Electronic Supplementary Information for:

Resonance Energy Transfer-enhanced Rhodamine-styryl Bodipy Dyad Triplet Photosensitizers

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1. General.

All the chemicals used in synthesis are analytical pure and were used as received. Solvents were dried and distilled before used for synthesis. All samples in flash photolysis experiments were deaerated with argon for ca. 15 min before measurement and the gas flow is kept during the measurement.

ESR spectra were recorded at room temperature using a Bruker ESP-300E spectrometer at 9.8 GHz, X-band, with 100 Hz field modulation. Samples were quantitatively injected into specially made quartz capillaries for ESR analysis in the dark and illuminated directly in the cavity of the ESR spectrometer. Triplet photosensitizers and superoxide radical anion ($O_2^{-\bullet}$) or singlet oxygen ($^1O_2$) scavengers (5,5-dimethyl-1-pyrroline-*N*-oxide (DMPO) or 2,2,6,6-tetramethylpiperidine (TEMP) in air-saturated CH_2Cl_2 was stirred in the dark, then the solution was injected into the quartz capillary. A diode pumped solid state (DPSS) laser (589 nm) irradiate the solution in quartz capillary 100 seconds.

Cyclic voltammetry was performed using a CHI610D Electrochemical workstation (Shanghai, China). Cyclic voltammograms were recorded at scan rates of 50 mV/s. A three electrodes cell was used. Electrochemical measurements were performed at RT using 0.1 M tetrabutylammonium hexafluorophosphate (TBAP) as supporting electrolyte, after purging with N_2. The working electrode was a glassy carbon electrode, and the counter electrode was platinum electrode. A nonaqueous $Ag/AgNO_3$ (0.1 M in DCM) reference electrode was contained in a separate compartment connected to the solution via frit. Dichloromethane was used as the solvent. Ferrocene was added the internal reference.

2. Synthesis and molecular structure characterization data

Compound 1

A mixture of *p*-hydroxybenzaldehyde (2.44 g, 20 mmol), 1,2-dibromoethane (7.43 g, 40 mmol) and K_2CO_3 (5.53 g, 40 mmol) were dissolved in DMF (40 mL), then the reaction mixture was stirred and refluxed for 6 h. The residue was poured into ice-water, yellow solid was obtained. Then the solid was dissolved in CH_2Cl_2, dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. Yield: 1.26 g (30.0 %). ^{1}H NMR (400 MHz, $CDCl_3$) : δ 9.90 (s, 1H, J = 8.0 Hz), 7.86 (d, 2H, J = 8.0

Hz), 7.03 (d, 2H, *J* = 8.0 Hz), 4.38 (t, 2H, *J* = 4.0 Hz, *J* = 8.0 Hz), 3.67 (t, 2H, *J* = 4.0 Hz, *J* = 8.0 Hz).

Compound 2

A mixture of compound **1** (1.26 g, 5.5 mmol), NaN_3 (0.45 g, 6.0 mmol) were dissolved in DMF (5 mL), then the reaction mixture was stirred and refluxed for 2 h. The solution was cooled to rt and diluted with CH_2Cl_2. The mixture was washed with water and the organic layer was dried over anhydrous Na_2SO_4, filtrated and the solvent was evaporated under reduced pressure to give the product as colorless oil. Yield: 0.82 g, 80.4%. ^{1}H NMR (400 MHz, $CDCl_3$) : δ 9.89 (s, 1H), 7.86 (d, 2H, *J* = 8.0 Hz), 7.04 (d, 2H, *J* = 8.0 Hz), 4.23 (t, 2H, *J* = 4.0 Hz), 3.65 (t, 2H, *J* = 4.0 Hz). MALDI-HRMS: calcd ($[C_9H_9N_3O_2+H]^+$) *m/z* = 192.0766, found *m/z* =192.0763.

Compound 3

A mixture of *p*-hydroxybenzaldehyde (2.44 g, 20 mmol), 3-bromo-1-propyne (3.54 g, 30 mmol) and potassium carbonate (5.53 g, 40 mmol) were dissolved in DMF(40 mL), then the reaction mixture was refluxed for 6 h. Then the solid was dissolved in CH_2Cl_2, dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure and then purified by column chromatography (silica gel, CH_2Cl_2). White solid was obtained, yield: 2.04 g, 63.8 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.91 (s, 1H), 7.88–7.85 (m, 2H), 7.12–7.08 (m, 2H), 4.79 (d, 2H), 2.58 (t, 1H, *J* = 4.0 Hz).

General synthetic procedure of compound 2a-2c [1, 2]

Aniline derivatives (5 mmol) were dissolved in THF (20 mL). Maleic anhydride (5.5 mmol) was dissolved in another portion of THF (20 mL). Maleic anhydride solution was added dropwise into the solution of aniline derivatives in THF at room temperature. The reaction mixture was stirred for 2 h and a lot of precipitation was produced. The precipitation was collected by filtration. The precipitation and sodium acetate (6 mmol) was dissolved in acetic anhydride (20 mL), then the mixture was heated at 120°C for 30 min with microwave irradiation. The solution was poured into water (25 mL), neutralized by saturated NaOH solution until a lot of precipitation appeared. The precipitation was collected and purified by column chromatography (silica gel, CH_2Cl_2).

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1 Y.-Q. Zou, L.-Q. Lu, L. Fu, N.-J. Chang, J. Rong, J.-R. Chen and W.-J. Xiao, *Angew. Chem. Int. Ed.,* 2011, **50**, 7171–7175.

2 L. Huang and J. Zhao, *Chem. Commun.*, 2013, **49**, 3751–3753.

2a. ^{1}H NMR (400 MHz, $CDCl_3$) : δ7.49 (2H, t, J = 8.0 Hz), 7.39–7.44 (m, 3H), 6.85 (s, 2H). **2b.** ^{1}H NMR (400 MHz, $CDCl_3$) : δ7.61 (2H, d, J = 8.0 Hz), 7.27–7.25 (d, 2H J = 8.0 Hz), 6.86 (2H, s). **2c.** ^{1}H NMR (400 MHz, $CDCl_3$) : δ7.30 (2H, t, J = 8.0 Hz), 6.85 (2H, d, J = 8.0 Hz), 6.68 (s, 2H), 3.78 (3H, s).

Compound of **2d**.[2]

p-Nitroaniline (5 mmol) and maleic anhydride (5.5 mmol) was dissolved in THF (40 mL). The mixture was stirred and refluxed for 6 h until a lot of precipitation was produced. The precipitation was collected by filtration. The solid was then dissolved in acetic anhydride (20 mL) and sodium acetate (6 mmol) was added. The mixture was heated by microwave irradiation at 120°C for 30 min. The resulting solution was poured into water (20 mL), neutralized with saturated NaOH solution. The solid was collected by filtration and purified by column chromatography (silica gel, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.35 (2H, d, J = 8.0 Hz), 7.70 (2H, d, J = 8.0 Hz), 6.93 (s, 2H).

General procedure for oxidation/[3+2] cycloaddition [1, 2]

To a dry flask, triplet photosensitizer (2 mol%), tetrahydroisoquinoline derivatives (0.15 mmol), *N*-substituted maleimides (0.1 mmol) and CH_2Cl_2 (3 mL) were added. The reaction mixture was stirred at rt under air atmosphere. The solution was then irradiated by a 35 W xenon lamp through a cut off filter (0.72 M $NaNO_2$ aqueous solution, which is transparent for light > 385 nm). Thin layer chromatography (TLC) was used to monitor the progress of the reaction. After the reaction is completed, 1.2 eqv. NBS was added into the mixture and stirred for further 10 min, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography (silica gel, CH_2Cl_2).

Compound **3a.** ^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.60 (1H, d, J = 4.0 Hz), 7.49 (t, 2H, J = 8.0 Hz), 7.42–7.38 (m, 5H), 7.30 (1H, d, J = 4.0 Hz), 4.79 (t, 2H, J = 8.0 Hz), 4.47–4.41 (m, 2H), 3.19 (t, 2H, J = 4.0 Hz), 1.47 (t, 3H, J = 8.0 Hz). H RMS (ESI): *m/z* calcd for [$C_{23}H_{18}N_2O_4Na$] 409.1164; found: 409.1153.

Compound **3b.** ^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.57 (1H, d, J = 8.0 Hz), 7.62 (2H, d, J = 12.0 Hz), 7.44–7.37 (m, 2H), 7.31 (t, 3H, J = 8.0 Hz), 4.78 (t, 2H, J = 8.0 Hz), 4.46–4.41 (m, 2H), 3.19 (t, 2H, J = 4.0 Hz), 1.47 (t, 3H, J = 8.0 Hz). H RMS (ESI): *m/z* calcd for [$C_{23}H_{17}N_2O_4NaBr$] 487.0269; found: 487.0260.

Compound **3c.** ^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.60 (1H, d, J = 4.0 Hz), 7.43–7.36 (m, 2H), 7.32–7.28 (m, 3H), 7.01 (2H, d, J = 8.0 Hz), 4.78 (t, 2H, J = 8.0 Hz), 4.46–4.40 (m, 2H), 3.84 (s, 3H), 3.19 (t, 2H, J = 4.0 Hz), 1.47 (t, 3H, J = 4.0 Hz). H RMS (ESI): *m/z* calcd for [$C_{24}H_{20}N_2O_5Na$] 439.1270; found: 439.1277.

Compound **3d.** ^{1}H NMR (400 MHz, $CDCl_3$) : δ8.57 (1H, d, J = 4.0 Hz), 8.36 (2H, d, J = 8.0 Hz), 7.73(2H, d, J = 8.0 Hz), 7.46–7.40 (2H, m), 7.33 (1H, d, J = 8.0 Hz), 4.80 (t, 2H, J = 8.0 Hz), 4.49–4.43 (m, 2H), 3.21(t, 2H, J = 4.0 Hz), 1.48 (t, 3H, J = 4.0 Hz). H RMS (ESI): *m/z* calcd for [431.1190]; found: 432.1188.

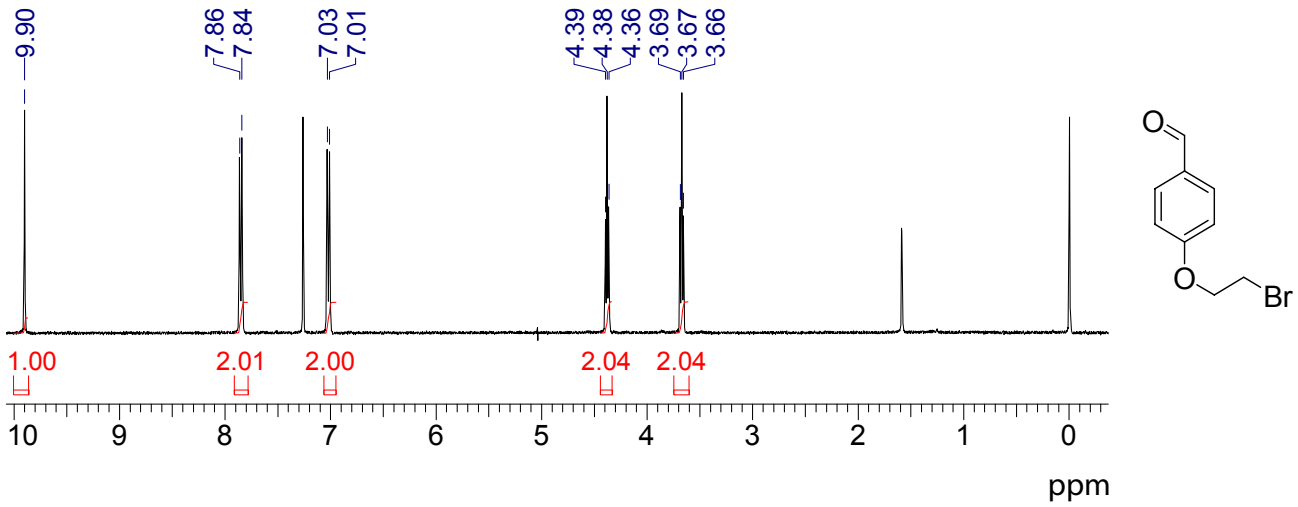


Figure S1. ^{1}H NMR of **1** (400 MHz, $CDCl_3$).

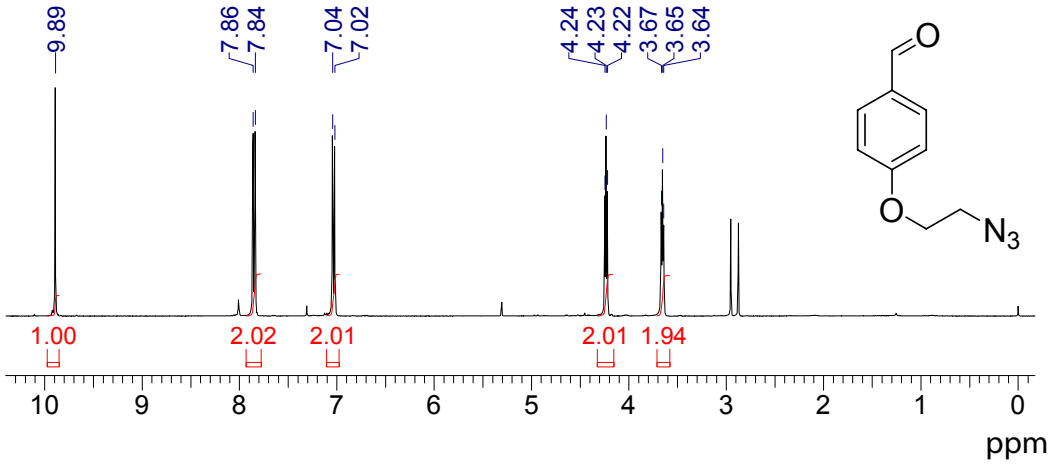


Figure S2. ^{1}H NMR of **2** (400 MHz , $CDCl_3$).

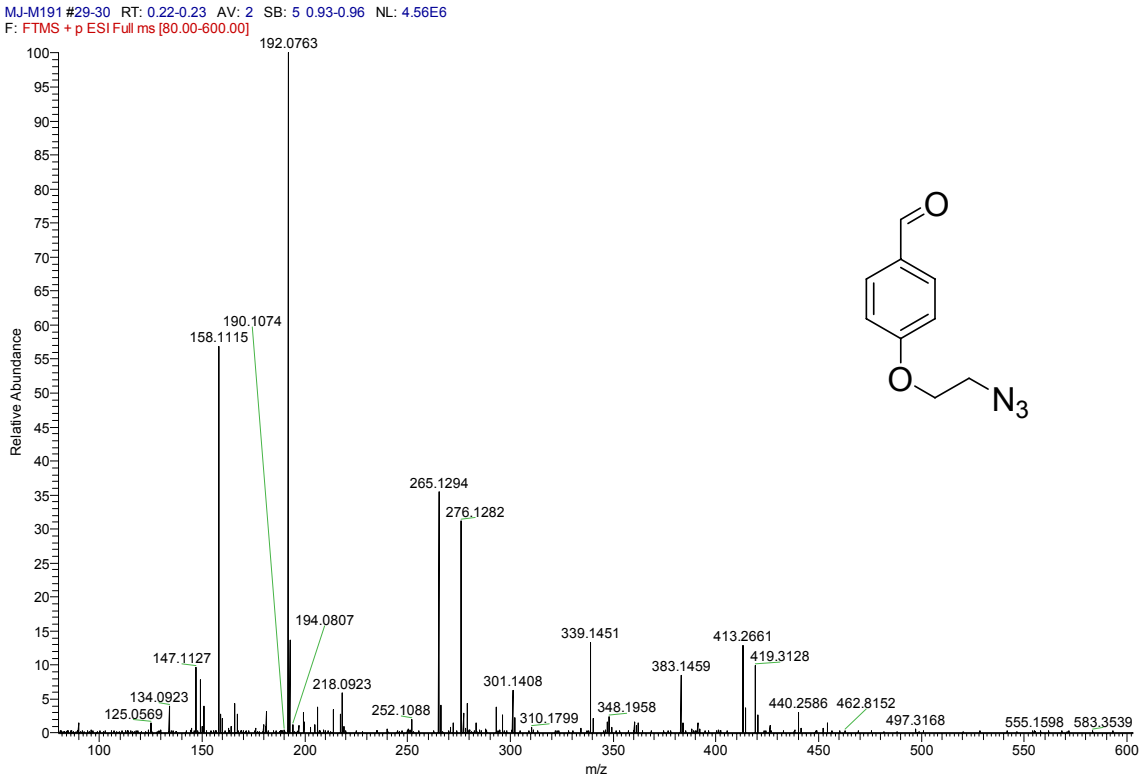


Figure S3. ESI-HRMS of **2**.

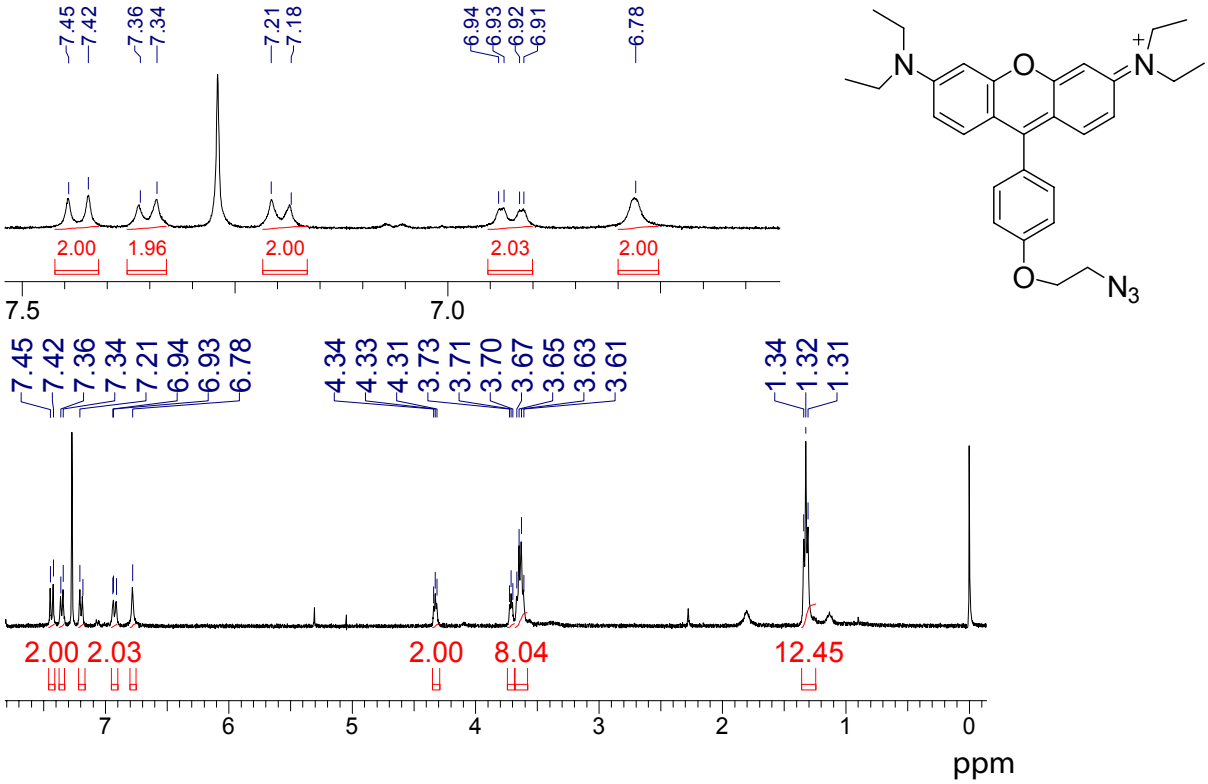


Figure S4. ^{1}H NMR of **R-0** (400 MHz, $CDCl_3$).

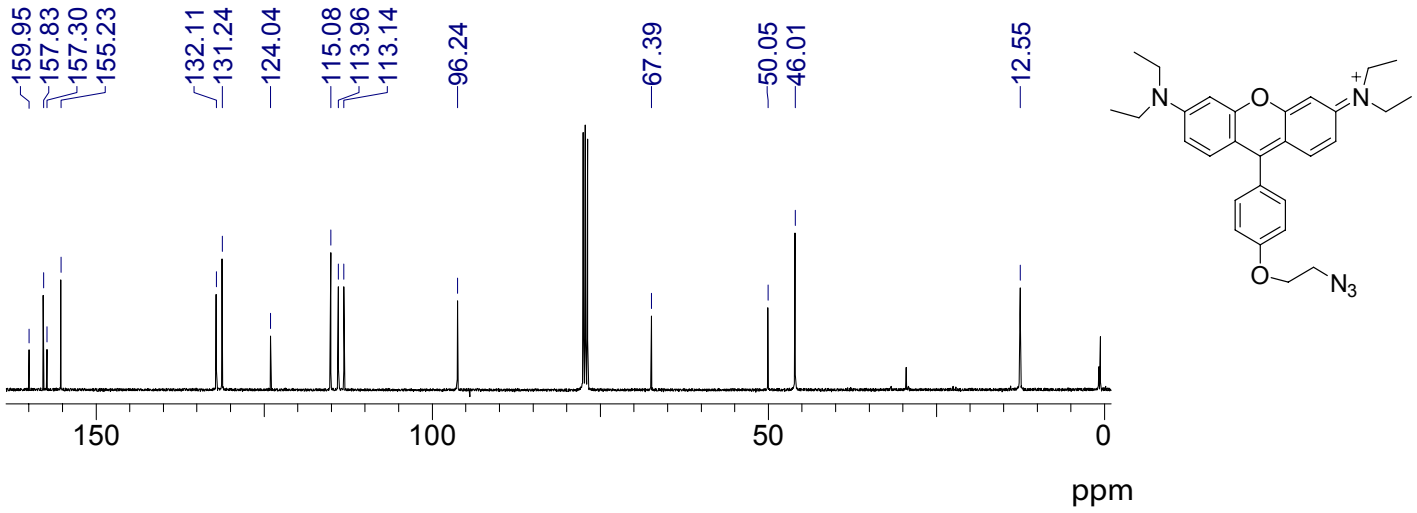


Figure S5. ^{13}C NMR of **R-0** (100 MHz, $CDCl_3$).

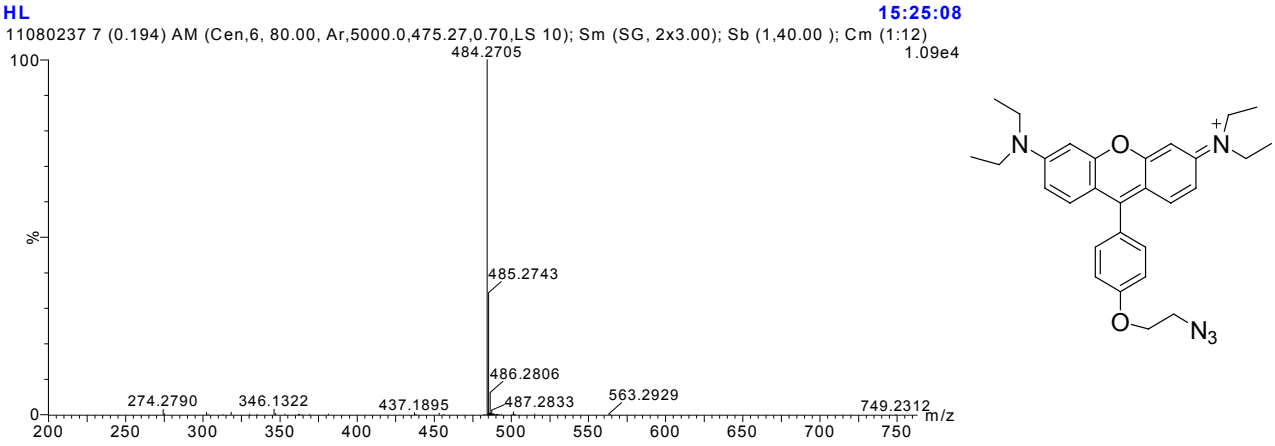


Figure S6. ESI-HRMS of **R-0.**

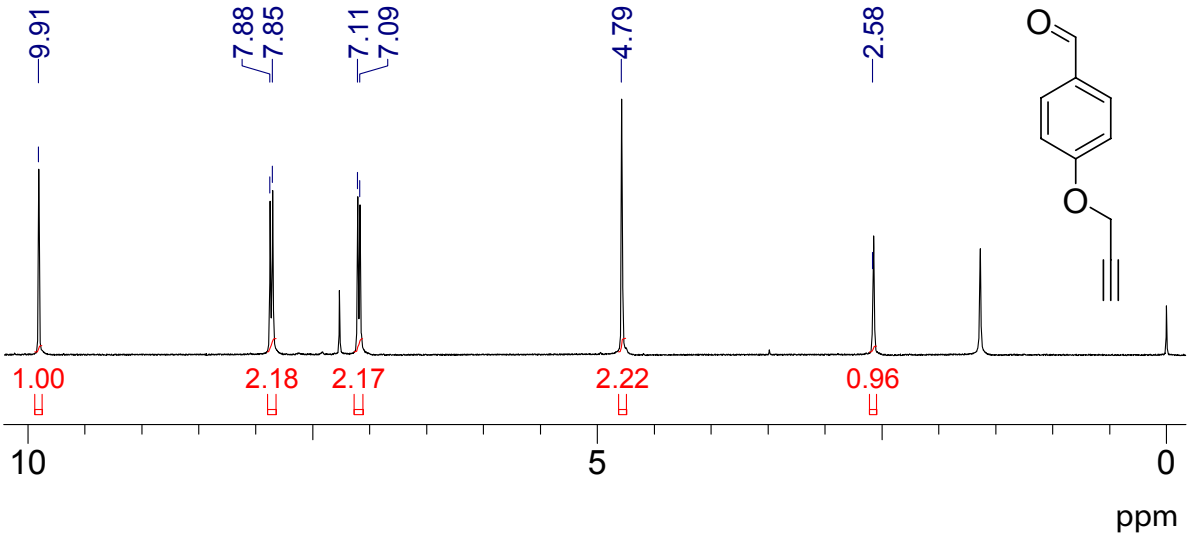


Figure S7. ^{1}H NMR of **3** (400 MHz, $CDCl_3$).

