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Intracellular Modulation of Excited-State Dynamics in a Chromophore Dyad: Differential Enhancement of Photocytotoxicity Targeting Cancer Cells**

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1. Experimental Section

1.1. General

All chemicals and solvents obtained from suppliers were used without further purification in the case of synthetic studies. During the photophysical characterizations, all solvents were dried and redistilled before use. Reactions were monitored by thin layer chromatography using Merck TLC Silica gel 60 F_{254}. Chromatography on silica gel was performed over Tirupati Industries (India) Limited silica gel 60 (200-400 mesh ASTM). ^{1}H NMR and ^{13}C NMR spectra were recorded at room temperature on Bruker DPX-400 (operating at 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR) in $CDCl_3$ with tetramethylsilane (TMS) as internal standard. Coupling constants (*J values*) are given in Hz and chemical shifts are reported in parts per million (ppm). Splitting patterns are designated as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and p (pentet). Electronic absorption spectra in solution were acquired using a Varian Cary-100 spectrophotometer and a StellarNet BLACK Comet C-SR diode array miniature spectrophotometer connected to deuterium and halogen lamp by optical fiber using 1 cm matched quartz cuvettes at room temperature. Fluorescence spectra were determined on Varian Eclipse and Edinburgh Instruments FLS920 fluorospectrometer. Fluorescence lifetime of S_1 state was measured by time-correlated single photon counting method (Edinburgh FLS920 spectrophotometer) with excitation at 509 nm by a portable diode laser (150 ps FWHM) and emission was monitored at 520 nm. The lifetime values were computed by the F900 software. All spectra were corrected for the sensitivity of the photo-multiplier tube. Mass spectra were recorded on Agilent Technologies 6530 Accurate-Mass Q-TOF LC/MS. Singlet oxygen phosphorescence at 1270 nm was determined by using Horiba Jobin-Yvon Fluoremeter with Hamamatsu NIR PMT module, model H-10330-75. The decays were analyzed with a multiexponential fitting function by iterative reconvolution and chi-square minimization.

1.2. Synthetic Pathways

Compound (1):

To a 1 L round-bottomed flask containing 400 mL argon-degassed dichloroethane, 2,4-Dimethyl pyrrole (9.56 mmol, 0.924 g) and benzoyl chloride (4,34 mmol, 0.611 g) were added. The solution was refluxed for 1 day at 90^{o}C. After that, 5 mL of Et_3N and 5 mL of $BF_3.OEt_2$ were successively added and after 30 min, the reaction mixture was washed three times with water (3 x 100 mL), which was then extracted into the CH_2Cl_2 (3 x 100 mL) and dried over anhydrous Na_2SO_4. The solvent was evaporated and the residue was purified by silica gel column chromatography using (5 Hexane: 1 EtOAc) as the eluent. Red solid (0.631 g, 45%). ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.51-7.49 (3H, m, Ar*H*), 7.30-7.28 (2H, m, Ar*H*), 6.00 (2H, s, Ar*H*), 2.58 (6H, s, CH_3), 1.39 (6H, s, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 155.5, 143.3, 141.9, 135.1, 131.5, 129.1, 128.9, 127.9, 121.2, 14.6, 14.4 ppm. MS (TOF- ESI): m/z: Calcd: 324.1718, Found: 324.1795 $[M+H]^+$, Δ=23.6 ppm.

Compound (2):

A mixture of DMF (2.5 mL) and $POCl_3$ (2.5 mL) was stirred under argon for 5 min in the ice bath. After warming solution up to room temperature, it was stirred for additional 30 min. **(1)** (1.24 mmol, 400.0 mg) in 60 mL dichloroethane was added to the solution and temperature raised to 50^{0}C. After stirring for 3 hrs, the mixture was cooled to room temperature and then poured in to iced cooled saturated aqueous solution of $NaHCO_3$ (150 mL). Then reaction mixture was stirred for 30 min after warming solution to rt. After 30 min. the mixture was washed with H_2O (2x100 mL). The product was extracted into the dichloromethane. Organic phase dried over Na_2SO_4. The solvent was evaporated and the residue was purified by silica gel column chromatography using CH_2Cl_2 as the eluent. Reddish-brown solid was obtained (388.0 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$, 300K) : δ_H 10.02 (1H, s, C*H*O), 7.55-7.53 (3H, m, Ar*H*), 7.30-7.28 (2H, m, Ar*H*), 6.12 (1H, s, Ar*H*), 2.83 (3H, s, CH_3), 2.62 (3H, s, CH_3), 1.66 (3H, s, CH_3), 1.43 (3H, s, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 186.2, 161.7, 156.7, 147.6, 143.6, 142.9, 134.2, 129.9, 129.5, 127.7, 126.8, 124.0, 15.1, 14.8, 13.0, 11.6 ppm; MS (TOF- ESI): m/z: : Calcd: 352.1668, Found: 352.1710 $[M+H]^+$, Δ=11.9 ppm

Compound (3):

To a 500 mL round-bottomed flask containing 250 mL argon-degassed CH_2Cl_2, were 2,4-Dimethyl pyrrole (1.87 mmol, 178.3 mg) and **(2)** (0.85 mmol, 0.300 g) were added. The solution was stirred under N_2 at room temperature for 1 day. After that, 1.5 mL of Et_3N and 2 mL of $BF_3.OEt_2$ were successively added and after 30 min, the reaction mixture was washed three times with water (3 x 100 mL), which was then extracted into the CH_2Cl_2 (3 x 100 mL) and dried over anhydrous Na_2SO_4. The solvent was evaporated and the residue was purified by silica gel column chromatography using CH_2Cl_2 as the eluent. Red solid (170.0 mg, 35%). ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.52-7.49 (3H, m, Ar*H*), 7.32-7.30 (2H, m, Ar*H*), 6.10 (1H, s, Ar*H*), 6.00 (2H, s, Ar*H*), 2.61 (3H, s, C*H*$_3$), 2.54 (6H, s, C*H*$_3$), 2.43 (3H, s, C*H*$_3$), 1.73 (6H, s, C*H*$_3$), 1.43 (3H, s, C*H*$_3$), 1.23 (3H, s, C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 158.8, 155.7, 150.4, 145.6, 142.5, 142.4, 138.2, 134.5, 133.7, 132.5, 131.8, 130.9, 129.4, 127.8, 125.6, 122.5, 121.2, 46.6, 31.7, 22.7, 14.6, 14.1, 13.9, 12.7, 12.1 ppm. MS (TOF- ESI): m/z: Calcd: 568.2822, Found: 568.2698 $[M]^+$, Δ=21.8 ppm.

Compound (4):

(3) (0.26 mmol, 150.0 mg) and 4-Pyridinecarboxaldehyde (0.79 mmol, 84.6 mg) were added to a 100 mL round-bottomed flask containing 50 mL benzene and to this solution piperidine (0.20 mL) and acetic acid (0.20 mL) were added. The mixture was heated under reflux by using a Dean Stark trap and reaction was monitored by TLC (CH_2Cl_2 : MeOH 95:5). When all the starting material had been consumed, the mixture was cooled to room temperature and solvent was evaporated. Water (100 mL) added to the residue and the product was extracted into the chloroform (3 x 100 mL). Organic phase dried over Na_2SO_4, evaporated and residue was purified by silica gel column chromatography using (CH_2Cl_2: MeOH 95:5) as the eluent. Purple solid was obtained (43.0 mg, 25%). ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.69 (2H, s, Ar*H*), 7.92 (1H, d, *J* = 16.2, C*H*), 7.56-7.54 (5H, m, Ar*H*), 7.36-7.33 (2H, m, Ar*H*), 7.19 (1H, d, *J* = 16.2, C*H*), 6.73 (1H, s, Ar*H*), 6.02 (2H, s, Ar*H*), 2.55 (6H, s, C*H*$_3$), 2.50 (3H, s, C*H*$_3$), 1.74 (6H, s, C*H*$_3$), 1.50 (3H, s, C*H*$_3$), 1.28 (3H, s, C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 156.1, 153.9, 151.7, 148.4, 145.3, 143.8, 142.7, 142.2, 140.5, 134.2, 133.8, 132.7, 132.5, 131.6, 129.7, 129.5, 128.8,

127.7, 127.1, 124.4, 121.8, 121.4, 118.7, 25.1, 24.7, 14.7, 13.9, 13.1, 12.4. MS (TOF-ESI): m/z: Calcd: 658.3160, Found: 658.3164 $[M+H]^+$, Δ=0.6 ppm.

Compound (5):

(4) (0.061 mmol, 40.0 mg) and excess iodomethane (0.61 mmol, 87.0 mg) were dissolved in 5 mL ethyl acetate. The reaction mixture was stirred for 1 day at room temperature. When all the starting material had been consumed, solution was poured in to the cold diethyl ether. Precipitate was filtered and dried. Dark blue solid was obtained (36.7 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 9.00 (2H, bs, Ar*H*), 8.07 (2H, s, Ar*H*), 7.99 (1H, bs, C*H*), 7.56-7.54 (3H, m, Ar*H*), 7.49 (1H, d, *J* = 16.2, C*H*), 7.34-7.32 (2H, m, Ar*H*), 6.98 (1H, s, Ar*H*), 6.02 (2H, s, Ar*H*), 4.55 (3H, s, CH_3), 2.54 (6H, s, CH_3), 2.50 (3H, s, CH_3), 1.73 (6H, s, CH_3), 1.49 (3H, s, CH_3), 1.30 (3H, s, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 156.1, 153.9, 151.7, 148.4, 145.3, 143.8, 142.7, 142.2, 140.5, 134.2, 133.8, 132.7, 132.5, 131.6, 129.7, 129.5, 128.8, 127.7, 127.1, 124.4, 121.8, 121.4, 118.7, 26.6, 25.1, 24.7, 14.7, 13.9, 13.1, 12.4. MS (TOF- ESI): m/z: Calcd: 672.3322, Found: 672.3236 $[M+H]^+$, Δ=12.8 ppm.

Compound (5r):

Excess amount of mercaptoethanol (5.0 mmol) and catalytic amount of K_2CO_3 were added on to **(5)** (0.024 mmol, 20 mg) in DCM. Solution was stirred for 1 hr. After that, the product was separated by silica gel column chromatography using (CH_2Cl_2: MeOH 90:10) as the eluent. Product was obtained as orange solid (17.3 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 9.15 (2H, d, *J* = 6.6, Ar*H*), 7.99 (2H, d, *J* = 6.6, Ar*H*), 7.55-7.52 (3H, m, Ar*H*), 7.34-7.32 (2H, m, Ar*H*), 6.17 (1H, s, Ar*H*), 6.01 (2H, s, Ar*H*), 4.68 (3H, s, CH_3), 3.41 (4H, s, CH_2), 2.54 (6H, s, CH_3), 2.43 (3H, s, CH_3), 1.73 (6H, s, CH_3), 1.44 (3H, s, CH_3), 1.25 (3H, s, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 161.5, 156.6, 156.0, 152.8, 145.4, 144.9, 143.9, 142.3, 140.4, 134.1, 132.9, 131.7, 129.6, 129.5, 128.2, 127.9, 126.7, 121.4, 120.8, 60.6, 49.0, 41.6, 34.7, 28.1, 14,7 14.6, 14.0, 12.9, 12.3. MS (TOF-ESI): m/z: Calcd: 674.3479, Found: 674.3511 $[M]^+$, Δ=4.9 ppm.

Compound (5m):

Excess amount of mercaptoethanol (5.0 mmol) were added on to **(5)** (0.024 mmol, 20 mg) in 90:10 (20 mM Hepes buffer:MeCN). Solution was stirred for 4 hr. Color change from dark blue to red was observed and solvent was evaporated under vacuum. Mass spectrum was acquired without any purification. MS (TOF- ESI): m/z: Calcd: 750.3461, Found: 750.3515 $[M]^+$, Δ=7.1 ppm.

Compound (5-GSH): Excess amount of GSH (2.4 mmol) were added on to **(5)** (0.012 mmol, 10 mg) in 90:10 (20 mM Hepes buffer:MeCN). Solution was stirred for 24 hours. Color change from dark blue to red was observed and solvent was evaporated under vacuum. Mass spectrum was acquired without any purification. MS (TOF- ESI): m/z: Calcd: 979.4160, Found: 979.3977 $[M]^+$, Δ=18.7 ppm.

1.3. NMR Spectra

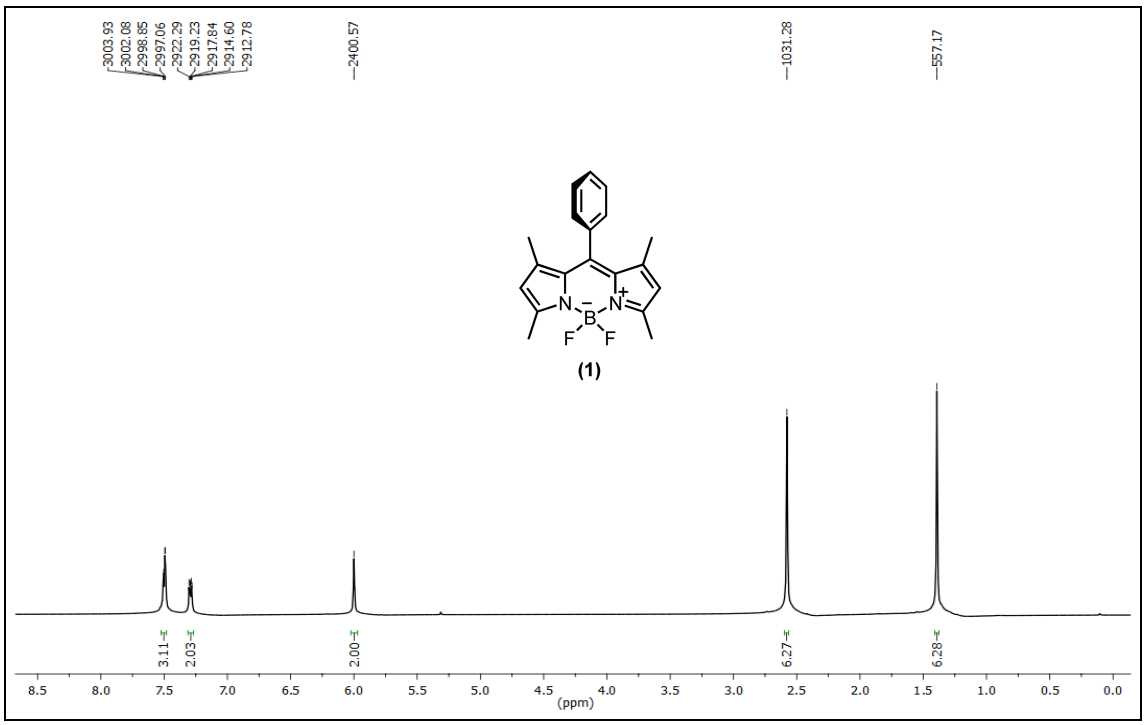


Figure S1. ^{1}H NMR spectrum of **(1)**.

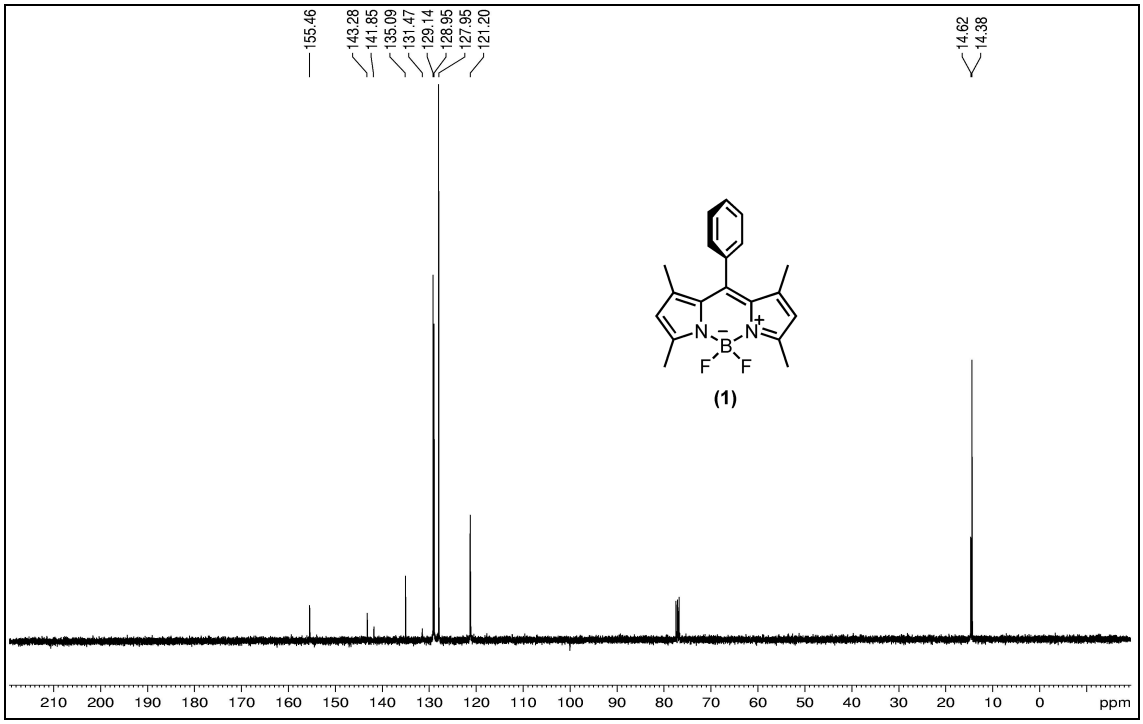


Figure S2. ^{13}C NMR spectrum of **(1)**.

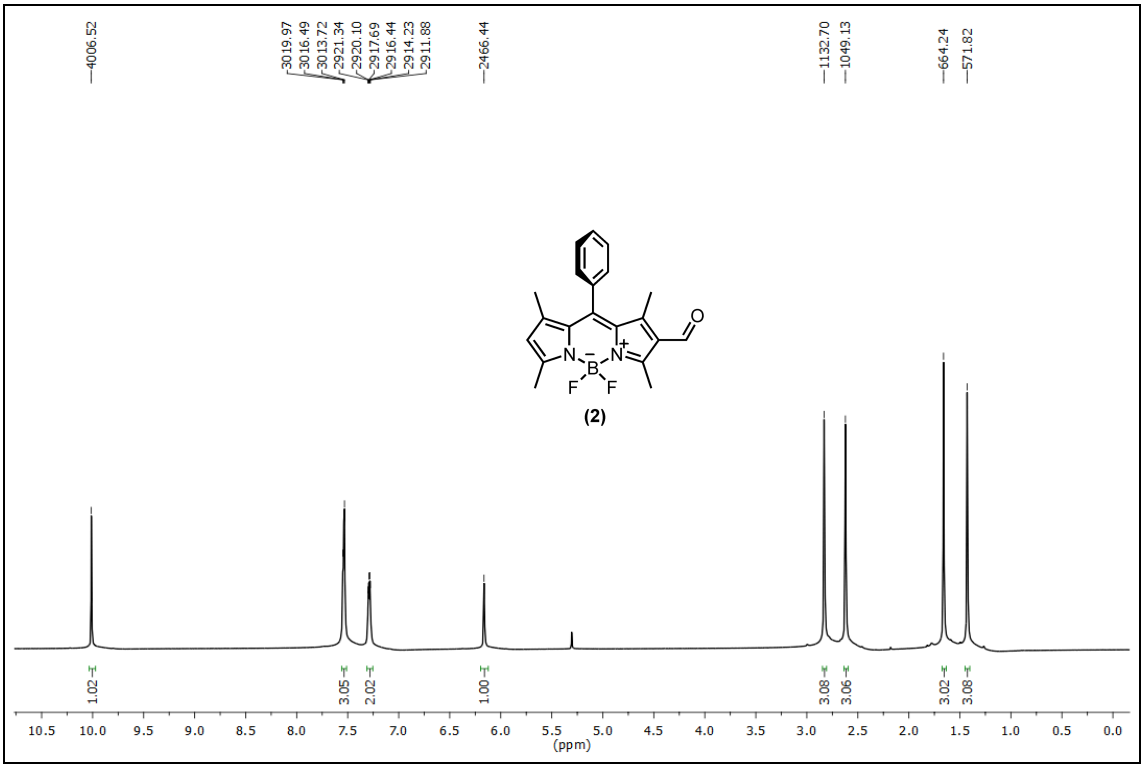


Figure S3. ^{1}H NMR spectrum of **(2)**.

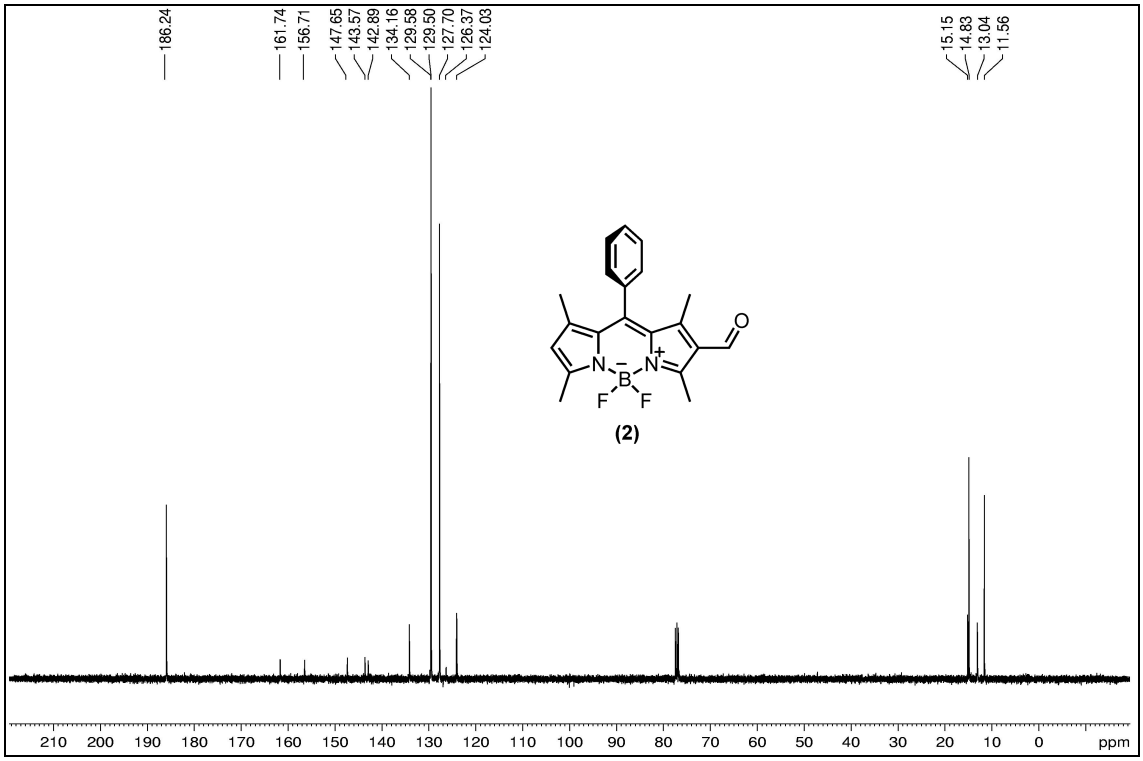


Figure S4. ^{13}C NMR spectrum of **(2)**.

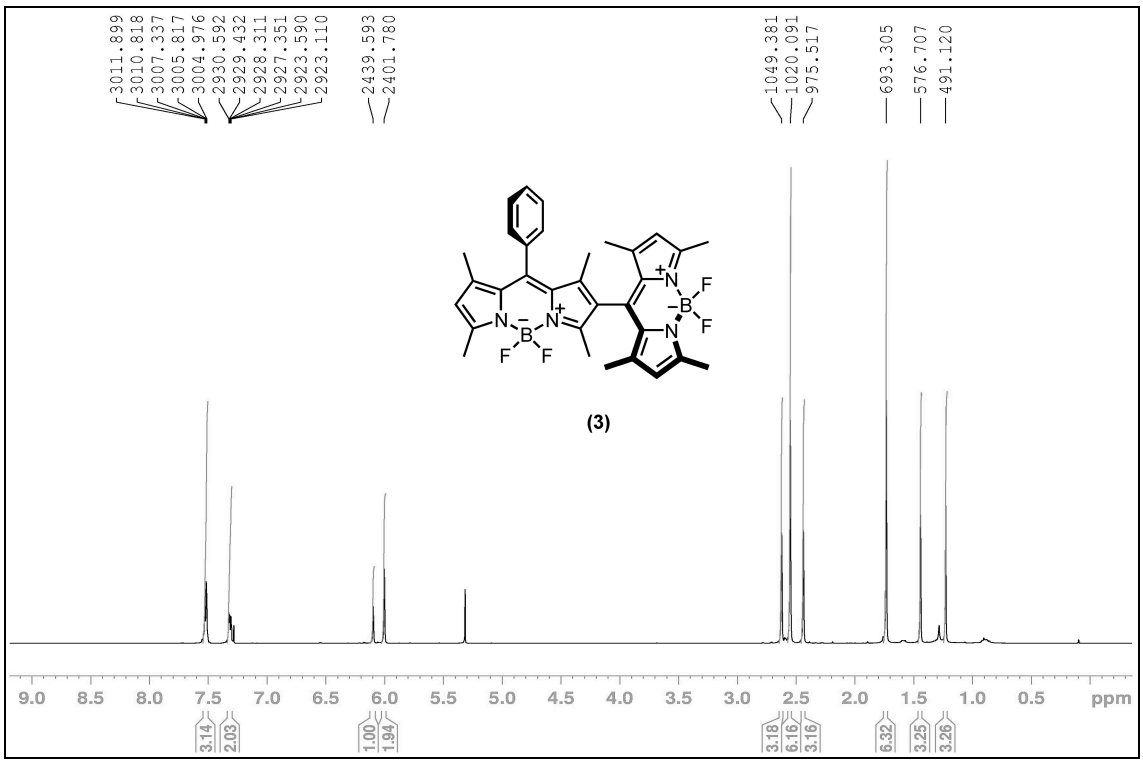


Figure S5. ^{1}H NMR spectrum of **(3)**.

