Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Support Information

β-Functionalized Push-Pull Opp-Dibenzoporphyrins as Sensitizers for Dye-Sensitized Solar Cells: The Push Group Effect

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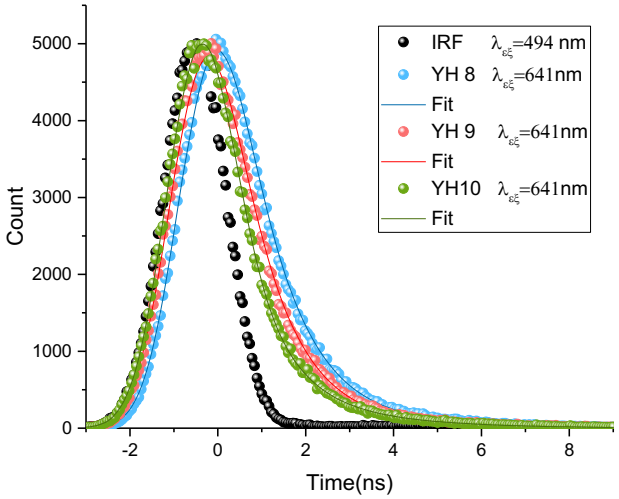
Figure S1. Fluorescence decay profiles of **YH8** – **YH10** in *o*-DCB



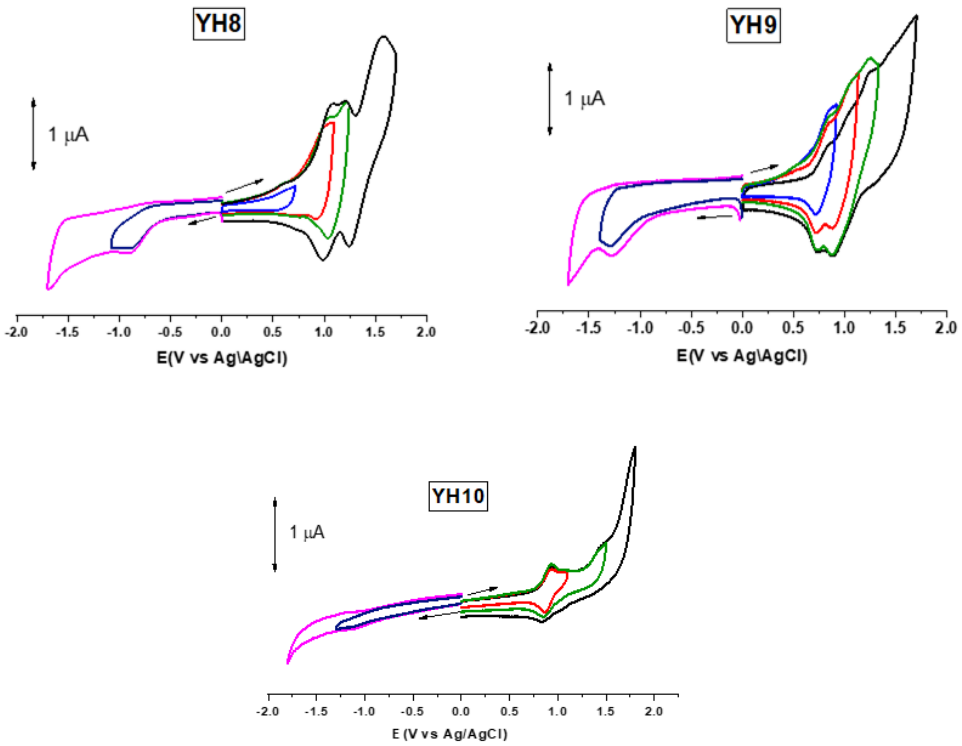
Compound	Solvent	λex (nm)	Time Constants (ns)		
YH8	DCB	641	τ_1= 1.18		
YH9	DCB	641	τ_1= 1.12		
YH10	DCB	641	τ_1= 0.37	τ_2=1.24	τ_{ave}= 0.58

1.2 Cyclic voltammograms of **YH7** -**YH10** in o-DCB.

Table S1. Cyclic voltammograms of investigated compounds in *o*-DCB containing 0.1 M (n-$Bu_4N)ClO_4$. Scan rate = 100 mV/s. The potentials were measured with respect to the Ag/AgCl reference electrode.

Dye	E_{ox} (V vs. Ag/Ag^+)		E_{red} (V vs. Ag/Ag^+)
	1st Oxidation	2nd Oxidation	1st Reduction
YH8	0.60	1.02	-0.90
YH9	0.78	0.99	-1.26
YH10	0.89	1.37	-1.21

Figure S2. Cyclic voltammograms of **YH8** – **YH10** in *o*-DCB containing 0.1 M $(TBA)ClO_4$.



1.3 Computational information

All calculations were carried out using Gaussian 09 program. The Calculations were performed by DFT B3LYP with a basis set 6-31G(d,p) for all atoms.[4]

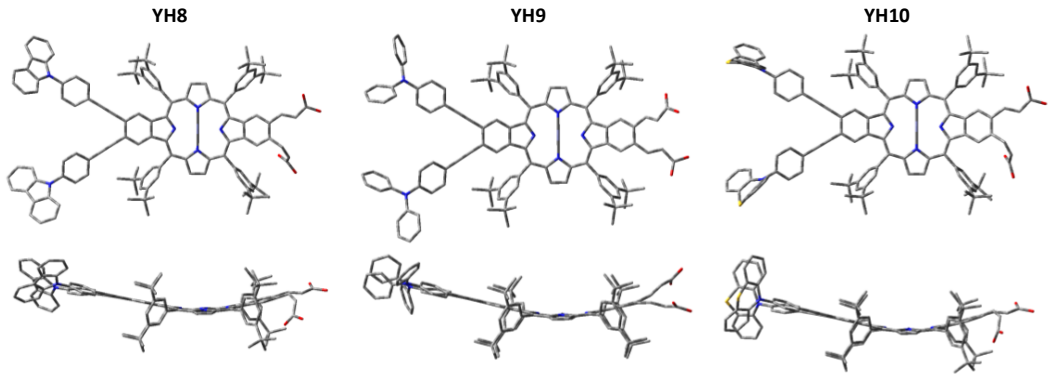


Figure S3 Geometry-optimized molecule structures of **YH8** – **YH10** (calculated by Gaussian09 DFT B3LYP/6-31G(d,p) in gas phase)

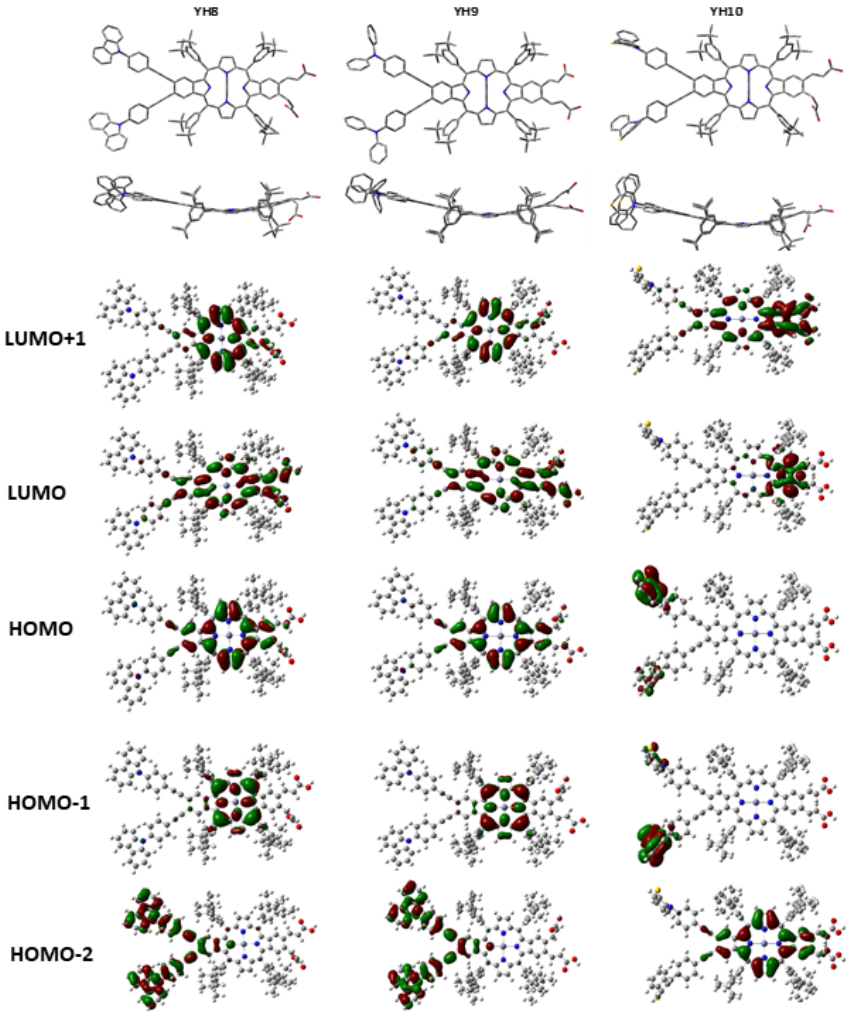


Figure S4 Geometry-optimized molecule structures of **YH8**-**YH10** (Top) and Isodensity surface of LUMO+1, LUMO, HOMO, HOMO-1 and HOMO-2 for Y**H8**-**YH10** calculated by Gaussian09 DFT B3LYP/6-31G(d,p) with acetonitrile as the solvent media. Hydrogen atoms were omitted for clarity

1.4 Solar cell condition optimization

Dye concentration, solvent ratio, CDCA concentration and soaking time using **YH10** were optimized to get the best solar cell performance. N719 dye solar cell was used as reference cell for comparison purpose. The condition for N719 dye solar cell is: soaking time 3 h, solvent ratio EtOH/MeCN (v/v) = 1/1, dye concentration 0.2 mM.

1.5 Photodegradation data

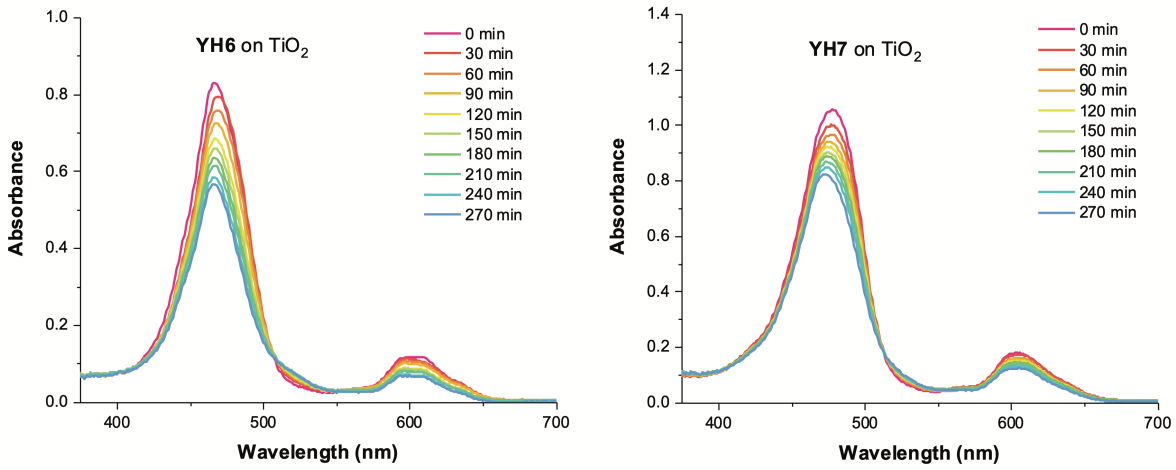


Figure S5. Decomposition study on TiO_2 (The TiO_2 films were soaked in a 0.05 mM dye solution for 10 min)

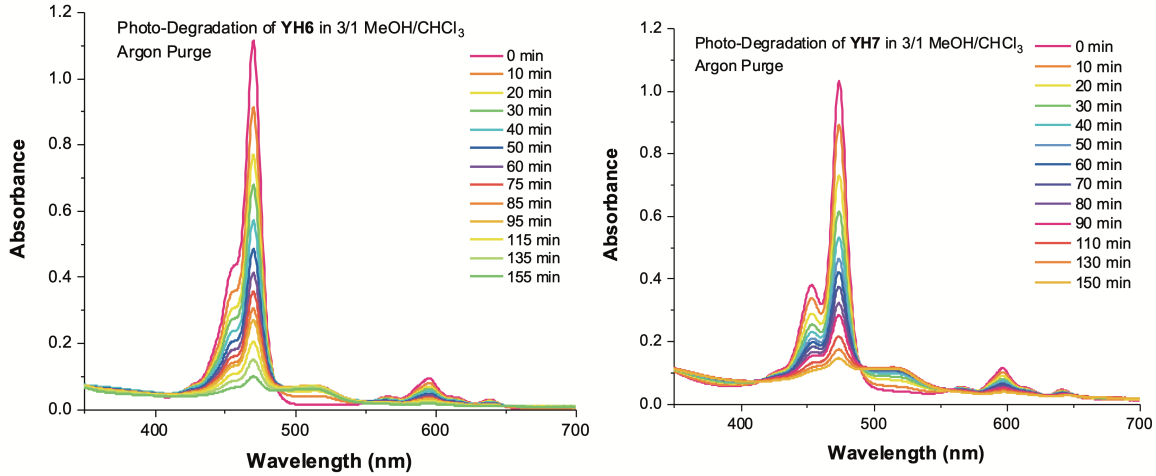


Figure S6. Decomposition study in solution (Incident light intensity: 100 mW/cm2, Solvent: MeOH/CHCl3 = 3/1 (v/v), Dye concentration: 2.14 * 10-6 mol/L)

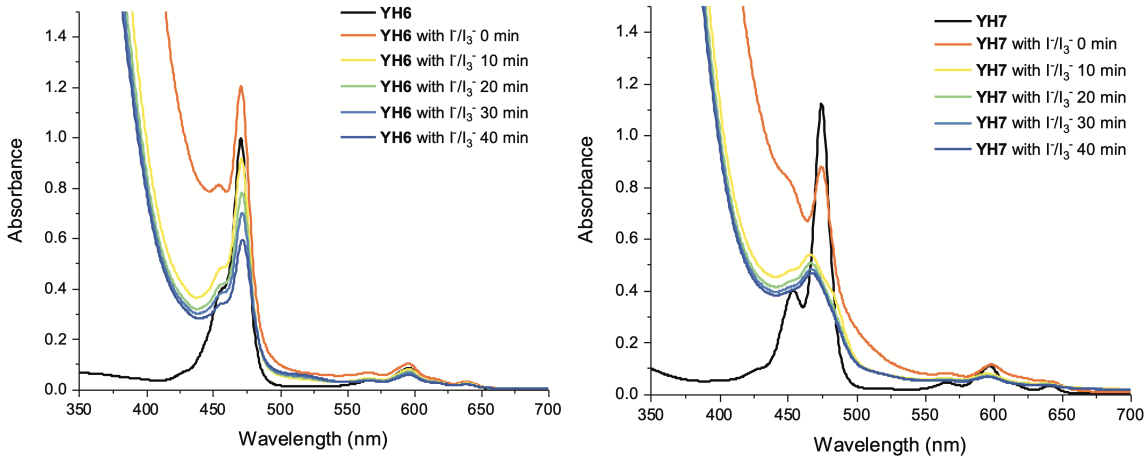


Figure S7. Decomposition study in solution in the presence of I^-/I_3^- electrolyte (Incident light intensity: 100 mW/cm^2, Solvent: MeOH/$CHCl_3$ = 2/1 (v/v), Dye concentration: 2.0 * 10^{-6} mol/L, 5 drops of I^-/I_3^- electrolyte)

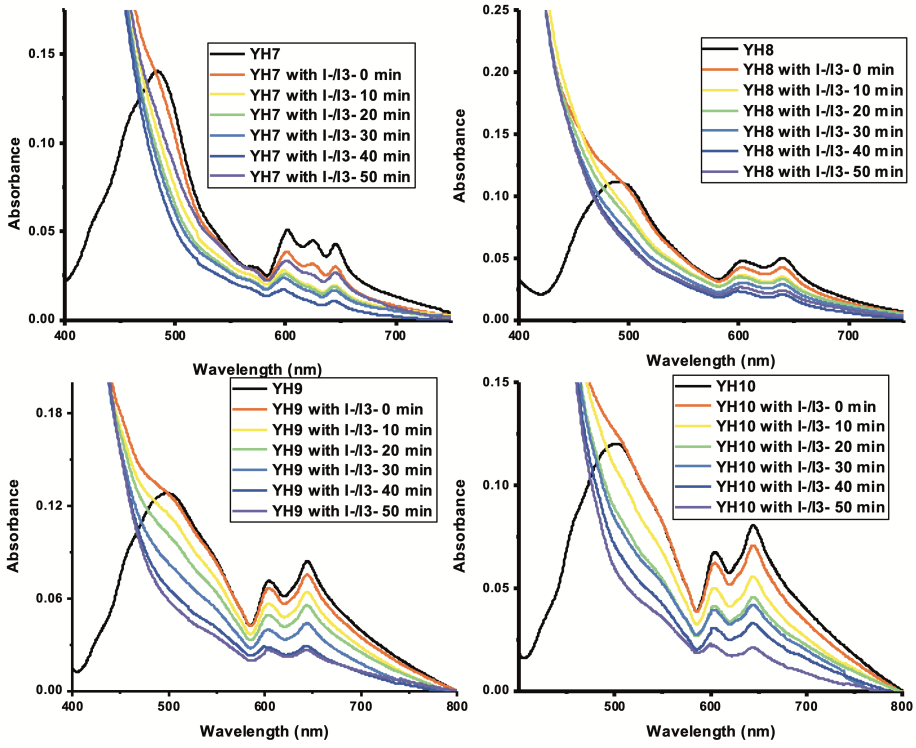


Figure S8. Decomposition study in solution in the presence of I^-/I_3^- electrolyte (Incident light intensity: 100 mW/cm^2, Solvent: ACN, Dye concentration: 2.0 * 10^{-6} mol/L, 5µl of I^-/I_3^- electrolyte)

Table S2. Photovoltaic performance of **YH10** with different dye concentration

Soaking time: 3 h Solvent ratio: $CHCl_3$/t-BuOH = 1/2 CDCA concentration: 0 mM					
Condition	Dye Concentration	J_{SC}	V_{OC}	FF	η
1	0.1 mM	-14.9	0.53	0.66	5.2%
2	0.2 mM	-14.5	0.59	0.65	5.6%
3	0.3 mM	-15.1	0.52	0.54	4.2%
N719	0.3 mM	-15.1	0.59	0.70	6.2%

Table S2 Photovoltaic performance of **YH10** with different solvent ratio

Dye concentration: 0.2 mM Soaking time: 3 h CDCA concentration: 0 mM					
Condition	$CHCl_3$/t-BuOH (v/v)	J_{SC}	V_{OC}	FF	η
1	1/1	-14.7	0.54	0.60	4.8%
2	2/1	-17.0	0.56	0.58	5.5%
3	3/1	-14.9	0.55	0.59	4.8%
4	4/1	-12.3	0.53	0.57	3.7%
5	5/1	-9.3	0.52	0.51	2.5%

Table S3 Photovoltaic performance of **YH10** with different CDCA concentration

Dye concentration: 0.2 mM Soaking time: 3 h Solvent ratio: $CHCl_3$/t-BuOH = 1/2					
Condition	CDCA Concentration	J_{SC}	V_{OC}	FF	η
1	0.0 mM	-18.1	0.57	0.61	6.3%
2	0.2 mM	-15.8	0.60	0.68	6.4%
3	0.4 mM	-6.2	0.56	0.68	2.4%
4	0.6 mM	-13.8	0.59	0.67	5.5%
5	0.8 mM	-7.7	0.58	0.70	3.1%
6	1.0 mM	-12.1	0.58	0.49	3.4%

Table S4 Photovoltaic performance of **YH10** with different soaking time

Dye concentration: 0.2 mM CDCA concentration: 0.2 mM Solvent ratio: $CHCl_3$/t-BuOH = 1/2					
Condition	Soaking Time	J_{SC}	V_{OC}	FF	η
1	15 h	-1.4	0.29	0.52	0.2%
2	12 h	-8.8	0.53	0.58	2.7%
3	9 h	-13.7	0.56	0.62	4.8%
4	6 h	-12.9	0.57	0.65	4.8%

5	3 h	-17.9	0.58	0.68	7.1%
N719 Dye (Reference)	16 h	-16.8	0.62	0.74	7.7%

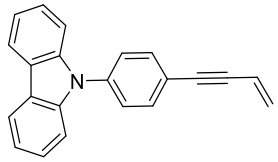
2. Experimental Section

2.1 General Experimental Information

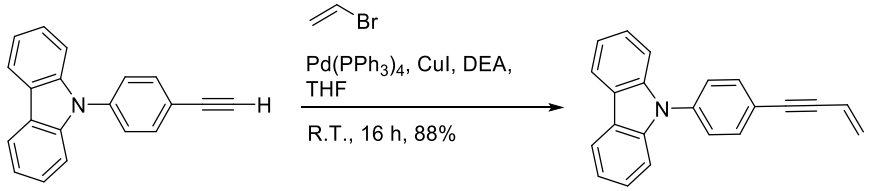
All reagents were purchased from Aldrich and Fisher and used without further purifications. Solvents used were dried through a commercially available solvent purification system. Column chromatography was performed on silica gel (43 – 63 µm). All NMR spectra were recorded on a 500 MHz or 400 MHz (^{1}H NMR)/126 MHz or 101 MHz (^{13}C NMR) spectrometer. All samples were prepared in $CDCl_3$ or $CDCl_3$ with one drop of d5-pyridine. $CDCl_3$ was used as internal standard (δ = 7.26 and 77.0 ppm, respectively. Mass spectra were obtained with a Thermoscientific MALDI-LTQ-XL-Orbitrap mass spectrometer.