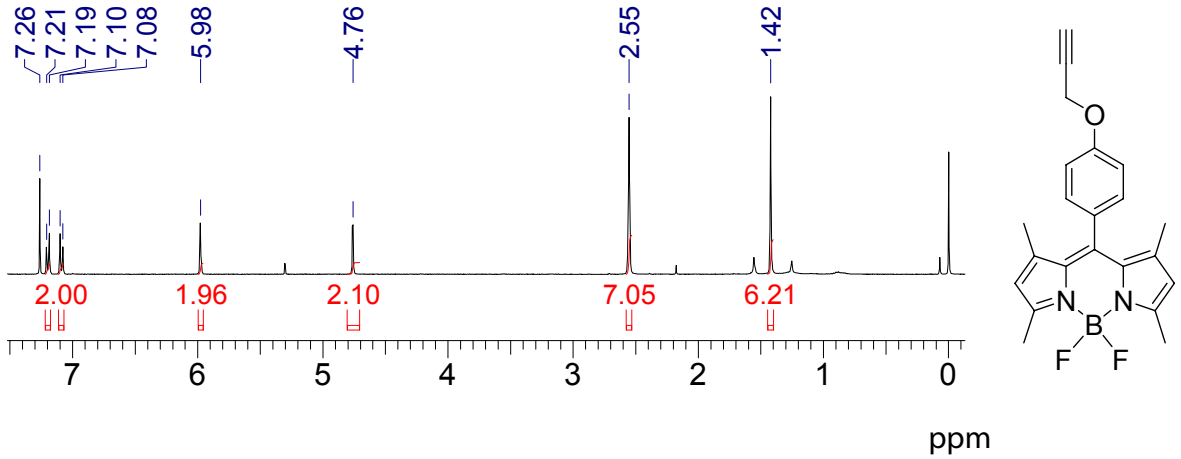


Figure S8. ^{1}H NMR of **4** (400 MHz, $CDCl_3$).

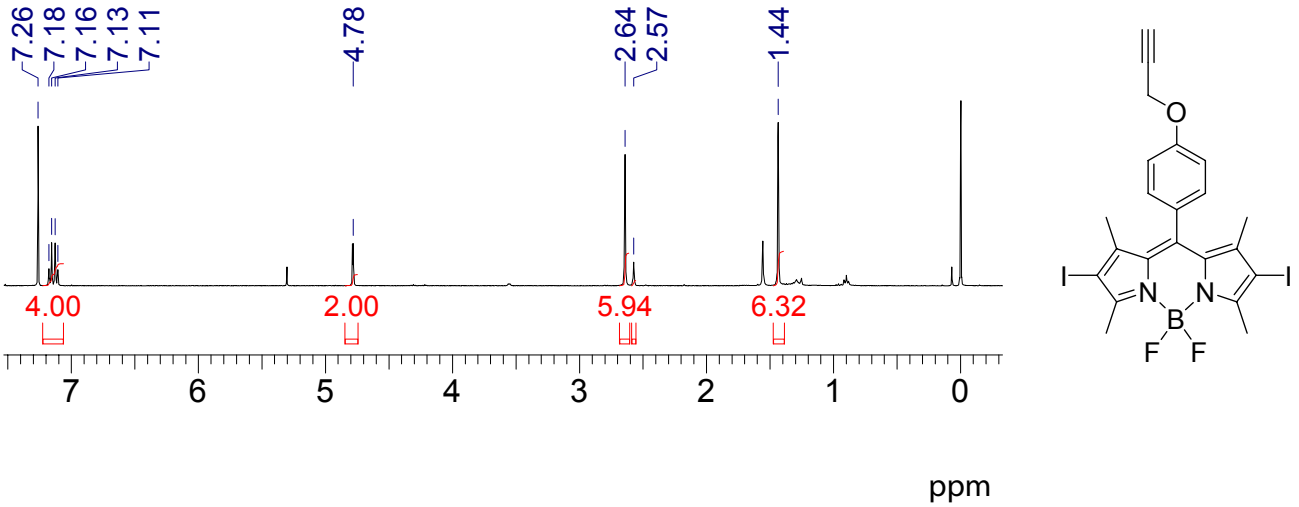


Figure S9. ^{1}H NMR of **5** (400 MHz, $CDCl_3$).

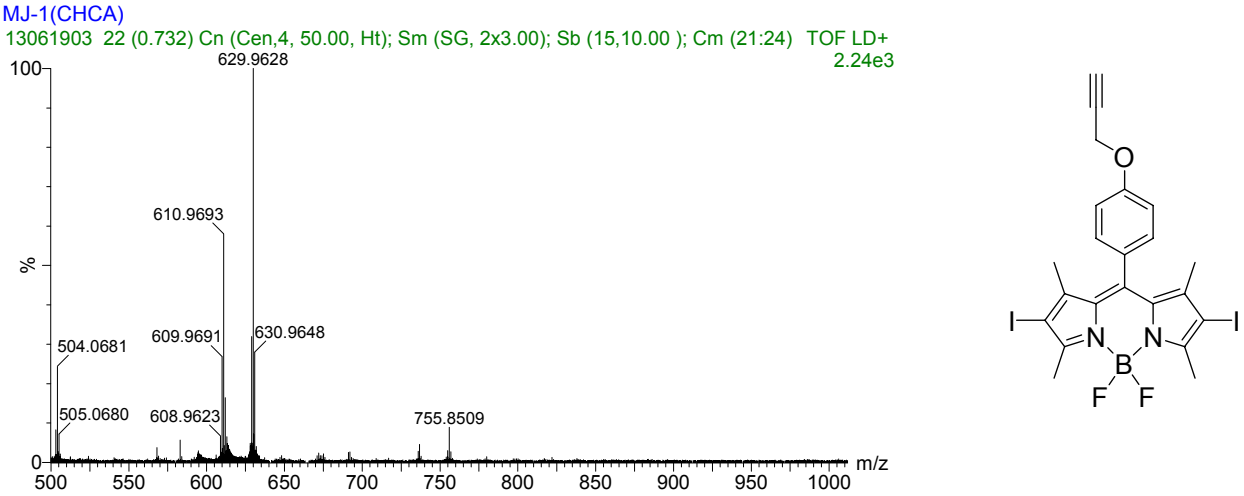


Figure S10. MALDI-HRMS of **5**.

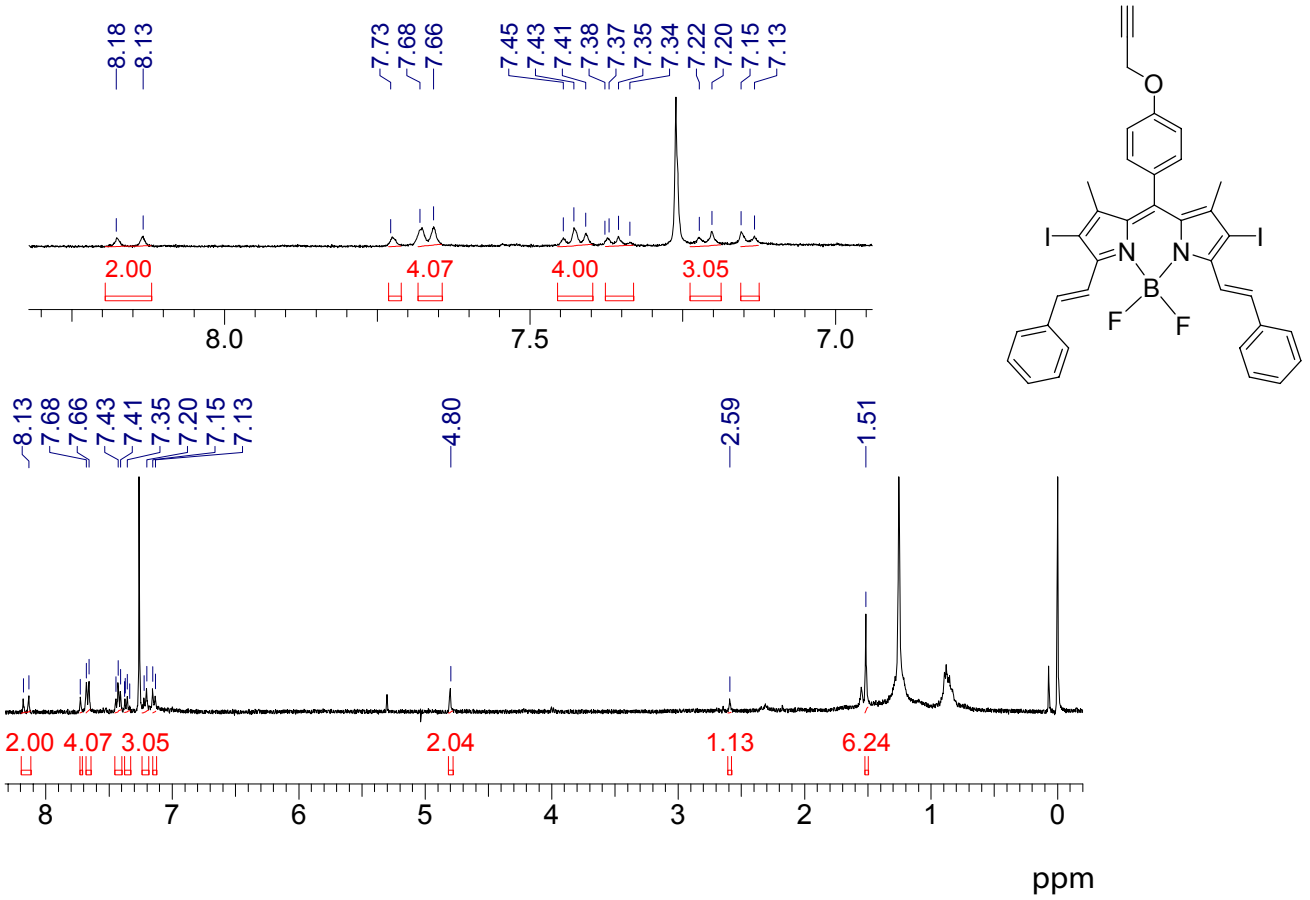


Figure S11. ^{1}H NMR of **6** (400 MHz, $CDCl_3$).

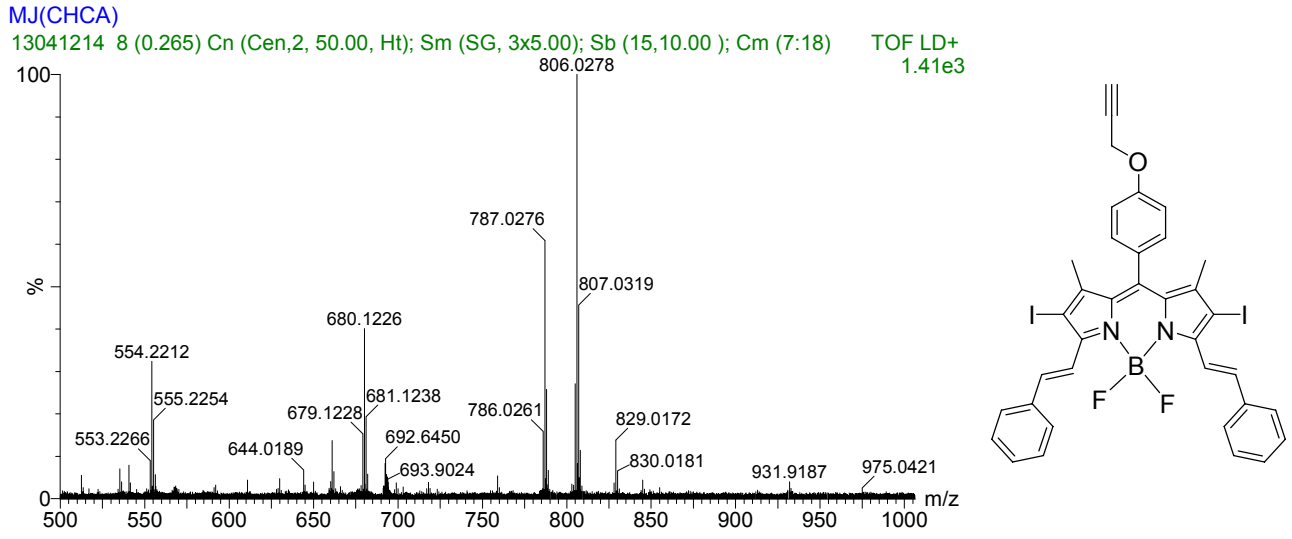


Figure S12. MALDI-HRMS of **6**.

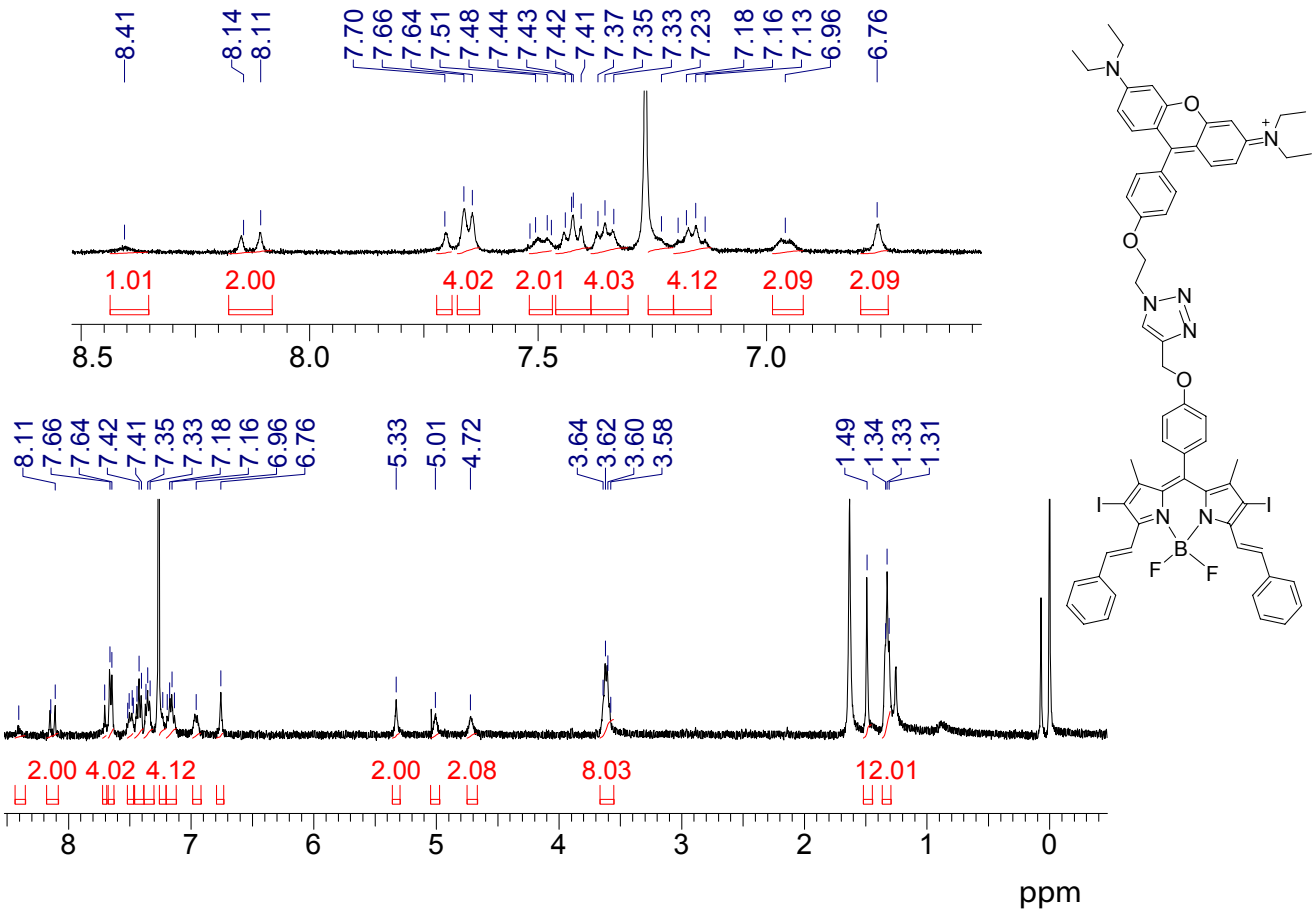


Figure S13. ^{1}H NMR of **R-1** (400 MHz, $CDCl_3$).

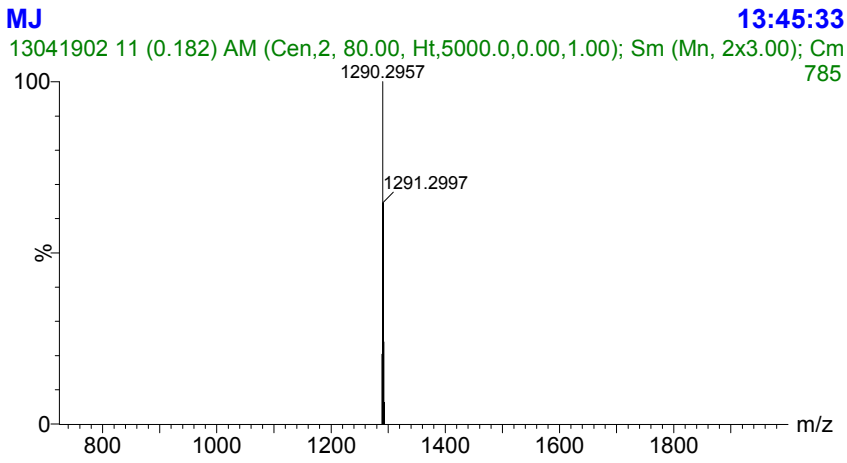


Figure S14. ESI-HRMS of **R-1**.

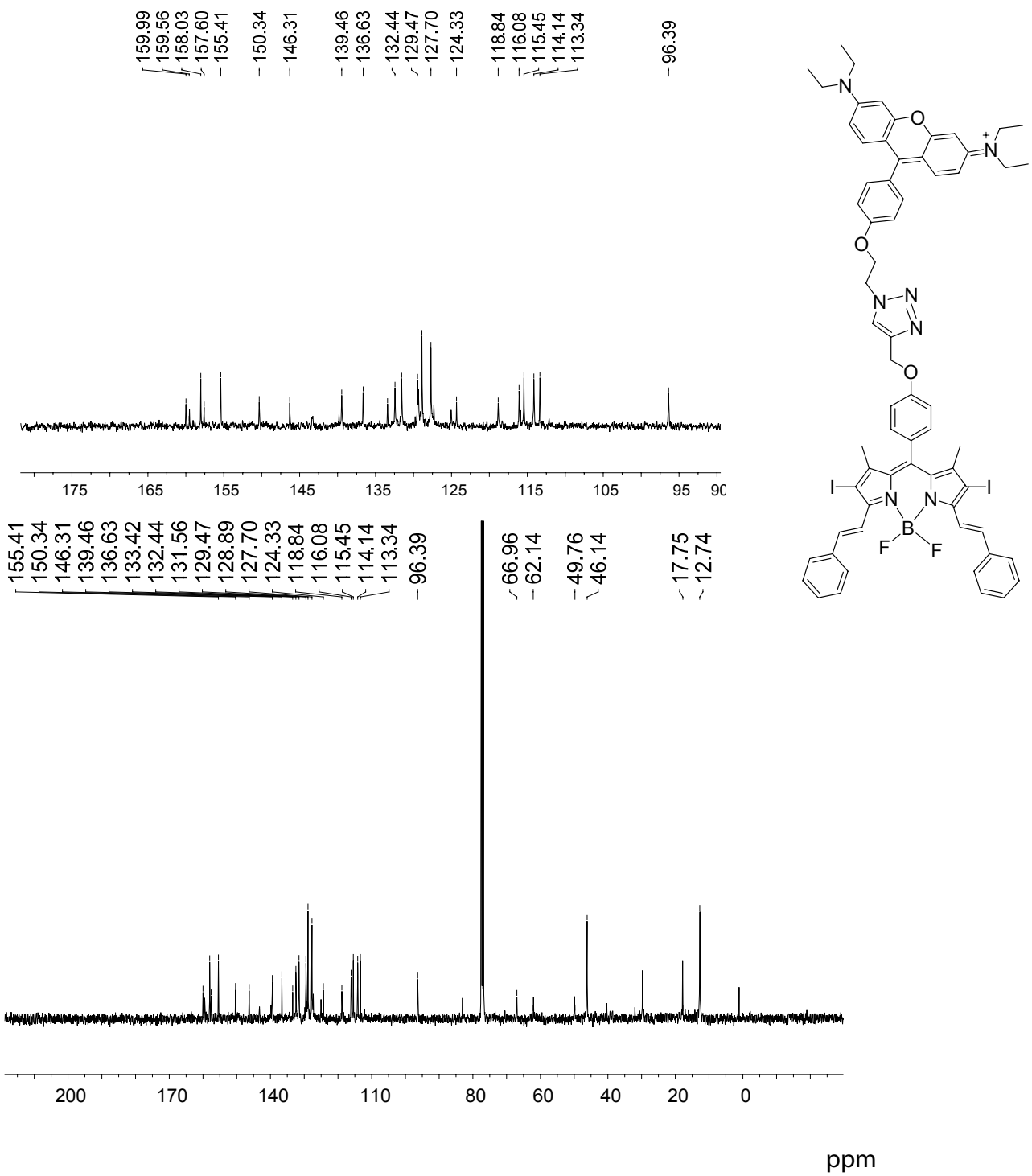


Figure S15. ^{13}C NMR of **R-1** (100 MHz, $CDCl_3$).

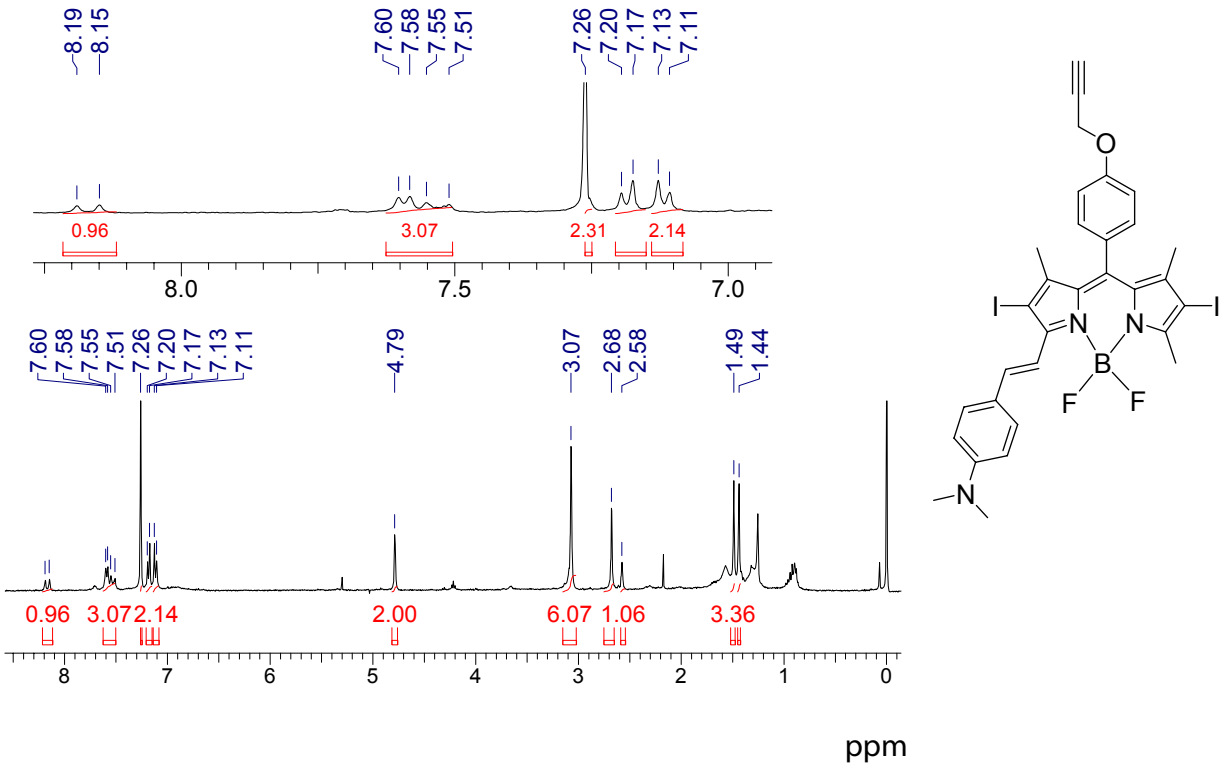


Figure S16. ^{1}H NMR of **B-2** (400 MHz, $CDCl_3$).