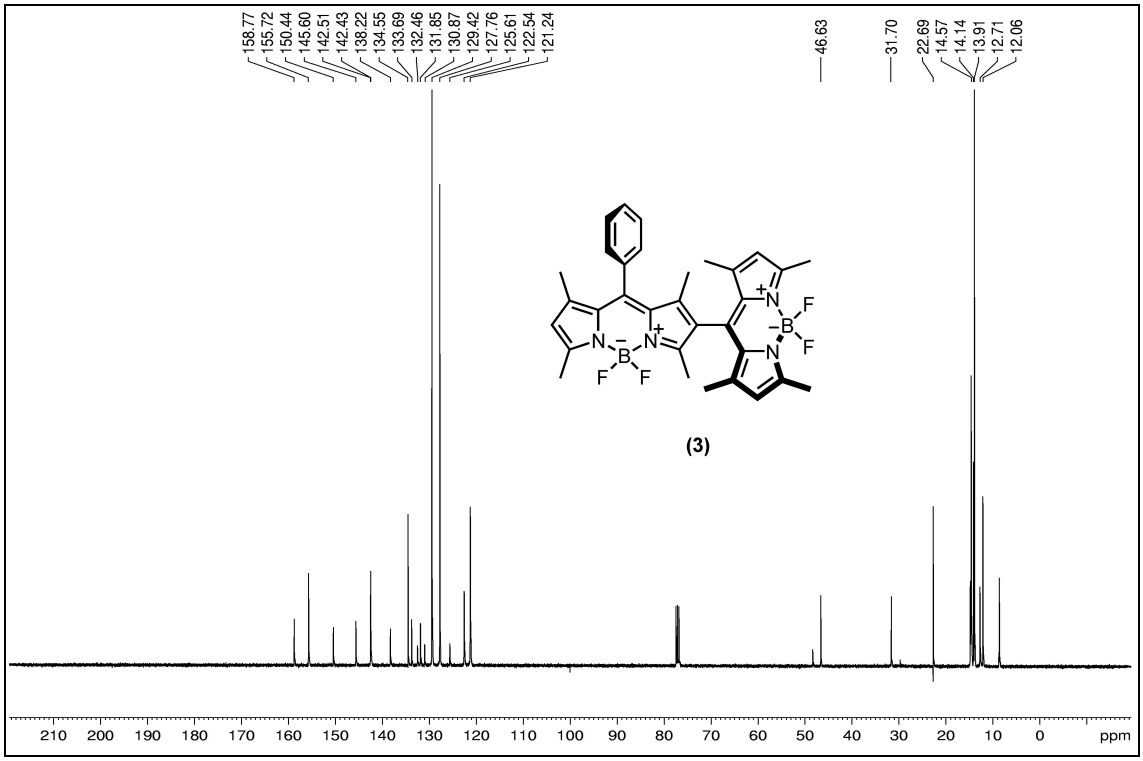


Figure S6. ^{13}C NMR spectrum of **(3)**.

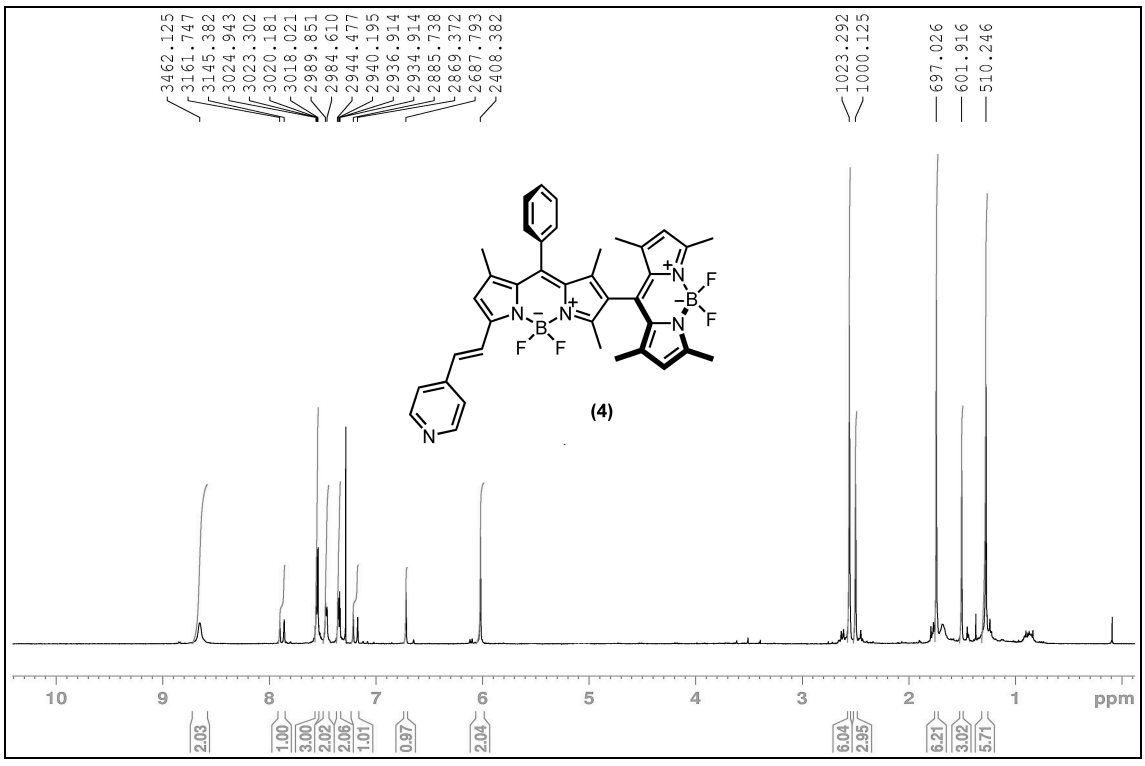


Figure S7. ^{1}H NMR spectrum of **(4)**.

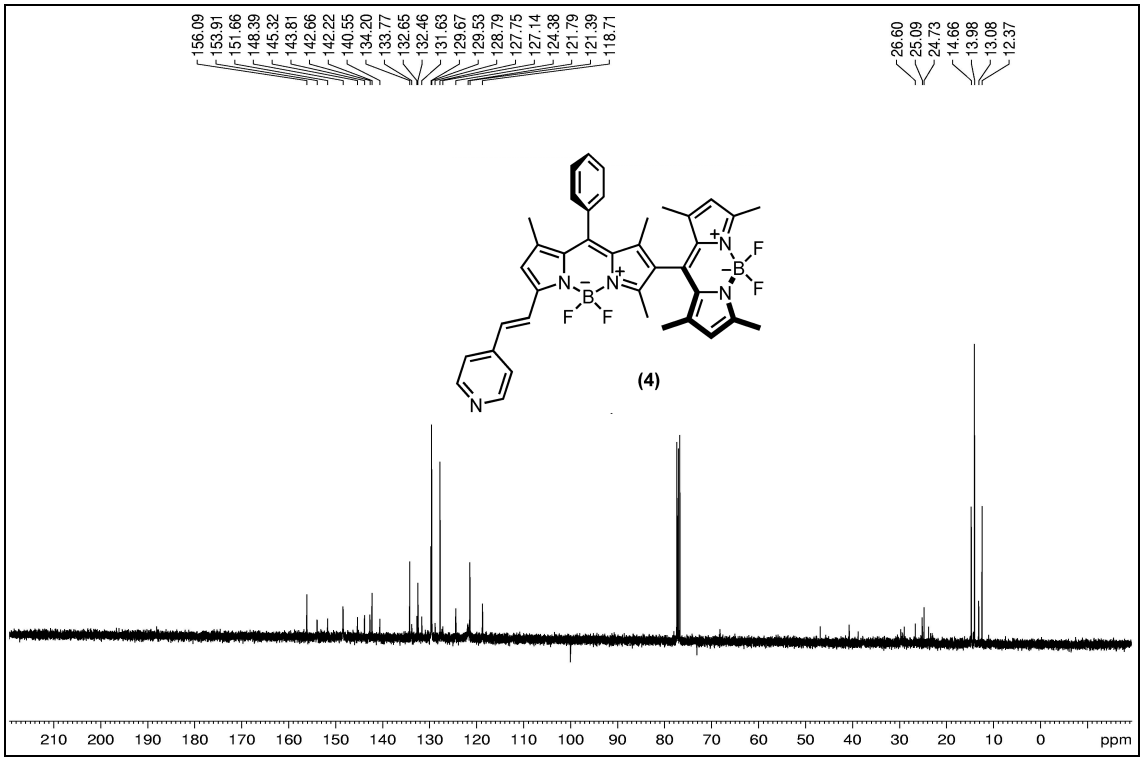


Figure S8. ^{13}C NMR spectrum of **(4)**.

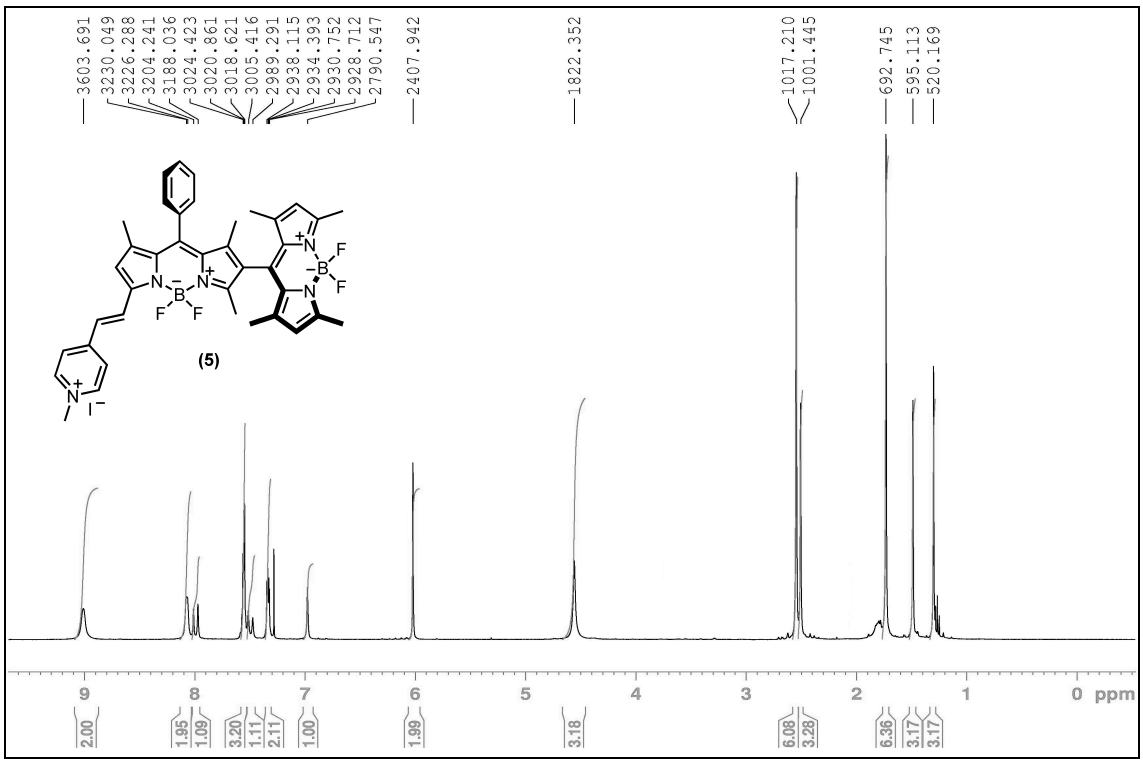


Figure S9. ^{1}H NMR spectrum of **(5)**.

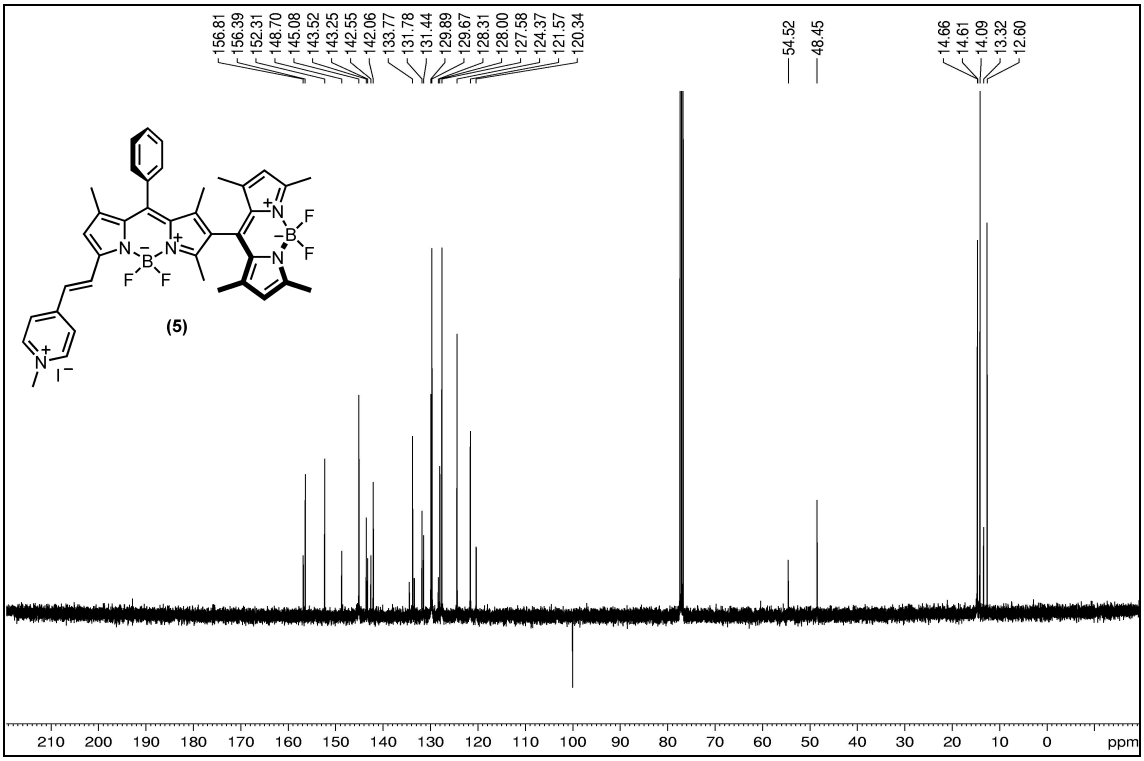


Figure S10. ^{13}C NMR spectrum of **(5)**.

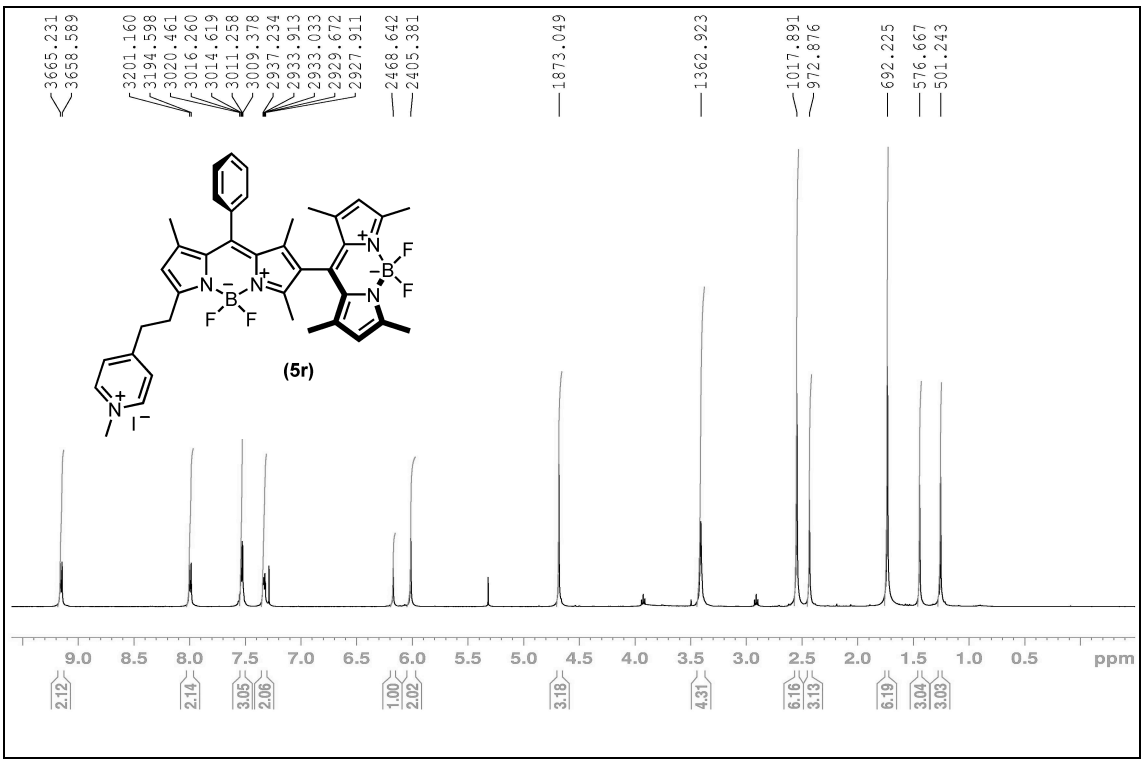


Figure S11. ^{1}H NMR spectrum of **(5r)**.

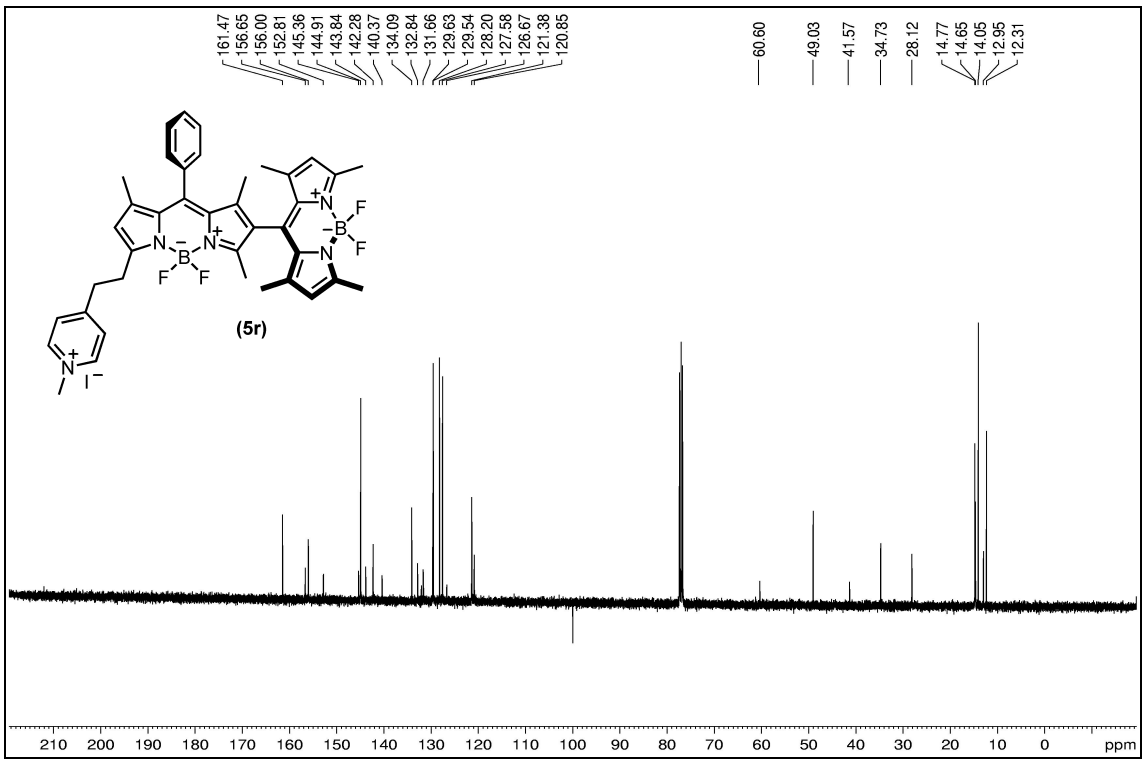


Figure S12. ^{13}C NMR spectrum of **(5r)**.

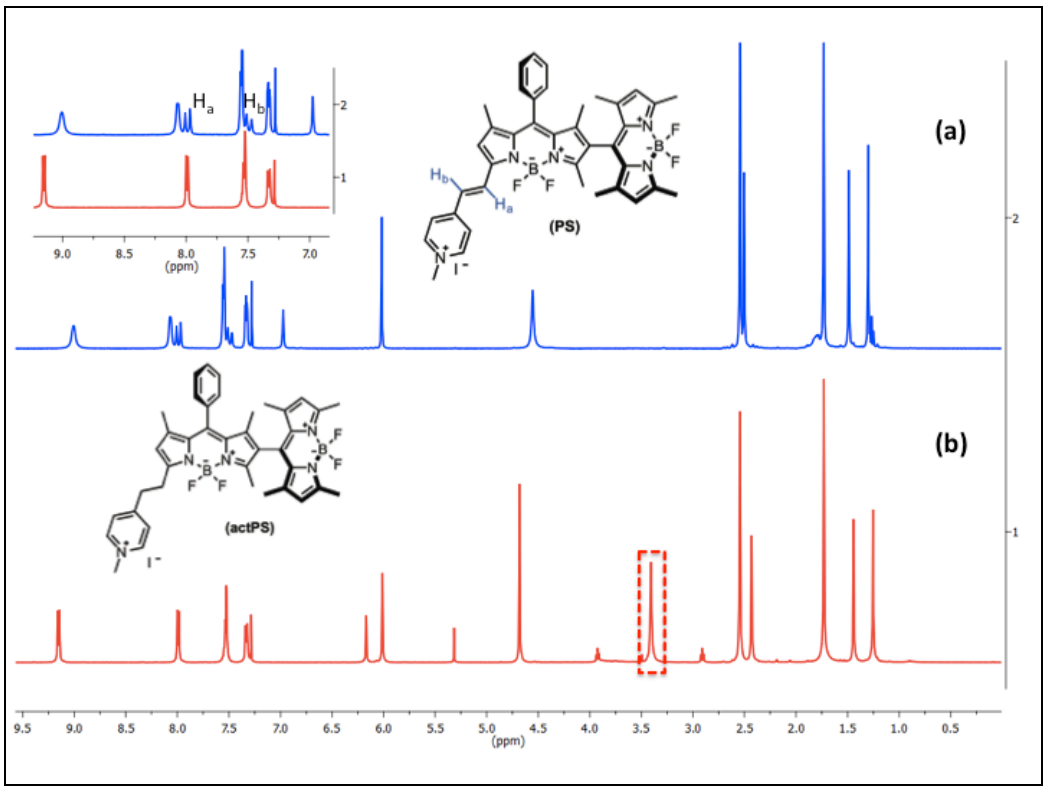


Figure S13. Combined ^{1}H NMR spectra of **(5)** and (**5r**).

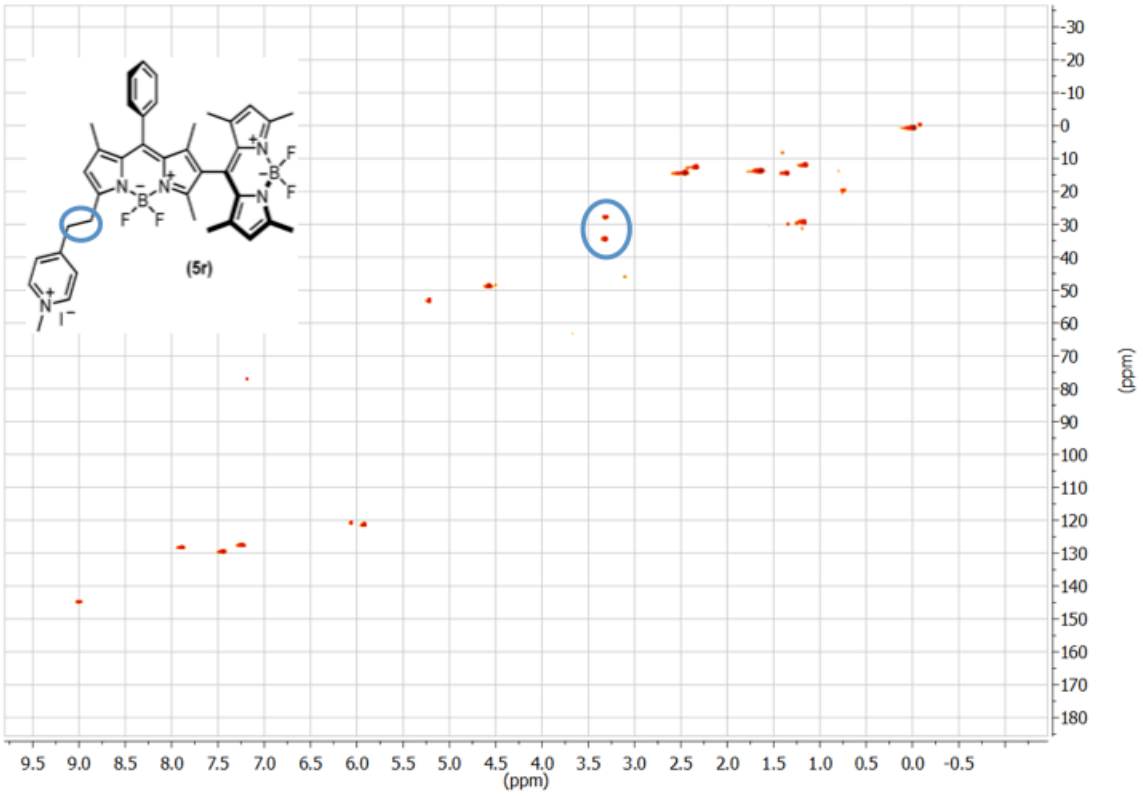


Figure S14. HSQC Analysis of **(5r)**.

