafa Hayvali,*[c] H. Gul Yaglioglu[b] and Ayhan Elmali[b]

[a] State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, E-208 Western Campus, 2 Ling Gong Road, Dalian 116024, P. R. China; [b] Department of Engineering Physics, Faculty of Engineering, Ankara University, 06100 Beşevler, Ankara, Turkey; [c] Department of Chemistry, Faculty of Science, Ankara University, 06100 Beşevler, Ankara, Turkey

E-mail: zhaojzh@dlut.edu.cn (J. Z.) and Mustafa.Hayvali@science.ankara.edu.tr (M. H.)

Group homepage: http://finechem.dlut.edu.cn/photochem

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1. Synthesis

Synthesis of 2. Under Ar atmosphere, phenol (1.32 g, 14.03 mmol) and anhydrous potassium carbonate (2.9 g, 20.98 mmol) were mixed in dry ethanol (80 mL), the mixture was stirred at 70 °C for 0.5 h. The mixture was then cooled to RT and 1,2-dibromoethane (4.0 g, 20.98 mmol) was added using syringe. The mixture was stirred at 79 °C for 8 h. The mixture was then cooled to RT. Potassium carbonate was removed by filtration and the filtrate was evaporated to dryness. The crude product was purified by column chromatography (silica gel, CH_2Cl_2/hexane, 1:2, v/v) to afford colourless oil. 0.45 g (21.1%). ^{1}H NMR (400 MHz, $CDCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$): 7.33–7.27 (m, 2H), 7.01–6.92 (m, 2H), 4.31 (d, 2H, J = 6.3 Hz), 3.65 (t, 2H, J = 6.4 Hz).

Synthesis of 3. A mixture of compound **2** (0.45 g, 2.23 mmol) and NaN_3 (0.4, 6.46 mmol) in DMF (20 mL) was heated at 100 °C. After 10 h, The mixture was poured to water and extracted with CH_2Cl_2. The solvent was evaporated under reduced pressure and the azide compound was obtained as colourless oil, 0.36 g (99 %). ^{1}H NMR (400 MHz, $CDCl_3$): 7.32–728 (m, 2H), 7.00–6.91 (m, 3H), 4.15 (t, 2H, J = 5.2 Hz), 3.59 (t, 2H, J = 4.9 Hz). TOF HRMS ESI$^+$: m/z calcd for $[C_{17}H_{17}NO+H]^+$: 163.0746; found: 163.0748.

Synthesis of 5. Mixture of carbazole (1.161 g, 6.95 mmol) and NaH (0.695 g, 17.35 mmol, 60% oil dispersion) in dry DMF (10 mL) was stirred at RT for 1 h. *n*-Butyl bromide (0.472 g, 3.47 mmol) was added, and the mixture was stirred for 1 h. The mixture was then poured into water (150 mL), and the precipitate was filtered, dissolved in dichloromethane (50 mL), dried over Na_2SO_4, and evaporated to dryness. The crude product was purified by column chromatography (silica gel, petroleum ether), to give **5** as white solid. Yield: 1.47 g (95%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.10 (d, 2H, J = 8 Hz), 7.44 (d, 1H, J = 7.2 Hz), 7.39 (d, 2H, J = 8 Hz), 7.21 (t, 2H, J = 7.2 Hz), 4.27 (t, 2H, J = 7.2 Hz), 1.87–1.79 (m, 2H), 1.43–1.33 (m, 2H,), 0.92–0.90 (m, 2H). TOF HRMS ESI$^+$: m/z calcd for $[C_{16}H_{17}N+H]^+$: 224.1434; found: 224.1435.

Synthesis of 6. $POCl_3$ (4.2 mL) was added dropwise into DMF (2 mL) while the mixture was cooled with ice-bath. Then the temperature of the mixture was warmed up to RT. The reaction mixture was stirred at RT for 2 h. 9-butyl-9*H*-carbazole (2.00 g, 8.96 mmol) was added into the reaction mixture at 60 °C. After 6 h, the reaction was quenched with $NaHCO_3$ solution (100 mL). Then the mixture was stirred for 1 h. The precipitate was collected with filtration and the solid was washed with cold ethanol (50 mL). The crude product was purified by column chromatography (silica gel, CH_2Cl_2 : petroleum ether = 1:1, v/v) to give the 9-butyl-9H-carbazole-3-carbaldehyde as colourless oil. Yield: 1.58 g (70%). ^{1}H NMR (400 MHz, $CDCl_3$): 10.08 (s, 1H), 8.58 (s, 1H), 8.14 (d, 2H, J = 7.8 Hz), 8.00 (d, 2H, J = 8.5 Hz), 7.52 (t, 1H, J = 8.3 Hz), 7.45 (d, 2H, J = 8.6 Hz), 7.31 (t, 1H, J = 7.2 Hz), 4.30 (t, 2H, J = 7.1 Hz), 1.89–1.81 (m, 2H), 1.44–1.35 (m, 2H), 0.95 (t, 3H, J = 8.7 Hz). TOF HRMS ESI$^+$: m/z calcd for $[C_{17}H_{17}NO+H]^+$: 252.1383; found: 252.1381.

Synthesis of 8. The synthesis procedure is similar to that of compound **2**. The product was purified by column chromatography (silica gel, CH_2Cl_2/hexane, 10:1, v/v) to afford colourless oil. Yield: 78.1% (1.45 g). ^{1}H NMR (400 MHz, $CDCl_3$): 9.90 (s, 1H), 7.87–7.85 (m, 2H), 7.04–7.01 (m, 2H), 4.40 (t, 2H, J = 12.0 Hz), 3.68 (t, 2H, J = 12.0 Hz). TOF HRMS ESI$^+$: m/z calcd for $[C_9H_9BrO_2+H]^+$: 228.9859; found: 228.9688.

Synthesis of 9. A mixture of compound **8** (1.65 g, 7.19 mmol) and NaN_3 (0.6 g, 9.46 mmol) in DMF (20 mL) was heated at 100 °C. After 10 h, The mixture was poured to water and extracted with CH_2Cl_2. The solvent was evaporated under reduced pressure and the azide compound was obtained as colourless oil. Colorless oil (1.36 g, 99 %), the compound was used without any further purification.

Synthesis of 13. A mixture of *p*-Hydroxyacetophenone (3.06 g, 22.4 mmol), 3-bromo-1-propyne (3.54 g, 30 mmol) and potassium carbonate (4.15 g, 30mmol) were dissolved in DMF (50 mL), then the reaction mixture was stirred and heated to reflux for 6 h. The solution was poured into ice water and filtered to afford white solid product. 3.45 g (88.1%). ^{1}H NMR (400 MHz, $CDCl_3$): 7.96 (d, 2H, *J* =8.8 Hz), 7.03 (d, 2H, *J* =8.8 Hz), 4.76 (d, 2H, *J* = 2.4 Hz), 2.56–2.55 (m, 4H).

Synthesis of 14. Compound **13** (2.23 g, 12.8 mmol) was dissolved in absolute ethyl alcohol (20 mL). Benzaldehyde (1.36g, 12.82 mmol) was added, followed by 10% NaOH aqueous solution (5 mL). The mixture was stirred at rt for 3 h. The precipitate was collected by filtration and the solid was washed with cold EtOH (50 mL) to afford yellow solid. Yield: 3.26 g (97.1%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.06 (d, 2H, *J* =8.8 Hz), 7.83 (d, 1H, *J* = 15.7 Hz), 7.65–7.63 (m, 5H), 7.58 (d, 1H, *J* = 15.7 Hz), 7.42–7.41 (m, 3H), 7.08 (d, 2H, *J* =8.8 Hz), 4.78 (d, 2H, *J* = 1.9 Hz), 2.27 (t, 1H, *J* = 2.3 Hz). TOF HRMS ESI$^+$: *m/z* calcd for $[C_{18}H_{14}O_2+H]^+$: 263.1067; found: 263.1063.

Synthesis of 15. Compound **14** (1.57 g, 6.0 mmol), diethylamine (3 mL, 30 mmol) and nitromethane (2 mL, 30 mmol, 5 eq) were added in methanol (100 mL). The solution was refluxed for 20 h. After cooled to 0 °C, the solution was quenched with HCl (100 mL, 2.5 M). The mixture was filtered and the crude product was recrystallized in methanol to give product **15** as a white solid. Yield: 1.82 g (93.8 %). ^{1}H NMR (400 MHz, $CDCl_3$): 7.93 (d, 2H, *J* =8.5 Hz), 7.35–7.29 (m, 5H), 7.02 (d, 2H, *J* = 8.7 Hz), 4.86–4.65 (m, 4H), 4.23–4.20 (m, 1H), 3.42–3.38 (m, 2H), 2.55 (t, 1H, *J* = 2.3 Hz). TOF HRMS ESI$^+$: *m/z* calcd for $[C_{19}H_{17}BF_{25}O_4+H]^+$: 324.1230; found: 342.1234.

Synthesis of 17. Compound **14** (1.57 g, 6.0 mmol) and ammonium acetate was dissolved in 40ml anhydrous butanol. The solution was heated under reflux for 24 h. The precipitation was filtered and washed with cold EtOH to afford blue solid product. Compound **16** was obtained. Yield: 0.43 g (25.3%). TOF HRMS ESI$^+$: *m/z* calcd for $[C_{38}H_{27}N_3O_2+H]^+$: 558.2176, found: 558.2177. This compound was used for the next step of synthesis without further purification. **16** (100 mg, 0.36 mmol) was dissolved in dry CH_2Cl_2 (70 mL), then diisopropylethylamine (0.77 mg, 4.3 mmol) was added. The solution was stirred for 15 min at rt. $BF_3{\cdot}Et_2O$ (0.83 mL, 6.5 mmol) was added dropwise. The solution was stirred 24 h at RT. Then the solution was washed with a saturated aqueous NH_4Cl solution, brine and water. The organic layer was dried over Na_2SO_4 and the solvent was evaporated under reduced pressure. The mixture was purified by column chromatography (silica gel, dichloromethane/hexanes, 1/1, v/v) to give blue solid (0.19 g, 87.2%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.11–8.05 (m, 84H), 7.48–7.44 (m, 6H), 7.11–7.04 (m, 6H), 4.78 (d, 4H, *J* = 2.4 Hz), 2.57 (t, 2H, *J* = 2.4 Hz). TOF HRMS ESI$^+$: *m/z* calcd for $[C_{19}H_{18}BF_{25}O_4]^+$: 605.2196, found: 605.2118.

2.0 NMR and HR-MS spectra

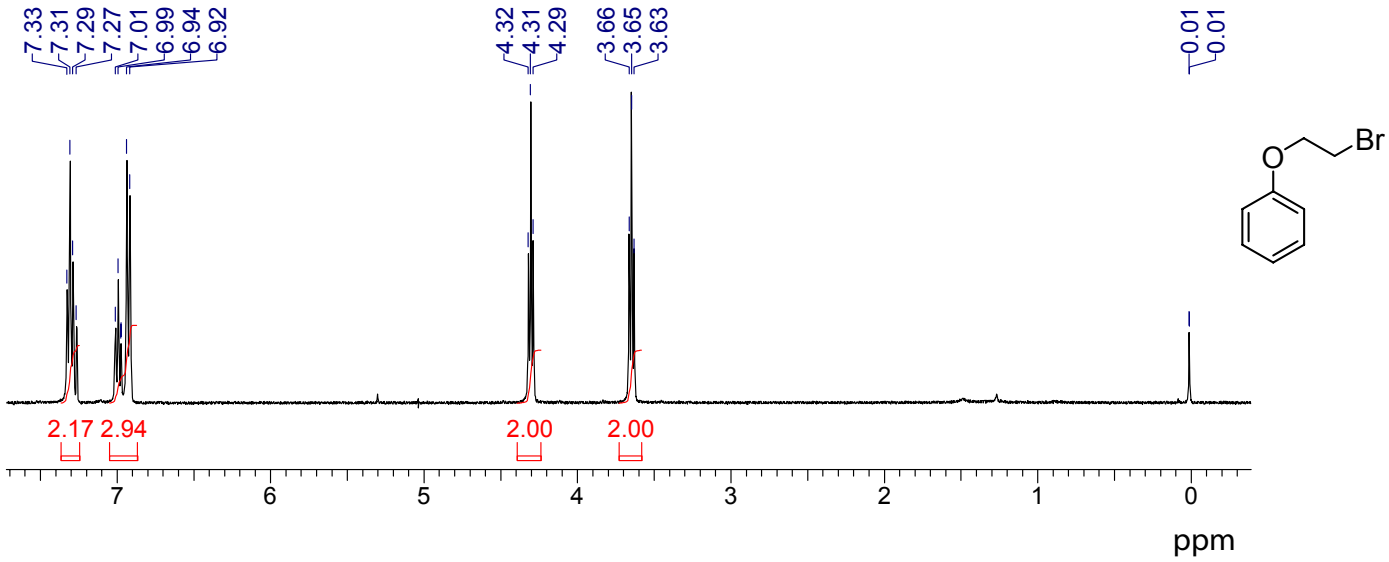


Figure S1. ^{1}H NMR of **2** (400 MHz, $CDCl_3$).

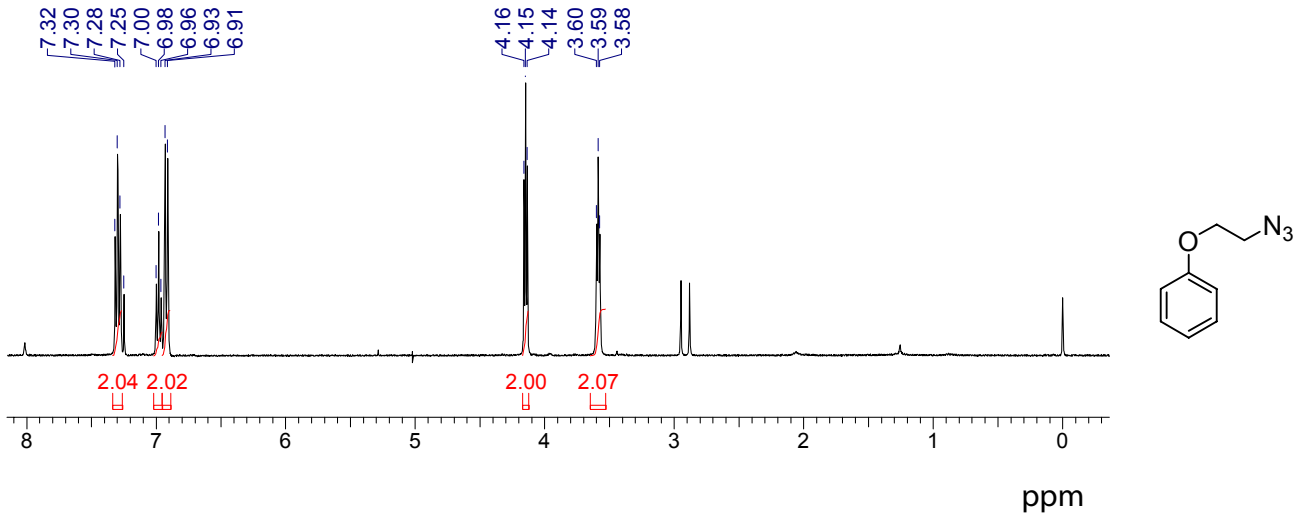


Figure S2. ^{1}H NMR of **3** (400 MHz, $CDCl_3$).

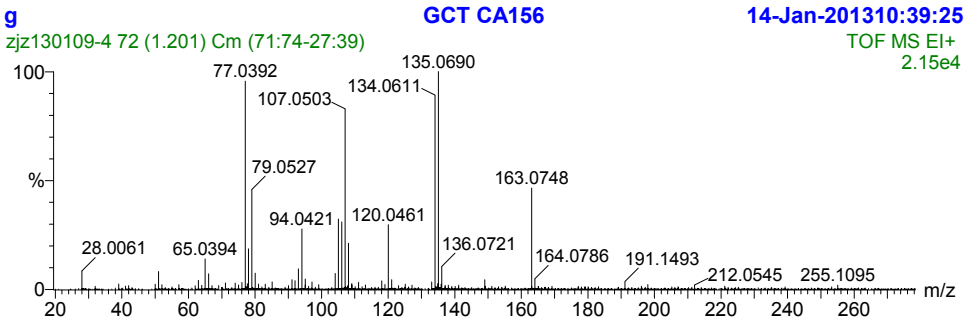
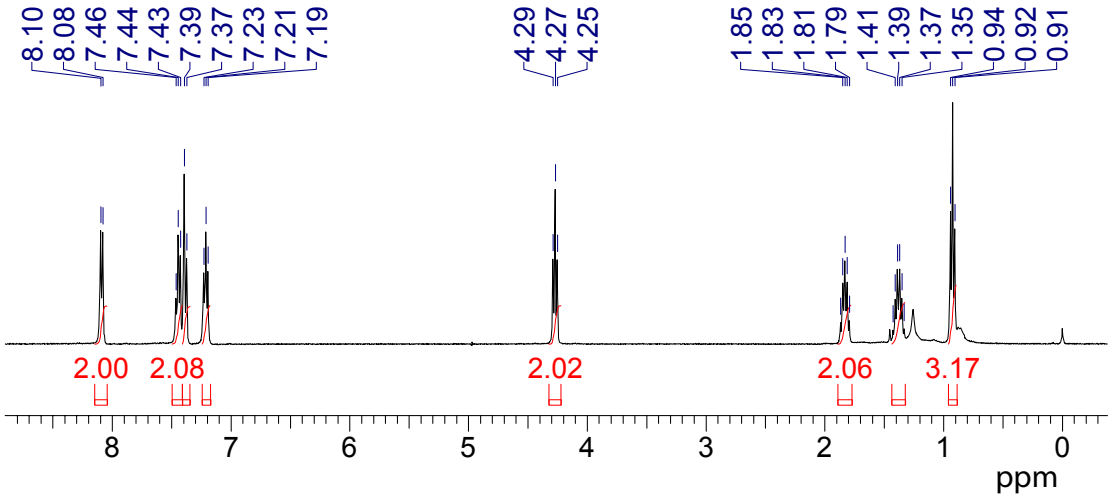


Figure S3. TOF MS EI+ of **3**.



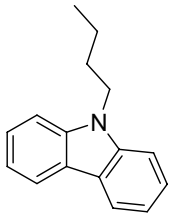
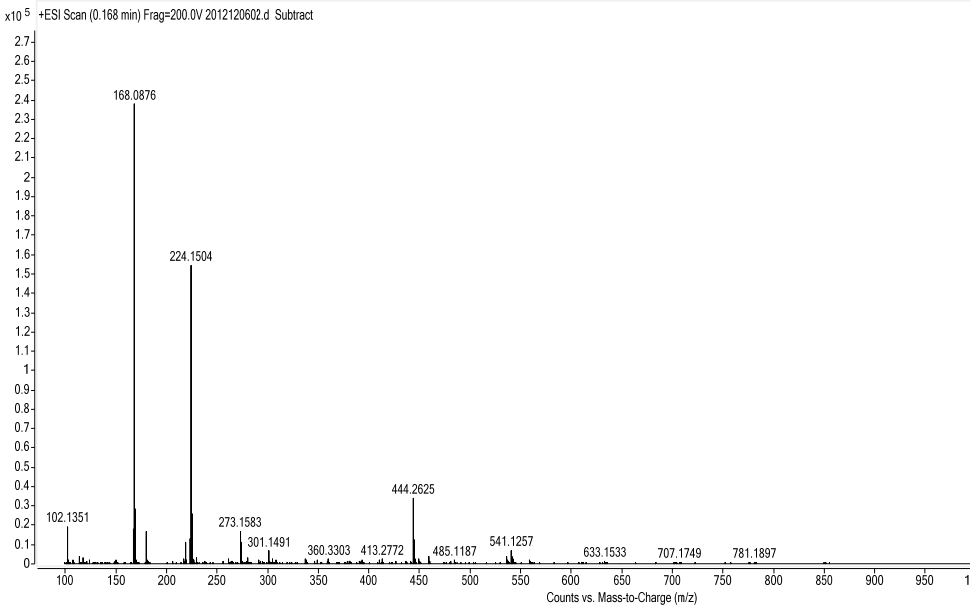


Figure S4. ^{1}H NMR of **5** (400 MHz, $CDCl_3$).



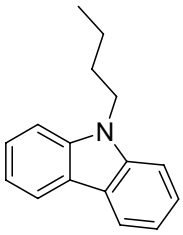
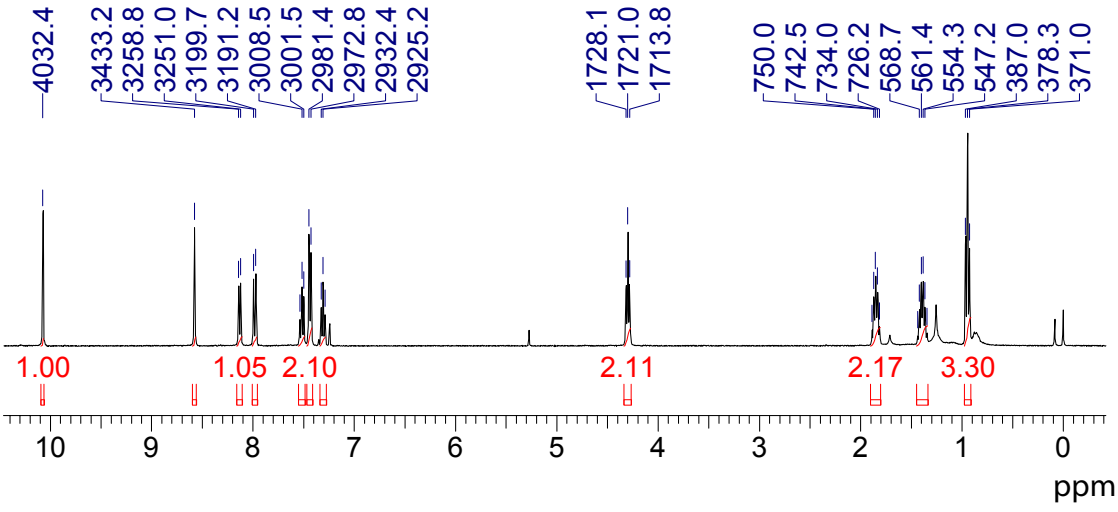


Figure S5. TOF HRMS ESI of **5**.



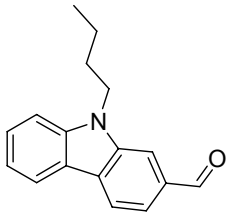


Figure S6. ^{1}H NMR of **6** ($CDCl_3$, 400 MHz).

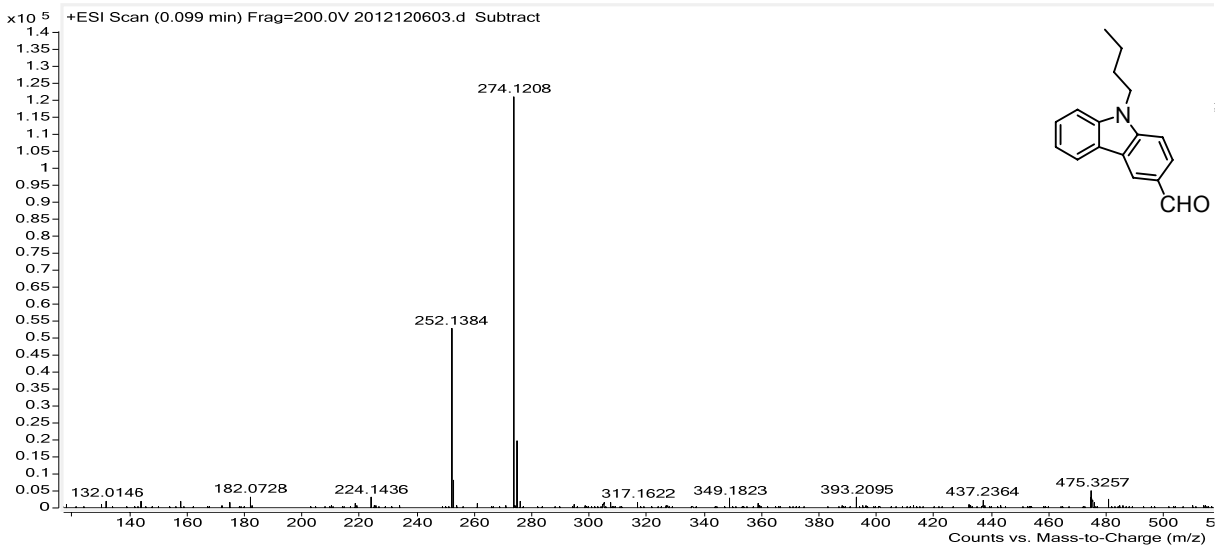


Figure S7. TOF HRMS ESI of **6**.