2.2 Synthesis

9-(4-(But-3-en-1-yn-1-yl)phenyl)-9H-carbazole



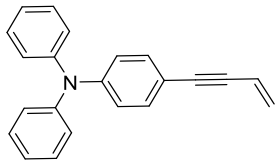
9-(4-(But-3-en-1-yn-1-yl)phenyl)-9H-carbazole was synthesized via Sonogashira coupling from the commercially available **9-(4-ethynylphenyl)-9H-carbazole** (see below).



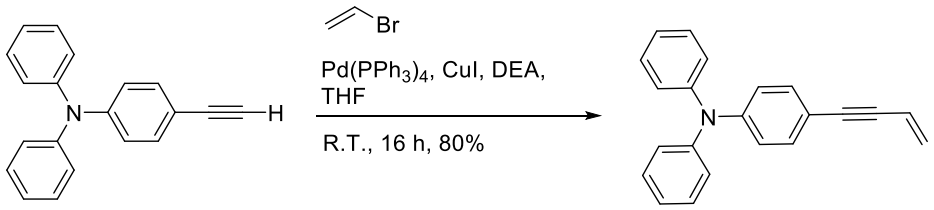
CuI (2.0 mol%) and $Pd(PPh_3)_4$ (0.3 mol%) were dissolved in anhydrous and degassed diethylamine (0.5 mL/1.0 mmol alkyne) and cooled to 0 °C. Then **9-(4-ethynylphenyl)-9H-carbazole** (660 mg, 2.5 mmol) and vinyl bromide (1 M in THF, 1.3 eq) were added dropwise and the resulting suspension were stirred at room temperature until complete conversion of the starting material. Water was added followed by extraction with CH_2Cl_2, the combined organic layers were washed with 1 M HCl, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography (Hexane/CH_2Cl_2 = 5/1) to afford **9-(4-(but-3-en-1-yn-1-yl)phenyl)-9H-carbazole** as a white solid.

9-(4-(But-3-en-1-yn-1-yl)phenyl)-9H-carbazole: $C_{22}H_{17}N$; white solid; yield: 635 mg (2.2 mmol, 87%); ^{1}H NMR (400 MHz, $CDCl_3$): 8.15 (d, *J* = 7.6 Hz, 2H), 7.71 – 7.63 (m, 2H), 7.58 – 7.51 (m, 2H), 7.46 – 7.38 (m, 5H), 7.35 – 7.27 (m, 2H), 6.08 (dd, *J* = 17.5, 11.1 Hz, 1H), 5.81 (dd, *J* = 17.6, 1.9 Hz, 1H), 5.65 – 5.57 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ140.40, 136.29, 133.02, 127.40, 126.79, 126.03, 123.52, 122.05, 120.35, 120.19, 109.74, 89.21, 88.97 ppm; HRMS (MALDI): m/z: calcd for $C_{22}H_{17}N$: 293.1204; found: 293.1204.

4-(But-3-en-1-yn-1-yl)-N,N-diphenylaniline



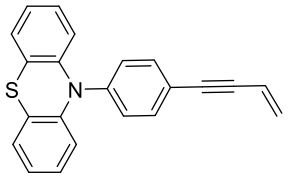
4-(But-3-en-1-yn-1-yl)-N,N-diphenylaniline was synthesized via Sonogashira coupling (see below) from **4-ethynyl-N,N-diphenylaniline**. **4-Ethynyl-N,N-diphenylaniline** was synthesized via a three-step pathway according to a published literature.[1]



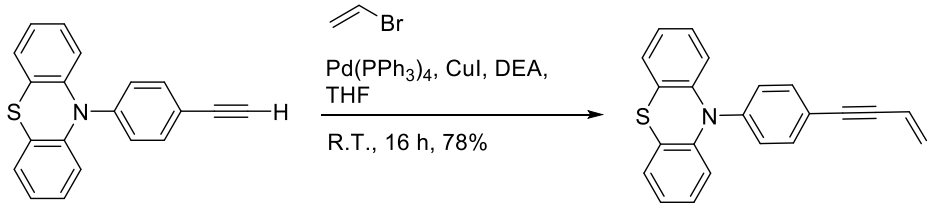
CuI (2.0 mol%) and $Pd(PPh_3)_4$ (0.3 mol%) were dissolved in anhydrous and degassed diethylamine (0.5 mL/1.0 mmol alkyne) and cooled to 0 °C. Then **4-ethynyl-N,N-diphenylaniline** (910 mg, 3.4 mmol) and vinyl bromide (1 M in THF, 1.3 eq) were added dropwise and the resulting suspension were stirred at room temperature until complete conversion of the starting material. Water was added followed by extraction with CH_2Cl_2, the combined organic layers were washed with 1 M HCl, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography (Hexane/CH_2Cl_2 = 5/1) to afford **4-(but-3-en-1-yn-1-yl)-N,N-diphenylaniline** as a white solid.

4-(But-3-en-1-yn-1-yl)-N,N-diphenylaniline: $C_{22}H_{15}N$; pale yellow solid; yield: 798 mg (2.7 mmol, 80%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30 – 7.26 (m, 2H), 7.26 – 7.23 (m, 1H), 7.12 – 7.03 (m, 7H), 6.99 – 6.93 (m, 2H), 6.01 (dd, J = 17.5, 11.2 Hz, 1H), 5.69 (dd, J = 17.5, 2.1 Hz, 1H), 5.53 – 5.45 (m, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 148.03, 147.25, 132.66, 129.52, 126.23, 125.07, 123.68, 122.37, 117.46, 115.97, 90.36, 87.55 ppm; HRMS (MALDI): m/z: calcd for $C_{22}H_{15}N$: 295.1361; found: 295.1364.

10-(4-(But-3-en-1-yn-1-yl)phenyl)-10H-phenothiazine



10-(4-(But-3-en-1-yn-1-yl)phenyl)-10*H*-phenothiazine was synthesized via Sonogashira coupling (see below) from **10-(4-ethynylphenyl)-10*H*-phenothiazine**. **10-(4-Ethynylphenyl)-10*H*-phenothiazine** was synthesized via a four-step pathway according to a published literature.[2]



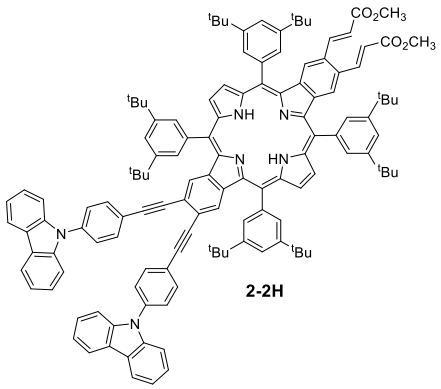
CuI (2.0 mol%) and $Pd(PPh_3)_4$ (0.3 mol%) were dissolved in anhydrous and degassed diethylamine (0.5 mL/1.0 mmol alkyne) and cooled to 0 °C. Then **10-(4-ethynylphenyl)-10*H*-phenothiazine** (1.3 g, 4.3 mmol) and vinyl bromide (1 M in THF, 1.3 eq) were added dropwise and the resulting suspension were stirred at room temperature until complete conversion of the starting material. Water was added followed by extraction with CH_2Cl_2, the combined organic layers were washed with 1 M HCl, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography (Hexane/CH_2Cl_2 = 3/1) to afford **10-(4-(but-3-en-1-yn-1-yl)phenyl)-10*H*-phenothiazine** as a white solid.

10-(4-(But-3-en-1-yn-1-yl)phenyl)-10*H*-phenothiazine: $C_{22}H_{15}NS$; white solid; yield: 1.1 g (3.4 mmol, 78%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 (d, J = 7.7 Hz, 2H), 7.33 (d, J = 7.7 Hz, 2H), 7.02 (dd, J = 70.2, 7.1 Hz, 6H), 6.40 (d, J = 7.4 Hz, 2H), 6.09 (dd, J = 17.3, 11.2 Hz, 1H), 5.82 (d, J = 17.4 Hz, 1H), 5.62 (d, J = 11.0 Hz, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.66, 141.57, 133.80, 128.92, 127.40, 127.10, 126.97, 123.15, 122.24, 122.15, 117.52, 117.09, 89.32, 89.15 ppm; HRMS (MALDI): m/z: calcd for $C_{22}H_{15}NS$: 325.0925; found: 325.0925.

Dibromomonobenzoporphyirn 1 was synthesized according to a previously published procedure.[3]

General procedure for the synthesis of dibenzoporphyrins 2-2H – 4-2H

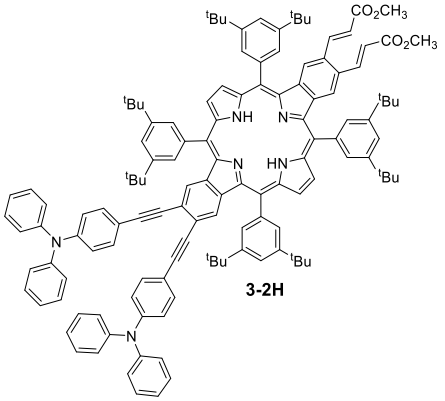
Dibromomobenzoporphyrin **1** (250 mg, 0.17 mmol) and K_2CO_3 (54 mg, 0.38 mmol) were added to a Schlenk flask and dried under vacuum. The vacuum was released under an argon atmosphere to allow the addition of dry THF (20 mL). The mixture was then degassed by three freeze-pump-thaw cycles before the addition of bis(tri-tert-butylphosphine)palladium (36 mg, 0.068 mmol) and the enyne (8-fold excess). The Schlenk flask was then sealed and heated at 45 °C for 48 h. Then the temperature was raised to reflux for 24 h. The progress of the reaction was monitored by UV-Vis spectroscopy and TLC. Upon completing of the reaction, solvent was removed under vacuum and the resulting residue was subjected to silica column chromatography (CH_2Cl_2). The band containing desired product was collected and the product was recrystallized using CH_2Cl_2/Hexane.



2-2H

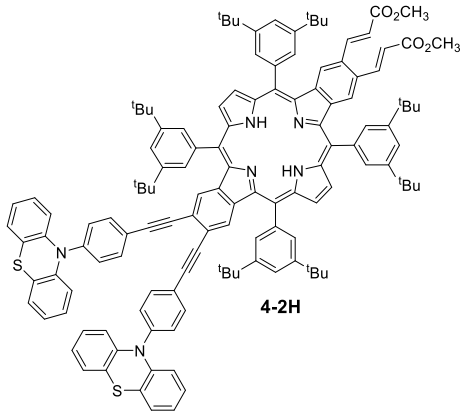
Dibenzoporphyrin **2-2H**: $C_{132}H_{128}N_6O_4$; purple solid; yield: 68 mg (0.036 mmol, 21%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.96 (d, J = 3.6 Hz, 2H), 8.91 (d, J = 4.6 Hz, 2H), 8.17 (d, J = 15.7 Hz, 2H), 8.03 (dd, J = 22.1, 13.2 Hz, 12H), 7.41 (d, J = 8.5 Hz, 4H), 7.30 (dd, J = 10.2, 5.4 Hz, 10H), 7.16 (d, J = 7.8 Hz, 8H), 7.11 – 7.02 (m, 8H), 6.79 (s, 2H), 3.91 (s, 3H), 1.50 (d, J = 8.4 Hz, 72H), -2.57 (s, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.26, 150.86, 150.69, 149.33, 149.20, 142.99, 141.51, 141.47, 141.41, 141.34, 140.71, 139.08, 138.94, 137.72, 133.04, 130.98, 128.41, 128.09,

127.85, 127.09, 126.24, 123.74, 123.68, 122.92, 122.70, 122.30, 120.55, 120.41, 110.15, 109.93, 92.12, 90.97, 51.84, 35.43, 35.35, 31.97, 31.80 ppm; UV-Vis (THF): λ_{max} = 466, 534, 576, 614 nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{128}N_6O_4$: 1860.9997; found: 1860.9999.



3-2H

Dibenzoporphyrin **3-2H**: $C_{132}H_{132}N_6O_4$; purple solid; yield: 78 mg (0.042 mmol, 24%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.96 (d, J = 4.9 Hz, 2H), 8.90 (d, J = 4.8 Hz, 2H), 8.16 (d, J = 15.7 Hz, 2H), 8.05 (d, J = 16.2 Hz, 12H), 7.49 (d, J = 8.5 Hz, 4H), 7.29 (s, 2H), 6.75 (d, J = 7.6 Hz, 6H), 6.10 (d, J = 15.6 Hz, 2H), 3.91 (s, 6H), 3.06 (s, 12H), 1.52 (s, 36H), 1.49 (s, 36H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.28, 150.77, 150.63, 149.74, 148.96, 147.89, 147.42, 142.95, 141.54, 141.39, 140.89, 138.96, 138.90, 132.55, 132.27, 130.84, 129.57, 129.37, 128.80, 128.41, 127.99, 127.87, 127.72, 125.21, 124.69, 123.68, 122.94, 122.65, 122.44, 122.23, 120.14, 119.81, 119.43, 116.97, 93.19, 89.44, 35.36, 35.34, 31.92, 31.79 ppm; UV-Vis (THF): λ_{max} = 646, 535, 578, 615 nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{132}N_6O_4$: 1865.0310; found: 1865.0366.



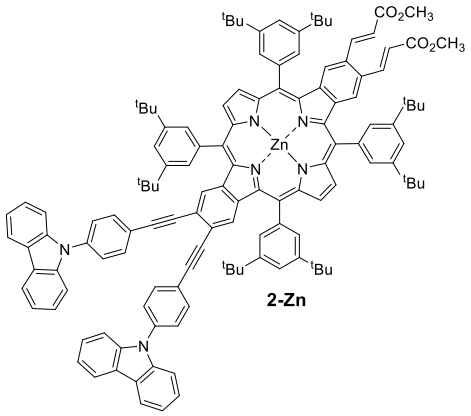
4-2H

Dibenzoporphyrin **4-2H**: $C_{132}H_{128}N_6O_4S_2$; purple solid; yield: 92 mg (0.047 mmol, 27%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.98 (dd, J = 5.0, 1.6 Hz, 2H), 8.92 (dd, J = 4.9, 1.6 Hz, 2H), 8.16 (d, J = 15.6 Hz, 2H), 8.08 – 8.02 (m, 12H), 7.73 (d, J = 8.3 Hz, 4H), 7.39 (d, J = 8.3 Hz, 4H), 7.30 (s, 2H), 7.12 (dd, J = 7.6, 1.6 Hz, 4H), 7.00 – 6.96 (m, 4H), 6.93 – 6.88 (m, 6H), 6.49 (dd, J = 8.2, 1.1 Hz, 4H), 6.10 (d, J = 15.6 Hz, 2H), 3.91 (s, 6H), 1.53 (s, 36H), 1.50 (s, 36H), -2.57 (s, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.25, 150.82, 150.75, 150.68, 149.33, 149.21, 143.78, 142.98, 141.78, 141.50, 141.47, 141.38, 141.28, 139.06, 138.93, 133.69, 132.27, 130.97, 129.29, 128.93, 128.65, 128.45, 128.40, 128.06, 128.01, 127.83, 127.34, 127.14, 123.67, 123.35, 122.90, 122.71, 122.29, 120.21, 119.90, 119.54, 118.03, 92.11, 91.00, 51.83, 35.40,

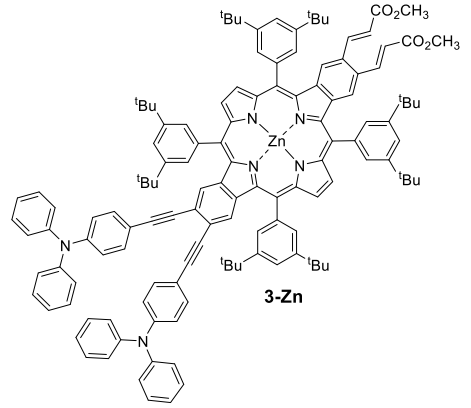
35.36, 31.94, 31.79 ppm; UV-Vis (THF): λ_{max} = 460, 535, 876, 614 nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{128}N_6O_4S_2$: 1924.9438; found: 1924.9463.

General procedure for the synthesis of dibenzoporphyrins 2-Zn – 4-Zn

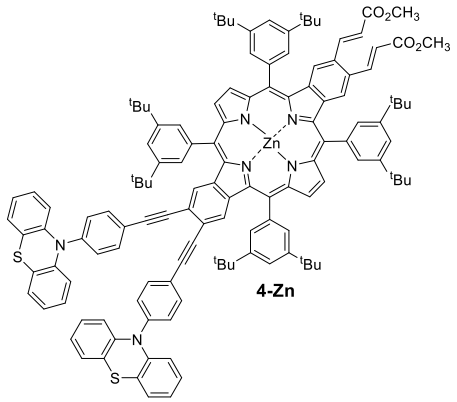
General procedure for the synthesis of dibenzoporphyrins **2-Zn** – **4-Zn**: dibenzoporphyrin **2-2H** – **4-2H** (50 mg) and zinc acetate (10 equiv.) were dissolved in MeOH/$CHCl_3$ (v/v = 1/3). The mixture was heated at reflux for 12 h. The progress of the reaction was monitored with TLC. Upon completion of the reaction, the solvent was removed and the resulting residue was recrystallized using CH_2Cl_2/MeOH to afford pure zinc product.