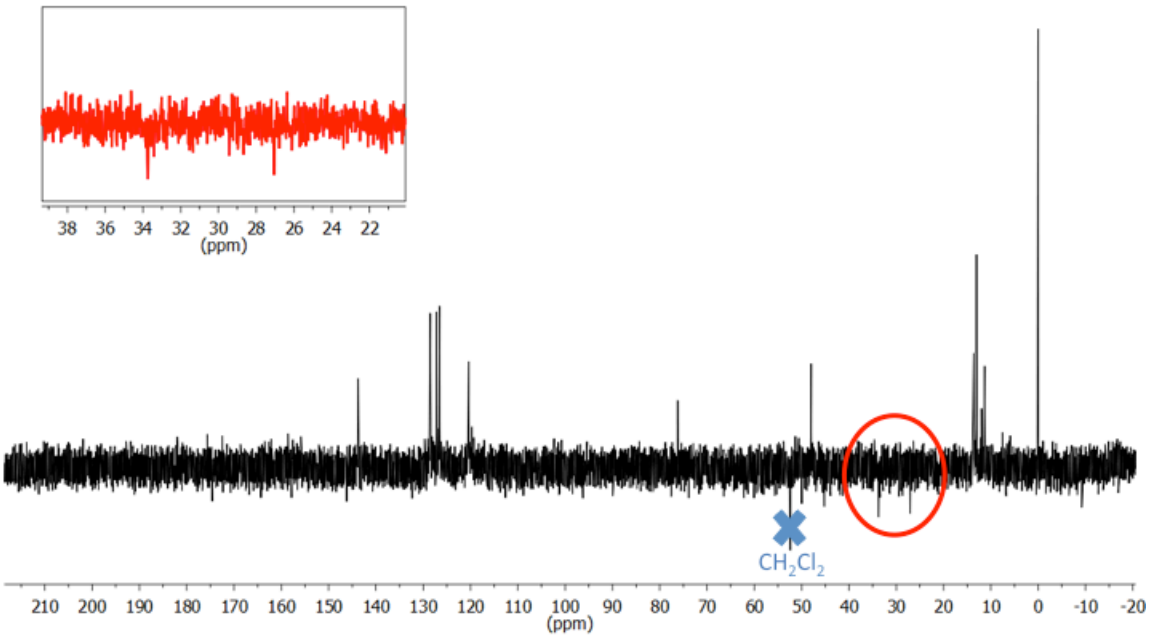


Figure S15. Depth 135 Analysis of **(5r)**.

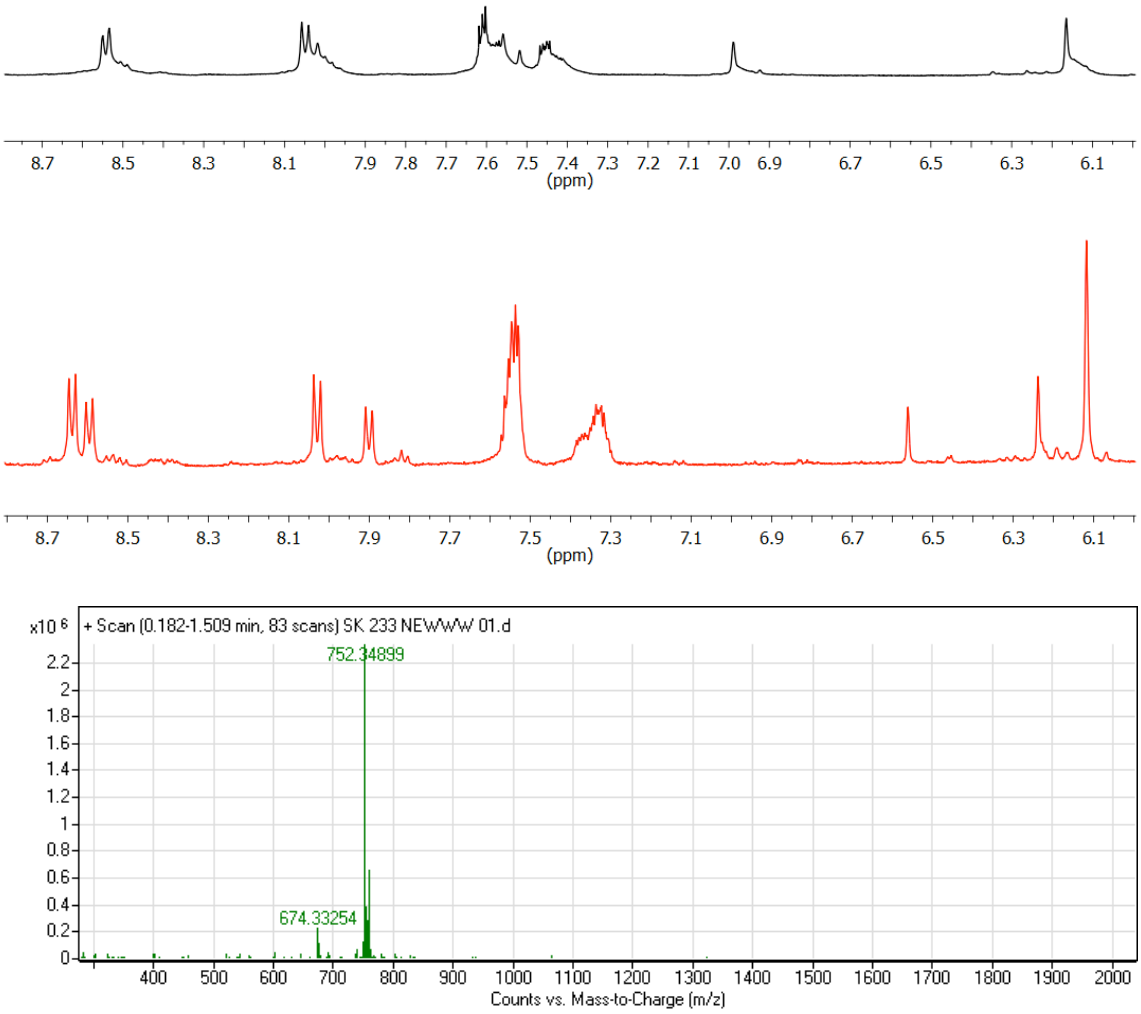


Figure S16. Partial ^{1}H NMR spectrum of **(5)** (top) and **(5m)*** (middle) which are acquired during the reaction of **(5)** with excess mercaptoethanol. Bottom: HRMS spectrum that is taken at the end of the reaction without any purification.

* A ^{1}H NMR experiment of **(5m)** was conducted in CD_3CN/buffer mixture, the reaction proceeds in such a way that the trans-coupled protons disappear, thiol nucleophile is likely to attack at both olefinic carbons, leading to two different sets of pyridine peaks. HRMS data scanning a very wide mass/charge ratio yields a single peak that corresponds to the adduct molecular ion. In addition, HRMS isotope distribution added is in perfect agreement with the adduct.

1.4. Mass Spectra

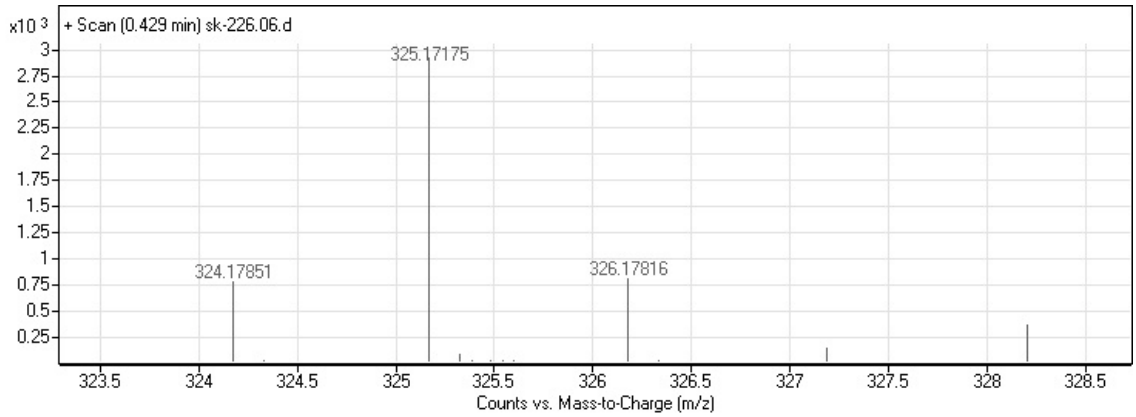


Figure S17. HRMS spectrum of **(1)**.

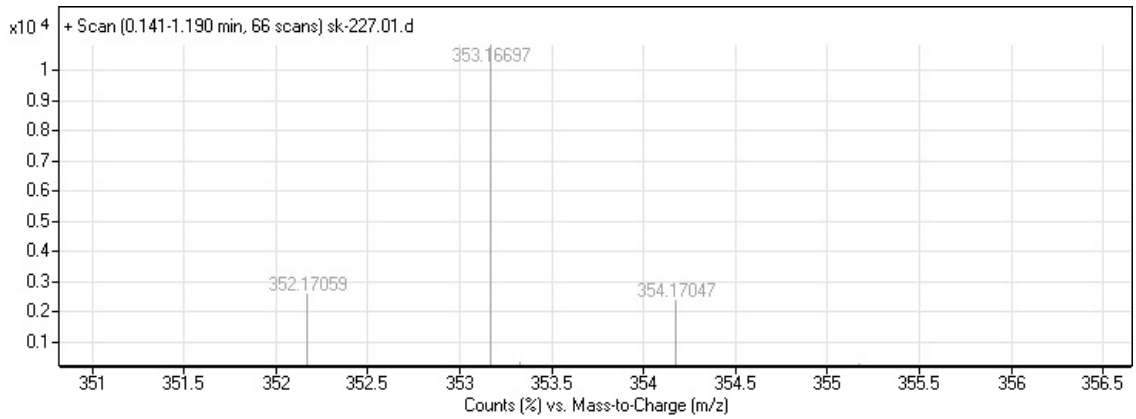


Figure S18. HRMS spectrum of **(2)**.

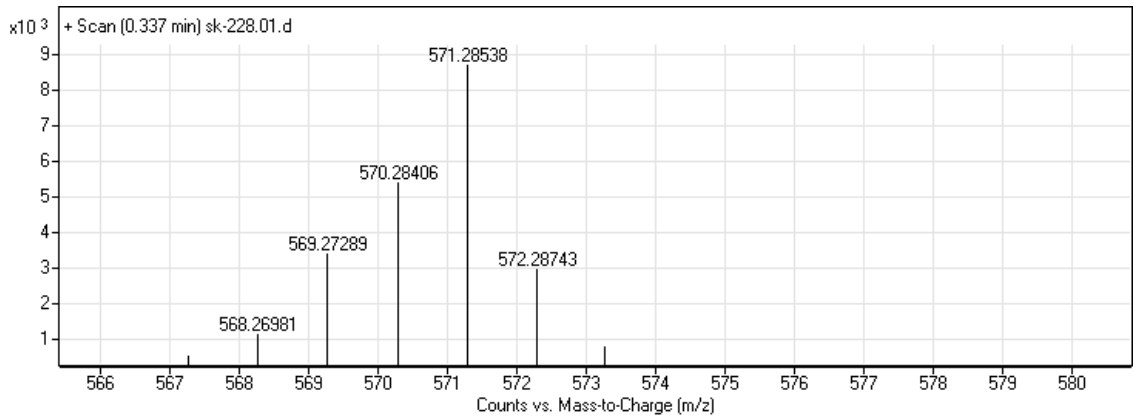


Figure S19. HRMS spectrum of **(3)**.

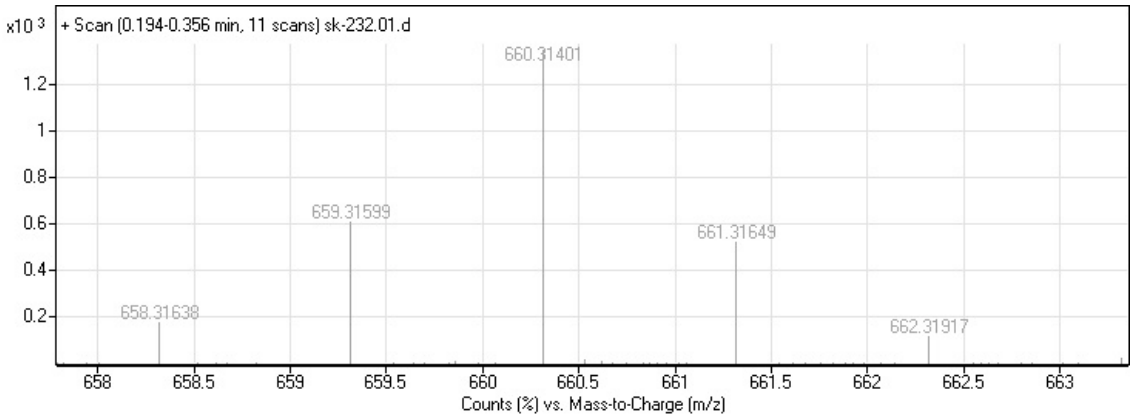
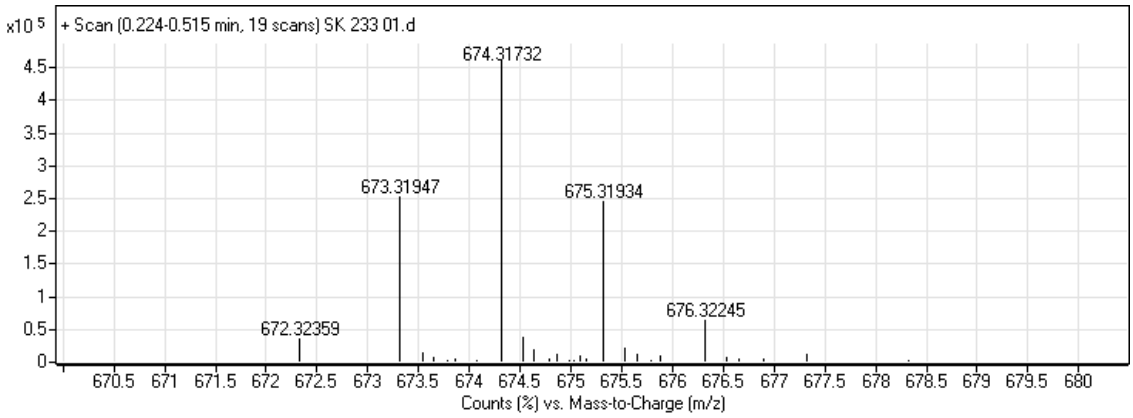
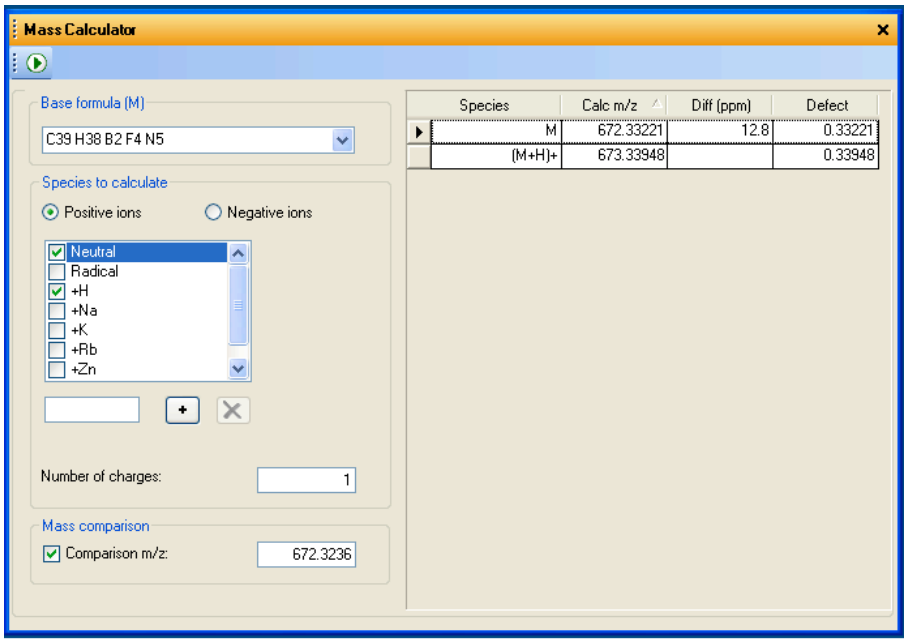


Figure S20. HRMS spectrum of **(4)**.





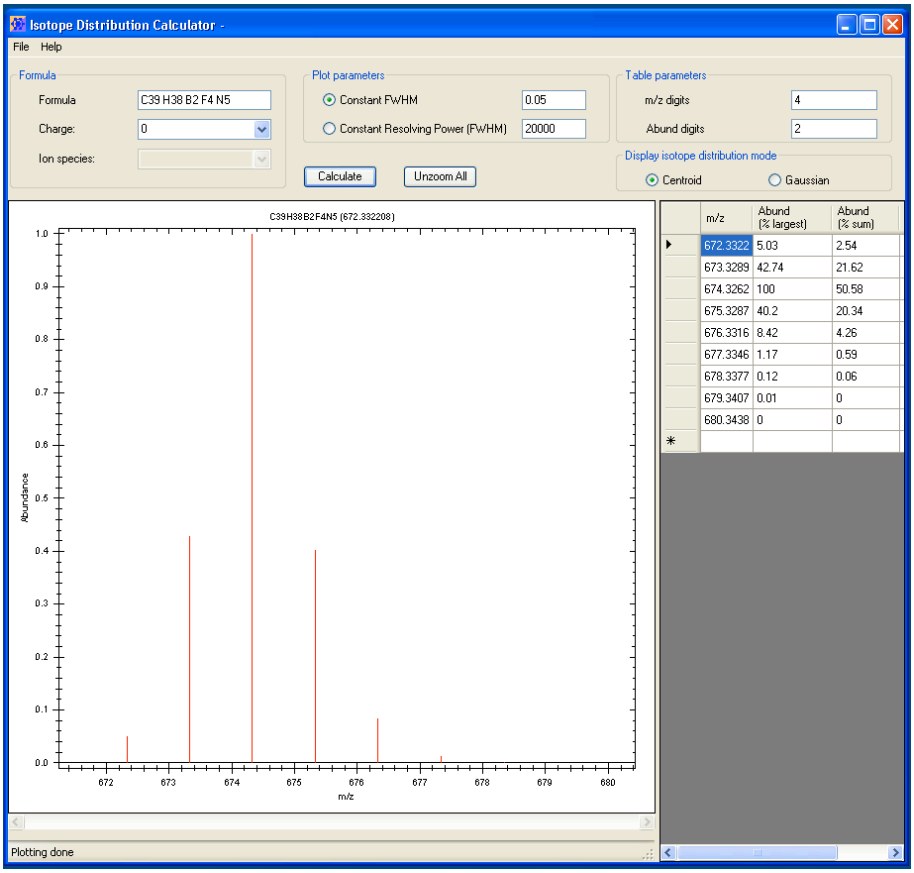
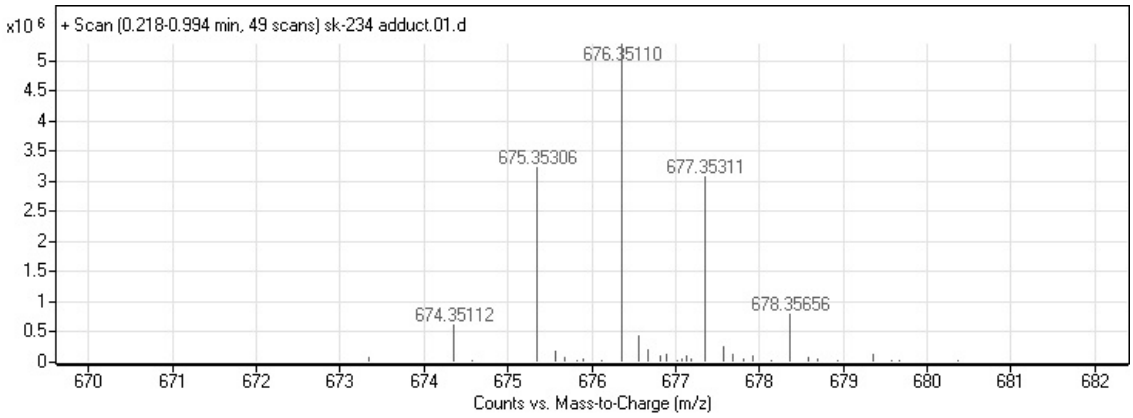


Figure S21. HRMS spectrum of **(5)**.



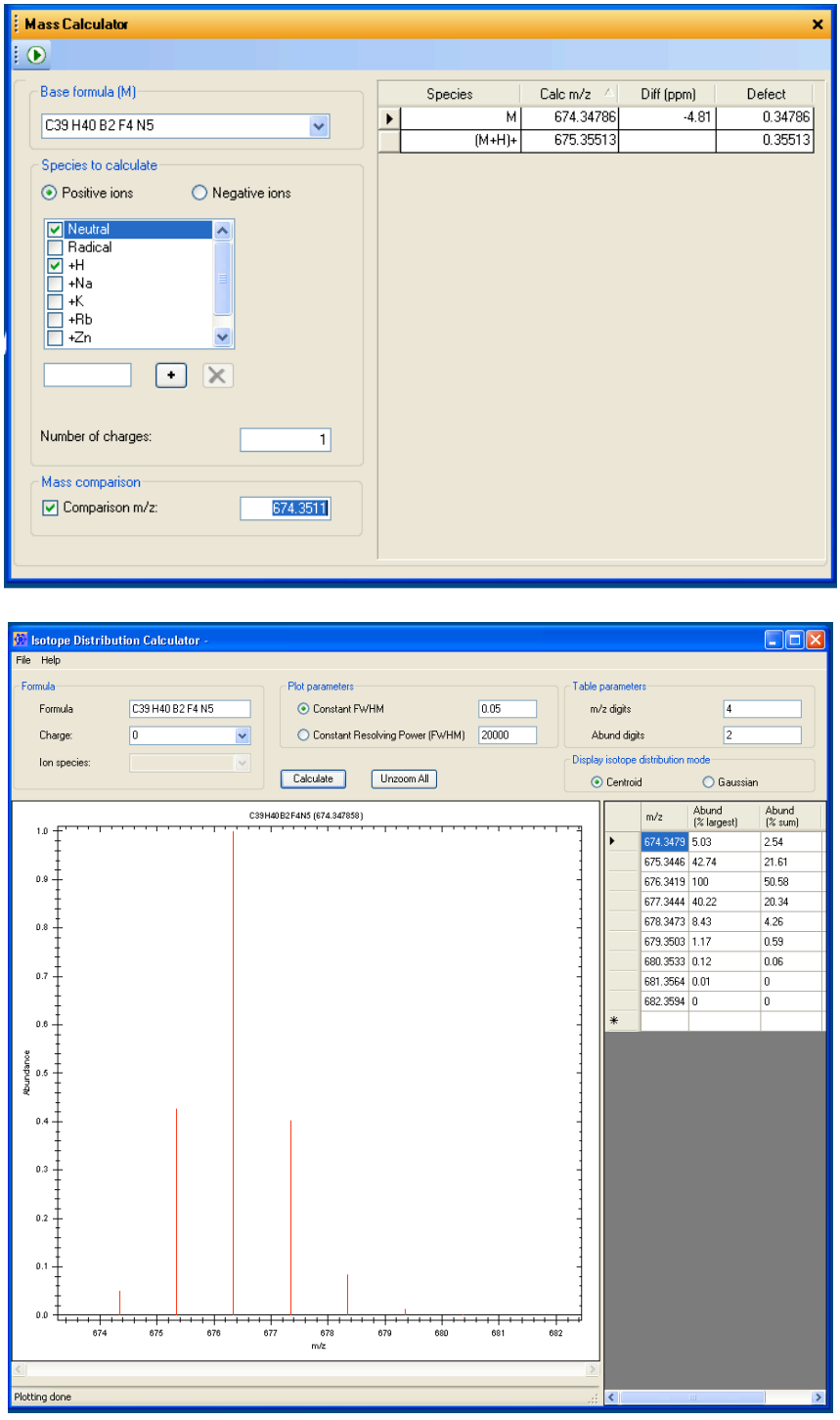


Figure S22. HRMS spectrum of **(5r)**.