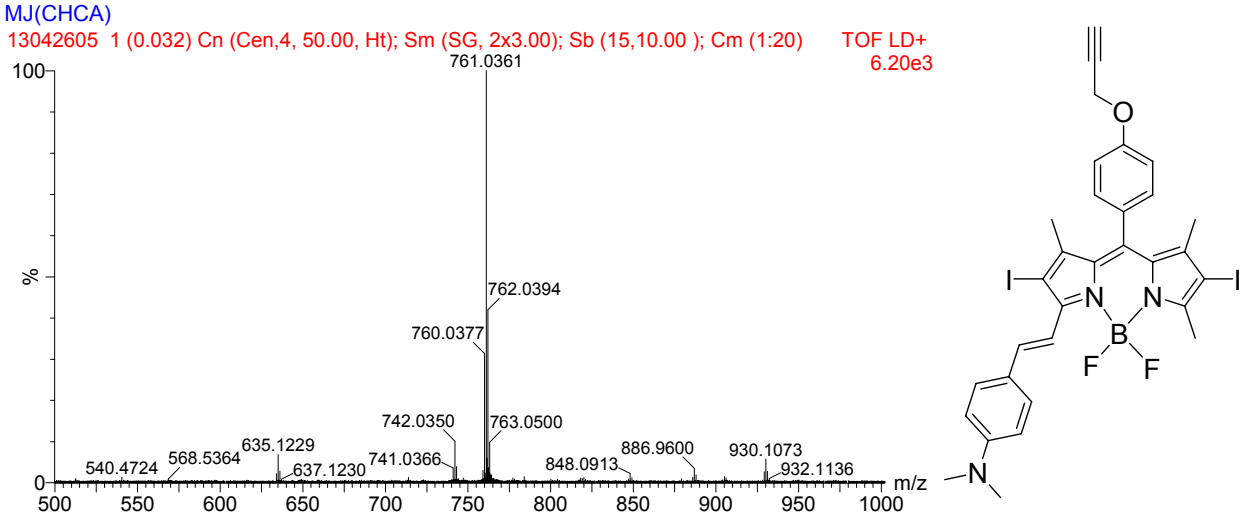


Figure S17. MALDI-HRMS of **B-2**.

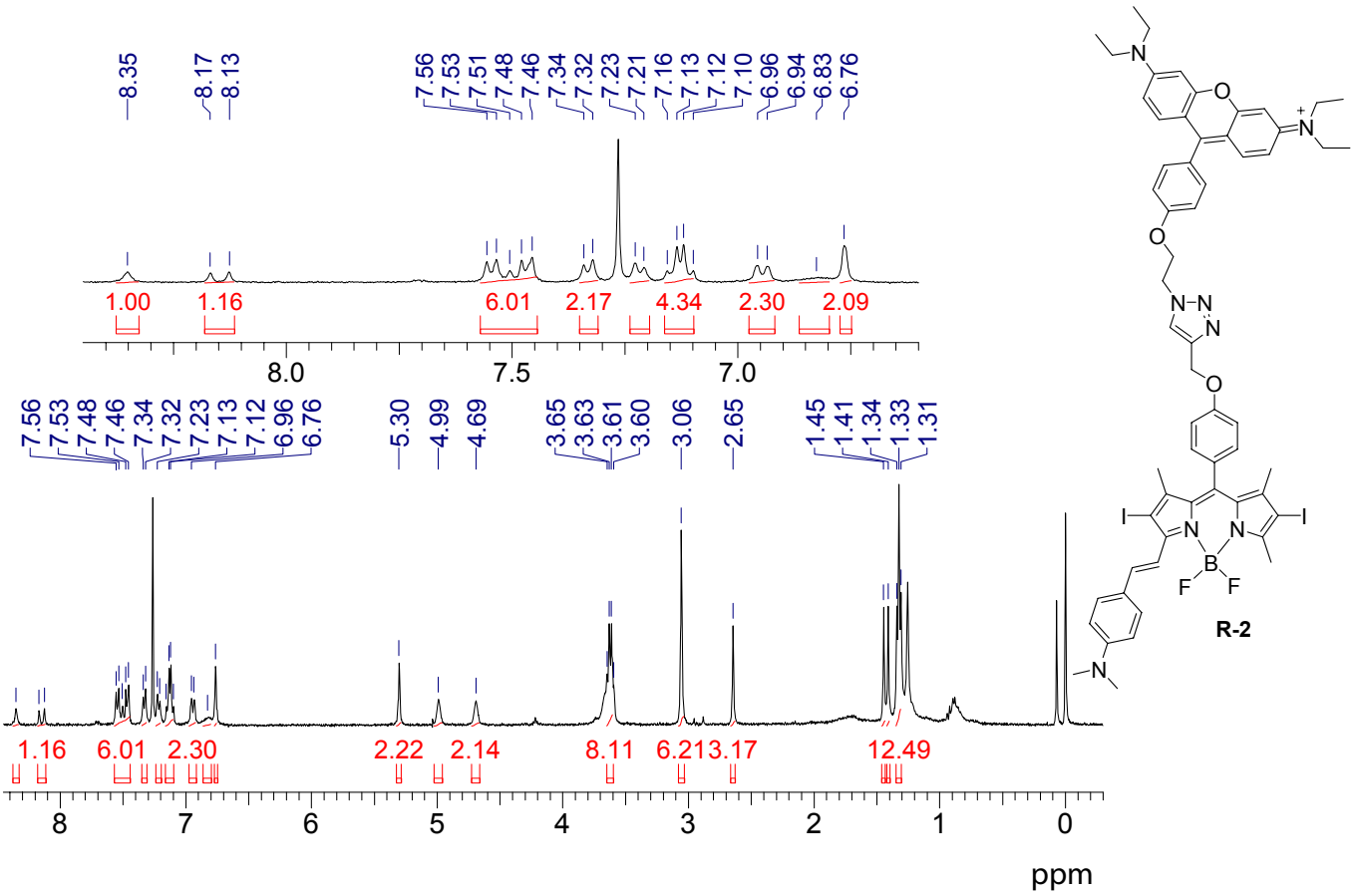


Figure S18. ^{1}H NMR of **R-2** (400 MHz, $CDCl_3$).

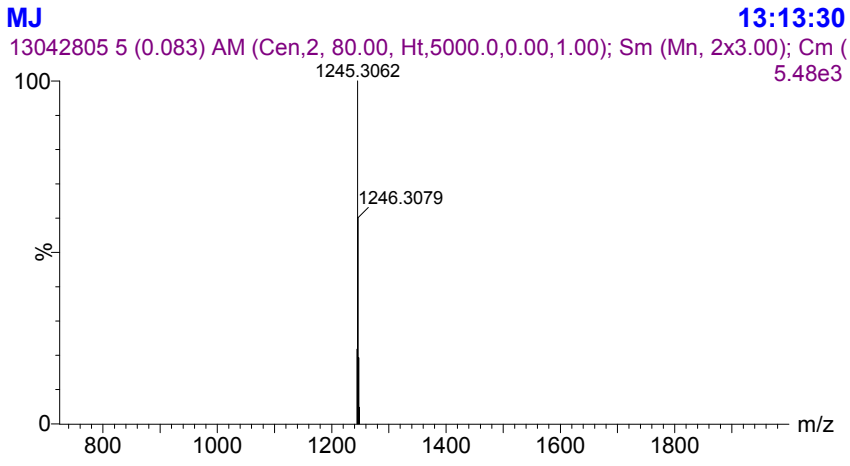


Figure S19. ESI-HRMS of **R-2**.

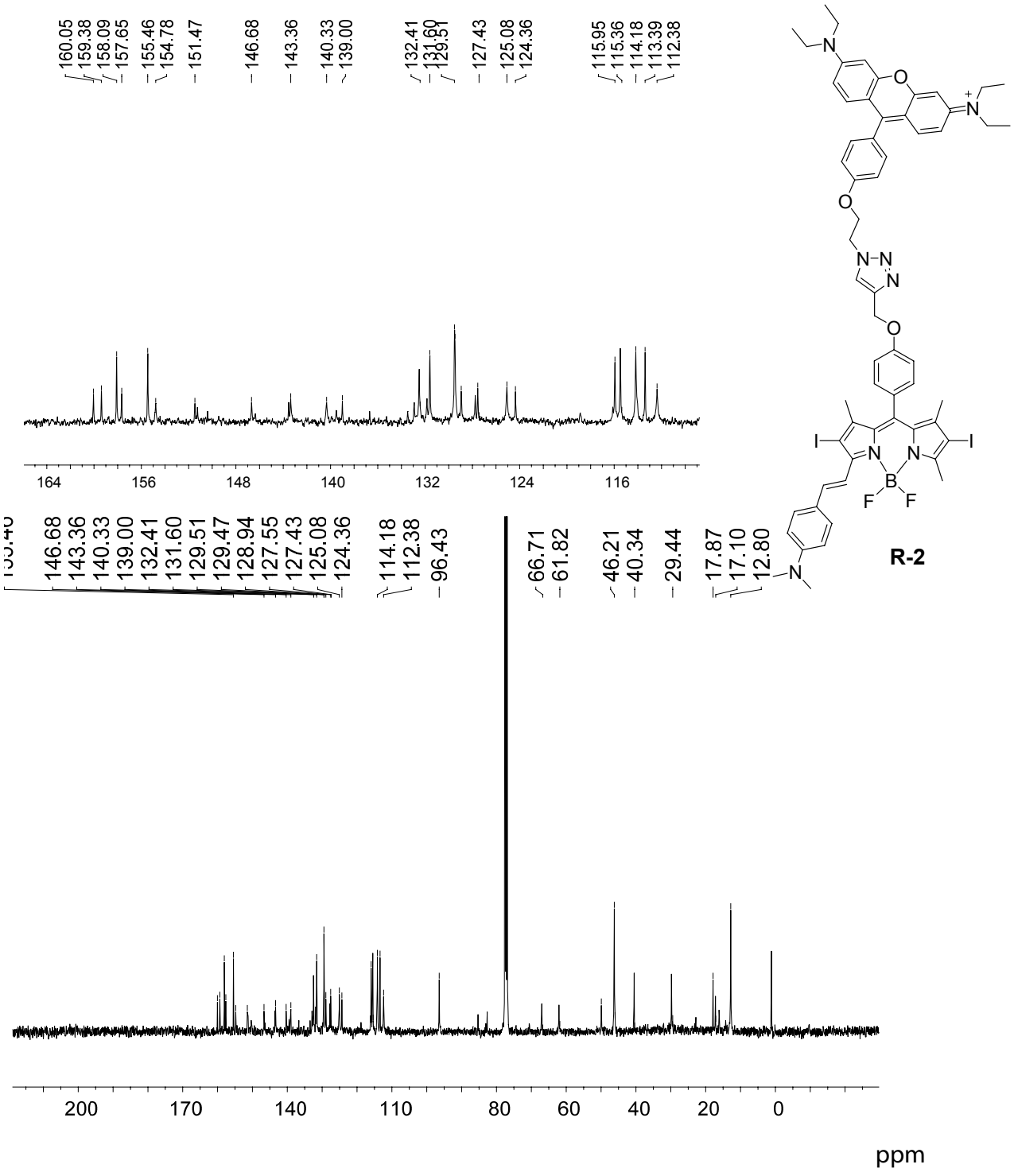


Figure S20. ^{13}C NMR of **R-2** (100 MHz, $CDCl_3$).

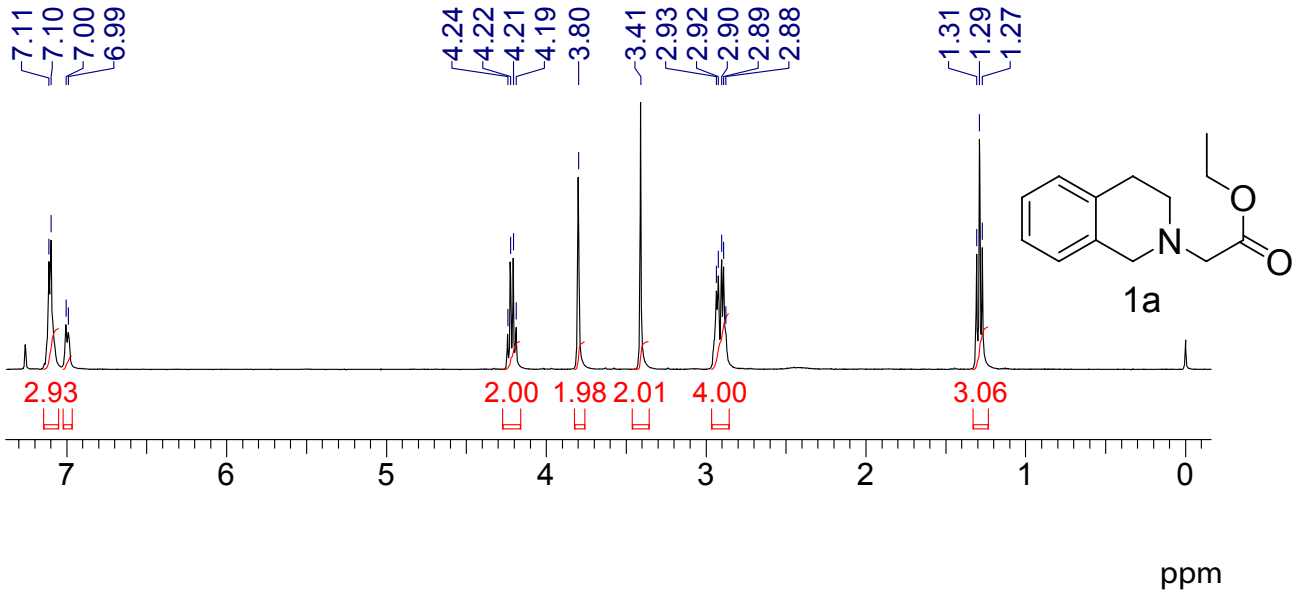


Figure S21. ^{1}H NMR of **1a** (400 MHz, $CDCl_3$).

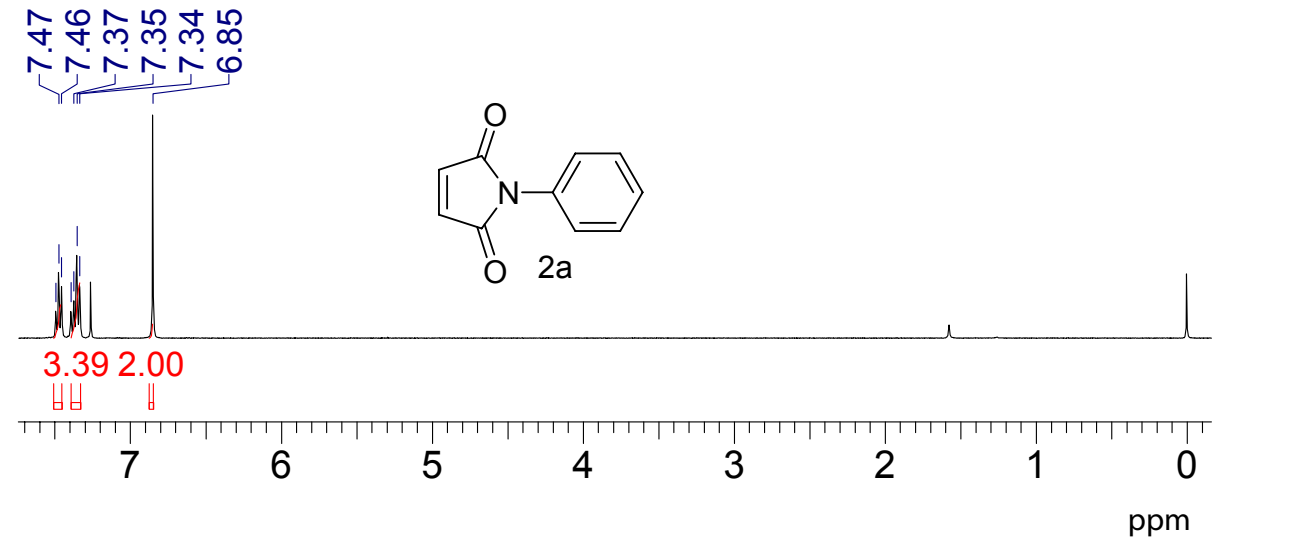


Figure S22. ^{1}H NMR of **2a** (400 MHz, $CDCl_3$).

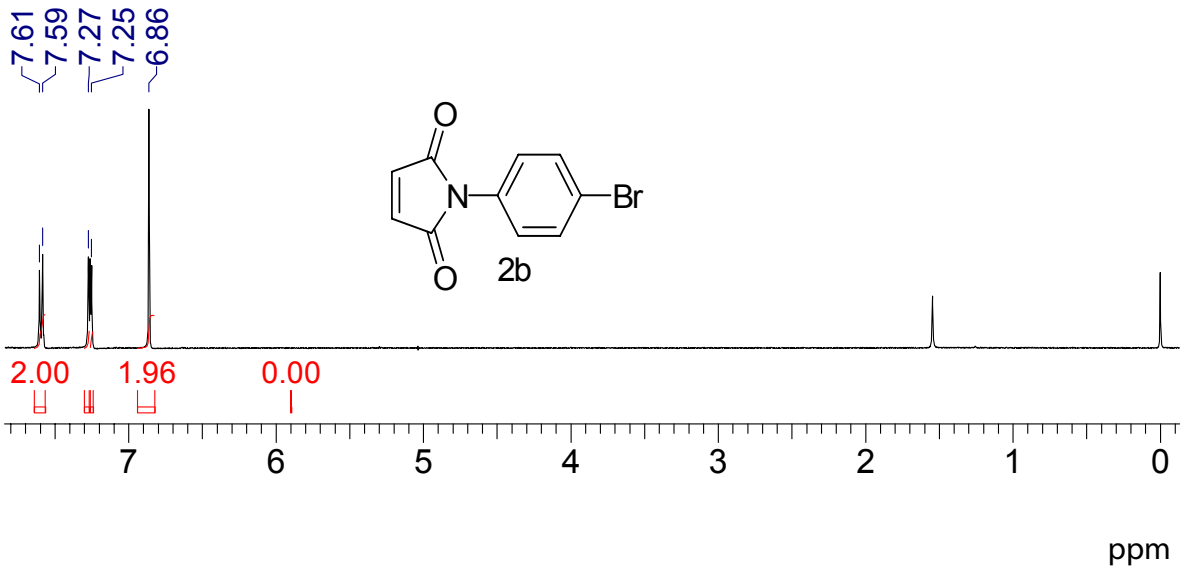


Figure S23. ^{1}H NMR of **2b** (400 MHz, $CDCl_3$).

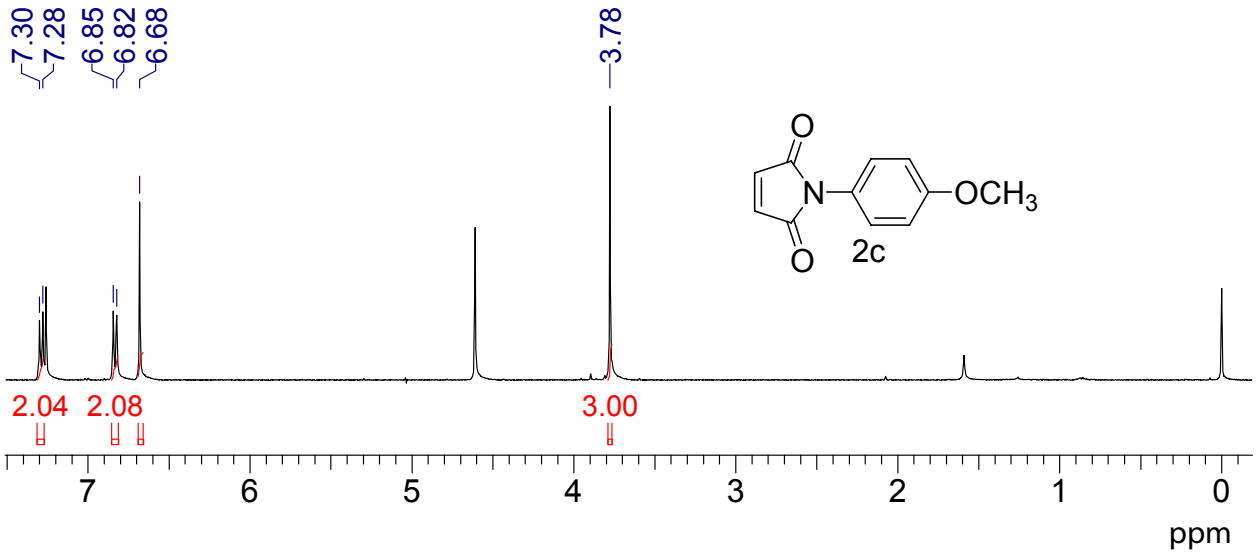


Figure S24. ^{1}H NMR of **2c** (400 MHz, $CDCl_3$).

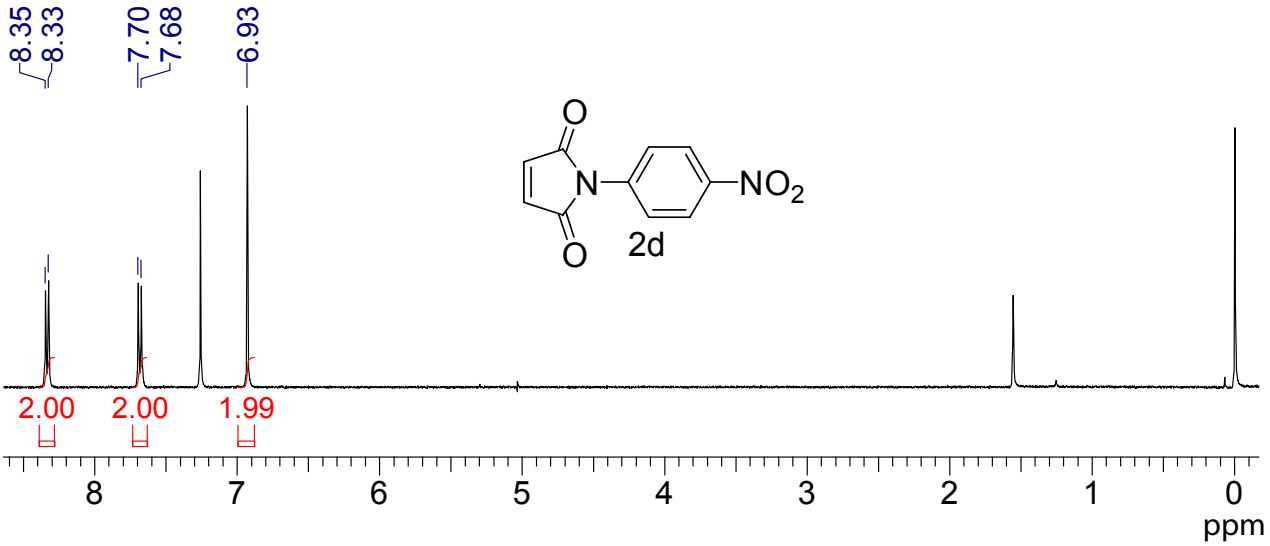


Figure S25. ^{1}H NMR of **2d** (400 MHz, $CDCl_3$).