Dibenzoporphyrin **2-Zn**: $C_{132}H_{128}N_6O_4Zn$; green solid; yield: 38 mg (0.019 mmol, 74%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.06 (d, J = 4.6 Hz, 2H), 8.99 (d, J = 4.6 Hz, 2H), 8.19 (dd, J = 23.1, 11.7 Hz, 6H), 8.11 – 8.04 (m, 12H), 7.86 (d, J = 8.4 Hz, 4H), 7.68 (d, J = 8.4 Hz, 4H), 7.52 (d, J = 9.0 Hz, 6H), 7.47 – 7.42 (m, 4H), 7.34 – 7.29 (m, 4H), 7.12 (s, 4H), 6.16 (d, J = 15.6 Hz, 6H), 3.93 (s, 6H), 1.57 (s, 36H), 1.50 (s, 36H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.21, 150.72, 150.53, 150.36, 145.01, 144.95, 142.21, 142.13, 141.56, 140.77, 140.71, 139.14, 137.75, 133.07, 131.69, 131.54, 130.78, 129.67, 128.12, 127.84, 127.10, 126.24, 123.99, 123.75, 122.92, 122.52, 122.10, 122.03, 121.05, 120.69, 120.55, 120.41, 109.93, 92.15, 90.97, 51.85, 35.43, 35.36, 31.98, 31.82 ppm; UV-Vis (THF): λ_{max} = 479, 596, 620 nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{128}N_6O_4Zn$: 1922.9132; found: 1922.9144.



Dibenzoporphyrin **3-Zn**: $C_{132}H_{130}N_6O_4Zn$; green solid; yield: 39 mg (0.020 mmol, 76%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.03 (d, J = 4.7 Hz, 2H), 8.96 (d, J = 4.8 Hz, 2H), 8.21 (d, J = 15.7 Hz, 2H), 8.09 – 7.99 (m, 12H), 7.50 (s, 2H), 7.43 (d, J = 8.4 Hz, 4H), 7.31 (t, J = 7.7 Hz, 8H), 7.17 (d, J = 7.6 Hz, 8H), 7.12 – 7.04 (m, 8H), 6.97 (s, 1H), 6.15 (d, J = 15.7 Hz, 2H), 3.92 (s, 6H), 1.50 (d, J = 8.8 Hz, 72H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.09, 150.48, 150.32, 150.22, 150.18, 147.77, 147.27, 145.22, 144.59, 142.11, 141.95, 141.45, 140.56, 138.57, 132.43, 131.40, 131.25, 130.51, 129.42, 128.88, 127.96, 127.60, 125.07, 123.80, 123.54, 122.60, 122.30, 121.87, 120.78, 120.44, 120.15, 116.80, 93.07, 89.28, 51.68, 35.21, 35.19, 31.79, 31.66 ppm; UV-Vis (THF): λ_{max} = 482, 597, 620, 639 nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{132}N_6O_4$: 1926.9445; found: 1926.9464.

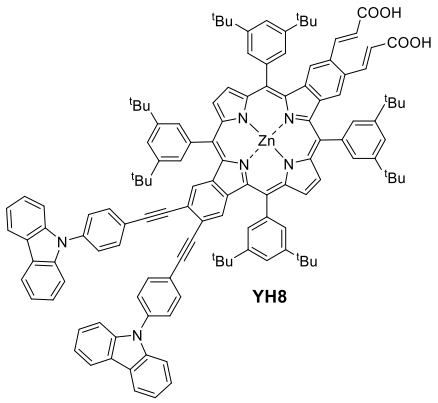


4-Zn

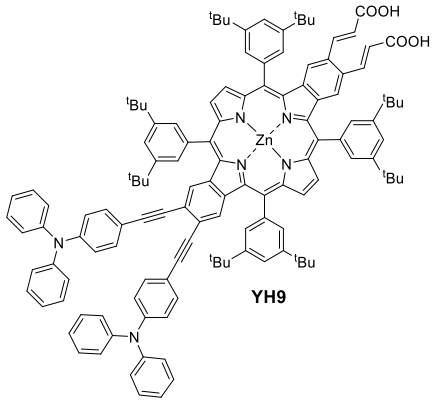
Dibenzoporphyrin **4-Zn**: $C_{132}H_{126}N_6O_4S_2Zn$; green solid; yield: 33 mg (0.017 mmol, 64%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.06 (d, J = 4.7 Hz, 2H), 8.99 (d, J = 4.7 Hz, 2H), 8.22 (d, J = 15.7 Hz, 2H), 8.11 – 8.03 (m, 14H), 7.79 – 7.73 (m, 4H), 7.52 (s, 2H), 7.41 (d, J = 8.4 Hz, 4H), 7.13 (dd, J = 7.6, 1.6 Hz, 4H), 7.08 (s, 2H), 7.02 – 6.96 (m, 4H), 6.92 (td, J = 7.4, 1.2 Hz, 4H), 6.51 (dd, J = 8.2, 1.2 Hz, 4H), 6.16 (d, J = 15.6 Hz, 2H), 3.93 (s, 6H), 1.55 (s, 36H), 1.51 (s, 36H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.24, 150.68, 150.52, 150.51, 150.35, 145.01, 144.94, 143.77, 142.19, 142.09, 141.79, 141.55, 140.75, 139.08, 133.72, 131.68, 131.52, 130.76, 129.57, 128.65, 128.11, 127.81, 127.33, 127.14, 123.98, 123.40, 122.89, 122.69, 122.52, 122.08, 122.06, 121.04, 120.68, 120.39, 119.51, 118.04, 92.13, 90.99, 51.85, 35.40, 35.35, 31.96, 31.81 ppm; UV-Vis (THF): λ_{max} = 479, 596, 620 nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{132}N_6O_4S_2$: 1986.8573; found: 1986.8529.

General procedure for the synthesis of porphyrin dye YH8 – YH10

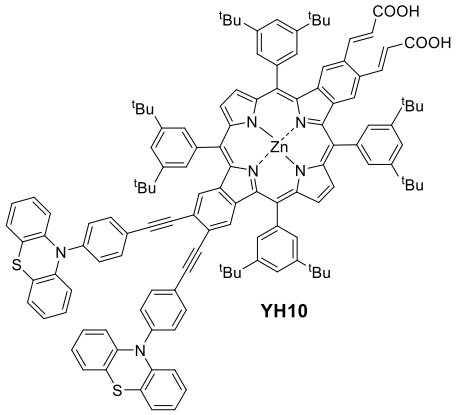
The zinc inserted product **2-Zn** – **4-Zn** (30 mg) was dissolved in THF (6 mL). A solution of 20% NaOH (aq) (1 mL) and MeOH (2 mL) were added. The mixture was heated at reflux for 12 h. The progress of the reaction was monitored by TLC. upon completion, the mixture was washed with 10% citric acid solution, water and extracted using ethyl acetate. The organic layer was separated and the solvent was removed under reduced pressure. Pure product **YH8** – **YH10** were obtained after recrystallization using CH_2Cl_2/MeOH.



Porphyrin Dye **YH8**: $C_{132}H_{128}N_6O_4Zn$; green solid; yield: 26 mg (0.014 mmol, 98%); ^{1}H NMR (500 MHz, $CDCl_3$/d5-pyridine): δ 8.99 (d, J = 4.4 Hz, 2H), 8.93 (d, J = 4.6 Hz, 2H), 8.27 (d, J = 15.6 Hz, 2H), 8.14 (d, J = 7.9 Hz, 12H), 8.05 (d, J = 21.3 Hz, 7H), 7.83 (d, J = 7.9 Hz, 4H), 7.64 (d, J = 8.2 Hz, 6H), 7.50 (d, J = 8.4 Hz, 6H), 7.45 – 7.39 (m, 4H), 7.32 – 7.27 (m, 4H), 7.06 (s, 2H), 4.75 (s, 2H), 1.53 (s, 36H), 1.50 (s, 36H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$/d5-pyridine): δ 169.17, 150.49, 150.25, 150.14, 144.67, 144.27, 142.77, 142.70, 141.05, 140.66, 139.48, 137.53, 132.98, 131.27, 130.83, 129.57, 128.09, 127.91, 127.02, 126.18, 123.66, 121.29, 120.47, 120.33, 120.20, 109.91, 91.66, 91.20, 35.31, 35.28, 31.93, 31.84 ppm; UV-Vis (THF): λ_{max}(log ε) = 477(5.64), 596(4.61), 618(4.42), 637(4.06) nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{128}N_6O_4Zn$: 1894.8819; found: 1894.8869.



Porphyrin dye **YH9**: $C_{132}H_{130}N_6O_4Zn$; green solid; yield: 26 mg (0.014 mmol, 87%); ^{1}H NMR (500 MHz, $CDCl_3$/d5-pyridine): δ 8.94 (d, J = 4.5 Hz, 2H), 8.89 (d, J = 4.7 Hz, 2H), 8.26 (d, J = 15.2 Hz, 2H), 7.99 (dd, J = 37.7, 13.1 Hz, 16H), 7.47 (s, 2H), 7.40 (d, J = 8.5 Hz, 4H), 7.13 (d, J = 7.6 Hz, 10H), 7.04 (dd, J = 14.3, 7.9 Hz, 10H), 6.91 (s, 2H), 6.17 (s, 2H), 4.72 (s, 2H), 1.47 (d, J = 6.8 Hz, 72H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$/d5-pyridine): δ 169.23, 150.25, 150.13, 150.11, 150.06, 147.72, 147.36, 144.59, 144.44, 142.74, 140.97, 139.10, 135.89, 132.45, 131.19, 131.10, 129.47, 128.89, 128.06, 127.80, 125.07, 123.55, 122.45, 122.34, 121.99, 120.28, 120.07, 92.73, 92.67, 89.61, 35.24, 35.22, 31.86, 31.81 ppm; UV-Vis (THF): λ_{max}(log ε) = 460(5.07), 480(5.47), 597(4.53), 618(4.32), 639(4.05) nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{132}N_6O_4$: 1898.9132; found: 1898.9163.



YH10

Porphyrin dye **YH10**: $C_{132}H_{126}N_6O_4S_2Zn$; green solid; yield: 30 mg (0.015 mmol, 99%); ^1H NMR (500 MHz, $CDCl_3$/d5-pyridine): δ 8.97 (d, J = 4.6 Hz, 2H), 8.93 (d, J = 4.7 Hz, 2H), 8.27 (d, J = 15.5 Hz, 2H), 8.02 (d, J = 9.2 Hz, 7H), 7.75 (d, J = 8.2 Hz, 3H), 7.48 (s, 2H), 7.39 (d, J = 8.3 Hz, 4H), 7.10 (d, J = 7.6 Hz, 4H), 7.02 (s, 2H), 6.92 (dt, J = 14.5, 7.0 Hz, 7H), 6.19 (d, J = 15.7 Hz, 2H), 1.51 (d, J = 4.6 Hz, 72H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$/d5-pyridine): δ 169.21, 150.19, 150.11, 149.84, 149.71, 144.23, 143.76, 142.68, 141.50, 141.01, 139.41, 133.62, 131.28, 130.82, 129.49, 128.84, 128.06, 127.86, 127.20, 127.06, 125.54, 123.72, 123.57, 122.53, 122.39, 121.83, 121.71, 121.29, 120.38, 120.17, 117.80, 91.62, 91.24, 35.26, 31.88, 31.82 ppm; UV-Vis (THF): λ_{max}(log ε) = 478(5.33), 598(4.60), 628(4.38) nm; HRMS (MALDI): m/z: calcd for $C_{132}H_{132}N_6O_4S_2$: 1958.8260; found: 1958.8244.

2.3 Instruments and measurement

The steady state fluorescence spectra were measured using a Horiba Jobin Yvon Nanolog UV-visible-NIR spectrofluorimeter equipped with a PMT (for UV-visible) and InGaAs (for NIR) detectors. Differential pulse and cyclic voltammograms were recorded on an EG&G 263A potentiostat/galvanostat using a three-electrode system. A platinum button electrode was used as the working electrode, while a platinum wire served as the counter electrode and an Ag/AgCl electrode was used as the reference electrode. Ferrocene/ferrocenium redox couple was used as an internal standard. All the solutions were purged prior to electrochemical and spectral measurements with nitrogen gas. Fluorescence lifetimes were measured using time correlated single photon counting (TCSPC) technique using nanoLED excitation sources. The emission was collected at emission peak maxima of a given compound.

2.3.1 Photovoltaic measurement

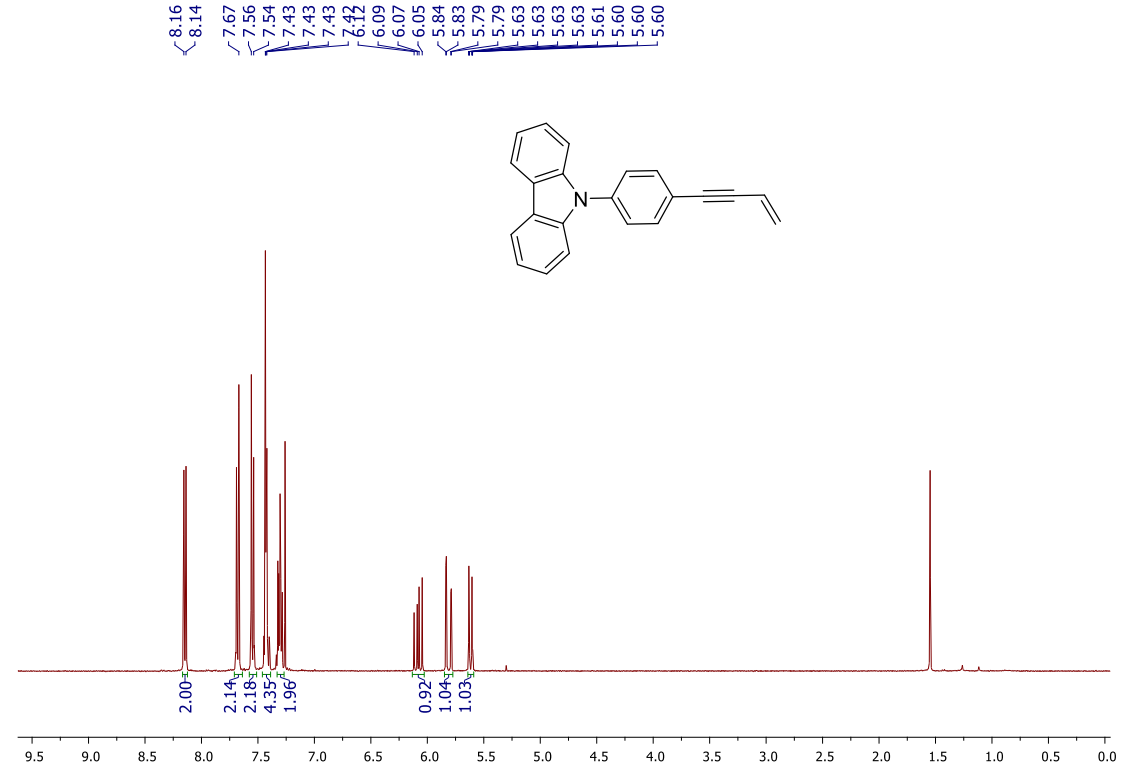
Photovoltaic measurements were performed using the Grätzel-type two-electrode system using FTO (~10-12 microns, tec7 grade from Pilkington) glass coated with thin film TiO2 as the working electrode and Pt-ized FTO as the counter electrode. The thin film TiO2 was prepared via the “Doctor blade” technique as reported earlier. A mediator solution containing 0.6 M PMII ionic liquid, 0.1 M LiI, 0.05 M I2, and 0.5 M 4-t-butylpyridine in acetonitrile was injected between the electrodes.

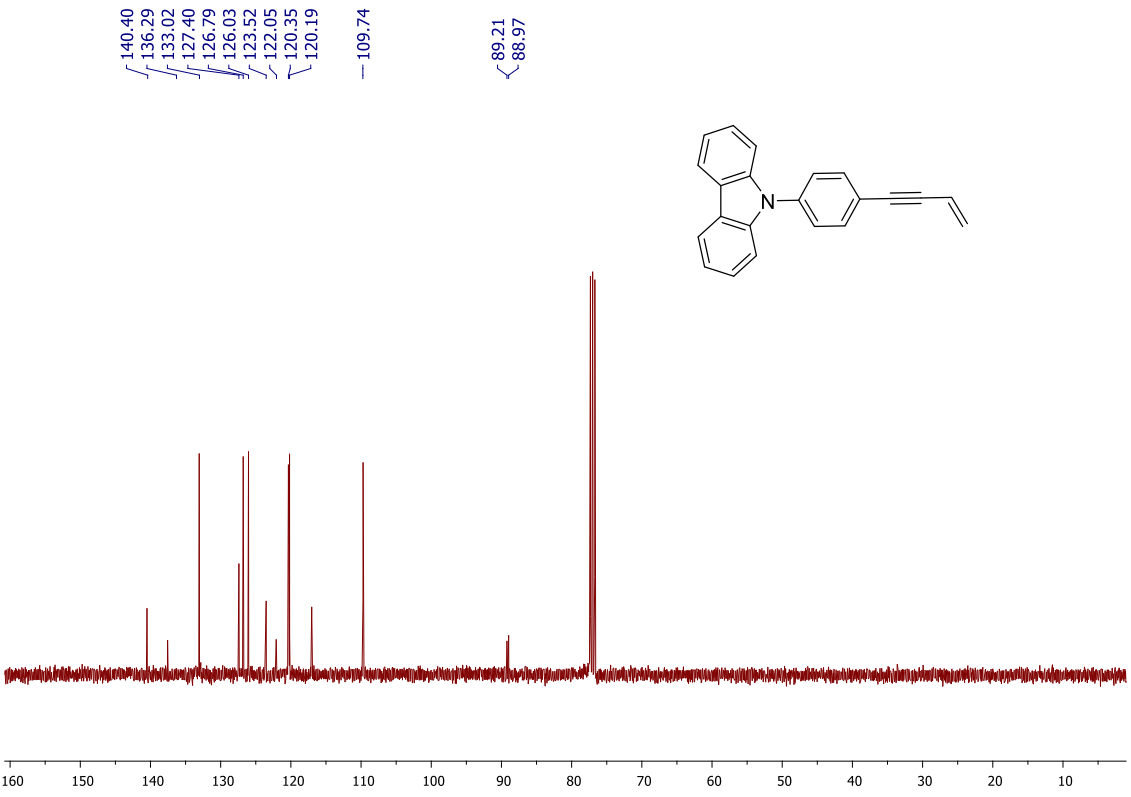
The photocurrent-photovoltage characteristics of the solar cells were measured with a Keithley 2400 source meter and solar simulator (SolarLight, Inc.). IPCE spectra were measured against a calibrated silicon photodiode using monochromatic light from a Xenon lamp (PV Measurements QEX7).