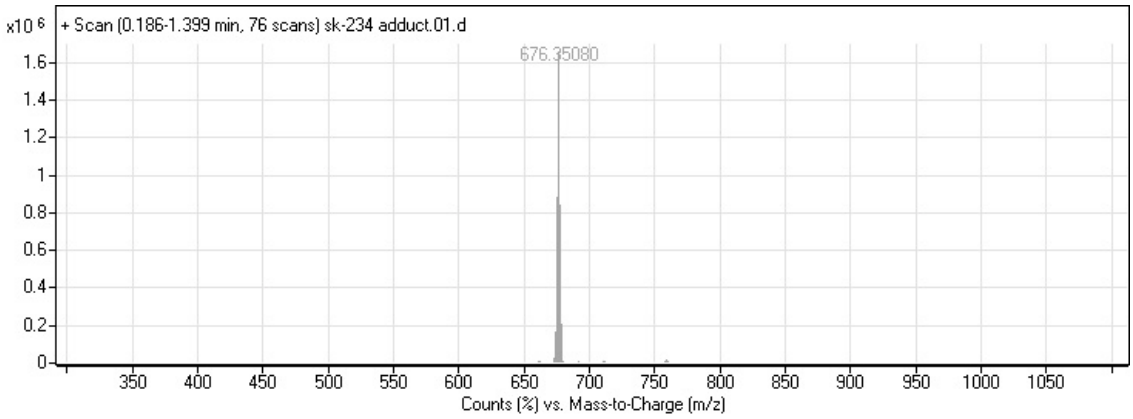
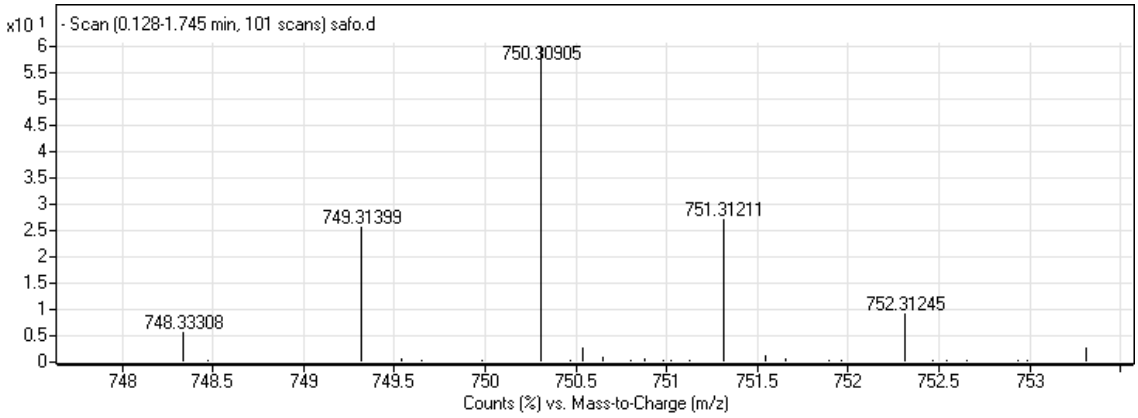
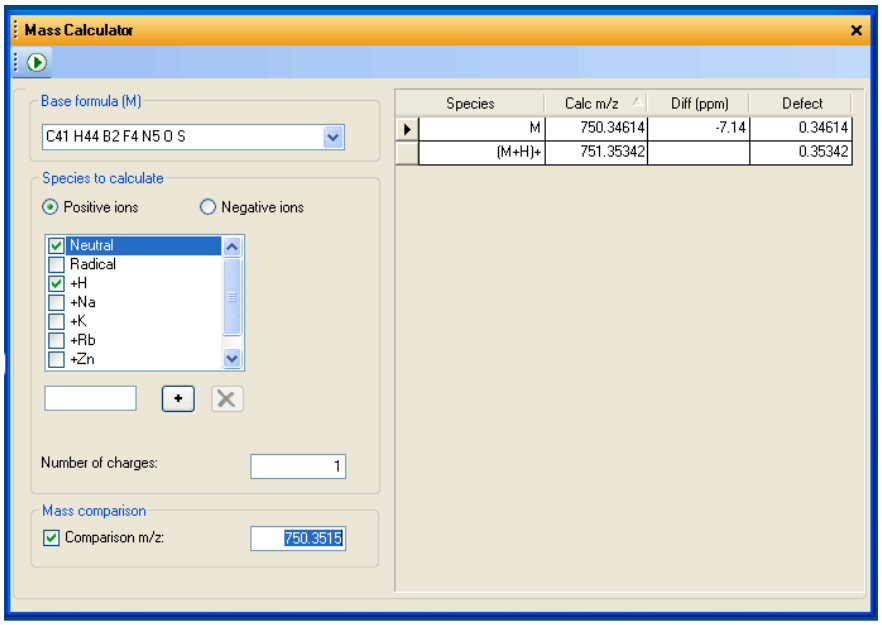


Figure S23. HRMS spectrum of **(5r)**-extended version.





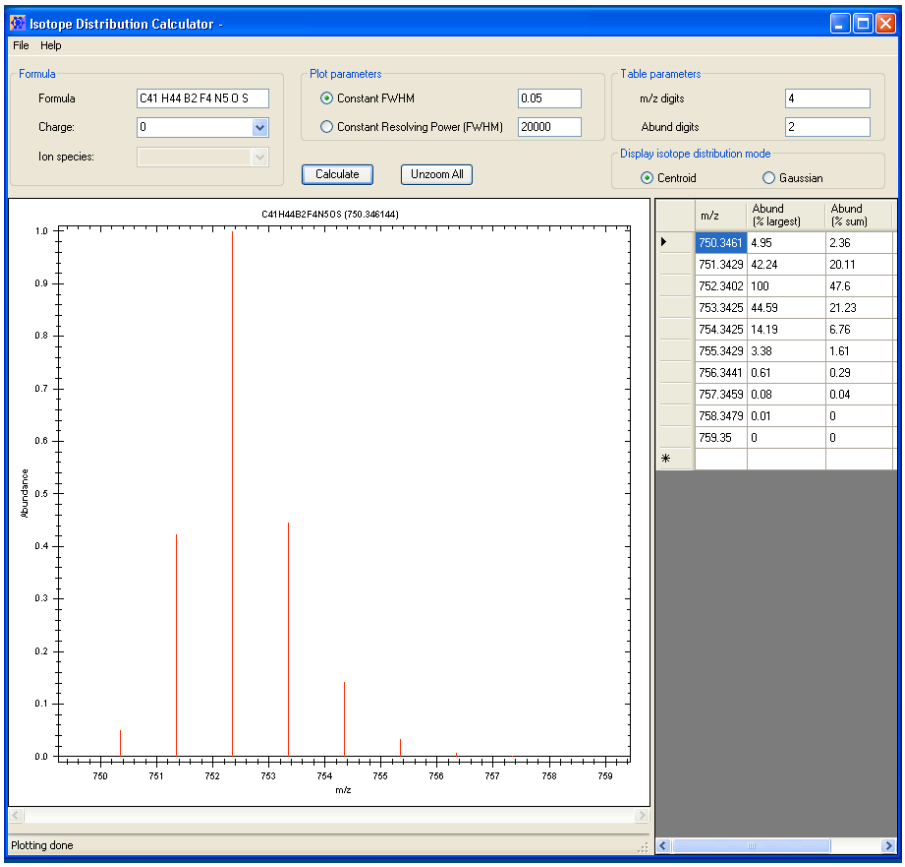
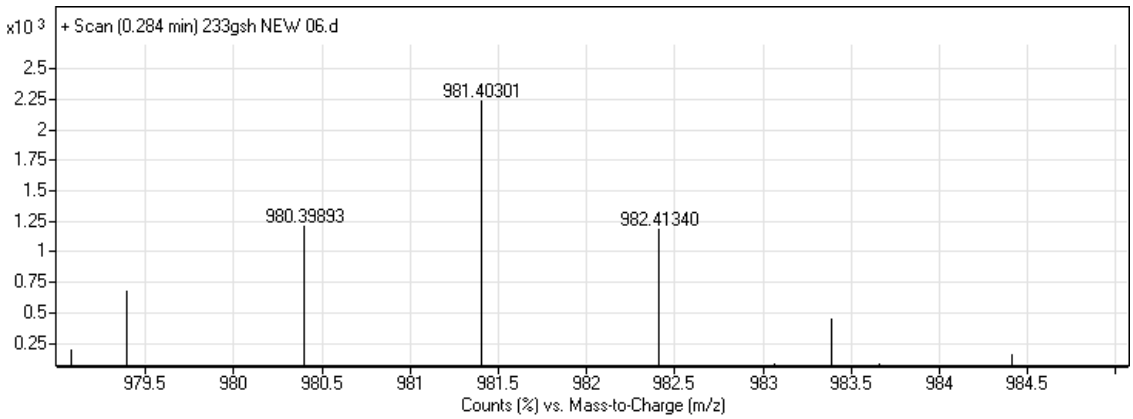


Figure S24. HRMS spectrum of **(5m)**.



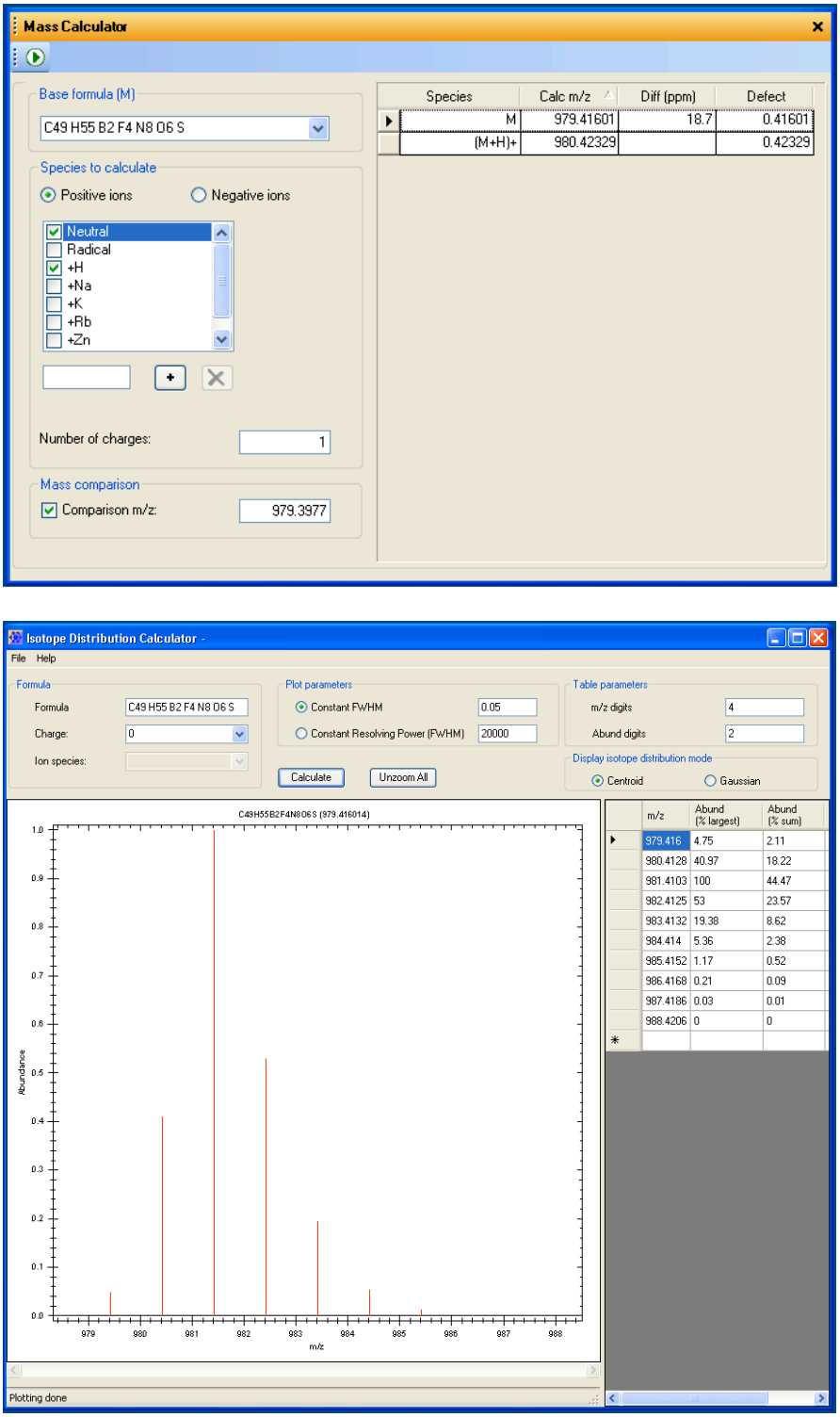


Figure S25. HRMS spectrum of **(5)** + GSH adduct.

1.5. Photophysical Characterization

1.5.1. Uv-Visible Measurements

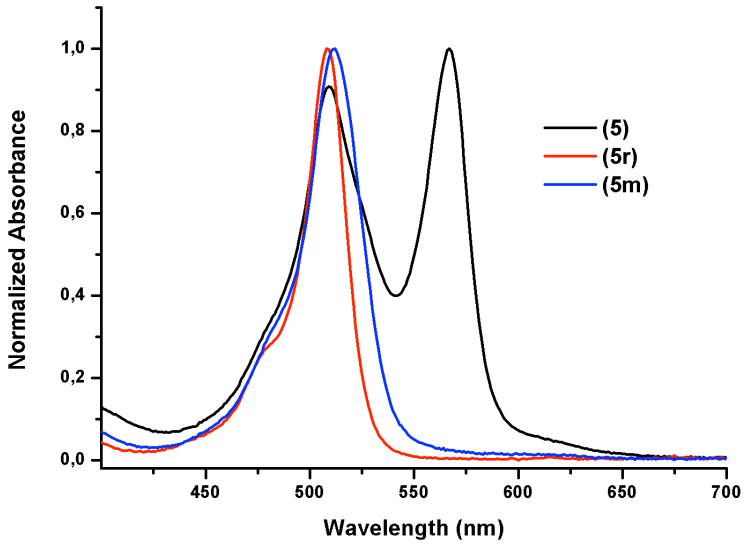


Figure S26. Normalized electronic absorption spectra of **(5), (5r)** and **(5m)** in DCM.

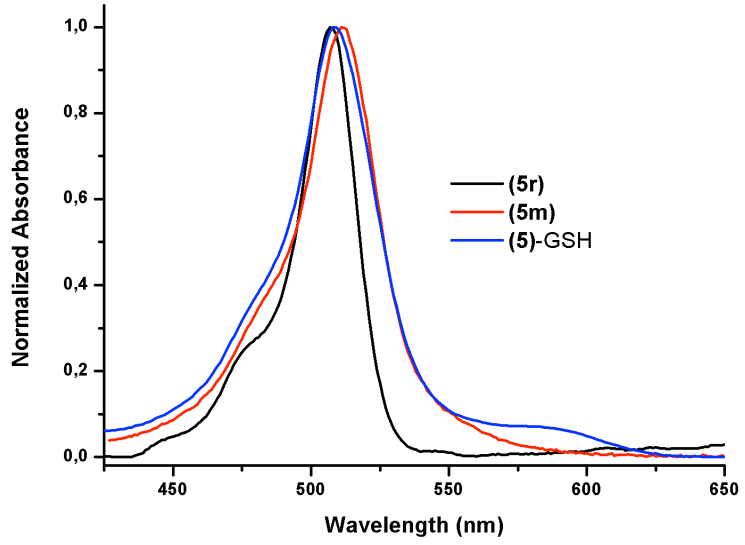


Figure S27. Normalized electronic absorption spectra of **(5r), (5m)** and **(5)**-GSH in 90:10 (Hepes buffer, pH 7.2, 20mM : MeCN

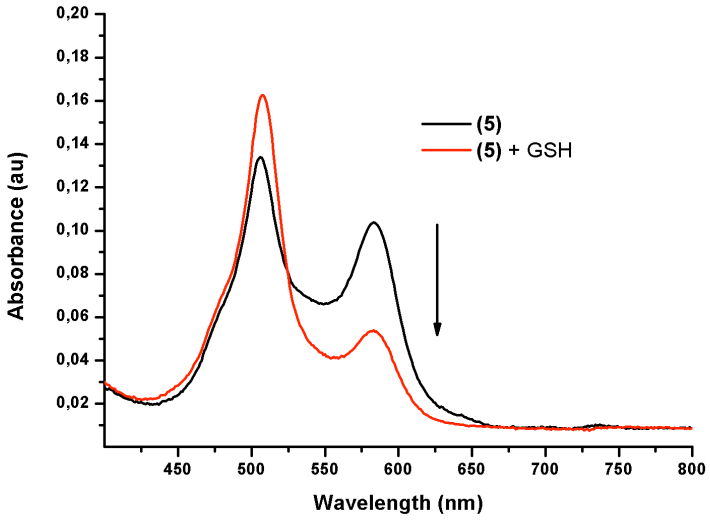


Figure S28. Reaction of 3.5 μM **(5)** with 5 mM GSH in 90:10 (Hepes buffer, pH 7.2, 20mM : MeCN) for 12 hours.

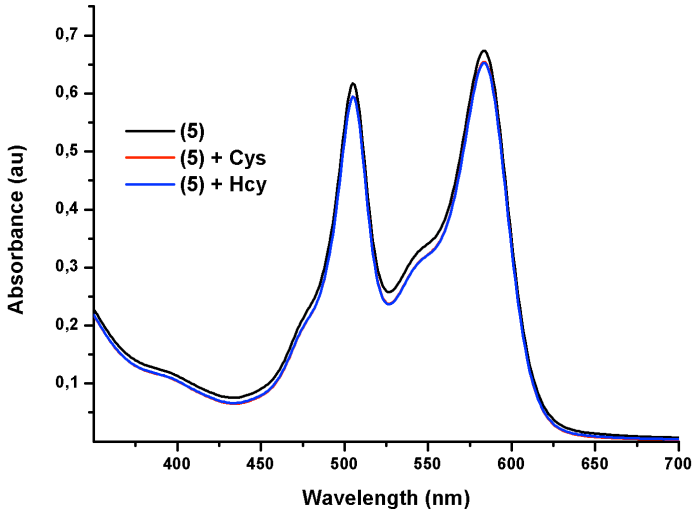


Figure S29. Electronic absorption spectra of **(5)** (20μM) and **(5)** (20μM) + Cys (20μM) & Hcy (20μM) in 90:10 (Hepes buffer, pH 7.2, 20mM : MeCN). Reaction time is 12 hours in all cases.

1.5.2. Fluorescence Measurements

The fluorescence quantum yield (Φ_f) was computed by using

$$\Phi_f = \Phi_f^0 \cdot \frac{F_s}{F_0} \cdot \frac{A_0}{A_s} \frac{n_s^2}{n_0^2} \qquad \text{Eq. (1)}$$

in which F is the integrated fluorescence intensity, A is the absorbance at excitation wavelength, n is the refractive index of the solvent used, the subscript "0" stands for a reference compound and "s" represents samples. A BODIPY monomer in CH_2Cl_2 was used as the reference (Φ_f=0.80).[1] The sample and reference solutions were prepared with the same absorbance (A_i) at the excitation wavelength (near 0.050 in a 1 cm quartz cell). All solutions were air saturated.

For **(5r)**, $\mathbf{\Phi_f}$ decreases with the increase of solvent polarity. The shape and emission maximum of fluorescence spectra is changed very slightly by solvent polarity. The fluorescence decay curves are bi-exponential except for water solvent (tri-exponential). The decay curves are decreased with the increase of solvent polarity, indicating that the percentage of the short-lived emission component is increased with the increase of solvent polarity.

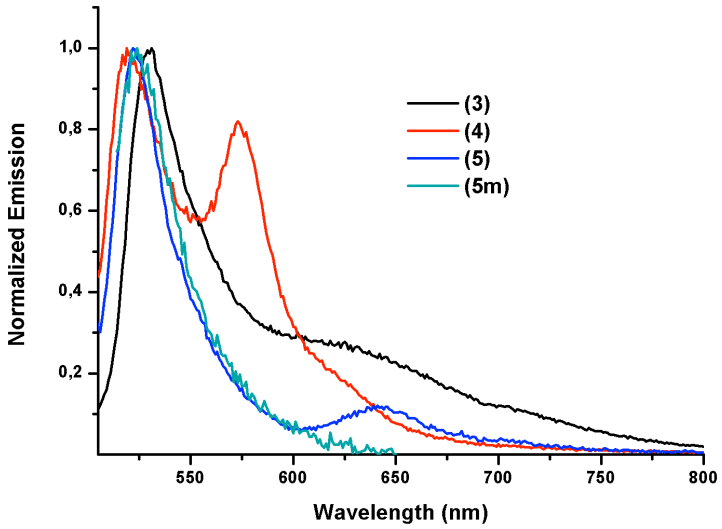


Figure S30. The normalized fluorescence emission spectra of **(3)**, **(4)**, **(5)** and **(5m)** in DCM.

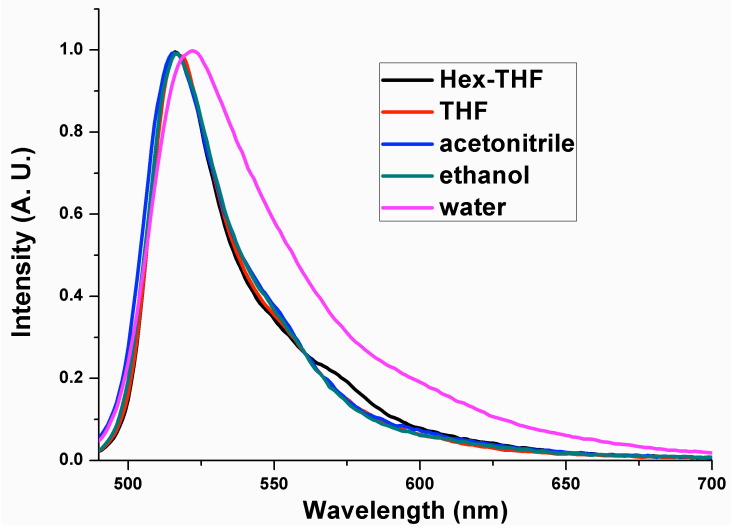


Figure S31. The normalized fluorescence emission spectra of **(5r)** in different solvents with excitation at 418 nm (absorbance 0.090).

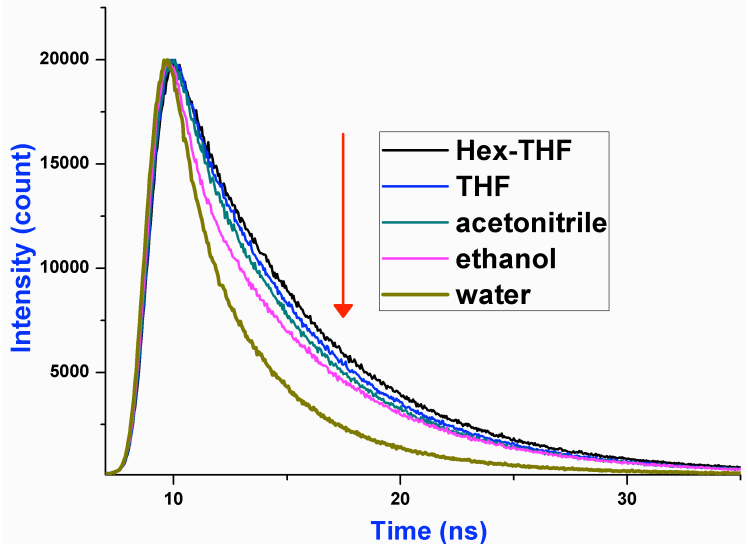


Figure S32. Fluorescence decay of **(5r)** in EtOH with excitation at 509 nm diode laser (150 *ps*), the emission was monitored at 520 nm, the concentration of dyes is ca. 3.0 μM. The decay curves are decreased with the increase of solvent polarity, indicating that the percentage of the short-lived emission component is increased with the increase of solvent polarity.

Table S1. Selected photophysical data for **(3)**, **(4)**, **(5)** and **(5r).**

sensitizer	λ_{abs}[a] / nm	ε_{max}[a] / M^{-1} cm^{-1}	λ_{ems}[a] / nm
3	508	140000	530
4	509 567	36000 30000	522 573
5	508 607 513[b] 590[b]	41000 38000 34000[b] 25000[b]	522 645 520[b] 606[b]
5r	511 508[b]	119000 90000[b]	535 533[b]
5m	513 509[b]	110000 98000[b]	525 523[b]

[a]Values were obtained in DCM. [b]Values were obtained in 90/10 (HEPES Buffer/ MeCN).

Table S2. Fluorescence quantum yield (Φ_f) and lifetime (τ_f) of **(5)** in THF and **(5r)** in different solvents.

Sample	**λ_{em}/nm**	**Φ_f**	**τ_f/ns**	**chi squared value**	**solvent**
5	517	0.088	1.60, 5.61(96%)	1.04	THF
5r	516	0.19	0.92, 5.95(98%)	1.03	Hexane-THF(5:1 v/v)
5r	517	0.15	1.35, 5.67(96%)	1.02	THF
5r	517	0.089	0.93, 5.89(90%)	1.09	ethanol
5r	516	0.073	2.11, 5.79(90%)	1.13	acetonitrile
5r	522	0.035	0.77, 2.99(57%), 6.43(31%)	1.14	water

1.5.3. Excited Triplet State Studies

Nanosecond transient absorption measurements were obtained using LP920 (Edinburgh Instruments Ltd.). The excitation source was a Q-switched Nd/YAG laser (BRIO) of 4 ns full width at half maximum with third harmonic (355 nm) generation. The 355 nm beam was directed onto one side of a 1 cm square silica cell containing the sample (absorbance 0.40) after bubbing Ar gas during 20 min. The transient transmission variations were monitored at right angles to the excitation in a crossbeam arrangement using a 450W xenon flash lamp, a monochromator, a photomultiplier and a digitized oscilloscope interfaced with a desktop computer. The power of the incident 355 nm laser pulse in the sample was about 5 mJ. The triplet quantum yield Φ_T was obtained by comparing the ΔA_T of the optically matched sample solution at peak maximum in a 1 cm cuvettes to that of the reference using the equation:[2]

$$\Phi_T = \Phi_T^{ZnPc} \cdot \frac{\Delta A_T}{\Delta A_T^{ZnPc}} \cdot \frac{\Delta \varepsilon_T^{ZnPc}}{\Delta \varepsilon_T} \qquad \text{Eq. (2)}$$

Where the superscript represents the reference, ΔA_T is the absorbance of the triplet transient difference absorption spectrum at the selected wavelength, and ZnPc is the reference compound (Φ_T=0.65 in 1-propanol).[2] $\Delta\varepsilon_T$ is the triplet state molar absorption coefficient, which is obtained by Eq. (3).

$$\Delta\varepsilon_T = \varepsilon_S \frac{\Delta A_T}{\Delta A_S} \qquad \text{Eq. (3)}$$

Where ΔA_S and ΔA_T are the absorbance change of the triplet transient difference absorption spectrum at the minimum of the bleaching band and the maximum of the positive band, respectively, and ε_S is the ground-state molar absorption coefficient at the UV-vis absorption band maximum. Both ΔA_S and ΔA_T were obtained from the triplet transient difference absorption spectra.

Table S3. The quantum yields for T_1 state formation of **(5r)** in different solvents.