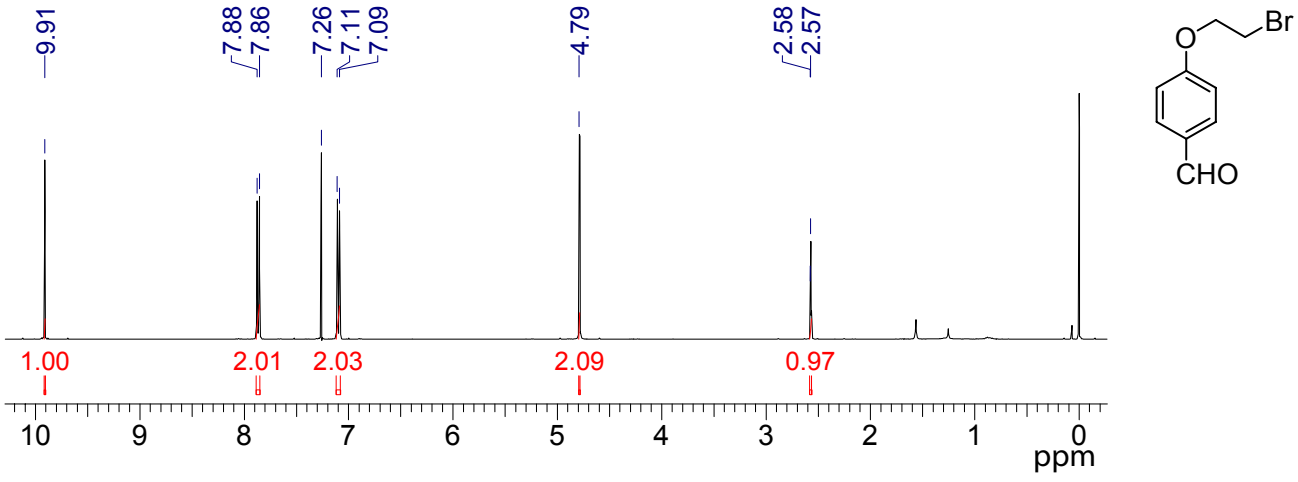


Figure S8. ^{1}H NMR of **8** (400 MHz, $CDCl_3$).

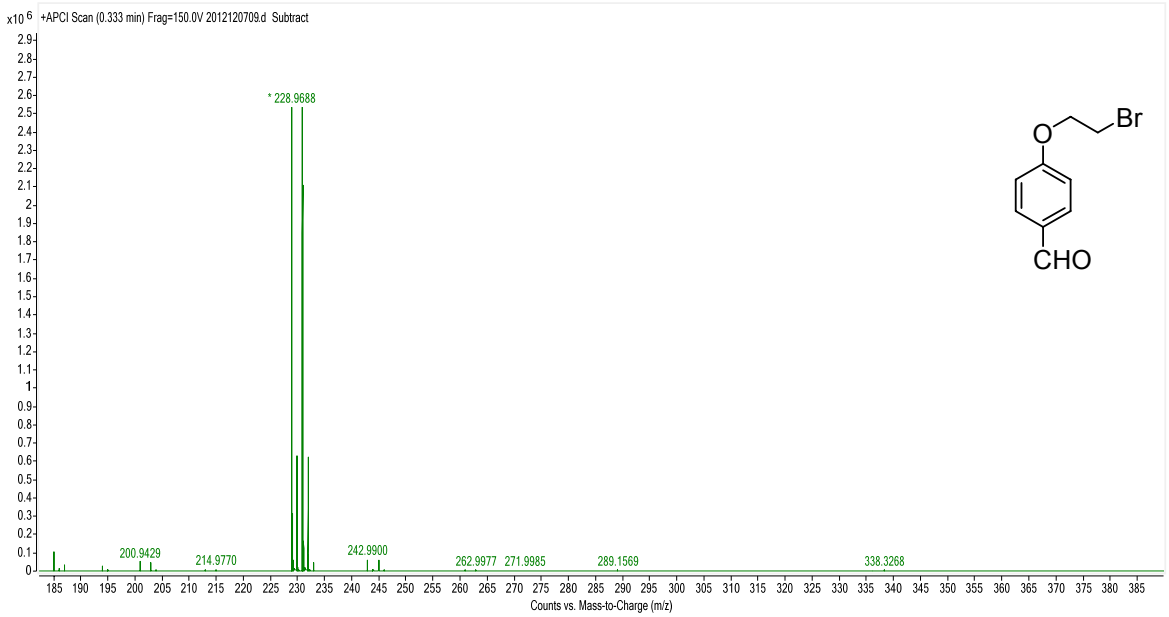


Figure S9. TOF MS EI$^+$ of **8.**

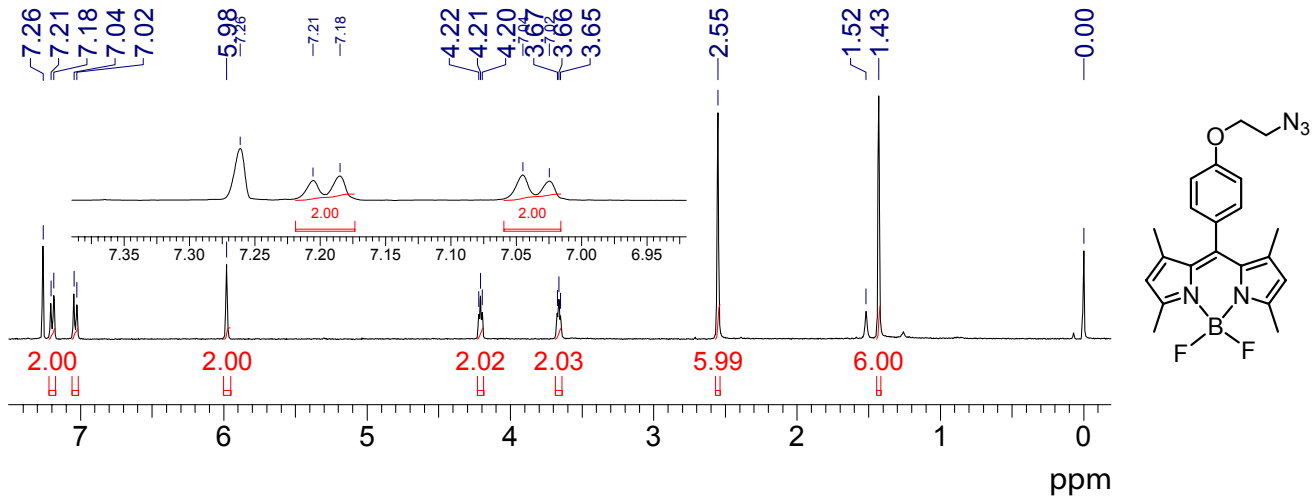


Figure S10. ^{1}H NMR of **10** (400 MHz, $CDCl_3$).

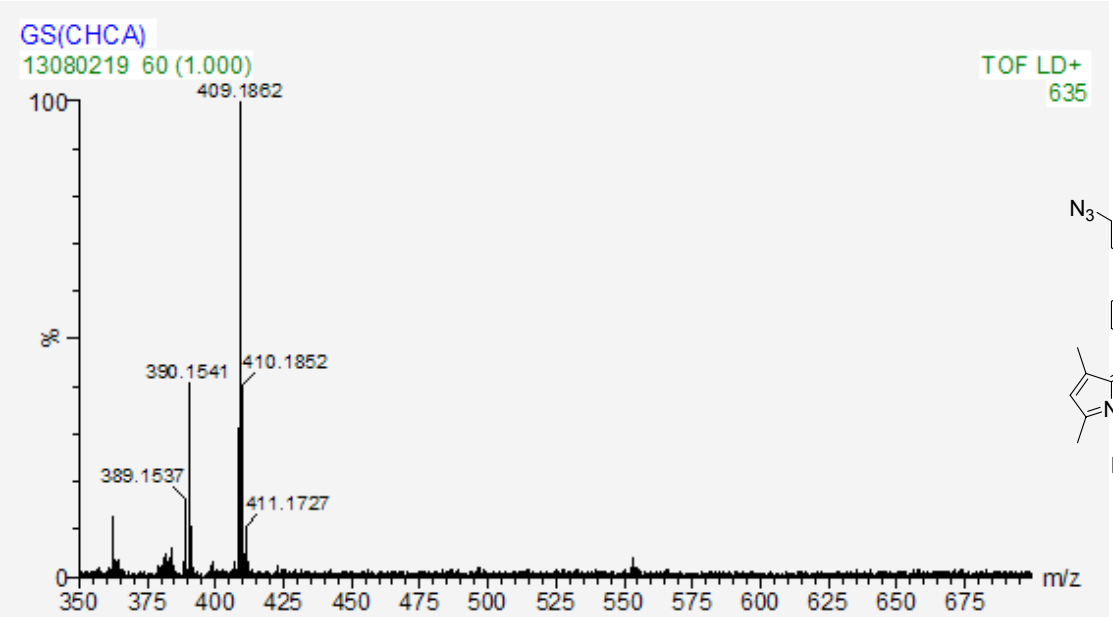


Figure S11. TOF MS EI⁺ of **10.**

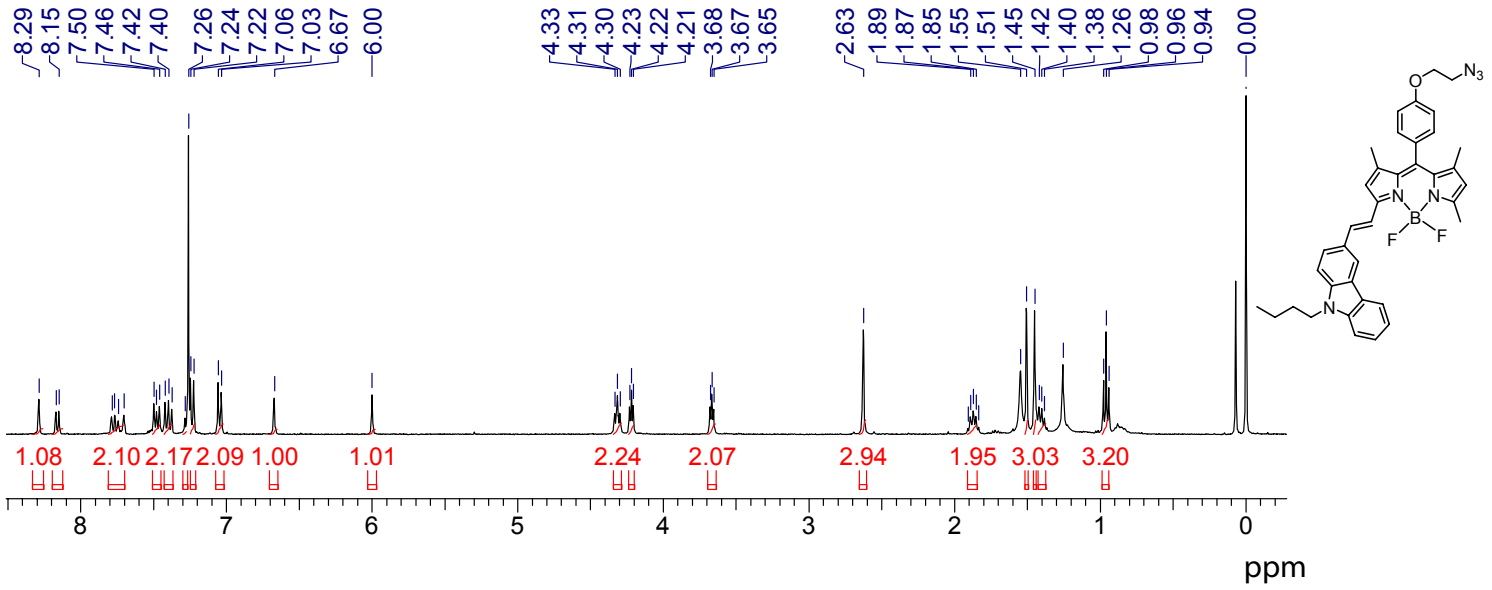


Figure S12. ^{1}H NMR of **11** (400 MHz, $CDCl_3$).

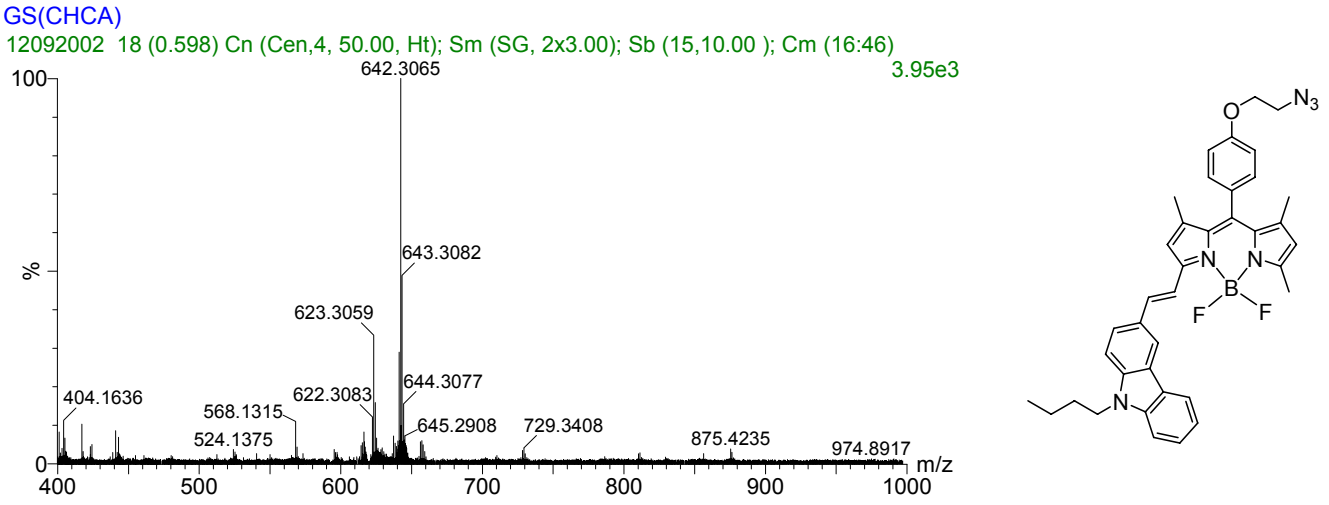


Figure S13. TOF HRMS (MALDI) ESI of **11**.

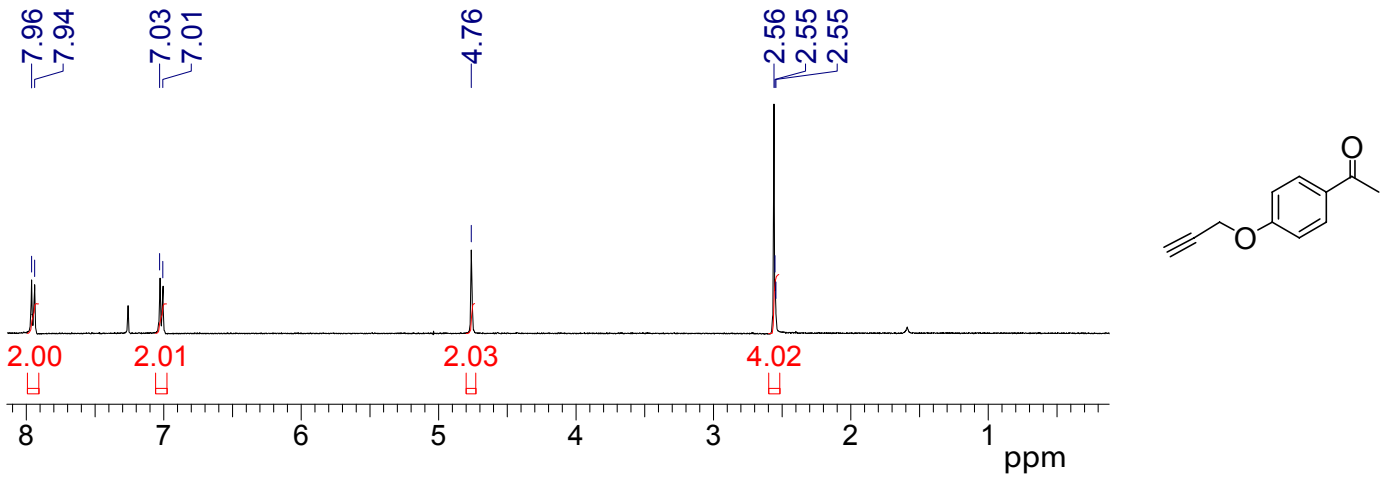


Figure S14. ^{1}H NMR of **13** (400 MHz, $CDCl_3$).

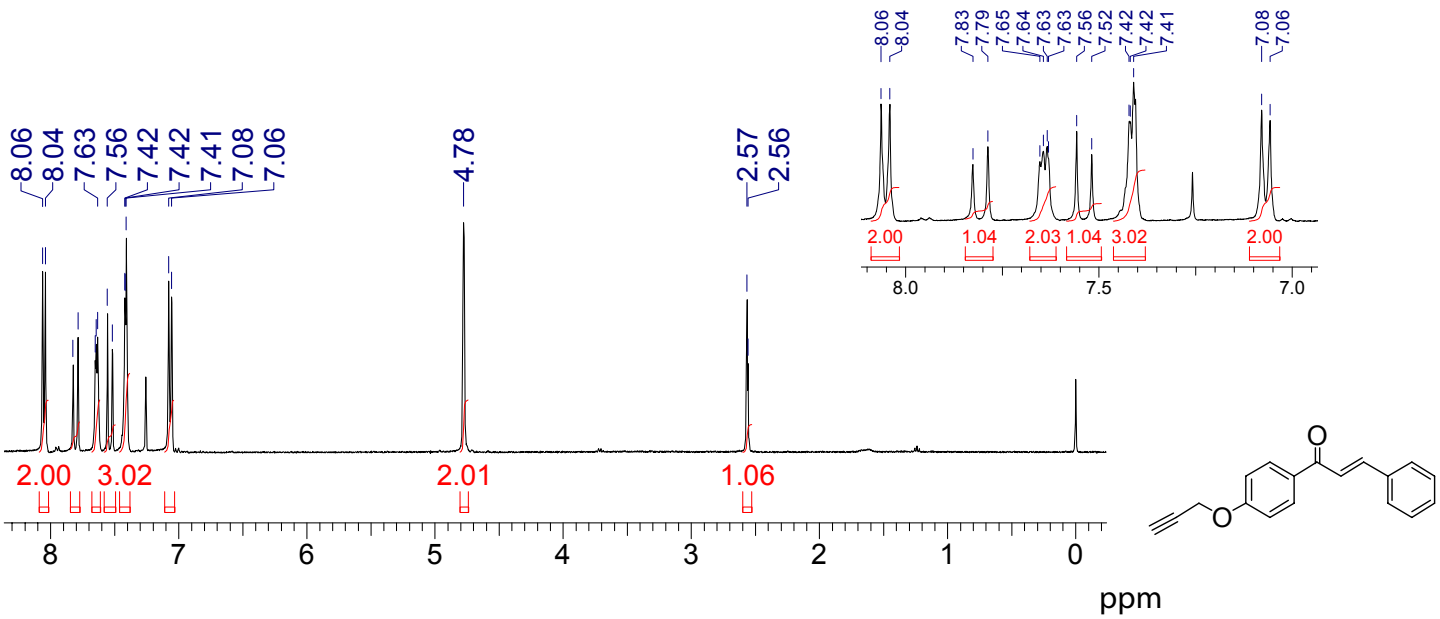


Figure S15. ^{1}H NMR of **14** (400 MHz, $CDCl_3$).

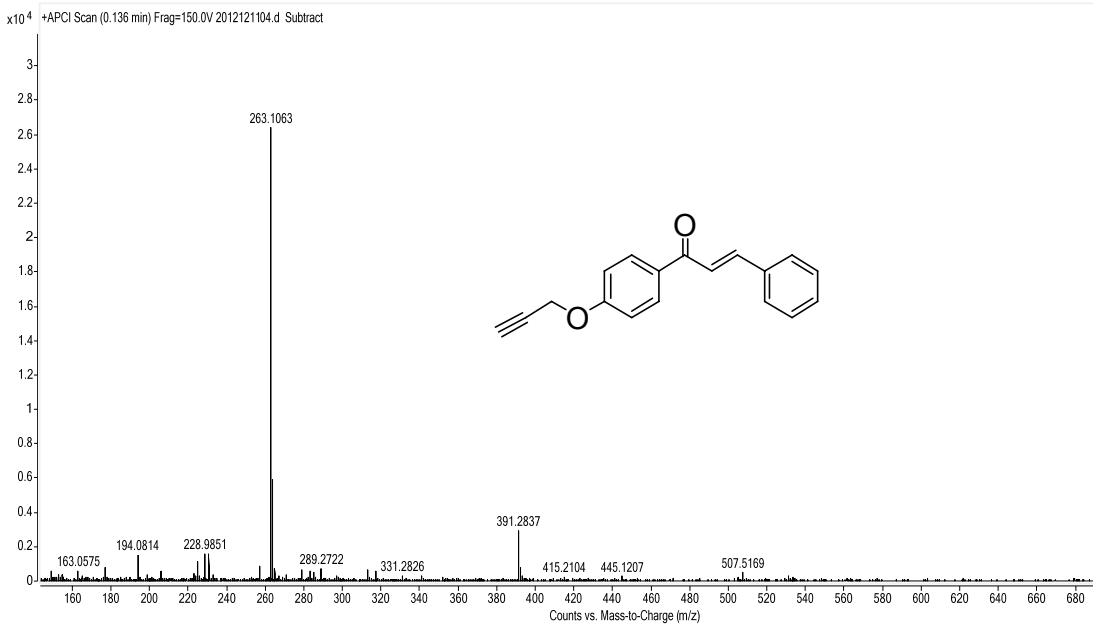


Figure S16. TOF MS EI^{+} of **14.**

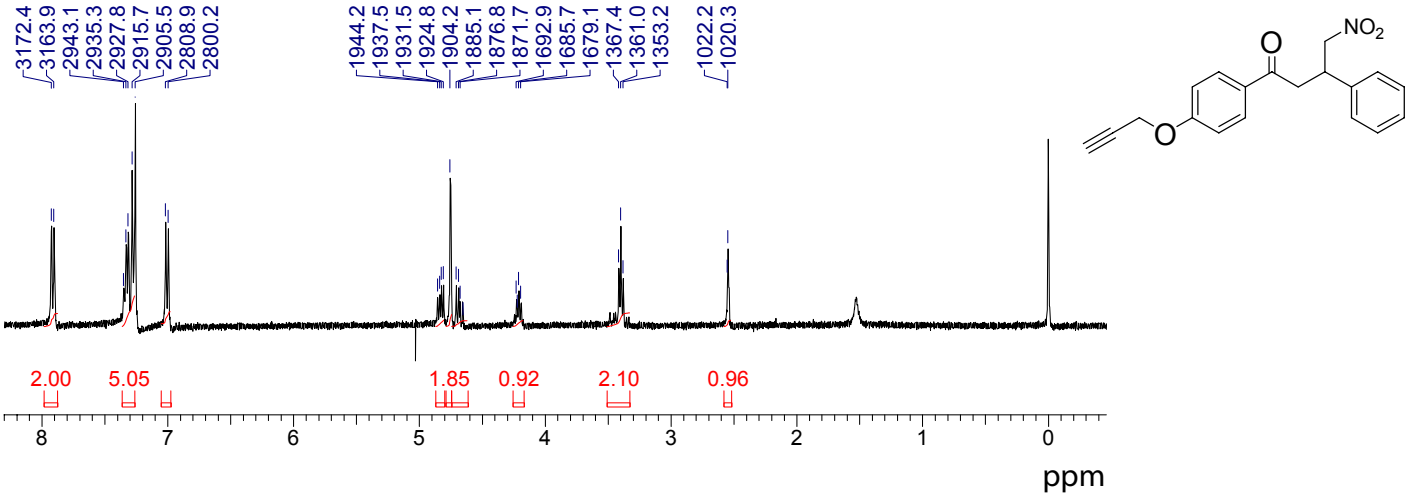


Figure S17. ^{1}H NMR of **15** (400 MHz, $CDCl_3$).

