Electronic Supplymentary Information for:

Red-light-absorbing Diimine Pt(II) Bisacetylide Complexes Showing Near-IR Phosphorescence and Long-lived ^{3}IL Excited State of Bodipy for Application in triplet-triplet annihilation Upconversion

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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 for synthesis. NMR spectra were recorded on a 400 MHz Varian Unity Inova NMR spectrophotometer. ^{13}C NMR spectra were recorded on the same instrument (100 MHz) with total proton decoupling. Mass spectra were recorded with Q-TOF Micro MS spectrometer. UV-vis absorption spectra were measured with a HP8453 UV-visible spectrophotometer. Fluorescence spectra were recorded on JASCO FP-6500 or a Sanco 970 CRT spectrofluorometer. Fluorescence/phosphorescence lifetimes were measured on a Horiba Jobin Yvon Fluoro Max-4 (TCSPC) instrument. The nanosecond time-resolved transient difference absorption spectra were detected by Edinburgh analytical instruments (LP900, Edinburgh Instruments, U.K.) and buffered on a Tektronix TDS 3012B oscilloscope. All samples in flash photolysis experiments were deaerated with argon or N_2 for ca. 15 min before measurement and the gas flow is kept during the measurement.

Diode pumped solid state laser (DPSSL) with 473 nm or 532 nm were used as excitation source for the upconversion experiments. The diameter of the laser spot is ca. 3 mm. The output power of the DPSS laser can be adjusted continuously. The laser power was measured with phototube. For 532 nm laser, the variation of the power is less than ±5% over eight hours. The noise of the 532 nm DPSS laser is 20%-25% in the range of 1 kHz- 1 MHz. The noise of the 473 nm DPSS laser is 20%-25% in the range of 1 kHz- 1MHz. For the upconversion experiments, the mixed solution of the complex (triplet sensitizer) and perylene (triplet acceptor) was degassed for at least 15 min with N_2 or Ar. Then the solution was excited with laser. The upconverted fluorescence of perylene was observed with spectrofluorometer. In order to repress the scattered laser, a black box with a small hole on it was put behind the fluorescent cell to trap the laser beam behind the cuvette (the small hole as the entrance of the laser into the black box).

The upconversion quantum yields were calculated with the following equation, where Φ_{UC}, A_{sam}, I_{sam} and η_{sam} represents the quantum yield, absorbance, integrated photoluminescence intensity and the refractive index of the samples and the solvents (**Eq. 1**). The equation is multiplied by factor 2 in order to made the maximum quantum yield to be unit.[1]

$$\Phi_{UC} = 2\Phi_{std}\left(\frac{A_{std}}{A_{sam}}\right)\left(\frac{I_{sam}}{I_{std}}\right)\left(\frac{\eta_{sam}}{\eta_{std}}\right)^2 \qquad \textbf{(Eq. 1)}$$

The density functional theory (DFT) calculations were used for optimization of the ground state geometries, for both singlet states and triplet states. The energy level of the T_1 state of the acetylide ligands **2-BDP** and **8-BDP** (energy gap between S_0 state and T_1 state) were calculated with the time-dependent DFT (TDDFT), based on the optimized T_1 state geometries. All the calculations were performed with Gaussian 09.[2]

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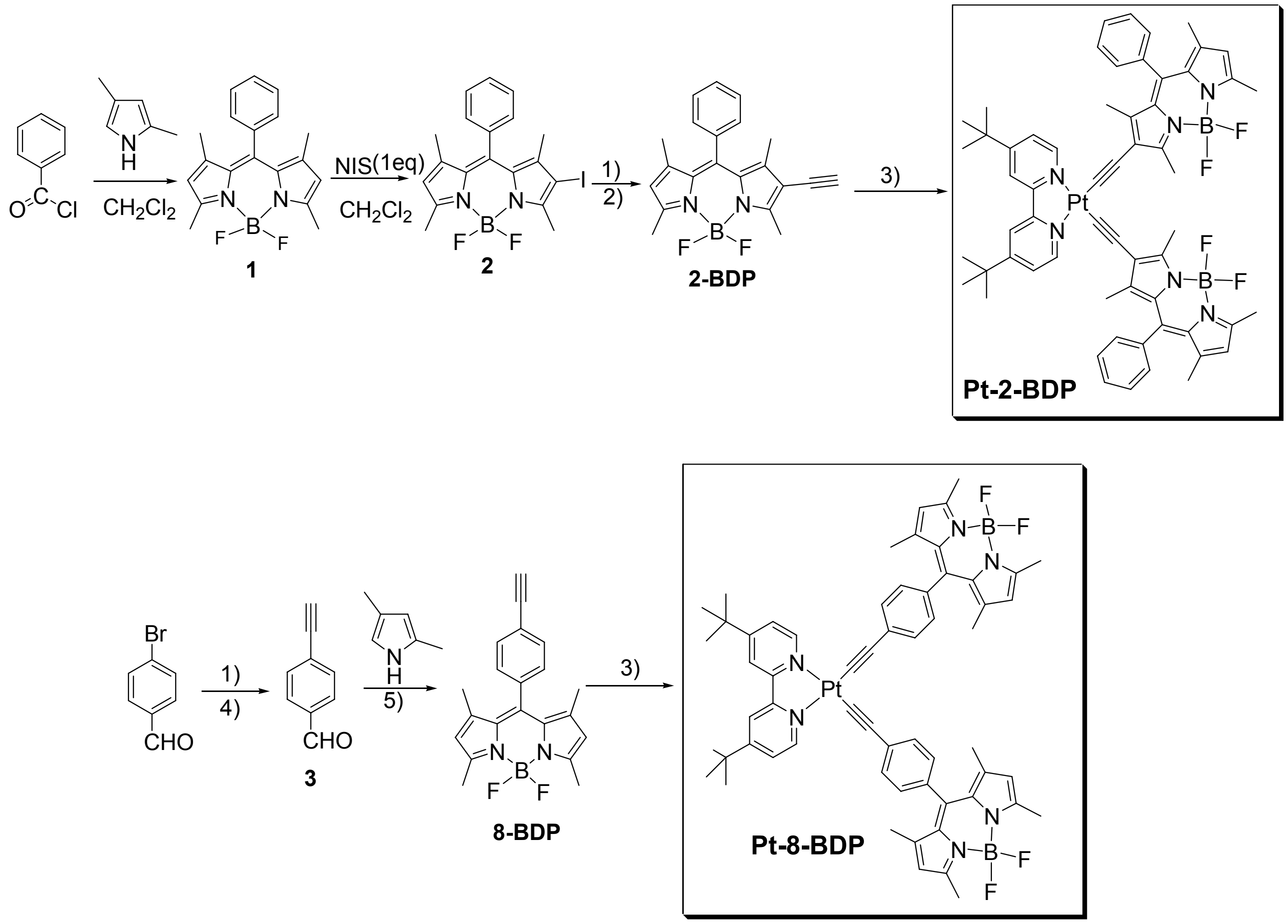
[1] T. N. Singh-Rachford, F. N. Castellano, *Coord. Chem. Rev.* 2010, **254**, 2560–2573.

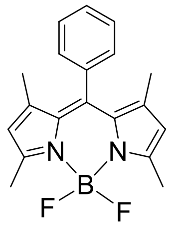
[2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, et al. Gaussian 09 Revision A.1, Gaussian Inc., Wallingford CT, 2009.

2. Synthesis and molecular structure characterization data



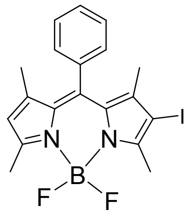
Scheme S1. Synthesis of the complexes **Pt-2-BDP** and **Pt-8-BDP**. Key: 1) Trimethylsilylacetylene, $Pd(PPh_3)_2Cl_2$, PPh_3, CuI, NEt_3, reflux, 8 h; 2) NaOH (aq), THF/MeOH; 3) $Pt(dbbpy)Cl_2$, CuI, r.t., overnight; 4) K_2CO_3, MeOH, r.t., 3h; 5) TFA, DDQ, r.t., overnight.

1, 3, 5, 7-tetramethyl-8-phenyl-4, 4-difluoroboradiazaindacene (**1**)



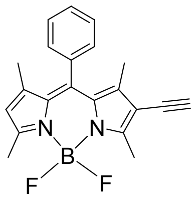
Under nitrogen atmosphere, benzoyl chloride (2.8 g, 0.021mol) and 2, 4-dimethylpyrrole (4 mL, 3.7 g, 0.04 mol) were added to 150 ml anhydrous CH_2Cl_2 via syringe, the mixture was stirred at room temperature over night, then Et_3N (20 mL) and $BF_3{\cdot}Et_2O$ (20 mL) were added under ice-cold condition, and reaction mixture was stirred for additional 1 h. After the reaction, the mixture was poured into water (200 mL), the organic layer was collected and dried over anhydrous $MgSO_4$ and evaporated under reduced pressure. The crude product was further purified using column chromatography (CH_2Cl_2:hexane = 1:1) to give **1** as green power. 2.3 g, Yield: 33.3 %. ^1H NMR (400 MHz, $CDCl_3$): 7.49–7.47 (m, 3H), 7.29–7.26 (m, 2H), 5.98 (s, 2H), 2.56 (s, 6H), 1.37 (s, 6H).

2- iodo-1, 3, 5, 7-tetramethyl-8-phenyl-4, 4-difluoroboradiazaindacene (**2**)



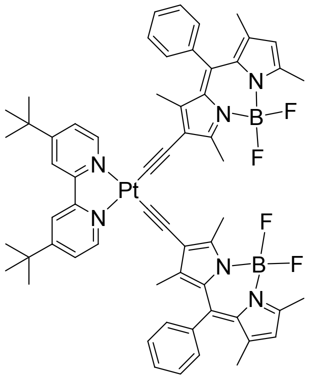
Under 10- 15 °C, *N*-iodo-succinimide (NIS) (140.0 mg, 0.62 mmol) in anhydrous CH_2Cl_2 (10 mL) was added dropwise into a solution of **1** (200 mg, 0.62 mmol) in CH_2Cl_2 (50 mL) in ca. 1 h, After the addition, the reaction mixture was allowed to stir at room temperature for additional 1 h. Crude product was then concentrated under vacuum, and purified by silica gel column chromatography (hexane/CH_2Cl_2, 2:1) , the second band was collected to give the product as a red solid. 191.7 mg, Yield: 68.7 %. ^{1}H NMR (400 MHz, $CDCl_3$): 7.51–7.48 (m, 3H), 7.27– 7.25 (m, 2H), 6.04 (s, 1H), 2.63 (s, 3H), 2.57 (s, 3H), 1.38 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.94, 154.65, 145.34, 143.42, 141.67, 134.96, 132.01, 131.07, 129.77, 129.45, 129.40, 128.00, 122.45, 84.41, 16.77, 15.95, 14.94, 14.73. MALDI-MS: calcd ($[C_{19}H_{18}BF_2IN_2]^+$), *m/z* = 450.0576, found, *m/z* = 450.0535.