Sample	Solvent	Φ_T (quantum yield for T_1 state formation)
5r	Hexane-THF(5/1 v/v)	0.47
5r	THF	0.14
5r	acetonitrile	0.084
5r	ethanol	not detected
5r	water	not detected

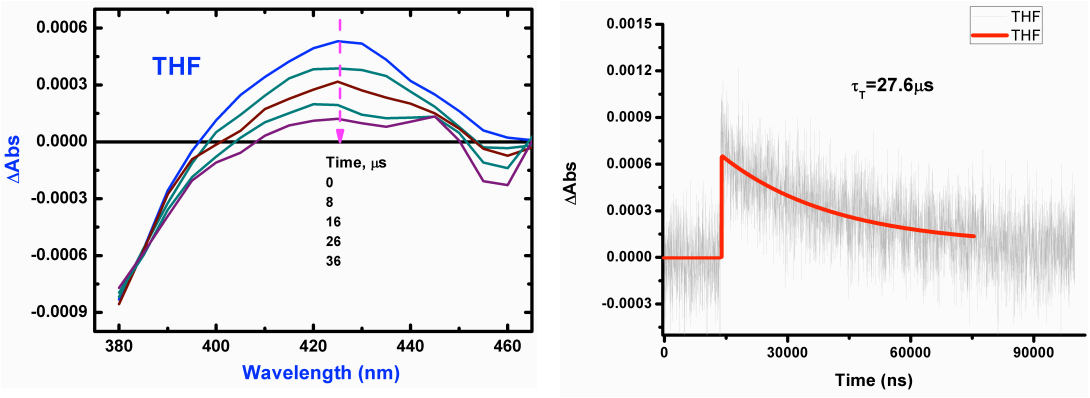


Figure S33. Left: the T_1-T_n transient absorption spectra, right: the decay of triplet state T_1 of **(5r)** at 425 nm in argon-saturated THF with laser excitation at 355 nm (the absorbance at 355 nm is 0.402).

1.6. Singlet Oxygen Trap Experiments

In singlet oxygen measurements 1,3-Diphenylisobenzofuran (DPBF) was used as a singlet oxygen trap in organic solvent and was purchased from a supplier. 2,2'-(Anthracene-9,10-diylbis(methylene))dimalonic acid (ADMDA) was used a singlet oxygen trap in aqueous solvent and was synthesized according to the literature.[3]

In a typical procedure for the detection of singlet oxygen generation by using trap molecules, a photosensitizer (~1 μM) and a trap molecule (O.D ~ 1.0) were mixed in O_2 bubbled solvent. Initially several dark measurements were taken followed by irradiation of the mixture at absorption maximum of a sensitizer. Absorbance decrease of trap molecules was monitored suggesting singlet oxygen generation in the presence of light and sensitizers. Irradiation of compounds was accomplished in Horiba Jobin-Yvon Time-

Resolved Fluorometer, Fluorolog FL-1057 by using monochromatic light system.

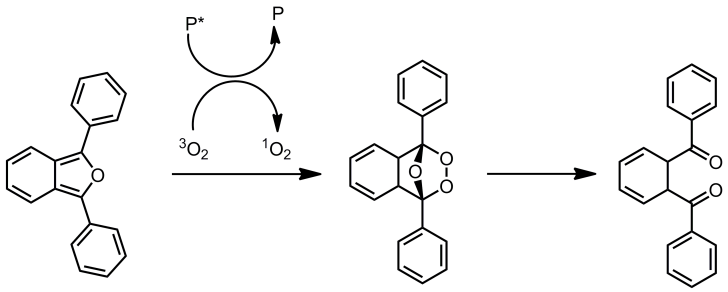


Figure S34. Reaction of singlet oxygen with 1,3-Diphenylisobenzofuran.

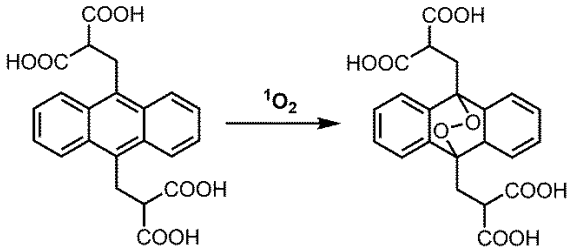


Figure S35. Reaction of singlet oxygen with 2,2'-(Anthracene-9,10-diylbis(methylene))dimalonic acid.

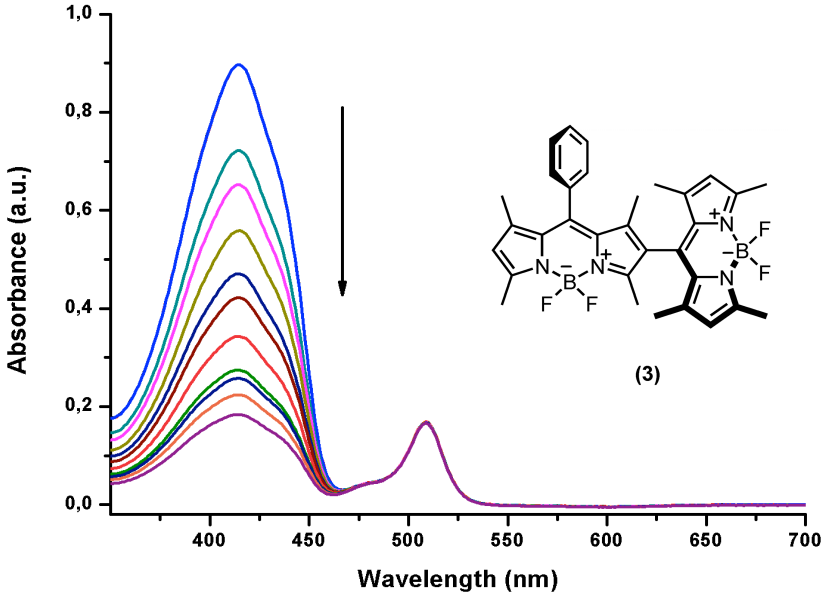


Figure S36. Decrease in absorbance of DPBF in ***DCM*** in the presence of ***(3) (1X10^{-6} M).*** *Excitation @508 nm.*

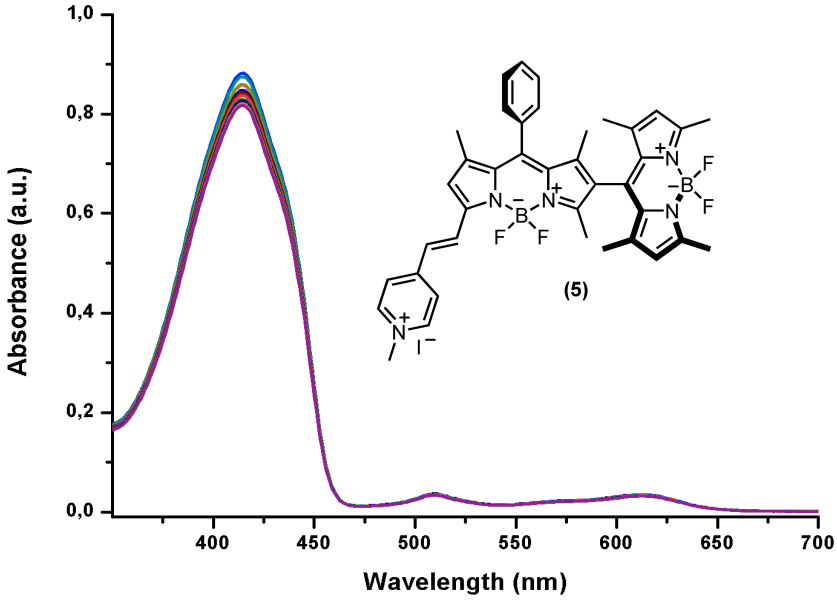


Figure S37. Decrease in absorbance of DPBF in ***DCM*** in the presence of ***(5) (1X10^{-6} M).*** *Excitation @508 nm.*

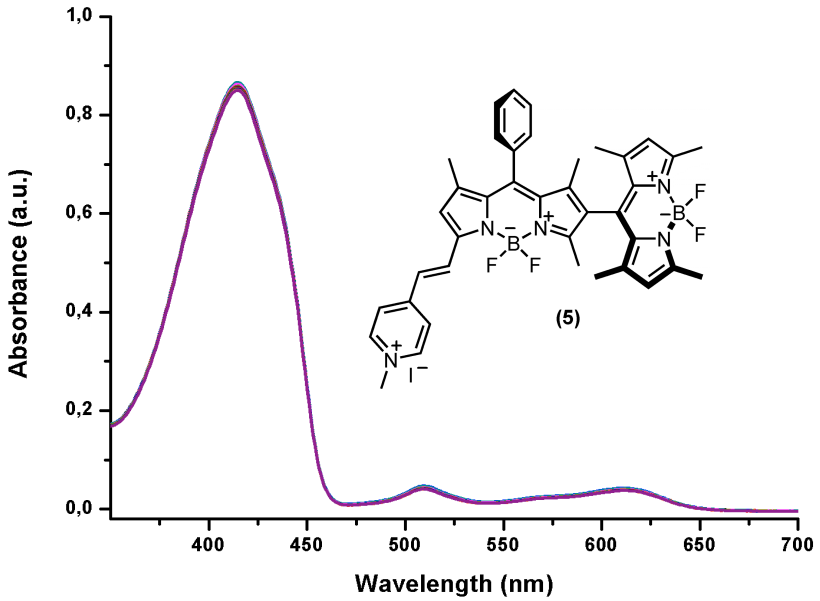


Figure S38. Decrease in absorbance of DPBF in ***DCM*** in the presence of ***(5) (1X10^{-6} M).*** *Excitation @607 nm.*

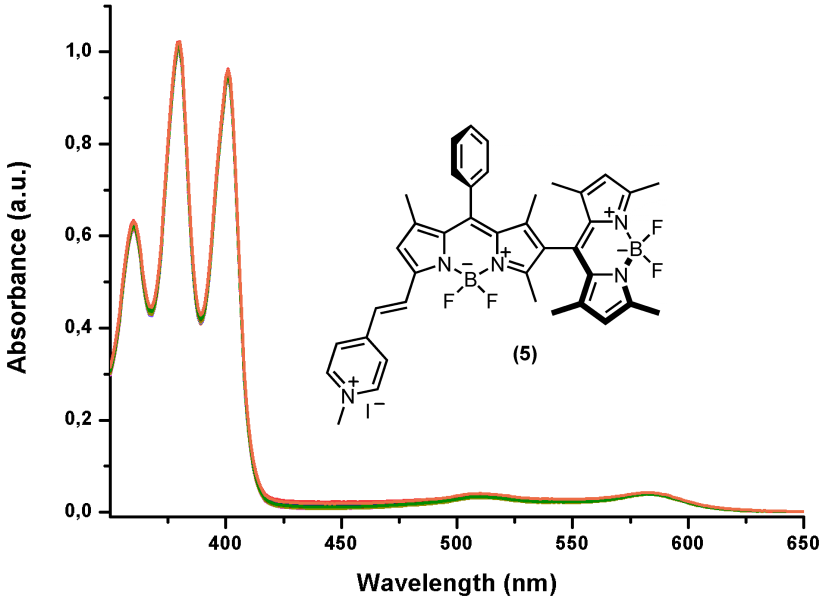


Figure S39. Decrease in absorbance of ADMDA in ***90:10 (20 mM Hepes buffer:MeCN)*** in the presence of ***(5) (1X10^{-6} M).*** *Excitation @513 nm.*

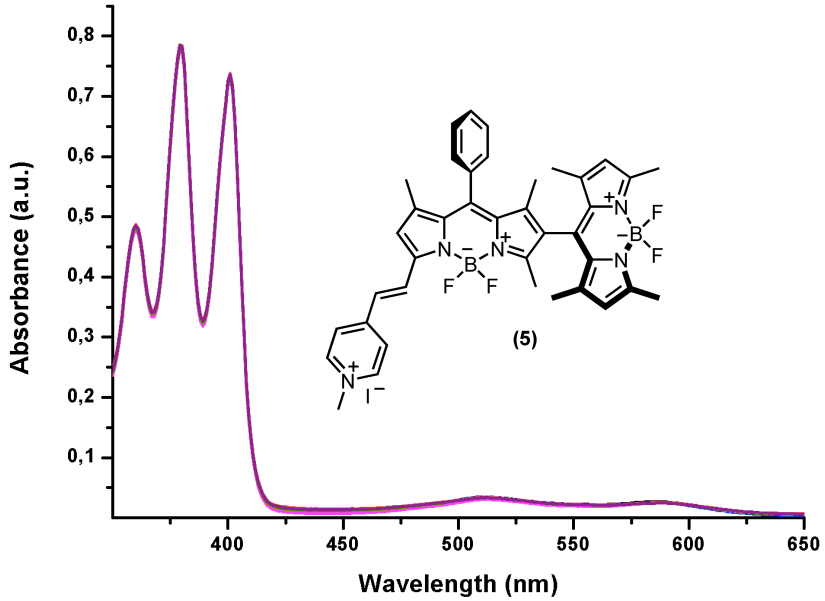


Figure S40. Decrease in absorbance of ADMDA in ***90:10 (20 mM Hepes buffer:MeCN)*** in the presence of ***(5) (1X10^{-6} M).*** *Excitation @590 nm.*

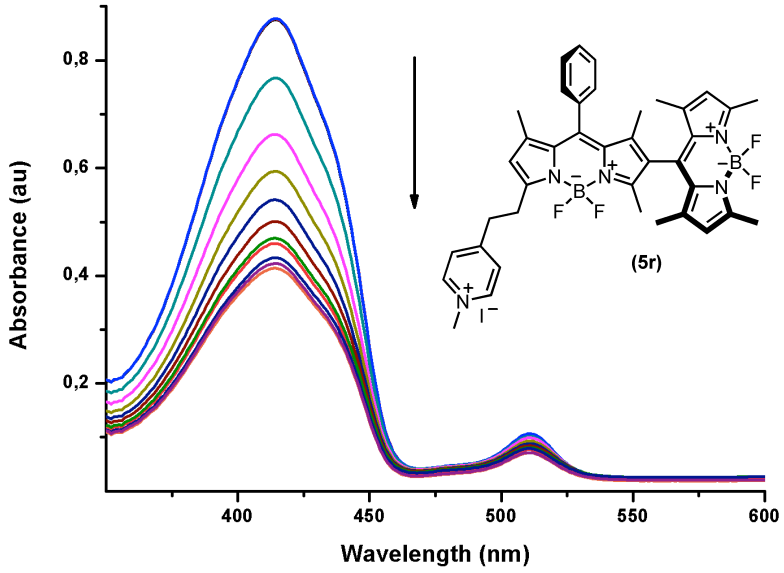


Figure S41. Decrease in absorbance of DPBF in ***DCM*** in the presence of ***(5r) (1X10^{-6} M).*** *Excitation @511 nm.*

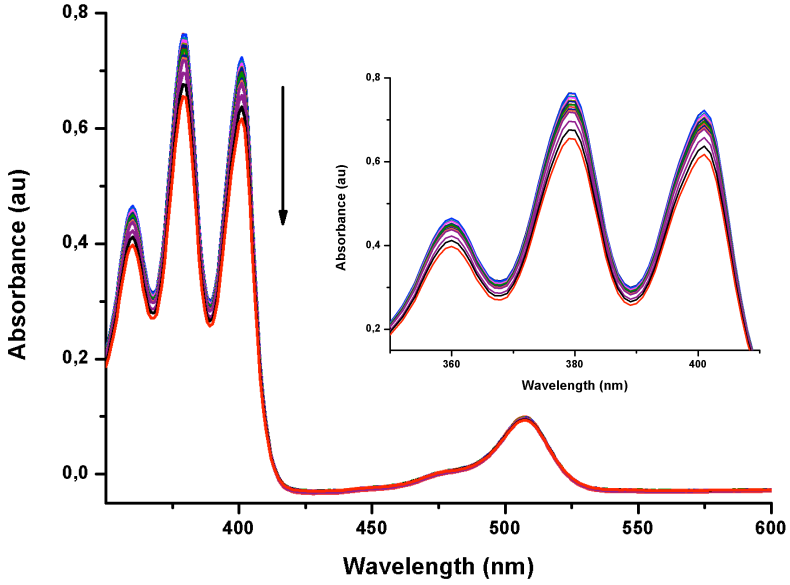


Figure S42. Decrease in absorbance of ADMDA in ***90:10 (20 mM Hepes buffer:MeCN)*** in the presence of ***(5r) (1X10^{-6} M).*** *Excitation @508 nm.*

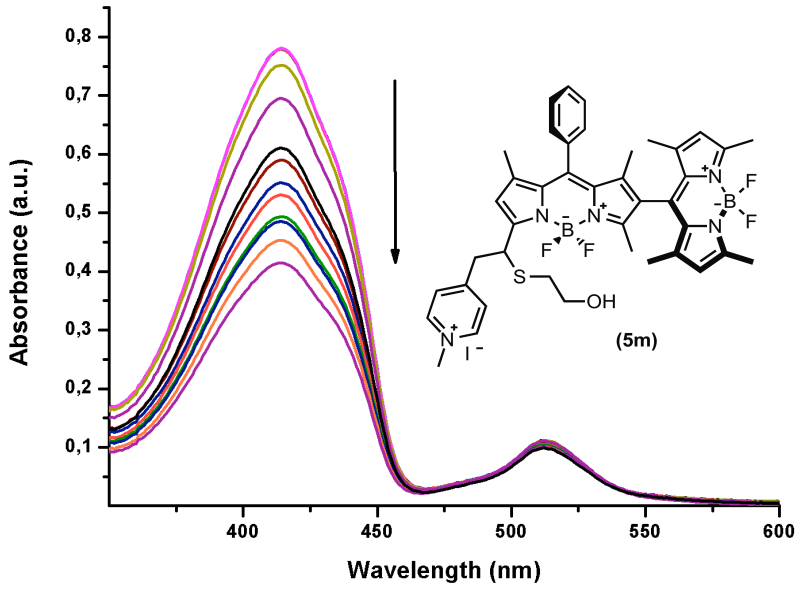


Figure S43. Decrease in absorbance of DPBF in ***DCM*** in the presence of ***(5m) (1X10^{-6} M).*** *Excitation @513 nm.*

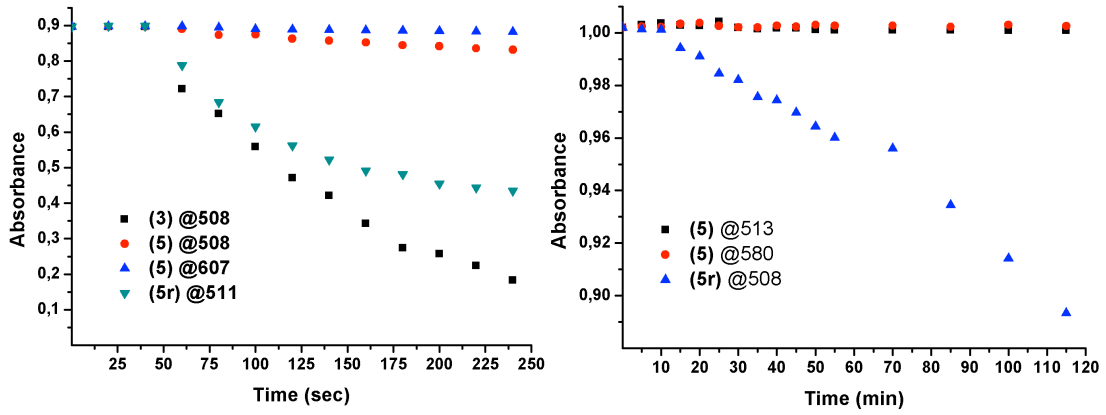


Figure S44. Left: Relative $^1O_2$ generation efficiency of the compounds **(3)**, **(5)** and **(5r)** in DCM as evidenced by the decreasing absorbance peak for the singlet oxygen trap DPBF at 414 nm and left: The same efficiency for **(5)** and **(5r)** in 90:10 (HEPES buffer, pH 7.2, 20 mM : MeCN) as revealed by ADMDA at 378 nm respectively with time. During first 60 seconds (left) and 15 minutes (right), the samples were kept in the dark to eliminate any possibility of a dark reaction.

1.7. Singlet Oxygen Quantum Yield Calculation

We have measured the singlet oxygen quantum yield (Φ_Δ) for **(5r)** in aqueous solution. Instead of pure water, we used aqueous micellar solution as solvents. Aqueous micellar or liposome solutions are generally considered good models for *in vitro* PDT, since aqueous phase acts as hydrophilic blood while micelles are similar to hydrophobic tissues. The photosensitizer **(5r)** intends to stay inside CTAB micelles, similar to the accumulation in cancer tissue. CTAB is cationic micelle, while SDS is anionic micelle. DPBF is also accumulated inside micelles. As shown in figure 44, with the excitation of **(5r)** at 510 nm, DPBF decomposes in first-order kinetics (figure 45). Using Rose Bengal as the reference, we obtained that Φ_Δ for **(5r)** is 0.36 in aqueous CTAB, and 0.24 in aqueous SDS solution.

Singlet oxygen quantum yield (Φ_Δ) determinations were carried out using the chemical trapping method.[3] 1,3-Diphenylisobenzofuran (DPBF) was used as a singlet oxygen trap in aqueous micellar solution (2 mM CTAB or 10 mM SDS) and was purchased from Sigma-Aldrich. In a typical procedure for the detection of singlet oxygen generation by using trap molecules, a photosensitizer (~6.7 mM) and a trap molecule (O.D. at 510 nm ~ 0.60) were mixed in O_2 bubbled solvent. Initially several dark measurements were taken followed by irradiation of the mixture at absorption maximum of a sensitizer. Absorbance decrease of trap molecules was monitored suggesting singlet oxygen generation in the presence of light and sensitizers. Irradiation of compounds was accomplished in Edinburgh Instruments Fluorometer, FLS920 by using monochromatic light system.

Typically, a 3 mL portion of the respective PS solutions that contained DPBF was irradiated at 510 nm in air saturated aq. micellar solution. Φ_Δ value was obtained by the relative method using methylene blue as the reference (Eq. 4):

$$\Phi_\Delta = \Phi_\Delta^{ref} \frac{k}{k^{ref}} \frac{I_a^{ref}}{I_a} \qquad \text{Eq. (4)}$$

where Φ_Δ^{ref} is the singlet oxygen quantum yield for the standard (rose bengal, 0.76),[4] k and k^{ref} are the DPBF photo-bleaching rate constants in the presence of the respective

samples and standard, respectively; I_a and I_a are the rates of light absorption at the irradiation wavelength of 510 nm by the samples and standard, respectively.

Table S4. Data for singlet oxygen quantum yield.

Compound	**Solvent**	**abs. (510 nm)**	**k, 10^{-3} s^{-1}**	**Φ_Δ**
5r	aq. 2 mM CTAB*	0.62	4.92	0.36
5r	aq. 10 mM SDS**	0.67	3.53	0.24
Rose Bengal	ethanol	0.49	8.18	0.76

* cmc of CTAB is 0.40 mM. ** cmc of SDS is 8 mM. k is the rate constant of DPBF decomposition.

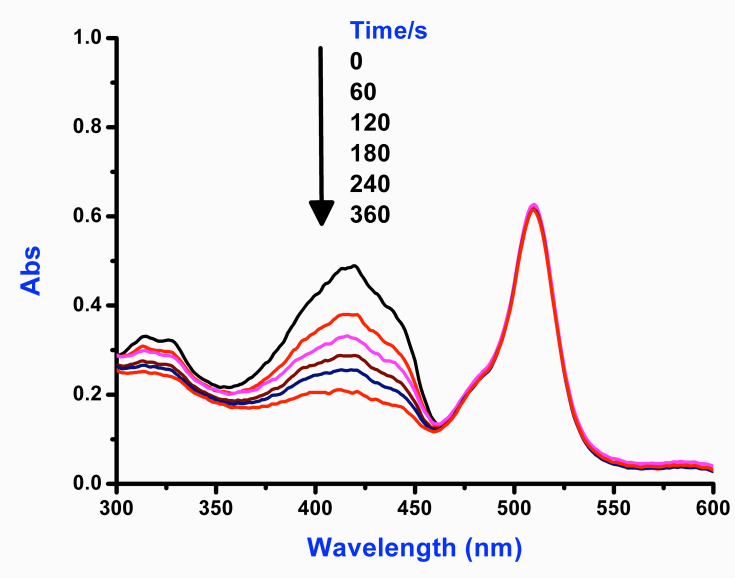


Figure S45. Decrease in absorbance of DPBF in aqueous CTAB micellar solution in the presence of **(5r)** ($6.7x10^{-6}$ M). Excitation @510 nm.

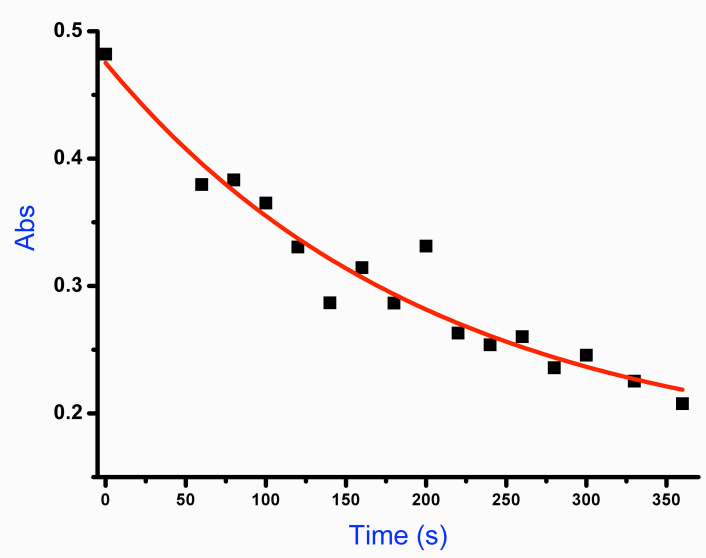


Figure S46. First order kinetics of DPBF decomposition in aqueous CTAB micellar solution in the presence of **(5r)** (6.7×10^{-6} M). Excitation @510 nm.