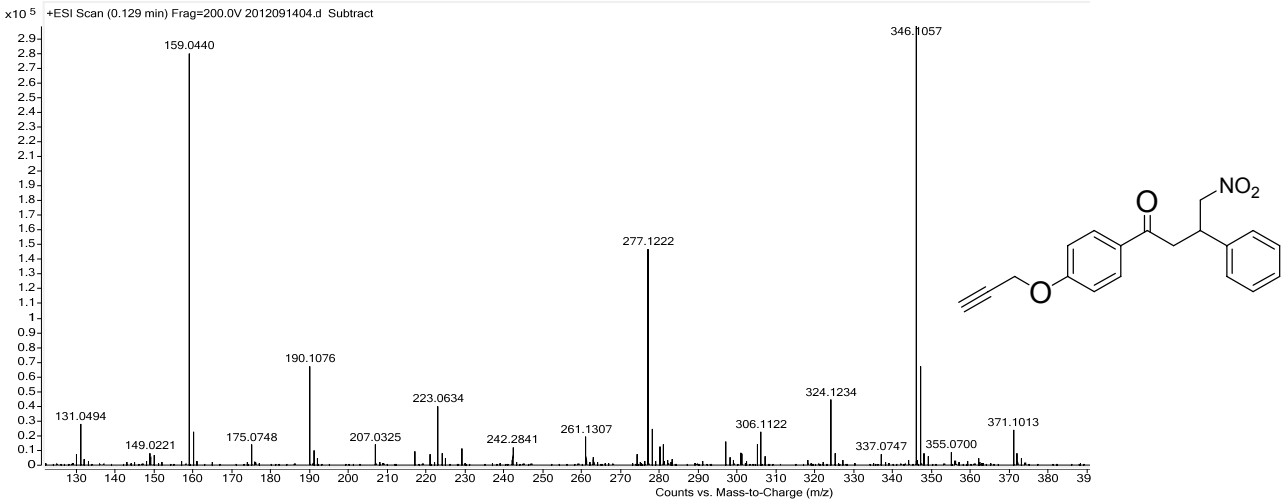


Figure S18. TOF MS EI^{+} of **15.**

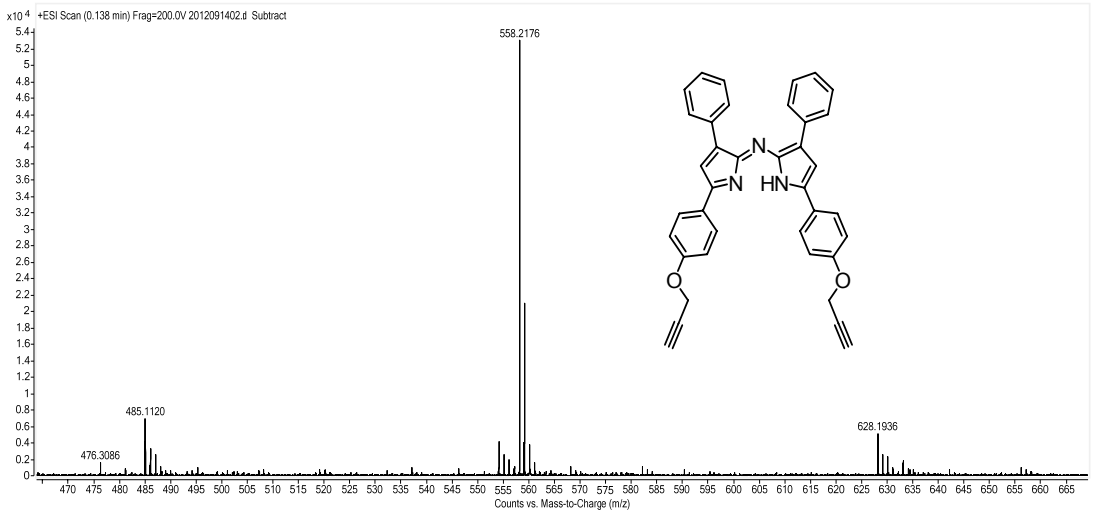


Figure S19. TOF MS EI$^+$ of **16.**

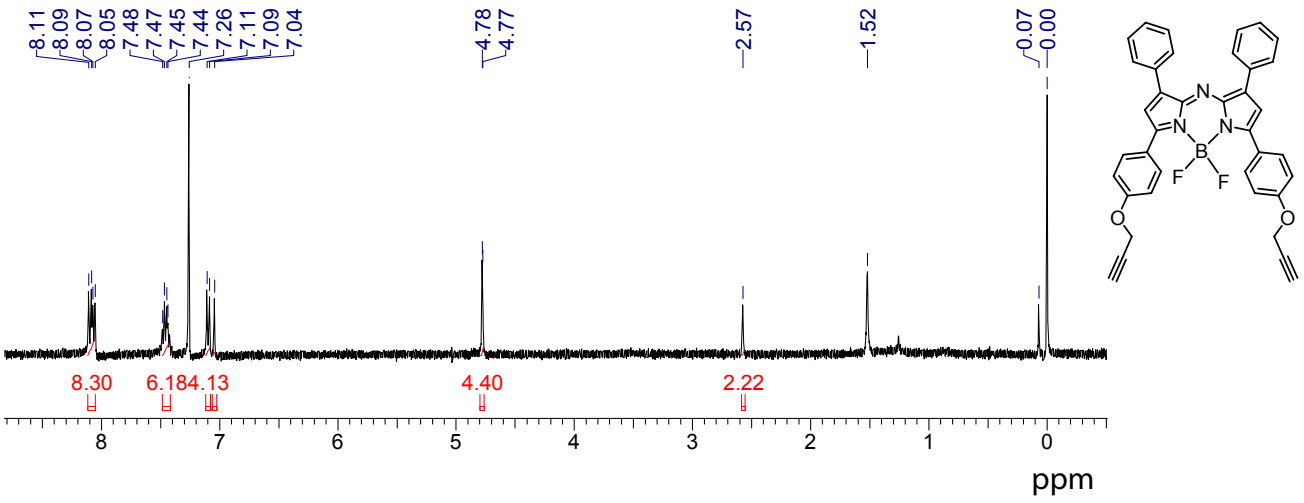


Figure S20. ^{1}H NMR of **17** (400 MHz, $CDCl_3$).

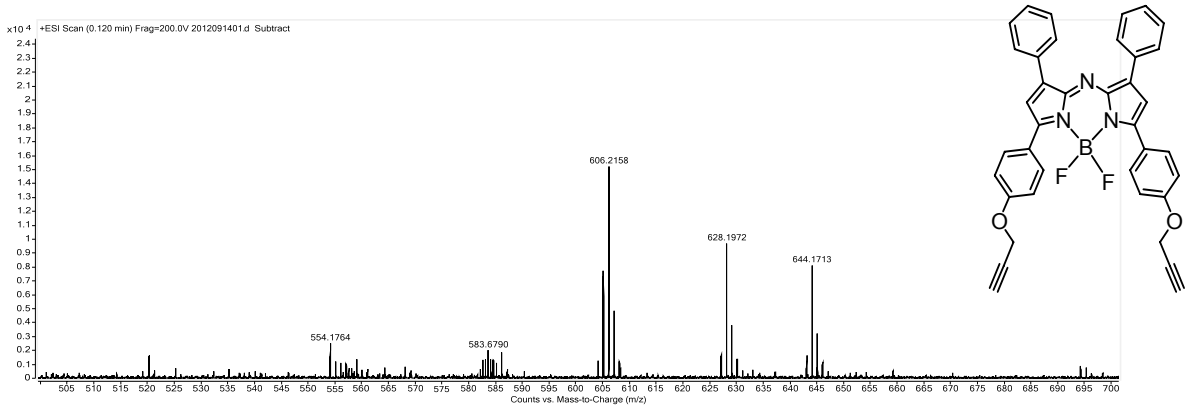


Figure S21. TOF MS EI$^+$ of **17.**

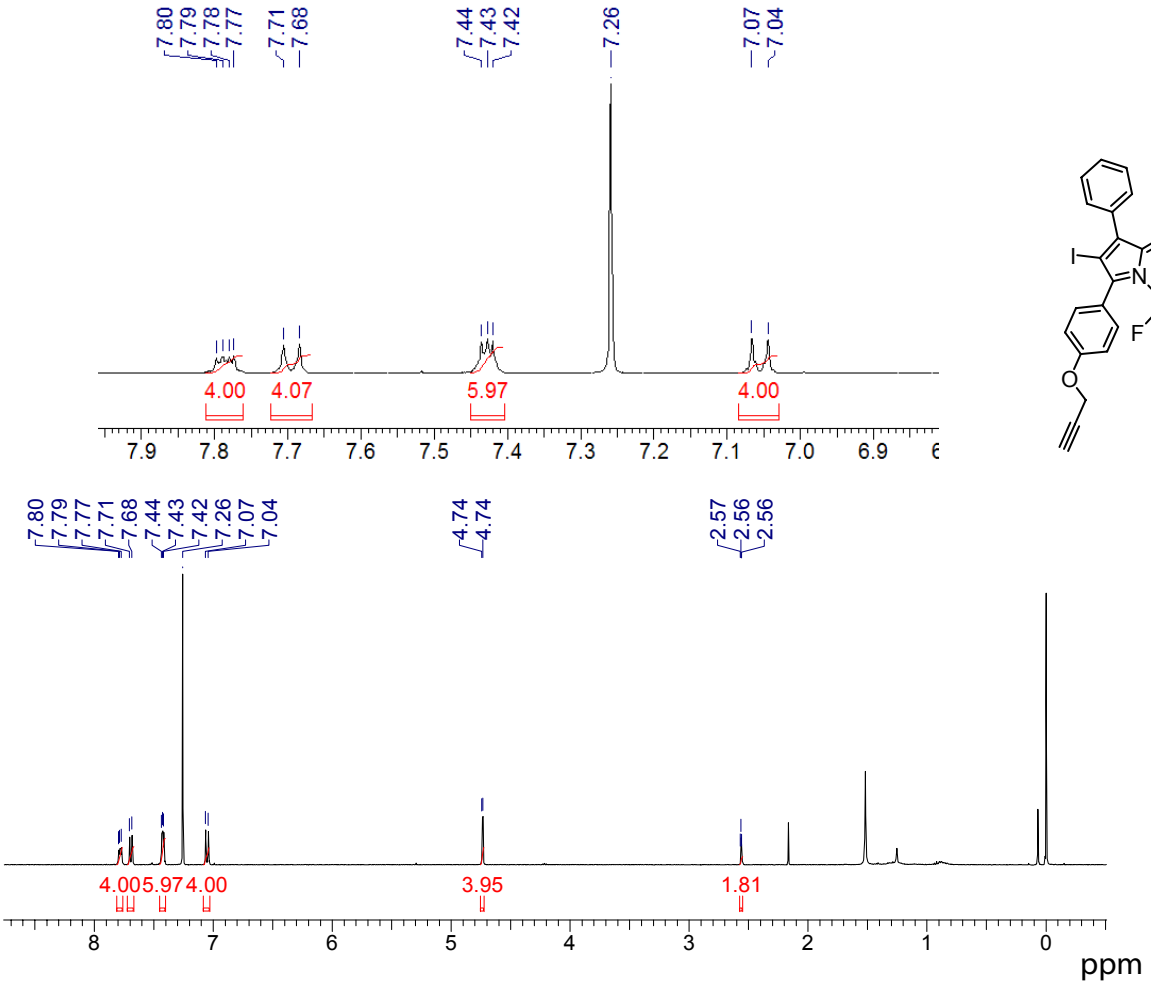


Figure S22. ^{1}H NMR of **18** (400 MHz, $CDCl_3$).

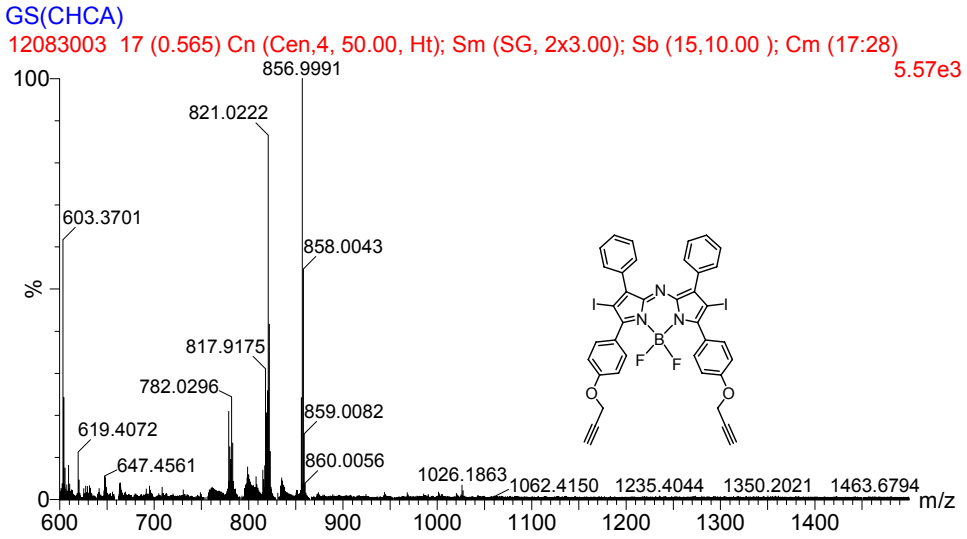


Figure S23. TOF HRMS (MALDI) ESI of **18**.

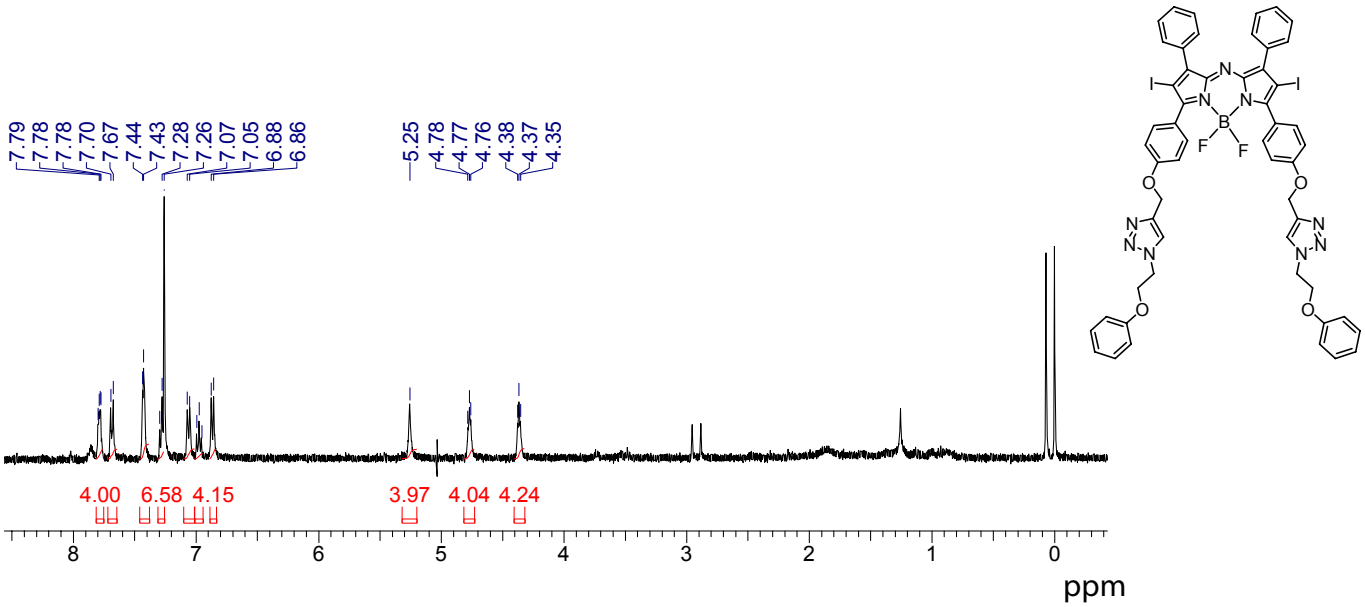


Figure S24. ^{1}H NMR of **B-1** (400 MHz, $CDCl_3$).

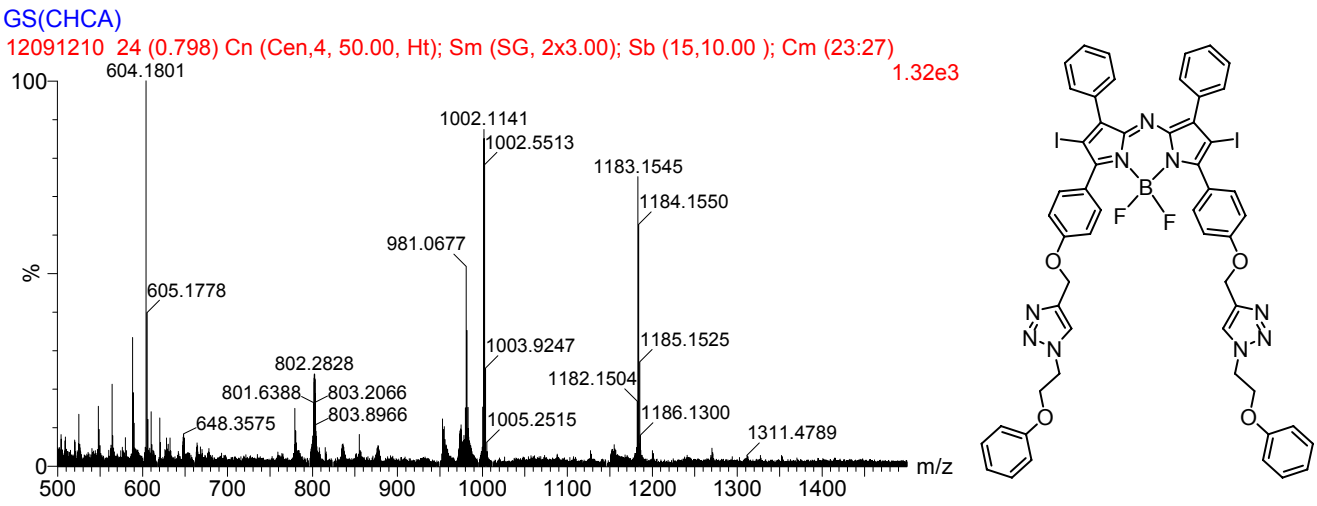


Figure S25. TOF HRMS (MALDI) ESI of **B-1**.

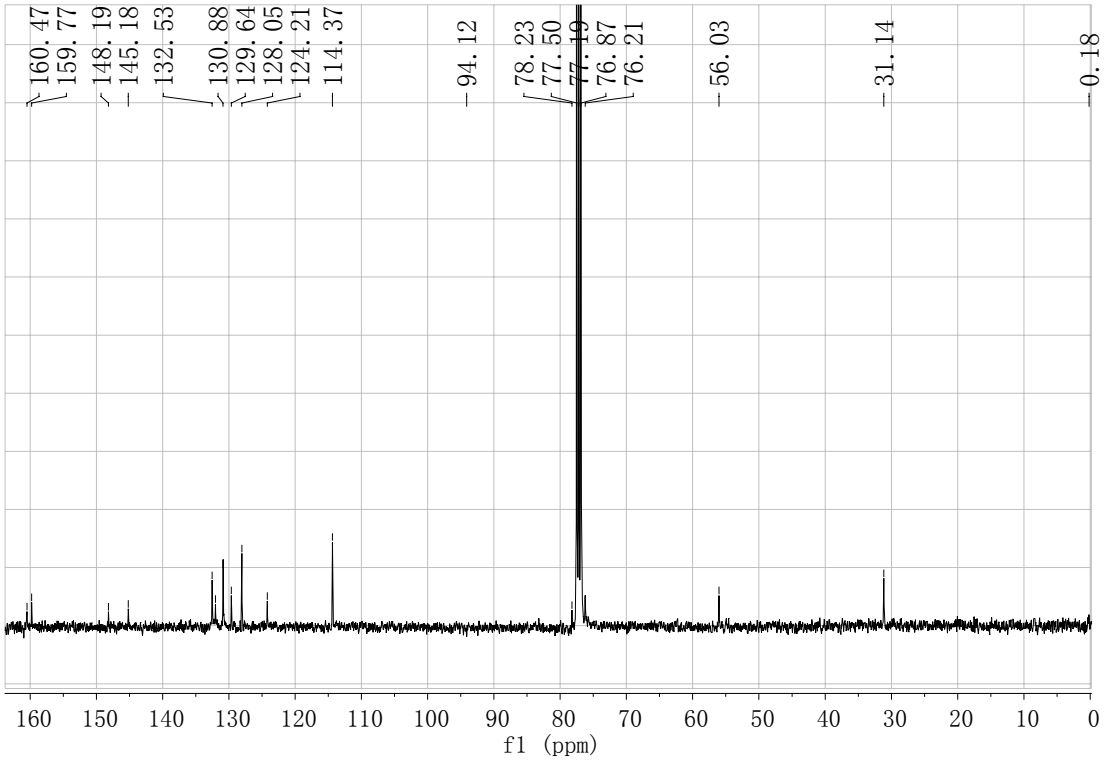


Figure S26. ^{13}C NMR of compound **B-1** in $CDCl_3$ (100 MHz), 25°C.

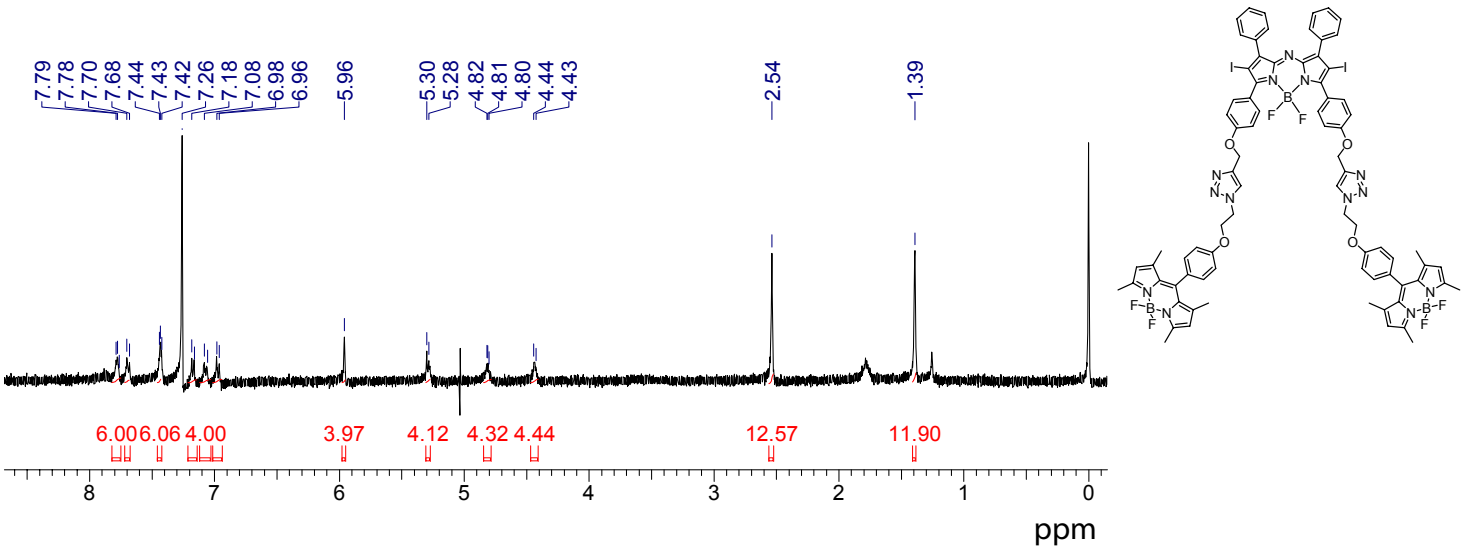


Figure S27. ^{1}H NMR of **B-2** (400 MHz, $CDCl_3$).