2-ethynyl-1, 3, 5, 7-tetramethyl-8-phenyl-4, 4-difluoroboradiazaindacene (**2-BDP)**



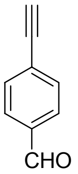
$Pd(PPh_3)_2Cl_2$ (29.5 mg, 0.042 mmol), PPh_3 (22.0 mg, 0.085 mmol) and CuI (17.0 mg, 0.085 mmol) were added to a solution of **2** (200 mg, 0.44 mmol) in a mixed solvent of $(i\text{-Pr})_2NH$ (5 mL) and THF (10 mL) that had been deaerated with argon. Trimethylsilylacetylene (65.0 mg, 0.67 mmol) was added via syringe. The mixture was then heated to 60 °C for 6 h. The solvent was removed under reduced pressure, water was added and the mixture was extracted with dichloromethane (DCM, 4×20 mL). The combined organic layer was dried over anhydrous Na_2SO_4. After removal the solvent the crude product was purified with column chromatography (silica gel, DCM: hexane = 1:1), red solid was abstained. NaOH (20% in water, 0.5 mL) was added to a solution of the above trimethylsilane protected intermediate (100 mg, 0.24 mmol) in 4ml tetrahydrofuran and 4ml MeOH, and the solution was stirred at room temperature under argon for 10 min. DCM (100 mL) and water (50 mL) were added. The organic layer was separated, and the aqueous layer was extracted with DCM (3×15 mL). The combined organic layers were washed with brine (200 mL), dried over anhydrous $MgSO_4$, and filtered, and then the solvent was completely removed. The residue was purified by passing through a silica plug using DCM as eluent to give a red solid. 70 mg, yield: 30.0 %. ^{1}H NMR (400 MHz, $CDCl_3$): 7.52–7.49 (m, 3H), 7.28– 7.25 (m, 2H), 6.04 (s, 1H), 3.28 (s, 1H), 2.64 (s, 3H), 2.57 (s, 3H), 1.44 (s, 3H), 1.39 (s, 3H). *m/z* = 348.1609, found, *m/z* = 348.1617.

Compound **Pt-2-BDP**



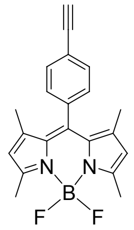
Under argon atmosphere, Pt(dbbpy)Cl_2 (20.4 mg, 0.038 mmol) and compound **3** (40 mg, 0.144 mmol) were dissolved in the a mixed solvent of diisopropylamine (1.0 mL) and CH_2Cl_2 (5 mL), the mixture was deaerated with argon for several times, then CuI (5 mg, 0.09mmol) was added, the mixture was stirred at room temperature for about 4 h. The mixture was evaporated to dryness, the residue was purified by column chromatography (silica gel, CH_2Cl_2 : CH_3OH = 100:1, v/v). The product was collected as the third fraction. 32.0 mg of purple powder was obtained, yield: 72.7 %. ^{1}H NMR (400 MHz, $CDCl_3$): 9.49 (s, 2H), 7.94 (s, 2H), 7.52– 7.48 (m, 8H), 7.26 (m, 4H), 5.95 (s, 2H), 2.73 (s, 6H), 2.54 (s, 6H), 1.53 (s, 6H), 1.43 (s, 18H), 1.36 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.99, 163.97, 156.08, 150.83, 150.76, 142.85, 142.19, 141.08, 135.17, 131.51, 130.89, 129.07, 128.85, 128.10, 126.02, 125.78, 124.58, 120.69, 119.05, 104.92, 86.29, 35.91, 30.25, 14.54, 14.32, 14.14, 13.84. MALDI-MS: calcd ($[C_{60}H_{60}B_2F_4N_6Pt+H]^+$), *m/z* = 1158.4728, found, *m/z* = 1158.4724.

4-ethynylbenzaldehyde **(3)**



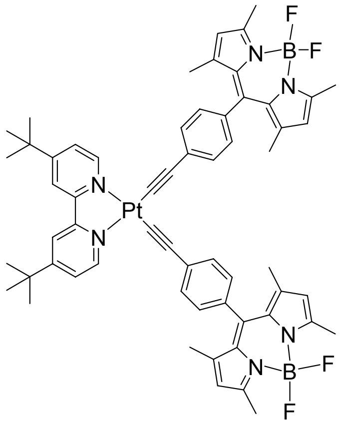
Under nitrogen atmosphere, 4-bromobenzaldehyde (1.0 g, 5.4 mmol), $Pd(PPh_3)_2Cl_2$ (37.8 mg, 0.054 mmol), PPh_3 (28.3 mg, 0.108 mmol), CuI (21.6 mg, 1.108 mmol) and KOH (160 mg) were dissolved in 30 ml Et$_3$N. The mixture was stirred at r.t. for about 10 min. Then ethynyltrimethylsilane (793.8 mg, 8.1mmol) was added via syringe. The solution was refluxed for 8 h. The solvent was removed under reduced pressure and the crude product was purified by column chromatography (silica gel, dichloromethane/petroleum ether = 3:1, V/V). Yellow solid was obtained, 763.9 mg, yield: 70%. The above trimethylsilane protected intermediate was dissolved in methanol (50 mL), K$_2$CO$_3$ (1.6 g) was added and the mixture was stirred at r.t. for 3 h. The solvent was removed under reduced pressure. Water was added and the mixture was extracted with diethyl ether. The organic layer was dried over anhydrous Na$_2$SO$_4$. After removal the solvent, compound **3** was obtained as light yellow solid, 470.0 mg, yield: 66.0 %. ^{1}H NMR (400 MHz, CDCl$_3$), 10.02 (s, 1H), 7.86 (d, 2H, *J* = 8.0 Hz), 7.65 (d, 2H, *J* = 8.0 Hz), 3.30 (s, 1H).

8-(4-ethynylphenyl)- 1, 3, 5, 7-tetramethyl- 4, 4-difluoroboradiazaindacene (**8-BDP)**



Under nitrogen atmosphere, to a solution of 4-ethynylbenzaldehyde (0.13 g, 1.0 mmol, compound **3**) and 2,4-dimethylpyrrole (0.22 g, 2.3 mmol) in CH$_2$Cl$_2$ (50 mL) was added trifluoroacetic acid (7.6 µL, 0.1 mmol). After the mixture was stirred at room temperature overnight, a solution of p-chloranil (0.246 g, 1.0 mmol) in CH$_2$Cl$_2$ (10 mL) was added. The mixture was stirred at room temperature for an additional 30 min. BF$_3$·OEt$_2$ (2.60 g, 18.6 mmol) and NEt$_3$ (1.7 g, 17.0 mmol) were added, followed by stirring at room temperature for 6 h. The reaction mixture was washed with water (4 ×60 mL) and dried with anhydrous Na$_2$SO$_4$. The solvent was removed under vacuum and the residue was purified by chromatography (hexanes/CH$_2$Cl$_2$ 1:1) to give compound **8-BDP** (104.8 mg, 30%). ^{1}H NMR (400 MHz, CDCl$_3$): 7.62 (s, 2H), 7.26 (s, 2H), 5.99 (s, 2H), 3.18 (s, 1H), 2.55 (s, 6H), 1.40 (s, 6H). EI-HRMS: calcd ([C$_{21}$H$_{19}$BF$_2$N$_2$]$^+$), *m/z* = 348.1609, found, *m/z* = 348.1617.

Compound **Pt-8-BDP**



Pt-8-BDP was obtained following a similar procedure outlined above for **Pt-2-BDP**, except compound **5** (50.0 mg, 0.144 mmol) and Pt(dbbpy)Cl$_2$ (25.7 mg, 0.048 mmol) was used. Yield: 80.2 %. ^{1}H NMR (400 MHz, CDCl$_3$): 9.76 (d, 2H, *J* = 6.1 Hz), 8.00 (s, 2H), 7.67 (d, 6H, *J* = 8.3 Hz), 7.16 (d, 4H, *J* = 8.1 Hz), 5.98 (s, 4H), 2.56 (s, 12 H), 1.48 (s, 12H), 1.47 (s, 18H) ^{13}C NMR (100 MHz, CDCl$_3$): δ 163.72, 156.24, 155.18, 151.23, 143.39, 142.35, 132.96, 131.78, 131.53, 127.32, 124.82, 121.05, 118.79, 101.73, 87.99, 35.90, 30.28, 14.76, 14.59. MALDI-MS: calcd ([C$_{60}$H$_{60}$B$_2$F$_4$N$_6$Pt+H]$^+$), *m/z* = 1158.4728, found, *m/z* = 1158.4777.

3. NMR and HRMS spectra.

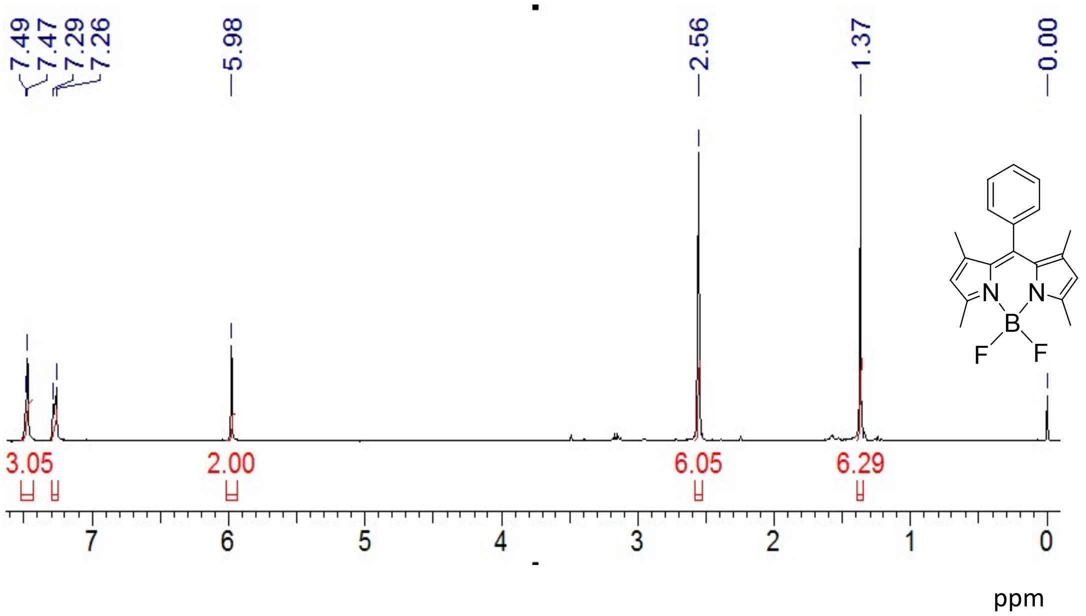


Figure S1. ^{1}H NMR of **1** (400 MHz, $CDCl_3$).

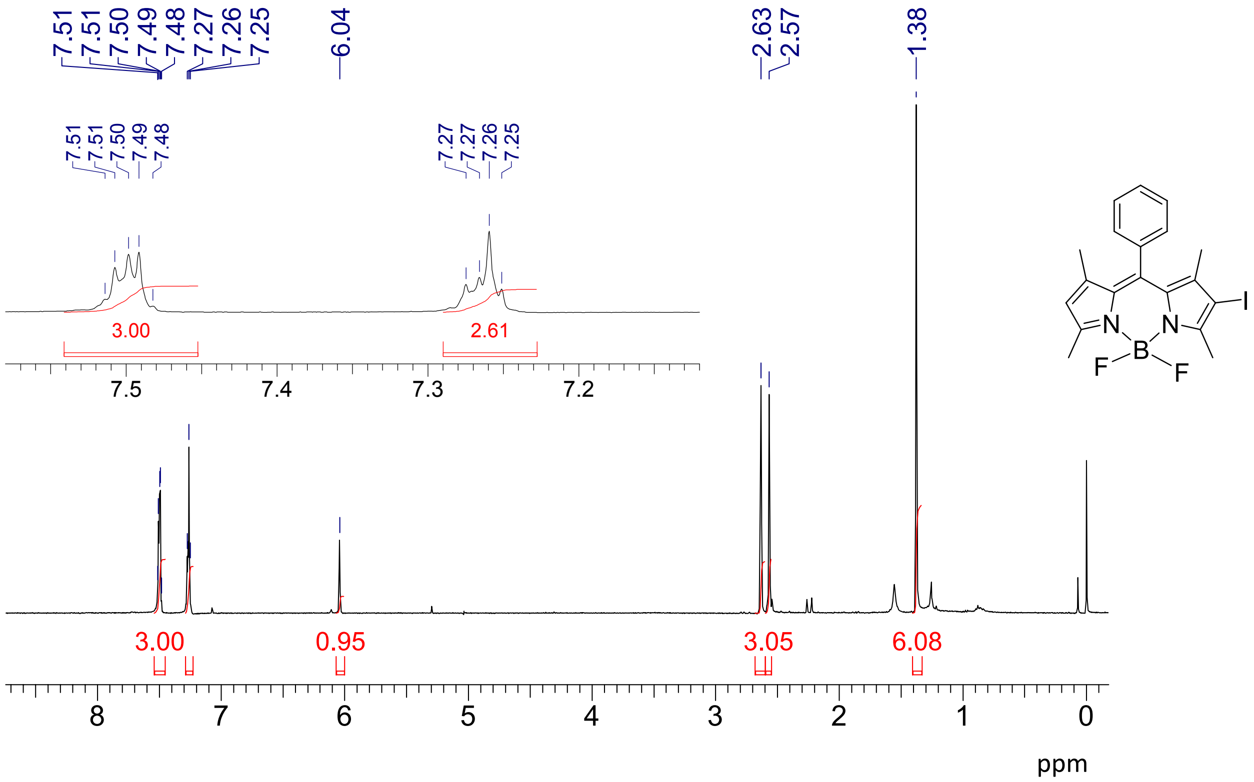


Figure S2. ^{1}H NMR of **2** (400 MHz, $CDCl_3$).