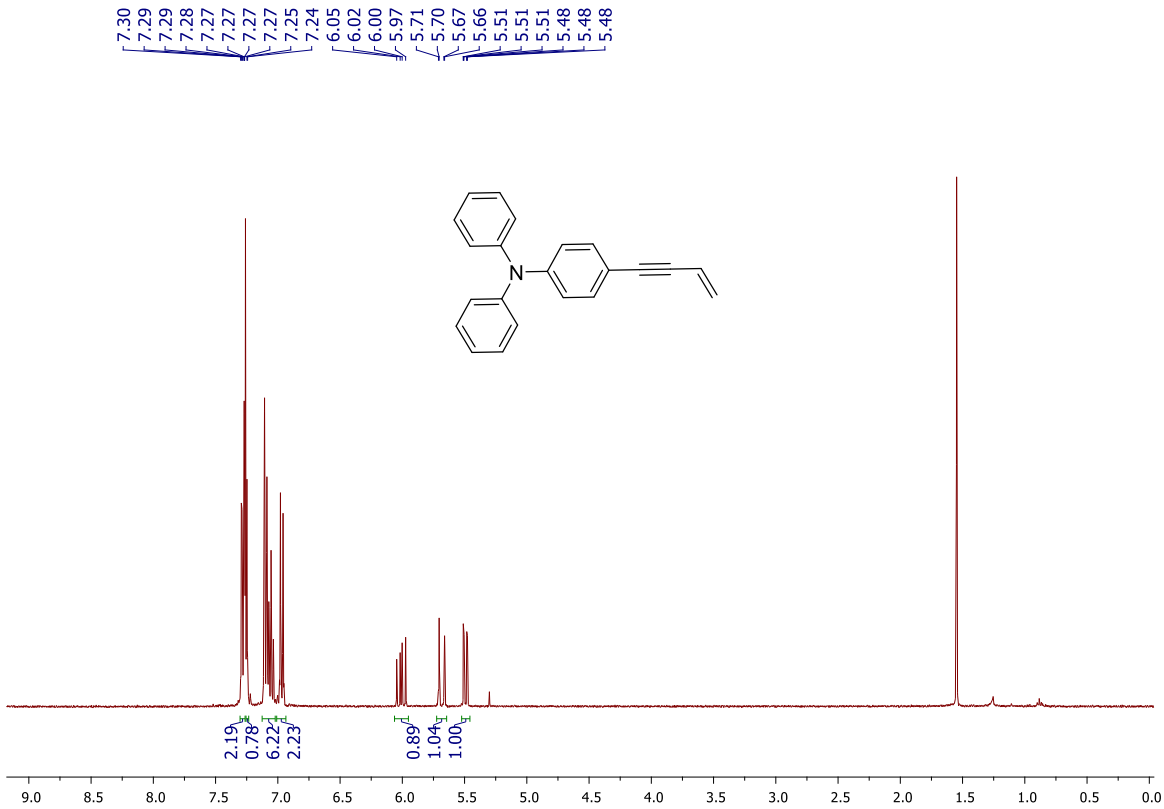
2.3.2 Electrochemical impedance measurement

Electrochemical impedance measurements were performed using EG&G PARSTAT 4000A potentiostat/galvanostat. Impedance data were recorded under forward bias condition from 100 kHz to 10 mHz with an AC amplitude of 10 mV. Data were recorded under dark and A.M 1.5 illumination conditions applying corresponding open circuit potential (VOC). The data were analyzed using ZSimpwin software from Princeton Applied Research. Solution resistance (Rs), charge transfer resistance (Rct), and capacitance due to constant phase element (Q) were deduced from the fitted data. CPE was considered as capacitance component of the double layer electrode interface due to roughness of the electrode.