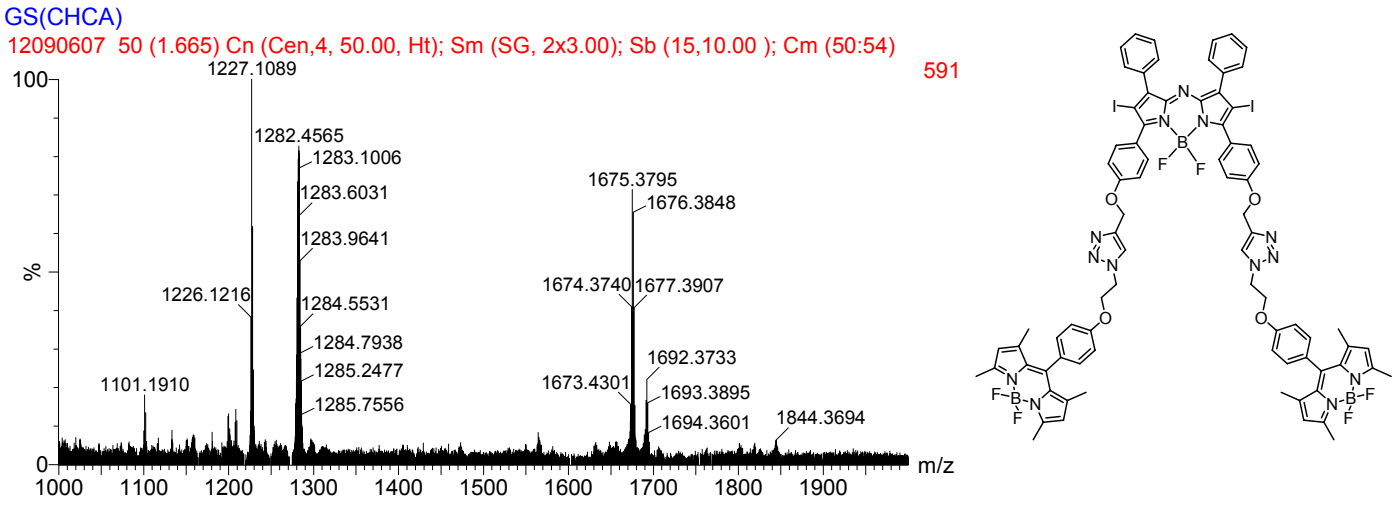


Figure S28. TOF HRMS (MALDI) ESI of **B-2**.

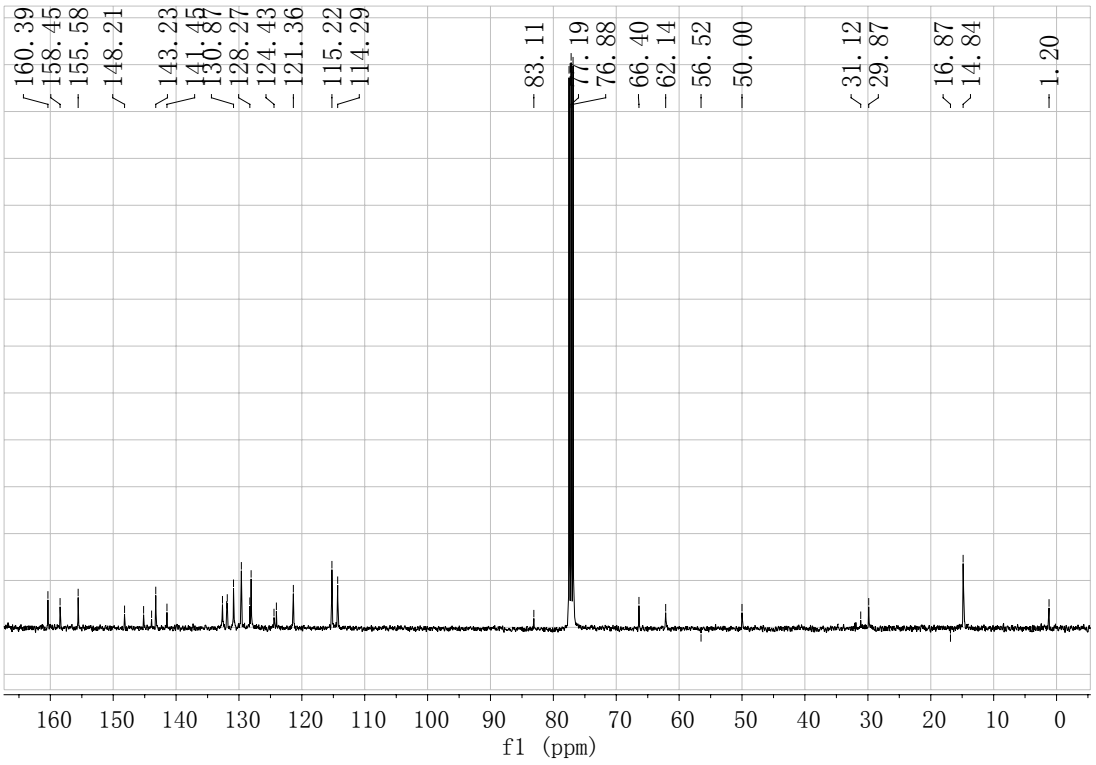


Figure S29. ^{13}C NMR of compound **B-2** in $CDCl_3$ (100 MHz), 25°C

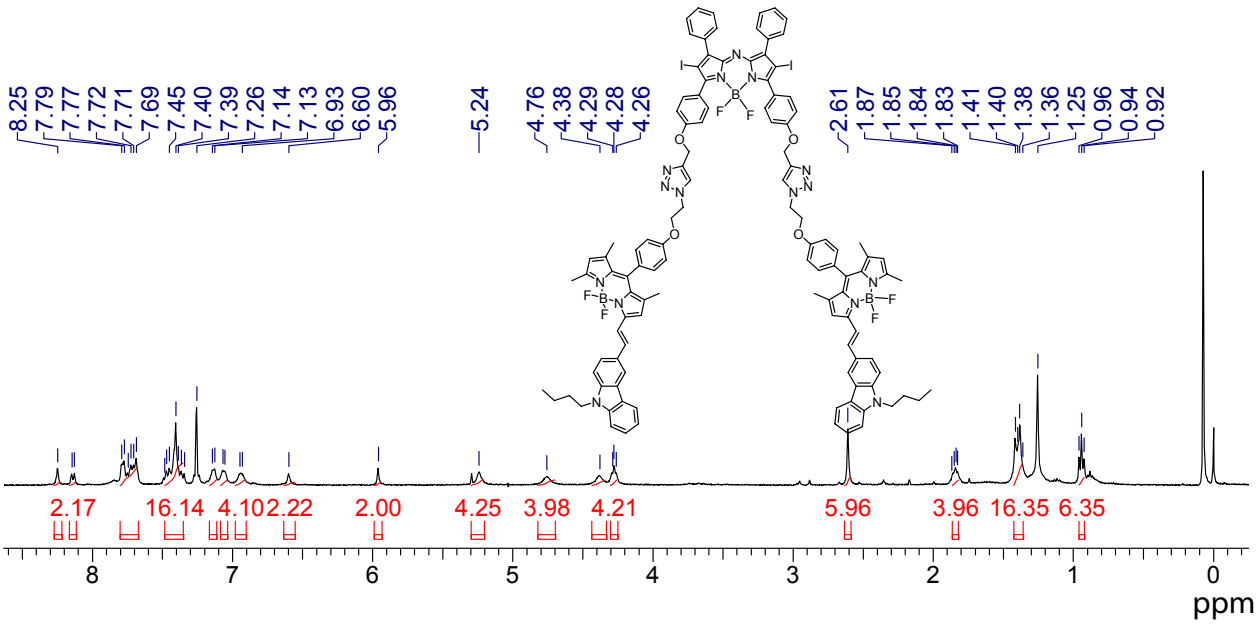


Figure S30. ^{1}H NMR of **B-3** (400 MHz, $CDCl_3$).

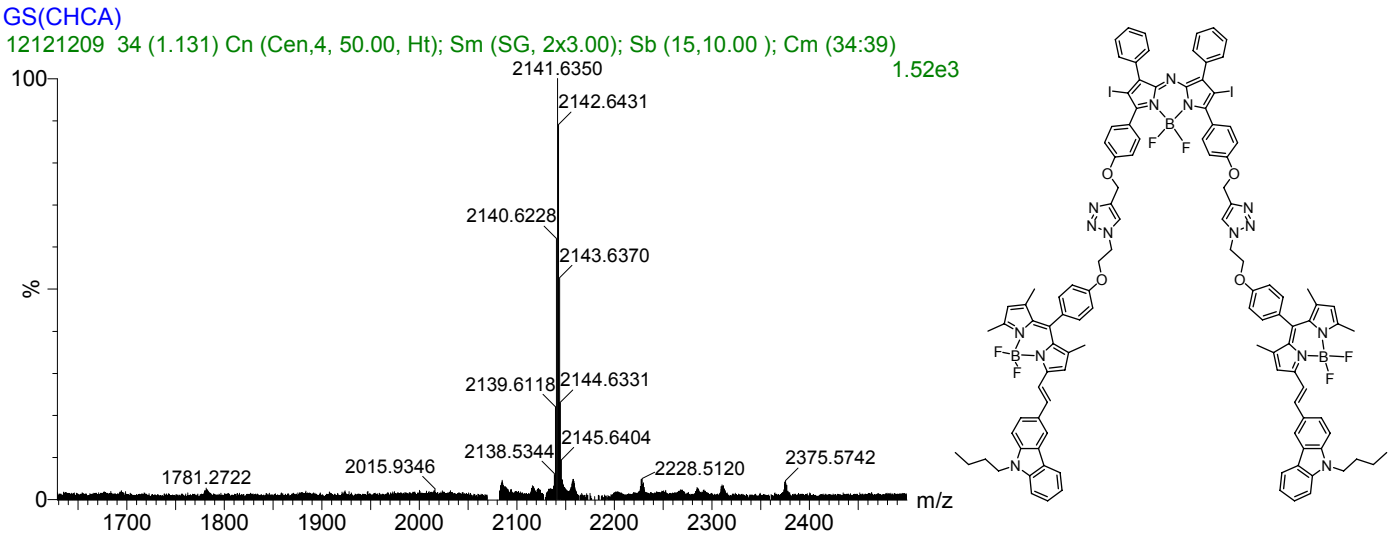


Figure S31. TOF HRMS ESI of **B-3**.

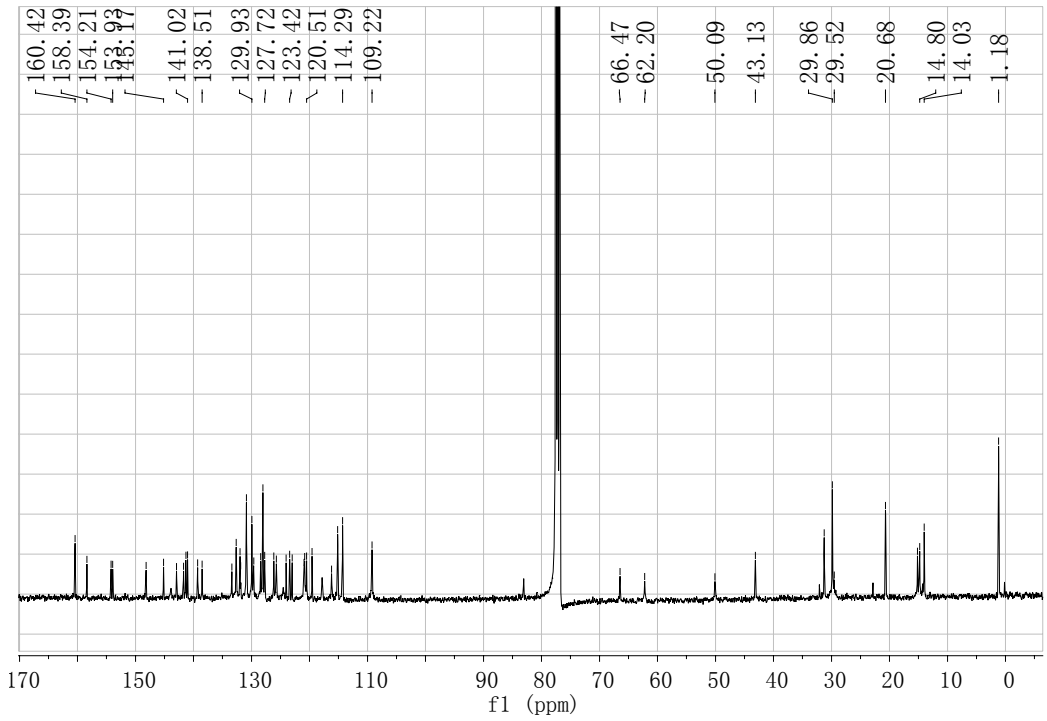


Figure S32. ^{13}C NMR of compound **B-3** in $CDCl_3$ (100 MHz), 25°C.

3.0 Absorption and Emission details.

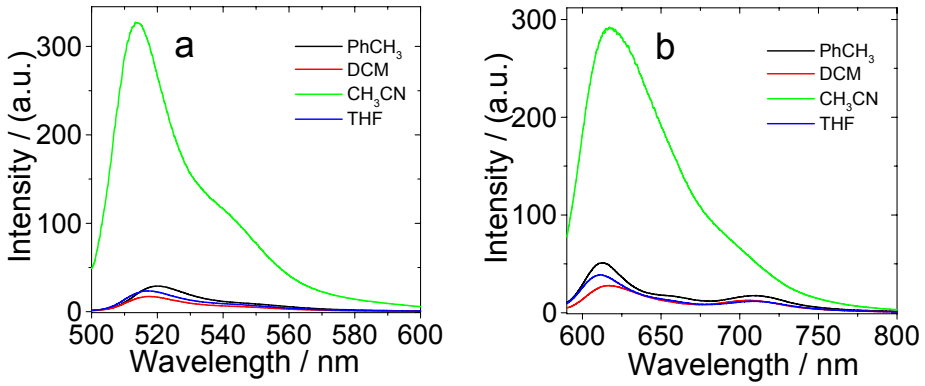


Figure S33. Fluorescence spectra of the triplet photosensitizers in different solvents. (a) **B-2**, λ_{ex} = 500 nm; (b) **B-3**, λ_{ex} = 585 nm. 25 °C.

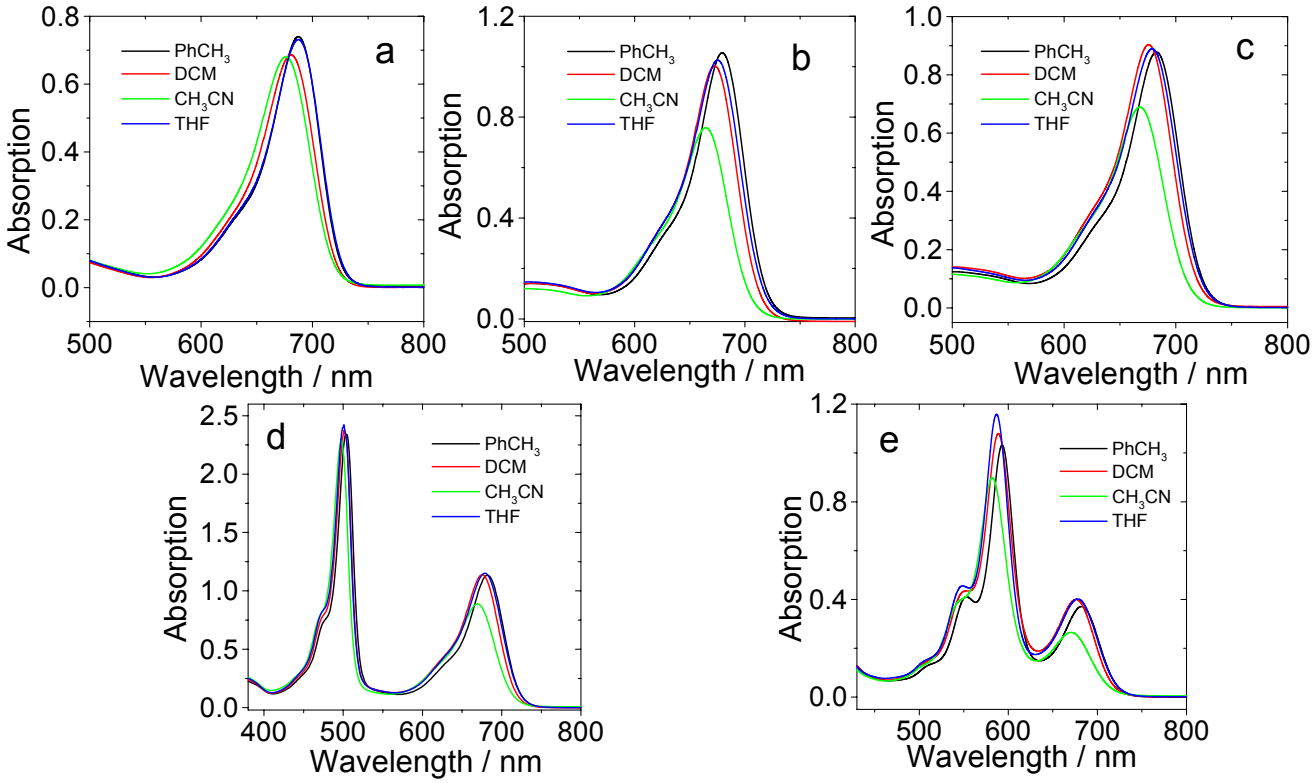


Figure S34. UV/Vis absorption spectra of the light-harvesting control compounds and the triplet photosensitizers in different solvents. (a) **17**, (b) **18**, (c) **B-1**, (d) **B-2** and (e) **B-3** in different solvents. $c = 1.0\times10^{-5}$ M^{-1}. 25 °C.

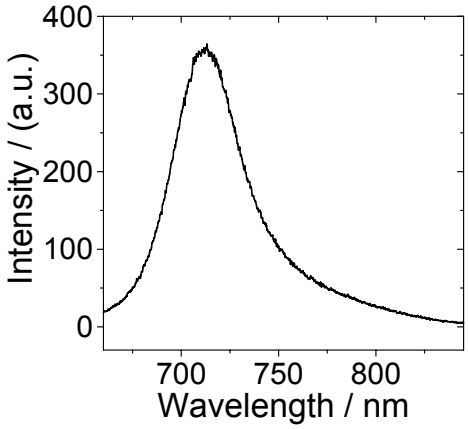


Figure S35. The fluorescence spectra of the **18**. c =1.0×10^{-5} M in toluene, 20 °C.

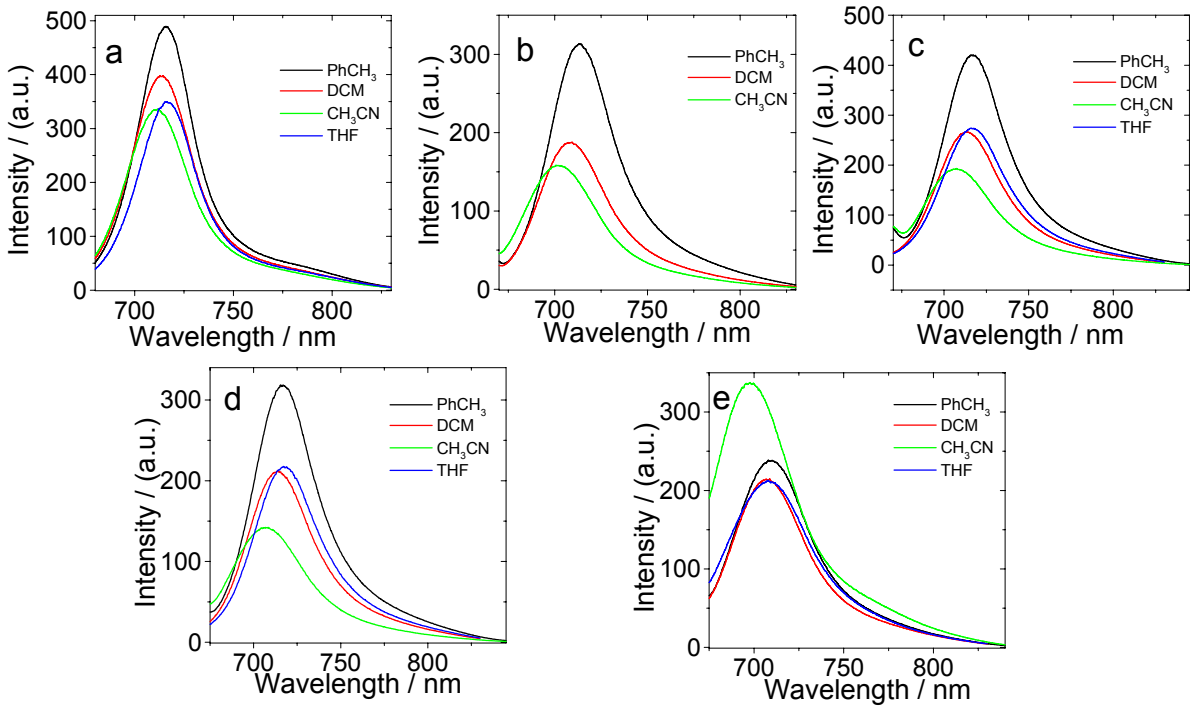


Figure S36. Fluorescence spectra: (a) **17**, λ_{ex} = 678 nm ; (b) **18**, λ_{ex} = 658 nm; (c) **B-1**, λ_{ex} = 530 nm; (d) **B-2**, λ_{ex} = 658 nm and (e) **B-3**, λ_{ex} = 664 nm, λ_{ex} = 653 nm in different solvents. λ_{ex} = 530 nm. c = 1.0×10^{-5} M^{-1}. 25 °C.

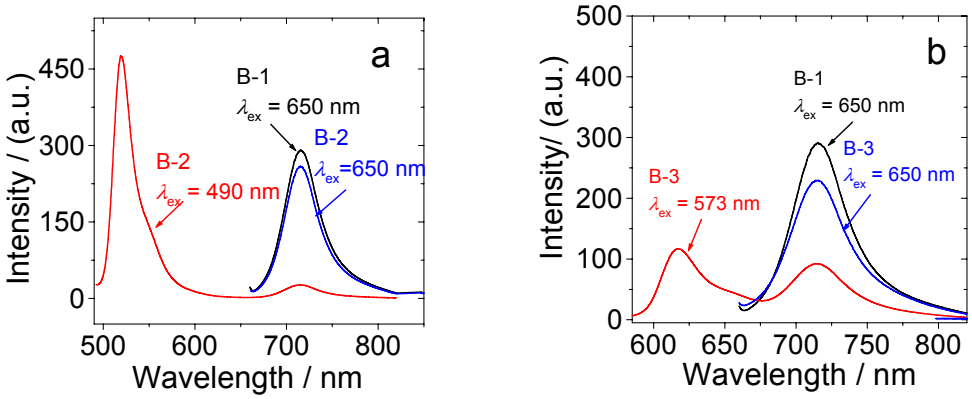


Figure S37. The fluorescence spectra of the **Bodipy** compounds. (a) The emission spectra of **B-1** and **B-2**, λ_{ex} = 650 nm; **B-2**, λ_{ex} = 490 nm; (b) The emission spectra of **B-1** and **B-3**, λ_{ex} = 650 nm; **B-3**, λ_{ex} =573 nm; in toluene, 20 °C. These results indicate that the excited state of energy acceptors in triads were not significantly quenched by electron transfer.