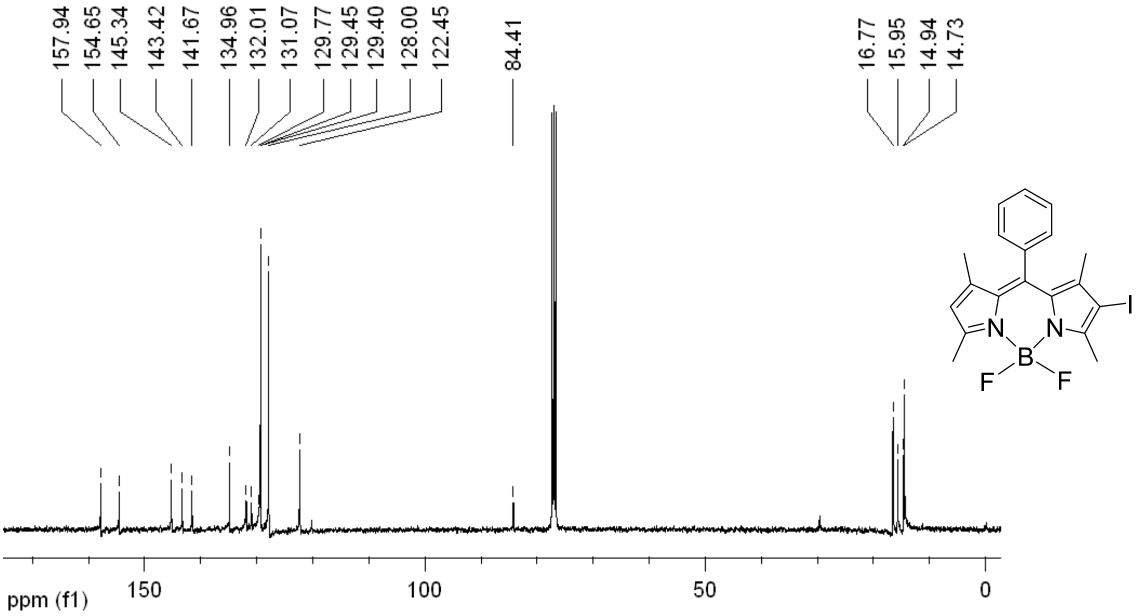


Figure S3. ^{13}C NMR of **2** (100 MHz, $CDCl_3$).

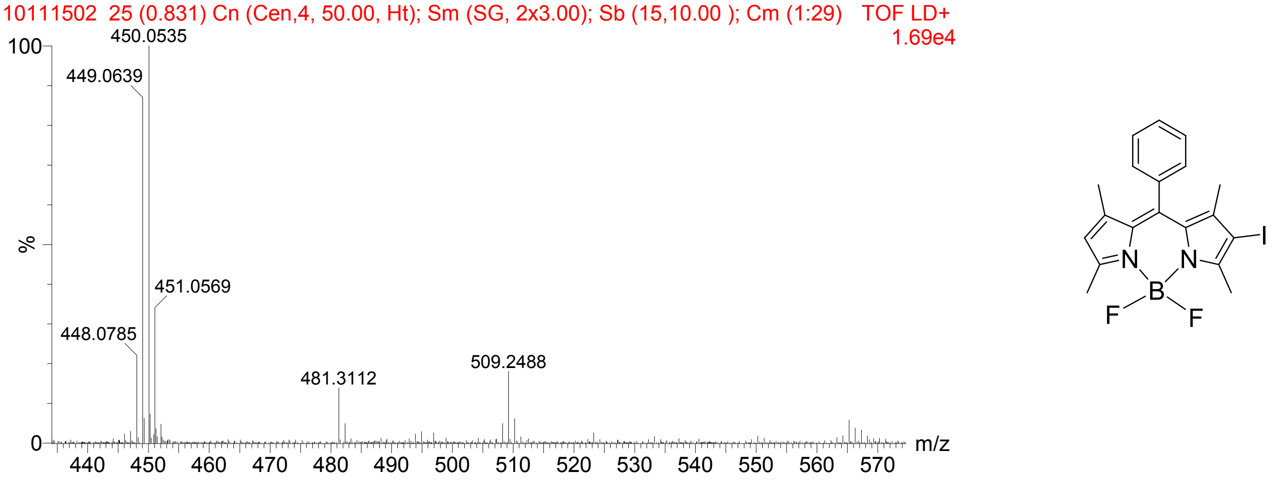


Figure S4. MALDI-HRMS of **2**

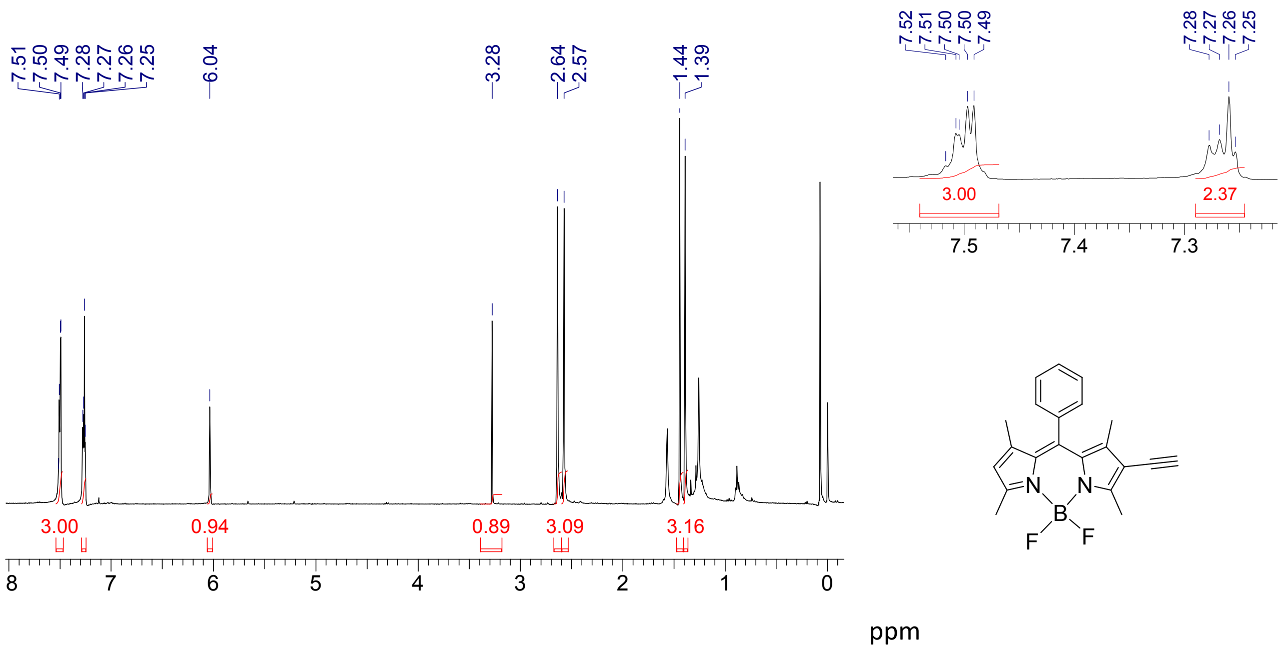


Figure S5. ^{1}H NMR of **2-BDP** (400 MHz, $CDCl_3$).

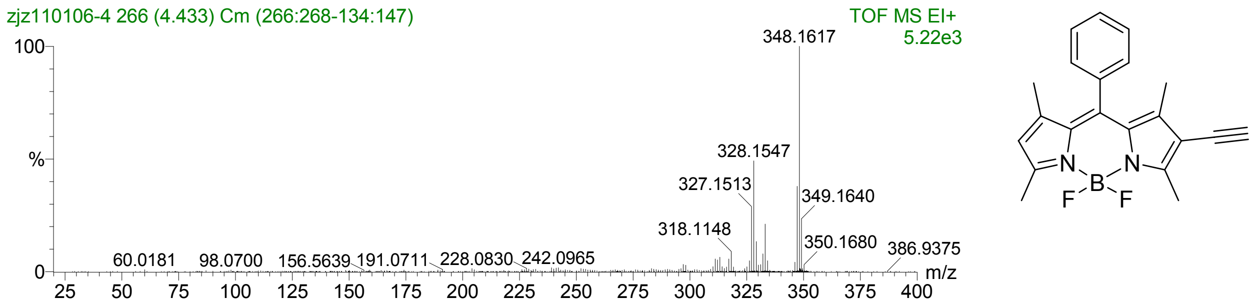


Figure S6. EI-HRMS of **2-BDP**.

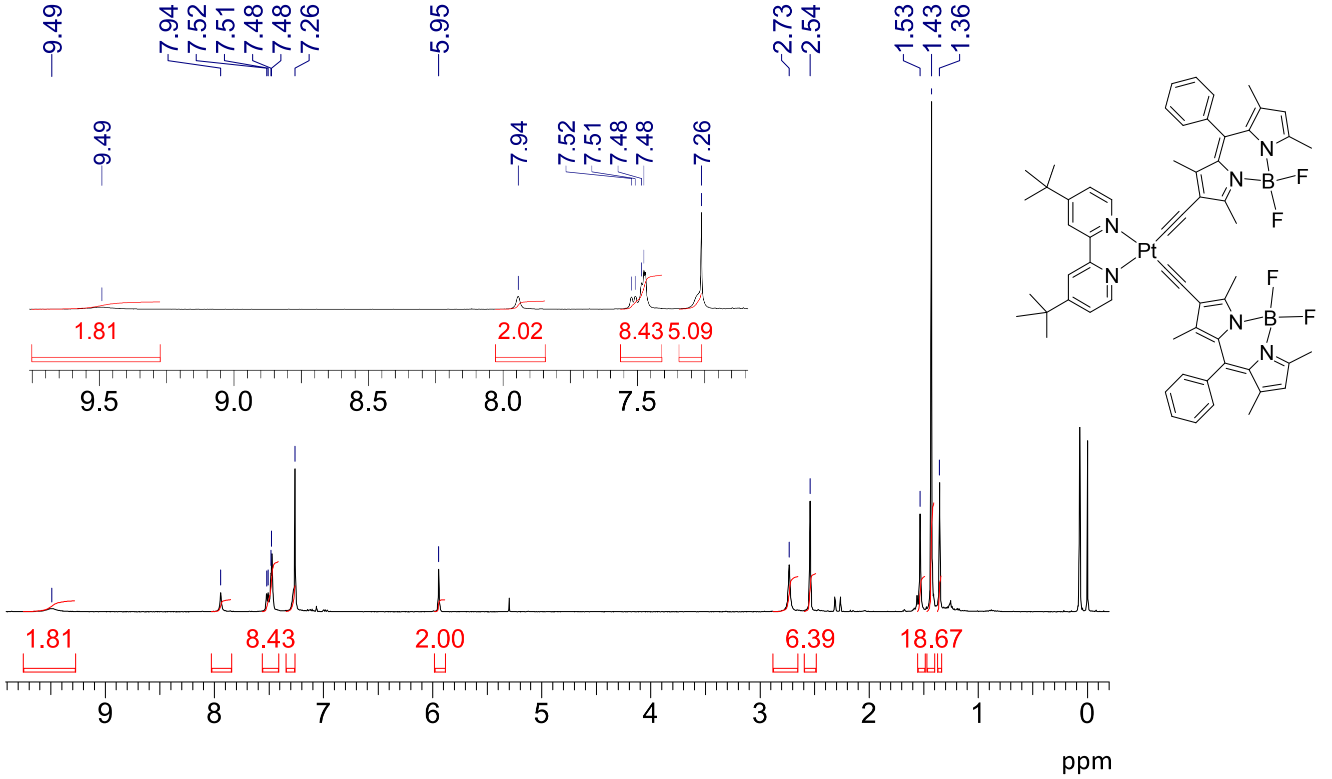


Figure S7. ^{1}H NMR of **Pt-2-BDP** (400 MHz, $CDCl_3$).