3. NMR Spectra



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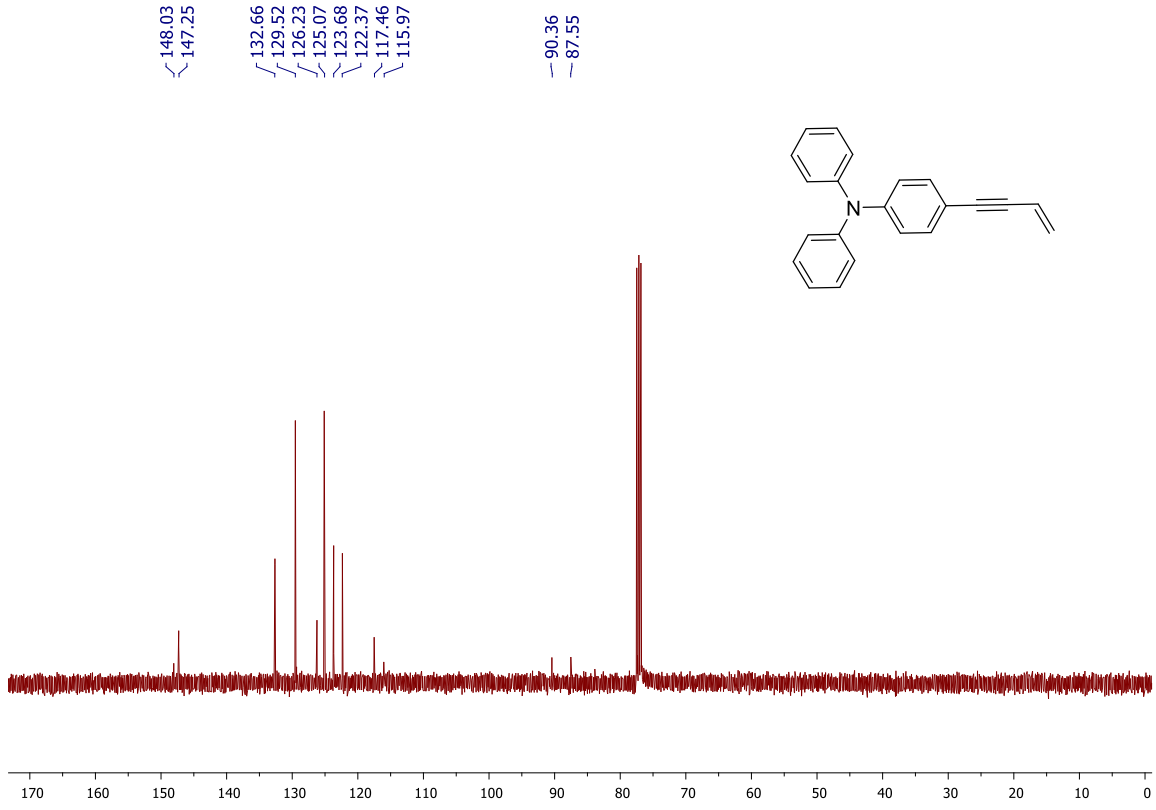
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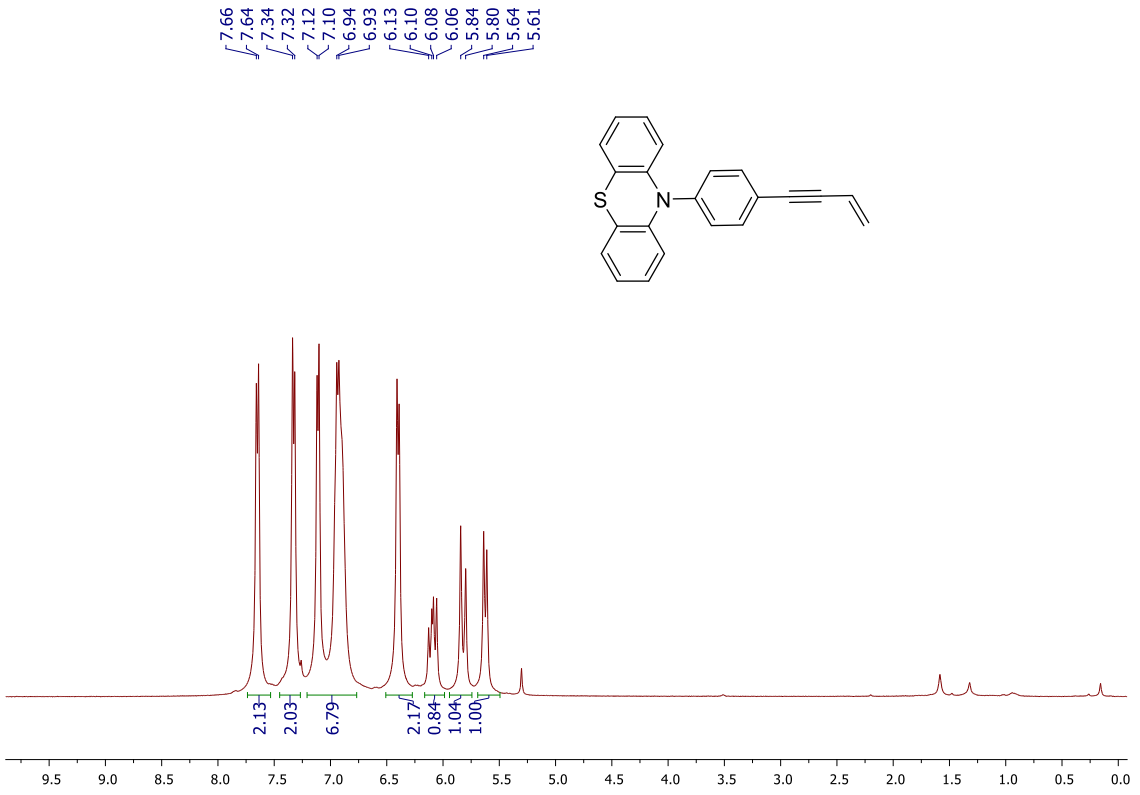
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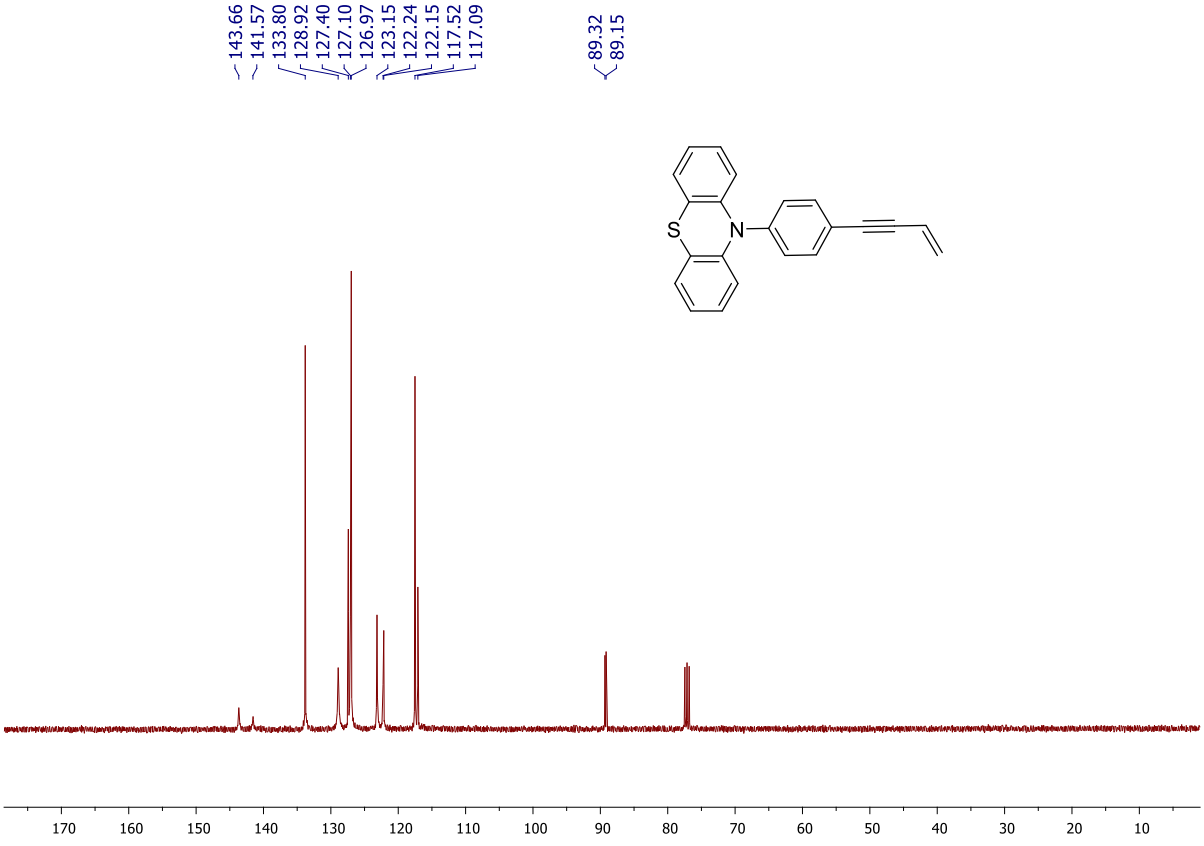
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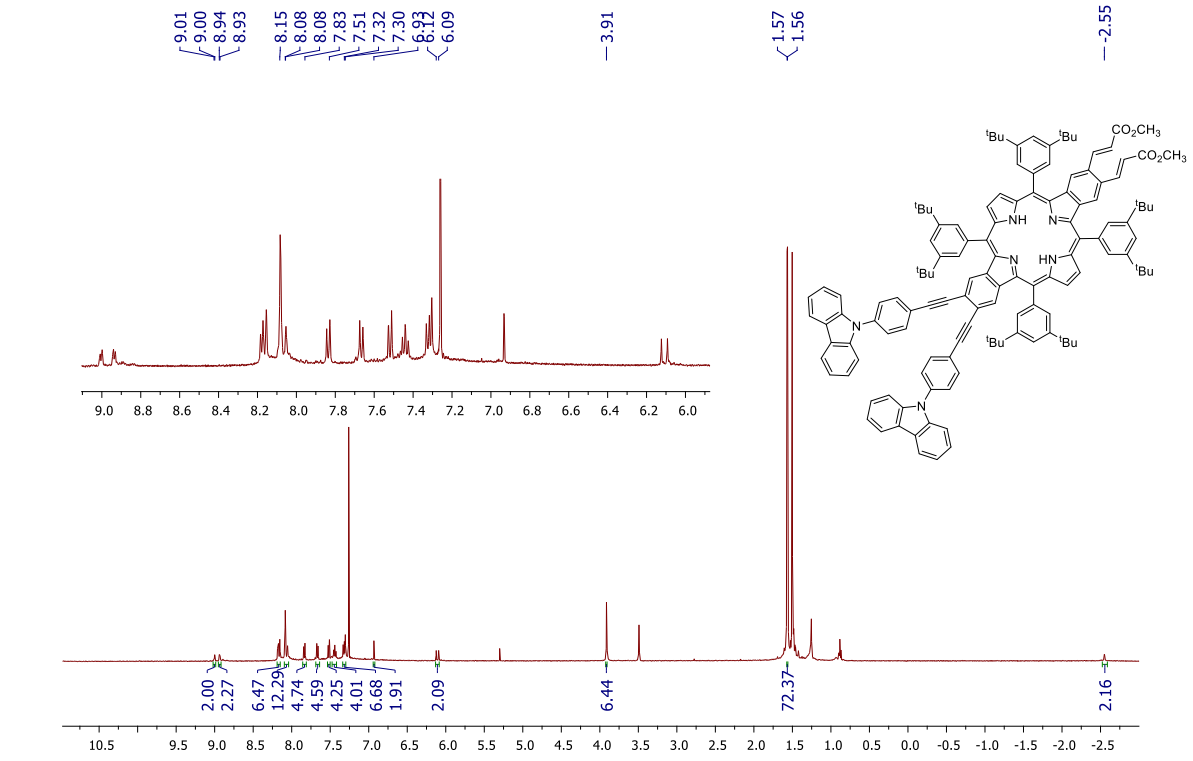
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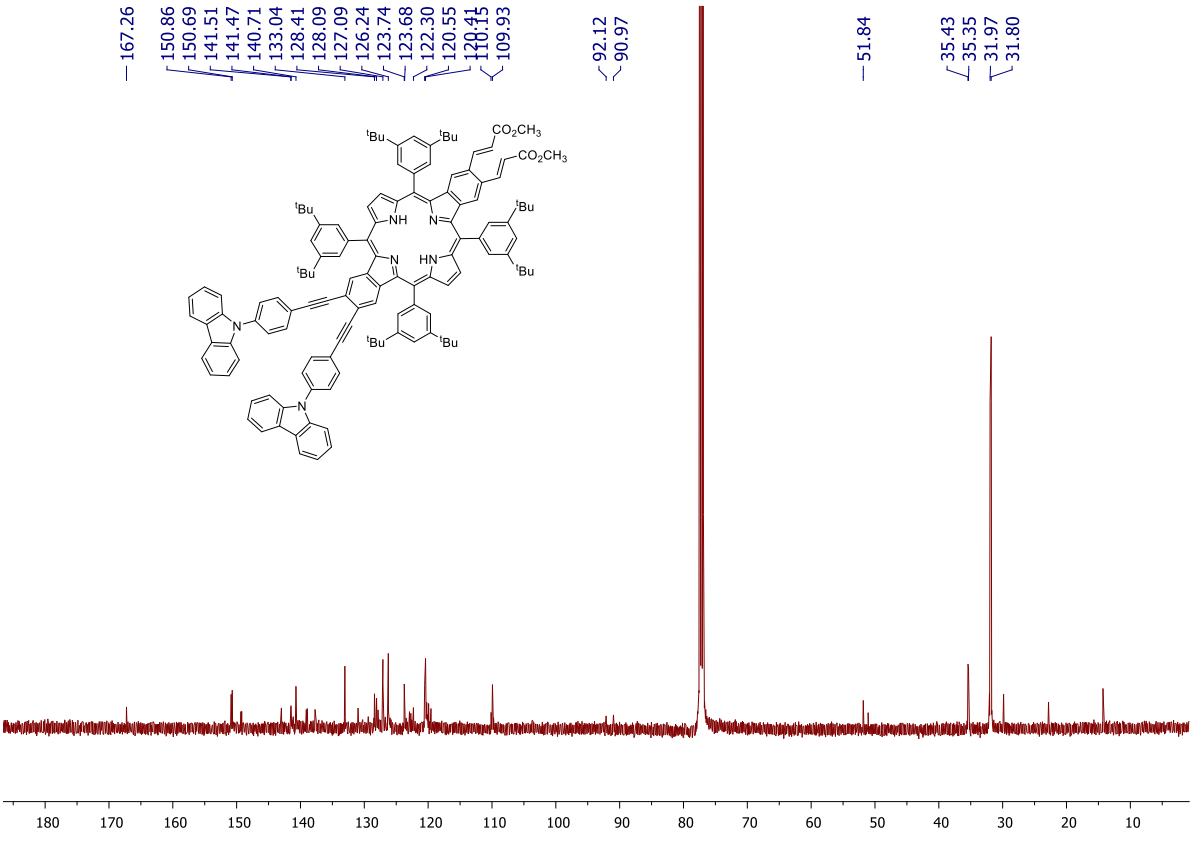
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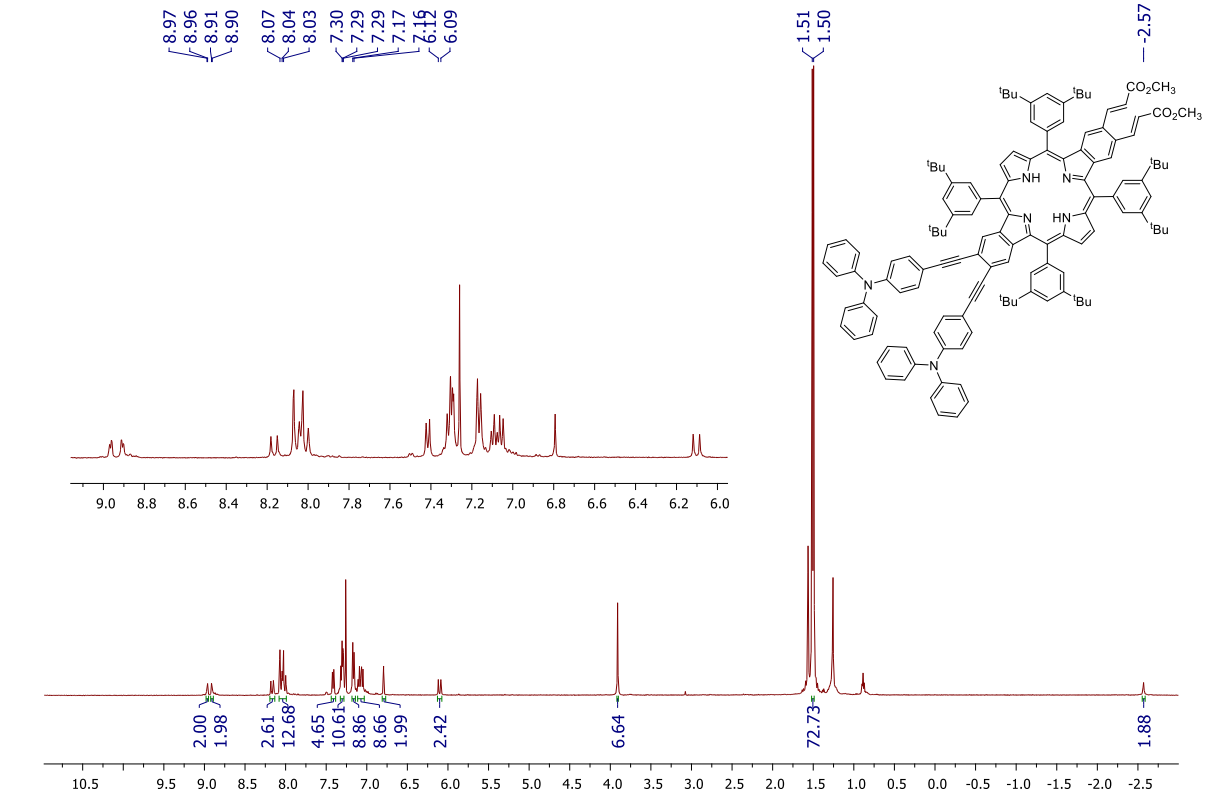
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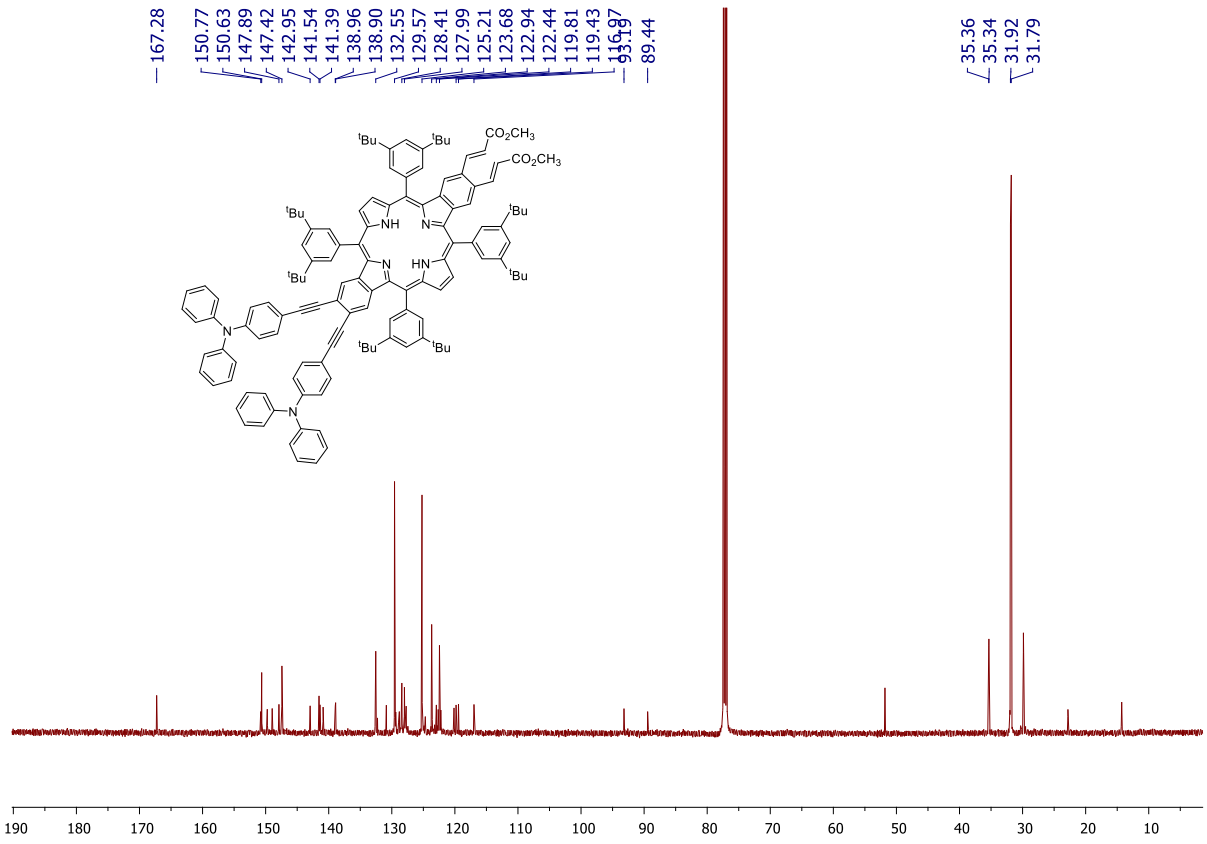
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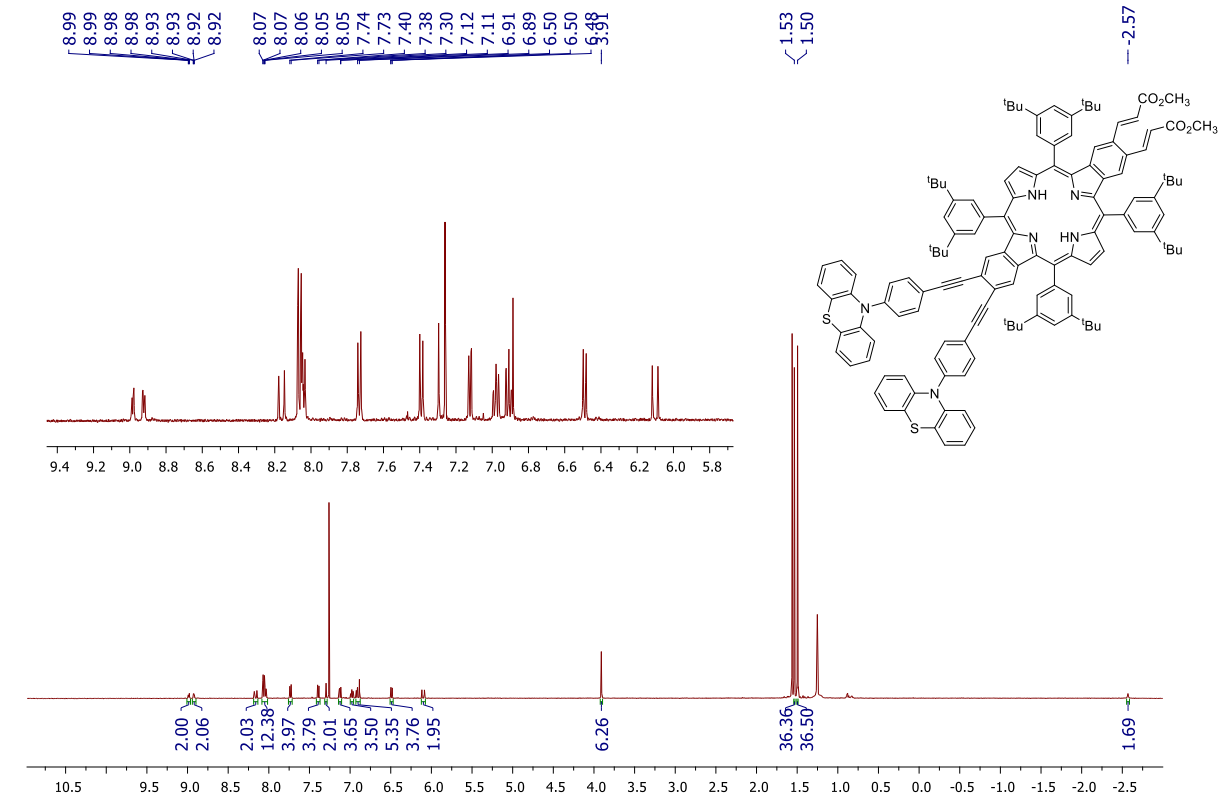
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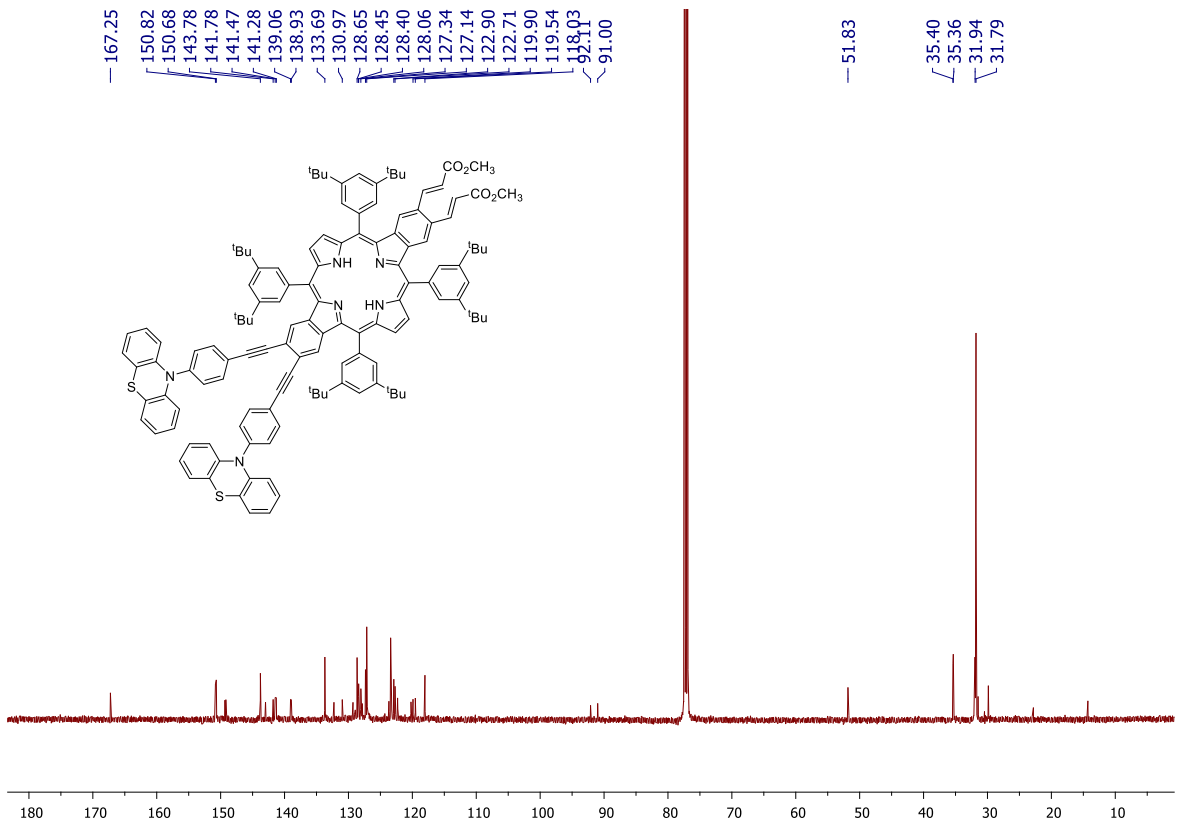
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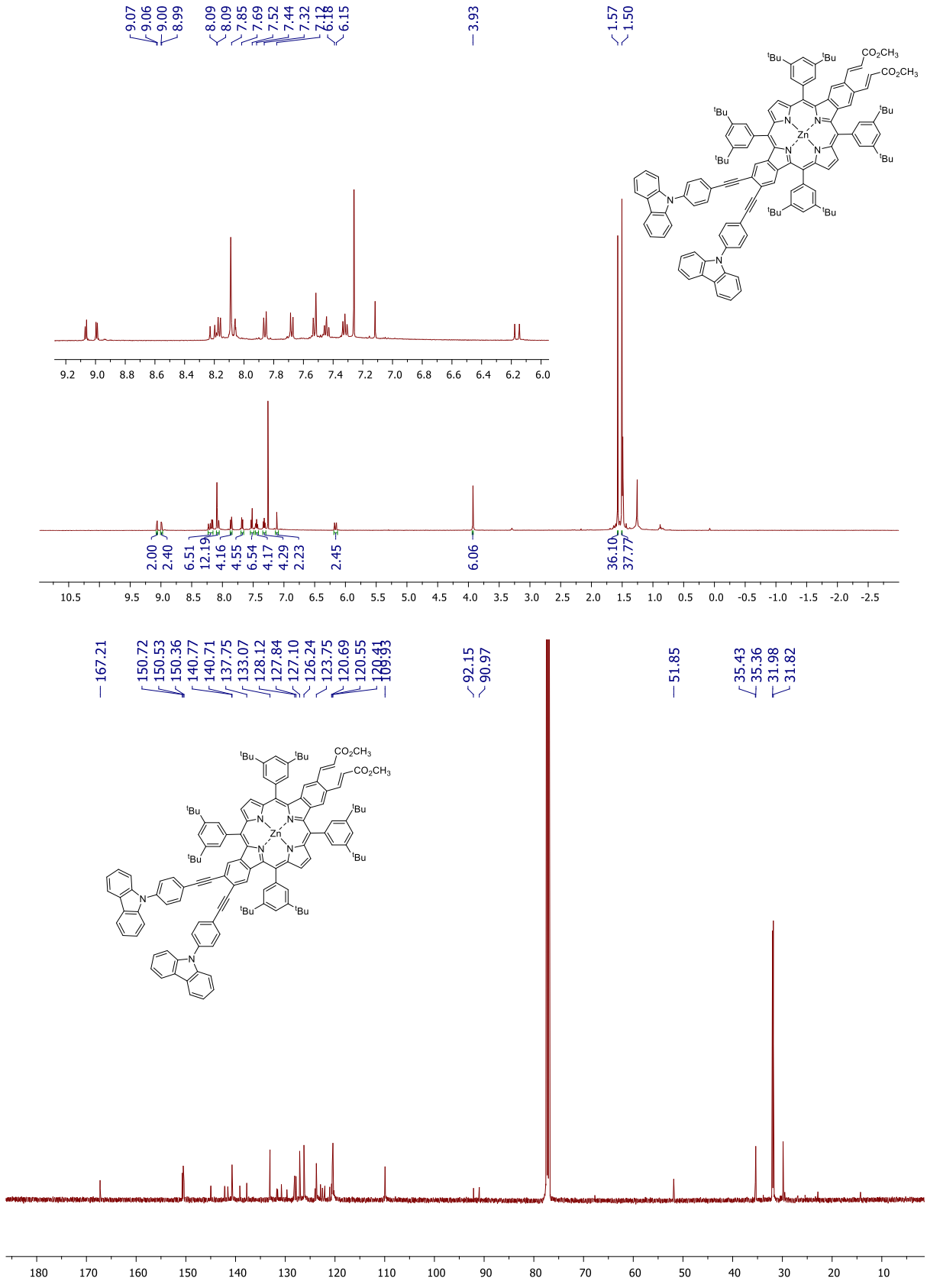
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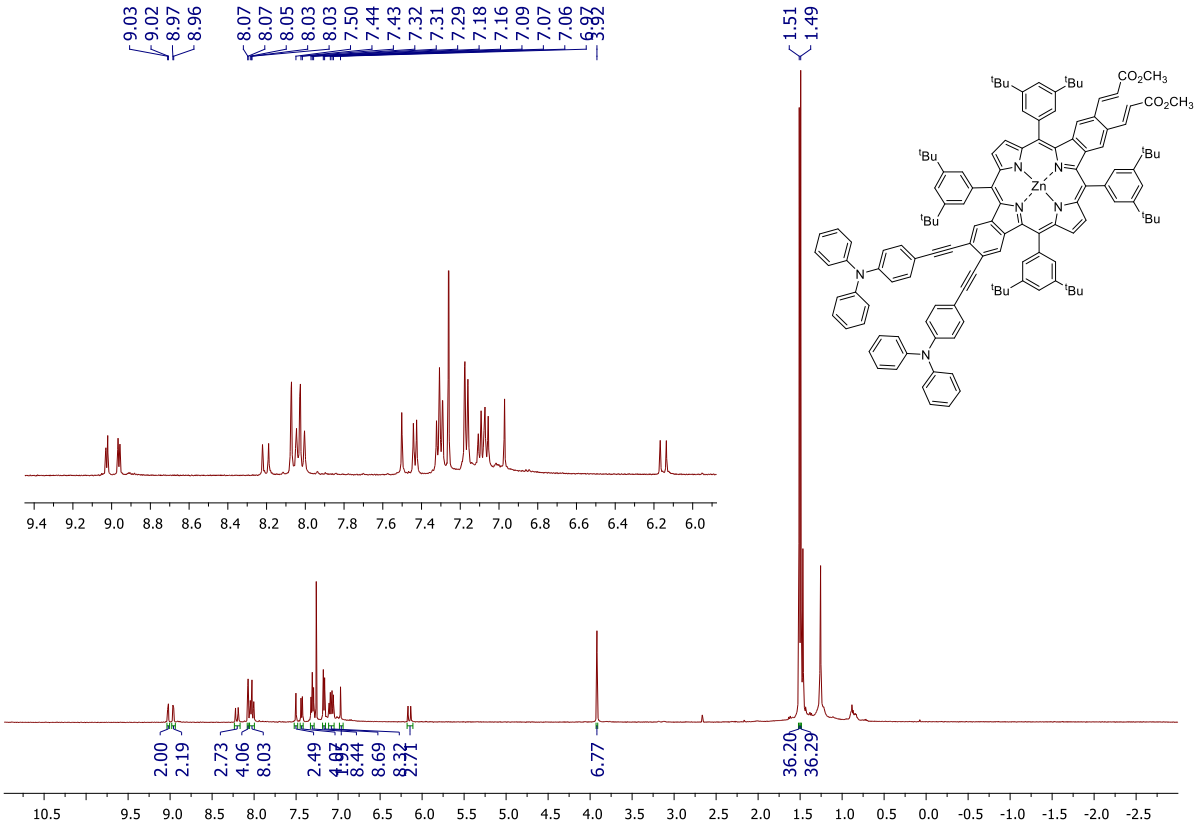
Zn
N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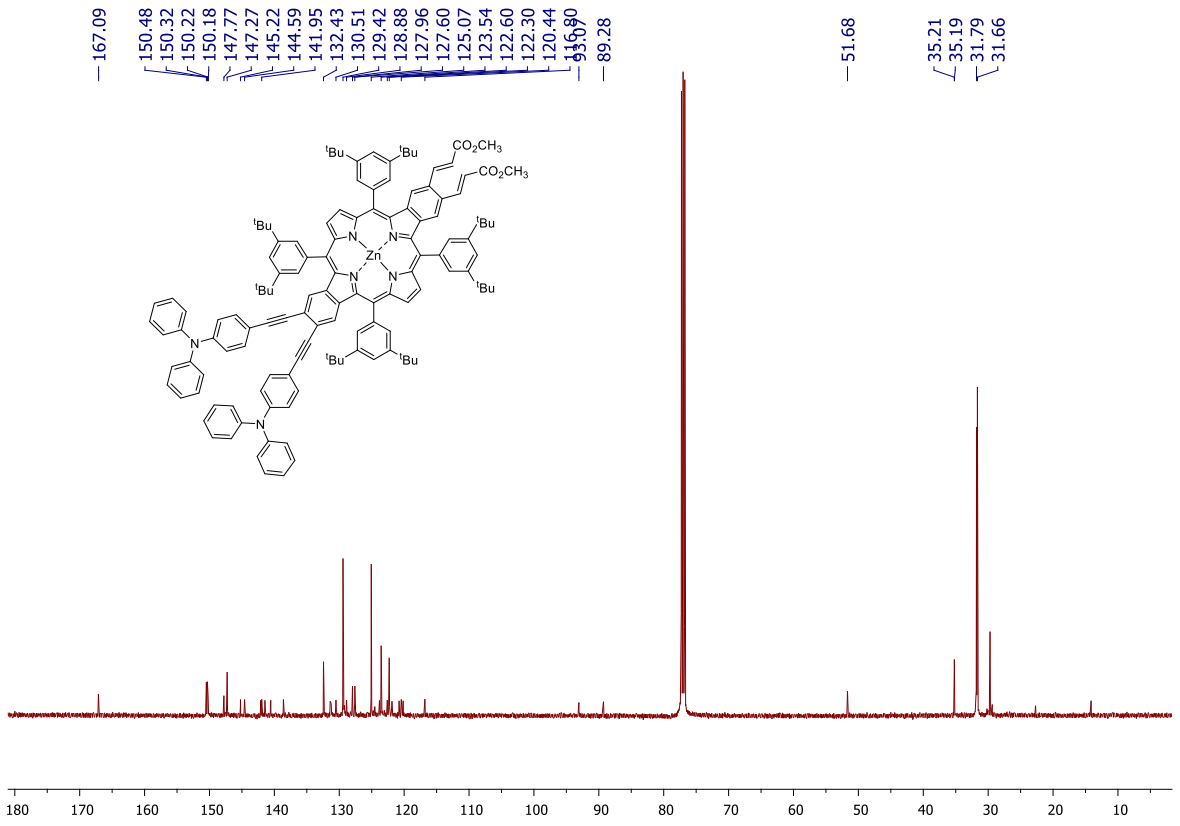
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128.88
127.96
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122.60
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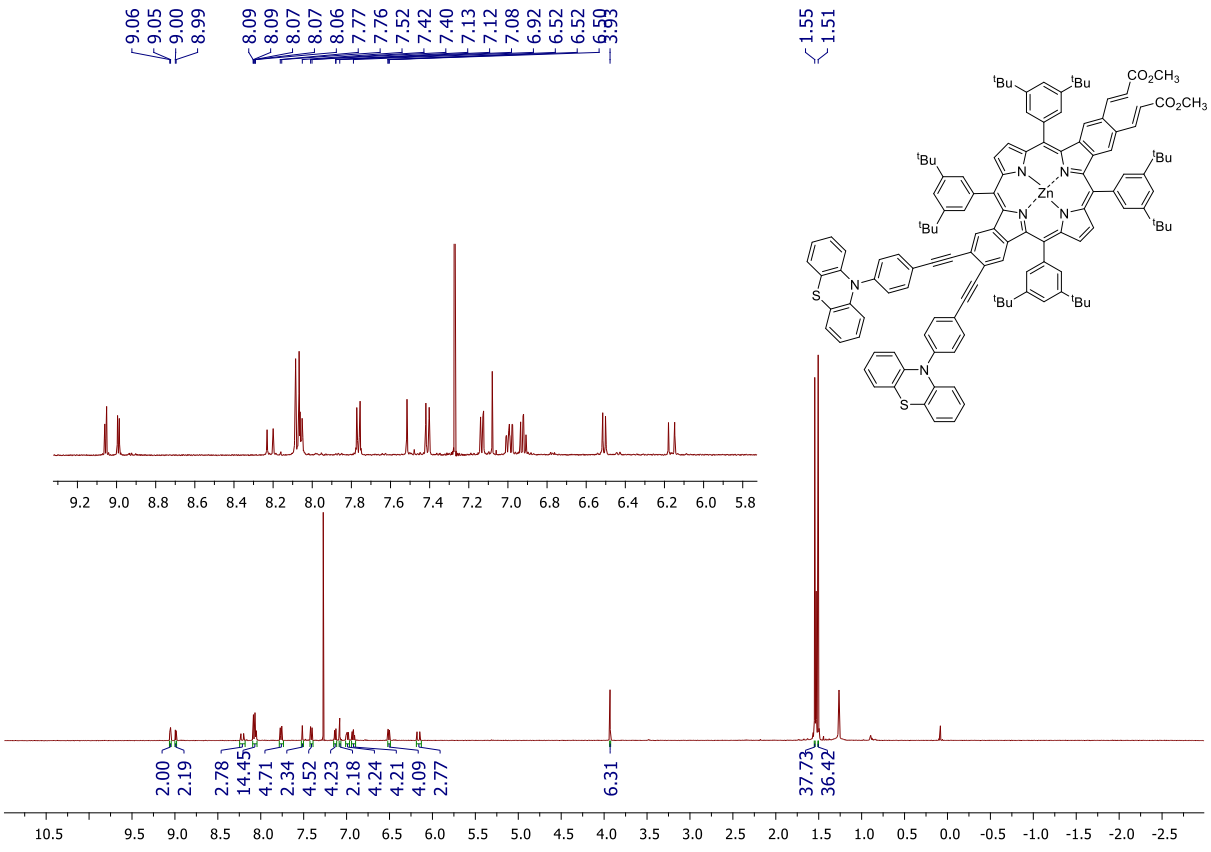
31.66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6.52
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3.93
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1.51