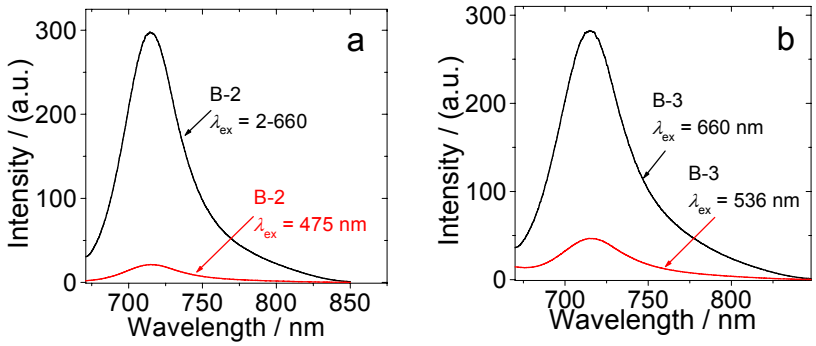


Figure S38. The fluorescence spectra of the Bodipy triads. (a) The emission spectra of **B-2**, λ_{ex} = 660 nm and λ_{ex} = 475 nm, at which **B-2** shows the same absorbance; (b) The emission spectra of **B-3**, λ_{ex} = 660 nm and λ_{ex} = 536 nm, at which **B-3** shows the same absorbance; *c* =1.0×10^{-5} M in toluene, 20 °C.

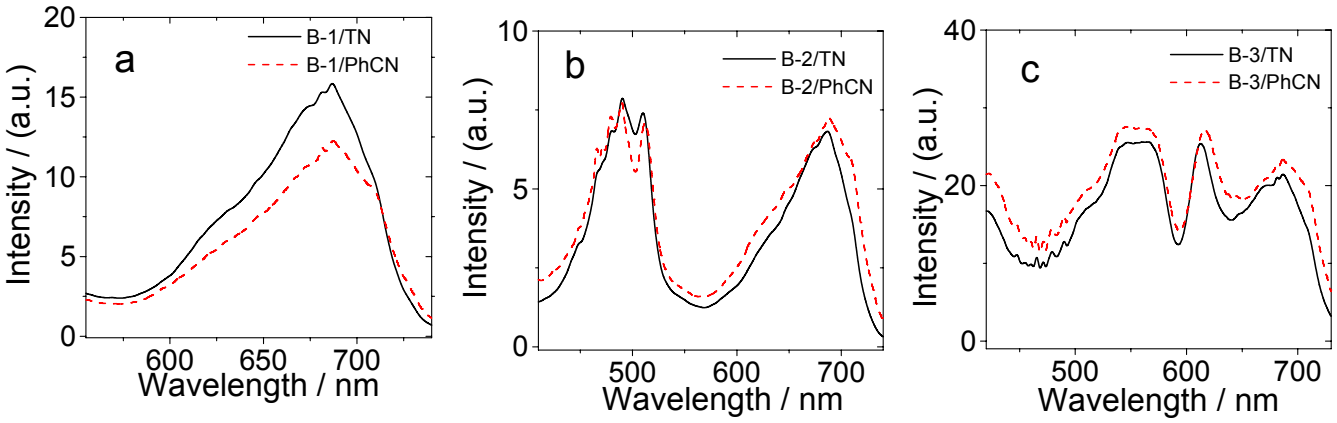


Figure S39. Excitation spectra of (a) **B-1**, (b) **B-2** and (c) **B-3** recorded by fixing the emission wavelength at 650 nm. $c = 1.0\times10^{-5}$ M. In toluene (TN) and benzonitrile (PhCN). 20 °C.

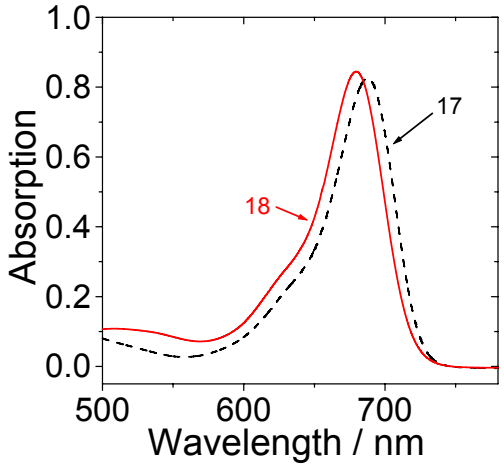


Figure S40. UV-vis absorption spectra of **17** and **18**. $c = 1.0\times10^{-5}$ M in toluene. 20 °C.

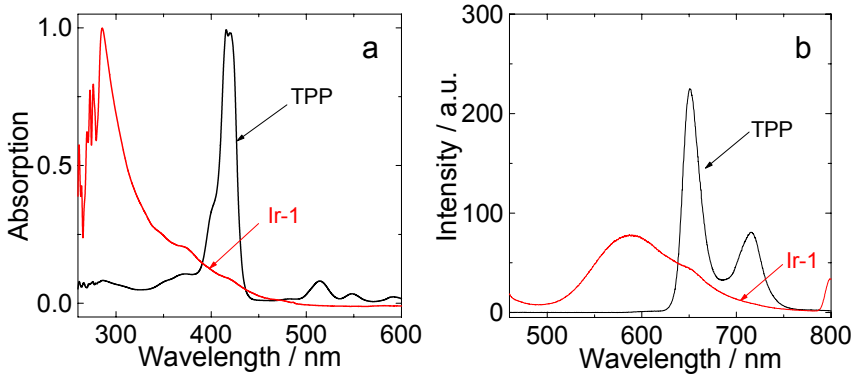


Figure S41. (a) UV/Vis absorption of $Ir(ppy)_2(phen)[PF_6]$ (**Ir-1**) (Normalized data) and **TPP**. (b). The emission spectra of **Ir-1**(Normalized data) and **TPP**. (c = 1.0×10^{-5} mol dm^{-3} in toluene). 20 ℃.

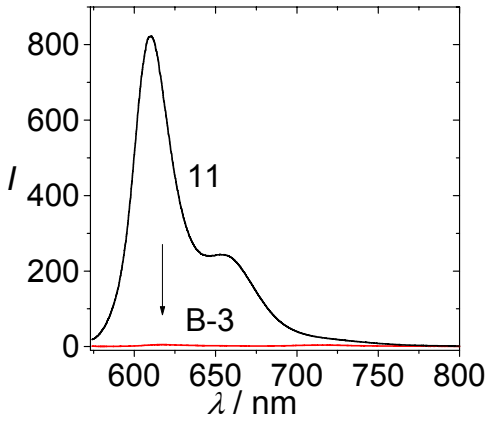


Figure S42. Fluorescence emission spectra of the Bodipys and the triplet photosensitizers: The emission spectra of **B-3** and **11**, λ_{ex} = 573 nm (toluene, 1.0×10^{-5} M, 20 ℃).

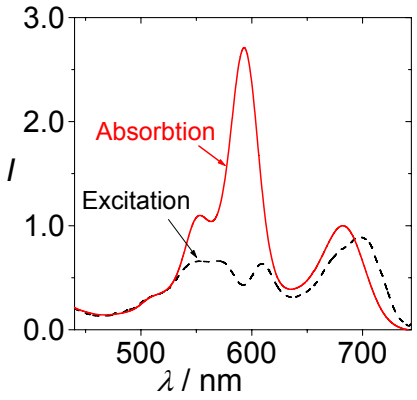


Figure S43. Normalized UV/Vis absorption and fluorescence excitation spectra: **B-3** (λ_{em} = 750 nm) (toluene, 1.0×10^{-5} M, 20 °C).

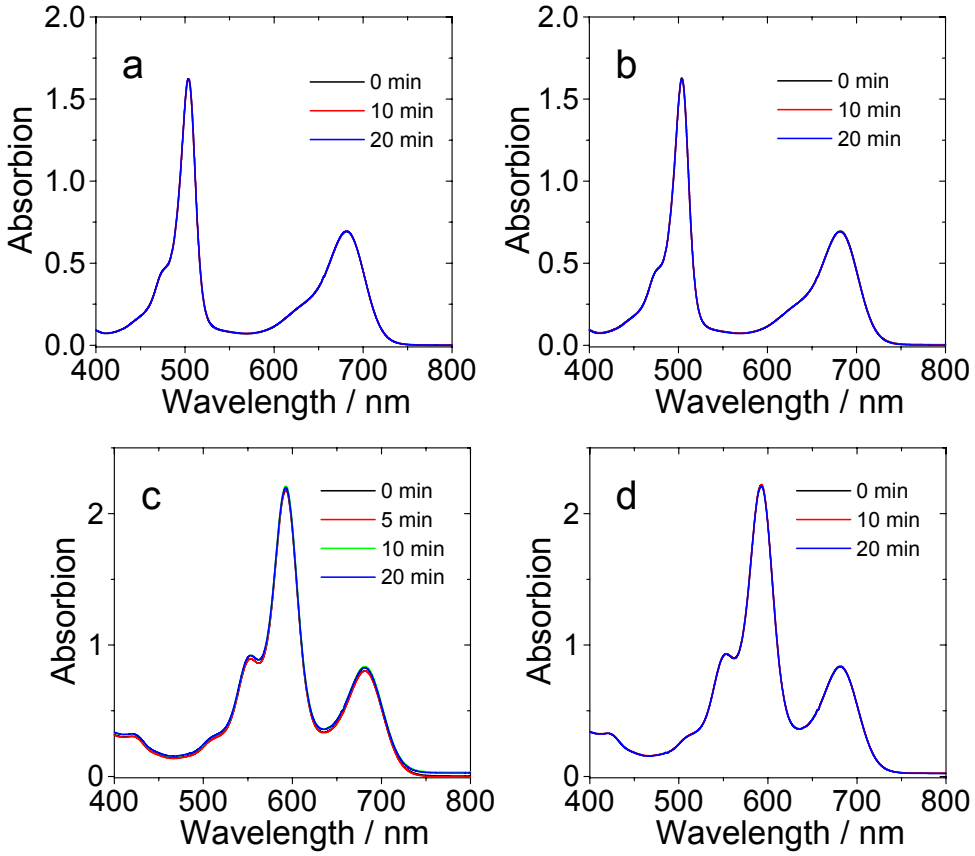


Figure S44. To clarify the possible C=C bond *cis-trans* isomerization by monitoring the UV/Vis absorption spectra of the triads upon manocromatic light irradiation. (a) **B-2**, λ_{ex}= 504 nm; (b) **B-2**, λ_{ex}=683 nm; (c) **B-3**, λ_{ex}= 593 nm; (d) **B-3**, λ_{ex}= 683 nm (c = 1.0×10^{-5} M in toluene, 20°C).

4.0 Photooxidation details.

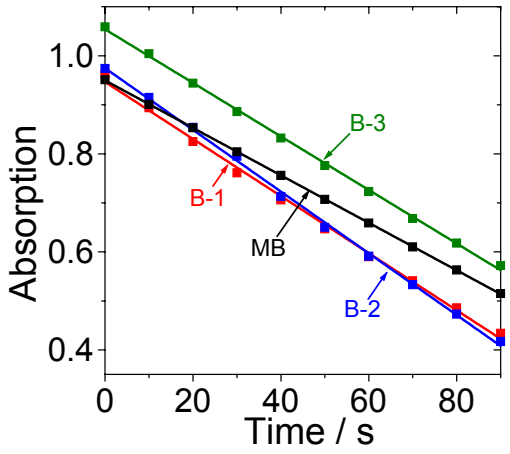


Figure S45. Comparison of the singlet oxygen generation of the different triplet photosensitizers, monitored by the decrease of the absorbance of DPBF against photoirradiation time. λ_{ex} = 673 nm. 20 °C.

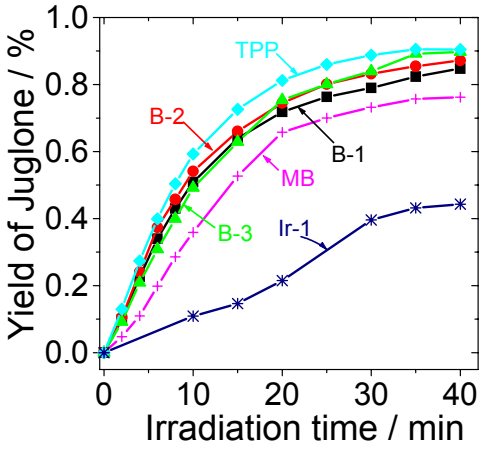


Figure S46. The yields of Juglone against irradiation time for the photooxidation of DHN using compounds **B-1**, **B-2**, **B-3**, **TPP**, **MB** and $Ir(ppy)_2(phen)[PF_6]$ (**Ir-1**) as singlet O_2 photosensitizer.

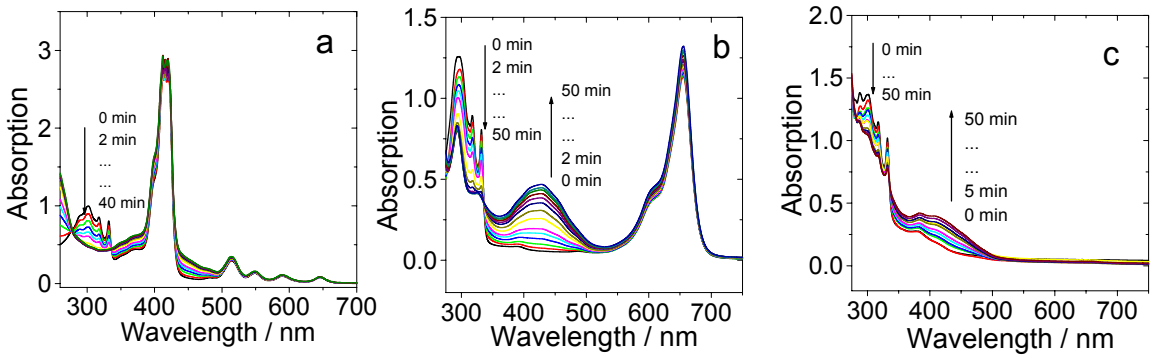


Figure S47. Absorption spectral change for the photooxidation of **DHN** using compounds as a sensitizer. (a) **TPP**. (b) **MB**. (c) $Ir(ppy)_2(phen)[PF_6]$ (**Ir-1**). Photoirradiation was carried out with 35 W xenon lamp (light power density: 170 W/m^2). *c* [DHN] = 1.0×10^{-4} M, *c* [photosensitizers] = 1.0×10^{-5} M. In CH_2Cl_2/CH_3OH=9/1 (v/v); 20 °C.

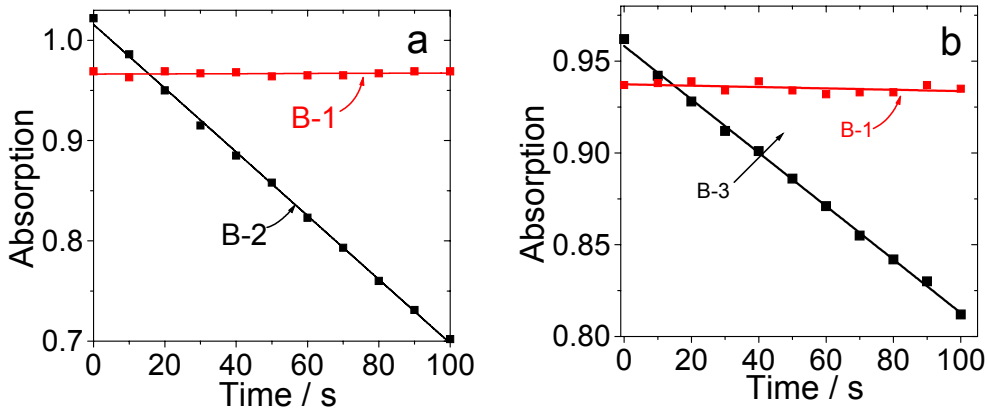


Figure S48. Comparative singlet oxygen generation experiment. Absorbance decrease of DPBF with time in the presence of photosensitizers: (a) **B-1** and **B-2**. The samples were irradiated with monochromatic light from spectrofluorometer (λ_{ex} = 501 nm); (a) **B-1** and **B-3**. The samples were irradiated with monochromatic light from spectrofluorometer (λ_{ex} = 560 nm), *c* [sensitizers] = 5.0×10^{-4} M. 20 °C.

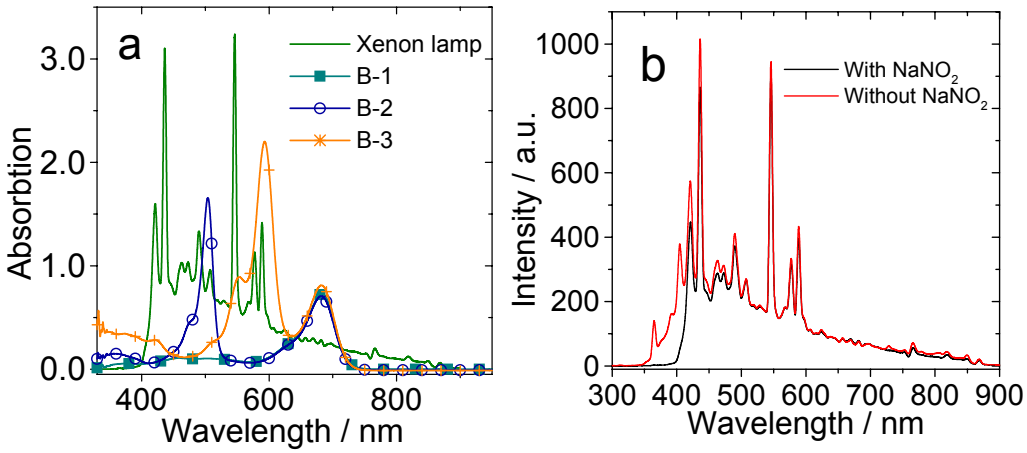


Figure S49. (a) Comparison of the UV-Vis absorption spectra of **B-1**, **B-2**, **B-3** and the emission spectra of the 35 W xenon lamp (measured with spectrofluorometer). In toluene, 1.0×10^{-5} M, 20°C. The excitation of xenon lamp with wavelength shorter than 387 nm was blocked by 0.72 M $NaNO_2$ solution. (b) The emission spectrum of the 35 W xenon lamp with and without the $NaNO_2$ solution filter. Xe lamp parameter: 35 W, color temperature: 8000 K.

5.0 Transient absorption (nanosecond and femtosecond)

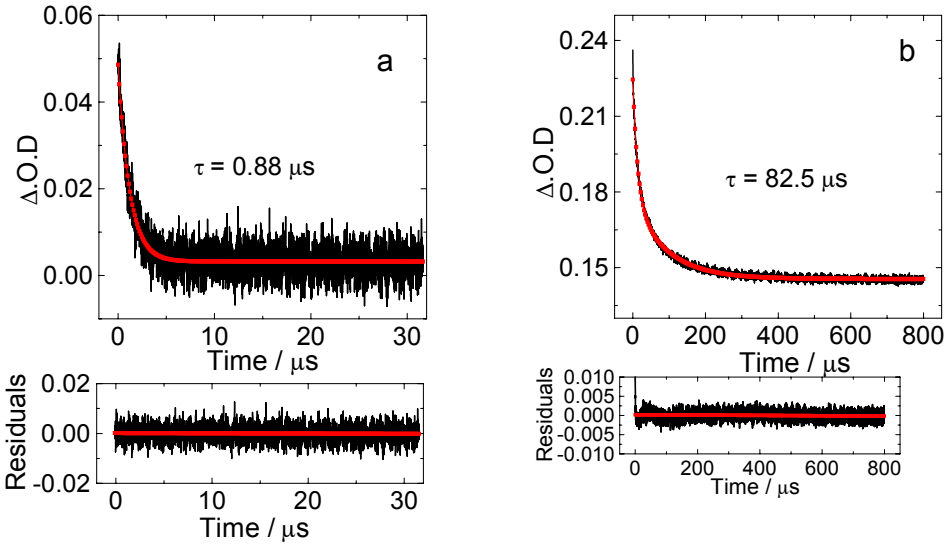


Figure S50. Nanosecond time-resolved transient absorption decay trace (a) $Ir(ppy)_2(phen)[PF_6]$ (**Ir-1)** at 310 nm. (b) Decay trace of **TPP** at 416 nm. In aerated toluene after pulsed excitation at 355 nm. $c = 1.0\times10^{-5}$ M. 20 °C.

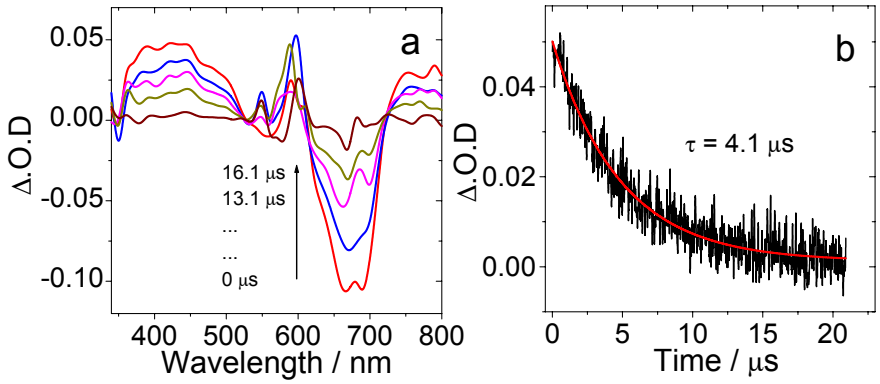


Figure S51. Nanosecond time-resolved transient absorption difference spectra of **B-3**. (a) Transient absorption with different delay times. (b) Decay trace at 430 nm. In deaerated toluene after pulsed excitation at 355 nm. $c = 2.0\times10^{-5}$ M; 20 °C.

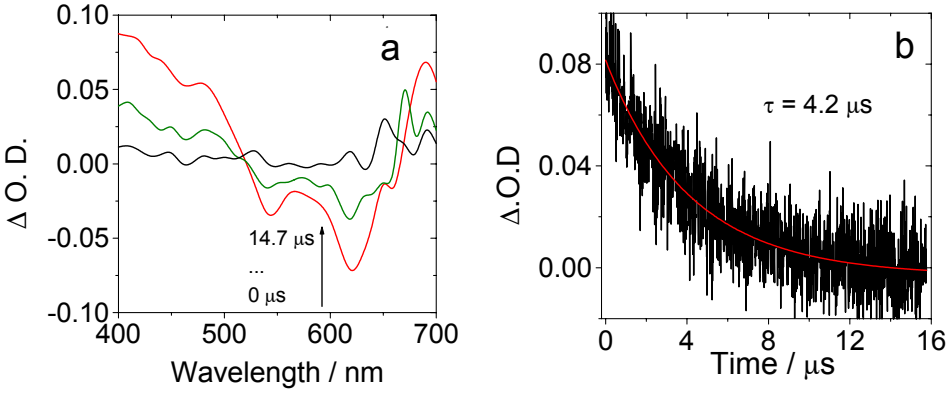


Figure S52. Nanosecond time-resolved transient absorption difference spectra of **18**. (a) Transient absorption with different delay times, (b) Decay trace at 470 nm. $c = 2.0\times10^{-5}$ M in deaerated toluene after pulsed excitation at 355 nm. 20 °C.