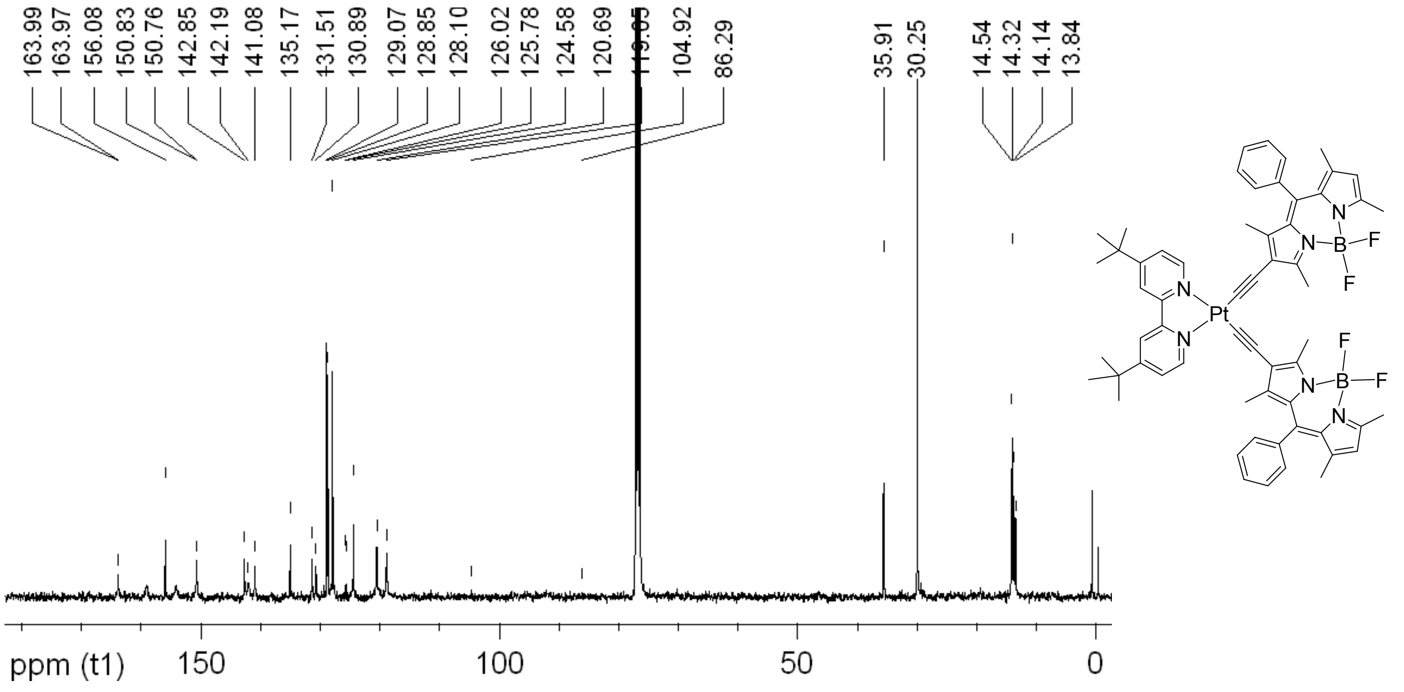


Figure S8. ^{13}C NMR of **Pt-2-BDP** (100 MHz, $CDCl_3$).

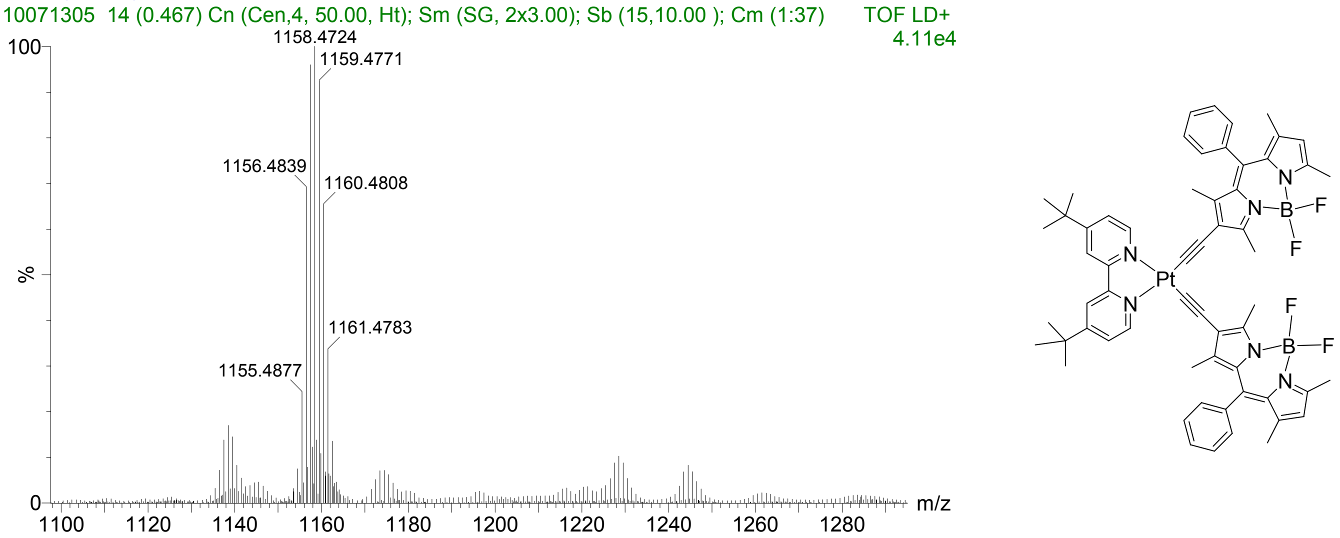


Figure S9. MALDI-HRMS of **Pt-2-BDP.**

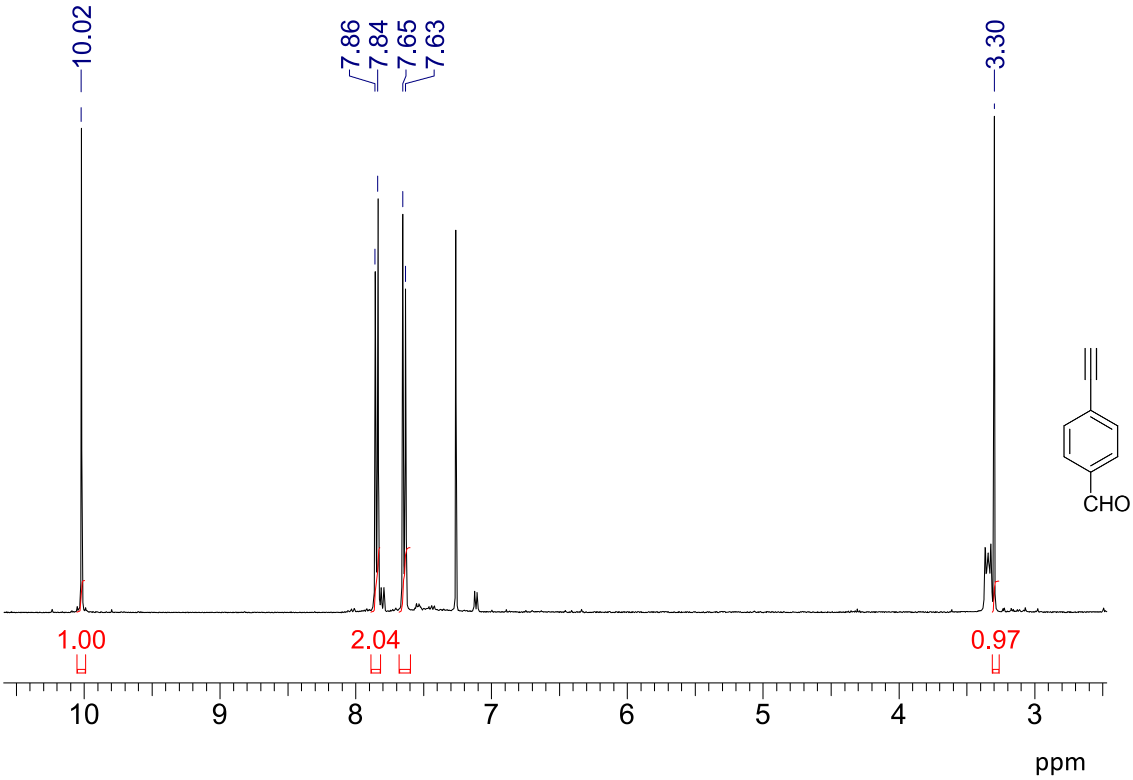


Figure S10. ^{1}H NMR of **3** (400 MHz, $CDCl_3$).

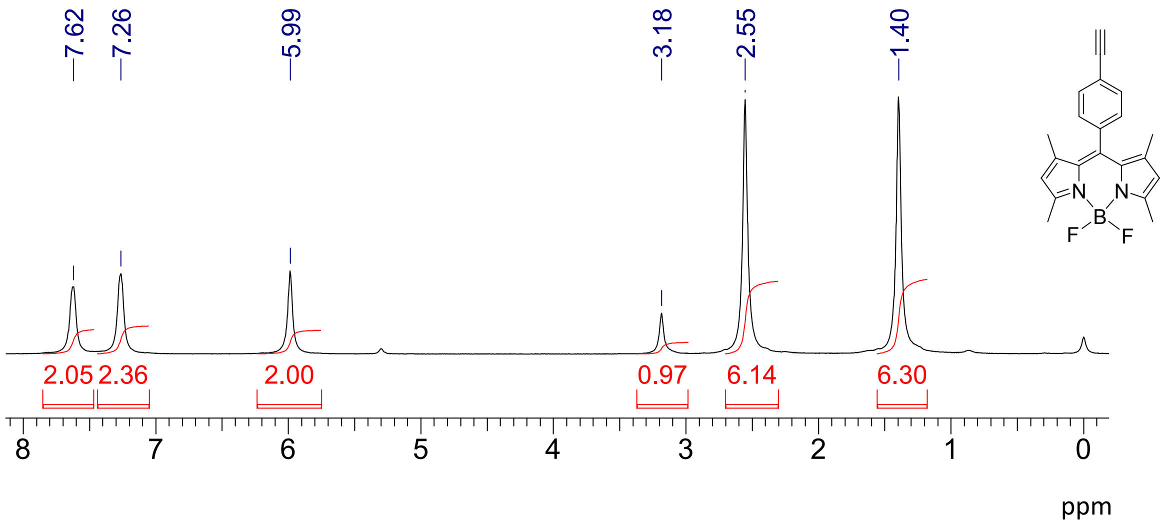


Figure S11. ^{1}H NMR of **8-BDP** (400 MHz, $CDCl_3$).