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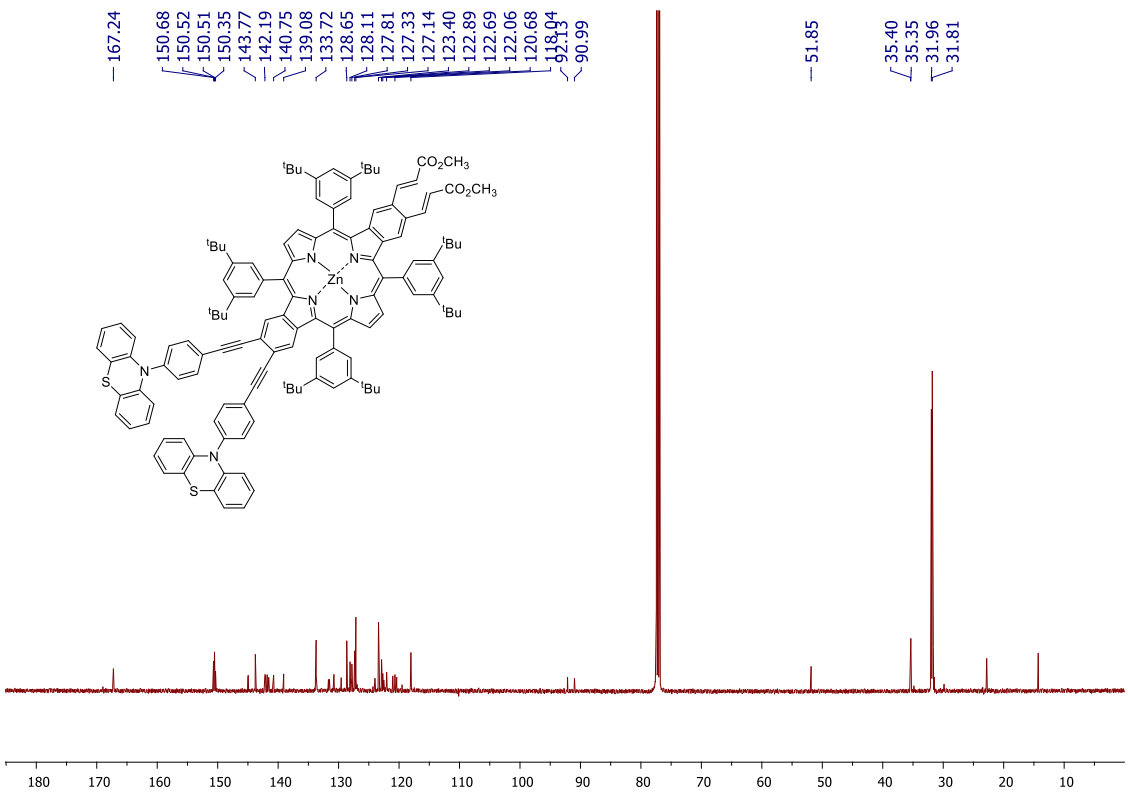
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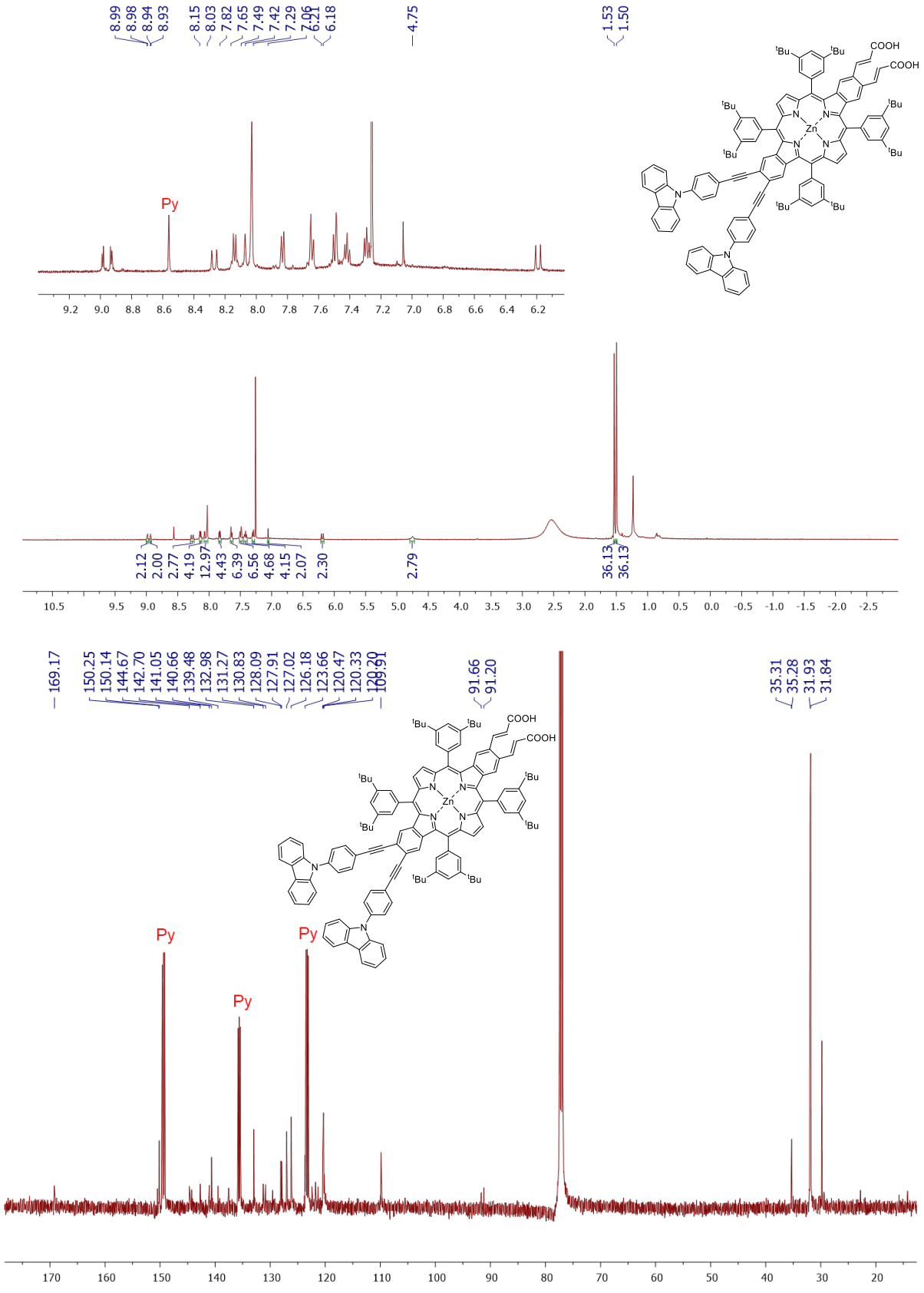
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6.18
4.75
1.53
1.50
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COOH
COOH
Zn
2.12
2.00
2.77
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12.97
4.43
6.39
6.56
4.68
4.15
2.07
2.30
2.79
36.13
36.13
169.17
150.25
150.14
144.67
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128.09
127.91
127.02
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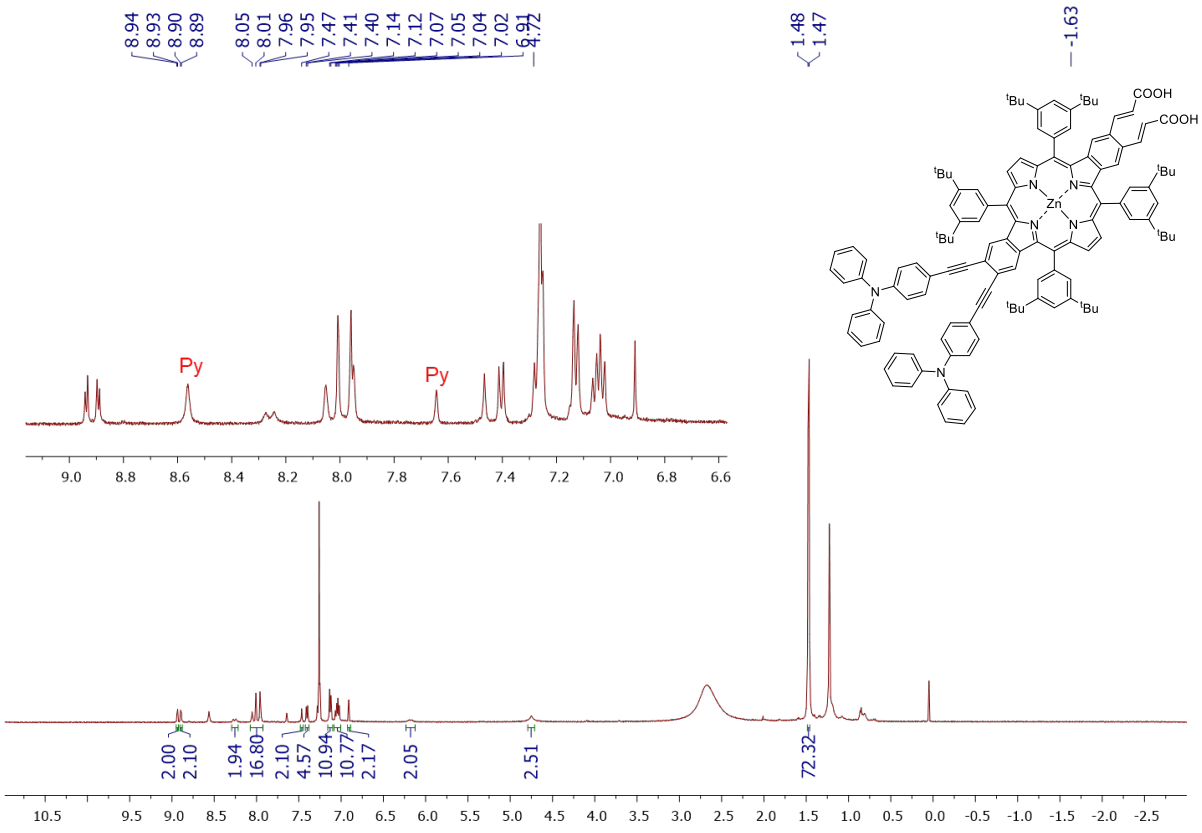
Py
Py
Py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7.07
7.05
7.04
7.02
6.91
6.72
1.48
1.47
-1.63
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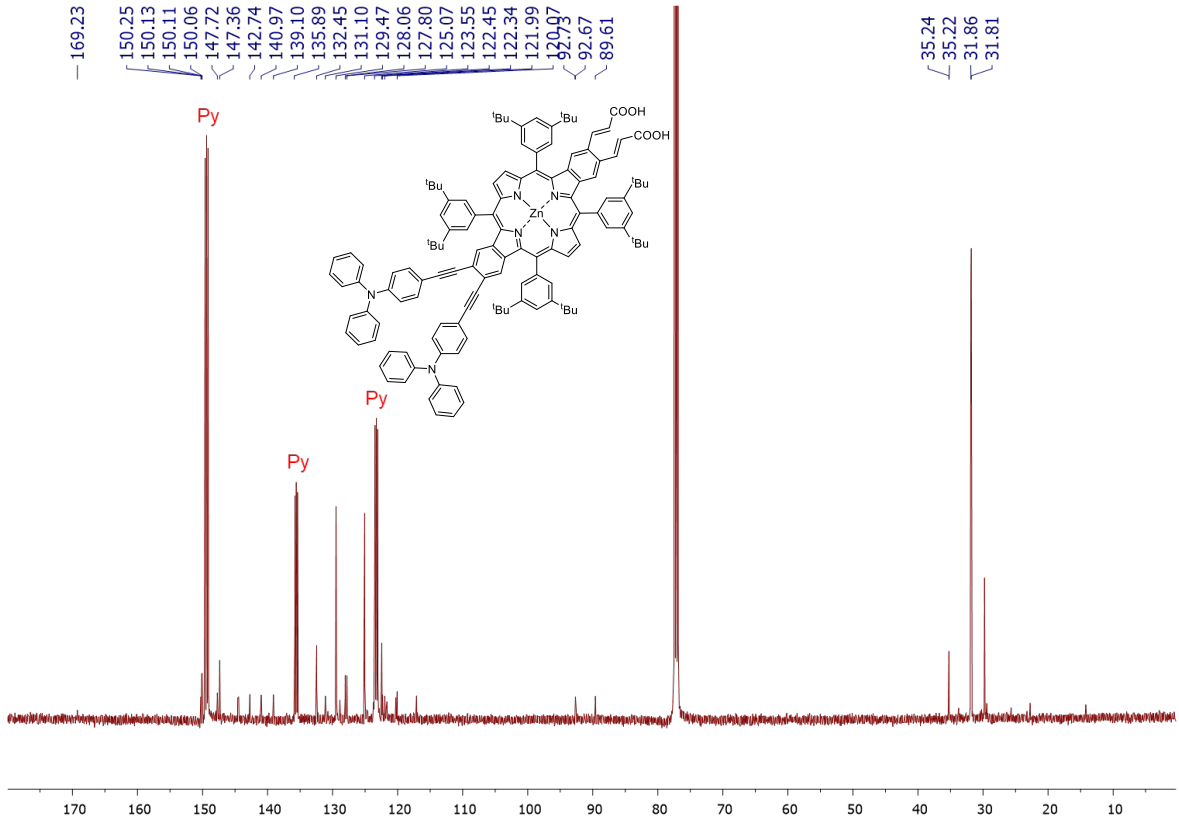
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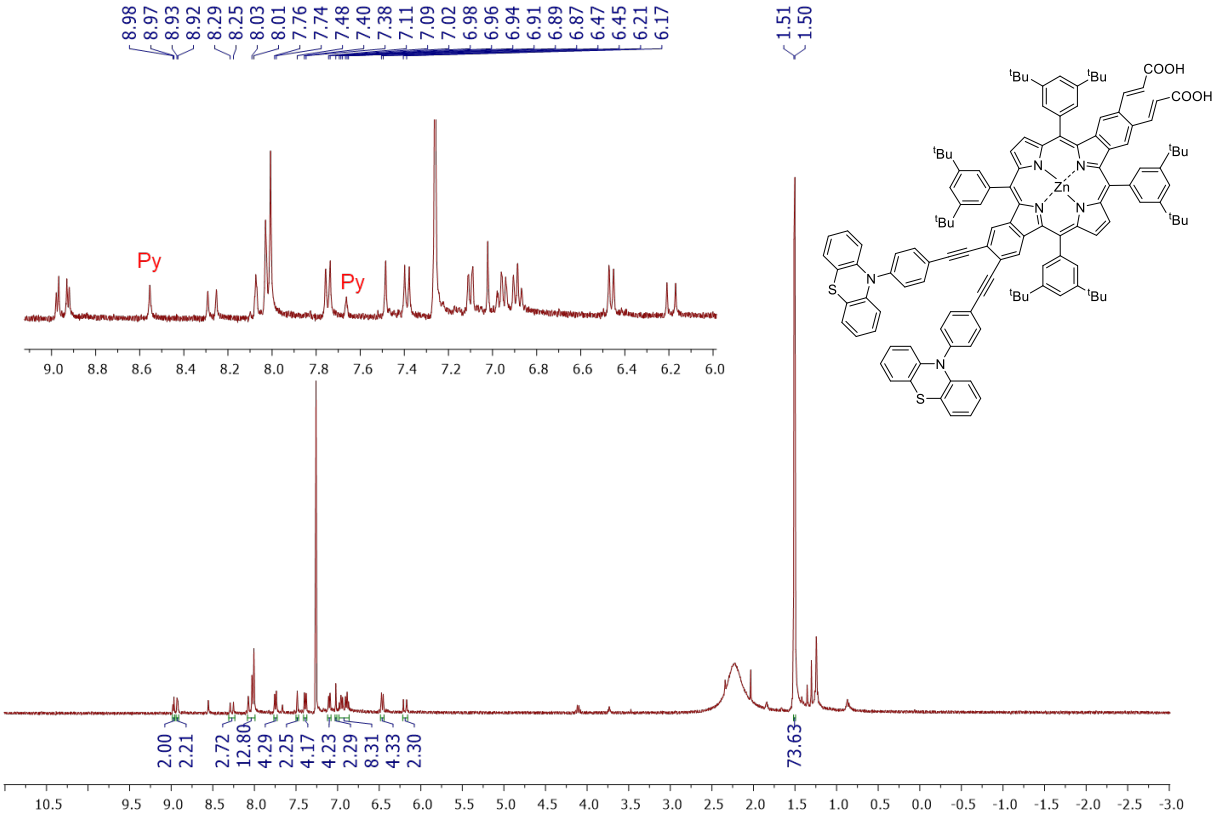
Py
COOH
COOH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6.96
6.94
6.91
6.89
6.87
6.47
6.45
6.21
6.17
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1.50
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Py
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COOH
Zn
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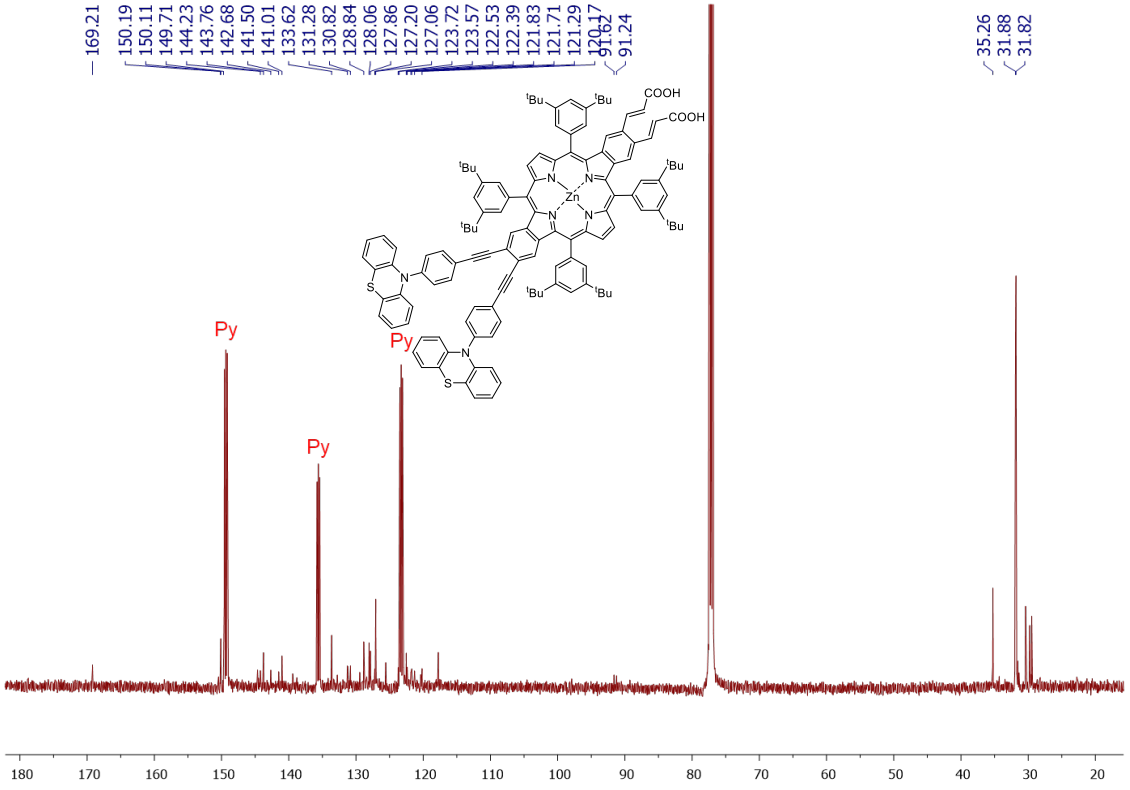
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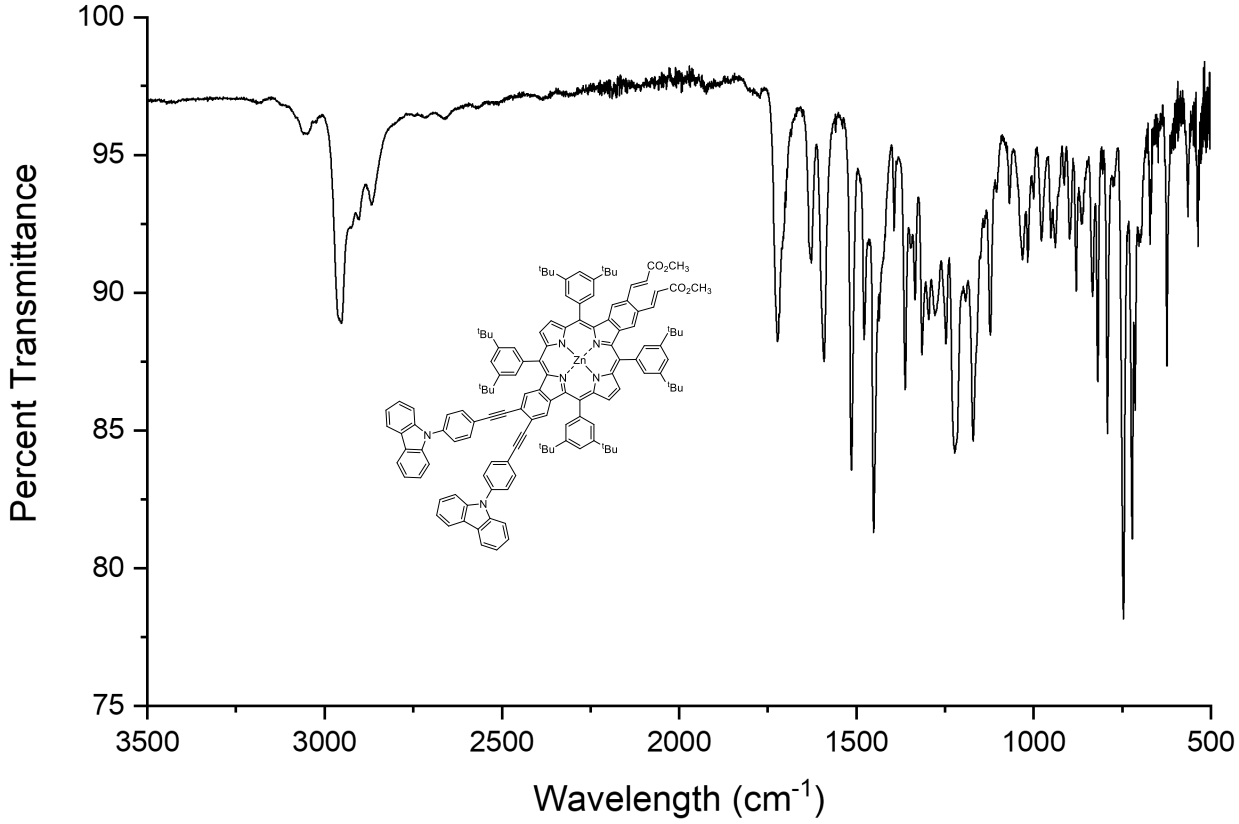
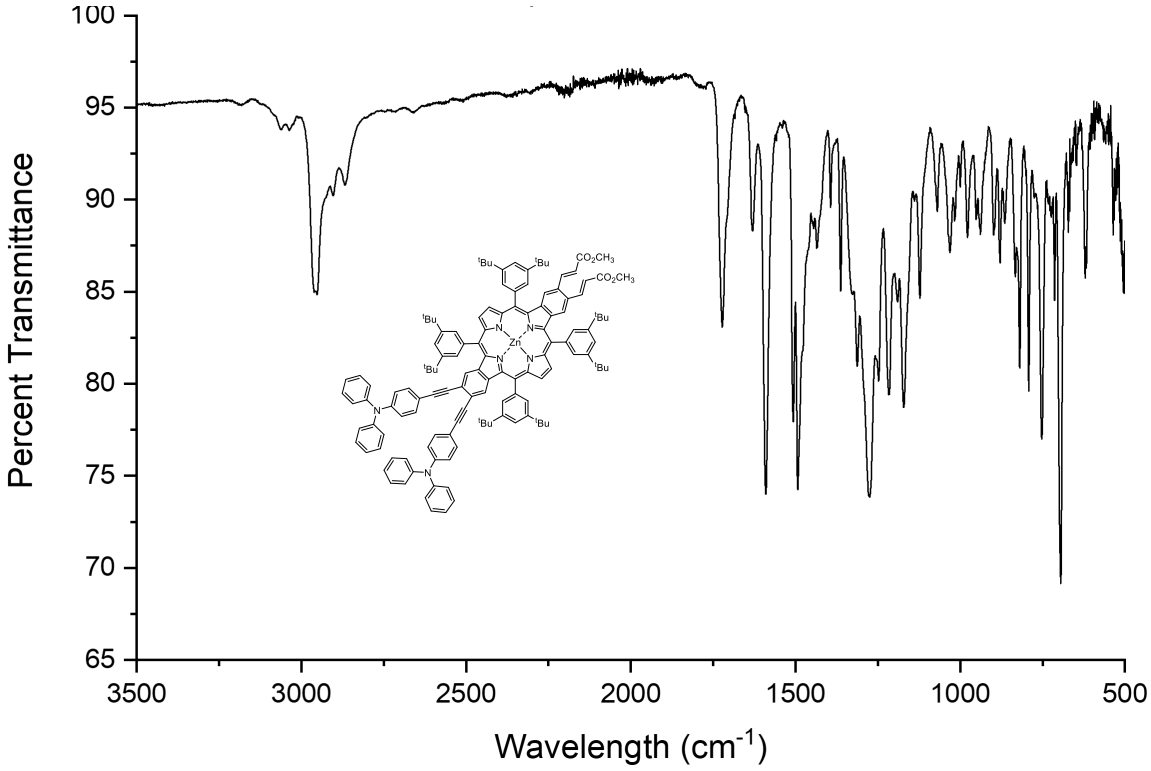
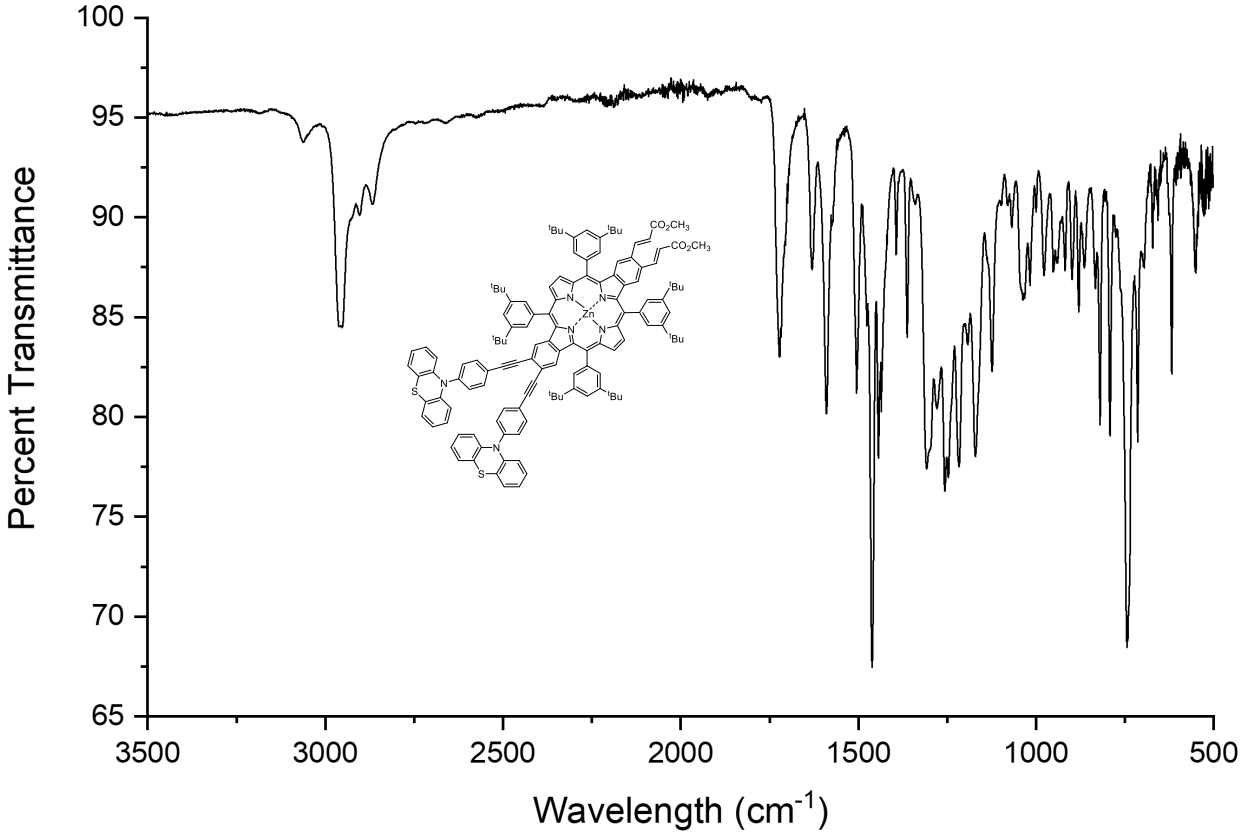
128.06
127.86
127.20
127.06
123.72
123.57
122.53
122.39
121.83
121.71
121.29
120.17
91.62
91.24
35.26
31.88
31.82
Py
Py
Py
COOH
COOH
Zn