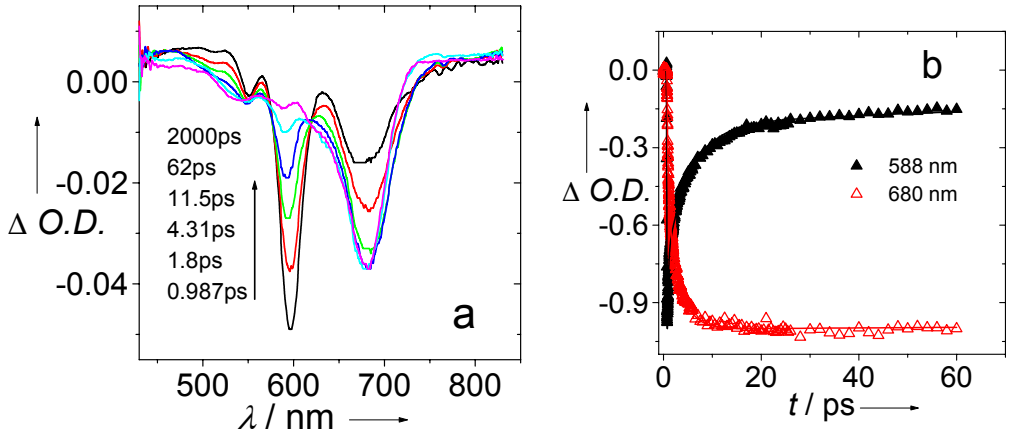


Figure S53. (a) Femtosecond transient absorption spectra of compound **B-3** upon femtosecond pulsed laser excitation at λ_{ex} = 592 nm) in toluene with several time delays between 0.987 and 2000 ps. (b) Decay profile at 588 nm and 680 nm. 20 °C.

The recovering of the bleaching band at 588 nm and the concomitant increasing of the bleaching band at 680 nm indicated the singlet energy transfer in **B-3**. The singlet energy transfer constant was calculated as $k_{ET} = (5.1\pm0.4)\times10^{11}$ s^{-1} with the increasing of the bleaching band at 680 nm.

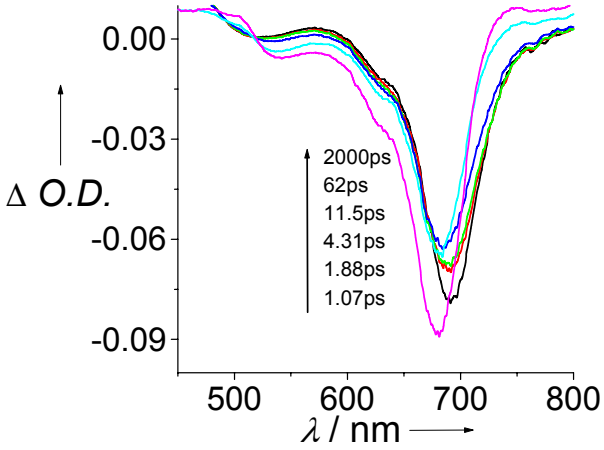


Figure S54. Femtosecond transient absorption spectra of compound **B-1** upon femtosecond pulsed laser excitation. c = 1.0 $\times 10^{-5}$ M in toluene with several time delays between 1.07 and 2000 ps. 20 °C.

6. DFT/TDDFT Calculation

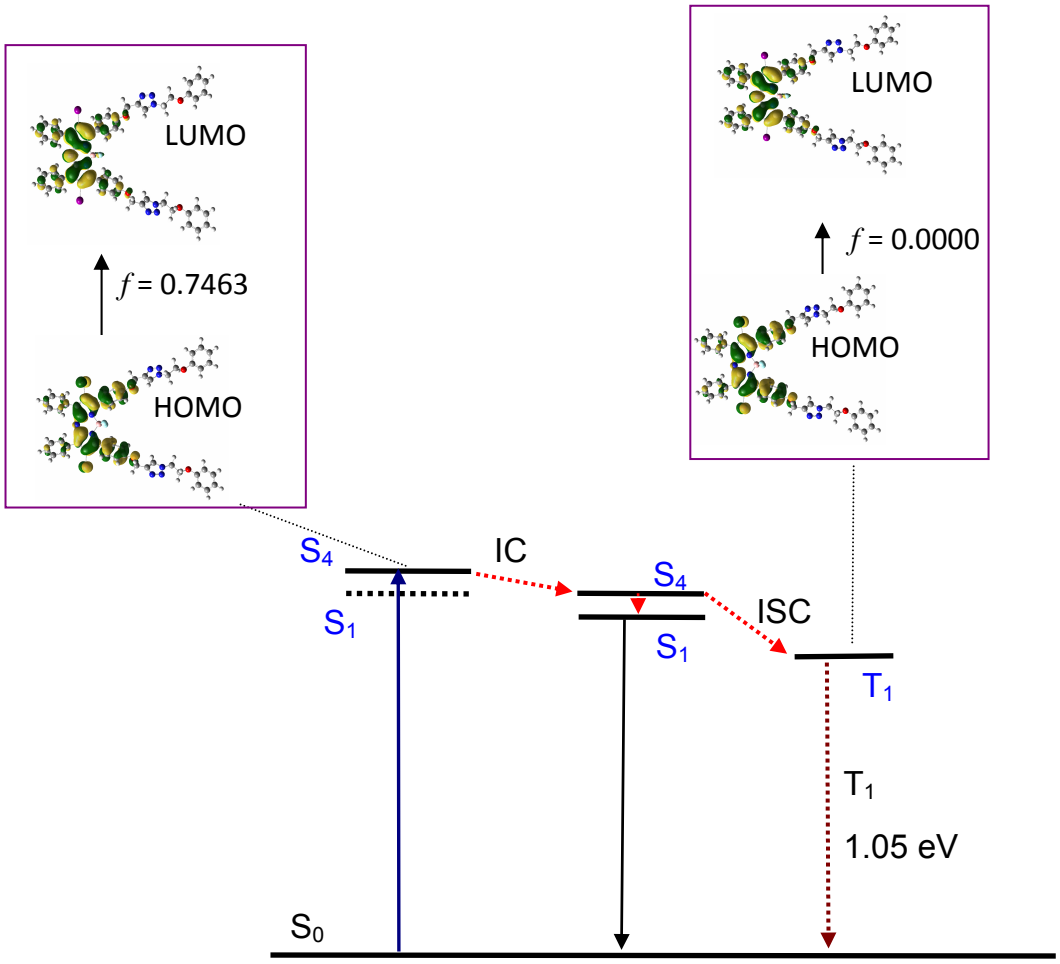


Figure S55. Selected frontier molecular orbitals involved in the excitation and emission of **B-1**. The charge transfer states were not denoted with molecular orbits (S_1 states). The left column is UV-Vis absorption (based on ground state geometry), the middle column is the fluorescence emission (based on the optimized S_1 state geometry) and the right column is the triplet excited state (based on ground state geometry). The calculations are at the B3LYP/genecp/ level using Gaussian 09W.

Table S1. Selected Electronic Excitation Energies (eV) and Corresponding Oscillator Strengths (*f*), Main Configurations and CI Coefficients of the Low-lying Electronically Excited States of **B-1.** [a]

Singlet	Electronic transition	TDDFT//B3LYP/6-31G(d)			
		Energy [b]	*f* [c]	Composition [d]	CI [e]
(UV-vis)	$S_0 \rightarrow S_1$	1.05 eV / 1183 nm	0.0000	H→L	0.6980
	$S_0 \rightarrow S_2$	1.99 eV / 622 nm	0.0000	H−2→L	0.6896
	$S_0 \rightarrow S_4$	2.09 eV / 593 nm	0.7463	H→L	0.7041
(FL)	$S_0 \rightarrow S_1$	1.95 eV / 637 nm	0.7150	H→L	0.7080
(Triplet)	$S_0 \rightarrow T_1$	1.05 eV / 1183 nm	0.0000	H→L	0.6980

[a] Calculated by TDDFT//B3LYP/ genecp. FL stands for fluorescence. [b] Only selected low-lying excited states are presented. [c] Oscillator strength. [d] H stands for HOMO and L stands for LUMO. Only the main configurations are presented. [e] CI coefficients are in absolute values.

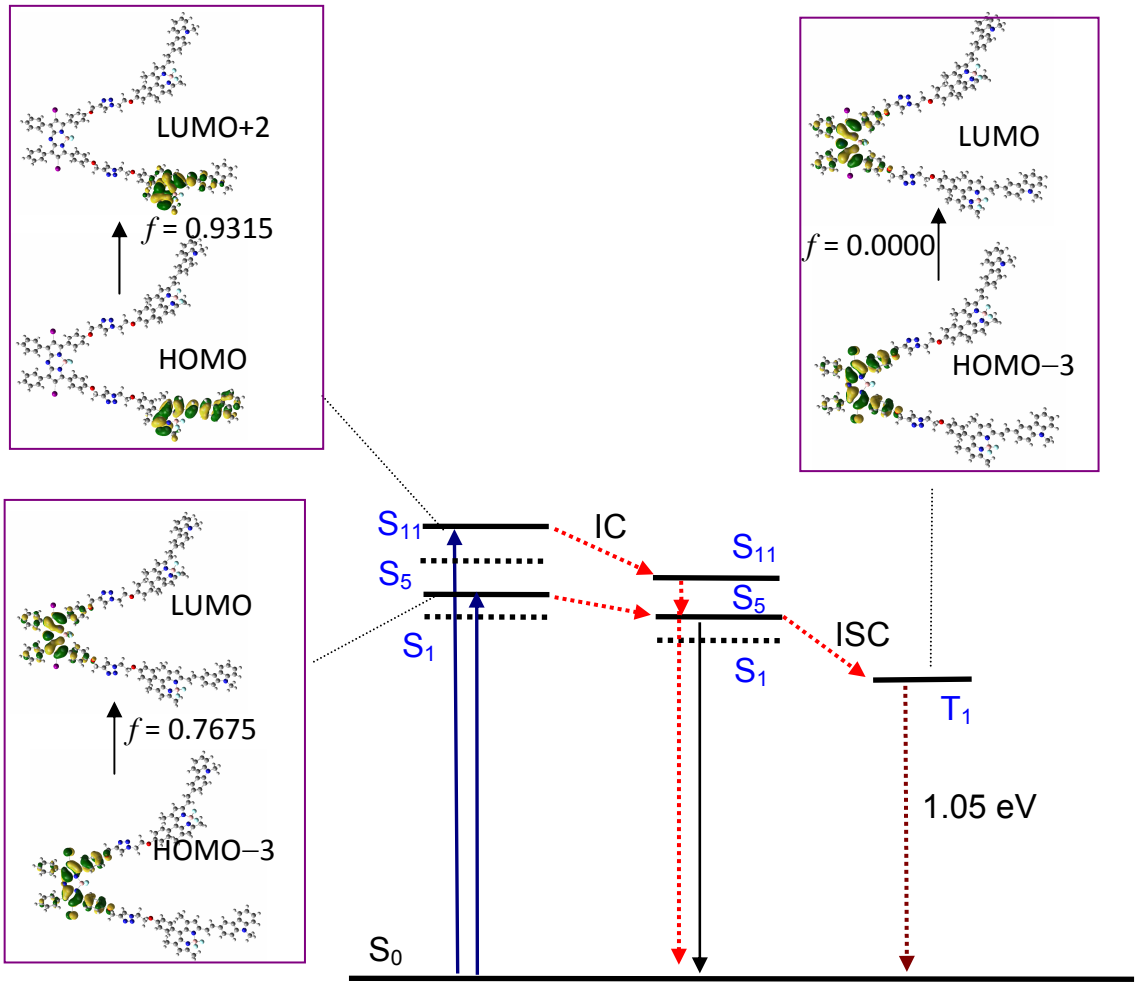


Figure S56. Selected frontier molecular orbitals involved in the excitation and emission of **B-3**. The charge transfer states were not denoted with molecular orbits. The left column is UV/Vis absorption (based on ground state geometry), the middle column is the fluorescence emission (based on the optimized S_1 state geometry) and the right column is the triplet excited state (based on ground state geometry). The calculations are at the B3LYP/ genecp / level using Gaussian 09W.

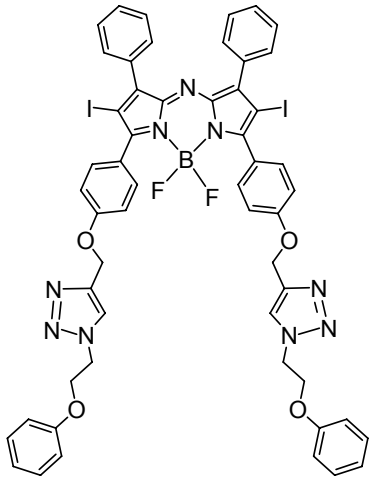
Table S2. Selected Electronic Excitation Energies (eV) and Corresponding Oscillator Strengths (*f*), Main Configurations and CI Coefficients of the Low-lying Electronically Excited States of **B-3.** [a]

Singlet	Electronic transition	TDDFT//B3LYP/6-31G(d)			
		Energy [b]	*f* [c]	Composition [d]	CI [e]
(UV-vis)	$S_0 \rightarrow S_1$	1.24eV 997 nm	0.0000	H→L	0.7070
	$S_0 \rightarrow S_2$	1.93 eV 990 nm	0.0000	H−1→L	0.7070
	$S_0 \rightarrow S_5$	2.10 eV 590 nm	0.7675	H−3→L	0.7038
	$S_0 \rightarrow S_{11}$	2.42 eV 512 nm	0.9315	H−2→L+2	0.1234
				H−1→L+1	0.1390
				H→L+2	0.6831
(Triplet)	$S_0 \rightarrow T_1$	1.05 eV 1177 nm	0.0000	H−3→L	0.6985
	$S_0 \rightarrow T_2$	1.27 eV 997 nm	0.0000	H→L	0.7070
	$S_0 \rightarrow T_3$	1.25 eV 990 nm	0.0000	H−1→L	0.7070

[a] Calculated by TDDFT//B3LYP/ genecp. FL stands for fluorescence. [b] Only selected low-lying excited states are presented. [c] Oscillator strength. [d] H stands for HOMO and L stands for LUMO. Only the main configurations are presented. [e] CI coefficients are in absolute values.

7. Coordinates of the optimized geometries of the compounds

Compound B-1. Ground state geometry.



Symbolic Z-matrix:

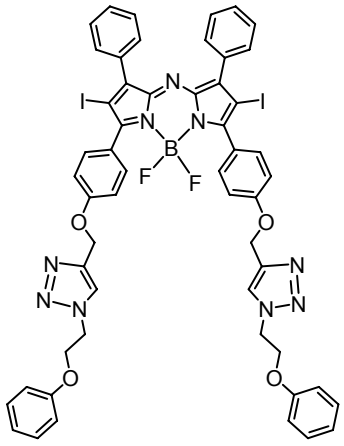
Charge = 0 Multiplicity = 1

C	-5.25883900	-1.19082200	0.02239700
C	-5.29502700	1.11502700	-0.02603000
C	-3.50275900	-2.59579300	0.15106100
C	-4.71290400	-3.37347500	0.16748400
C	-5.81263600	-2.51752900	0.09091500
C	-3.58264900	2.57518100	-0.12413700
C	-4.81641100	3.31409700	-0.16152300
C	-5.88932900	2.42352500	-0.10420300
B	-2.92443900	-0.00034200	0.01806600
F	-2.12479600	0.01855000	-1.14039200
F	-2.14271000	0.00611800	1.18856300
C	-7.33583000	2.65989100	-0.12216700
C	-8.19359500	1.88570300	0.68450600
C	-7.89911000	3.63510700	-0.96666600
C	-9.56957000	2.10210400	0.66128300
H	-7.77488200	1.11548700	1.31592300
C	-9.27643900	3.84334600	-0.98860200
H	-7.25721600	4.21038500	-1.62008100
C	-10.11578500	3.08316000	-0.17009000
H	-10.21540300	1.50370200	1.29292000
H	-9.69501600	4.59391600	-1.64877500
H	-11.18654600	3.25037000	-0.18450700
C	-2.22742700	3.11879200	-0.18507000
C	-1.19893200	2.66143900	0.66799100
C	-1.92663300	4.13593500	-1.10791100
C	0.06062400	3.23180400	0.61382500
H	-1.39356500	1.83633300	1.33526200
C	-0.65513300	4.69562500	-1.17355700
H	-2.68535200	4.47218700	-1.80135900
C	0.34577500	4.25787100	-0.29956600
H	0.85333300	2.89563700	1.26853400
H	-0.45544300	5.46463900	-1.90661600
C	-2.13241700	-3.09635400	0.23494400
C	-1.10353000	-2.60375800	-0.59786500
C	-1.81642000	-4.10778400	1.15901700
C	0.17115300	-3.13726300	-0.52562900

H	-1.31186700	-1.78221200	-1.26543800
C	-0.53036800	-4.63049100	1.24290800
H	-2.57574500	-4.46860700	1.83928100
C	0.47121800	-4.15979000	0.38695800
H	0.96417900	-2.77474100	-1.16574000
H	-0.31964500	-5.39493200	1.97771800
C	-7.25112000	-2.79958200	0.08376400
C	-8.11933900	-2.04976400	-0.73477000
C	-7.79775200	-3.79497800	0.91568400
C	-9.48803000	-2.30925500	-0.73540200
H	-7.71468100	-1.26407900	-1.35616100
C	-9.16803100	-4.04636200	0.91370600
H	-7.14956400	-4.35248700	1.57816500
C	-10.01705500	-3.31000000	0.08354100
H	-10.14162800	-1.72890400	-1.37583600
H	-9.57379500	-4.81201500	1.56449300
H	-11.08213300	-3.51071600	0.07945000
N	-5.92101400	-0.04809700	-0.00754500
N	-3.89062100	1.24386800	-0.02171300
N	-3.85118100	-1.27486400	0.04260200
I	-4.96135500	5.43142200	0.04842300
I	-4.78724800	-5.49472900	-0.04380200
C	2.01893800	5.78117200	-1.24525000
H	1.90431800	5.39451000	-2.26601400
H	1.39855600	6.67948300	-1.13934800
O	1.63232100	4.75947600	-0.26773500
C	4.26563500	5.44248300	-0.04118000
H	4.05195200	4.62343200	0.61798800
N	4.14557300	7.09486500	-1.57096400
N	5.40459300	7.11332700	-1.09324500
N	5.47053500	6.07211700	-0.13270500
C	3.44663900	6.08868700	-0.94259000
C	6.72301700	5.82601400	0.59610500
C	7.79403900	6.84505500	0.19151800
H	7.09176800	4.82106600	0.37499800
H	6.54813700	5.91180700	1.67167000
H	8.03605800	6.76820100	-0.87137200
H	7.46924400	7.86543100	0.40918200
O	8.93581400	6.44293200	1.03198800
C	10.10177900	7.21498700	0.87014000
C	10.19103800	8.50427800	1.39882200
C	11.18514100	6.66162000	0.18656900
C	11.36976000	9.23556100	1.24927300
H	9.34714600	8.91891100	1.93609500
C	12.36525500	7.39210800	0.04411800
H	11.09140500	5.65976400	-0.21215500
H	11.43904600	10.23413400	1.66480500
H	13.20736900	6.95709900	-0.48142000
C	2.14996600	-5.69935700	1.29472000
H	2.04348800	-5.37110100	2.33612600
H	1.51644900	-6.58174500	1.13918600

O	1.77159000	-4.62515300	0.37223300
C	4.35004100	-5.42805200	-0.00910900
H	4.10387000	-4.66251300	-0.71924300
N	4.30837200	-6.95072700	1.65370600
N	5.54778400	-6.99838300	1.12896100
N	5.56484200	-6.03803900	0.08586900
C	3.57418900	-6.00505200	0.97365700
C	6.78628700	-5.83950600	-0.70721200
C	7.91185900	-6.75087800	-0.20565700
H	7.11484900	-4.80002400	-0.62842900
H	6.58976200	-6.07136900	-1.75725600
H	8.16457300	-6.53577900	0.83570400
H	7.63534000	-7.80423100	-0.29364900
O	9.02055700	-6.39898200	-1.11044200
C	10.20756900	-7.13121900	-0.91909400
C	10.30964200	-8.45819800	-1.34150500
C	11.29773000	-6.50172300	-0.31719500
C	11.50792000	-9.15138300	-1.16826600
H	9.45995500	-8.93221600	-1.81697500
C	12.49731700	-7.19474900	-0.15113500
H	11.19380200	-5.47206200	-0.00022600
H	11.58713100	-10.17954400	-1.50177300
H	13.34456200	-6.70119600	0.31053600
C	12.45934600	8.68261100	0.57106700
H	13.37429500	9.25152400	0.45720700
C	12.60431500	-8.52259000	-0.57209000
H	13.53446400	-9.06210600	-0.43975500

Compound B-1. Triplet state geometry.
Charge = 0 Multiplicity = 3



C	5.25999700	1.13618100	0.10576500
C	5.25315300	-1.16095300	-0.09207100
C	3.54009300	2.60181600	0.23922800
C	4.76244800	3.33211800	0.37126800
C	5.84755700	2.45465500	0.31028800
C	3.52451600	-2.61511500	-0.23693000
C	4.74276900	-3.35338500	-0.36215400
C	5.83327000	-2.48315200	-0.29353000
B	2.93796000	-0.00484100	-0.00040800
F	2.14120100	-0.00689200	-1.16615300
F	2.13369900	0.00235300	1.16001900
C	7.27043200	-2.72752500	-0.39595700
C	8.18524200	-1.96913800	0.36690000
C	7.77956800	-3.70031300	-1.28121800
C	9.55426600	-2.20332400	0.26610100
H	7.81261300	-1.18987200	1.01481900
C	9.14993800	-3.92492900	-1.38012100
H	7.09852600	-4.25774400	-1.90945500

C	10.04331500	-3.18405400	-0.60120500
H	10.24056200	-1.61676100	0.86568900
H	9.52220400	-4.67172600	-2.07170900
H	11.10958200	-3.36316400	-0.67688600
C	2.16384800	-3.10849700	-0.30187300
C	1.13790300	-2.60020400	0.53447200
C	1.82851100	-4.13903000	-1.20714300
C	-0.13352700	-3.13776600	0.49133600
H	1.35302600	-1.76706100	1.18553600
C	0.54543500	-4.66613300	-1.25931300
H	2.57293400	-4.50242600	-1.90118100
C	-0.44459300	-4.18365100	-0.39386200
H	-0.91804900	-2.76534500	1.13629100
H	0.32383400	-5.44236700	-1.97850700
C	2.18219000	3.10368500	0.29745900
C	1.15651100	2.59990300	-0.54194500
C	1.84916500	4.13743800	1.19991700
C	-0.11233900	3.14385200	-0.50368000
H	1.36994400	1.76580700	-1.19235200
C	0.56857700	4.67106700	1.24721600
H	2.59298800	4.49799300	1.89605000
C	-0.42173100	4.19068700	0.38094000
H	-0.89658600	2.77458100	-1.15078500
H	0.34826700	5.44856300	1.96547300
C	7.28555900	2.68946800	0.42263900
C	8.20073600	1.92437800	-0.33304800
C	7.79481300	3.65936400	1.31100500
C	9.57054500	2.14936000	-0.22238000
H	7.82757000	1.14712800	-0.98307300
C	9.16590600	3.87476400	1.41978400
H	7.11298900	4.22164800	1.93405000
C	10.05989600	3.12732200	0.64787200
H	10.25721500	1.55771400	-0.81651700
H	9.53817100	4.61941200	2.11368700
H	11.12677700	3.29919300	0.73128500
N	5.93579400	-0.01456300	0.00907800
N	3.87727300	-1.26021200	-0.04468000
N	3.88507900	1.24451100	0.04977000
I	4.87713800	-5.48159000	-0.24017900
I	4.91197500	5.45927300	0.24779200
C	-2.15496400	-5.69318400	-1.29592900
H	-2.06029100	-5.32622600	-2.32574500
H	-1.53643000	-6.59180800	-1.18472600
O	-1.73993200	-4.65277100	-0.34804100
C	-4.37351800	-5.32421800	-0.04660300
H	-4.14632800	-4.48950200	0.58800300
N	-4.28663500	-7.01275300	-1.53884400
N	-5.53252000	-7.02397800	-1.02805300
N	-5.57742500	-5.96099000	-0.09066500
C	-3.57582500	-5.98914100	-0.95346100
C	-6.81296800	-5.69964300	0.66185100