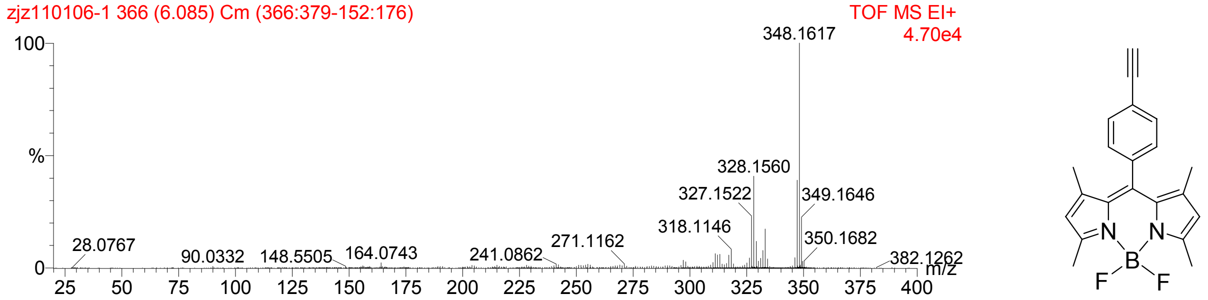


Figure S12. EI-HRMS of **8-BDP.**

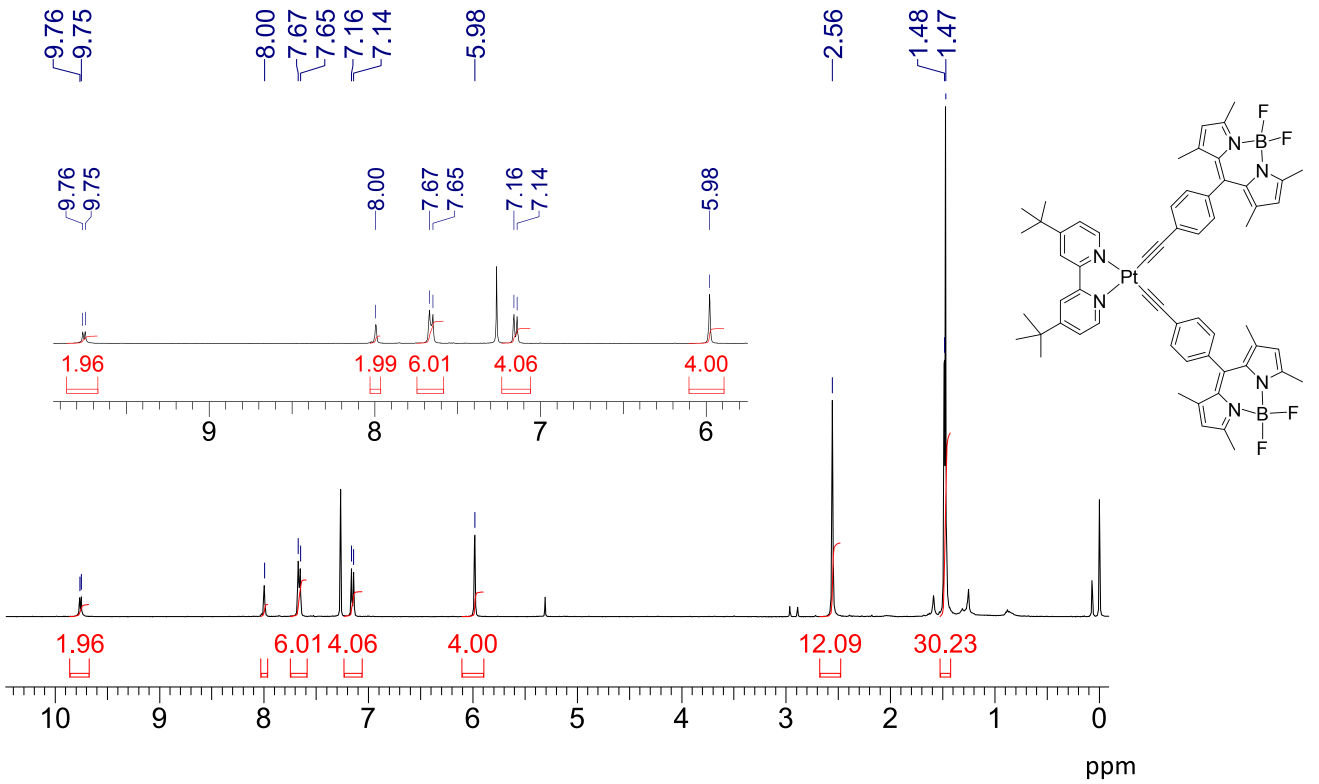


Figure S13. ^{1}H NMR of **Pt-8-BDP** (400 MHz, $CDCl_3$).

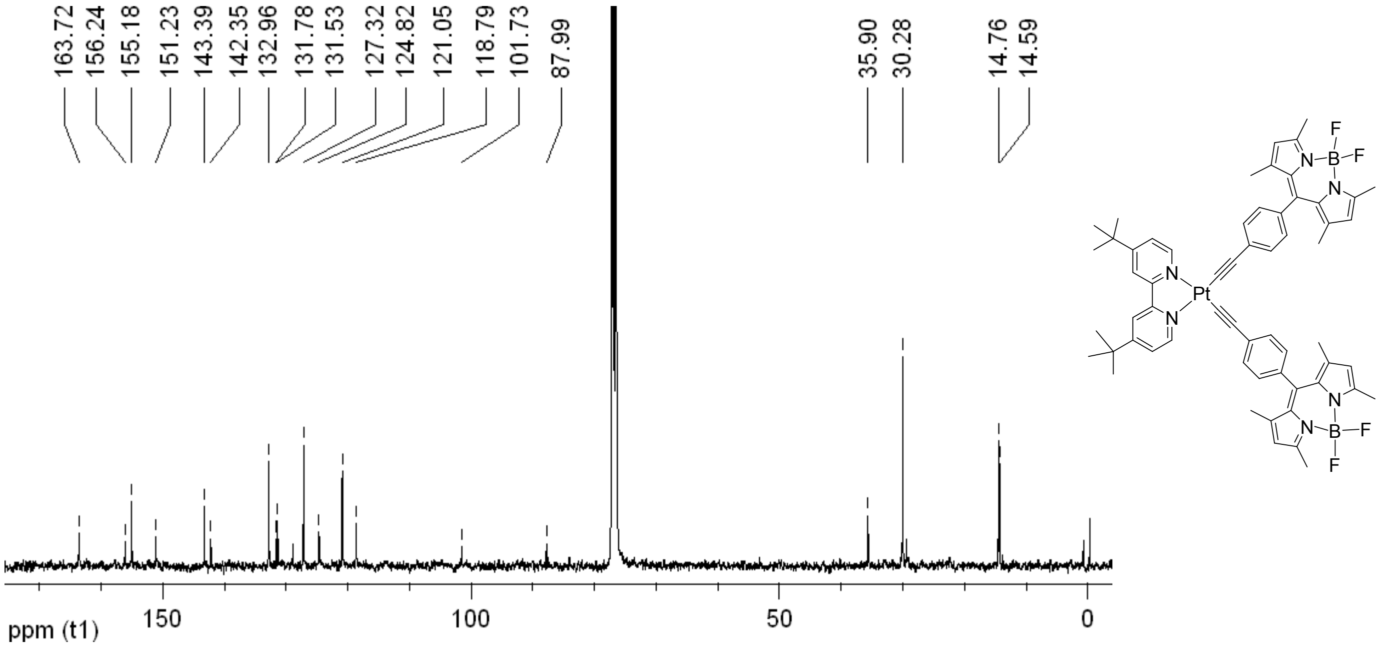


Figure S14. MALDI-HRMS of **Pt-8-BDP.**

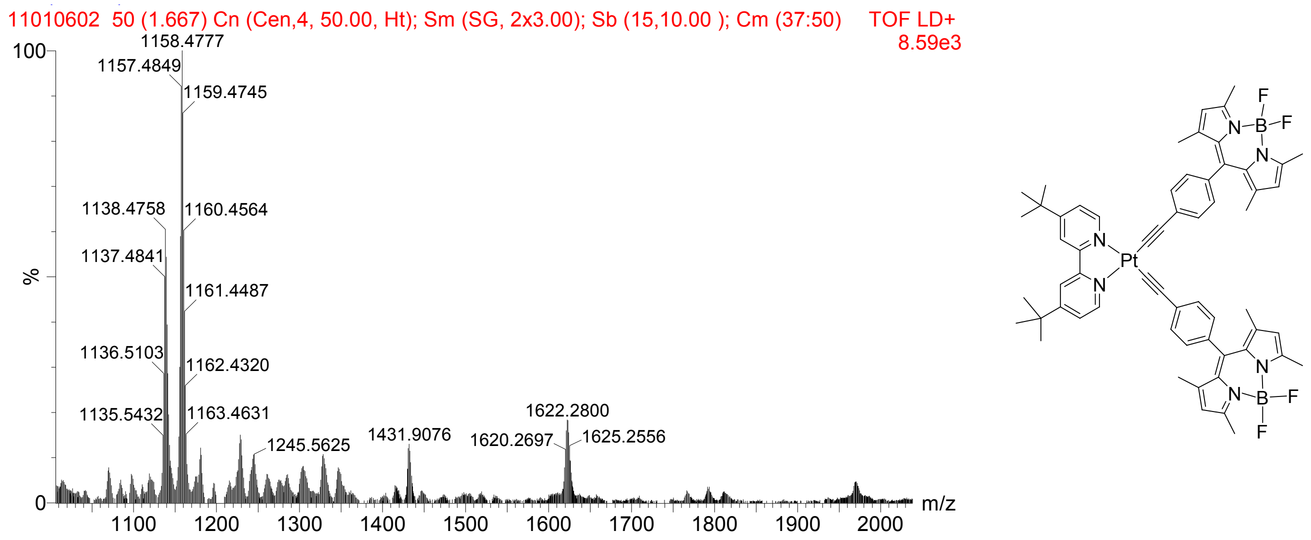


Figure S15. MALDI-HRMS of **Pt-8-BDP.**

4. Photophysical properties of Pt-2-BDP and Pt-8-BDP.

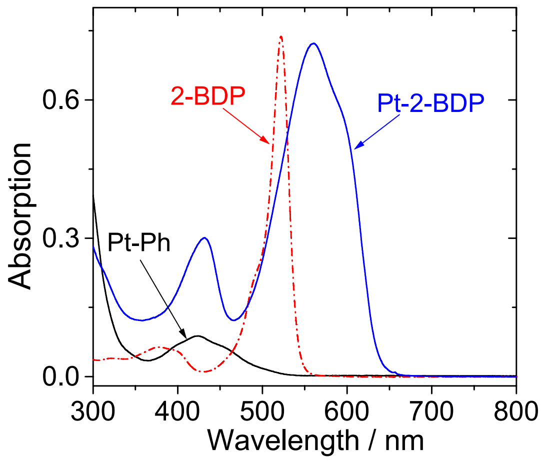


Figure S16. Absorption spectra of the parent complex **Pt-Ph**, the ligand **2-DBP** and complex **Pt-2-BDP**. In toluene (1.0×10^{-5} M; 20 °C).

Please note: the UV-vis absorption spectrum of **Pt-2-BDP** is *not* the sum of the ligand and the parent complex (**Pt-Ph**), which is an indication of the strong interaction between the two subunits in **Pt-2-BDP**.