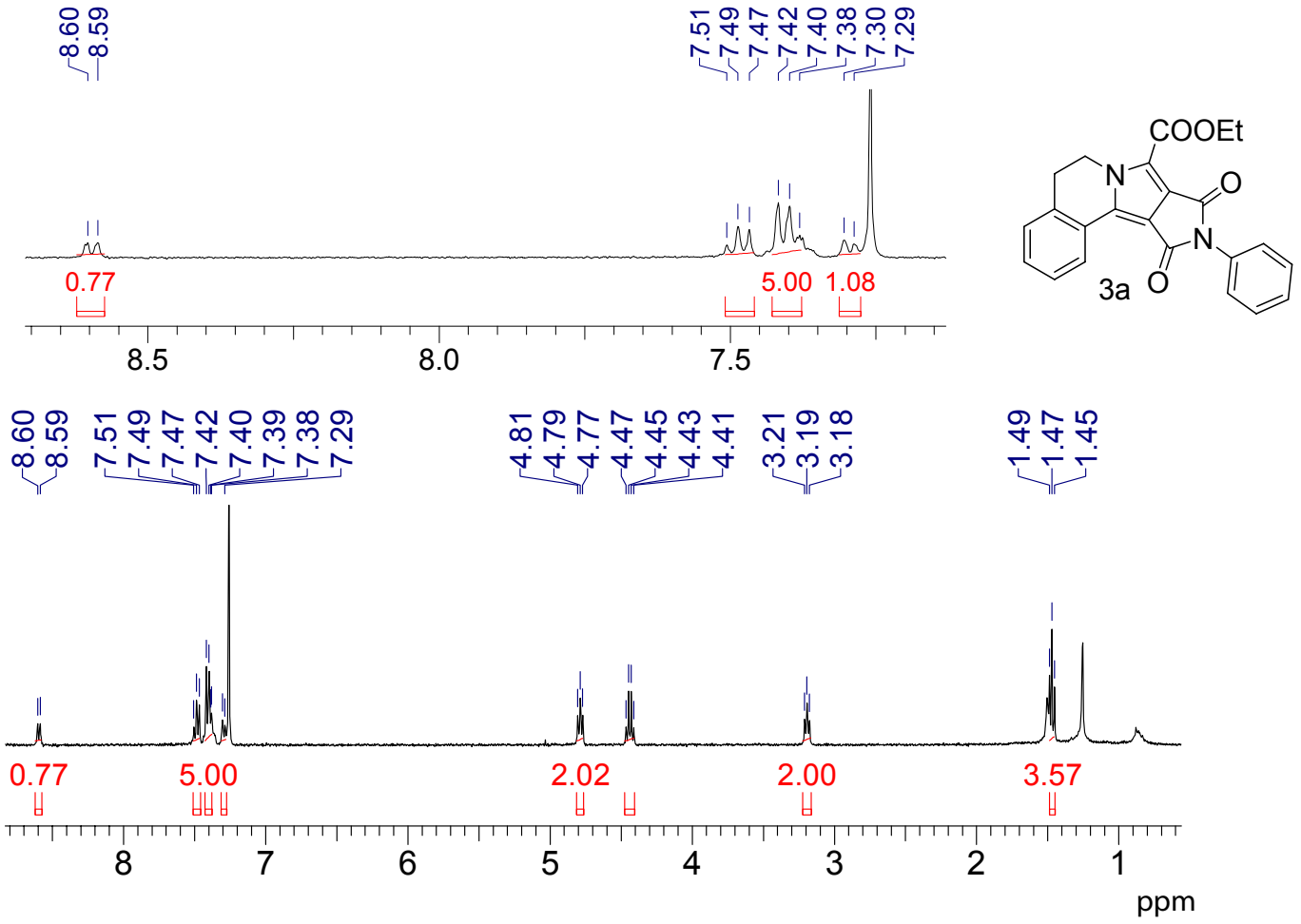


Figure S26. ^{1}H NMR of **3a** (400 MHz, $CDCl_3$).

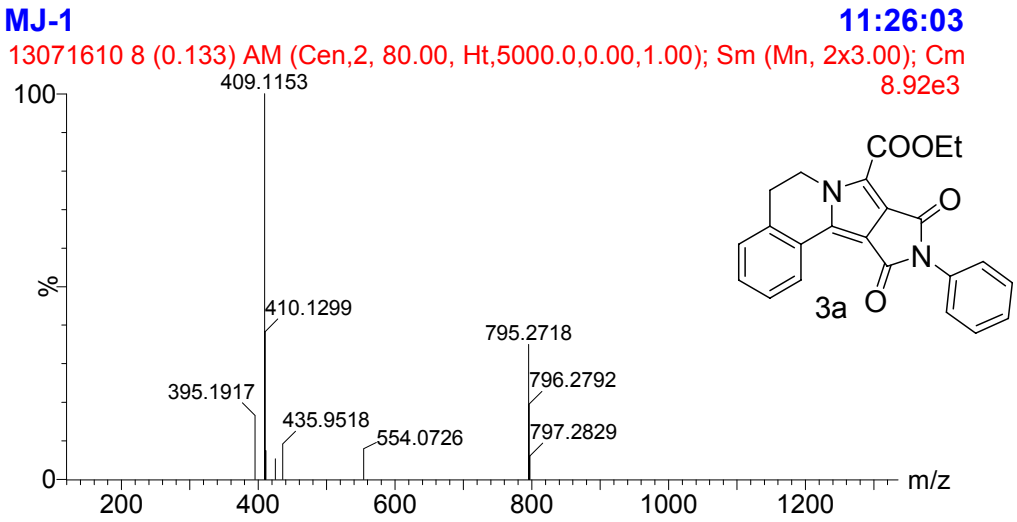


Figure S27. ESI-HRMS of **3a**.

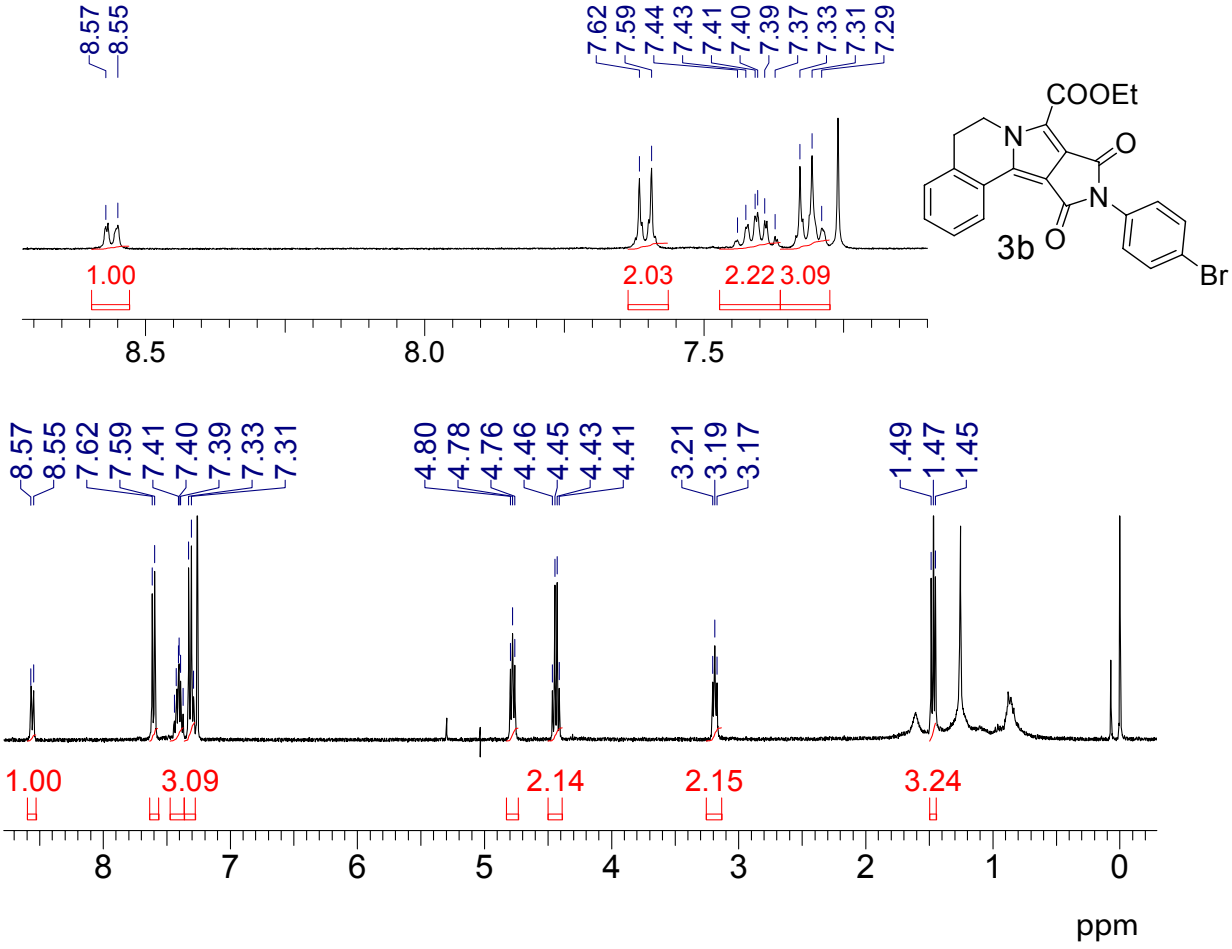


Figure S28. ^{1}H NMR of **3b** (400 MHz, $CDCl_3$).

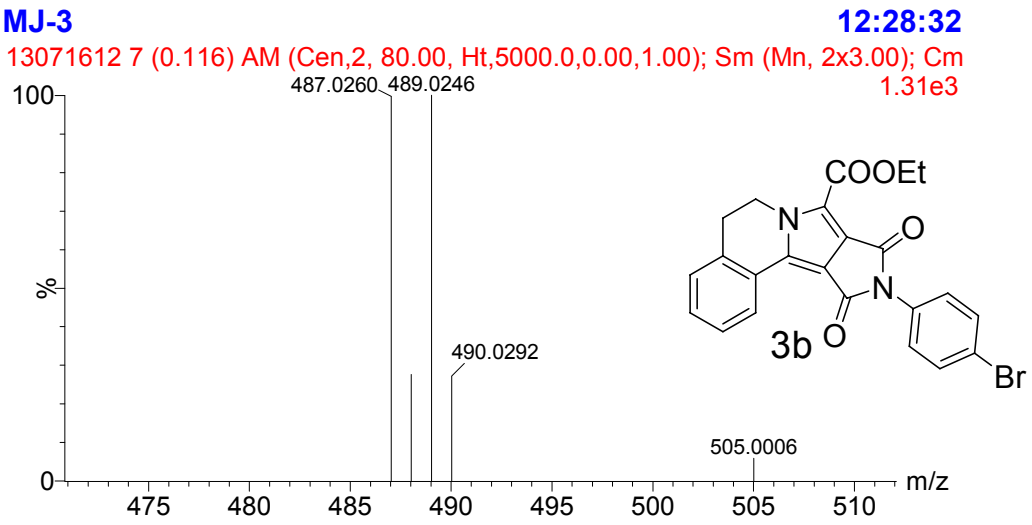


Figure S29. ESI-HRMS of **3b**.

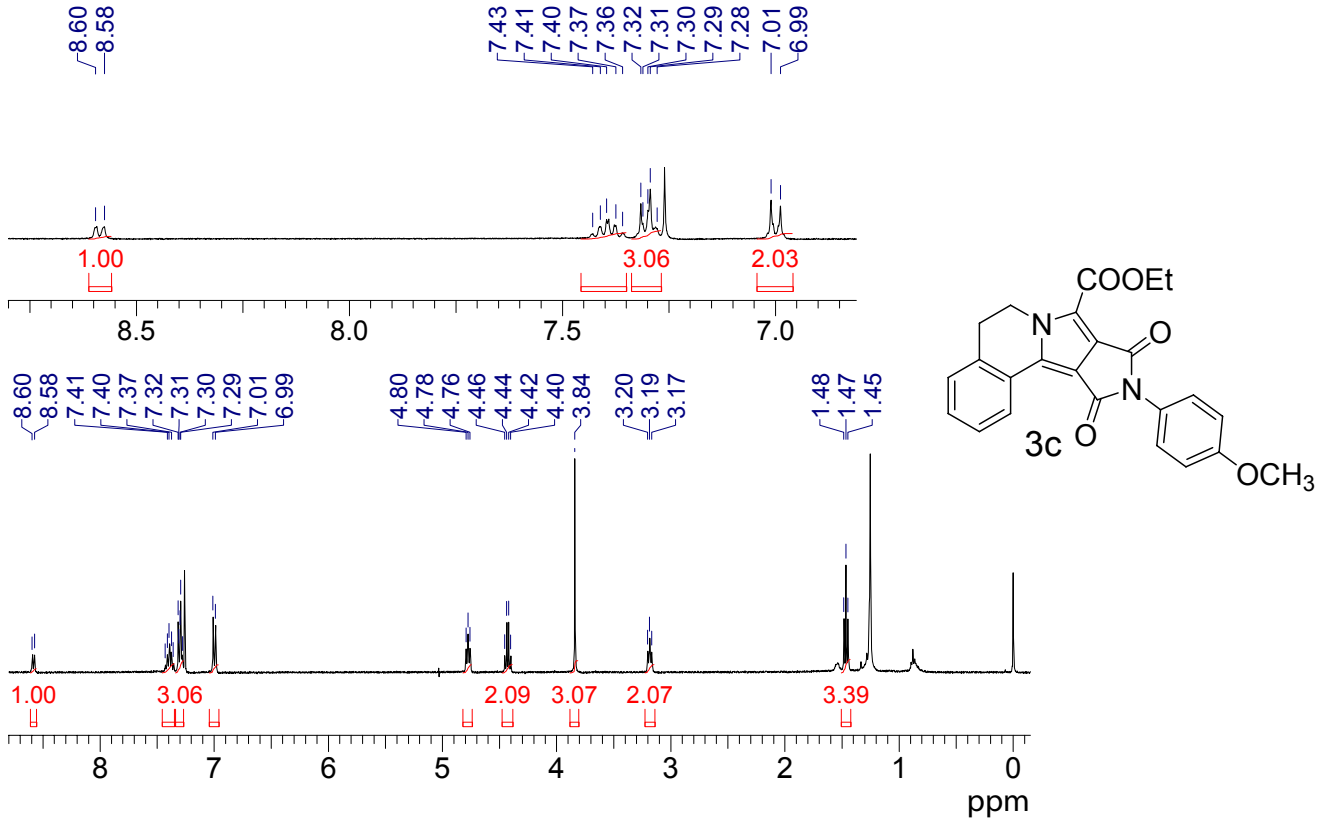


Figure S30. ^{1}H NMR of **3c** (400 MHz, $CDCl_3$)

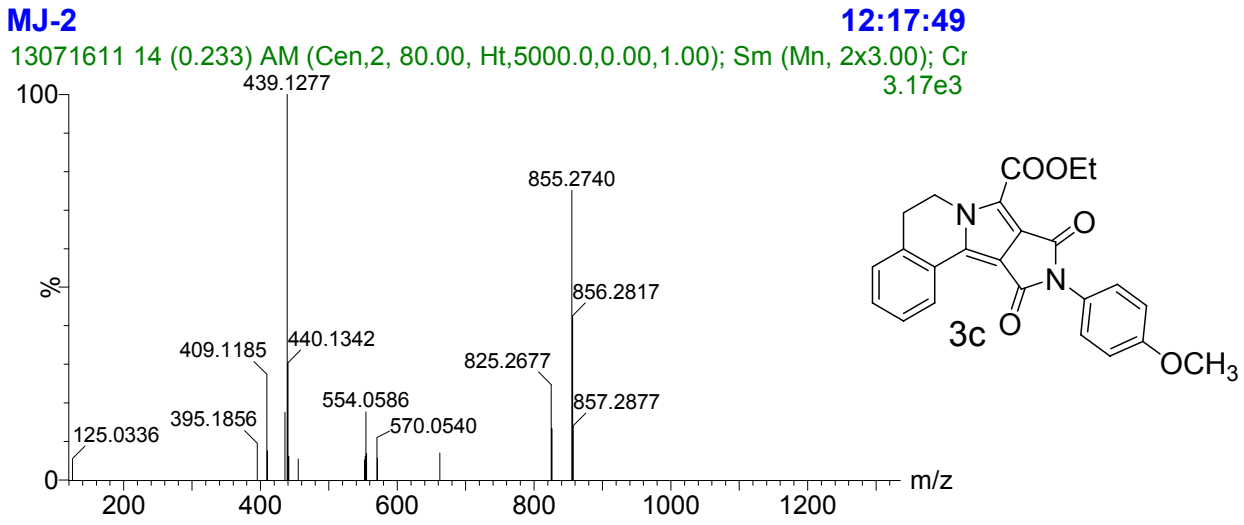


Figure S31. ESI-HRMS of **3c**.

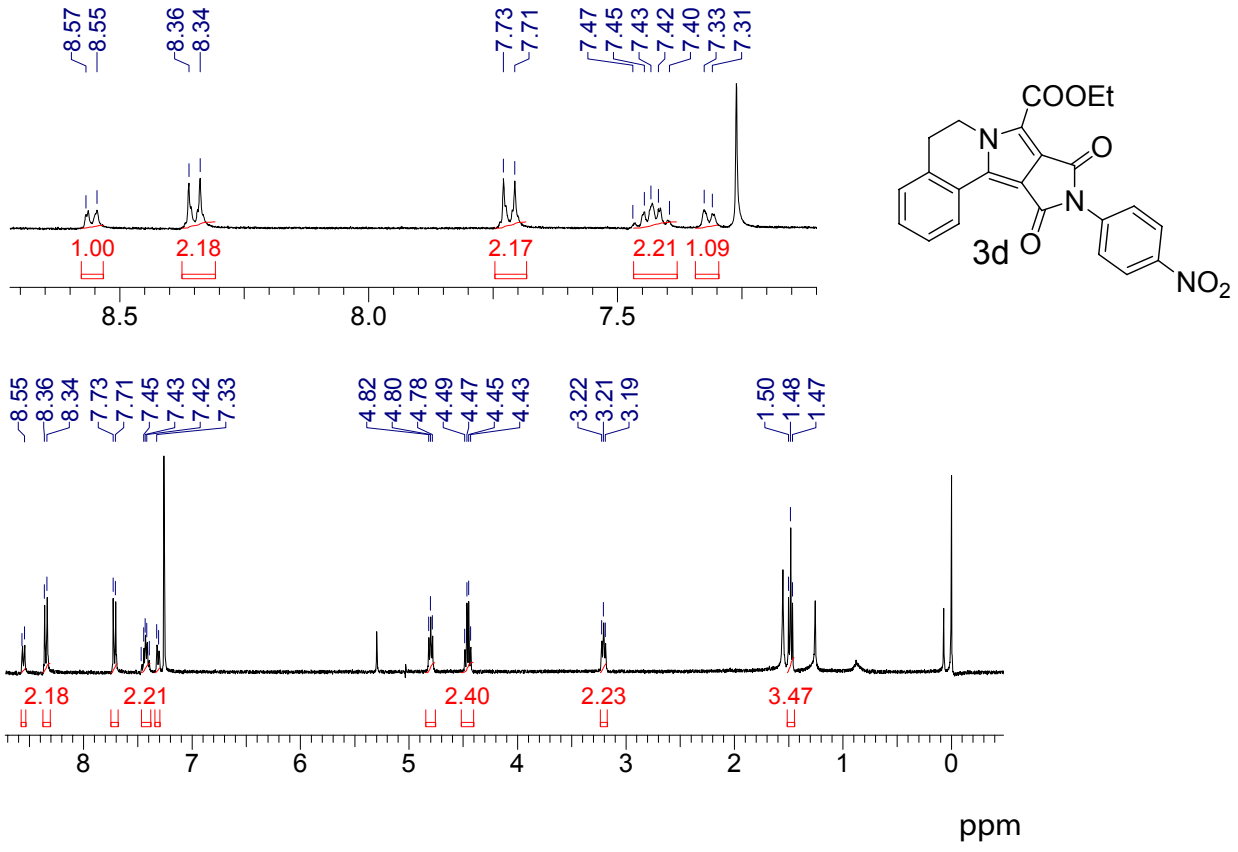


Figure S32. ^{1}H NMR of **3d** (400 MHz, $CDCl_3$).

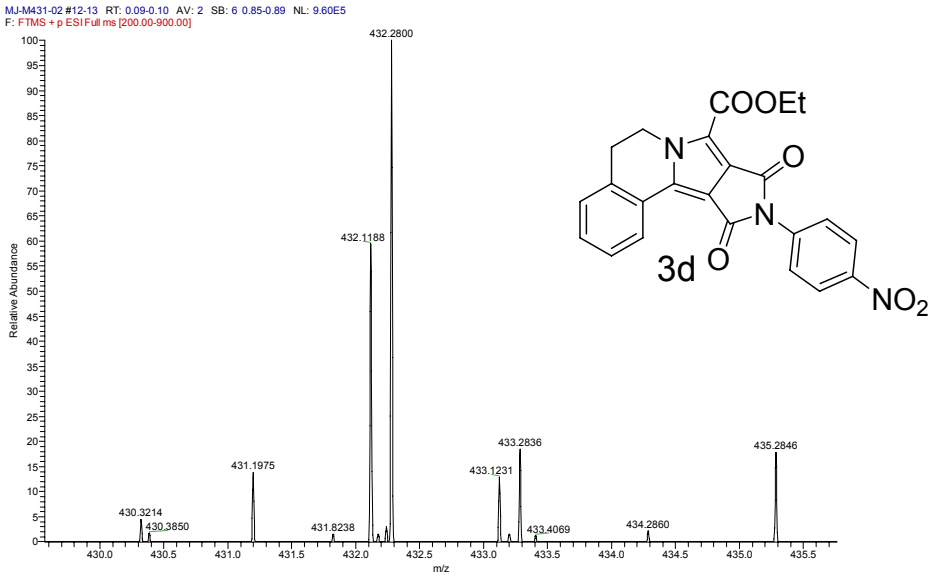


Figure S33. ESI-HRMS of **3d**.

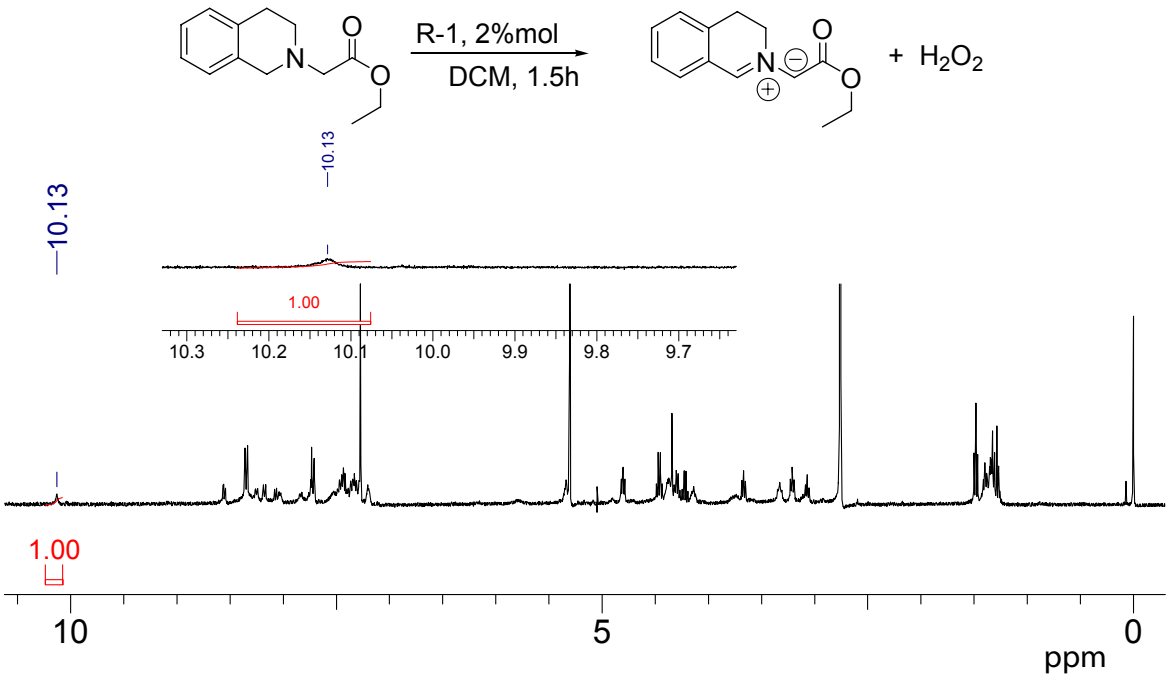


Figure S34. Experimental evidence for the photocatalytic reaction mechanism: the detection of H_2O_2 by ^1H NMR spectroscopy after reaction in $CDCl_3$. The peak at 10.13 ppm is due to H_2O_2.[3]

3. J. H. Park, K. C. Ko, E. Kim, N. Park, J. H. Ko, D. H. Ryu, T. K. Ahn, J. Y. Lee, S. U.Son, *Org. Lett.*, 2012, **14**, 5502–5505.

3. Electrochemical studies on the dyad triplet photosensitizers

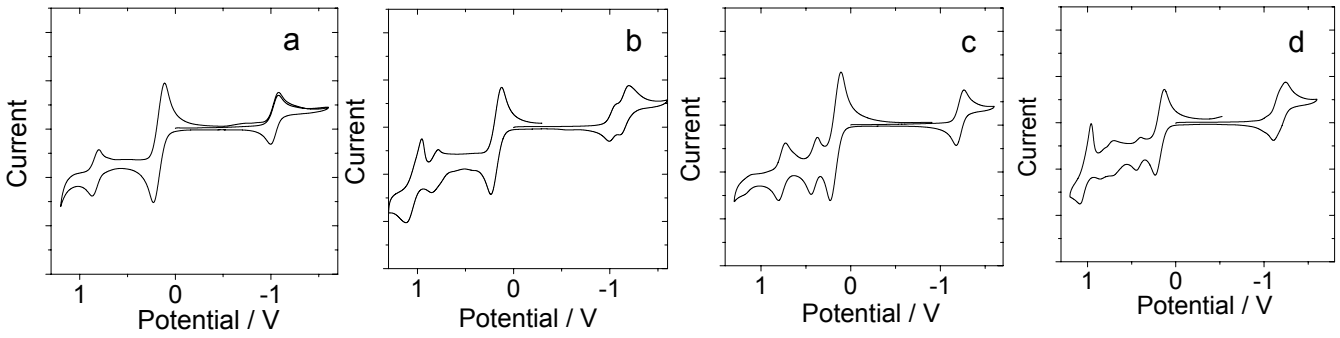


Figure S35. Cyclic voltammogram of (a) **B-1**, (b) **R-1**, (c) **B-2** (d) **R-2** respectively in deaerated CH_2Cl_2 solutions containing 1.0 mM photosensitizers with the ferrocene, 0.10 M Bu_4NPF_6 as supporting electrode, $Ag/AgNO_3$ reference electrode, Scan rates: 50 mV/s. Ferrocene (Fc) was used as internal reference.