C	-7.88859200	-6.73408900	0.31218000
H	-7.19154000	-4.70254100	0.42230800
H	-6.61090200	-5.75501300	1.73454800
H	-8.15156600	-6.69556300	-0.74773300
H	-7.55574200	-7.74535500	0.55884300
O	-9.01584400	-6.30788200	1.16000700
C	-10.13685300	-7.15943400	1.14187700
C	-10.11834200	-8.38300300	1.81435900
C	-11.28335500	-6.75278300	0.45857000
C	-11.25265400	-9.19515500	1.80927700
H	-9.22622900	-8.68210400	2.35055100
C	-12.41910700	-7.56362200	0.46056200
H	-11.27328500	-5.79932700	-0.05356400
H	-11.23836700	-10.14179600	2.33679000
H	-13.31057100	-7.24222100	-0.06531100
C	-2.10617300	5.76074600	1.22525800
H	-2.02176400	5.45251800	2.27451800
H	-1.46277500	6.63445600	1.06275600
O	-1.71526900	4.66447700	0.33212900
C	-4.27942600	5.48769700	-0.12455300
H	-4.02261200	4.71641500	-0.82469000
N	-4.26606600	7.02038100	1.52966800
N	-5.49400400	7.06959200	0.97906600
N	-5.49351000	6.10294000	-0.05813800
C	-3.52183900	6.06780000	0.87058400
C	-6.69950100	5.90443100	-0.87497900
C	-7.83126400	6.82332200	-0.40172400
H	-7.03371200	4.86675300	-0.79662600
H	-6.48046300	6.12931400	-1.92205200
H	-8.10649100	6.61453000	0.63522800
H	-7.54823000	7.87499700	-0.48908000
O	-8.92215900	6.47157400	-1.32769600
C	-10.11409000	7.20091600	-1.15546400
C	-10.21120700	8.52924900	-1.57466000
C	-11.21338700	6.56700500	-0.57527800
C	-11.41368200	9.21953600	-1.41979200
H	-9.35424300	9.00671300	-2.03331100
C	-12.41705600	7.25712800	-0.42773000
H	-11.11299400	5.53636100	-0.26037600
H	-11.48899800	10.24882800	-1.75067900
H	-13.27134300	6.76024200	0.01706300
C	-12.40543400	-8.78866900	1.13192900
H	-13.28590900	-9.41995100	1.13030200
C	-12.51914300	8.58641400	-0.84536100
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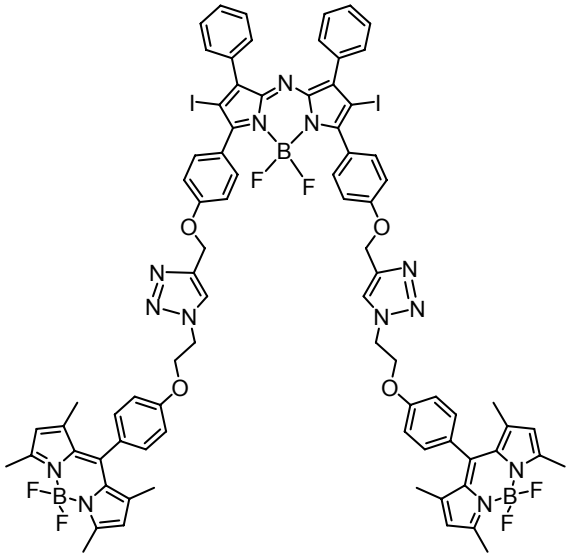
Compound B-2. Ground state geometry.
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1



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C	-9.90162100	1.11360400	0.16356200
C	-8.16910200	-2.57257100	-0.22182100
C	-9.37901700	-3.33451100	-0.27031800
C	-10.46832300	-2.46755200	-0.24647200
C	-8.20382200	2.55147600	0.24339200
C	-9.42286200	3.29814500	0.28415000
C	-10.50122300	2.41759000	0.25122900
B	-7.54512000	-0.00419900	-0.00086900
F	-6.79220400	0.20330100	-1.14445400
F	-6.76220800	-0.19812700	1.12358100
C	-11.94834000	2.66302300	0.28122100
C	-12.79403900	1.84080600	1.04978500
C	-12.52371400	3.70342100	-0.47092300
C	-14.16882700	2.06447800	1.07428200
H	-12.36631200	1.03146300	1.62999200
C	-13.89979700	3.91935200	-0.44865800
H	-11.89178200	4.32859800	-1.09210800
C	-14.72699500	3.10440000	0.32754900
H	-14.80484000	1.42419300	1.67926600
H	-14.32648000	4.72327600	-1.04227500
H	-15.79971700	3.27714200	0.34797500
C	-6.83304800	3.07611600	0.25147100
C	-5.85071900	2.59689900	1.14177700
C	-6.47811300	4.10120600	-0.63935400
C	-4.57301300	3.13356100	1.13957500
H	-6.09372400	1.79820100	1.82981200
C	-5.19095700	4.63302900	-0.66204500
H	-7.21005600	4.47433100	-1.34756300
C	-4.23120300	4.15285100	0.23811300
H	-3.81658000	2.77412500	1.82983500
H	-4.95314200	5.41185100	-1.37694500
C	-6.79229700	-3.08043800	-0.21936300
C	-5.80400500	-2.57726900	-1.08997100
C	-6.43573300	-4.11304700	0.66238300
C	-4.52063100	-3.09977400	-1.07965400
H	-6.04750200	-1.77173700	-1.76983200
C	-5.14323200	-4.63122200	0.69304500
H	-7.17078900	-4.50302500	1.35803000
C	-4.17833400	-4.12848800	-0.18908200
H	-3.76015800	-2.72233600	-1.75573100
H	-4.90474500	-5.41558700	1.40165900
C	-11.91215500	-2.73070000	-0.28565400
C	-12.76249500	-1.91990400	-1.06119500
C	-12.48005500	-3.77660100	0.46452200
C	-14.13432600	-2.16000500	-1.09441000
H	-12.34064900	-1.10631900	-1.63976200
C	-13.85329100	-4.00898300	0.43352200
H	-11.84489000	-4.39316700	1.09099900
C	-14.68497700	-3.20528000	-0.34958600
H	-14.77389700	-1.52828800	-1.70462200

H	-14.27430200	-4.81691600	1.02574300
H	-15.75540600	-3.39084700	-0.37678300
N	-10.55157900	-0.02546000	0.00065600
N	-8.51364900	1.23008200	0.18499600
N	-8.49629200	-1.25498600	-0.16798100
I	-9.53076600	5.38012000	0.66451600
I	-9.46216400	-5.41770600	-0.65216200
C	-2.52055000	5.59040200	-0.62309000
H	-2.65796700	5.22201200	-1.64980100
H	-3.11207300	6.51048300	-0.51870000
O	-2.94836700	4.60746800	0.31394900
C	-0.19748000	5.25816900	0.50654600
H	-0.31279100	4.44622000	1.20651700
N	-0.41460600	6.86347200	-1.01973600
N	0.82588800	6.89110400	-0.61405500
N	0.97325100	5.92158200	0.31576400
C	-1.07639100	5.87423100	-0.35615600
C	2.26027900	5.69433000	0.96600000
C	3.31211000	6.70586800	0.51526200
H	2.60991400	4.68259400	0.73479400
H	2.13213000	5.76649400	2.05105500
H	3.48936100	6.63756400	-0.56398500
H	2.99285900	7.72964000	0.74082700
O	4.49208700	6.35725800	1.24435400
C	5.60183500	7.12855400	0.96104600
C	5.71568200	8.43038800	1.45719500
C	6.63448100	6.57454600	0.20147500
C	6.86347300	9.17540000	1.18716000
H	4.91425800	8.84747300	2.05988900
C	7.78253600	7.32312600	-0.05908700
H	6.53070400	5.55919100	-0.16873200
C	7.90711900	8.63240800	0.42466100
H	6.95394300	10.18680100	1.57361100
H	8.58779800	6.89115600	-0.64680500
C	9.13243100	9.43712000	0.13044200
C	10.21445600	9.40432700	1.02586900
C	9.18145800	10.21183300	-1.04049600
C	10.41449300	8.70400400	2.26353300
C	12.25071500	9.94803900	1.76383800
C	11.68516500	9.05875900	2.70152700
H	12.16998900	8.71658200	3.60704500
C	10.11796500	11.61658400	-2.50234500
C	8.83506800	11.29231100	-2.99075100
H	8.40381800	11.66898300	-3.90958600
C	8.22959300	10.41731400	-2.09634800
F	12.70751600	10.60070700	-1.19972700
F	11.81903400	12.38015300	-0.06465300
C	6.85200200	9.84657400	-2.26913200
H	6.86143500	8.75327400	-2.33707500
H	6.18881700	10.10385400	-1.43621800
H	6.40437100	10.23668300	-3.18859700

C	9.49343200	7.76965800	2.99254000
H	8.56353400	8.26065000	3.30000800
H	9.20531300	6.90908000	2.37944000
H	9.98796500	7.39256900	3.89329800
C	13.59592800	10.59756600	1.79618100
H	14.18706800	10.30182500	0.92256300
H	13.49682500	11.68730000	1.75376300
H	14.13494700	10.31895000	2.70538900
C	11.14228700	12.51721600	-3.11230800
H	11.40476500	13.32371800	-2.41954100
H	12.06633400	11.96566000	-3.31676600
H	10.76773600	12.94914600	-4.04390400
B	11.61197700	11.06348100	-0.47352500
N	10.32013000	10.96989200	-1.33839100
N	11.36962300	10.15113700	0.76567300
C	-2.48505900	-5.61926100	0.61424200
H	-2.61636300	-5.32332500	1.66459700
H	-3.09813600	-6.51531900	0.44296800
O	-2.88932800	-4.56645700	-0.25466300
C	-0.18617500	-5.33539400	-0.57593300
H	-0.31526800	-4.54965200	-1.30285500
N	-0.37002900	-6.87428500	1.02152400
N	0.85961800	-6.92466400	0.58597300
N	0.98744000	-5.99379600	-0.38524900
C	-1.04504800	-5.91108600	0.33346700
C	2.25719100	-5.80214400	-1.07932700
C	3.34313800	-6.73535200	-0.54792000
H	2.58223200	-4.76389100	-0.95538000
H	2.11561800	-5.98501400	-2.14977300
H	3.51852600	-6.56930100	0.52126900
H	3.05967700	-7.78484700	-0.68410100
O	4.51020600	-6.40983100	-1.30771400
C	5.63119000	-7.15721500	-1.00503600
C	5.75213600	-8.47785700	-1.44686600
C	6.66866800	-6.56043100	-0.28554100
C	6.91175000	-9.19875200	-1.16253400
H	4.94698900	-8.92829700	-2.01989300
C	7.82821600	-7.28563200	-0.00977700
H	6.55943800	-5.53114500	0.04219700
C	7.96017500	-8.61293700	-0.43936700
H	7.00806500	-10.22464600	-1.50707000
H	8.63704600	-6.82084300	0.54719900
C	9.19875000	-9.39174600	-0.13107000
C	10.27215000	-9.37312500	-1.03724700
C	9.26855500	-10.12865700	1.06304900
C	10.45196000	-8.71011900	-2.29834800
C	12.30901200	-9.91336500	-1.77625700
C	11.72357600	-9.06154400	-2.73625400
H	12.19582700	-8.74197900	-3.65656100
C	10.23550300	-11.47595600	2.55875200
C	8.95463500	-11.14902500	3.05077200

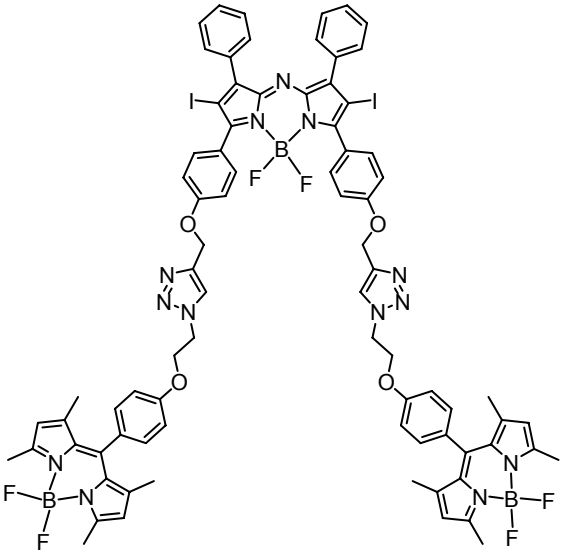
H	8.53749100	-11.49978300	3.98624000
C	8.33051400	-10.30927200	2.13564400
F	12.80090600	-10.47961400	1.19882100
F	11.91662100	-12.29710700	0.12234600
C	6.94973600	-9.74566000	2.30602100
H	6.94819500	-8.65043500	2.32413800
H	6.27570900	-10.04741000	1.49697500
H	6.52171200	-10.09861000	3.24951300
C	9.51180200	-7.81260200	-3.04898600
H	8.58320200	-8.32386000	-3.32588700
H	9.22260100	-6.93276700	-2.46439900
H	9.99074300	-7.46403200	-3.96945200
C	13.66222100	-10.54637900	-1.80058900
H	14.25828800	-10.21352100	-0.94385400
H	13.57766000	-11.63516600	-1.72009500
H	14.18837400	-10.29217500	-2.72436900
C	11.27576700	-12.34544500	3.18673000
H	11.54675000	-13.16618400	2.51426700
H	12.19267400	-11.77552900	3.37243600
H	10.91179000	-12.75795300	4.13124400
B	11.70217700	-10.97157200	0.49731000
N	10.41841200	-10.86483900	1.37256000
N	11.43936400	-10.09629700	-0.76427000

Compound B-2. Triplet state geometry.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	9.87801700	-1.26778000	-0.15278800
C	9.95403100	1.01515900	0.15833600
C	8.10672300	-2.65771000	-0.38506600
C	9.30221000	-3.42764700	-0.53332500
C	10.41868700	-2.59695200	-0.41131900
C	8.27874500	2.52624500	0.33851100
C	9.51953400	3.20836100	0.53598100
C	10.57794200	2.30120100	0.44572000
B	7.59914000	-0.04307500	-0.04059700
F	6.77533300	-0.06018600	1.10600000
F	6.82400500	0.03288200	-1.21802300
C	12.02031600	2.48253500	0.59393200
C	12.92255700	1.73517800	-0.19452700
C	12.54537400	3.37944800	1.54722700
C	14.29679900	1.90839400	-0.05135400
H	12.53490500	1.01154800	-0.89606100
C	13.92073800	3.54255000	1.68847100
H	11.87181600	3.92529600	2.19355000
C	14.80269500	2.81489100	0.88446300
H	14.97395600	1.33227800	-0.67107300
H	14.30543700	4.23090400	2.43191500



H	15.87300400	2.94650600	0.99323100
C	6.93535200	3.06775800	0.38754200
C	5.92430400	2.64838200	-0.51339800
C	6.60412000	4.05573800	1.34019400
C	4.67117100	3.22802800	-0.48098400
H	6.13299300	1.84635800	-1.20426000
C	5.33791500	4.62411700	1.38137000
H	7.33586000	4.35159500	2.07845400
C	4.36336900	4.22700100	0.45754300
H	3.89805300	2.92297200	-1.17334800
H	5.11710100	5.36508300	2.13705700
C	6.73176000	-3.10491900	-0.48095900
C	5.71787600	-2.60702800	0.37578300
C	6.37066900	-4.08162800	-1.43449700
C	4.43222200	-3.10668300	0.30583700
H	5.95374800	-1.81128700	1.06517300
C	5.07321900	-4.56963400	-1.51355400
H	7.10725400	-4.43277000	-2.14311600
C	4.09492600	-4.10029200	-0.62816400
H	3.65657500	-2.74327200	0.96649700
H	4.83144500	-5.30305600	-2.27029200
C	11.84862400	-2.88178500	-0.50860100
C	12.77587900	-2.19177600	0.30274800
C	12.33923600	-3.82463500	-1.43570500
C	14.13818100	-2.46392000	0.20694500
H	12.41845500	-1.43437400	0.98435600
C	13.70323600	-4.08681900	-1.52952100
H	11.64982900	-4.32866800	-2.09902700
C	14.60834800	-3.41467100	-0.70321400
H	14.83411600	-1.93021100	0.84362600
H	14.06173900	-4.80915600	-2.25357800
H	15.66948300	-3.62326900	-0.77511200
N	10.59506200	-0.15037500	0.01330300
N	8.58482600	1.17063800	0.08273900
N	8.49914900	-1.32506700	-0.12569800
I	9.73586100	5.33258200	0.54540000
I	9.36824400	-5.56244700	-0.51538400
C	2.66537700	5.73229300	1.39404400
H	2.73894500	5.31192800	2.40499300
H	3.29395900	6.62920400	1.33951400
O	3.08433200	4.73914900	0.39909400
C	0.46886100	5.43875800	0.09147800
H	0.70863700	4.64142200	-0.58510600
N	0.52805400	7.04047000	1.67797000
N	-0.71092300	7.07588200	1.15223500
N	-0.73875600	6.06607200	0.15626100
C	1.25158200	6.05493300	1.04479200
C	-1.95992200	5.84915300	-0.63117800
C	-3.04433000	6.85570100	-0.23128100
H	-2.33861500	4.83779600	-0.46238500
H	-1.74205800	5.97436400	-1.69497300

H	-3.33190200	6.73683800	0.81609200
H	-2.71048400	7.88280900	-0.39610100
O	-4.15165600	6.48909500	-1.13529900
C	-5.34031100	7.21617900	-0.96793800
C	-5.45232300	8.53501300	-1.41456900
C	-6.43256800	6.59101800	-0.36359100
C	-6.65827100	9.22027200	-1.26977000
H	-4.60348500	9.01096100	-1.88920800
C	-7.64110000	7.27225700	-0.22478300
H	-6.32450700	5.56890300	-0.02471400
C	-7.76072000	8.59294200	-0.67529100
H	-6.75265100	10.24077100	-1.62204300
H	-8.49379900	6.78658800	0.23492800
C	-9.05665400	9.32241500	-0.53155600
C	-10.00766500	9.24770300	-1.55293800
C	-9.31069900	10.06870100	0.62254200
C	-10.01496100	8.56576600	-2.82055300
C	-11.98114100	9.69018100	-2.54848600
C	-11.24293600	8.85260300	-3.41860900
H	-11.57940800	8.49959100	-4.37966000
C	-10.53325100	11.39376100	1.97592300
C	-9.30672300	11.13023300	2.63157800
H	-9.02545000	11.50384200	3.60251100
C	-8.53289200	10.31040500	1.80892400
F	-12.88228700	10.29292400	0.32723100
F	-11.93146400	12.13333700	-0.67231100
C	-7.15626300	9.80203500	2.13618200
H	-7.12445000	8.70755900	2.13883100
H	-6.41997400	10.14376900	1.40095900
H	-6.85343100	10.16192500	3.12401700
C	-8.93921600	7.70356300	-3.42100000
H	-7.99614600	8.25053800	-3.52029500
H	-8.73695700	6.82517900	-2.79873700
H	-9.25067600	7.36199400	-4.41266700
C	-13.34409200	10.28430100	-2.70307700
H	-13.96237900	9.98221700	-1.85046100
H	-13.26604000	11.37684200	-2.65915800
H	-13.80920300	9.97508000	-3.64051300
C	-11.70716500	12.21038300	2.41143800
H	-11.87442200	13.01355000	1.68435200
H	-12.60445200	11.58186800	2.39306900
H	-11.55415900	12.62805400	3.40791500
B	-11.69958500	10.80922600	-0.24568800
N	-10.53228000	10.75945600	0.77732400
N	-11.24110700	9.92447600	-1.43679800
C	2.36313800	-5.57783800	-1.54479900
H	2.43421300	-5.21701400	-2.57809800
H	2.99326300	-6.46980600	-1.43963800
O	2.78685600	-4.53645100	-0.60299900
C	0.22770500	-5.34635900	-0.13104700
H	0.51698100	-4.62163700	0.60521600

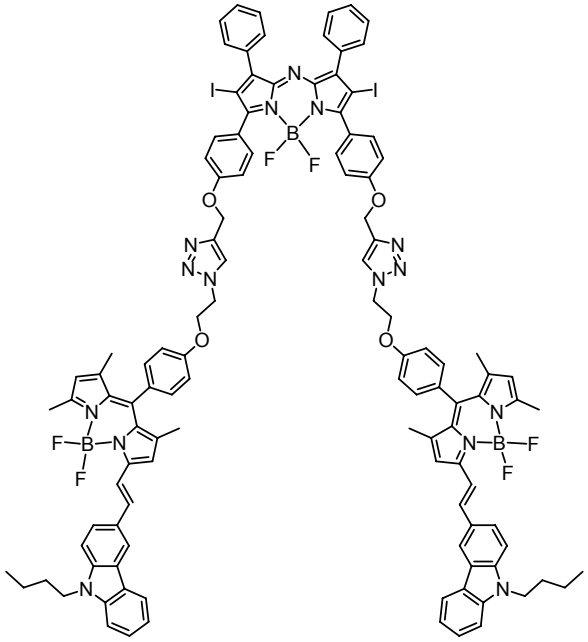
N	0.17175600	-6.78086600	-1.87040100
N	-1.04224000	-6.84218800	-1.29167100
N	-0.99811500	-5.93723200	-0.20026500
C	0.94936500	-5.88029700	-1.17749900
C	-2.17911600	-5.76899000	0.65749000
C	-3.33482500	-6.64260800	0.15768200
H	-2.49893500	-4.72383500	0.64899600
H	-1.93853200	-6.05892400	1.68365100
H	-3.63116300	-6.36995800	-0.85814500
H	-3.06711100	-7.70154700	0.17903000
O	-4.40196900	-6.32993000	1.12785800
C	-5.59552800	-7.05127400	0.96916500
C	-5.68297100	-8.39373700	1.34558800
C	-6.71500900	-6.40055200	0.44758500
C	-6.89040000	-9.07845000	1.21283600
H	-4.81287400	-8.88903500	1.75791900
C	-7.92498100	-7.08195900	0.32064800
H	-6.62627200	-5.36040700	0.16224800
C	-8.01932200	-8.42687500	0.69985500
H	-6.96490500	-10.11770800	1.51082200
H	-8.79835400	-6.57740500	-0.07560200
C	-9.31487800	-9.15877900	0.56561300
C	-10.23198700	-9.13996500	1.62000200
C	-9.60045300	-9.85490200	-0.61218800
C	-10.20183400	-8.51804900	2.91761100
C	-12.16573500	-9.64991800	2.66022300
C	-11.40590600	-8.84539400	3.54287000
H	-11.71211300	-8.54147600	4.53044600
C	-10.85390200	-11.13340000	-1.98186100
C	-9.65465300	-10.82336300	-2.66696600
H	-9.40349800	-11.14805800	-3.66340700
C	-8.86240600	-10.03102200	-1.83502000
F	-13.15672800	-10.13545700	-0.21197200
F	-12.15519600	-12.00492300	0.67794700
C	-7.50665500	-9.48541600	-2.18857800
H	-7.49175800	-8.39152800	-2.14154500
H	-6.73787800	-9.84786100	-1.49800300
H	-7.23613600	-9.79411600	-3.20276400
C	-9.11220800	-7.67608200	3.52165400
H	-8.16402900	-8.22152000	3.56791800
H	-8.93319400	-6.77048200	2.93232700
H	-9.39412200	-7.38003600	4.53652700
C	-13.51516800	-10.26883200	2.83507800
H	-14.17340100	-9.92473100	2.02944800
H	-13.42698100	-11.35554900	2.72188200
H	-13.94307000	-10.02209900	3.80808700
C	-12.03241500	-11.94538600	-2.41356800
H	-12.16044100	-12.78726300	-1.72313600
H	-12.93647800	-11.33240100	-2.32830900
H	-11.91246700	-12.30947900	-3.43525700
B	-11.95100500	-10.66127400	0.30085600

N	-10.81856400	-10.55390500	-0.75637800
N	-11.46267800	-9.82352900	1.51391800

Compound B-3. Ground state geometry.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