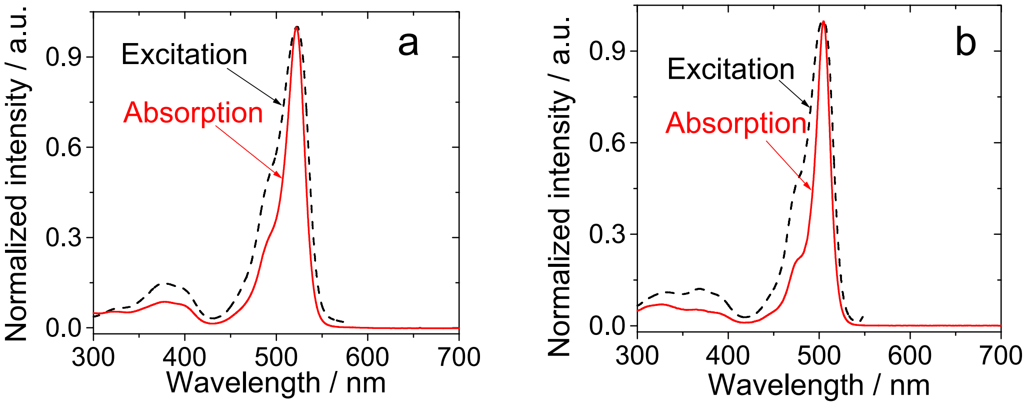


Figure S17. Comparison of the normalized UV-vis absorption and the excitation spectra of the ligands. (a) **2-BDP** (for excitation spectrum, λ_{em} = 580 nm), (b) **8-BDP** (for excitation spectrum, λ_{em} = 550 nm). c = 1.0×10^{-5} M in deaerated toluene solution. 20 °C.

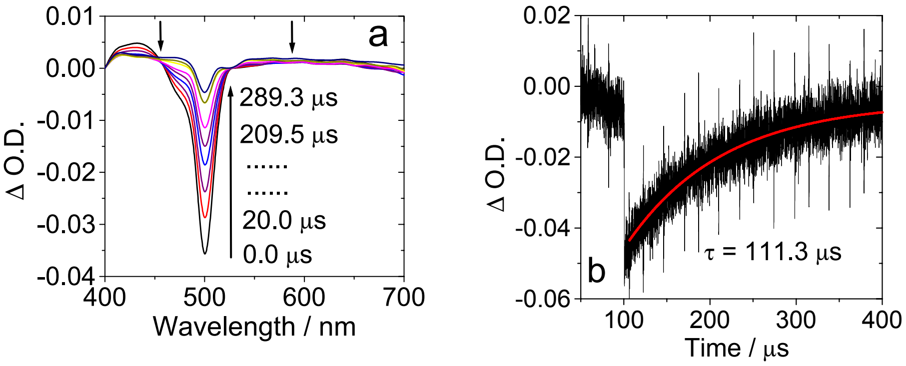


Figure S18. (a) **Pt-8-BDP** after pulsed excitation (λ_{ex} = 532 nm). (b) Decay trace of **Pt-8-BDP** at 500 nm. In deaerated toluene; c = 1.0×10^{-5} M; 20 °C.

5. Concentration dependency of the T_1 state lifetime of the complexes

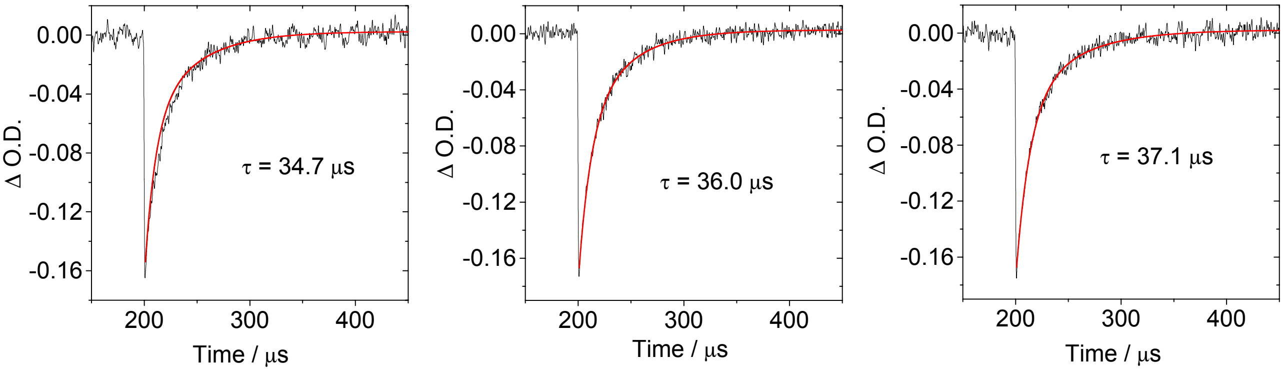


Figure S19. Decay trace of **Pt-2-BDP** at 560 nm after pulsed excitation (λ_{ex} = 532 nm). The decay curve was measured for three times. $c = 1.0 \times 10^{-5}$ M in deaerated toluene; 20 °C. The mean result is 35.9 μs.

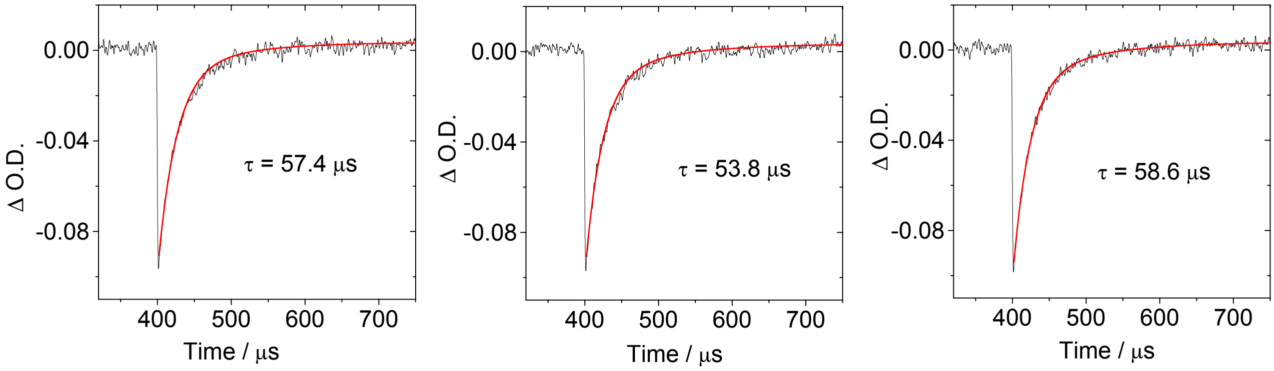


Figure S20. Decay trace of **Pt-2-BDP** at 560 nm after pulsed excitation (λ_{ex} = 532 nm). The decay curve was measured for three times. $c = 5.0 \times 10^{-6}$ M in deaerated toluene; 20 °C. The mean result is 56.6 μs.

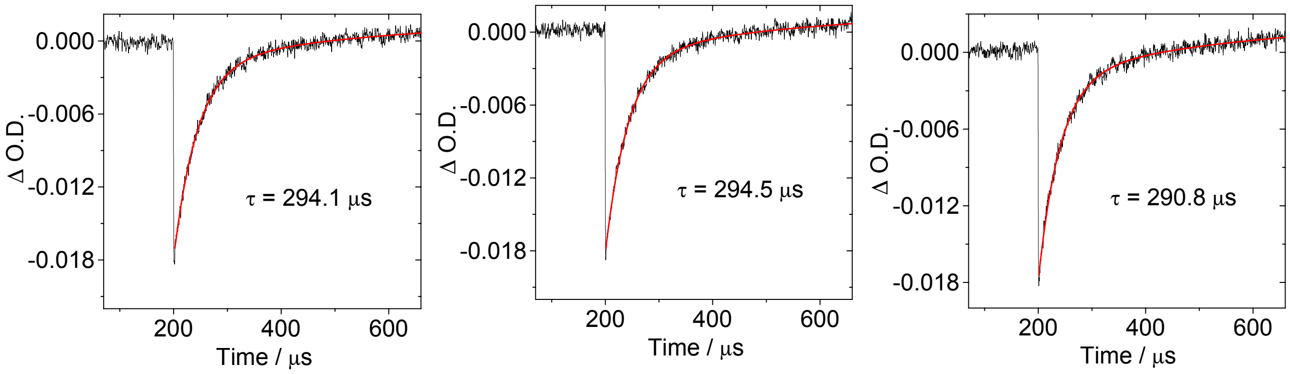


Figure S21. Decay trace of **Pt-2-BDP** at 560 nm after pulsed excitation (λ_{ex} = 532 nm). The decay curve was measured for three times. $c = 1.0 \times 10^{-6}$ M in deaerated toluene; 20 °C. The mean result is 293.1 μs.

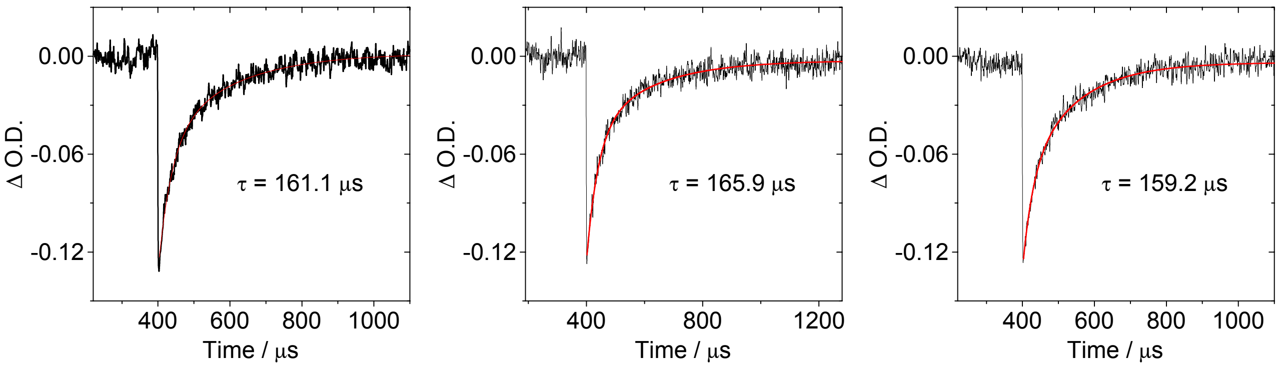


Figure S22. Decay trace of **Pt-8-BDP** at 560 nm after pulsed excitation (λ_{ex} = 532 nm). The decay curve was measured for three times. *c* =1.0×10^{-5} M in deaerated toluene; 20 °C. The mean result is 162.1 μs.

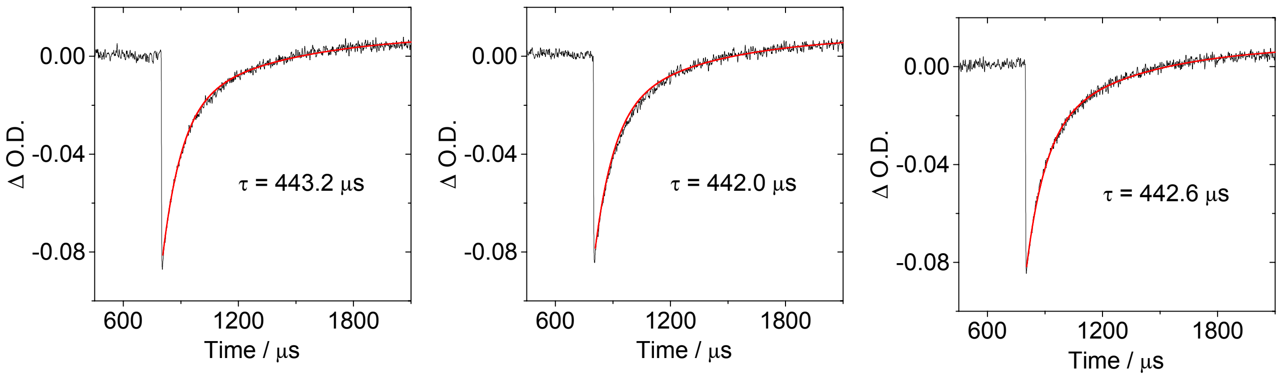


Figure S23. Decay trace of **Pt-8-BDP** at 560 nm after pulsed excitation (λ_{ex} = 532 nm). The decay curve was measured for three times. *c* =5.0×10^{-6} M in deaerated toluene; 20 °C. The mean result is 442.6 μs.