Table S1. Electrochemical data of **B-1**, **R-1**, **B-2, R-2** and **R-0.**

Compd	Oxidation (V)			Reduction (V)	
	I	II	III	I	II
B-1	+0.84	–[b]	–[b]	−1.03	–[b]
R-1	+0.82	+1.04	–[b]	−1.02	−1.16
B-2	+0.41	+0.71	–[b]	−1.22	–[b]
R-2	+0.43	+0.79	+1.03	−1.18	–[b]
R-0	+1.08	–[b]	–[b]	−1.13	–[b]

[a] Recorded with $[Bu_4N][PF_6]$ as the electrolyte in CH_2Cl_2 (0.1 M) at ambient temperature with a scan rate of 50 mV/s. Potentials are expressed as the half-wave potentials ($E_{1/2}$) in volts vs SCE using ferrocene as an internal reference. [b] Not determined.

In order to study the possibility of the intramolecular electron transfer, the redox potentials of the triplet photosensitizers were studied (Figure S35).[4–8] The redox potential ($E_{1/2}$) of Rhodamine was determined as +1.08 V and −1.13 V, respectively (Table S1). For the Bodipy reference compounds **B-1** and **B-2,** the redox potentials are +0.84 V/−1.03 V, and +0.41 V, +0.71 V /−1.03 V, respectively. The redox potentials show little shifts in the dyad **R-1** and **R-2** (Table S1). Therefore, we propose that the interaction of the chromophores in **R-1** or **R-2** is weak at the ground states.

The possibility of the photo-induced electron transfer can be evaluated by the free energy changes of the electron transfer, calculated by the Weller equation (Eq. 1):

$$\Delta G^{0}{}_{\mathrm{CS}} = e[E_{OX} - E_{RED}] - E_{00} + \Delta G_{\mathrm{S}} \qquad \textbf{(Eq. 1)}$$

$$\Delta G_{\mathrm{S}} = -\frac{e^2}{4\pi\varepsilon_{\mathrm{S}}\varepsilon_0 R_{\mathrm{CC}}} - \frac{e^2}{8\pi\varepsilon_0}\left(\frac{1}{R_D} + \frac{1}{R_{\mathrm{A}}}\right)\left(\frac{1}{\varepsilon_{REF}} - \frac{1}{\varepsilon_S}\right) \qquad \textbf{(Eq. 2)}$$

Where ΔG_S is the static Coulombic energy, which is described by eq. 2. e = electronic charge, E_{OX} = half-wave potential for one-electron oxidation of the electron-donor unit, E_{RED} = half-wave potential for one-electron reduction of the electron-acceptor unit; note herein the anodic and cathodic peak potentials were used because in some cases the oxidation is irreversible therefore the formal potential $E_{1/2}$ cannot be derived; E_{00} = energy level approximated with the fluorescence emission wavelength (for the singlet excited state), or for the T_1 state energy. ε_S = static dielectric constant of the solvent, R_{CC} = (21.0 Å) center-to-center separation distance determined by DFT optimization of the geometry, R_D is the radius of the Rhodamine-based donor, R_A is the radius of the electron acceptor, ε_{REF} is the static dielectric constant of the solvent used for the electrochemical studies, ε_0 permittivity of free space. The solvents used in the calculation of free energy of the electron transfer is CH_2Cl_2 (ε= 8.9).

Based on these parameters, for **R-1** in CH_2Cl_2, ΔG_S is calculated as −0.08 eV. For **R-1**, we assume that the singlet energy transfer from the energy donor to the energy acceptor is much more fast than any electron transfer.[9] E_{00} of compound **B-1** was approximated by the T_1 state energy level (1.13 eV). At triplet excited state of the styryl-Bodipy, the iodo-styryl Bodipy part as electron acceptor, $\Delta G_{(CS)}$ = 1.04 − (−1.02) − 1.13 −0.08 = 0.85 eV; With reference **B-1** as electron donor, $\Delta G_{(CS)}$ = 0.82 − (−1.16) − 1.13 − 0.08 = 0.77 eV. Therefore the triplet excited state localized on the energy acceptor part (compound **B-1**) is unlikely to reduce or oxidize the energy donor part (compound **R-0**).

If the electron transfer from the energy donor to the acceptor occurs at the singlet excited state of energy donor (reference unit **R-0**), then E_{00} of the Rhodamine part is approximated as 2.37 eV.

With Rhodamine part as electron donor, $\Delta G_{(CS)}$ = 1.04– (–1.02) – 2.37– 0.08 = – 0.39 eV. Instead, with Rhodamine part as electron acceptor, $\Delta G_{(CS)}$ = 0.82 – (–1.16) –2.37 – 0.08 = –0.47 eV. Therefore, the exergonic electron transfer process are possible for **R-1**. However, the luminscence emission and lifetime studies (no significant quenching of the energy acceptor emission was observed), as well as the comparison of the excitation and absorption spectra (Fig. 5) indicated that the electron transfer will not be significant. Therefore, we propose that the singlet energy transfer from the Rhodamine part to the iodo-styryl Bodipy part can strongly compete with the electron transfer process.

Similar studies were carried out for **R-2**. We found that at the singlet excited state of the energy donor Rhodamine, the electron transfer between the Rhodamine and iodo-styryl Bodipy parts is more exergonic than **R-1**. For example, the free energy changes of **R-2** is –0.88 eV with Rhodamine part as the electron acceptor. This is in agreement with the more significantly quenched emission of the energy acceptor in **R-2**, as well as the lower energy transfer calculated by the comparison of the fluorescence excitation spectrum and the UV/Vis absorption of **R-2**.

4. J. Liu, M. E. El-Khouly, S. Fukuzumi, and D. K. P. Ng, *Chem. Asian J.*, **2011**, *6*, 174–179.
5. R. Ziessel, B. D. Allen, D. B. Rewinska, and A. Harriman, *Chem. Eur. J.*, **2009**, *15*, 7382–7393.
6. P. A. Hal, J. Knol, B. M. W. Langeveld-Voss, S. C. J. Meskers, J. C. Hummelen, and R. A. J. Janssen, *J. Phys. Chem. A*, **2000**, *104*, 5974–5988.
7. C. C. Hofmann, S. M. Lindner, M. Ruppert, A. Hirsch, S. A. Haque, M. Thelakkat, and J. Köhler, *J. Phys. Chem. B*, **2010**, *114*, 9148–9156.
8. A. N. Amin, M. E. El-Khouly, N. K. Subbaiyan, M. E. Zandler, S. Fukuzumi and F. D'Souza, *Chem. Commun.*, **2012**, *48*, 206–208.
9. M. E. El-Khouly, A. N. Amin, M. E. Zandler, S. Fukuzumi, and F. D'Souza, *Chem. Eur. J.*, 2012, **18,** 5239 –5247.

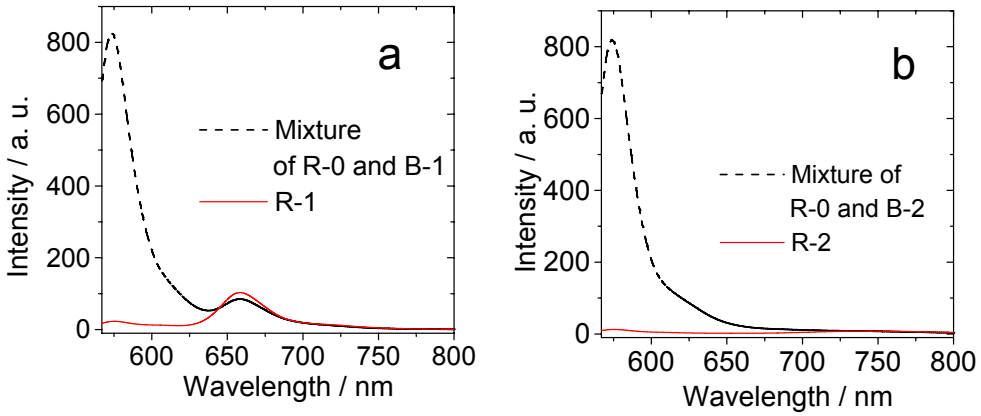


Figure S36. Emission spectra of (a) mixture of **R-0** and **B-1** (molar ratio is 1:1) and **R-1,** λ_{ex}=557 nm, at which A=0.96. (b) mixture of **R-0** and **B-2** (molar ratio is 1:1) and **R-2,** λ_{ex}=557 nm, at which A =1.01. c = 1.0×10^{-5} M in DCM. 20 °C.

4. Nanosecond time-resolved transient difference absorption spectra

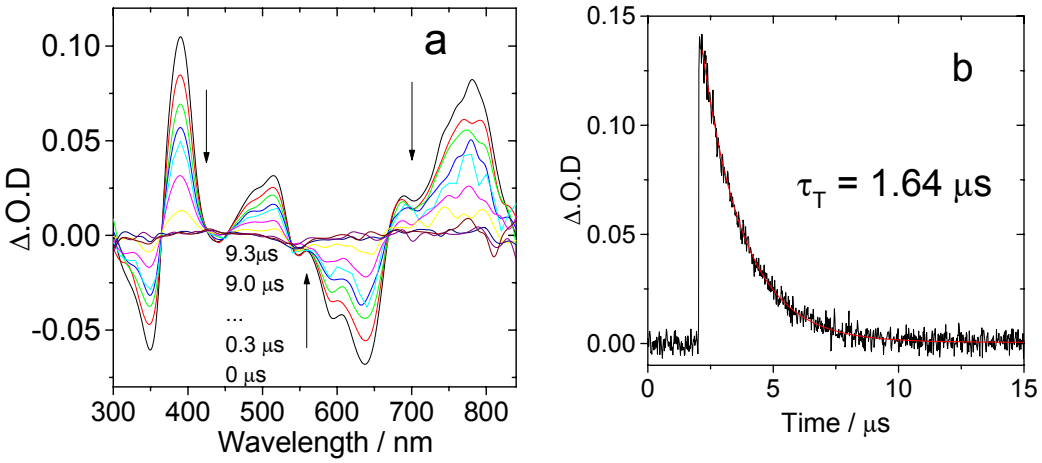


Figure S37. (a) Nanosecond time-resolved transient difference absorption of **R-1** after pulsed laser excitation (λ_{ex} = 532 nm) and (b) decay trace at 390 nm. c = 1.0×10^{-5} M in deaerated toluene. 20 °C.

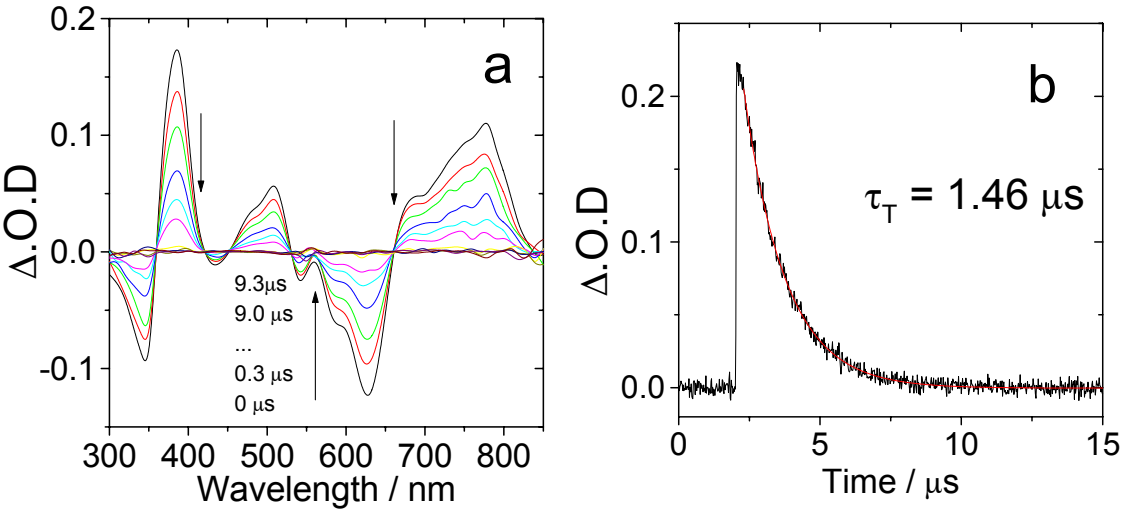


Figure S38. (a) Nanosecond time-resolved transient difference absorption of **R-1** after pulsed laser excitation (λ_{ex} = 532 nm) and (b) decay trace at 390 nm. c = 1.0×10^{-5} M in deaerated CH_3CN. 20 °C.

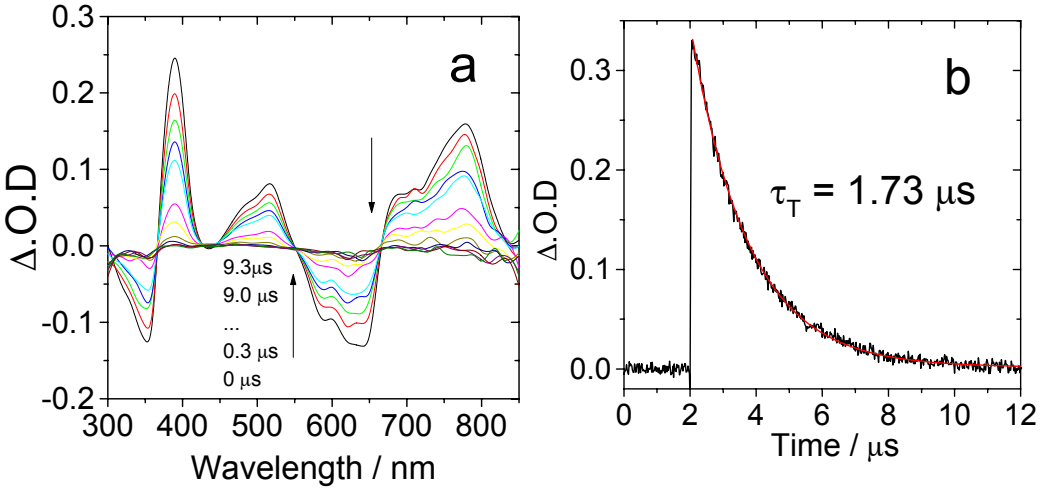


Figure S39. Nanosecond time-resolved transient difference absorption of **B-1** after pulsed laser excitation (λ_{ex} = 532 nm) and decay trace at 390 nm. c = 1.0×10^{-5} M in deaerated toluene. 20 °C.

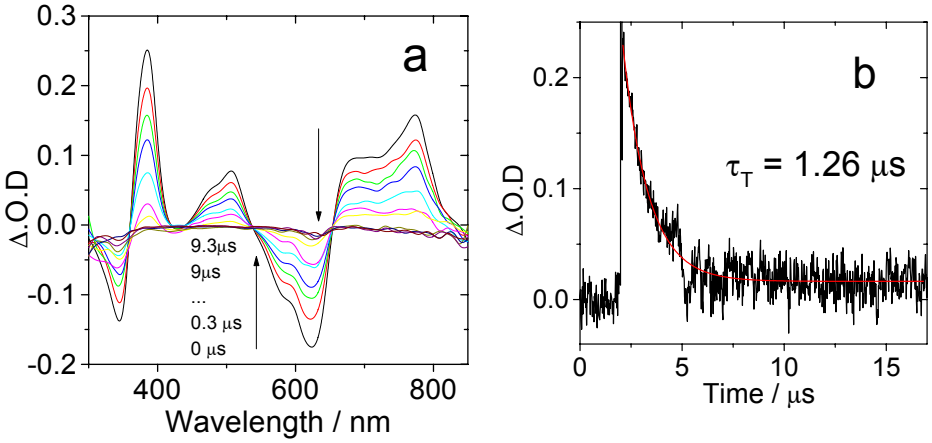


Figure S40. (a) Nanosecond time-resolved transient difference absorption of **B-1** after pulsed laser excitation (λ_{ex} = 532 nm) and (b) decay trace at 390 nm. $c = 1.0\times10^{-5}$ M in deaerated CH_3CN. 20 °C.

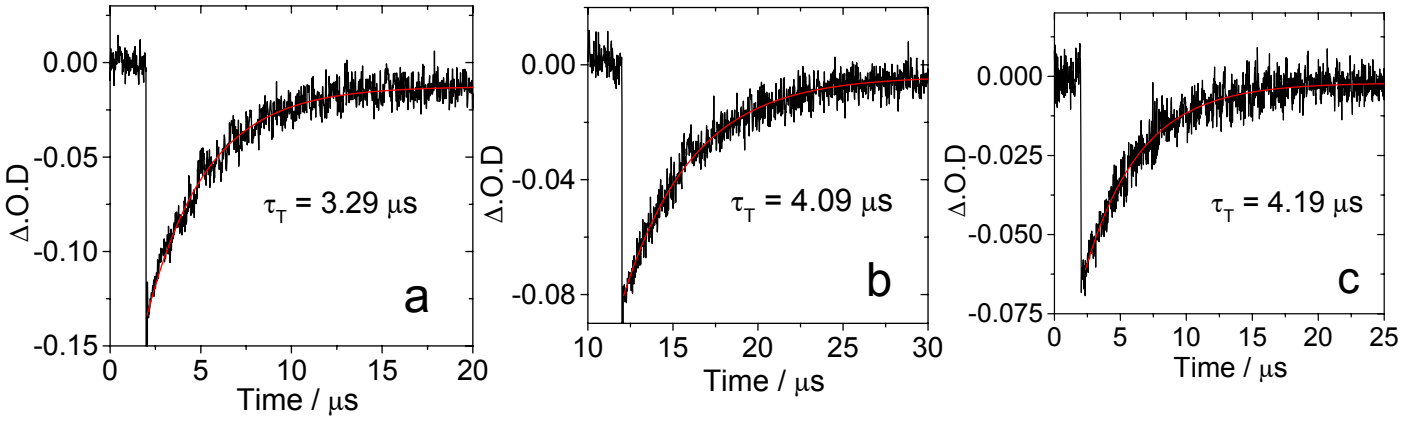


Figure S41. Decay trace of **R-2** at 650 nm in deaerated (a) $PhCH_3$, (b) DCM, (c) CH_3CN. $c = 1.0\times10^{-5}$ M. 20 °C.

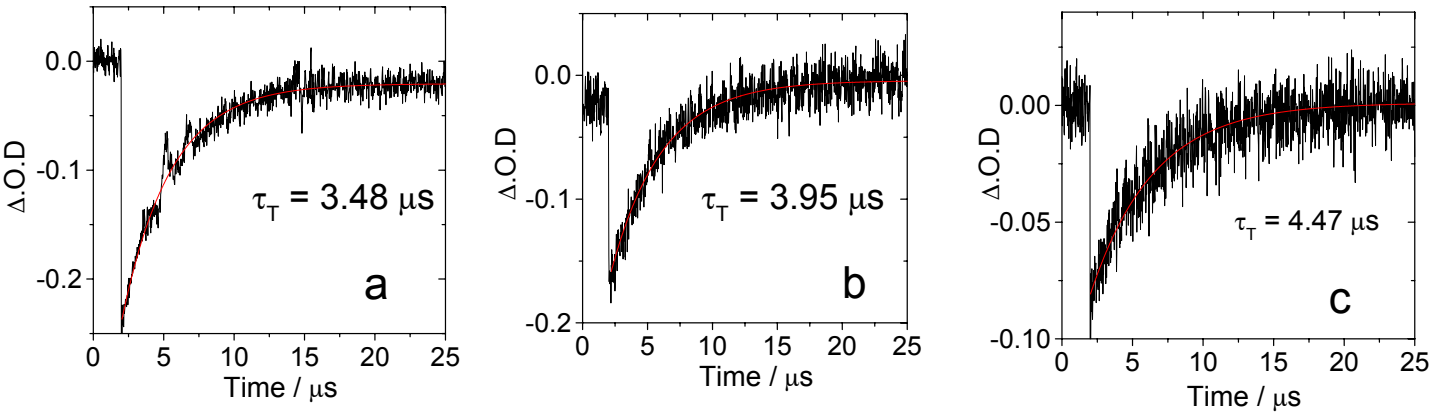


Figure S42. Decay trace of **B-2** at 630 nm in deaerated (a) $PhCH_3$, (b) DCM, (c) CH_3CN. $c = 1.0\times10^{-5}$ M. 20 °C.

5. ESR spectra of the mixture of R-1 and the substrate

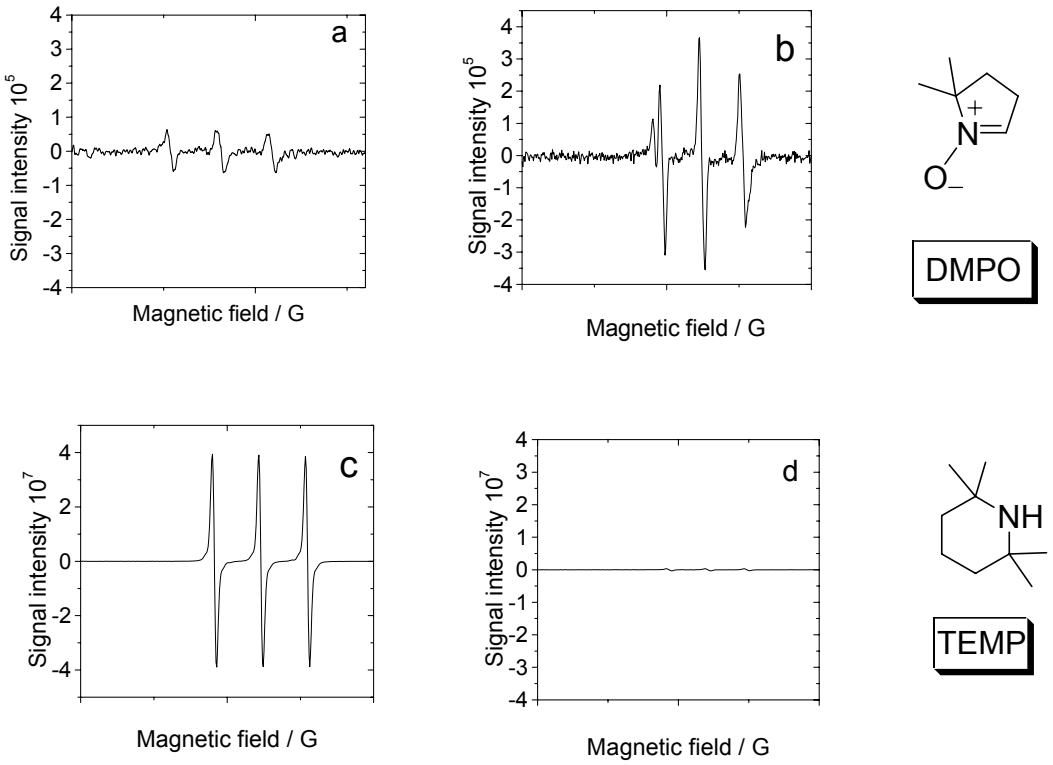
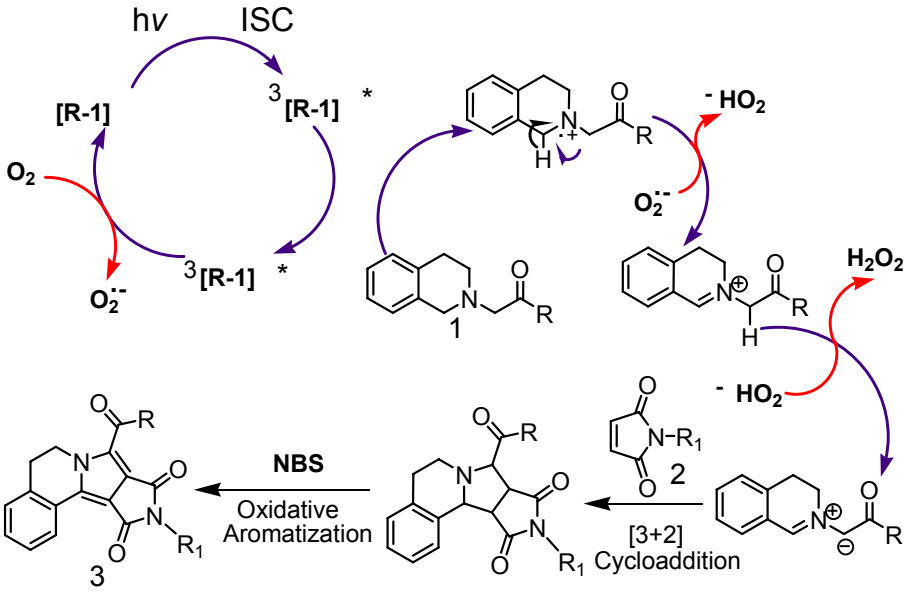


Figure S43. (a) ESR spectra of the mixture **R-1** (4.0×10^{-4} M) and DMPO (1.0×10^{-2} M) in air-saturated CH_2Cl_2 upon irradiation; (b) ESR spectrum of the mixture **R-1** (4.0×10^{-4} M), **1a** (3.0×10^{-3} M) and DMPO (1.0×10^{-2} M) in air-saturated CH_2Cl_2 upon irradiation; (c) ESR spectrum of a solution of **R-1**(4.0×10^{-4} M), TEMP (0.10 M), in air-saturated CH_2Cl_2 (d) ESR spectrum of **R-1**(4.0×10^{-4} M), TEMP(0.10 M), **1a** (3.0×10^{-3} M) in air-saturated CH_2Cl_2 upon irradiation. All the irradiations were performed with 589 nm continuous laser and the duration of the irradiation is 100 s (140 mW/cm^2). 25 °C.