C	-13.21506500	-0.40521300	-0.61680400
C	-12.81492000	-2.64597800	-0.24559400
C	-11.75734300	1.30255600	-0.79157300
C	-13.08363200	1.80811200	-1.02592800
C	-14.00072000	0.76124000	-0.92238800
C	-10.87846300	-3.70195900	0.21052900
C	-11.94551000	-4.66602700	0.25052400
C	-13.15425400	-4.02759200	-0.02997300
B	-10.71162300	-1.08382900	-0.24483800
F	-10.05402900	-0.79959300	0.96709600
F	-9.82053900	-1.07132300	-1.33462200
C	-14.52245100	-4.54794300	-0.10743900
C	-15.40516700	-4.07838400	-1.10055600
C	-14.99277400	-5.49343200	0.82299000
C	-16.70955900	-4.56221000	-1.17110000
H	-15.06370800	-3.33199300	-1.80333600
C	-16.30001900	-5.96964100	0.74998500
H	-14.33965600	-5.83417800	1.61500500
C	-17.16079200	-5.51168600	-0.25087500
H	-17.37397300	-4.19659100	-1.94505700
H	-16.64870500	-6.69290000	1.47779400
H	-18.17569900	-5.88742100	-0.30925600
C	-9.45875800	-3.94558800	0.45855700
C	-8.45251500	-3.39666500	-0.36651300
C	-9.06830200	-4.75873100	1.53682400
C	-7.12005400	-3.68808800	-0.13327100
H	-8.72957900	-2.71661900	-1.15692800
C	-7.72741800	-5.03786000	1.77950100
H	-9.81726200	-5.15306300	2.20991300
C	-6.74273500	-4.51765000	0.93316200
H	-6.34181300	-3.28092300	-0.76462300
H	-7.46298900	-5.65517600	2.62664800
C	-10.50677300	2.05805300	-0.82371700
C	-9.50921300	1.89360100	0.16232600
C	-10.28198700	2.99047600	-1.85150700
C	-8.35946800	2.66286400	0.13003900
H	-9.63455900	1.13602100	0.92022400
C	-9.11794100	3.75075000	-1.89235700
H	-11.01082600	3.10222400	-2.64266100
C	-8.15360300	3.60387500	-0.88975000
H	-7.59375000	2.55209700	0.88602700
H	-8.97183600	4.44602700	-2.70748800
C	-15.45816700	0.73828400	-1.07841900
C	-16.25041600	-0.05959600	-0.22883700

C	-16.09066600	1.47787100	-2.09535000
C	-17.63464900	-0.09358300	-0.38112500
H	-15.77307400	-0.65339800	0.53726000
C	-17.47509300	1.43531200	-2.24565600
H	-15.49337900	2.06469900	-2.78006100
C	-18.25259100	0.65558400	-1.38552300
H	-18.23069500	-0.70639400	0.28469800
H	-17.94627400	2.00546100	-3.03767800
H	-19.32990700	0.62818300	-1.50079300
N	-13.64554500	-1.64686100	-0.48349100
N	-11.42047700	-2.48481800	-0.11029400
N	-11.85658100	-0.03796700	-0.52560900
I	-11.66668500	-6.77754000	0.35351900
I	-13.58624800	3.87746600	-1.13827000
C	-4.91678700	-5.54767200	2.20680500
H	-5.20354500	-5.07130800	3.15313600
H	-5.34186900	-6.55842400	2.18060000
O	-5.38759800	-4.75091900	1.07074800
C	-2.66939400	-4.91310200	1.13332200
H	-2.97141000	-4.23728200	0.35676300
N	-2.62077200	-6.36491100	2.85831400
N	-1.34210700	-6.19175600	2.47545000
N	-1.38236300	-5.27917800	1.38930300
C	-3.43366300	-5.59723700	2.05481100
C	-0.13360400	-4.87743700	0.72774100
C	1.05484000	-5.62343300	1.34631200
H	0.02230700	-3.80181400	0.84431100
H	-0.18460700	-5.11852300	-0.33701000
H	1.16241000	-5.38429000	2.40713900
H	0.93797100	-6.70433000	1.23300000
O	2.18096900	-5.11708900	0.56150400
C	-6.70119500	5.33132900	-1.85084600
H	-6.62147100	4.86408200	-2.84032500
H	-7.50102600	6.08174100	-1.88088200
O	-6.97628200	4.32396300	-0.82318700
C	-4.64866800	5.63898400	-0.33588200
H	-4.82491000	4.91262000	0.43365100
N	-4.79433100	6.95492900	-2.16143400
N	-3.65325200	7.30159700	-1.53710800
N	-3.57031000	6.46962700	-0.39048600
C	-5.40609400	5.95086400	-1.44493300
C	-2.42625300	6.59465300	0.52212500
C	-1.45540500	7.66737700	0.01403800
H	-1.89623500	5.64089000	0.58652700
H	-2.77419800	6.87830100	1.51869900
H	-1.06694800	7.41205900	-0.97510100
H	-1.94176900	8.64497800	-0.03309500
O	-0.40554200	7.63436800	1.03293200
C	9.30456100	-9.87427500	0.02778300
C	7.18228600	-9.09112600	-0.30860200
C	8.06051400	-10.11383000	-0.63043600

C	7.89240000	-8.19622100	0.57394800
C	7.47558300	-7.06404100	1.27925300
C	8.34428000	-6.42162400	2.16957500
C	8.14815600	-5.33573300	3.08969600
C	9.35319300	-5.17556800	3.77563500
N	9.19411100	-8.70849200	0.73529800
N	9.67409200	-6.87320300	2.32774400
B	10.36113200	-7.92868500	1.41414000
F	11.14239900	-8.82116200	2.19826900
F	11.17989200	-7.30336000	0.46254100
C	6.07731400	-6.56340100	1.11794600
C	5.77644800	-5.59615000	0.14642900
C	5.04881600	-7.05202900	1.92767000
C	4.47482800	-5.13630300	-0.01033100
H	6.56848800	-5.21079300	-0.48482900
C	3.73817600	-6.59285000	1.77522800
H	5.27317800	-7.79834400	2.68107500
C	3.44502500	-5.63361000	0.80169500
H	4.22393800	-4.39358700	-0.75595900
H	2.96096900	-6.98757600	2.41562800
H	9.55193100	-4.45255200	4.55001600
H	7.83427700	-10.96728900	-1.24777000
C	10.49942000	-10.67244800	0.05739100
H	11.22494200	-10.36413400	0.79817600
C	10.70873300	-11.74636500	-0.73839100
H	9.94753400	-12.01387900	-1.46880900
C	5.76224100	-8.98450600	-0.79213100
H	5.05258400	-9.01919500	0.04056700
H	5.59203300	-8.04037100	-1.31972400
H	5.54184700	-9.81096500	-1.47467700
C	6.90629300	-4.51770000	3.31337900
H	6.56497400	-4.04764600	2.38550400
H	6.08086300	-5.13578800	3.68253300
H	7.10842900	-3.73317600	4.04912300
C	10.28023200	-6.12644600	3.28867500
C	11.71117900	-6.32695900	3.67748800
H	11.95447100	-7.38827700	3.60780100
H	12.36888400	-5.78921900	2.98095400
H	11.89296500	-5.95230900	4.68796900
C	11.88107800	-12.61338400	-0.73586400
C	12.97307200	-12.41368400	0.15079600
C	11.93291800	-13.68945500	-1.64165100
C	14.08192200	-13.24559800	0.15022300
H	12.93874100	-11.58741900	0.84954500
C	13.03709600	-14.53546000	-1.65959900
H	11.10561100	-13.85357400	-2.32408800
C	14.12010300	-14.30901600	-0.75917700
H	14.89386500	-13.07015800	0.84471700
C	13.38885300	-15.70434400	-2.45000400
C	14.66857200	-16.13581700	-1.99401600
C	12.74804200	-16.40074500	-3.47710100

C	15.29592800	-17.25183400	-2.54960600
C	13.37736900	-17.51215500	-4.03624600
H	11.77543200	-16.08145000	-3.83352300
C	14.63734300	-17.93075200	-3.57457100
H	16.26274100	-17.58915400	-2.19745100
H	15.10661900	-18.79985100	-4.02071900
N	15.09821100	-15.27444100	-0.97845300
C	16.36102000	-15.39723000	-0.24869200
H	16.28094200	-16.10892400	0.58133000
H	17.14532800	-15.73142400	-0.93368500
H	16.64486900	-14.41865300	0.14496300
H	12.89199200	-18.06233600	-4.83331500
C	7.36938700	11.15929200	-0.08541800
C	5.61858300	9.69317500	-0.20726000
C	6.96173900	9.85741500	-0.50648700
C	5.17983700	10.91678300	0.42028000
C	3.96329900	11.27395400	1.00792100
C	3.82218800	12.50807100	1.65440900
C	2.74985900	13.07274200	2.42635800
C	3.20296500	14.31007800	2.88727500
N	6.28321300	11.79140300	0.45535700
N	4.88718800	13.43656000	1.67044100
B	6.18752100	13.30253500	0.82709100
F	7.31713300	13.67875400	1.60416700
F	6.12007600	14.10864700	-0.31885700
C	2.81420400	10.31968900	0.98604400
C	1.87140700	10.37212200	-0.04351900
C	2.65785400	9.36474100	2.00309200
C	0.78629600	9.49161100	-0.06603500
H	1.98400800	11.10678000	-0.83235600
C	1.58090400	8.48769600	1.98629800
H	3.38401500	9.31809300	2.80630000
C	0.63490600	8.54667000	0.95220400
H	0.07150700	9.55263100	-0.87558100
H	1.44253600	7.74756100	2.76327700
H	2.65099900	14.99739000	3.50764700
H	7.60259600	9.11632200	-0.95461400
C	8.66648400	11.77701900	-0.12650800
H	8.74229100	12.69600400	0.43906300
C	9.72984200	11.25608900	-0.78080200
H	9.60189500	10.32672000	-1.33250900
C	4.81396100	8.45329100	-0.48333000
H	4.45283800	7.99562000	0.44331500
H	3.93403300	8.67959400	-1.09401500
H	5.43132300	7.72331100	-1.01576600
C	1.39904500	12.48047200	2.72016700
H	0.85481200	12.25015500	1.79864900
H	1.48491900	11.54563700	3.28424800
H	0.80664400	13.18779400	3.30865700
C	4.51651600	14.51813800	2.40617400
C	5.40852600	15.70507900	2.58914300

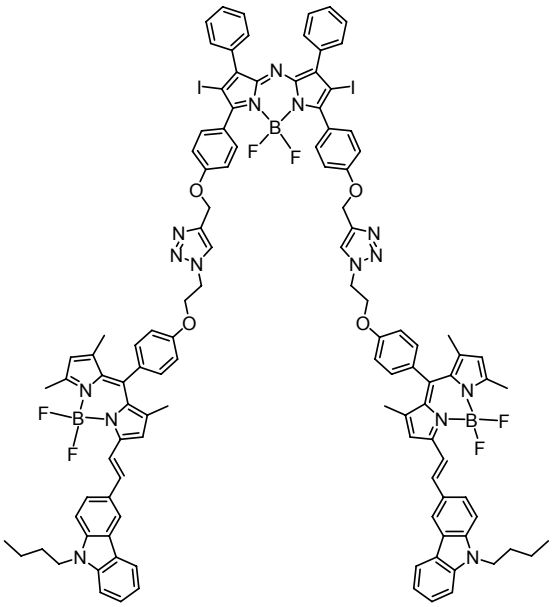
H	6.44352700	15.36624200	2.65635100
H	5.33446600	16.36768500	1.71600000
H	5.12501300	16.26913400	3.48117400
C	11.07257700	11.82099000	-0.84346600
C	11.41506100	13.04214000	-0.20299400
C	12.06594600	11.13398700	-1.56607700
C	12.69390900	13.57286200	-0.26920500
H	10.65470500	13.57611800	0.35274400
C	13.35563800	11.64958000	-1.64547600
H	11.81757100	10.20048400	-2.05999200
C	13.66963000	12.88010600	-0.99527500
H	12.92301600	14.50267800	0.23591700
C	14.57586300	11.19715200	-2.29460700
C	15.57515500	12.17288400	-2.01053500
C	14.89816800	10.08190700	-3.07129800
C	16.87898200	12.03482200	-2.48855600
C	16.19954900	9.94606200	-3.55299100
H	14.14736600	9.33293300	-3.29569300
C	17.17696100	10.91363300	-3.26281200
H	17.64234000	12.76974200	-2.26532900
H	18.18310000	10.78613900	-3.64491200
N	15.00658300	13.18636500	-1.23154200
C	15.72367800	14.35808700	-0.72672300
H	16.30026700	14.12059600	0.17492600
H	16.40270500	14.73173000	-1.49876300
H	15.00400700	15.14553700	-0.49353700
H	16.46387900	9.08572100	-4.15596100

Compound B-3. Triplet state geometry.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-12.89720900	-0.12304400	0.89754900
C	-12.73036000	2.13241000	0.45149400
C	-11.30061700	-1.72589400	0.96942500
C	-12.54791400	-2.31933300	1.33893900
C	-13.55646300	-1.35323700	1.31893700
C	-10.92266800	3.39496300	-0.05817100
C	-12.08351200	4.22619300	-0.13095600
C	-13.22295400	3.47489000	0.16669900
B	-10.52355600	0.77873300	0.39087900
F	-9.88174400	0.60212100	-0.85423200



F	-9.58450600	0.80191000	1.44476700
C	-14.63784200	3.83858800	0.21170300
C	-15.49511800	3.26033600	1.17354600
C	-15.18743300	4.74447200	-0.71876900
C	-16.84360400	3.60472900	1.21648600
H	-15.09737800	2.53077800	1.86317000
C	-16.53823000	5.07874800	-0.67341300
H	-14.55850100	5.16249100	-1.49272200
C	-17.37085600	4.51773300	0.29901300
H	-17.48430400	3.15695500	1.96714800
H	-16.94374100	5.77074800	-1.40229400
H	-18.42119400	4.78267900	0.33493100
C	-9.54194000	3.74819700	-0.32060500
C	-8.47759800	3.24144900	0.46680900
C	-9.22342800	4.63375400	-1.37287000
C	-7.17776600	3.64423200	0.23191000
H	-8.68864900	2.50987100	1.23116900
C	-7.91321100	5.02386200	-1.61698000
H	-10.00731100	4.98878000	-2.02671200
C	-6.87895800	4.54578800	-0.80305600
H	-6.36132400	3.27276300	0.83652100
H	-7.70618800	5.69013400	-2.44303800
C	-9.99455500	-2.34901400	0.89458800
C	-9.06973400	-2.03210500	-0.13229100
C	-9.61525000	-3.31672900	1.85021800
C	-7.85973100	-2.69255000	-0.21520200
H	-9.30732300	-1.24605100	-0.83197100
C	-8.39102100	-3.96721300	1.77344700
H	-10.27208700	-3.53166800	2.68095800
C	-7.50896800	-3.67493200	0.72576200
H	-7.15517500	-2.46777600	-1.00463400
H	-8.12847500	-4.68812000	2.53515900
C	-14.98211800	-1.43723500	1.63009700
C	-15.92076200	-0.67385400	0.90167300
C	-15.45131900	-2.25327100	2.68019700
C	-17.27905700	-0.75397000	1.19755400
H	-15.57137800	-0.01010500	0.12489200
C	-16.81046700	-2.32320700	2.97385300
H	-14.74483200	-2.80951700	3.28092000
C	-17.73159800	-1.58126700	2.22903600
H	-17.98520700	-0.16700300	0.62194500
H	-17.15076000	-2.95007000	3.78981600
H	-18.78956700	-1.64056000	2.45680000
N	-13.48452400	1.07147800	0.76070600
N	-11.35623500	2.10664200	0.32742400
N	-11.55619700	-0.36653200	0.67909200
I	-12.03163800	6.35656000	-0.26846700
I	-12.88400400	-4.42305500	1.48819200
C	-5.14751000	5.76216000	-2.04869800
H	-5.41430300	5.30916400	-3.01192100
H	-5.64016100	6.73878100	-1.97075000

O	-5.54957500	4.88422600	-0.94475400
C	-2.85196700	5.22716200	-1.02510900
H	-3.10064300	4.50141000	-0.27514000
N	-2.91540900	6.75045700	-2.68687300
N	-1.62324800	6.63944300	-2.32630900
N	-1.59317100	5.68064800	-1.28060300
C	-3.66902400	5.90175400	-1.90761800
C	-0.31467900	5.32855200	-0.64813600
C	0.82126800	6.16693400	-1.24658800
H	-0.09682100	4.26977700	-0.81047800
H	-0.36740600	5.52256100	0.42608400
H	0.92567200	5.98225400	-2.31857300
H	0.64801300	7.23356900	-1.08179800
O	1.98368800	5.68651800	-0.49957400
C	-5.85200200	-5.32260400	1.47759900
H	-5.71533000	-4.90376900	2.48219000
H	-6.59593600	-6.12708900	1.53018400
O	-6.28426400	-4.28083500	0.54015300
C	-3.92821200	-5.40967300	-0.22597500
H	-4.21398700	-4.65563200	-0.93356300
N	-3.83167300	-6.83033200	1.52297700
N	-2.73367000	-7.06940100	0.78164900
N	-2.80199200	-6.17148100	-0.31436900
C	-4.56279000	-5.82918200	0.92392800
C	-1.74808800	-6.18765000	-1.33809200
C	-0.68530600	-7.23741100	-0.99345000
H	-1.27179700	-5.20579700	-1.39832500
H	-2.17928500	-6.43489700	-2.31164200
H	-0.18861400	-7.01214100	-0.04685000
H	-1.13326600	-8.23102900	-0.93370400
O	0.24713500	-7.11402600	-2.12512300
C	8.92958800	10.72216700	0.11264600
C	6.84310900	9.85276700	0.45944500
C	7.69304900	10.89130700	0.80564800
C	7.56368200	9.01949000	-0.47373000
C	7.17114900	7.90243600	-1.21590400
C	8.04189600	7.32764100	-2.14963000
C	7.86472000	6.27074500	-3.10694700
C	9.05929800	6.18158500	-3.82355200
N	8.84322300	9.58342400	-0.64059400
N	9.35054400	7.83371400	-2.31813300
B	10.02078900	8.87795600	-1.37989300
F	10.74588400	9.83095000	-2.14644200
F	10.88870300	8.24731900	-0.47652500
C	5.79710600	7.34175500	-1.04583700
C	5.55762800	6.32151200	-0.11221400
C	4.73317800	7.81785000	-1.81626500
C	4.28138600	5.79538100	0.04418500
H	6.37794400	5.94536500	0.48764300
C	3.44770500	7.29215600	-1.66382500
H	4.91070300	8.60427000	-2.54079600

C	3.21643100	6.27754700	-0.73073800
H	4.07788300	5.00953700	0.75941900
H	2.64224300	7.67740000	-2.27445600
H	9.26684000	5.49606100	-4.62911300
H	7.45181700	11.71090000	1.46206700
C	10.09590300	11.56163800	0.09036200
H	10.81087900	11.31143900	-0.68191000
C	10.29152300	12.60517000	0.92892200
H	9.54226600	12.81379900	1.69023200
C	5.43815300	9.67852600	0.96706700
H	4.71090700	9.70679000	0.14957700
H	5.31482000	8.71569600	1.47392100
H	5.20021800	10.47814700	1.67522100
C	6.64942100	5.41542900	-3.33685000
H	6.34331200	4.90146600	-2.42005100
H	5.79497400	6.01463600	-3.66941700
H	6.86620400	4.66499300	-4.10331900
C	9.96177200	7.14705200	-3.31961300
C	11.37567400	7.41480300	-3.72949600
H	11.57789400	8.48337500	-3.63984800
H	12.06734200	6.88989700	-3.05649400
H	11.55345500	7.07007100	-4.75116100
C	11.43549000	13.50941300	0.93559800
C	12.50852700	13.38340900	0.01301300
C	11.47862800	14.54612700	1.88674500
C	13.59092700	14.24931000	0.02162700
H	12.48026000	12.58776500	-0.72053800
C	12.55644400	15.42542300	1.91350700
H	10.66534500	14.65382800	2.59677800
C	13.62072200	15.27282100	0.97595100
H	14.38878600	14.13071900	-0.70067200
C	12.89381600	16.57013500	2.74476600
C	14.14621600	17.06194100	2.27400200
C	12.26061200	17.20122500	3.81789300
C	14.75296900	18.17365100	2.86007000
C	12.86986900	18.30808100	4.40736600
H	11.30897900	16.83542200	4.18602000
C	14.10240400	18.78691500	3.93047300
H	15.69808900	18.55772300	2.49710400
H	14.55634500	19.65143500	4.40072400
N	14.57413600	16.25858800	1.21117200
C	15.81076800	16.45065800	0.45214500
H	15.67378700	17.15941800	-0.37298300
H	16.59099600	16.82471900	1.12051000
H	16.13832300	15.48971200	0.04837400
H	12.38987200	18.80807800	5.23996100
C	7.24833100	-11.72632000	-0.13463700
C	5.38377000	-10.41879100	0.07488300
C	6.46038700	-10.94892000	0.76744700
C	5.50585600	-10.86972200	-1.29122200
C	4.76789300	-10.56643800	-2.43820900

C	5.16133500	-11.05886900	-3.68845300
C	4.67047000	-10.81509700	-5.01670500
C	5.50732200	-11.52012200	-5.88313200
N	6.65303500	-11.68324200	-1.36556800
N	6.27766000	-11.91830300	-3.80240700
B	7.01333300	-12.57054800	-2.59620300
F	8.41893900	-12.54960200	-2.80882900
F	6.58783300	-13.89412000	-2.41210400
C	3.57468000	-9.67214300	-2.34020700
C	2.30087500	-10.21409100	-2.13301800
C	3.71505900	-8.28281300	-2.45623600
C	1.18312800	-9.38416000	-2.04511300
H	2.18752200	-11.28828800	-2.04496600
C	2.60093400	-7.45240400	-2.35844600
H	4.69995900	-7.85819000	-2.61210900
C	1.32867600	-7.99945900	-2.16667400
H	0.20256400	-9.81791500	-1.89642200
H	2.69162800	-6.37732500	-2.44021800
H	5.42962900	-11.54831000	-6.95785900
H	6.68533900	-10.77956800	1.80732900
C	8.48481200	-12.42336800	0.09020800
H	8.97284500	-12.77161400	-0.81022200
C	9.03267200	-12.60840500	1.31343300
H	8.50163000	-12.23480200	2.18688500
C	4.32184700	-9.53436000	0.66779000
H	4.31139700	-8.54751800	0.19430200
H	3.32525000	-9.96706500	0.53219600
H	4.50353600	-9.40646000	1.73922500
C	3.50181100	-9.96789300	-5.43895300
H	2.57424800	-10.29954400	-4.96112100
H	3.64660600	-8.91764600	-5.16451600
H	3.37587400	-10.02850200	-6.52429300
C	6.48506400	-12.19661500	-5.11701000
C	7.57451400	-13.11054000	-5.58257000
H	8.43767400	-13.00086900	-4.92445000
H	7.24065500	-14.15544200	-5.52185200
H	7.84567100	-12.89158700	-6.61849500
C	10.29284400	-13.27890700	1.60943800
C	11.10929000	-13.84737900	0.59516900
C	10.71840400	-13.36444900	2.94834800
C	12.30852200	-14.47918400	0.88565400
H	10.78551100	-13.78617000	-0.43610600
C	11.91834400	-13.99462700	3.26156500
H	10.10431800	-12.93414700	3.73247500
C	12.71659300	-14.55869300	2.22225100
H	12.91049800	-14.89632300	0.08816700
C	12.62180000	-14.24326400	4.50991000
C	13.81474300	-14.94667600	4.17306900
C	12.34986400	-13.94021700	5.84593600
C	14.72757200	-15.33504700	5.15468500
C	13.25902600	-14.33284700	6.82734800

H	11.44530700	-13.40703000	6.11506200
C	14.43435200	-15.02218600	6.48187200
H	15.64024700	-15.85955500	4.90075500
H	15.12903800	-15.31477000	7.26058200
N	13.84970300	-15.13603300	2.78727800
C	14.92667300	-15.80783900	2.05842800
H	15.77012500	-15.13297600	1.87154300
H	15.27629200	-16.66798100	2.63654800
H	14.54096700	-16.17128300	1.10356500
H	13.06159700	-14.10399600	7.86765600