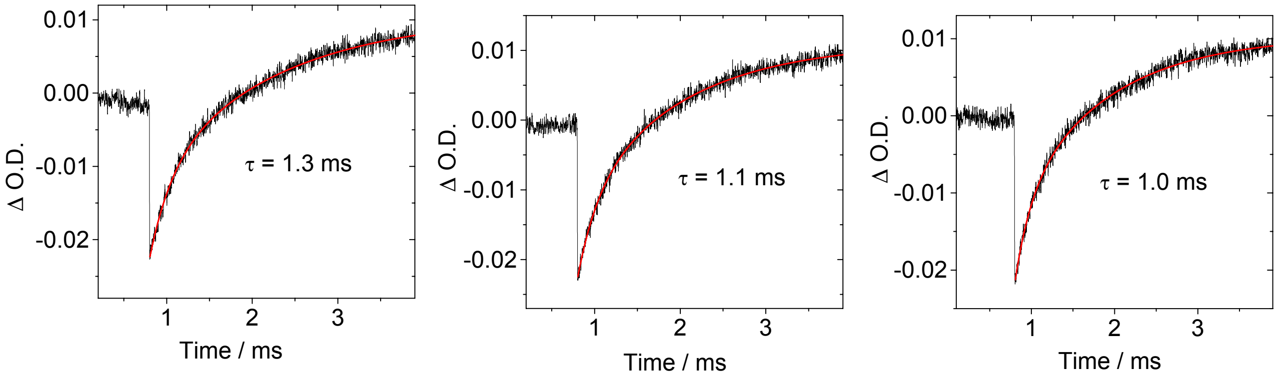


Figure S24. Decay trace of **Pt-8-BDP** at 560 nm after pulsed excitation (λ_{ex} = 532 nm). The decay curve was measured for three times. *c* =1.0×10^{-6} M in deaerated toluene; 20 °C. The mean result is 1.1 ms.

6. Upconversion details

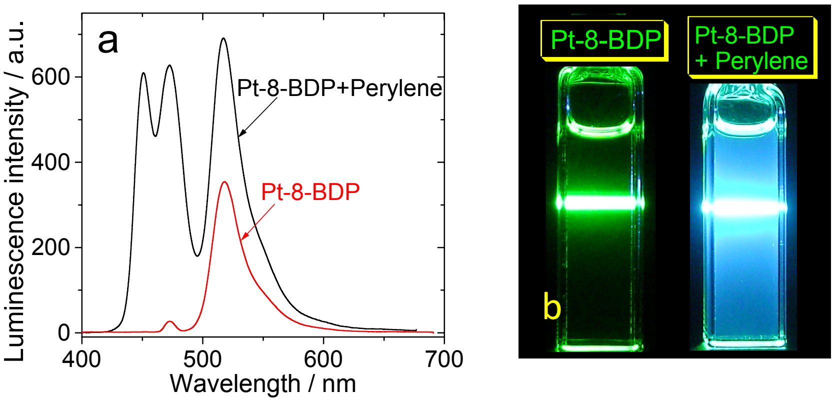


Figure S25. Emission of the **Pt-8-BDP** sensitizer alone and the upconverted perylene fluorescence following selective excitation at 473 nm. (b) Photographs of the emission of the sensitizer alone and the upconversion (data are from a). In deaerated toluene (**Pt-BDP** is at 1.0 × 10^{-5} mol L^{-1} and perylene is at 1.5 × 10^{-4} mol L^{-1}. 20 °C).

Please note that the fluorescence of **Pt-8-BDP** at 520 nm is intensified with the acceptor (perylene) added, this is due to the spectra overlap of the emission of perylene and the absorption of **Pt-8-BDP**, that is, part of the upconverted emission of perylene is absorbed by **Pt-8-BDP** (to produce the emission at 520 nm)**,** in other words, the upconversion quantum yield (Φ_{UC}) should be much higher than the value we determined (Φ_{UC} = 7.4%).

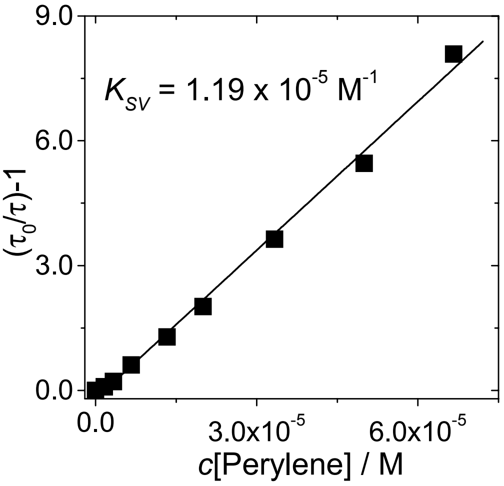


Figure S26. The Stern-Volmer plot of **Pt-2-BDP** with perylene as the triplet acceptor. *c* [photosensitizer] = 1.0 × 10^{-5} M. In deaerated toluene. 25 °C.

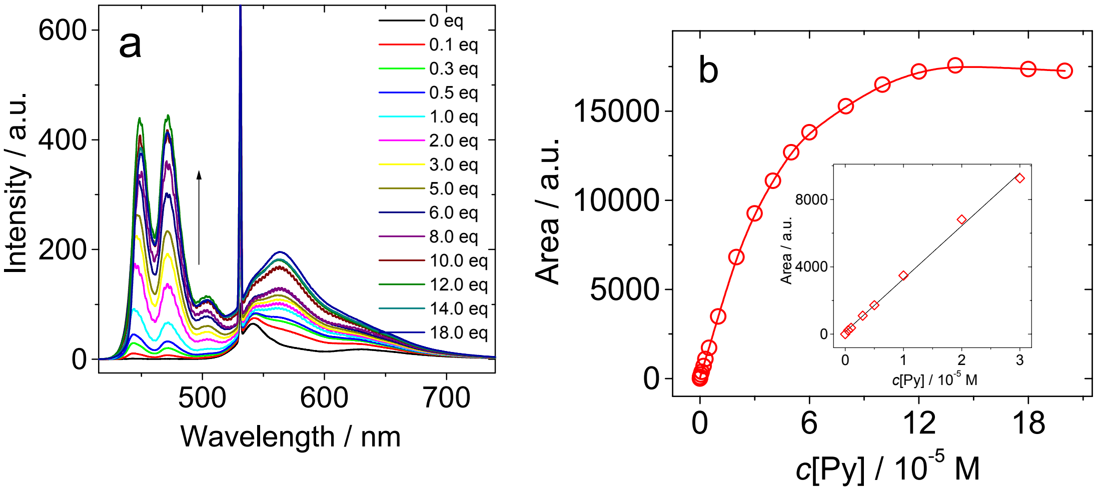


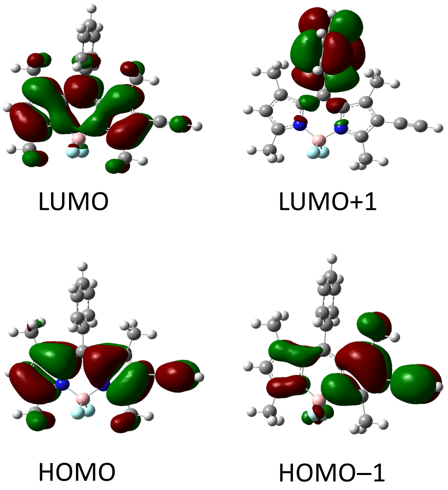
Figure S27. Upconverted emission of perylene with increasing perylene concentration. (a) Emission spetra; (b) Integrated area of the upconvertion intensity with **Pt-2-BDP** as triplet sensitizer with increasing perylene concentration; Excited with 532 nm laser (7.2 mW). c[sensitizer] = 1.0×10^{-5} M. In deaerated toluene at 20 °C.

7. Calculation details

Table S1. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of **2-BDP** and **8-BDP,** Calculated by TDDFT//B3LYP/6-31G(d), based on the DFT//B3LYP/6-31G(d) Optimized Ground State Geometries.

Compounds	**Electronic transition**	**TDDFT//B3LYP/6-31G(d)**			
		Energy (eV / nm) [a]	***f*** [b]	**Composition**	**CI** [c]
2-BDP	$S_0 \rightarrow T_1$	1.52 eV 817 nm	0.0000	HOMO−1→ LUMO	0.1595
				HOMO→ LUMO	0.6947
				HOMO← LUMO	0.1057
	$S_0 \rightarrow T_2$	2.43 eV 510 nm	0.0000	HOMO−1→ LUMO	0.6704
				HOMO→ LUMO	0.1571
	$S_0 \rightarrow T_3$	2.80 eV 443 nm	0.0000	HOMO−2→ LUMO	0.6832
	$S_0 \rightarrow T_4$	3.36 eV 369 nm	0.0000	HOMO-7→ LUMO	0.1238
				HOMO−6→ LUMO	0.6695
	$S_0 \rightarrow T_5$	3.73 eV 332 nm	0.0000	HOMO−4→ LUMO+2	0.4528
				HOMO−3→ LUMO+1	0.5316
8-BDP	$S_0 \rightarrow T_1$	1.51 eV 821 nm	0.0000	HOMO→ LUMO	0.7109
				HOMO←LUMO	0.1191
	$S_0 \rightarrow T_2$	2.71 eV 458 nm	0.0000	HOMO−1→ LUMO	0.6925
	$S_0 \rightarrow T_3$	2.86 eV 433 nm	0.0000	HOMO−3→ LUMO	0.6851
	$S_0 \rightarrow T_4$	3.16 eV 392 nm	0.0000	HOMO−4→ LUMO+2	0.2376
				HOMO−2→ LUMO+1	0.6574
	$S_0 \rightarrow T_5$	3.54 eV 351 nm	0.0000	HOMO→ LUMO+1	0.7054

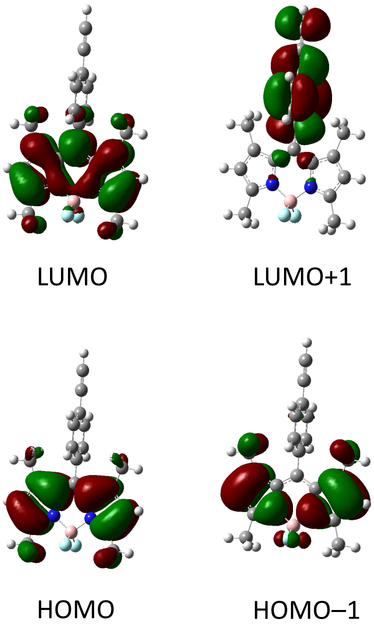
[a] Only the selected low-lying excited states are presented. [b] Oscillator strength. No spin-orbit coupling was considered, thus the *f* value is zero. [c] The CI coefficients are in absolute values.



LUMO LUMO+1

HOMO HOMO–1

Figure S27. Frontier molecular orbitals for **2-BDP** Calculated by DFT at the B3LYP/6-31G(d) level using Gaussian 09.

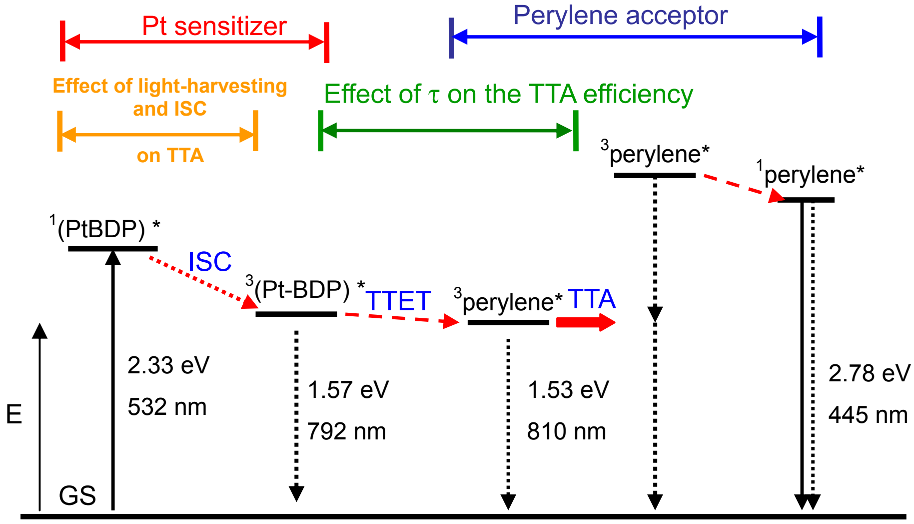


LUMO LUMO+1

HOMO HOMO–1

Figure S28. Frontier molecular orbitals for **8-BDP** Calculated by DFT at the B3LYP/6-31G(d) level using Gaussian 09.