DMPO is a superoxide anion radical ($O_2^{\bullet-}$) scavenger. TEMP is a scavenger of singlet oxygen ($^1O_2$).

6. Photocatalytic oxidation



Scheme S1. Photocatalytic oxidation–cycloaddition–aromatization sequence with the organic triplet photosensitizers.

Table S2. Optimization of the reaction conditions of the oxidation/[3+2] cycloaddition/oxidative aromatization with tetrahydroisoquinoline [a]

	Catalyst	Time / h	Solvents	Power / W/m^2	Yield %[b]
1	1%	1h	DCM	300	44
2	1%	1.5 h	DCM	200	30
3	2%	1.5 h	DCM	300	80

[a] Reaction conditions: 1 (0.12 mmol), 2 (0.10 mmol), NBS (1.2 equiv) were mixed in CH_2Cl_2 (3.0 mL), the mixture was irradiated with 35 W Xe lamp(λ > 385 nm), 20 °C. [b] Yield of the isolated product.

7. Femto-second transient difference absorption

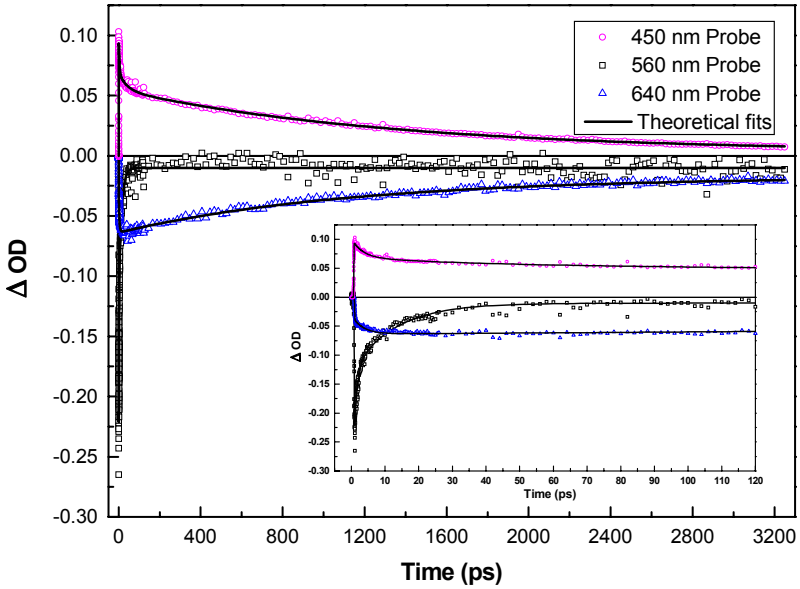


Figure S44. Decay trace of **R-1** at 450 nm, 560 nm and 640 nm probe wavelength (λ_{ex}= 555 nm).

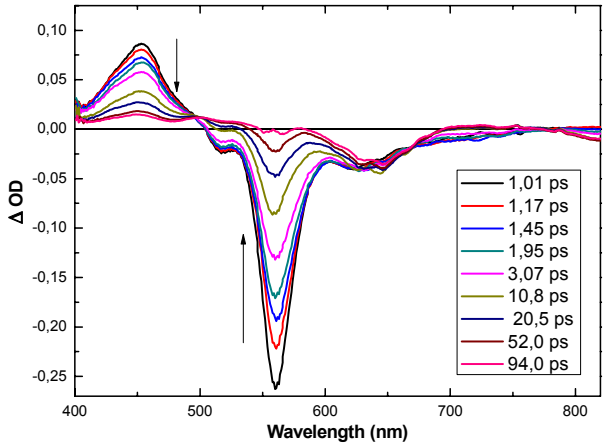


Figure S45. Femtosecond time-resolved transient absorption spectra of compound **R-2** upon excitation 555 nm wavelength in DCM.

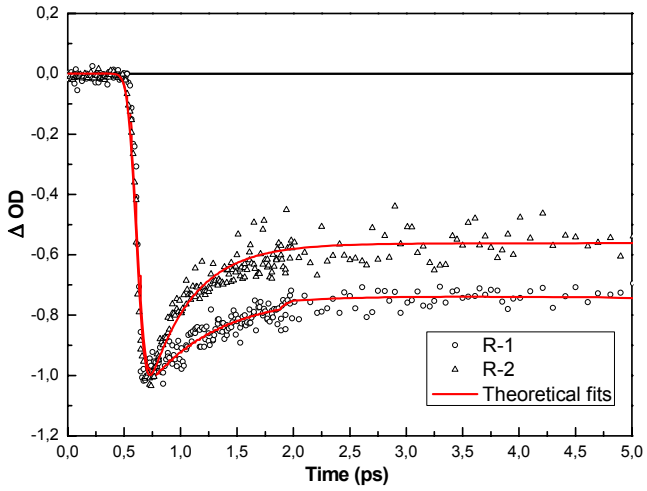


Figure S46. Decay trace of **R-1** and **R-2** at 640 nm probe wavelength (λ_{ex}= 640 nm).

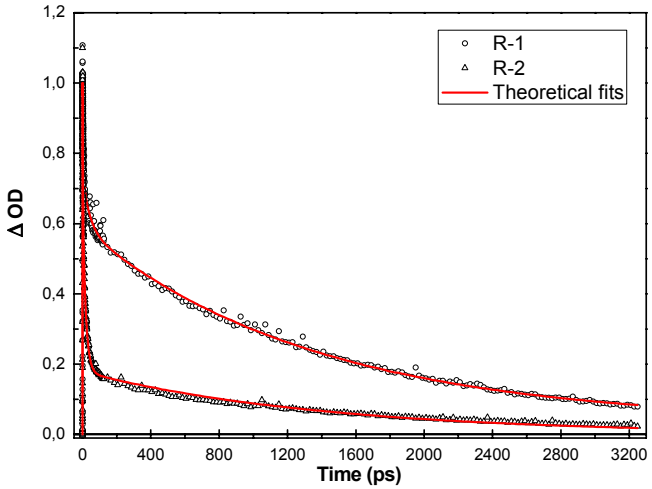


Figure S47. Decay trace of **R-1** and **R-2** at 450 nm probe wavelength (λ_{ex}= 555 nm).

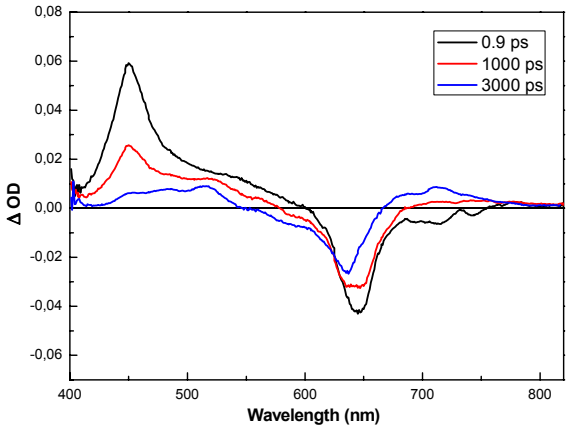


Figure S48. Transient absorption spectra of **R-1** with different time delays upon excitation at 640 nm.

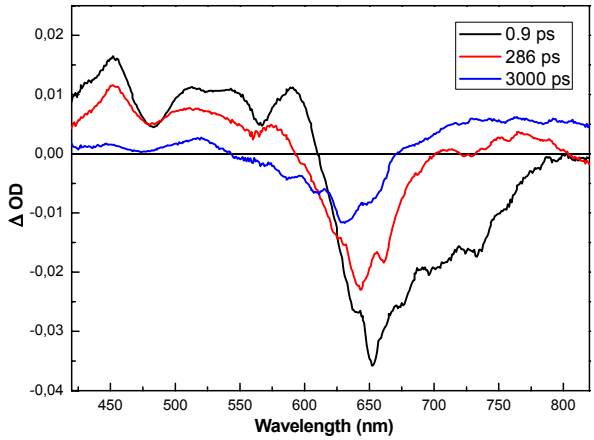


Figure S49. Transient absorption spectra of **R-2** with different time delays upon excitation at 640 nm.

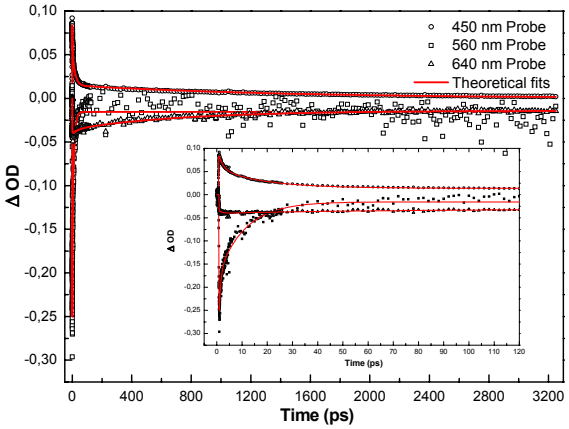


Figure S50. Decay trace of **R-2** at 450 nm, 560 nm and 640 nm probe wavelength (λ_{ex}= 555 nm).

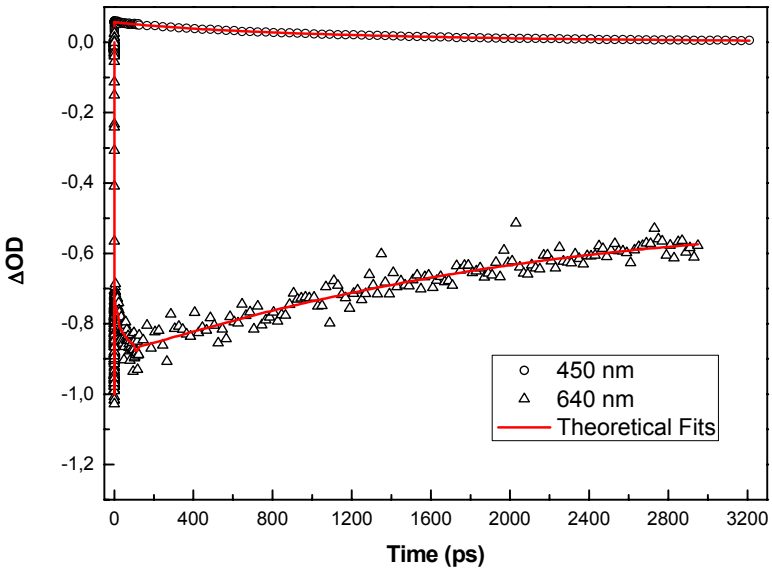


Figure S51. Decay trace of **R-1** at 450 nm and 640 nm probe wavelength (λ_{ex}= 640 nm).

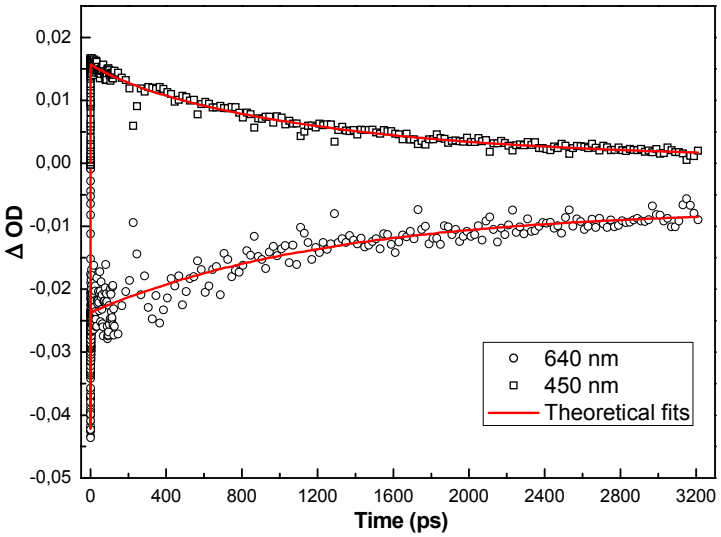


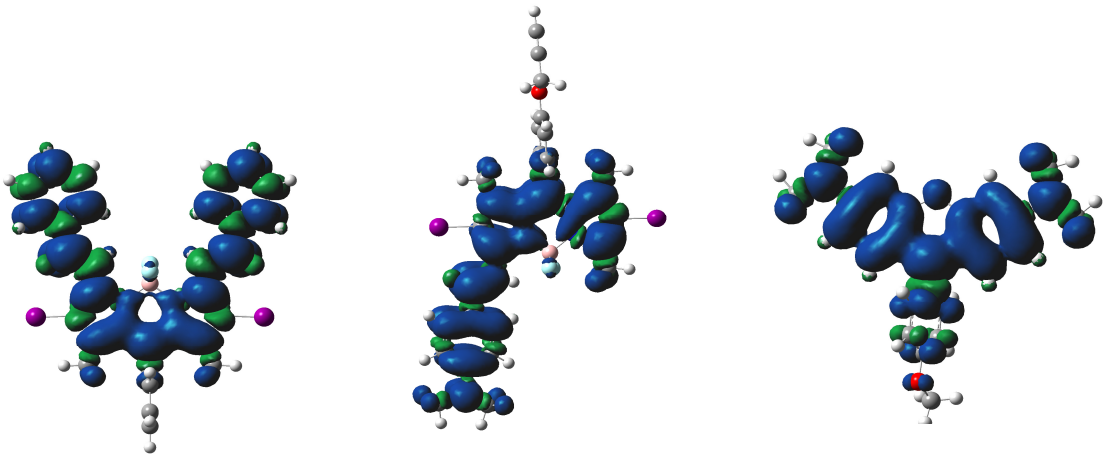
Figure S52. Decay trace of **R-2** at 450 nm and 640 nm probe wavelength (λ_{ex}= 640 nm).

8. DFT calculation results

Table S3. 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.** Based on the optimized ground state geometries and the optimized S_1 state geometries. Calculated by TDDFT//B3LYP/ genecp.[a] (DCM was employed as solvent in all the calculation).

	Electronic transition[a]	Excitation energy	TDDFT/B3LYP/6-31G(d)		
			f [b]	Composition[c]	CI[d]
Absorption	$S_0 \rightarrow S_1$	2.06 eV (603 nm)	0.9465	H → L	0.7076
	$S_0 \rightarrow S_2$	2.88 eV (431 nm)	0.3785	H−1 → L	0.6803
	$S_0 \rightarrow S_3$	2.92 eV (424 nm)	0.0185	H−2 → L	0.7027
Emission	$S_0 \rightarrow S_1$	1.75 eV (710 nm)	1.0990	H →L	0.7082
	$S_0 \rightarrow S_2$	2.70 eV (459 nm)	0.5251	H−1 → L	0.6783
				H → L+1	0.1917
Triplet	$S_0 \rightarrow T_1$	1.13 eV (1094 nm)	0.0000	H → L	0.7014
				H-1 → L	0.6119
				H → L+1	0.2646
	$S_0 \rightarrow T_2$	2.12 eV (584 nm)	0.0000	H-1 → L	0.6119

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



B-1 **B-2** **R-0**

Figure S53. Isosurfaces of spin density of compounds **B-1**, **B-2,** and **R-0**. At the optimized triplet state geometries. DCM was used as solvents in the calculations. Calculation was performed at B3LYP/6-31G(d)/genecp level with Gaussian 09W.

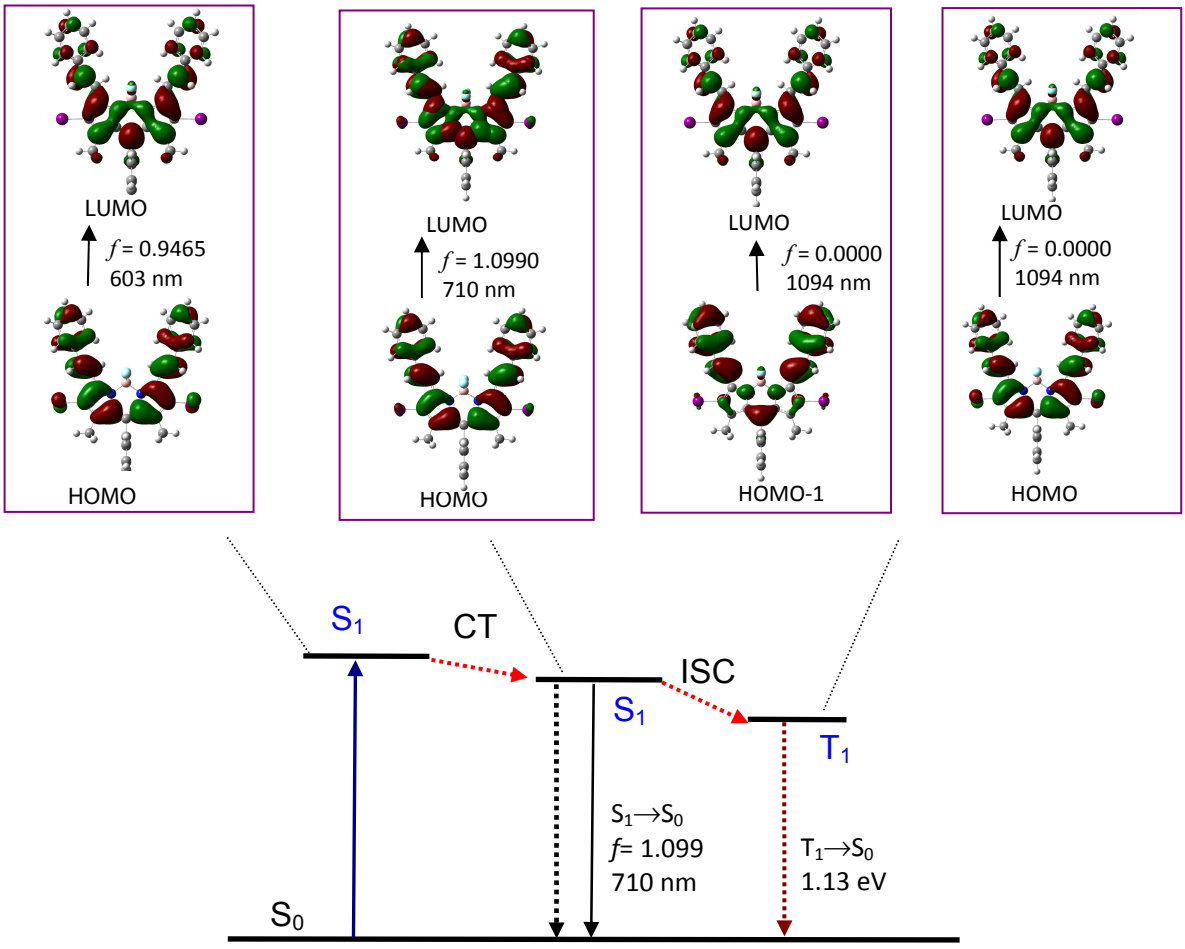


Figure S54. Selected frontier molecular orbitals involved in the excitation, emission and triplet excited states of **B-1**. CT stands for conformation transformation. Dichloromethane was employed as solvent in all the calculation. The calculations are at the B3LYP/6-31G(d)/genecp level using Gaussian 09W.

Table S4. Selected parameters for the vertical excitation (UV-vis absorption and fluorescence emission) of the compounds. Electronic excitation energies (eV) and oscillator strengths (*f*), configurations of the low-lying excited states of **R-1** and its fluorescent precursors. DCM was employed as solvent in the calculation. Calculated by TDDFT//B3LYP/6-31G(d) /Genecp, based on the optimized ground state geometries.

Electronic		TDDFT/B3LYP/6-31G(d)			
		Excitation energy	f^b	Composition[c]	CI[d]
Absorption	$S_0 \rightarrow S_1$	2.05 eV (604 nm)	0.9401	H → L+1	0.7077
	$S_0 \rightarrow S_2$	2.09 eV (594 nm)	0.0000	H→ L	0.7071
	$S_0 \rightarrow S_3$	2.61 eV (475 nm)	0.9289	H−1 →L	0.7050
	$S_0 \rightarrow S_6$	2.88 eV (430 nm)	0.5218	H−2 →L+1	0.6224
	$S_0 \rightarrow S_{18}$	3.54 eV (350 nm)	0.5688	H−10 →L+1	0.5225
				H →L+2	0.4395
Emission	$S_0 \rightarrow S_1$	1.75 eV (710 nm)	1.0861	H→ L	0.7082
	$S_0 \rightarrow S_2$	1.99 eV (624 nm)	0.0000	H→ L+1	0.7071
	$S_0 \rightarrow S_3$	2.45 eV (506 nm)	1.1510	H−1 → L+1	0.7061
	$S_0 \rightarrow S_6$	2.68V (462 nm)	0.5614	H−2 →L	0.5973
Triplet	$S_0 \rightarrow T_1$	1.13 eV (1099 nm)	0.0000	H → L+1	0.7016
	$S_0 \rightarrow T_2$	1.74 eV (712 nm)	0.0000	H−1→L	0.7055

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

Table S5. Selected Electronic Excitation Energies (eV) and Corresponding Oscillator Strengths (*f*), Main Configurations and CI Coefficients of the Low-lying Electronically Excited States of **B-2.** Based on the optimized ground state geometries and the optimized S_1 state geometries. Calculated by TDDFT//B3LYP/ genecp.[a] (DCM was employed as solvent in all the calculation).

	Electronic transition[a]	Excitation energy	TDDFT/B3LYP/6-31G(d)		
			f [b]	Composition[c]	CI[d]
Absorption	$S_0 \rightarrow S_1$	1.96 eV (633 nm)	1.1091	H → L	0.7088
	$S_0 \rightarrow S_2$	2.74 eV (453 nm)	0.2678	H−3 → L	0.1578
				H−1 → L	0.6711
				H → L+1	0.1398
	$S_0 \rightarrow S_3$	2.90 eV (427 nm)	0.0330	H−2 → L	0.7022
Emission	$S_0 \rightarrow S_1$	1.71 eV (720 nm)	1.1761	H →L	0.7078
	$S_0 \rightarrow S_2$	2.65 eV (468 nm)	0.3676	H−3 → L	0.1421
				H−1 → L	0.6801
				H → L+1	0.1172
	$S_0 \rightarrow S_3$	2.85 eV (434 nm)	0.1121	H−2 → L	0.6994
Triplet	$S_0 \rightarrow T_1$	1.14 eV (1084 nm)	0.0000	H−1 →L	0.2209
				H→L	0.6693
	$S_0 \rightarrow T_2$	2.05 eV (606 nm)	0.0000	H−1→L	0.6374
				H → L	0.1959
				H → L+1	0.1713

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

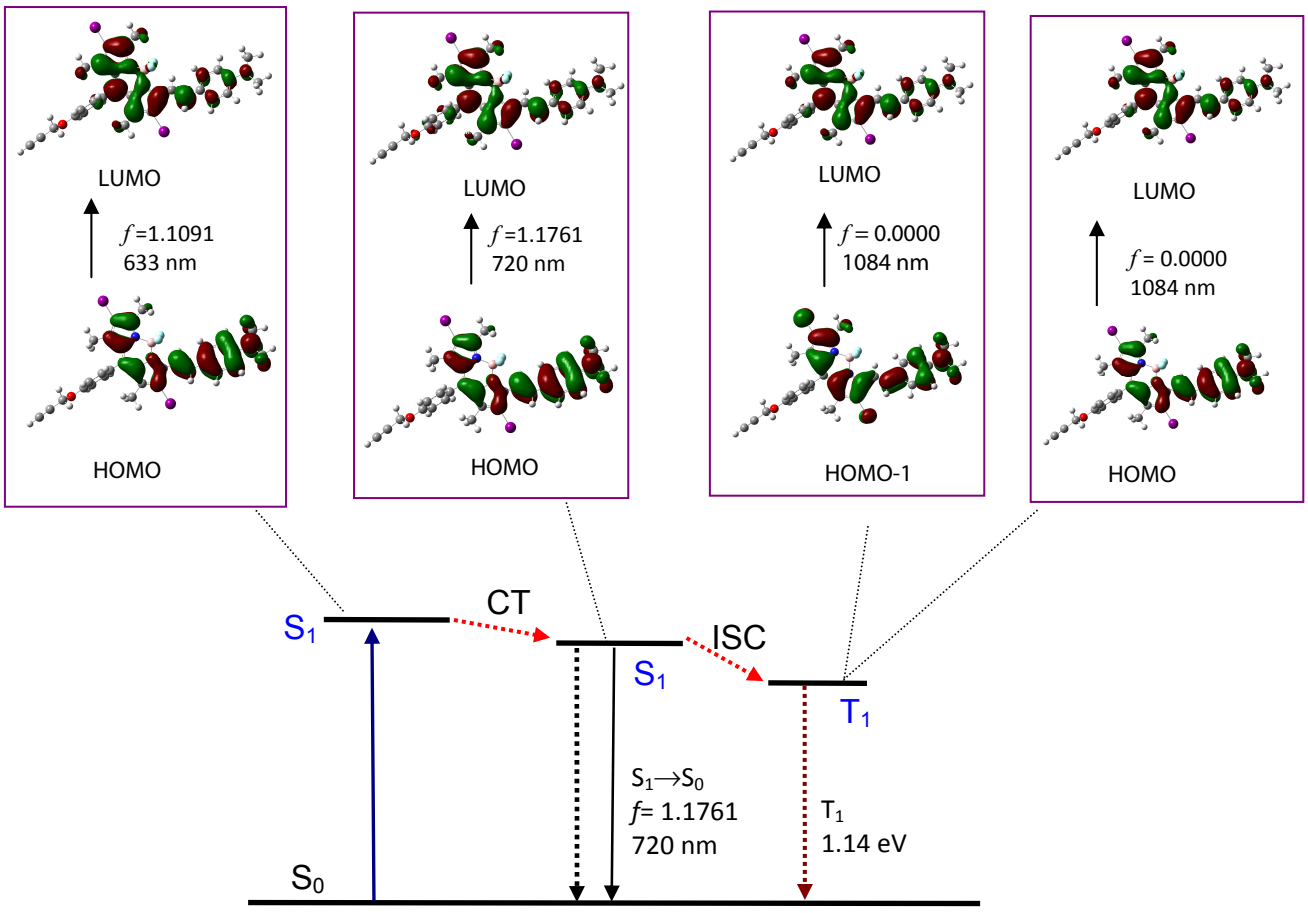


Figure S55. Selected frontier molecular orbitals involved in the excitation, emission and triplet excited states of **B-2**. CT stands for conformation transformation. DCM was used as solvent in all the calculation. The calculations are at the B3LYP/6-31G(d)/ genecp level using Gaussian 09W.