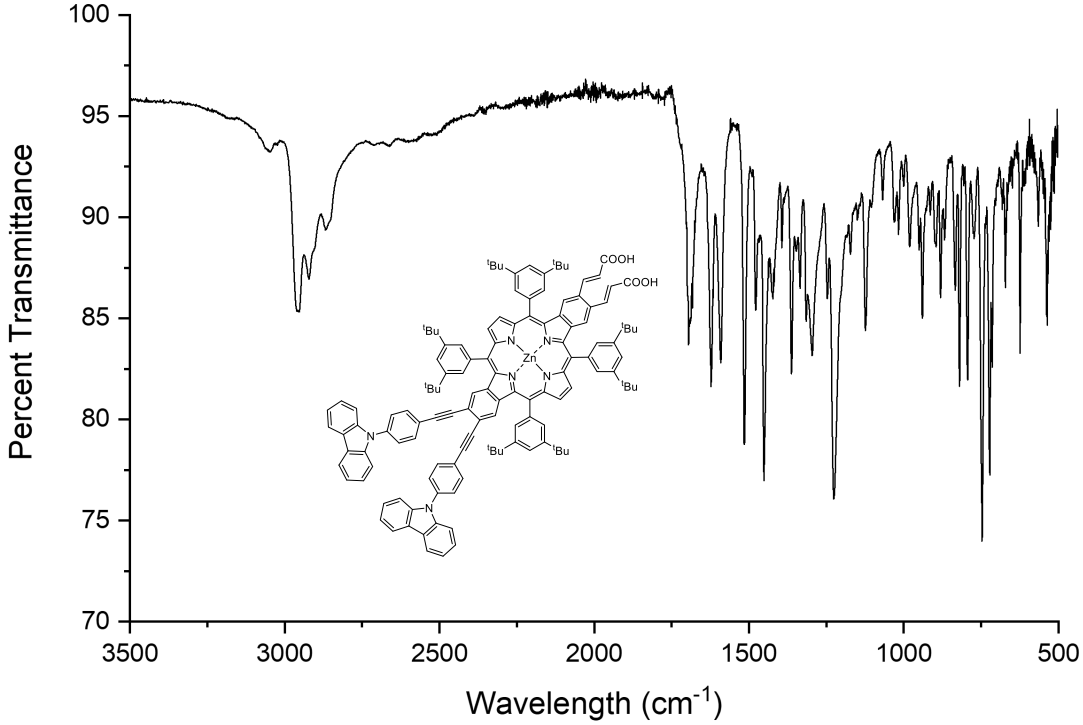
4. IR Spectra


Percent Transmittance
100
95
90
85
80
75
3500
3000
2500
2000
1500
1000
500
Wavelength (cm-1)

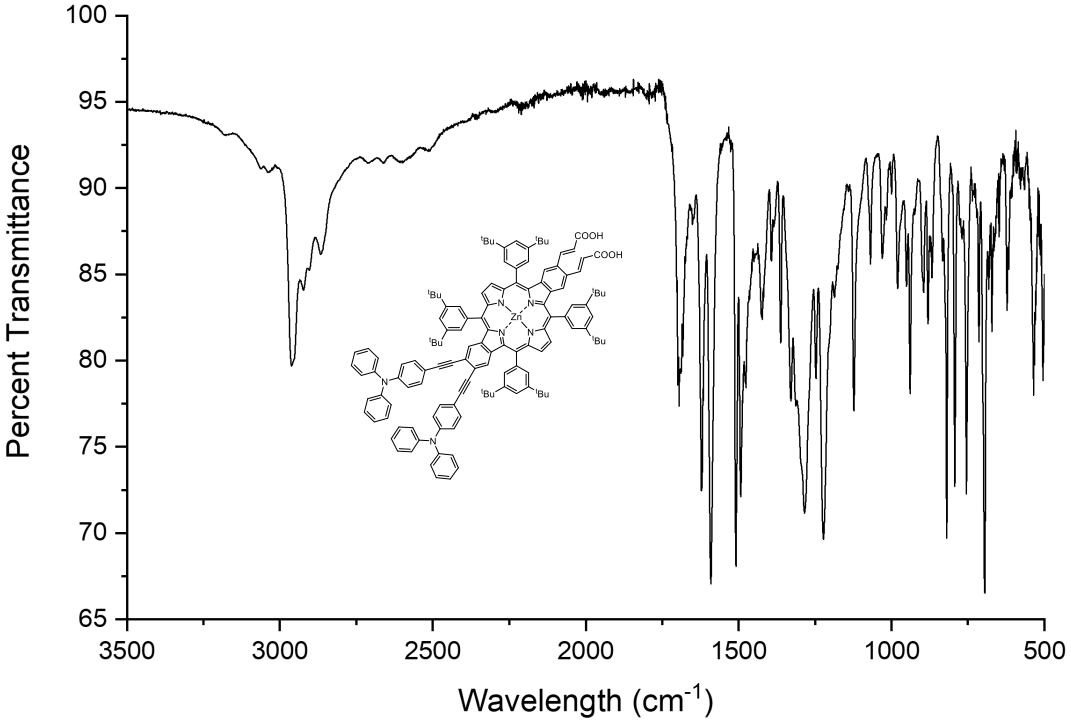

Percent Transmittance
100
95
90
85
80
75
70
65
3500
3000
2500
2000
1500
1000
500
Wavelength (cm-1)