1.8. Singlet Oxygen Phosphorescence

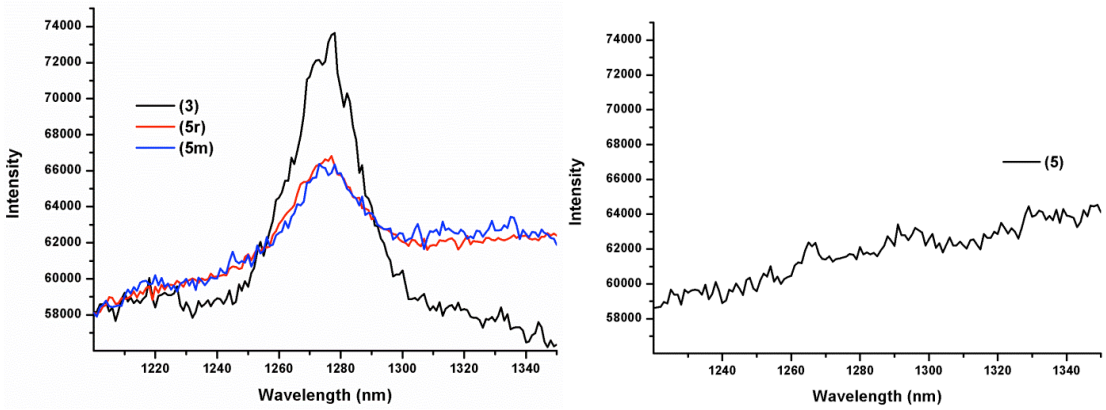


Figure S47. Singlet oxygen phosphorescence with sensitization from Bodipy derivatives; left: **(3)**, **(5r)**, **(5m)** right: **(5)** in O_2 bubbled DCM at equal absorbances (0.2) at the wavelength of the maximum of their respective absorbances.

1.9. Cell Culture Studies

1.9.1. Cell culture

HeLa cells (human epithelial adenocarcinoma), SK Hep-1 (human liver adenocarcinoma), NIH-3T3 (mouse embryo fibroblast) and WI38 VA-13 (human lung epithelial cell) were obtained from Korean Cell Line Bank (Seoul, Korea). All cells were grown in DMEM (Dulbecco's Modified Eagle's Medium, high glucose) supplemented with 10 % fetal bovine serum, 100 U/ml penicillin and 100 U/ml streptomycin. All cells were kept in 5 % CO_2 at 37 ℃.

1.9.2. Confocal microscopy imaging

Cells were seeded in a 35-mm glass bottomed dishes at a density of 3 X 105 cells per dish in culture media. After 24 hr, 1 μg/mL sample **(5)**, **(5r)** were added to the medium and the cells were incubated for 4 h at 37 ℃. After washing with the DPBS twice, cells were irradiated with green LED for 30 min. Another 3 hrs incubation, cells were stained with Annexin V AF-594 (apoptosis marker) followed by manufacturer's instructions (Molecular probe). To stain nucleus, 1 μg/mL DAPI were added to the media for 30 min. After washing with the DPBS, the cells were imaged by confocal laser scanning microscope (Super resolution confocal microscope, STED-SP8, Leica, Germany). DAPI (ex. 405 nm, em. 434-501 nm); **(5)**, **(5r)** (ex. 458 nm, em. 470-540 nm); Annexin V-AF594 (ex. 561 nm, em. 575-675 nm).

1.9.3. Flow Cytometry

To detect apoptotic cells, flow cytometry was used. Cells were incubated with sample **(5)**, **(5r)** and irradiated green LED for 30 min. Cells were harvested and washed in cold PBS and incubated Annexin V AF-594 in annexin-binding buffer (10 mM Hepes, 140 mM NaCl and 2.5 mM $CaCl_2$, pH 7.4) for 15 min, room temperature, in the dark. Cells were transferred to ice and add DAPI solution and analyzed with LSRFortessa flow cytometer (Becton Dickinson, Franklin Lakes, NJ, USA) immediately. At least 10,000 cells were acquired for each sample.

1.9.4. Cell viability

Cells were seeded in a 96-well plate with culture media. After 24 h, cells were incubated with sample **(5)**, **(5r)** for 4 h and washed with DPBS. After irradiation with green LED for 30 min, cells were incubated another 3 hrs. To identify cell viability, 0.5 mg/mL of MTT (Sigma) media was added to the cells for 4 hrs, and the produced formazan was dissolved in 0.1 mL of dimethylsulfoxide (DMSO) and read at OD 650 nm with a Spectramax Microwell plate reader.

1.9.5. Determination of intracellular GSH level

Cells were cultured for 24 hr in culture media and harvested cell and re-suspended 5 % MPA (metaphosphoric acid, to remove interfering protein and enzyme). Homogenize cell suspension and centrifuge at 12,000 rpm for 5 min at 4℃. Supernatant were used for GSH detection and followed manufacturer's instruction (OxiselectTM Total GSH Assay Kit, CellBioLabs, INC.). Protein concentrations were determined by BCA Protein assay kit (Pierce).

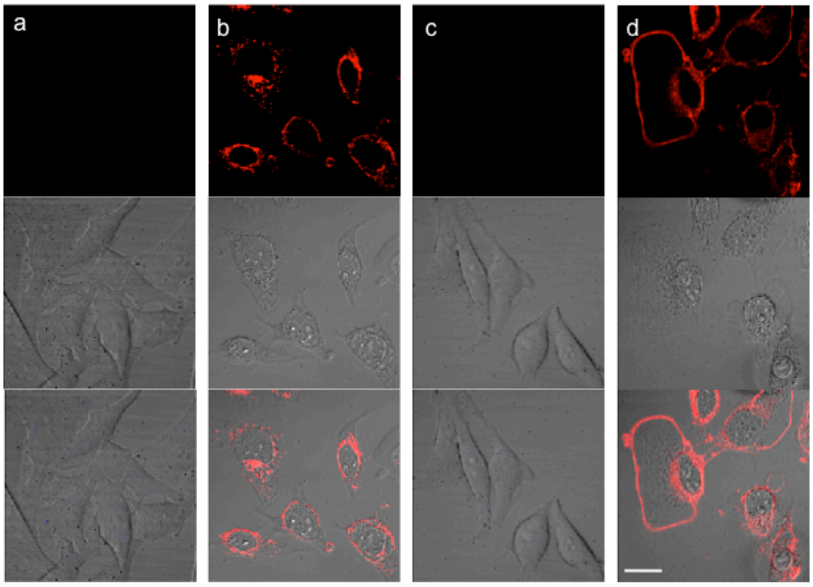


Figure S48: Apoptotic effect of sample **(5)**, **(5r)**: HeLa cells were incubated with sample **(5)**, **(5r)** and illuminated with a green (520 nm) LED array and stained with Annexin V-AF594 (Apoptotic marker, red fluorescence). (a) **(5)**, (b) **(5)** + LED, (c) **(5r)** and (d) **(5r)** + LED. Confocal images were acquired by ex. 559 nm Em. 575 - 675 nm. Top : fluorescence, middle : DIC, bottom : merge. Scale bar: 10 μm.

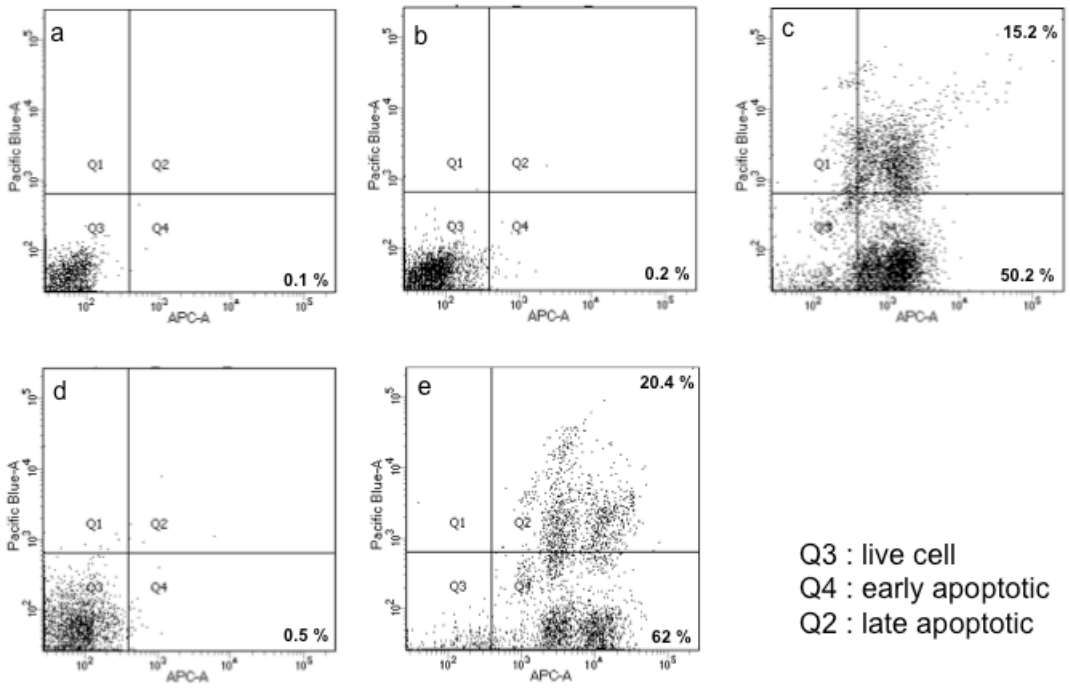


Figure S49. FACs analysis of sample **(5)**, **(5r)**: HeLa cells were incubated with sample **(5)**, **(5r)** stained with Annexin V-AF594 (Apoptotic marker) and DAPI. (a) Control (b) **(5)**, (c) **(5)** + LED, (d) **(5r)** and (e) **(5r)** + LED.

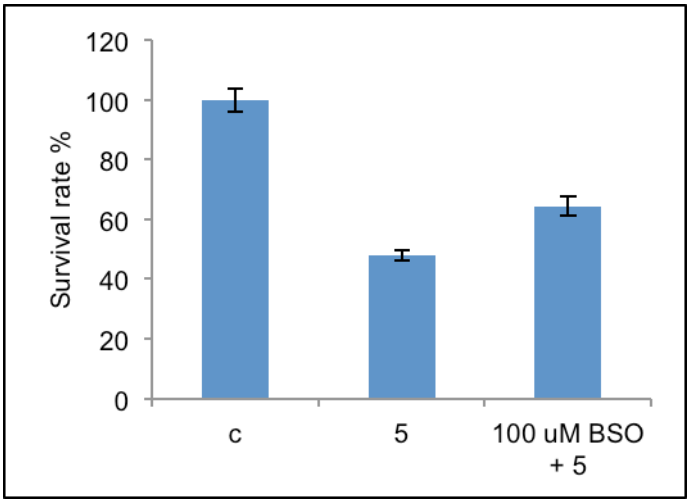


Figure S50. Photocytotoxic effects of compound **(5)**. HeLa cells were incubated with 0, 100 μM BSO (Buthionine sulfoximine, inhibitor of GSH synthesis) for 4hr and removed BSO and then incubated with 280 ng/mL **(5)** for 4hr and irradiated with green LED. Cell viability was identified by MTT assay. Results are expressed as mean ± standard deviation of three independent experiments. (c: control)

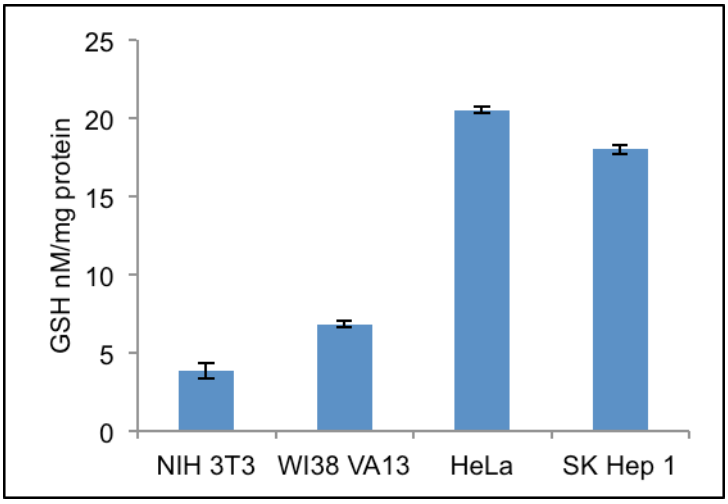
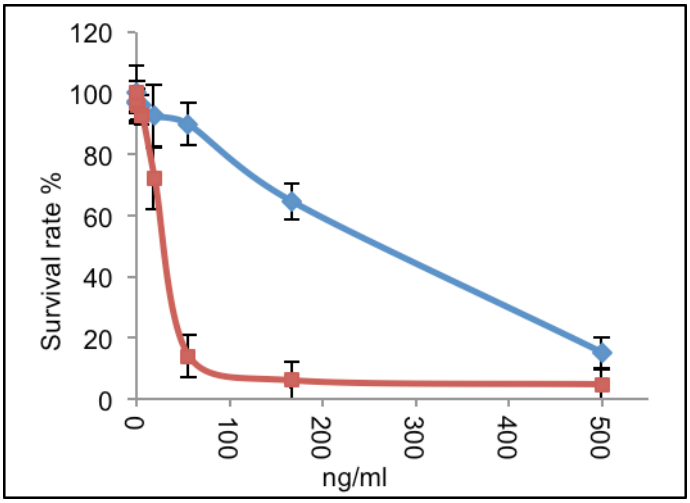


Figure S51. GSH levels in each cell were determined by Oxiselect Total glutathione assay kit (Cell Biolabs, INC.). Cells were cultured for 24 hr and harvested and assayed by manufacturer's Instructions. Results are expressed as mean ± standard deviation of three independent experiments.



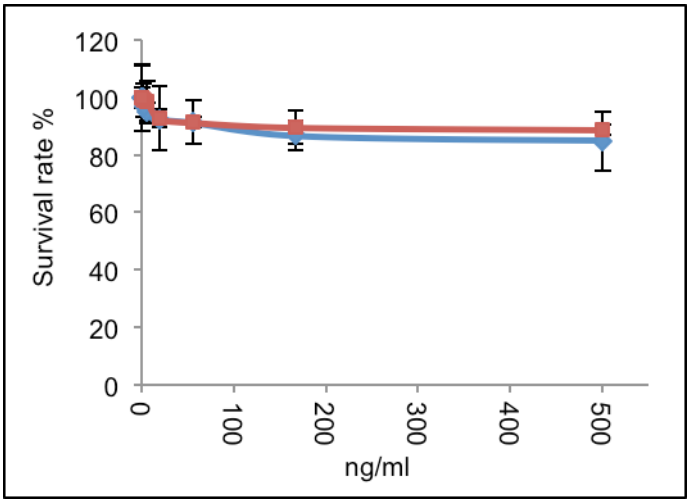


Figure S52. Concentration-dependent photocytotoxicity of the sensitizer **(5)** (blue) and **(5r)** (red). The HeLa cells were incubated with each concentration of **(5)**, **(5r)** for 24 hr. After removal of **(5)**, **(5r)**, cells were kept either in the dark (bottom), or under illumination with a green (520 nm) LED array (top). Cell viability was identified by MTT assay. Results are expressed as mean ± standard deviation of three independent experiments.

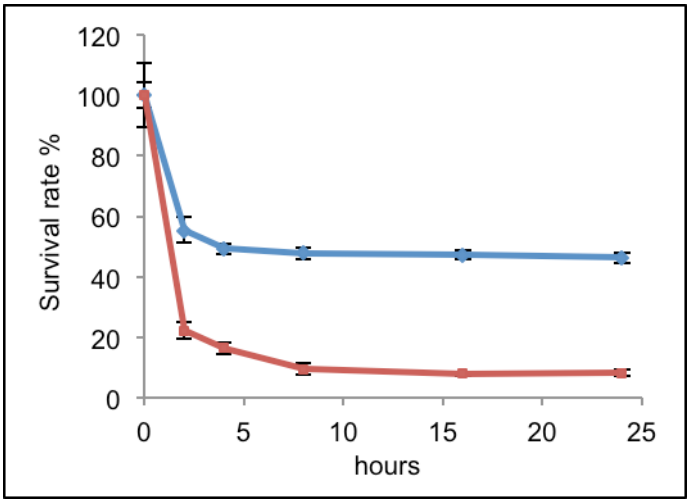


Figure S53. Time-dependent photocytotoxicity of the sensitizer **(5)** (blue) and **(5r)** (red). The HeLa cells were incubated with 280 ng/mL (IC_{50}) of **(5)**, **(5r)** for 2, 4, 8, 16, 24 hr. After removal of **(5)**, **(5r)**, cells were illuminated with a green (520 nm) LED array. Cell viability was identified by MTT assay. Results are expressed as mean ± standard deviation of three independent experiments.

1.10. Computational Details:

Geometry optimizations were performed using Density Functional Theory (DFT),[5-8] No restrictions on symmetry were imposed. Becke's three-parameter exchange in conjunction with Lee-Yang-Parr correlation functional, B3LYP,[7-13] was used as implemented in Gaussian 09. Stevens-Basch-Krauss split valence effective core potentials (ECP) CEP-31G[14] was employed. Several other basis sets and functionals were previously tested, and this level of theory was confirmed to have reliable results compared with the experimental data[1,15-17]. Spin contamination of the unrestricted Kohn-Sham wave functions were checked and found to be negligible in all cases. Harmonic vibrational frequency calculations ensured that Hessian matrix does not contain any negative eigenvalues, i.e. all reported geometries correspond to minimum points on the potential energy surface. All computations were carried out using Gaussian 09[18].

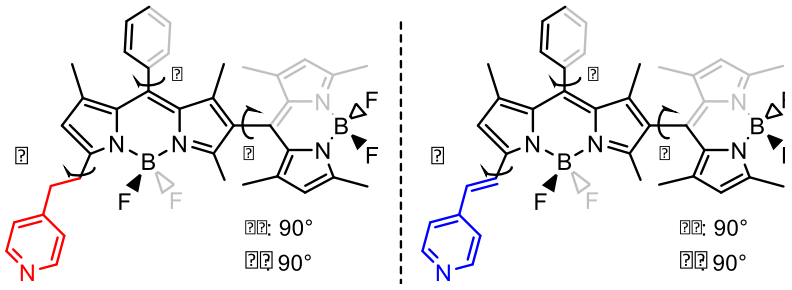


Figure S54. Molecular structures and important dihedral angles of **(5)** and **(5r)**.

1.10.1. Molecular Orbitals and Energies

Table S4. Relative energies for **(5)** and **(5r)** of S_0 and T_1 states at UB3LYP/CEP-31G level of theory.

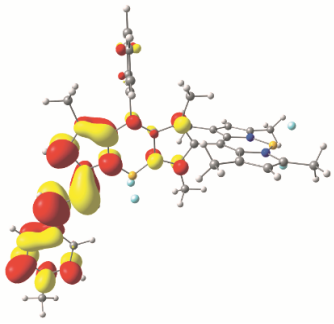
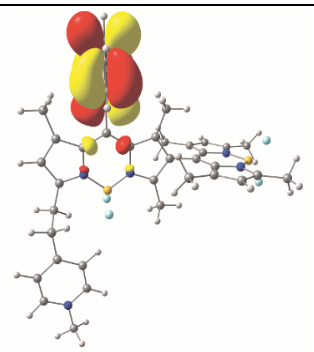
Molecule	$E(T_1\text{-}S_0)$ (eV)
5	1.1
5r	1.4

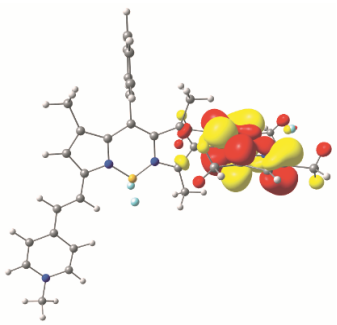
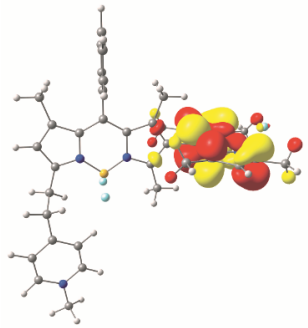
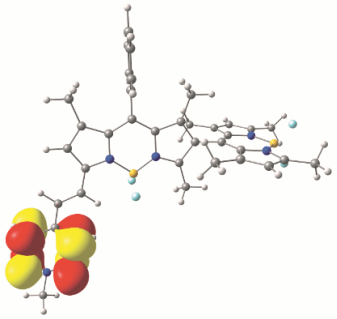
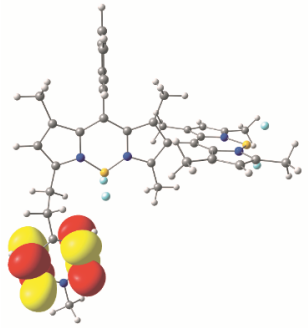
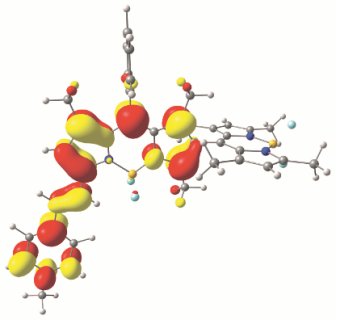
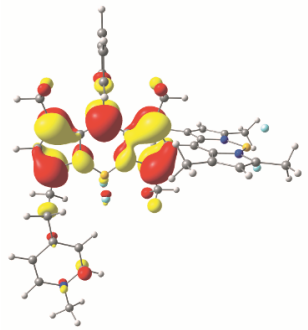
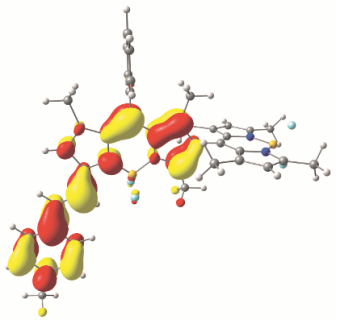
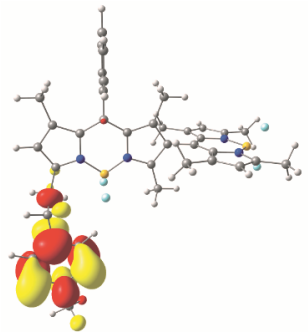
Table S5. Excited State DFT Results for $S_0 \rightarrow S_1$ Absorption Spectra of **(5)** and **(5r)** at TD-UCAM-B3LYP/CEP-31G Level of Theory.