Table S6. Selected Electronic Excitation Energies (eV) and Corresponding Oscillator Strengths (*f*), Main Configurations and CI Coefficients of the Low-lying Electronically Excited States of **R-2.** Based on the optimized ground state geometries and the optimized S_1 state geometries. Calculated by TDDFT//B3LYP/ genecp.[a] (DCM was employed as solvent in all the calculation).

	Electronic transition[a]	Excitation energy	TDDFT/B3LYP/6-31G(d)		
			f [b]	Composition[c]	CI[d]
Absorption	$S_0 \rightarrow S_1$	1.71 eV (726 nm)	0.0000	H →L	0.7070
	$S_0 \rightarrow S_2$	1.95 eV (635 nm)	1.1129	H → L+1	0.7087
	$S_0 \rightarrow S_4$	2.61 eV (476 nm)	0.9155	H–2 → L	0.7050
Emission	$S_0 \rightarrow S_1$	1.27 eV (978 nm)	0.0000	H →L	0.7071
	$S_0 \rightarrow S_2$	1.76 eV (704 nm)	1.3753	H → L+1	0.7083
	$S_0 \rightarrow S_4$	2.39 eV (520 nm)	1.0503	H–2 → L	0.7060
Triplet	$S_0 \rightarrow T_1$	1.14 eV (1084 nm)	0.0000	H–1 →L+1	0.2194
excited states				H→ L+1	0.6696
	$S_0 \rightarrow T_2$	1.71 eV (726 nm)	0.0000	H→ L	0.7070

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

Table S7. Selected Electronic Excitation Energies (eV) and Corresponding Oscillator Strengths (*f*), Main Configurations and CI Coefficients of the Low-lying Electronically Excited States of **R-0.** Based on the optimized ground state geometries and the optimized S_1 state geometries. Calculated by TDDFT//B3LYP. DCM was employed as solvent in all the calculation.

	Electronic transition[a]	Excitation energy	TDDFT/B3LYP/6-31G(d)		
			f [b]	Composition[c]	CI[d]
Absorption	$S_0 \rightarrow S_1$	2.59 eV (478 nm)	0.9641	H → L	0.7057
	$S_0 \rightarrow S_2$	2.81 eV (441 nm)	0.2674	H–2 → L	0.1110
				H–1 → L	0.6932
Emission	$S_0 \rightarrow S_1$	2.37 eV (523 nm)	1.0792	H →L	0.7064
	$S_0 \rightarrow S_2$	2.71 eV (458 nm)	0.4223	H–2 → L	0.1170
				H–1 → L	0.6918
Triplet	$S_0 \rightarrow T_1$	1.72 eV (722 nm)	0.0000	H → L	0.7058
excited states	$S_0 \rightarrow T_2$	2.36 eV (526 nm)	0.0000	H–3 → L	0.1333
				H–2 → L	0.3162
				H–1 → L	0.6063

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

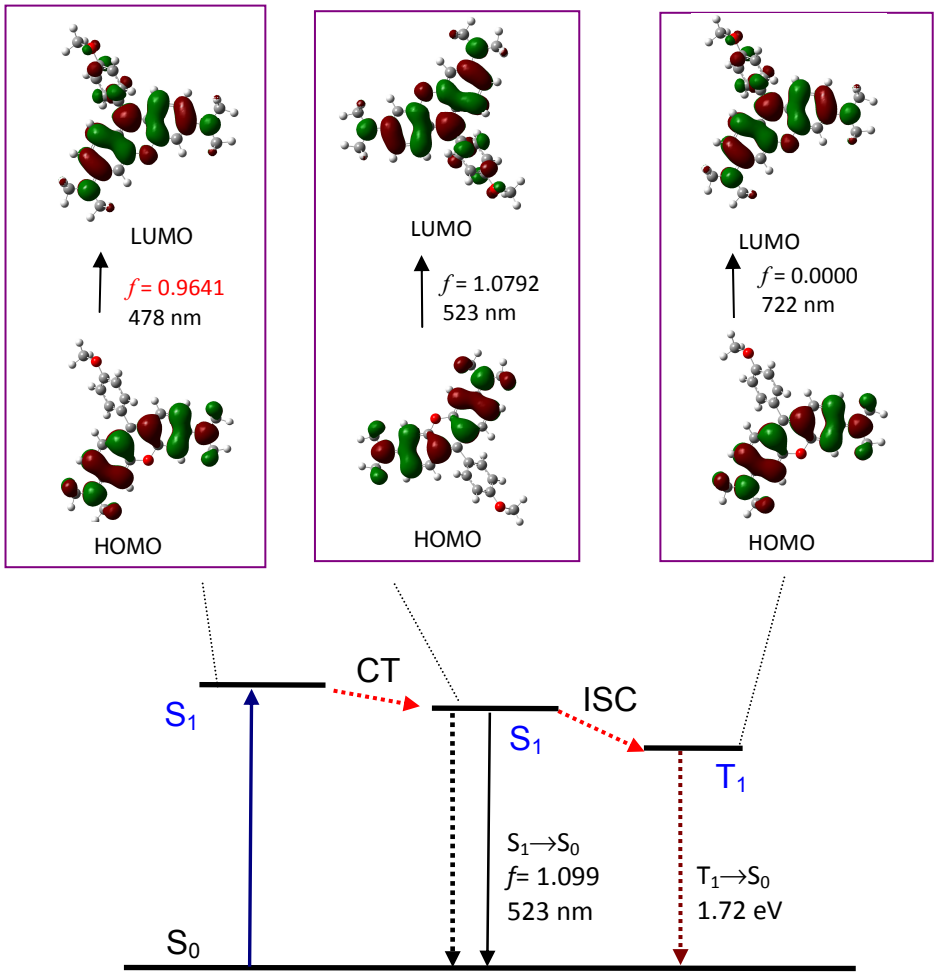
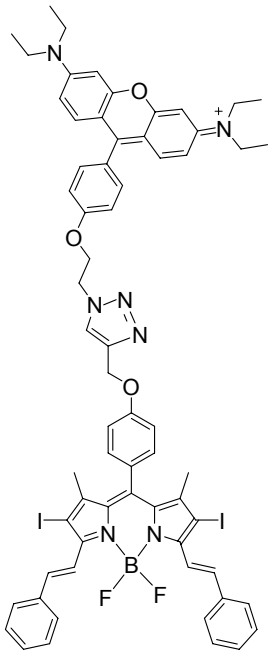


Figure S56. Selected frontier molecular orbitals involved in the excitation, emission and triplet excited states of **R-0**. CT stands for conformation transformation. DCM was employed as solvent in all the calculation. The calculations are at the B3LYP/6-31G(d) level using Gaussian 09W.

Compound R-1 (DFT//B3LYP/6-31G(d) / genecp)

Charge = 1 Multiplicity = 1



C	8.29262	-2.21828	0.12417
C	6.09062	-2.75048	-0.28557
C	6.23981	-1.33024	-0.12667
C	5.28983	-0.29191	-0.18954
C	5.67759	1.04827	0.00762
C	4.90329	2.25863	0.0153
C	7.12876	2.7292	0.37032
N	7.58064	-1.05553	0.12856
N	7.00945	1.37737	0.24302
B	8.19667	0.37075	0.2283
F	8.92263	0.4865	1.42588
F	9.03044	0.61784	-0.85851
C	4.83726	-3.52815	-0.54978
H	4.13978	-3.46865	0.29229
H	4.30796	-3.15339	-1.42978
H	5.07431	-4.58067	-0.71686
C	3.4218	2.41158	-0.15207
H	2.86965	1.82538	0.58829
H	3.13278	3.45871	-0.04123
H	3.09117	2.07159	-1.13845
C	3.86003	-0.61205	-0.47892
C	3.38015	-0.59961	-1.79952
C	2.97132	-0.9289	0.55236
C	2.05094	-0.89522	-2.07527
C	1.63042	-1.22425	0.28962
H	3.32326	-0.94542	1.58012
H	1.67645	-0.88783	-3.09409
H	0.97195	-1.4649	1.11565
C	1.16416	-1.20803	-1.03147
H	4.05463	-0.35742	-2.61599
C	7.36834	-3.27525	-0.12452
C	5.82047	3.28011	0.23832
I	5.28651	5.31874	0.49353
I	7.79772	-5.35417	-0.10072
O	-0.11723	-1.47945	-1.40884
C	-1.08671	-1.75115	-0.38238
H	-0.79581	-2.64131	0.18696
H	-1.14034	-0.89688	0.3032
C	-3.29811	-1.106	-1.59368
H	-3.29561	-0.03094	-1.68883
C	-2.40383	-1.99876	-1.03706
N	-2.90554	-3.25855	-1.19977
N	-4.05317	-3.18969	-1.81813
N	-4.29957	-1.88252	-2.07082
C	-5.5441	-1.48917	-2.71932
H	-5.80219	-2.26815	-3.43911
H	-5.37478	-0.55499	-3.25861

C	-6.67065	-1.3204	-1.69784
H	-6.84051	-2.26196	-1.16199
H	-6.41931	-0.53851	-0.97071
O	-7.82195	-0.95273	-2.4538
C	-11.32419	-0.11875	-2.05072
C	-10.42671	-0.59781	0.13871
C	-10.0845	-0.3758	-2.61726
C	-9.17047	-0.83914	-0.41777
H	-10.54705	-0.67393	1.21512
H	-9.93556	-0.30731	-3.68998
H	-8.34612	-1.10461	0.23327
C	-8.9965	-0.73263	-1.80387
H	-12.15779	0.14707	-2.69356
C	8.42238	3.32738	0.62346
C	8.80163	4.58951	0.31201
H	9.14155	2.64999	1.06911
H	8.10014	5.24504	-0.19405
C	9.71674	-2.20154	0.38053
C	10.62119	-3.12866	-0.01519
H	10.05686	-1.32122	0.91324
H	10.2896	-3.97643	-0.60581
C	-11.52084	-0.22981	-0.65934
C	10.11637	5.18202	0.55899
C	10.3707	6.47676	0.06349
C	11.1462	4.52847	1.26807
C	11.60466	7.09472	0.25985
H	9.58788	6.99659	-0.48338
C	12.37763	5.14633	1.46404
H	10.98263	3.53441	1.67281
C	12.6144	6.43125	0.96072
H	11.77724	8.0928	-0.13313
H	13.15749	4.62633	2.0135
H	13.57728	6.90938	1.11692
C	12.06014	-3.0959	0.24696
C	12.87098	-4.08782	-0.34064
C	12.68272	-2.12605	1.06091
C	14.24913	-4.10956	-0.13235
H	12.40807	-4.84519	-0.9685
C	14.05847	-2.14876	1.26861
H	12.08862	-1.35361	1.53947
C	14.84928	-3.13891	0.67316
H	14.85322	-4.88362	-0.59737
H	14.51834	-1.39339	1.89983
H	15.92274	-3.15282	0.8393
C	-12.84845	0.036	-0.05644
C	-13.47788	1.29501	-0.21669
C	-13.51925	-0.96218	0.6918
C	-12.90224	2.41313	-0.8907
C	-14.76117	1.5186	0.36425
C	-14.79208	-0.67291	1.26725
C	-13.03968	-2.29147	0.89072
C	-13.56	3.60724	-1.01287
H	-11.90835	2.31463	-1.31005
C	-15.44636	2.71248	0.25304
C	-15.51077	-1.58408	2.01559
H	-12.1004	-2.5809	0.43533

C	-13.73366	-3.21304	1.62726
C	-14.87089	3.79626	-0.45521
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H	-16.41513	2.78792	0.7277
C	-14.99469	-2.88544	2.23371
H	-16.46705	-1.27335	2.41344
H	-13.32316	-4.2078	1.73917
C	-16.85044	5.15527	-0.00327
H	-17.21548	6.15259	-0.2443
H	-17.56018	4.42232	-0.40381
H	-16.81863	5.05276	1.08813
C	-16.96447	-3.45233	3.56324
H	-17.33812	-4.30594	4.12697
H	-16.87253	-2.60062	4.24727
H	-17.69838	-3.202	2.78802
O	-15.37593	0.54286	1.08635
C	-15.13099	-5.14234	3.18314
H	-15.8097	-5.69752	3.82908
H	-14.14984	-5.10488	3.66902
H	-15.03571	-5.68624	2.23622
C	-14.90575	6.09646	-1.30479
H	-15.60058	6.93499	-1.31178
H	-14.68031	5.83039	-2.34345
H	-13.98075	6.42095	-0.81444
N	-15.67057	-3.79725	2.97528
N	-15.5235	4.97683	-0.59162

Complex R-1 (DFT//B3LYP/6-31G(d) / genecp)

Charge = 1 Multiplicity = 3

C	8.29214	-2.21834	0.12411
C	6.09011	-2.75035	-0.2857
C	6.2394	-1.33014	-0.12671
C	5.28952	-0.29172	-0.18959
C	5.67741	1.04841	0.00765
C	4.90321	2.25882	0.01559
C	7.12875	2.72918	0.37039
N	7.58025	-1.05553	0.12852
N	7.00932	1.3774	0.24292
B	8.19643	0.37066	0.22842
F	8.92214	0.48631	1.42617
F	9.03047	0.61769	-0.85819
C	4.83668	-3.52793	-0.54982
H	4.13932	-3.46837	0.29236
H	4.30728	-3.15313	-1.42974
H	5.07361	-4.58047	-0.71692
C	3.42167	2.41187	-0.1514
H	2.86974	1.8265	0.5898
H	3.13289	3.45915	-0.04143
H	3.09053	2.07097	-1.13728
C	3.85969	-0.61171	-0.47904

C	3.37991	-0.59934	-1.79967
C	2.9709	-0.92847	0.5522
C	2.05073	-0.89498	-2.07552
C	1.63004	-1.2239	0.28936
H	3.32276	-0.94492	1.57999
H	1.67632	-0.88767	-3.09437
H	0.97147	-1.46447	1.11535
C	1.16388	-1.20775	-1.03177
H	4.05445	-0.35718	-2.6161
C	7.36779	-3.27523	-0.12466
C	5.82046	3.28021	0.23867
I	5.28662	5.31883	0.49418
I	7.79705	-5.35416	-0.10107
O	-0.11745	-1.47931	-1.40925
C	-1.08701	-1.75111	-0.38292
H	-0.79596	-2.64106	0.18667
H	-1.14102	-0.89673	0.3025
C	-3.29847	-1.10681	-1.59463
H	-3.29617	-0.03178	-1.69018
C	-2.404	-1.99921	-1.03773
N	-2.90535	-3.25916	-1.20021
N	-4.05292	-3.19075	-1.81875
N	-4.29966	-1.88371	-2.07174
C	-5.54433	-1.49077	-2.72023
H	-5.80233	-2.26999	-3.4398
H	-5.37521	-0.5567	-3.25979
C	-6.67088	-1.32197	-1.69876
H	-6.84071	-2.26349	-1.16284
H	-6.41959	-0.54002	-0.97168
O	-7.82221	-0.95434	-2.45473
C	-11.3243	-0.11984	-2.05126
C	-10.42665	-0.59911	0.13804
C	-10.08475	-0.3772	-2.61799
C	-9.17053	-0.84065	-0.4186
H	-10.54689	-0.67518	1.21447
H	-9.93594	-0.30871	-3.69073
H	-8.34615	-1.1063	0.23233
C	-8.9967	-0.73415	-1.80473
H	-12.15793	0.14618	-2.69399
C	8.42248	3.32724	0.62337
C	8.80169	4.58938	0.31191
H	9.1417	2.64977	1.06881
H	8.10012	5.24491	-0.19403
C	9.71625	-2.20171	0.38064
C	10.62066	-3.12899	-0.01482
H	10.05636	-1.32134	0.91326
H	10.28909	-3.97678	-0.60544
C	-11.52077	-0.23081	-0.65986
C	10.11647	5.18191	0.55862
C	10.37062	6.47669	0.06316
C	11.14651	4.52833	1.26736
C	11.60462	7.09468	0.25918
H	9.58762	6.99654	-0.48345
C	12.37799	5.14622	1.46299
H	10.98309	3.53423	1.67207
C	12.61459	6.43118	0.9597

H	11.77704	8.0928	-0.13377
H	13.15803	4.62619	2.01218
H	13.57751	6.90932	1.11566
C	12.05956	-3.09636	0.24762
C	12.87042	-4.08847	-0.33965
C	12.68206	-2.12645	1.06155
C	14.24852	-4.11029	-0.13108
H	12.40755	-4.8459	-0.96747
C	14.05777	-2.14926	1.26954
H	12.08791	-1.35391	1.53989
C	14.8486	-3.13956	0.67439
H	14.85264	-4.88448	-0.59585
H	14.51758	-1.39384	1.90075
H	15.92203	-3.15356	0.84076
C	-12.84821	0.03566	-0.0568
C	-13.47689	1.29505	-0.21684
C	-13.51939	-0.96214	0.6916
C	-12.90072	2.41287	-0.89093
C	-14.7599	1.51942	0.36445
C	-14.79196	-0.67216	1.26725
C	-13.04049	-2.29167	0.89054
C	-13.55767	3.60746	-1.01266
H	-11.90705	2.3137	-1.31066
C	-15.44431	2.71378	0.25361
C	-15.51109	-1.58294	2.01565
H	-12.10135	-2.58158	0.43517
C	-13.73489	-3.21285	1.62719
C	-14.86821	3.79734	-0.45445
H	-13.06805	4.42132	-1.53077
H	-16.41292	2.78982	0.72851
C	-14.99571	-2.8846	2.23369
H	-16.46714	-1.27165	2.41363
H	-13.32479	-4.20776	1.73922
C	-16.84636	5.15789	-0.00101
H	-17.21057	6.15571	-0.24124
H	-17.55708	4.42588	-0.40151
H	-16.81392	5.05472	1.0903
C	-16.96585	-3.45058	3.56303
H	-17.33982	-4.30393	4.12693
H	-16.87369	-2.59875	4.24687
H	-17.69962	-3.20016	2.78769
O	-15.37508	0.54401	1.08664
C	-15.13332	-5.14154	3.18274
H	-15.81241	-5.69648	3.82849
H	-14.15216	-5.10487	3.66864
H	-15.03839	-5.68517	2.23563
C	-14.90137	6.09797	-1.30291
H	-15.59511	6.93743	-1.30843
H	-14.67729	5.83261	-2.34204
H	-13.9755	6.42067	-0.81306
N	-15.67201	-3.79604	2.9753
N	-15.51995	4.97846	-0.59029

R-2 (DFT//B3LYP/6-31G(d) / genecp)

Charge = 1 Multiplicity = 1

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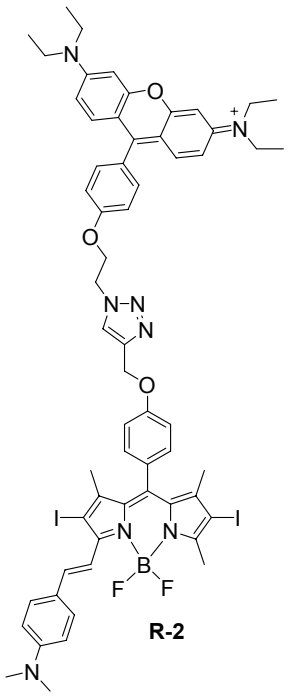
C	-6.48357	2.39572	-0.29048
C	-5.66733	1.24419	-0.34892
C	-6.22566	-0.03659	-0.19127
C	-5.61922	-1.33966	-0.25335
C	-7.87354	-1.53163	0.19306
N	-7.86681	2.26807	-0.14422
N	-7.58587	-0.20182	0.0738
B	-8.64739	0.93475	-0.00464
F	-9.41644	0.97328	1.16639
F	-9.47944	0.7414	-1.11049
C	-4.81951	4.44782	-0.44112
H	-4.08368	3.98315	0.2198
H	-4.41834	4.38883	-1.45941
H	-4.89861	5.5056	-0.17744
C	-4.18915	-1.68842	-0.53675
H	-3.54941	-1.52637	0.33825
H	-4.10804	-2.74136	-0.81626
H	-3.78095	-1.08435	-1.34984
C	-4.20102	1.40097	-0.57105
C	-3.6946	1.67977	-1.85226
C	-3.29938	1.28343	0.49173
C	-2.32917	1.82534	-2.06083
C	-1.9242	1.44115	0.29887
H	-3.67142	1.07171	1.49017
H	-1.9334	2.03214	-3.05024
H	-1.25838	1.35079	1.14879
C	-1.43251	1.71068	-0.98529
H	-4.37712	1.77429	-2.69206
C	-7.39245	4.44451	-0.22479
C	-6.64623	-2.23924	-0.00387
I	-6.33946	-4.33036	0.2028
I	-7.69958	6.54303	-0.21883
O	-0.11614	1.87942	-1.29615
C	0.85494	1.74718	-0.244
H	0.66079	2.4863	0.54161
H	0.78803	0.74353	0.19246
C	3.03738	1.13952	-1.52609
H	2.94396	0.10618	-1.82345
C	2.20812	1.98993	-0.822
N	2.82341	3.20638	-0.73508
N	3.97836	3.15001	-1.34019
N	4.11733	1.89651	-1.83318
C	5.34486	1.52144	-2.52355
H	5.66991	2.38046	-3.11378
H	5.12281	0.69454	-3.20078
C	6.43702	1.12546	-1.52804
H	6.63944	1.95592	-0.84138
H	6.13076	0.24835	-0.9444
O	7.5885	0.82988	-2.31511



R-2

C	11.0834	-0.06566	-1.98009
C	10.13893	0.05346	0.23837
C	9.85455	0.27854	-2.52371
C	8.89421	0.38241	-0.29787
H	10.23542	-0.04711	1.31511
H	9.72859	0.38471	-3.5963
H	8.05561	0.53917	0.37002
C	8.74945	0.50278	-1.68631
H	11.93113	-0.22174	-2.64017
C	-9.21512	-1.95385	0.49886
C	-9.75865	-3.18805	0.30996
H	-9.84152	-1.16182	0.89161
H	-9.15062	-3.9722	-0.12961
C	11.25174	-0.17938	-0.58497
C	-11.11864	-3.5843	0.61586
C	-11.53584	-4.90096	0.32094
C	-12.08358	-2.73217	1.20082
C	-12.81983	-5.34902	0.5836
H	-10.82441	-5.58947	-0.1296
C	-13.37036	-3.16006	1.4709
H	-11.82193	-1.70847	1.45227
C	-13.78483	-4.48789	1.16956
H	-13.07831	-6.37076	0.33358
H	-14.06584	-2.46211	1.92089
C	12.56735	-0.53331	-0.0025
C	13.22138	-1.7382	-0.3617
C	13.20325	0.32651	0.92757
C	12.68599	-2.72657	-1.241
C	14.49045	-2.04689	0.2114
C	14.46359	-0.04655	1.48195
C	12.70204	1.59809	1.3383
C	13.36921	-3.87111	-1.553
H	11.70278	-2.56858	-1.6674
C	15.19909	-3.1941	-0.08624
C	15.1505	0.72832	2.39558
H	11.77253	1.9552	0.91204
C	13.3641	2.38468	2.24193
C	14.66627	-4.14008	-0.99611
H	12.90974	-4.58697	-2.2217
H	16.15481	-3.33991	0.39826
C	14.61287	1.9688	2.81851
H	16.10021	0.36106	2.75979
H	12.9379	3.34184	2.51152
C	16.64961	-5.53812	-0.71485
H	17.03383	-6.48055	-1.10254
H	17.36905	-4.74687	-0.95589
H	16.57054	-5.61979	0.37575
C	16.54256	2.31958	4.27518
H	16.88684	3.06291	4.99289
H	16.44809	1.35831	4.79323
H	17.30017	2.22125	3.48838
O	15.06846	-1.20772	1.11289
C	-9.89924	3.7077	0.04071
H	-10.21251	3.53458	1.07696
H	-10.45394	3.00672	-0.58858
H	-10.1703	4.72853	-0.23471