8. Qualitative Jablonski Diagram for the triplet-triplet-annihilation (TTA) based upconversion



Scheme S2. Qualitative Jablonski diagram of the triplet-triplet-annihilation (TTA) based upconversion. Exemplified by **Pt-2-BDP**. For **Pt-2-BDP**, the energy levels will change. The excitation wavelength is 532 nm, due to the available DPSSL laser, actually the excitation wavelength can be longer (the absorption maximum of **Pt-2-BDP** is 561 nm).

E is energy. GS is ground state (S_0). ^{1}(Pt-BDP)* is the singlet excited state of the sensitizers. ^{3}(Pt-BDP)* is the triplet excited state. TTET is the triplet-triplet-energy-transfer. TTA is triplet-triplet annihilation. ^{3}perylene* is the triplet excited state of perylene. ^{1}perylene* is the singlet excited state of perylene. The typical power density of the laser used in the upconversion is 140 mW cm^{-2}, too low to observe simultaneous two-photon absorption.

9. The *x-y-z* coordinates of the optimized geometries of the triplet state of the complexes

Complex Pt-2-BDP (DFT//B3LYP/6-31G(d) / LanL2DZ)

Charge = 0 Multiplicity = 3

C	3.38256866	4.82153547	-0.23988400
C	2.81142569	6.10547528	-0.22745716
C	1.41362862	6.17536911	-0.18032756
C	0.63126679	5.02173785	-0.14394457
C	2.57217091	3.69566815	-0.20502421
C	-0.83609685	5.01898625	-0.09649391
C	-1.62200317	6.17063800	-0.07792735
C	-3.01995619	6.09763842	-0.04220682
C	-3.58695104	4.81251114	-0.02540590
C	-2.77182669	3.68892238	-0.04117329

H	4.45314847	4.68678003	-0.27721769
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H	-4.65737548	4.67393411	0.00056853
H	-3.17667051	2.68673722	-0.02772197
N	-1.42202751	3.77637257	-0.07514725
N	1.22186748	3.78146620	-0.15529430
Pt	-0.09041589	2.15207975	-0.09417030
C	-1.43095443	0.74480575	-0.02042433
C	-2.29488685	-0.13622871	0.03992506
C	1.29809571	0.76505131	-0.12637733
C	2.19284644	-0.07182008	-0.15670051
H	-1.13612779	7.13572565	-0.09194912
H	0.92532648	7.13932241	-0.17271875
C	-3.85940349	7.38513165	-0.02077125
C	3.64715007	7.39496688	-0.26750204
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H	-2.43929330	8.47360813	1.26181658
H	-4.09197532	9.12242489	1.27472952
H	-3.71854834	7.61962183	2.15290952
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H	-4.13284797	9.14311472	-1.27938453
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H	-5.68512005	6.52867113	-0.89069488
H	-5.66030767	6.52175420	0.89420690
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C	3.33323598	8.24414756	0.99451288
H	3.92283934	9.16748243	0.97017276
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H	3.58857911	7.68855008	1.90288069
C	5.16503876	7.10124155	-0.29434908
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C	6.87214706	-3.91995865	-0.24507970
C	6.45105188	-2.67957720	0.25055420
C	5.16724573	-2.20291928	-0.01757822
C	4.49567391	-0.98921435	0.34192560

C	3.10691070	-2.29595477	-0.92515876
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H	1.14087321	-2.11562292	-1.73526164
H	2.29245299	-3.10590601	-2.70376258
H	1.61229719	-3.77261058	-1.22620144
C	5.00615670	0.15428511	1.16928099
H	5.88356522	0.62375271	0.71032553
H	4.21088679	0.89913813	1.27057090
H	5.30429976	-0.17720038	2.16934602
C	5.96085822	-6.89562999	-2.20694290
H	5.62354382	-6.44166068	-3.14552569
H	6.62048603	-7.74142023	-2.40867818
H	5.05915505	-7.23302182	-1.68298727
C	7.39389165	-1.85209960	1.06360401
C	7.43256466	-1.98585455	2.45720778
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C	8.31893618	-1.21185080	3.21030019
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H	8.34499350	-1.31936497	4.28849817
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H	9.85799783	0.29561383	3.16245704
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C	-4.63835408	-1.09940385	0.03350324
C	-2.86068556	-2.55887400	0.33499393
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N	-3.99371859	-3.28191220	0.37049024
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F	-3.43871244	-5.15407061	1.82696424
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H	-5.97573128	0.14888874	-1.12316688
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C	-7.61049485	-2.05993301	-0.01587285
C	-8.07948607	-1.77666097	-1.30733279
C	-8.26154347	-1.48392056	1.08526562
C	-9.17929594	-0.93561046	-1.49414419
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H	-9.53460084	-0.72598498	-2.49683577
H	-9.85895437	-0.20597273	1.75718437
C	-9.82280823	-0.36799272	-0.39138120
H	-10.67798269	0.28235399	-0.53603307
H	-7.57691067	-2.22214709	-2.15819660
H	8.69262650	-6.60301572	-0.95517576
H	-8.02838940	-7.34180997	0.70035398
C	-3.21659273	-1.16506168	0.12299007
C	3.20908564	-1.04649793	-0.22772827

Complex Pt-8-BDP (DFT//B3LYP/6-31G(d) / LanL2DZ)

Charge = 0 Multiplicity = 3

C	-3.53237783	5.61293212	-0.00038518
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C	-0.78474019	5.83137681	-0.00004840
C	-2.71199118	4.49159838	-0.00022333
C	0.68954663	5.83943395	0.00008973
C	1.46508673	6.99538726	0.00023203
C	2.86620677	6.92979955	0.00032281
C	3.43930364	5.64987107	0.00028230

C	2.63086368	4.51990645	0.00014929
H	-4.60280316	5.47078305	-0.00051323
H	-3.10232406	3.48281640	-0.00024733
H	4.51113632	5.51875487	0.00037967
H	3.03148012	3.51509471	0.00010833
N	1.28077596	4.60345852	0.00006174
N	-1.36275579	4.58901844	-0.00005161
Pt	-0.03171908	2.96712949	0.00002295
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C	2.25712342	0.75329186	0.00002759
C	-1.39947421	1.56303450	0.00003133
C	-2.28831685	0.72056056	0.00003758
H	0.97387900	7.95776430	0.00027965
H	-1.09125931	7.94639619	-0.00028109
C	3.69791400	8.22232101	0.00047743
C	-3.81744732	8.18280650	-0.00066225
C	3.35254550	9.04623242	-1.27015222
H	2.29113733	9.31364547	-1.29560717
H	3.93954865	9.97137596	-1.27631903
H	3.58947963	8.47441661	-2.17338177
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H	3.93962318	9.97103740	1.27773195
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H	-5.62820603	7.31638914	0.89147235
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C	-6.48312992	-3.55944316	2.58070204
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C	-6.79983049	-3.87364152	1.21327112
C	-6.31145969	-3.37916696	0.00006025
C	-6.79968391	-3.87384978	-1.21312523

C	-6.48265186	-3.56005048	-2.58056892
C	-7.28973596	-4.37876705	-3.37352017
C	-8.08757661	-5.18019340	-2.52345715
H	-7.30646193	-4.40277107	-4.45089274
N	-7.79349535	-4.87656182	1.23486599
N	-7.79324907	-4.87687277	-1.23466823
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F	-8.23021824	-6.93297715	0.00031797
F	-9.85223552	-5.30292924	-0.00005640
C	-5.48688845	-2.55894160	3.09667639
H	-4.47433847	-2.78753472	2.74855211
H	-5.72075643	-1.54698862	2.75016145
H	-5.48987809	-2.56417843	4.19089023
C	-9.11386572	-6.21685608	-2.85186325
H	-9.22376112	-6.34089978	-3.93056240
H	-8.82472623	-7.16552388	-2.38569188
H	-10.07048711	-5.92771194	-2.40174336
C	-5.48644018	-2.55954393	-3.09659341
H	-4.47386510	-2.78809901	-2.74850348
H	-5.48946205	-2.56480339	-4.19080616
H	-5.72032817	-1.54759865	-2.75008056
C	-9.11473044	-6.21585906	2.85212038
H	-8.82537458	-7.16480748	2.38664734
H	-9.22520884	-6.33929203	3.93082923
H	-10.07108994	-5.92693521	2.40130929
C	-5.26526561	-2.31387427	0.00003143
C	-5.63411117	-0.96213377	-0.00011998
C	-3.90484998	-2.65190603	0.00017929
C	-4.66148888	0.03380317	-0.00013316
C	-2.93003869	-1.65822936	0.00017971
H	-3.61690446	-3.69721369	0.00028606
H	-4.95221166	1.07742057	-0.00022058
H	-1.87945252	-1.92024116	0.00030950
H	-7.30752352	-4.40149069	4.45107124
C	-3.28717357	-0.29106619	0.00001750
H	-6.68581349	-0.69838685	-0.00023381
C	8.18416775	-5.07897995	2.54930896
C	6.55022986	-3.48979461	2.61184336
C	7.37465605	-4.29557273	3.39523114
C	6.87692352	-3.80110493	1.20844297
C	6.35175040	-3.28682982	-0.00002564
C	6.87687304	-3.80111850	-1.20851456
C	6.55002443	-3.48989934	-2.61190248
C	7.37445491	-4.29564038	-3.39532553
C	8.18408547	-5.07896074	-2.54943982
H	7.39385185	-4.32176731	-4.47276252

N	7.86636544	-4.76324491	1.22411887
N	7.86636014	-4.76320124	-1.22423164
B	8.54881088	-5.41371139	-0.00006990
F	9.93965528	-5.15363835	-0.00009170
F	8.35479270	-6.81528162	-0.00007979
C	5.53422547	-2.50613339	3.10647244
H	5.75254755	-1.49209728	2.75235942
H	4.52892867	-2.75237501	2.74605045
H	5.52295225	-2.50142135	4.20076187
C	9.23054448	-6.09671919	-2.83867816
H	9.36660098	-6.24017650	-3.91189243
H	10.17231033	-5.78381467	-2.36965965
H	8.95237378	-7.04186855	-2.35538124
C	5.53374768	-2.50649260	-3.10647697
H	5.75188724	-1.49237497	-2.75249681
H	5.52229983	-2.50189984	-4.20076394
H	4.52855745	-2.75293076	-2.74587435
C	9.23059608	-6.09678312	2.83850781
H	10.17234616	-5.78393887	2.36941218
H	9.36672751	-6.24020634	3.91171633
H	8.95234690	-7.04192893	2.35525611
C	5.28985897	-2.23947603	-0.00001432
C	3.93055239	-2.59128310	0.00026610
C	5.62903657	-0.87749124	-0.00029013
C	2.93841661	-1.61460735	0.00028784
C	4.64186859	0.10445947	-0.00028756
H	6.67649568	-0.59640151	-0.00051418
H	1.89192908	-1.89329885	0.00049799
H	4.91570815	1.15290865	-0.00049315
H	7.39410803	-4.32169568	4.47266721
C	3.27313272	-0.24205995	0.00001686
H	3.65885514	-3.64117021	0.00045133