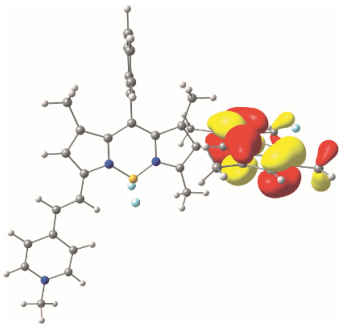
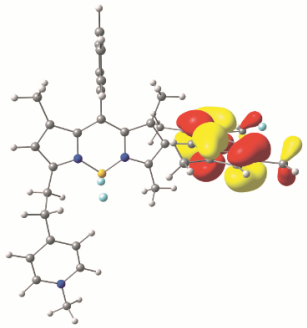
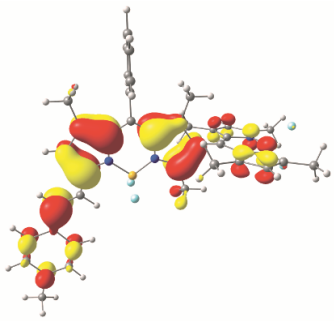
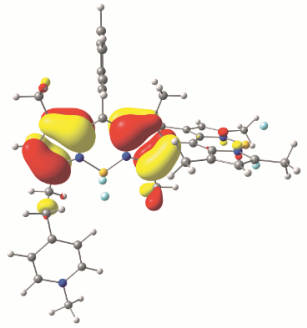
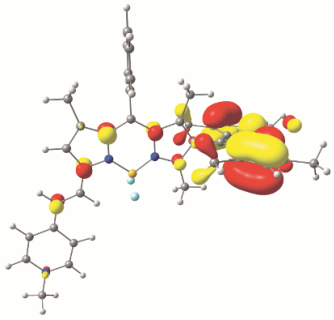
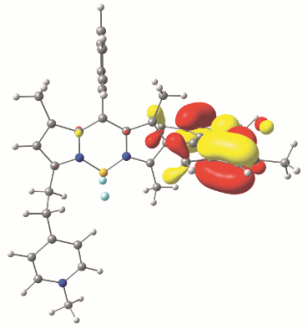
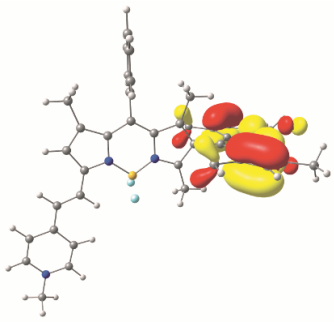
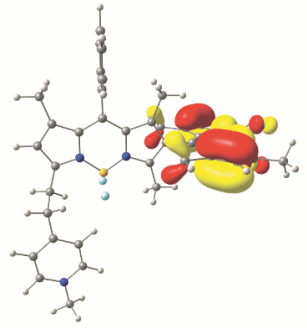
Molecule	Transitions with large oscillator strength (nm)	
5	438	530
5r	438	440

* Two distinct absorption peaks are observed for compound **(5)** where the transitions are of BOD1→BOD1 and BOD2→BOD2 type at 438 nm and 530 nm respectively. Hence (i) a BODIPY like and (ii) a slightly red shifted absorption (due to conjugation with the MP π-system) are calculated as predicted. Similarly, calculations on **(5r)** shows two essentially isoenergetic transitions at 438 nm and 440 nm, the calculated signature of unconjugated BODIPY core also seen above for **(5)**. Therefore absorption spectra of **(5)** ad **(5r)** are matched with TD-DFT calculations apart from numerical deviations that are within the limitations of quantum chemical calculations on excited states for similar systems.[17]

Table S6. Kohn-Sham orbitals and energies for S_0 state of **(5)** and **(5r)** using UB3LYP/CEP-31G level of theory. Orbital shapes are obtained using iso value of 0.3

5			**5r**		
	MO	Energy (eV)		MO	Energy (eV)
LUMO+4		-3.25	LUMO+4		-2.64

LUMO+3		-4.35	LUMO+3		-4.24
LUMO+2		-4.42	LUMO+2		-4.85
LUMO+1		-4.96	LUMO+1		-5.02
LUMO		-6.04	LUMO		-5.79

HOMO		-7.23	HOMO		-7.13
HOMO-1		-8.25	HOMO-1		-8.02
HOMO-2		-8.35	HOMO-2		-8.25
HOMO-3		-8.54	HOMO-3		-8.44

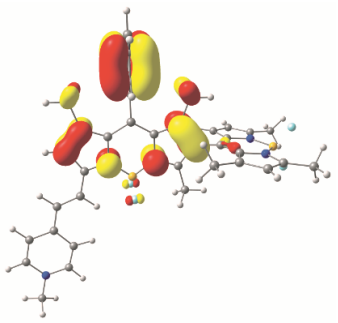
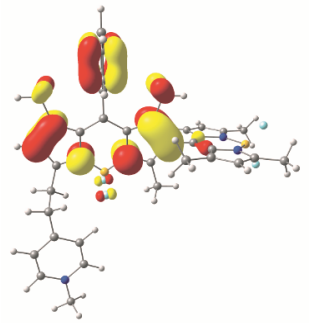
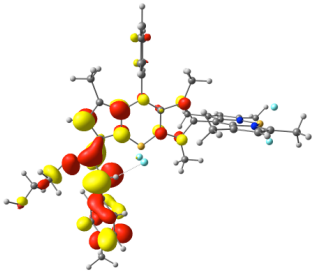
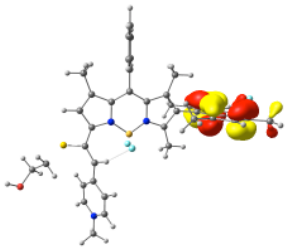
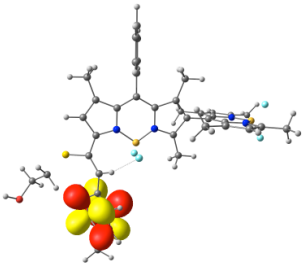
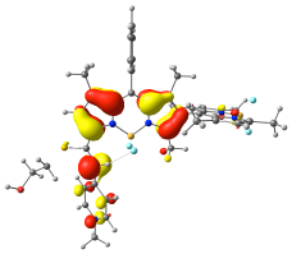
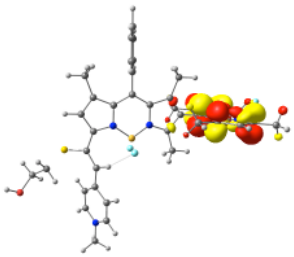
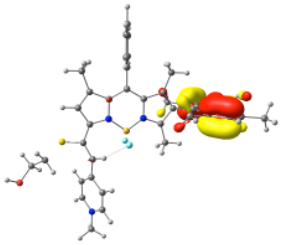
HOMO-4		-9.20	HOMO-4		-8.93

Table S7. Kohn-Sham orbitals and energies for S_0 state of **(5m)** using UB3LYP/CEP-31G level of theory. Orbital shapes are obtained using iso value of 0.3

5m

MO		Energy (eV)	MO		Energy (eV)
LUMO+4		-3.22	HOMO		-7.25
LUMO+3		-4.24	HOMO-1		-8.23
LUMO+2		-4.37	HOMO-2		-8.37

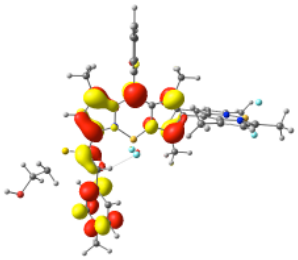
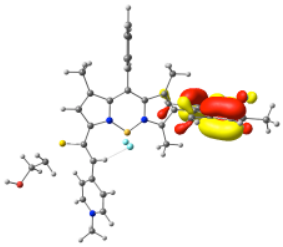
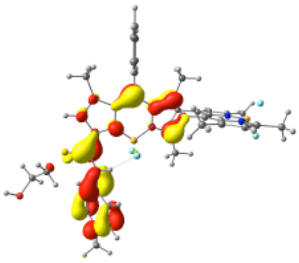
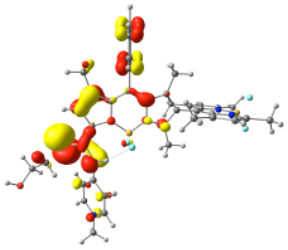
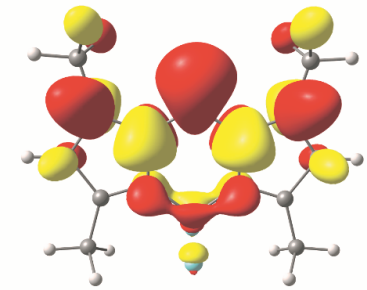
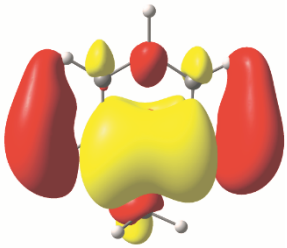
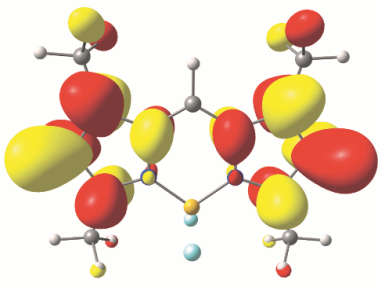
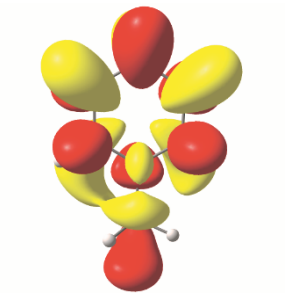
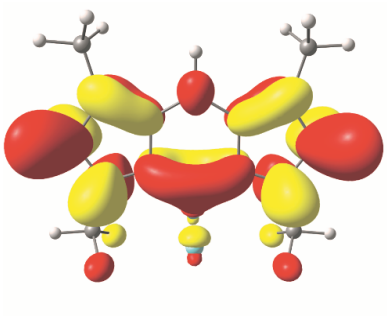
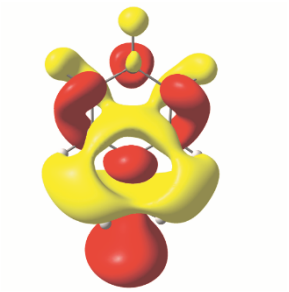
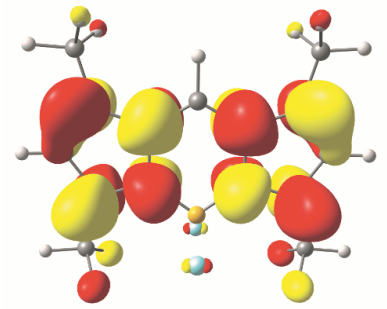
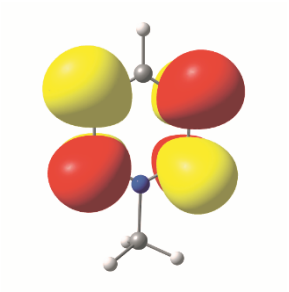
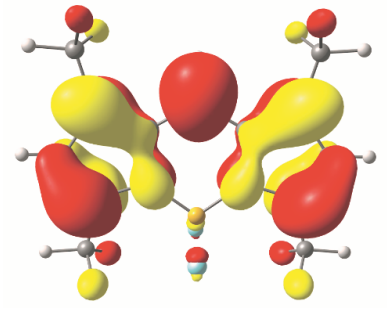
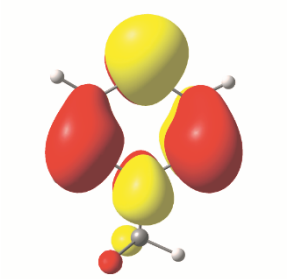
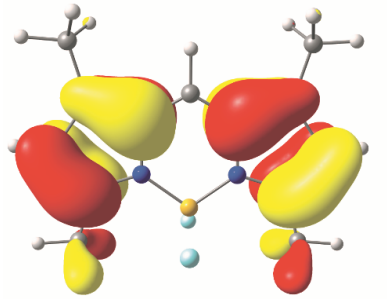
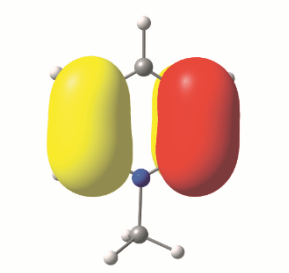
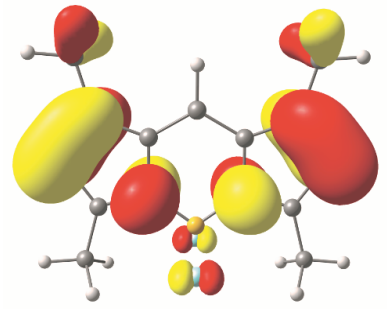
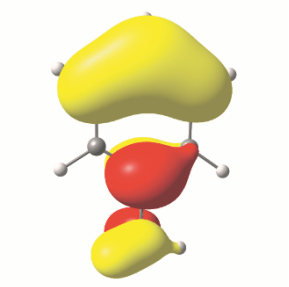
LUMO+1		-4.97	HOMO-3		-8.56
LUMO		-5.96	HOMO-4		-9.11

Table S8. Kohn-Sham orbitals and energies for S_0 state of **BODIPY** and **MePy** using UB3LYP/CEP-31G level of theory. Orbital shapes are obtained using iso value of 0.3

BODIPY			**MePy**		
MO		Energy (eV)	MO		Energy (eV)
LUMO+4		2.65	LUMO+4		-1.25
LUMO+3		1.61	LUMO+3		-2.19

LUMO+2		0.96	LUMO+2		-2.30
LUMO+1		0.50	LUMO+1		-5.80
LUMO		-2.78	LUMO		-6.86
HOMO		-5.69	HOMO		-12.68
HOMO-1		-6.85	HOMO-1		-13.21

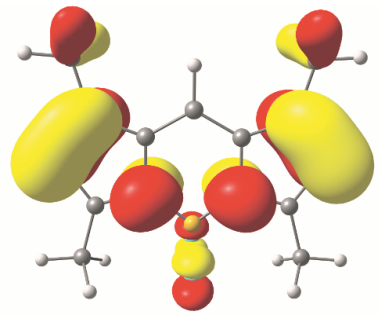
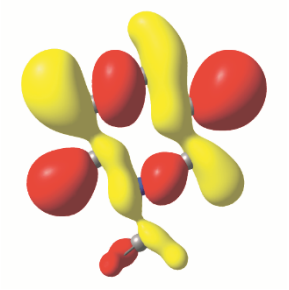
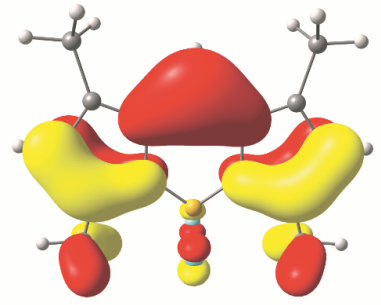
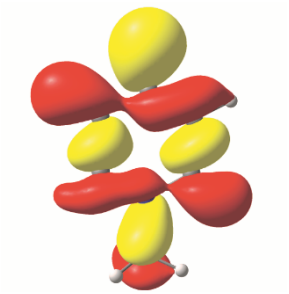
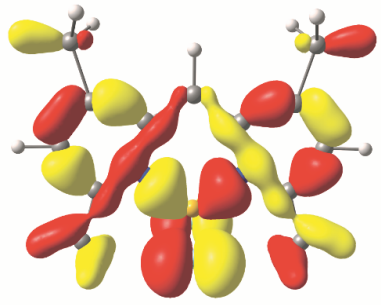
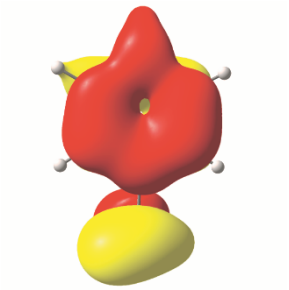
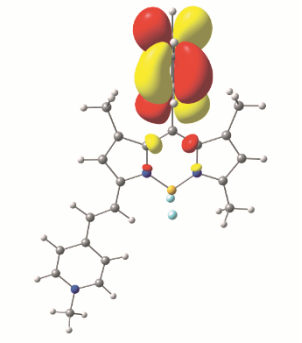
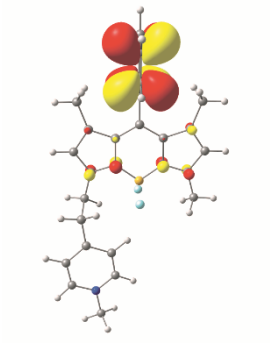
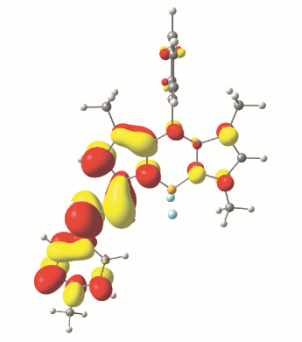
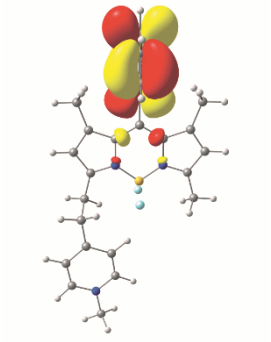
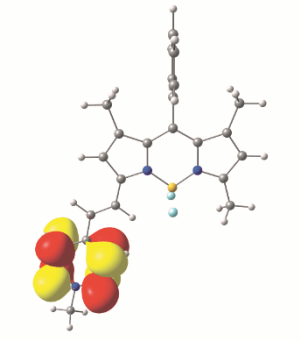
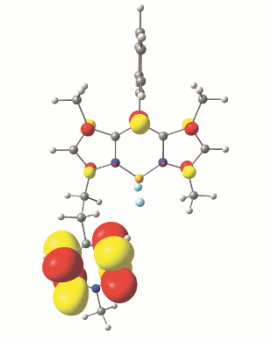
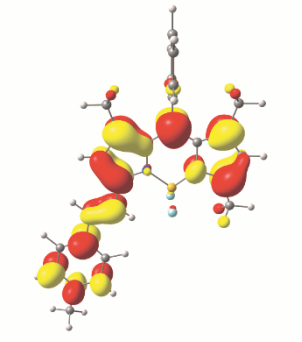
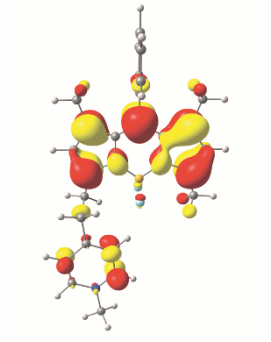
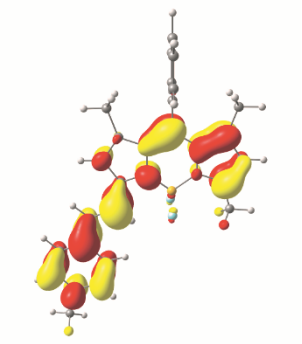
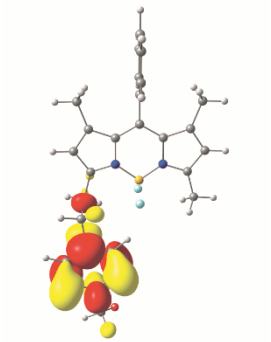
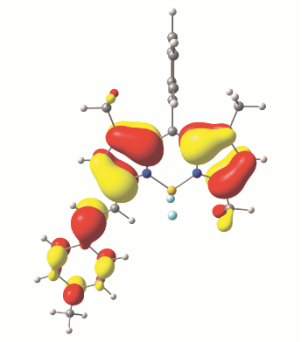
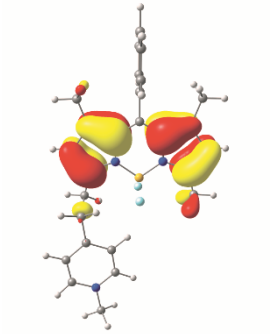
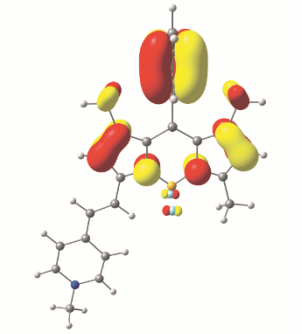
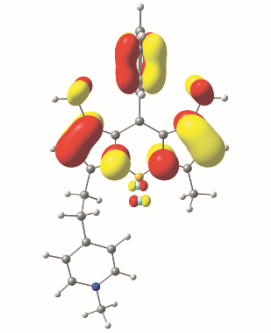
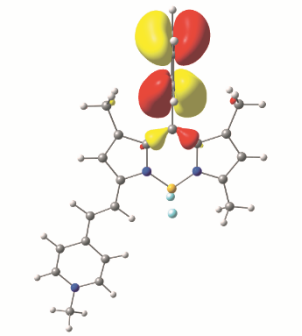
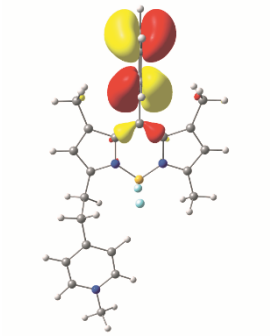
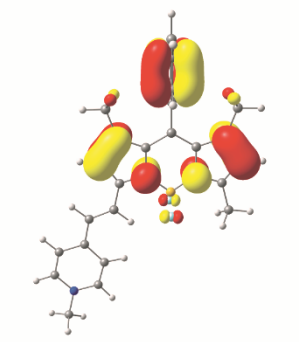
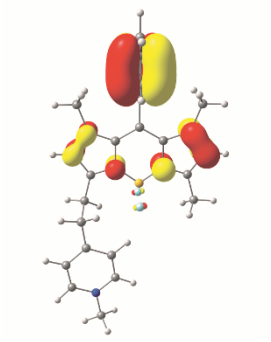
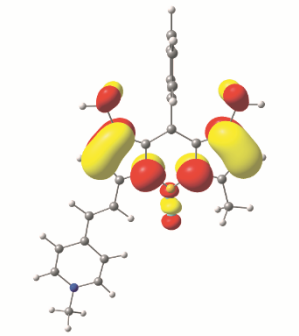
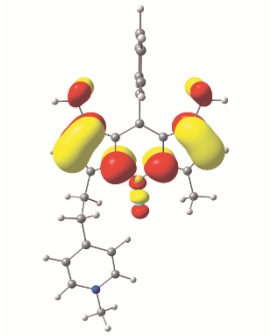
HOMO-2		-7.04	HOMO-2		-15.31
HOMO-3		-7.97	HOMO-3		-15.47
HOMO-4		-8.92	HOMO-4		-15.60

Table S9. Kohn-Sham orbitals and energies for S_0 state of **MD1** and **MD2** using UB3LYP/CEP-31G level of theory. Orbital shapes are obtained using iso value of 0.3

MD1		**MD2**	
MO	Energy (eV)	MO	Energy (eV)

LUMO+4		-2.76	LUMO+4		-2.47
LUMO+3		-3.15	LUMO+3		-2.51
LUMO+2		-4.33	LUMO+2		-4.76
LUMO+1		-4.83	LUMO+1		-4.82

LUMO		-5.92	LUMO		-5.70
HOMO		-8.16	HOMO		-7.85
HOMO-1		-9.13	HOMO-1		-8.81
HOMO-2		-9.16	HOMO-2		-8.91

HOMO-3		-9.33	HOMO-3		-9.03
HOMO-4		-9.45	HOMO-4		-9.09

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Cartesian Coordinates

5, Singlet, UB3LYP/CEP-31G, E(SCF)=-394.651428, MB_bv2_P504

	x	y	z
C	5.179982000	-4.065971000	-0.246731000
N	5.615809000	-2.732662000	-0.277718000
B	4.700211000	-1.484240000	-0.291314000
N	3.237110000	-1.964713000	-0.230377000
C	2.820845000	-3.333063000	-0.180610000
C	3.767084000	-4.377991000	-0.193996000
C	2.129126000	-1.162556000	-0.205531000
C	0.945459000	-1.994178000	-0.133185000
C	1.353122000	-3.344046000	-0.116364000
C	6.349702000	-4.937502000	-0.274341000
C	7.474644000	-4.080024000	-0.317972000
C	7.010558000	-2.718556000	-0.318567000
C	6.421552000	-6.457847000	-0.263576000
C	7.746808000	-1.472943000	-0.348331000
C	0.419089000	-4.538104000	-0.038376000
F	4.939431000	-0.705056000	-1.489296000
F	5.010041000	-0.627485000	0.837122000
C	-0.454236000	-1.466236000	-0.077456000
C	-1.024418000	-1.120041000	1.181419000
N	-2.342342000	-0.581061000	1.249830000
B	-3.268932000	-0.321240000	0.034387000
N	-2.517444000	-0.767655000	-1.246162000
C	-1.193211000	-1.294628000	-1.283179000
C	-3.007719000	-0.699079000	-2.527743000
C	-1.999475000	-1.184869000	-3.432506000
C	-0.860825000	-1.559946000	-2.679727000
C	-0.508499000	-1.203307000	2.544606000
C	-1.535658000	-0.708691000	3.384003000
C	-2.655916000	-0.330473000	2.563829000
C	0.423450000	-2.126428000	-3.270447000
C	0.839662000	-1.716936000	3.032869000
F	-4.499313000	-1.065573000	0.177717000
F	-3.599398000	1.084373000	-0.047981000
C	9.134420000	-1.369792000	-0.383405000
C	9.852754000	-0.103387000	-0.403548000
C	11.298558000	-0.096345000	-0.438064000

C	12.013012000	1.106437000	-0.456237000
N	11.361383000	2.328841000	-0.444004000
C	9.973463000	2.364594000	-0.412189000
C	9.210005000	1.195829000	-0.392230000
H	8.510774000	-4.402088000	-0.346018000
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H	5.995142000	-6.883327000	0.658613000
H	5.869356000	-6.902253000	-1.106357000
H	7.138478000	-0.568832000	-0.337052000
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H	0.637140000	-5.168199000	0.838706000
H	-2.108667000	-1.245587000	-4.510964000
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H	1.004900000	-2.771665000	2.754247000
H	1.684024000	-1.135522000	2.625264000
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H	11.852079000	-1.035374000	-0.452019000
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H	9.516651000	3.353958000	-0.403782000
H	8.126127000	1.291687000	-0.370202000
C	-3.982550000	0.250428000	3.002881000
H	-4.816090000	-0.386562000	2.665546000
H	-4.013625000	0.341859000	4.098273000
H	-4.140323000	1.243550000	2.550898000
C	-4.391377000	-0.184200000	-2.860485000
H	-4.546088000	-0.187542000	-3.949207000
H	-5.164104000	-0.808649000	-2.382486000
H	-4.528435000	0.839159000	-2.475264000
C	2.195293000	0.345631000	-0.252707000
H	2.695903000	0.678705000	-1.177049000
H	1.186124000	0.775538000	-0.209385000
H	2.795402000	0.731285000	0.587779000
C	3.320522000	-5.817330000	-0.154154000
C	3.027711000	-6.504704000	-1.366202000
C	3.192095000	-6.490006000	1.093880000

C	2.605516000	-7.861908000	-1.328722000
C	2.767948000	-7.846704000	1.129555000
C	2.474066000	-8.534445000	-0.081308000
H	3.129496000	-5.988636000	-2.323411000
H	3.418259000	-5.961964000	2.022864000
H	2.381112000	-8.385709000	-2.260349000
H	2.666973000	-8.357985000	2.089232000
H	2.147216000	-9.576074000	-0.053396000
C	12.139191000	3.610777000	-0.418666000
H	12.180710000	4.004133000	0.608506000
H	13.157534000	3.422014000	-0.780976000
H	11.654836000	4.343621000	-1.078111000

5, Triplet, UB3LYP/CEP-31G, E(SCF)=-394.611740, MB_bv2_P505

	x	y	z
C	5.152202000	-3.962724000	-0.209255000
N	5.593516000	-2.628088000	-0.256453000
B	4.684462000	-1.384660000	-0.260537000
N	3.224079000	-1.871844000	-0.187264000
C	2.808995000	-3.220947000	-0.139602000
C	3.771689000	-4.295107000	-0.150227000
C	2.105630000	-1.050176000	-0.164520000
C	0.930741000	-1.884315000	-0.099952000
C	1.342973000	-3.240801000	-0.083911000
C	6.358771000	-4.844929000	-0.232752000
C	7.461743000	-3.999818000	-0.292851000
C	7.000102000	-2.608042000	-0.308010000
C	6.408983000	-6.362676000	-0.199045000
C	7.750936000	-1.402819000	-0.361837000
C	0.414525000	-4.441786000	-0.023035000
F	4.899364000	-0.598105000	-1.461473000
F	4.992970000	-0.521140000	0.864447000
C	-0.482142000	-1.389852000	-0.060039000
C	-1.128189000	-1.180060000	1.192890000
N	-2.498038000	-0.798883000	1.250084000
B	-3.418199000	-0.563325000	0.023028000
N	-2.572488000	-0.810909000	-1.254373000
C	-1.202696000	-1.195751000	-1.274744000
C	-3.023053000	-0.696457000	-2.548422000