C	-8.42916	3.49645	-0.11112
C	-15.45741	-6.28057	1.11915
H	-16.49889	-6.42608	1.40657
H	-15.36701	-6.49108	0.0451
H	-14.84776	-7.01432	1.66302
N	-15.06168	-4.91439	1.43451
C	14.69966	4.03635	4.13433
H	15.35609	4.4811	4.88083
H	13.70683	3.91442	4.58108
H	14.62355	4.72847	3.28763
C	14.78312	-6.23886	-2.25965
H	15.50638	-7.03826	-2.41462
H	14.57275	-5.77542	-3.22971
H	13.8585	-6.68225	-1.87188
N	15.25746	2.74662	3.72282
N	15.34635	-5.26732	-1.32049
C	-16.03167	-4.00559	2.03153
H	-16.98154	-4.52682	2.15143
H	-15.707	-3.65751	3.0211
H	-16.20425	-3.12486	1.39907

R-2 (DFT//B3LYP/6-31G(d) / genecp)

Charge = 1 Multiplicity = 3

C	-6.16252	3.78994	-0.33233
C	-6.48389	2.39519	-0.29085
C	-5.66732	1.24382	-0.34835
C	-6.2254	-0.037	-0.19027
C	-5.61855	-1.33998	-0.25081
C	-7.87319	-1.53225	0.1939
N	-7.86716	2.26728	-0.14534
N	-7.5858	-0.20244	0.07374
B	-8.64752	0.93381	-0.00643
F	-9.41808	0.97246	1.1637
F	-9.47819	0.73994	-1.11318
C	-4.82007	4.44751	-0.44065
H	-4.08519	3.9843	0.22239
H	-4.41717	4.38659	-1.45812
H	-4.89989	5.50576	-0.17911
C	-4.18816	-1.68875	-0.53265
H	-3.54974	-1.52823	0.34362
H	-4.10701	-2.74136	-0.81345
H	-3.7785	-1.08374	-1.34426
C	-4.201	1.401	-0.57002
C	-3.69449	1.67949	-1.85128
C	-3.29944	1.28397	0.49287
C	-2.32909	1.82531	-2.05977
C	-1.92426	1.44183	0.30007
H	-3.67152	1.07247	1.49134
H	-1.93327	2.0319	-3.0492
H	-1.25849	1.35177	1.15006
C	-1.43251	1.7111	-0.98412
H	-4.37697	1.77358	-2.69117
C	-7.39317	4.44383	-0.22585
C	-6.64543	-2.23962	-0.00124

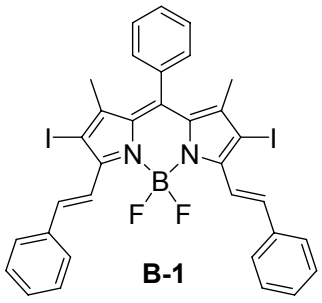
I	-6.33789	-4.33046	0.20718
I	-7.70071	6.5423	-0.21975
O	-0.11615	1.88	-1.29495
C	0.85499	1.74825	-0.24277
H	0.66039	2.48724	0.54285
H	0.78863	0.74454	0.19365
C	3.03811	1.1425	-1.52487
H	2.94562	0.10917	-1.82259
C	2.20805	1.99204	-0.82066
N	2.82251	3.20886	-0.73302
N	3.97766	3.15355	-1.33784
N	4.11764	1.90036	-1.83133
C	5.34546	1.52665	-2.52196
H	5.67068	2.38693	-3.11023
H	5.12368	0.70117	-3.20101
C	6.4373	1.12861	-1.52694
H	6.63954	1.95766	-0.83853
H	6.13089	0.25031	-0.94519
O	7.589	0.83463	-2.31433
C	11.08392	-0.06134	-1.98069
C	10.13918	0.0532	0.2379
C	9.85508	0.28382	-2.52374
C	8.89448	0.38306	-0.2978
H	10.23561	-0.04947	1.31445
H	9.72923	0.39214	-3.59614
H	8.05581	0.53835	0.37034
C	8.74987	0.50627	-1.68602
H	11.93173	-0.21595	-2.641
C	-9.21504	-1.95454	0.49836
C	-9.75771	-3.18945	0.31156
H	-9.84243	-1.16198	0.88844
H	-9.14846	-3.9746	-0.1245
C	11.25212	-0.17785	-0.58578
C	-11.11814	-3.58543	0.6158
C	-11.53346	-4.90379	0.32596
C	-12.08541	-2.73133	1.19405
C	-12.81769	-5.3518	0.5876
H	-10.82035	-5.59376	-0.11965
C	-13.37249	-3.1591	1.46286
H	-11.8255	-1.70604	1.44078
C	-13.78491	-4.48885	1.16714
H	-13.07457	-6.37496	0.34175
H	-14.0699	-2.45953	1.90732
C	12.56768	-0.53265	-0.00373
C	13.22217	-1.73664	-0.36511
C	13.20307	0.32548	0.92827
C	12.68744	-2.72337	-1.24666
C	14.49092	-2.04633	0.20817
C	14.46325	-0.0484	1.48245
C	12.70147	1.59617	1.34123
C	13.37099	-3.86719	-1.56054
H	11.70438	-2.56477	-1.67317
C	15.19981	-3.19293	-0.09124
C	15.14961	0.72481	2.3979
H	11.77215	1.95403	0.91515
C	13.36294	2.38112	2.24673

C	14.66773	-4.13715	-1.00332
H	12.91177	-4.58201	-2.23051
H	16.15536	-3.33945	0.3934
C	14.61154	1.96435	2.823
H	16.09897	0.35677	2.76224
H	12.93661	3.33782	2.51774
C	16.64879	-5.53793	-0.71963
H	17.03234	-6.48076	-1.10703
H	17.37075	-4.74794	-0.9573
H	16.56582	-5.62066	0.3706
C	16.54082	2.31305	4.28073
H	16.88721	3.05769	4.99605
H	16.4459	1.353	4.8011
H	17.29713	2.21198	3.49312
O	15.06832	-1.2089	1.11164
C	-9.90015	3.70643	0.03707
H	-10.21496	3.53384	1.07293
H	-10.45365	3.00492	-0.59266
H	-10.17114	4.72697	-0.23947
C	-8.42977	3.49556	-0.11258
C	-15.45627	-6.28286	1.1199
H	-16.4983	-6.42789	1.40556
H	-15.36336	-6.49724	0.04682
H	-14.84743	-7.01426	1.6678
N	-15.06194	-4.91536	1.43131
C	14.69462	4.02692	4.14674
H	15.34815	4.46809	4.89789
H	13.70078	3.90043	4.58993
H	14.61964	4.72415	3.30412
C	14.78596	-6.23343	-2.27103
H	15.51235	-7.02873	-2.43236
H	14.5705	-5.76634	-3.23811
H	13.8645	-6.68271	-1.88235
N	15.25575	2.7407	3.72882
N	15.34819	-5.26369	-1.32941
C	-16.03479	-4.00411	2.01998
H	-16.98376	-4.52642	2.14225
H	-15.71233	-3.64831	3.00748
H	-16.20806	-3.12829	1.38087

B-1 (DFT//B3LYP/6-31G(d) / genecp)

Charge = 0 Multiplicity = 1

C	-9.80211	-0.93032	-0.23915
C	-7.76929	-1.97681	-0.03711
C	-7.60203	-0.55116	-0.05878
C	-6.44797	0.25052	0.0119
C	-6.5405	1.65475	-0.02459
C	-5.52746	2.67122	-0.01191
C	-7.61472	3.61726	-0.13877
N	-8.8663	0.03644	-0.17643
N	-7.78836	2.28161	-0.10652
B	-9.16864	1.56413	-0.17655
F	-9.83374	1.92126	-1.34657
F	-9.93729	1.89638	0.94081



B-1

C	-6.72493	-3.04338	0.09325
H	-6.11567	-3.12725	-0.81369
H	-6.03931	-2.84284	0.92068
H	-7.19924	-4.01214	0.26746
C	-4.0389	2.51373	0.05173
H	-3.6705	1.81967	-0.70879
H	-3.55433	3.48064	-0.10213
H	-3.71334	2.12465	1.02266
C	-5.10554	-0.39401	0.11985
C	-4.4893	-0.55815	1.37153
C	-4.43321	-0.84166	-1.02081
C	-3.2667	-1.15927	1.45993
C	-3.16979	-1.43312	-0.93227
H	-4.89555	-0.72652	-1.99723
H	-2.80729	-1.28803	2.43491
H	-2.67927	-1.76916	-1.83812
H	-4.99713	-0.21896	2.27003
C	-9.14306	-2.17888	-0.15806
C	-6.22589	3.87556	-0.0807
I	-5.37676	5.81659	-0.10632
I	-10.13372	-4.05038	-0.22776
C	-8.79388	4.6023	-0.24299
C	-8.62833	5.91745	-0.27508
H	-9.78303	4.12723	-0.28857
H	-7.63918	6.39252	-0.22951
C	-11.30361	-0.61932	-0.3819
C	-12.22896	-1.5669	-0.44411
H	-11.54586	0.4509	-0.42801
H	-11.98671	-2.63712	-0.39799
C	-9.8075	6.90249	-0.37927
C	-9.56841	8.27625	-0.40872
C	-11.11545	6.42051	-0.44384
C	-10.63669	9.16854	-0.50392
H	-8.53777	8.65635	-0.35822
C	-12.18345	7.31267	-0.53854
H	-11.30372	5.33732	-0.42055
C	-11.94406	8.68678	-0.56898
H	-10.44794	10.25157	-0.52757
H	-13.21439	6.93312	-0.58944
H	-12.78616	9.38991	-0.64383
C	-13.73046	-1.25591	-0.58688
C	-14.656	-2.29753	-0.64698
C	-14.16502	0.0683	-0.65652
C	-16.01634	-2.01567	-0.77553
H	-14.31389	-3.34115	-0.59176
C	-15.52499	0.35001	-0.78551
H	-13.43507	0.88941	-0.60917
C	-16.45078	-0.69202	-0.84462
H	-16.74593	-2.83703	-0.82244
H	-15.86779	1.39354	-0.84043
H	-17.52288	-0.4697	-0.94612
H	-1.49108	-2.06795	0.4167
C	-2.56491	-1.58812	0.32166

Complex B-1 (DFT//B3LYP/6-31G(d) / genecp)

Charge = 0 Multiplicity = 3

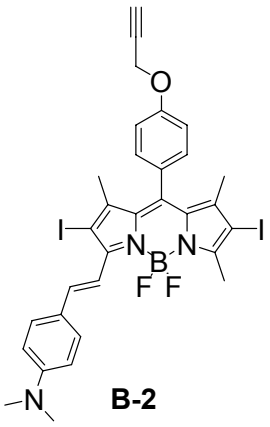
C	-2.54327	0.07534	-0.09402
C	-2.57946	-2.22334	0.02032
C	-1.22438	-1.74546	-0.00518
C	-0.0001	- 2.44074	0.03862
C	1.22421	-1.74553	-0.00518
C	2.57927	-2.2235	0.02023
C	2.5432	0.07519	-0.094
N	-1.2505	-0.35604	-0.0873
N	1.25041	-0.35613	-0.08729
B	-0.00002	0.56899	-0.0314
F	0.00001	1.42638	-1.14502
F	0.00001	1.31664	1.14274
C	-3.06135	-3.64115	0.07241
H	-2.72692	-4.2129	-0.79879
H	-2.68609	-4.16129	0.95844
H	-4.15237	-3.66968	0.09863
C	3.06105	-3.64135	0.07222
H	2.72602	-4.21318	-0.79868
H	4.15209	-3.66999	0.09779
H	2.68628	-4.16132	0.95856
C	-0.00016	-3.93319	0.12773
C	0.00009	-4.57018	1.37681
C	-0.00045	-4.70878	-1.04009
C	0.00004	-5.96466	1.45474
C	-0.00049	-6.10292	-0.95907
H	-0.00064	-4.21937	-2.01006
H	0.00022	-6.44871	2.42725
H	-0.00072	-6.69457	-1.87012
H	0.00032	-3.97334	2.28466
C	-3.37292	-1.08238	-0.03359
C	3.37279	-1.08258	-0.03364
I	5.49112	-1.11517	-0.16454
I	-5.49126	-1.11488	-0.16457
C	2.83904	1.48887	-0.18932
C	3.95617	2.11158	0.25531
H	2.04108	2.07596	-0.62908
H	4.72219	1.53174	0.76009
C	-2.83897	1.48905	-0.18934
C	-3.95605	2.11189	0.25522
H	-2.04091	2.07604	-0.62907
H	-4.72223	1.53212	0.75984
C	4.23969	3.54393	0.16201
C	5.38904	4.04345	0.80699
C	3.42464	4.45517	-0.542
C	5.70979	5.39925	0.76111
H	6.03082	3.35518	1.35149
C	3.74627	5.80829	-0.5883
H	2.53867	4.10386	-1.06188
C	4.88869	6.28823	0.06349
H	6.60002	5.76075	1.26824
H	3.10603	6.49348	-1.13704

H	5.13582	7.34535	0.0238
C	-4.23935	3.54431	0.16207
C	-5.38898	4.04382	0.80652
C	-3.42379	4.45561	-0.5413
C	-5.70959	5.39966	0.7607
H	-6.03112	3.35551	1.35055
C	-3.74527	5.80875	-0.58754
H	-2.5375	4.10433	-1.06065
C	-4.88803	6.28868	0.06368
H	-6.60006	5.76115	1.26742
H	-3.10465	6.49399	-1.13577
H	-5.13504	7.34583	0.02404
H	-0.00029	-7.81772	0.34997
C	-0.00026	-6.73324	0.28782

B-2 (DFT//B3LYP/6-31G(d) / genecp)

Charge = 0 Multiplicity = 1

C	-8.00533	-1.99341	-0.04025
C	-7.83806	-0.56776	-0.06192
C	-6.684	0.23391	0.00876
C	-6.77653	1.63815	-0.02772
C	-5.76349	2.65462	-0.01504
C	-7.85075	3.60066	-0.14191
N	-9.10233	0.01984	-0.17957
N	-8.02439	2.26501	-0.10966
B	-9.40467	1.54753	-0.17969
F	-10.06977	1.90465	-1.34971
F	-10.17332	1.87978	0.93767
C	-6.96096	-3.05998	0.09011
H	-6.3517	-3.14385	-0.81683
H	-6.27534	-2.85944	0.91754
H	-7.43527	-4.02874	0.26432
C	-4.27493	2.49713	0.04859
H	-3.90653	1.80306	-0.71193
H	-3.79036	3.46404	-0.10527
H	-3.94938	2.10804	1.01952
C	-5.34157	-0.41062	0.11671
C	-4.72533	-0.57476	1.36839
C	-4.66924	-0.85826	-1.02395
C	-3.47333	-1.16788	1.47141
C	-3.40582	-1.44973	-0.93541
H	-5.13158	-0.74312	-2.00037
H	-2.85764	-1.01513	2.38342
H	-3.05253	-2.07245	-1.78587
H	-5.23316	-0.23557	2.26689
C	-9.37909	-2.19548	-0.1612
C	-6.46192	3.85896	-0.08384
I	-5.6128	5.79999	-0.10946
I	-10.32294	-4.03871	-0.69463
C	-9.02992	4.5857	-0.24613
C	-8.86436	5.90085	-0.27822
H	-10.01906	4.11063	-0.2917
H	-7.87521	6.37592	-0.23265
C	-10.04353	6.88589	-0.38241



B-2

C	-9.80444	8.25964	-0.41186
C	-11.35148	6.40391	-0.44698
C	-10.87272	9.15193	-0.50706
H	-8.7738	8.63975	-0.36136
C	-12.41948	7.29606	-0.54168
H	-11.53975	5.32072	-0.42369
C	-12.18009	8.67017	-0.57212
H	-10.68397	10.23497	-0.53071
H	-13.45042	6.91652	-0.59258
C	-11.08769	-0.76148	-0.33693
H	-11.26265	0.29383	-0.36131
H	-11.60217	-1.18912	0.49814
H	-11.44781	-1.20373	-1.24227
C	-10.03814	-0.94693	-0.24229
C	-14.56914	8.93458	-1.21479
C	-12.96647	10.81842	-1.55059
H	-14.83997	8.07833	-0.55124
H	-15.44456	9.62565	-1.27416
H	-14.36766	8.5374	-2.23904
H	-12.06947	11.33494	-1.1318
H	-12.72309	10.4703	-2.58358
H	-13.80018	11.55855	-1.61876
N	-13.35945	9.65491	-0.67695
C	-0.71373	-1.03258	0.30023
H	-0.81567	-0.28016	1.11967
H	-0.77234	-0.49421	-0.67688
C	-2.80095	-1.60473	0.31852
O	-1.78991	-2.07322	0.3985
C	0.68014	-1.67794	0.41077
C	1.76175	-2.17872	0.49654
H	2.72208	-2.62335	0.5727

B-2 (DFT//B3LYP/6-31G(d) / genecp)

Charge = 0 Multiplicity = 3

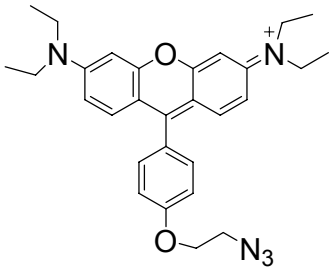
C	-3.1649	2.04581	-0.08349
C	-2.02023	1.18723	-0.0245
C	-1.9023	-0.22007	-0.05757
C	-0.63692	-0.83172	-0.07289
C	-0.26488	-2.22183	-0.07511
C	1.61952	-0.89338	-0.10319
N	-0.87656	1.98492	0.05808
N	0.53147	-0.06884	-0.08856
B	0.5871	1.47413	0.10772
F	1.31924	2.07547	-0.92522
F	1.16811	1.78446	1.34033
C	-4.61312	1.67866	-0.20512
H	-4.78172	0.94509	-0.99811
H	-5.00069	1.24166	0.72187
H	-5.20869	2.56736	-0.42903
C	-1.16138	-3.42249	-0.05173
H	-1.64486	-3.58694	-1.02114
H	-0.5844	-4.31799	0.1891
H	-1.9569	-3.31609	0.68932

C	-3.13992	-1.05379	-0.08083
C	-3.85577	-1.2996	1.09501
C	-3.61887	-1.59831	-1.28438
C	-5.01829	-2.07578	1.08871
C	-4.77916	-2.36198	-1.30756
H	-3.08035	-1.41575	-2.20993
H	-5.54015	-2.24913	2.02231
H	-5.15578	-2.77975	-2.23588
H	-3.50292	-0.88619	2.03556
C	-2.64389	3.34113	-0.01928
C	1.12252	-2.23487	-0.10268
I	2.27302	-4.01117	-0.28222
I	-3.75713	5.14589	-0.05888
C	2.94545	-0.33474	-0.14448
C	4.11174	-0.94926	0.19565
H	2.97109	0.70385	-0.45198
H	4.08313	-1.97329	0.55364
C	5.43598	-0.36162	0.16092
C	6.54046	-1.12491	0.59898
C	5.71295	0.95052	-0.28737
C	7.83341	-0.62805	0.59845
H	6.37132	-2.14005	0.95121
C	6.99645	1.46486	-0.29623
H	4.90494	1.58542	-0.63895
C	8.10477	0.69119	0.14933
H	8.63808	-1.26386	0.94688
H	7.14794	2.47707	-0.65093
C	-0.24535	4.3989	0.15177
H	0.26617	4.536	-0.80811
H	0.52039	4.17283	0.89868
H	-0.73918	5.33545	0.41703
C	-1.23811	3.28673	0.06964
C	9.62666	2.55826	-0.32388
C	10.49425	0.38719	0.60947
H	9.08794	3.30029	0.28019
H	10.69317	2.7716	-0.24973
H	9.32561	2.6874	-1.37194
H	10.36549	0.08518	1.65735
H	10.61317	-0.52153	0.00449
H	11.4147	0.96667	0.535
N	9.37893	1.20072	0.14414
C	-7.36849	-3.65523	0.9301
H	-7.7136	-2.71724	1.38624
H	-6.74351	-4.17625	1.66827
C	-5.48513	-2.60915	-0.11926
O	-6.60664	-3.37652	-0.25134
C	-8.50995	-4.48717	0.55981
C	-9.46046	-5.17677	0.28125
H	-10.30039	-5.78631	0.02979

R-0 (DFT//B3LYP/6-31G(d))

Charge = 1 Multiplicity = 1

C	-2.54125	-1.0103	2.07279
C	-1.17662	-1.0103	2.07279
C	-0.44373	0.22092	2.07279
C	-1.16773	1.45267	2.06727
C	-2.59997	1.41118	2.06597
C	-3.26375	0.21889	2.06934
C	0.95517	0.24381	2.07769
C	0.93159	2.68672	2.07118
C	1.65556	1.45502	2.0786
C	3.08774	1.49664	2.08571
H	3.63361	0.54112	2.09231
C	3.75148	2.689	2.08675
C	1.66435	3.91797	2.07121
H	-3.10712	-1.95358	2.07519
H	-0.6073	-1.95203	2.0759
H	-3.14578	2.36673	2.06137
H	4.85088	2.7249	2.09291
H	1.09481	4.85958	2.06494
C	3.02899	3.91811	2.07858
N	3.63136	5.06291	2.07784
C	2.79522	6.05701	2.76597
H	1.78692	5.97813	2.41666
H	2.82245	5.8774	3.82044
H	3.16766	7.03908	2.5617
C	4.91957	4.93922	2.77508
H	5.60423	4.38858	2.16439
H	5.31675	5.91421	2.96617
H	4.77539	4.42482	3.70217
N	-4.73296	0.17056	2.06743
C	-5.20096	-0.55343	3.25811
H	-6.24292	-0.36041	3.40627
H	-5.0489	-1.60349	3.11973
H	-4.6517	-0.22338	4.11502
C	-5.19884	-0.52274	0.85781
H	-4.96554	-1.56439	0.93153
H	-6.25747	-0.40026	0.7619
H	-4.71263	-0.10821	-0.00048
C	1.73528	-1.08397	2.08373
C	2.06294	-1.69495	3.29443
C	2.11418	-1.67582	0.87887
C	2.76993	-2.89718	3.30019
H	1.76475	-1.2277	4.24417
C	2.82053	-2.87892	0.88444
H	1.85585	-1.1945	-0.07545
C	3.14857	-3.48957	2.09482
H	3.02879	-3.3785	4.25446
H	3.11879	-3.34555	-0.06571
C	5.27713	-4.45074	2.07537
H	5.81924	-5.37299	2.09712
H	5.52048	-3.91496	1.18172
H	5.54202	-3.86112	2.92806
O	3.87338	-4.72226	2.10105
O	-0.46735	2.66384	2.06555



R-0

Complex R-0 (DFT//B3LYP/6-31G(d))

Charge = 1 Multiplicity = 3

C	3.4598	1.36502	-0.0765
C	2.09256	1.48086	-0.04098
C	1.23452	0.33863	0.01566
C	1.89603	-0.9269	-0.0181
C	3.26753	-1.07405	-0.053
C	4.09985	0.07638	-0.06814
C	-0.18526	0.39655	0.05519
C	-0.22988	-2.06958	-0.00821
C	-0.92002	-0.82033	0.04889
C	-2.34366	-0.90989	0.14533
H	-2.9176	0.00213	0.24147
C	-3.00115	-2.11482	0.13439
C	-0.86367	-3.29515	-0.02202
H	4.05915	2.26316	-0.12374
H	1.64746	2.46667	-0.06735
H	3.67263	-2.07469	-0.07602
H	-4.07879	-2.12306	0.21612
H	-0.25335	-4.18477	-0.06729
C	-2.28124	-3.35648	0.03424
N	-2.93775	-4.54988	0.01141
C	-2.18228	-5.81105	-0.06891
H	-1.57529	-5.84925	-0.98042
H	-1.52264	-5.9333	0.79785
H	-2.88242	-6.64412	-0.0875
C	-4.40896	-4.60563	0.07976
H	-4.86498	-4.057	-0.75114
H	-4.72433	-5.64547	0.01541
H	-4.78067	-4.1913	1.02357
N	5.45746	-0.03372	-0.09018
C	6.31294	1.16618	-0.11277
H	7.35575	0.85451	-0.10034
H	6.14226	1.76032	-1.0173
H	6.13282	1.79713	0.76401
C	6.09485	-1.36086	-0.10037
H	5.8076	-1.93127	-0.99115
H	7.17602	-1.23569	-0.10674
H	5.81893	-1.93762	0.78963
C	-0.88603	1.70257	0.10355
C	-0.63798	2.6191	1.15117
C	-1.81298	2.06276	-0.8933
C	-1.29866	3.8412	1.19999
H	0.05714	2.35769	1.94154
C	-2.46803	3.29683	-0.86244
H	-2.00721	1.38467	-1.71741
C	-2.21362	4.1883	0.1905
H	-1.12448	4.54002	2.0095
H	-3.16094	3.54887	-1.65455
C	-3.77949	5.86402	-0.68035
H	-4.09728	6.85314	-0.35579
H	-3.31534	5.9271	-1.66948
H	-4.63919	5.18751	-0.71253
O	-2.81052	5.4283	0.32398
O	1.15622	-2.09982	-0.03528