C	-1.936385000	-1.008802000	-3.445964000
C	-0.794596000	-1.324104000	-2.678261000
C	-0.635114000	-1.284539000	2.570459000
C	-1.729627000	-0.962131000	3.401636000
C	-2.869937000	-0.666862000	2.567190000
C	0.565759000	-1.706667000	-3.237368000
C	0.760119000	-1.648677000	3.050552000
F	-4.540314000	-1.469604000	0.060024000
F	-3.922158000	0.788526000	0.031801000
C	9.165096000	-1.365175000	-0.416397000
C	9.953750000	-0.159231000	-0.470816000
C	11.403446000	-0.234817000	-0.528037000
C	12.184018000	0.919770000	-0.583761000
N	11.601776000	2.186423000	-0.589180000
C	10.213632000	2.301896000	-0.533499000
C	9.386699000	1.182000000	-0.476803000
H	8.498899000	-4.317765000	-0.322899000
H	7.457024000	-6.698827000	-0.230818000
H	5.941660000	-6.766887000	0.712996000
H	5.874758000	-6.808308000	-1.053201000
H	7.183168000	-0.473714000	-0.359035000
H	-0.633420000	-4.107036000	-0.005026000
H	0.549690000	-5.108344000	-0.889977000
H	0.596737000	-5.055236000	0.874250000
H	-2.003683000	-0.995659000	-4.529213000
H	-1.731044000	-0.932396000	4.486646000
H	0.540303000	-1.667269000	-4.337184000
H	1.361806000	-1.026037000	-2.891129000
H	0.862638000	-2.725944000	-2.936398000
H	0.809450000	-1.567449000	4.147291000
H	1.035942000	-2.679716000	2.769888000
H	1.530593000	-0.984275000	2.624312000
H	9.720228000	-2.307446000	-0.419110000
H	11.901472000	-1.205146000	-0.530719000
H	13.272228000	0.887929000	-0.626536000
H	9.815669000	3.316348000	-0.538786000
H	8.310096000	1.338780000	-0.440105000
C	-4.263939000	-0.272168000	2.996541000
H	-5.003380000	-0.998213000	2.619683000
H	-4.327201000	-0.222764000	4.092638000

H	-4.538480000	0.706140000	2.568958000
C	-4.439361000	-0.303773000	-2.899717000
H	-4.561140000	-0.247698000	-3.990570000
H	-5.155651000	-1.035533000	-2.490007000
H	-4.694358000	0.670233000	-2.451117000
C	2.188088000	0.456608000	-0.201382000
H	2.736735000	0.793550000	-1.096782000
H	1.182154000	0.898729000	-0.200888000
H	2.753401000	0.835019000	0.667196000
C	3.312483000	-5.730987000	-0.096427000
C	3.047335000	-6.445604000	-1.299963000
C	3.131020000	-6.378852000	1.159216000
C	2.604669000	-7.796172000	-1.248785000
C	2.688679000	-7.729526000	1.212057000
C	2.424013000	-8.440179000	0.007610000
H	3.186067000	-5.951653000	-2.264443000
H	3.335104000	-5.833523000	2.083573000
H	2.403508000	-8.337550000	-2.175859000
H	2.552707000	-8.219387000	2.178766000
H	2.083179000	-9.477093000	0.047200000
C	12.461579000	3.409062000	-0.591222000
H	12.728417000	3.690034000	0.440141000
H	13.376314000	3.210348000	-1.165924000
H	11.916729000	4.235668000	-1.066261000

5r, Singlet, UB3LYP/CEP-31G, E(SCF)=-395.868982, MB_bv2_P506

	x	y	z
C	5.307963000	-4.477852000	-0.562599000
N	5.875875000	-3.178753000	-0.717140000
B	5.080533000	-1.860779000	-0.687572000
N	3.595894000	-2.180395000	-0.483662000
C	3.055666000	-3.493833000	-0.319577000
C	3.900492000	-4.635656000	-0.358229000
C	2.567812000	-1.268844000	-0.419756000
C	1.332973000	-1.971615000	-0.209537000
C	1.616430000	-3.360922000	-0.143007000
C	6.380842000	-5.451188000	-0.668195000
C	7.573015000	-4.703268000	-0.886973000

C	7.236794000	-3.317120000	-0.914509000
C	6.318019000	-6.969286000	-0.585260000
C	8.152770000	-2.122336000	-1.086973000
C	0.576532000	-4.448888000	0.068392000
F	5.299334000	-1.091375000	-1.900030000
F	5.576579000	-0.997727000	0.404139000
C	-0.009283000	-1.318349000	-0.091016000
C	-0.491001000	-0.920004000	1.190023000
N	-1.757478000	-0.277586000	1.316506000
B	-2.705587000	0.070166000	0.141197000
N	-2.059815000	-0.449769000	-1.167990000
C	-0.789237000	-1.090899000	-1.261042000
C	-2.604825000	-0.351881000	-2.425491000
C	-1.689392000	-0.934743000	-3.370188000
C	-0.551846000	-1.400929000	-2.667480000
C	0.080278000	-1.039134000	2.526889000
C	-0.864748000	-0.463607000	3.411426000
C	-1.988763000	-0.000718000	2.642604000
C	0.645209000	-2.089553000	-3.308973000
C	1.407400000	-1.653559000	2.951335000
F	-3.996657000	-0.546418000	0.341595000
F	-2.898264000	1.503342000	0.065491000
C	8.628824000	-1.538889000	0.313029000
C	9.035023000	-0.082095000	0.176578000
C	10.401468000	0.335648000	0.126924000
C	10.721138000	1.698338000	-0.036311000
N	9.728623000	2.647664000	-0.150368000
C	8.396595000	2.274650000	-0.106128000
C	8.024197000	0.930454000	0.052715000
H	8.568785000	-5.114937000	-1.021720000
H	7.331483000	-7.387616000	-0.688684000
H	5.897762000	-7.313250000	0.373029000
H	5.687319000	-7.397515000	-1.380966000
H	7.620634000	-1.340984000	-1.647246000
H	-0.417747000	-3.995826000	0.194308000
H	0.534565000	-5.144307000	-0.785484000
H	0.796785000	-5.058586000	0.959116000
H	-1.857738000	-0.999894000	-4.440805000
H	-0.772244000	-0.381453000	4.490123000
H	0.495453000	-2.151367000	-4.398404000

H	1.587487000	-1.546030000	-3.126985000
H	0.784043000	-3.114993000	-2.926249000
H	1.526922000	-1.556325000	4.042109000
H	1.464706000	-2.725713000	2.697736000
H	2.268965000	-1.161101000	2.469732000
H	9.461578000	-2.144670000	0.703033000
H	11.212171000	-0.387191000	0.215796000
H	11.749437000	2.056438000	-0.075588000
H	7.665125000	3.077119000	-0.199530000
H	6.970219000	0.652806000	0.088595000
C	-3.243813000	0.683653000	3.140488000
H	-4.137926000	0.094533000	2.879003000
H	-3.199568000	0.810394000	4.232093000
H	-3.364293000	1.670432000	2.664256000
C	-3.953028000	0.279490000	-2.699009000
H	-4.157455000	0.284261000	-3.779602000
H	-4.754029000	-0.273414000	-2.181187000
H	-3.983615000	1.312901000	-2.317396000
C	2.767422000	0.225262000	-0.551118000
H	3.306766000	0.465914000	-1.480875000
H	1.796183000	0.738360000	-0.550368000
H	3.373431000	0.610458000	0.286652000
C	3.318511000	-6.016354000	-0.187328000
C	2.864220000	-6.745494000	-1.322063000
C	3.226575000	-6.593413000	1.110852000
C	2.318078000	-8.048149000	-1.158470000
C	2.679366000	-7.895685000	1.273359000
C	2.224019000	-8.624965000	0.139115000
H	2.937496000	-6.302892000	-2.317847000
H	3.577611000	-6.033910000	1.980664000
H	1.970267000	-8.603709000	-2.032055000
H	2.608935000	-8.333787000	2.271328000
H	1.803412000	-9.625056000	0.264255000
C	10.080656000	4.104840000	-0.290346000
H	9.918137000	4.615704000	0.669887000
H	11.133798000	4.194428000	-0.583001000
H	9.449510000	4.555810000	-1.067443000
H	7.784002000	-1.606511000	1.011949000
H	9.036418000	-2.417266000	-1.674742000

5r, Triplet, UB3LYP/CEP-31G, E(SCF)=-395.818527, MB_bv2_P507

	x	y	z
C	5.311636000	-4.471056000	-0.543636000
N	5.872674000	-3.173108000	-0.730778000
B	5.071172000	-1.858181000	-0.729798000
N	3.588718000	-2.180513000	-0.505815000
C	3.054915000	-3.492555000	-0.309636000
C	3.906941000	-4.631086000	-0.327953000
C	2.556047000	-1.273692000	-0.466226000
C	1.318956000	-1.972728000	-0.237105000
C	1.616604000	-3.361870000	-0.138071000
C	6.391623000	-5.440436000	-0.621285000
C	7.578951000	-4.691488000	-0.857070000
C	7.234696000	-3.307814000	-0.921902000
C	6.338990000	-6.955982000	-0.493912000
C	8.145565000	-2.112595000	-1.109590000
C	0.582050000	-4.451026000	0.091709000
F	5.271415000	-1.124434000	-1.967283000
F	5.569841000	-0.963636000	0.332778000
C	-0.020721000	-1.324930000	-0.108317000
C	-0.569333000	-0.995866000	1.183123000
N	-1.822998000	-0.386244000	1.313362000
B	-2.749650000	0.030025000	0.151939000
N	-2.059565000	-0.385574000	-1.164402000
C	-0.809141000	-1.007602000	-1.272732000
C	-2.599633000	-0.203009000	-2.451881000
C	-1.661814000	-0.727829000	-3.408745000
C	-0.540685000	-1.236825000	-2.720158000
C	-0.010938000	-1.180421000	2.551907000
C	-0.980147000	-0.668332000	3.440418000
C	-2.097693000	-0.177325000	2.679542000
C	0.672211000	-1.894052000	-3.357453000
C	1.327511000	-1.782360000	2.940651000
F	-4.037670000	-0.617544000	0.276706000
F	-2.972146000	1.461975000	0.172956000
C	8.628114000	-1.520825000	0.284953000
C	9.066248000	-0.075149000	0.134963000
C	10.442421000	0.313552000	0.079635000
C	10.793108000	1.665237000	-0.098245000
N	9.819748000	2.638838000	-0.223784000

C	8.477127000	2.292954000	-0.174918000
C	8.077881000	0.959332000	-0.001333000
H	8.577913000	-5.099985000	-0.977201000
H	7.359399000	-7.366936000	-0.547520000
H	5.886347000	-7.275618000	0.457982000
H	5.742882000	-7.414548000	-1.299543000
H	7.608885000	-1.334022000	-1.669140000
H	-0.423845000	-4.005200000	0.113003000
H	0.609308000	-5.216489000	-0.699837000
H	0.744882000	-4.981029000	1.044748000
H	-1.811384000	-0.728953000	-4.484107000
H	-0.909119000	-0.639489000	4.523450000
H	0.521942000	-1.969514000	-4.445961000
H	1.598707000	-1.320031000	-3.183830000
H	0.845644000	-2.909093000	-2.962533000
H	1.457146000	-1.723396000	4.032988000
H	1.406002000	-2.842658000	2.643725000
H	2.172936000	-1.255882000	2.465212000
H	9.445809000	-2.140636000	0.685406000
H	11.237070000	-0.426216000	0.176112000
H	11.828881000	2.000721000	-0.140937000
H	7.762973000	3.109726000	-0.277246000
H	7.018040000	0.705427000	0.035912000
C	-3.373365000	0.465533000	3.163781000
H	-4.251883000	-0.107950000	2.822434000
H	-3.379137000	0.524305000	4.261765000
H	-3.482542000	1.479433000	2.742141000
C	-3.943455000	0.439955000	-2.688142000
H	-4.154876000	0.498466000	-3.765577000
H	-4.742889000	-0.134295000	-2.189339000
H	-3.972060000	1.453429000	-2.253039000
C	2.753572000	0.217565000	-0.628798000
H	3.295022000	0.441198000	-1.561650000
H	1.779459000	0.725930000	-0.637866000
H	3.357949000	0.623108000	0.200508000
C	3.333127000	-6.010485000	-0.122353000
C	2.928765000	-6.790109000	-1.242572000
C	3.199173000	-6.537215000	1.193313000
C	2.389616000	-8.091227000	-1.047281000
C	2.661766000	-7.839243000	1.387732000

C	2.255227000	-8.617989000	0.268003000
H	3.034422000	-6.386199000	-2.251808000
H	3.513786000	-5.940167000	2.052058000
H	2.079201000	-8.684669000	-1.910034000
H	2.562022000	-8.239585000	2.399043000
H	1.841769000	-9.617743000	0.417650000
C	10.206891000	4.082933000	-0.370053000
H	10.142747000	4.585583000	0.606738000
H	11.234168000	4.144692000	-0.750275000
H	9.529324000	4.568939000	-1.084474000
H	7.778427000	-1.565193000	0.979914000
H	9.026500000	-2.408270000	-1.701312000

MD1, Singlet, UB3LYP/CEP-31G, E(SCF)=-242.421635, MB_bv2_P541

	x	y	z
C	5.180600000	-4.061542000	-0.232867000
N	5.613115000	-2.727848000	-0.259008000
B	4.695388000	-1.479188000	-0.254019000
N	3.232032000	-1.962286000	-0.204536000
C	2.820163000	-3.334831000	-0.175599000
C	3.766751000	-4.376743000	-0.189489000
C	2.118364000	-1.164920000	-0.181323000
C	0.941628000	-2.003563000	-0.135461000
C	1.346898000	-3.351648000	-0.131080000
C	6.351054000	-4.931274000	-0.257531000
C	7.474717000	-4.072200000	-0.297950000
C	7.008561000	-2.711325000	-0.298334000
C	6.424630000	-6.451647000	-0.245703000
C	7.744368000	-1.466704000	-0.330942000
C	0.412720000	-4.548520000	-0.087383000
F	4.937643000	-0.679954000	-1.438875000
F	5.003958000	-0.639899000	0.887136000

C	9.132858000	-1.365863000	-0.370743000
C	9.853951000	-0.102742000	-0.401887000
C	11.300151000	-0.099897000	-0.443541000
C	12.017931000	1.100111000	-0.475648000
N	11.370144000	2.325052000	-0.470710000
C	9.982191000	2.364998000	-0.431376000
C	9.215381000	1.199109000	-0.397580000
H	8.511391000	-4.392763000	-0.324192000
H	7.478139000	-6.769537000	-0.289151000
H	5.974789000	-6.878393000	0.664628000
H	5.895471000	-6.896274000	-1.103121000
H	7.136895000	-0.561920000	-0.321720000
H	-0.631387000	-4.202732000	-0.047246000
H	0.532250000	-5.191097000	-0.974449000
H	0.603849000	-5.183118000	0.792712000
H	9.742018000	-2.273156000	-0.379978000
H	11.850627000	-1.040795000	-0.452597000
H	13.106695000	1.125505000	-0.506189000
H	9.528476000	3.355830000	-0.428963000
H	8.131868000	1.298166000	-0.370912000
C	2.178705000	0.344763000	-0.201766000
H	2.704728000	0.697121000	-1.104327000
H	1.165021000	0.768024000	-0.182563000
H	2.747065000	0.719082000	0.665678000
C	3.322434000	-5.817092000	-0.157931000
C	3.063289000	-6.509769000	-1.374564000
C	3.161349000	-6.484815000	1.089175000
C	2.642790000	-7.867727000	-1.342778000
C	2.740272000	-7.842657000	1.118935000
C	2.480561000	-8.535981000	-0.096625000
H	3.187025000	-5.996326000	-2.330558000
H	3.359979000	-5.951761000	2.021532000
H	2.443482000	-8.395323000	-2.278001000
H	2.615605000	-8.350477000	2.077714000
H	2.156215000	-9.578571000	-0.073256000
C	12.152230000	3.604012000	-0.460450000
H	12.208584000	4.001871000	0.564348000
H	13.165218000	3.410464000	-0.835247000
H	11.662057000	4.335946000	-1.116635000
H	-0.079076000	-1.635805000	-0.109055000

MD1, Triplet, UB3LYP/CEP-31G, E(SCF)=-242.381120, MB_bv2_P542

	x	y	z
C	5.144565000	-4.010852000	-0.230107000
N	5.554089000	-2.664434000	-0.256380000
B	4.615898000	-1.440483000	-0.247031000
N	3.167200000	-1.968853000	-0.200731000
C	2.789825000	-3.325631000	-0.175945000
C	3.775761000	-4.379266000	-0.189350000
C	2.019082000	-1.177863000	-0.179567000
C	0.867423000	-2.049088000	-0.140108000
C	1.306932000	-3.385904000	-0.137062000
C	6.379671000	-4.865541000	-0.253596000
C	7.458033000	-3.993953000	-0.292475000
C	6.958889000	-2.609163000	-0.294674000
C	6.462059000	-6.381098000	-0.239116000
C	7.680063000	-1.386078000	-0.327610000
C	0.412442000	-4.612187000	-0.101771000
F	4.828190000	-0.628311000	-1.428240000
F	4.892219000	-0.596920000	0.898373000
C	9.093923000	-1.318815000	-0.367134000
C	9.858554000	-0.093546000	-0.401737000
C	11.308425000	-0.138036000	-0.443782000
C	12.063797000	1.035110000	-0.480554000
N	11.452055000	2.287026000	-0.480541000
C	10.062033000	2.371890000	-0.439195000
C	9.259898000	1.232215000	-0.401523000
H	8.503418000	-4.283736000	-0.317231000
H	7.516790000	-6.695608000	-0.264281000
H	5.992487000	-6.805777000	0.662366000
H	5.944549000	-6.824969000	-1.104397000
H	7.091189000	-0.470607000	-0.321187000
H	-0.642479000	-4.298760000	-0.080152000
H	0.565653000	-5.256140000	-0.982767000
H	0.607716000	-5.236470000	0.785086000
H	9.669623000	-2.248727000	-0.373184000
H	11.828405000	-1.096734000	-0.449799000
H	13.152728000	1.028609000	-0.511868000
H	9.641285000	3.377018000	-0.439709000

H	8.179701000	1.364063000	-0.375047000
C	2.059529000	0.329293000	-0.197527000
H	2.580458000	0.691062000	-1.100232000
H	1.040587000	0.739625000	-0.174662000
H	2.628156000	0.710873000	0.667413000
C	3.348480000	-5.825696000	-0.157352000
C	3.107901000	-6.529734000	-1.372262000
C	3.170863000	-6.491640000	1.089495000
C	2.694751000	-7.890273000	-1.340787000
C	2.757894000	-7.852223000	1.121812000
C	2.519236000	-8.553541000	-0.093629000
H	3.239390000	-6.019947000	-2.329469000
H	3.351027000	-5.952308000	2.022279000
H	2.511463000	-8.423886000	-2.275945000
H	2.623440000	-8.356296000	2.081319000
H	2.200552000	-9.597915000	-0.069415000
C	12.284196000	3.530078000	-0.464852000
H	12.529090000	3.810330000	0.571909000
H	13.210975000	3.354551000	-1.027318000
H	11.726906000	4.346063000	-0.943502000
H	-0.163176000	-1.709426000	-0.117246000

MD2, Singlet, UB3LYP/CEP-31G, E(SCF)=-243.638132, MB_bv2_P543

	x	y	z
C	5.448480000	-4.177751000	-0.541830000
N	6.155603000	-2.952003000	-0.717105000
B	5.532559000	-1.549176000	-0.590794000
N	4.042556000	-1.693268000	-0.262828000
C	3.360881000	-2.940381000	-0.085116000
C	4.051786000	-4.171347000	-0.222079000
C	3.140182000	-0.668573000	-0.085158000
C	1.853579000	-1.229138000	0.213957000
C	1.964327000	-2.640995000	0.220696000
C	6.380086000	-5.268464000	-0.758719000
C	7.633583000	-4.663246000	-1.064260000
C	7.468728000	-3.247392000	-1.034559000
C	6.140000000	-6.770239000	-0.699547000
C	8.505751000	-2.167563000	-1.265328000

C	0.817252000	-3.600233000	0.496992000
F	5.742622000	-0.771391000	-1.800449000
F	6.224497000	-0.784773000	0.469198000
C	9.173361000	-1.688979000	0.096364000
C	9.735049000	-0.286495000	-0.050165000
C	11.131350000	-0.028271000	-0.218759000
C	11.592465000	1.291713000	-0.391729000
N	10.711651000	2.351920000	-0.400989000
C	9.354318000	2.134189000	-0.239895000
C	8.842549000	0.838548000	-0.066691000
H	8.556285000	-5.188148000	-1.293353000
H	7.078112000	-7.303387000	-0.920350000
H	5.785749000	-7.092291000	0.292766000
H	5.380646000	-7.094394000	-1.429020000
H	8.026286000	-1.310558000	-1.758591000
H	-0.100353000	-3.028834000	0.706019000
H	0.622846000	-4.264242000	-0.360662000
H	1.024978000	-4.250553000	1.361783000
H	9.960128000	-2.399703000	0.393838000
H	11.855944000	-0.842251000	-0.215809000
H	12.647855000	1.530124000	-0.520464000
H	8.716488000	3.017718000	-0.255404000
H	7.770633000	0.681182000	0.059240000
C	3.509637000	0.795122000	-0.196660000
H	3.961322000	1.009636000	-1.178401000
H	2.615339000	1.420885000	-0.065661000
H	4.251320000	1.067072000	0.573201000
C	3.319360000	-5.476730000	-0.037099000
C	2.691206000	-6.105211000	-1.149226000
C	3.256488000	-6.082424000	1.249608000
C	2.001186000	-7.336016000	-0.974037000
C	2.565721000	-7.313135000	1.423659000
C	1.936955000	-7.941734000	0.312297000
H	2.740538000	-5.639022000	-2.135617000
H	3.738835000	-5.598577000	2.101678000
H	1.519987000	-7.814237000	-1.830000000
H	2.518696000	-7.773472000	2.413015000
H	1.405564000	-8.886526000	0.446263000
C	11.221151000	3.760736000	-0.547176000
H	11.262363000	4.241110000	0.441364000

H	12.224474000	3.736852000	-0.989724000
H	10.547805000	4.321064000	-1.208874000
H	8.393815000	-1.679745000	0.870461000
H	9.291157000	-2.548166000	-1.937430000
H	0.952122000	-0.653882000	0.400273000

MD2, Triplet, UB3LYP/CEP-31G, E(SCF)=-243.584956, MB_bv2_P544

	x	y	z
C	5.448482000	-4.161443000	-0.532316000
N	6.141545000	-2.949591000	-0.713277000
B	5.518576000	-1.552787000	-0.613245000
N	4.031362000	-1.710297000	-0.299803000
C	3.365023000	-2.928274000	-0.115014000
C	4.053297000	-4.194125000	-0.222574000
C	3.102714000	-0.649837000	-0.144862000
C	1.820280000	-1.219171000	0.147869000
C	1.934465000	-2.626375000	0.177375000
C	6.421189000	-5.273438000	-0.739638000
C	7.658015000	-4.661093000	-1.043730000
C	7.488081000	-3.239672000	-1.034068000
C	6.164344000	-6.766952000	-0.662208000
C	8.510507000	-2.152294000	-1.240468000
C	0.808129000	-3.605055000	0.453037000
F	5.735835000	-0.785484000	-1.830424000
F	6.191756000	-0.764625000	0.443278000
C	9.142228000	-1.659327000	0.144141000
C	9.722803000	-0.268564000	-0.006292000
C	11.124525000	-0.029761000	-0.170611000
C	11.604325000	1.279627000	-0.361331000
N	10.736292000	2.354110000	-0.395117000
C	9.373187000	2.154413000	-0.241065000
C	8.844937000	0.868894000	-0.051018000
H	8.587724000	-5.178680000	-1.261220000
H	7.097159000	-7.315285000	-0.867621000
H	5.794109000	-7.070060000	0.331088000
H	5.403919000	-7.091117000	-1.391799000
H	8.033042000	-1.297707000	-1.740075000
H	-0.123757000	-3.051054000	0.645823000
H	0.636871000	-4.285361000	-0.397635000

H	1.020506000	-4.242399000	1.327190000
H	9.910370000	-2.377652000	0.470408000
H	11.839021000	-0.852575000	-0.148602000
H	12.663752000	1.502824000	-0.483971000
H	8.746514000	3.045341000	-0.275326000
H	7.769926000	0.728376000	0.067092000
C	3.491845000	0.801298000	-0.279977000
H	3.949944000	0.993064000	-1.264770000
H	2.607374000	1.443091000	-0.159531000
H	4.241456000	1.075907000	0.482790000
C	3.319850000	-5.497642000	-0.027789000
C	2.699075000	-6.147967000	-1.133820000
C	3.238045000	-6.091523000	1.265346000
C	2.005096000	-7.375853000	-0.950470000
C	2.544570000	-7.319409000	1.451947000
C	1.926376000	-7.963666000	0.343497000
H	2.758579000	-5.696597000	-2.126944000
H	3.711535000	-5.596358000	2.116377000
H	1.532432000	-7.866080000	-1.804612000
H	2.486999000	-7.765893000	2.447257000
H	1.392467000	-8.906042000	0.485370000
C	11.267433000	3.751097000	-0.553757000
H	11.359554000	4.226820000	0.434064000
H	12.251075000	3.710713000	-1.038089000
H	10.579788000	4.329992000	-1.184103000
H	8.336098000	-1.634653000	0.889424000
H	9.319881000	-2.522000000	-1.889678000
H	0.913330000	-0.646873000	0.316592000

MePy, Singlet, UB3LYP/CEP-31G, E(SCF)=-48.294264, YD_bv2a_P101

	x	y	z
H	8.501723000	-1.243590000	0.310060000
C	8.793296000	-0.197888000	0.212114000
C	10.159741000	0.219855000	0.162460000
C	10.479412000	1.582545000	-0.000775000
N	9.486896000	2.531871000	-0.114832000
C	8.154868000	2.158857000	-0.070592000
C	7.782470000	0.814661000	0.088251000
H	10.970445000	-0.502984000	0.251332000

H	11.507711000	1.940645000	-0.040052000
H	7.423398000	2.961326000	-0.163994000
H	6.728492000	0.537013000	0.124131000
C	9.838929000	3.989047000	-0.254810000
H	9.676410000	4.499911000	0.705423000
H	10.892072000	4.078635000	-0.547465000
H	9.207783000	4.440017000	-1.031907000