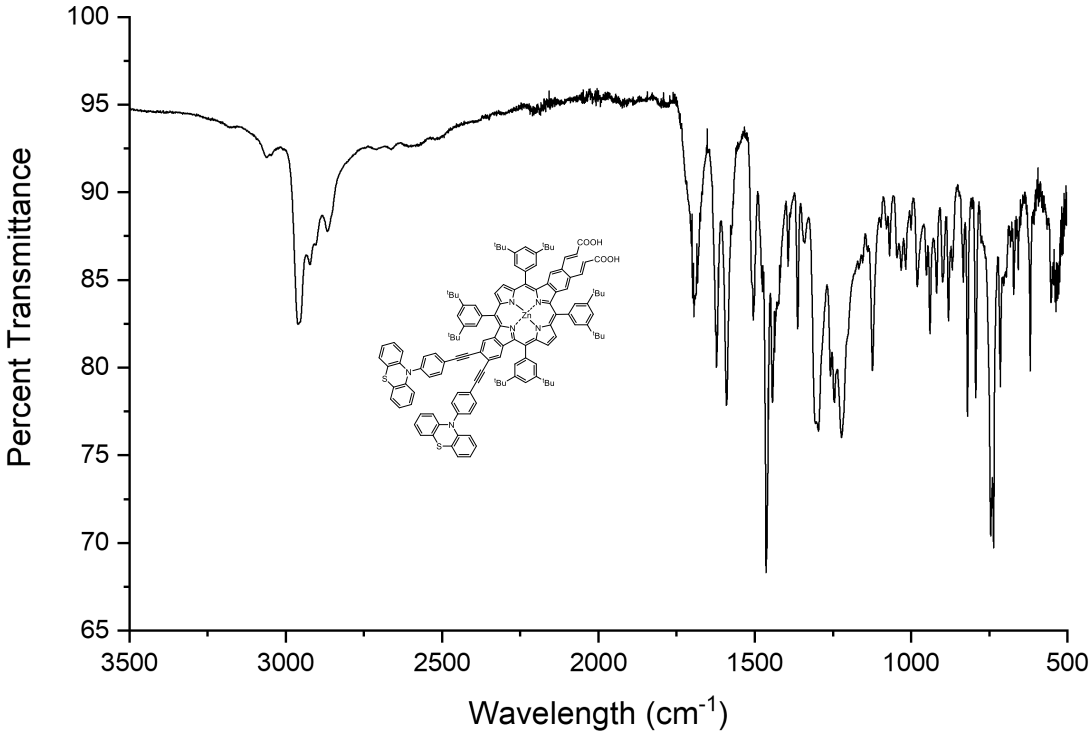
IR Spectrum of **YH8**



IR Spectrum of **YH9**



IR Spectrum of **YH10**



5. Atom Coordinates for Optimized (in Vacuo) Structures **YH8** – **YH10**

Atom coordinates for optimized structure **YH8**

	X	Y	Z
C	-1.22551100	-0.75195600	0.27496400
C	-1.21628600	0.66345800	0.28489000
C	0.18725900	1.06346500	0.39134800
N	0.98136700	-0.05922800	0.38190700
C	0.17368000	-1.17147900	0.36698100
C	3.78593700	-4.24933700	0.32964800
C	2.43871700	-4.24424600	0.51223800
C	1.99933400	-2.87435900	0.40964200
N	3.09135700	-2.05389700	0.20605800
C	4.19297200	-2.88162000	0.12439100
C	0.64632400	-2.49180900	0.45837300
C	7.39292800	0.63281400	-0.41530200
C	7.34984400	-0.77028400	-0.57846000
C	5.98251300	-1.18351300	-0.26516700
N	5.21800000	-0.06716000	-0.02722800
C	6.02829500	1.04489000	-0.07682900
C	5.52082300	-2.50489600	-0.14363400
C	2.48122200	4.09728800	0.73489000
C	3.83652400	4.09086800	0.63195700
C	4.24079000	2.72698200	0.39337000
N	3.12496000	1.91318600	0.37241800
C	2.03335400	2.73883000	0.55456200
C	0.67457700	2.37283300	0.53456400
C	5.57921200	2.35265600	0.16905800
C	-0.34145000	-3.60805600	0.63981100
C	6.50694400	-3.63210700	-0.25735300
C	6.56301900	3.48946600	0.19007200

C	-0.30263200	3.49902800	0.71722700
C	-0.93964100	-3.81291900	1.88853900
C	-1.86945300	-4.84076900	2.08679400
C	-2.16937700	-5.66482200	0.99184700
C	-1.58267200	-5.49998500	-0.27124300
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C	-0.60406200	4.35883600	-0.34553100
C	-1.51056800	5.41540700	-0.18703600
C	-2.09949700	5.58155400	1.07490200
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C	8.01534800	4.99085000	1.45155300
C	7.13539500	3.89761900	1.39513000
C	7.34989700	-3.93371000	0.81846300
C	8.29339800	-4.96445500	0.73147200
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C	6.58768000	-4.38727700	-1.43325000
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C	9.68172700	-0.77237700	-1.27100800
C	8.48212200	-1.45390300	-1.02747200
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C	7.36581700	-7.75639600	-2.51137400
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C	-2.09796200	3.96010000	4.58454800
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C	8.92120200	4.28992400	3.72770300
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C	11.39648700	2.79424400	0.58700500
O	12.24888400	3.80773200	0.91169200
O	10.64182000	2.30377100	1.40414100
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C	13.07606500	-2.37103300	-2.14516500
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H	7.70028600	4.43275200	-3.69852200
H	7.99427700	8.08634100	-3.01010400
H	8.22381400	7.99822100	-1.25966200
H	6.64426700	7.62168800	-1.95959600
H	9.94658600	6.48265500	-3.39119500
H	9.97478100	4.90112000	-2.58803000
H	10.21851400	6.37610600	-1.64722900
H	9.61839100	3.60034900	3.24381600
H	8.03485800	3.71849300	4.01773400
H	9.37573300	4.66213500	4.65245200
H	9.64035200	7.28105100	2.11543000
H	10.60918200	5.80312000	2.05290000
H	10.26196800	6.58491100	3.60711200
H	7.22481200	7.21250800	2.87291400
H	7.84280000	6.71366400	4.45920600
H	6.57271100	5.76916100	3.66235700
H	-3.76427900	-7.03338500	-2.51039600
H	-3.76967200	-5.34461200	-1.97019000
H	-4.06690600	-6.65086500	-0.81176200
H	-1.86204300	-8.59532600	-1.83785900
H	-2.11687600	-8.22699300	-0.12725500
H	-0.51840000	-7.99927800	-0.84722800
H	-1.52351800	-6.80973800	-3.51725600
H	-0.13815700	-6.18112500	-2.62083400
H	-1.46618000	-5.09925900	-3.08202900
H	-2.56393800	-7.27545600	3.24467100
H	-2.73308400	-6.69301900	4.90526000
H	-1.15725000	-6.62575100	4.09634300

H	-4.49073500	-5.67994900	2.55008800
H	-4.35956500	-3.94907500	2.88004100
H	-4.61033100	-5.09270500	4.21270000
H	-2.35251300	-3.04201900	4.22835800
H	-1.04437000	-4.13809600	4.71309900
H	-2.64112800	-4.28033000	5.45388600
H	-9.63065900	8.54761500	-3.66185700
H	-8.87447200	6.51370600	-2.46466600
H	-13.59444400	8.13733400	-2.03476000
H	-11.95862200	9.36155300	-3.44634700
H	-14.88265100	6.35661700	-0.34135100
H	-15.48110700	4.49181300	1.18573300
H	-13.78286400	2.81626100	1.84584000
H	-11.46135000	2.94702700	0.98826100
H	-8.29159300	5.98672400	-0.01176500
H	-10.33543300	2.42698400	-1.27292000
H	-8.24080100	1.12645100	-1.00483300
H	-6.18343200	4.69972100	0.21305300
H	-10.49109000	-2.34621500	0.30098600
H	-8.35027500	-1.09548700	0.36060800
H	-8.37145400	-5.93060700	-0.74801300
H	-6.22414200	-4.69624800	-0.64031300
H	-11.31056500	-2.79502000	-2.09952100
H	-13.49367500	-2.58599400	-3.25405800
H	-15.30423700	-4.22818700	-2.86265600
H	-14.95869200	-6.13685400	-1.31191500
H	-13.94874600	-7.98516300	0.49463600
H	-12.54586600	-9.27702500	2.08544300
H	-10.25053300	-8.52634300	2.62954500
H	-9.29439900	-6.48992500	1.58968100

H	1.83720000	4.94483800	0.90983800
H	4.50663700	4.93296600	0.70479900
H	4.45029500	-5.09943400	0.33544500
H	1.79448800	-5.08993300	0.69503300
H	-2.43367100	2.45433700	0.12888700
H	-2.47051800	-2.52444000	0.12338000
H	8.64830300	2.39349000	-0.52046100
H	8.45762800	-2.51983000	-1.20096700
H	12.10709000	3.98048200	1.85715300
H	14.91132000	-2.69044800	-2.34232000
H	-2.80223100	6.39694300	1.21502400
H	-0.12270700	4.18132300	-1.29958700
H	-0.65362300	3.02457000	2.77028100
H	6.40006400	3.85370500	-1.91208000
H	8.98899000	6.48843600	0.26616100
H	6.87946900	3.35300200	2.29677600
H	5.91928700	-4.13783500	-2.24866500
H	7.26364500	-3.33795000	1.71910800
H	9.08971000	-6.48288800	-0.55556800
H	-0.18391500	-4.27794700	-1.38301900
H	-2.88636800	-6.46807900	1.12921800
H	-0.67291900	-3.14516600	2.69887900
H	10.53144800	-2.58395400	-2.08009000
H	11.29743400	1.17001400	-2.46111800
H	12.39747600	2.90272400	-1.33290200
H	12.55628400	-0.44319700	-1.24797500

Atom coordinates for optimized structure **YH9**

	X	Y	Z
C	-1.28387500	-0.72467100	0.42813000
C	-1.28247300	0.68932800	0.47950800

C	0.11683900	1.09318400	0.62955500
N	0.91740800	-0.02515100	0.60385200
C	0.11459300	-1.14107800	0.55189200
C	3.74599900	-4.19724800	0.67124400
C	2.39304800	-4.19940700	0.80737900
C	1.94659900	-2.83555800	0.65534000
N	3.03595400	-2.01243700	0.46368000
C	4.14762400	-2.83265400	0.43562300
C	0.58919300	-2.45889000	0.65743900
C	7.25259600	0.70204800	-0.39451600
C	7.24882500	-0.70868900	-0.42727800
C	5.90884700	-1.12845200	-0.03126200
N	5.12899000	-0.01396400	0.16721800
C	5.91099000	1.10749500	0.01592500
C	5.47227100	-2.45065100	0.16953000
C	2.40125500	4.12980000	1.04360100
C	3.75177800	4.13561000	0.88494700
C	4.14980100	2.78498400	0.57471400
N	3.03850000	1.96406400	0.57643600
C	1.95214200	2.77585900	0.82530200
C	0.59447700	2.40059300	0.81783100
C	5.47199100	2.41879300	0.27460100
C	-0.39921500	-3.57763100	0.81625500
C	6.48791900	-3.55647500	0.13462400
C	6.47827700	3.53289100	0.24725700
C	-0.39104900	3.50748400	1.05707500
C	-1.04928800	-3.76330800	2.04190400
C	-1.98315700	-4.79114400	2.21846800
C	-2.23418000	-5.63462400	1.12609000
C	-1.59520700	-5.48930800	-0.11371600

C	-0.67097000	-4.44514600	-0.24860000
C	-0.67638700	4.43811300	0.05064500
C	-1.59784900	5.47240800	0.26109900
C	-2.21775200	5.54376000	1.51710800
C	-1.95221600	4.63581800	2.55276900
C	-1.02400200	3.61871000	2.30056600
C	6.57067200	4.37272800	-0.86898000
C	7.53788100	5.38456900	-0.93511500
C	8.40220200	5.52812700	0.16018600
C	8.32372500	4.72350400	1.30665300
C	7.34209600	3.72515800	1.33194000
C	7.31940300	-3.76819900	1.24061900
C	8.29229000	-4.77502400	1.23243700
C	8.40840400	-5.55698400	0.07389200
C	7.59118000	-5.38053600	-1.05259800
C	6.61873600	-4.37242900	-0.99590100
C	8.41724000	1.39651800	-0.75060600
C	9.57962200	0.72022400	-1.13847600
C	9.54017500	-0.70986100	-1.27108800
C	8.38796000	-1.39429600	-0.87011300
C	-2.47790400	1.39986700	0.33124200
C	-3.68532800	0.71336900	0.14891700
C	-3.68819800	-0.72024300	0.10653800
C	-2.48144500	-1.42054400	0.23428800
C	-4.90252600	-1.43914200	-0.05599400
C	-5.93629500	-2.07141300	-0.17548300
C	-7.15191600	-2.79491900	-0.31031700
C	-8.39901400	-2.14854900	-0.18173500
C	-7.15026100	-4.18045100	-0.57284900
C	-8.33777600	-4.88451200	-0.71122400

C	-9.58735700	-2.85426800	-0.30460700
C	-9.57831900	-4.23491500	-0.57562700
C	-4.89128200	1.44784400	-0.00786600
C	-5.91191700	2.09634400	-0.15047200
C	-7.10900600	2.84308100	-0.32111600
C	-7.17607300	4.20355200	0.04320700
C	-8.26749700	2.24689900	-0.86132200
C	-9.43541700	2.97624500	-1.03227800
C	-8.34775200	4.93022700	-0.11204600
C	-9.49888800	4.33054700	-0.65526500
C	7.78187500	-6.28639300	-2.28529300
C	6.86562400	-5.87983200	-3.45480800
C	7.45038700	-7.74694500	-1.89557600
C	9.24822600	-6.20940100	-2.77346500
C	9.22558400	-5.03891300	2.43028300
C	9.03003000	-6.49151000	2.92555700
C	10.69566000	-4.84095600	1.99027600
C	8.94689600	-4.08934600	3.61075600
C	-1.94407500	6.51022200	-0.82454900
C	-3.45928600	6.45115000	-1.13192400
C	-1.57904500	7.92595900	-0.31835200
C	-1.17981600	6.25862200	-2.13801700
C	-2.68423800	4.77631900	3.90126600
C	-2.26693200	3.68793000	4.90843600
C	-4.20957300	4.65734500	3.66904100
C	-2.36516200	6.15640400	4.52305000
C	7.68647100	6.31767700	-2.15312700
C	6.63331000	6.03243100	-3.24029000
C	7.52118700	7.78772400	-1.69967800
C	9.08912600	6.12823600	-2.77797300

C	9.31280900	4.94775700	2.46708100
C	9.05279200	3.99508300	3.64944000
C	10.75584200	4.70701400	1.96210200
C	9.18344900	6.39989500	2.98437800
C	-1.92526500	-6.45977400	-1.26475500
C	-3.43416100	-6.37283900	-1.59724600
C	-1.57852800	-7.90524400	-0.83591800
C	-1.13478100	-6.13758100	-2.54717500
C	-2.73882600	-5.00920900	3.54338900
C	-2.43198500	-6.42390400	4.08852600
C	-4.25958700	-4.87297900	3.29081900
C	-2.33722700	-3.98318300	4.61968900
Zn	3.02471500	-0.02208000	0.45237500
C	10.76056700	1.58002800	-1.25597400
C	12.05814700	1.29045700	-1.03849200
C	13.06581000	2.37811900	-1.09392300
O	14.34920900	2.00673900	-0.81884000
O	12.82389800	3.53539400	-1.35953700
C	10.54293800	-1.56226800	-1.91630300
C	11.42487800	-1.27079400	-2.89141000
C	12.24000500	-2.36192000	-3.47965300
O	13.08964300	-1.99049200	-4.47935600
O	12.19578100	-3.52351900	-3.13610200
N	-10.69185800	5.07312700	-0.81924500
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C	-10.53468600	9.14960300	-1.95334000
C	-9.72391500	8.20859500	-2.59115800
C	-9.77725900	6.86469500	-2.22710200
C	-11.39678700	8.73212000	-0.93747400
C	-10.63552700	6.44452100	-1.19886800

C	-11.44393400	7.39331700	-0.55397900
C	-12.16126200	3.61015600	0.49744100
C	-13.40261700	3.01112100	0.70122600
C	-13.02490900	4.70497500	-1.48026900
C	-14.26778100	4.11606900	-1.25710100
C	-14.46447800	3.26262000	-0.16988300
N	-10.78918000	-4.95572500	-0.70692000
C	-10.89145500	-6.28061400	-0.19543800
C	-11.91572800	-4.36022000	-1.34136700
C	-10.37515700	-6.59695700	1.07103500
C	-10.47286500	-7.89641800	1.56417800
C	-11.10064600	-8.89434100	0.81608900
C	-11.51526500	-7.28717200	-0.94900200
C	-11.62425400	-8.57952200	-0.43939100
C	-11.75957100	-3.61750200	-2.52251100
C	-12.86587900	-3.03264000	-3.13506500
C	-14.14386600	-3.19282900	-2.59589300
C	-13.20057600	-4.51337800	-0.79698500
C	-14.30303100	-3.94032600	-1.42754800
H	4.41709400	-5.04085100	0.72079900
H	1.74931000	-5.04559200	0.99009500
H	1.76073300	4.96488400	1.28077200
H	4.42404900	4.97566900	0.96755300
H	-0.82033000	-3.07966800	2.85043300
H	-2.95592300	-6.43633000	1.24591400
H	-0.15399700	-4.28199600	-1.18638300
H	-0.17297500	4.33116200	-0.90257100
H	-2.93502400	6.33863200	1.69623200
H	-0.78478200	2.88752100	3.06321500
H	5.88474700	4.20875500	-1.69135900

H	9.16661000	6.29716500	0.11952000
H	7.24636400	3.06709600	2.18714700
H	7.19675700	-3.12618400	2.10447600
H	9.16475300	-6.33470100	0.04751600
H	5.96251200	-4.19048700	-1.83852200
H	8.45275800	2.47472100	-0.70103800
H	8.37704100	-2.47027200	-0.96857300
H	-2.50293400	2.47878300	0.33706700
H	-2.50975400	-2.49764100	0.17298500
H	-8.42197200	-1.08649900	0.04025900
H	-6.20160700	-4.69551600	-0.68434000
H	-8.31364700	-5.94656800	-0.92921200
H	-10.53508400	-2.34060700	-0.18677500
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H	-8.23142000	1.20653800	-1.16819100
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H	7.04483900	-6.54081400	-4.30865400
H	7.05952600	-4.85423200	-3.78539000
H	5.80539000	-5.96134100	-3.19384100
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H	9.69021200	-6.69579500	3.77582300
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H	11.37300600	-5.03222400	2.83014800
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H	9.10103600	-3.04064200	3.33680400
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H	-3.71853300	7.17838900	-1.90954300
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H	-0.50772200	8.00206600	-0.10506900
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H	-1.41842800	5.28006000	-2.56659700
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H	-2.80970900	3.82954300	5.84848500
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H	-2.89091800	6.27519400	5.47706800
H	6.77463100	6.72226800	-4.07835700
H	5.61327500	6.17056700	-2.86705000
H	6.71853200	5.01483400	-3.63491700
H	7.62509400	8.46307600	-2.55617300
H	8.27312600	8.07462700	-0.95898400
H	6.53401600	7.95254800	-1.25544200
H	9.21603400	6.79659400	-3.63700900

H	9.22629400	5.09981300	-3.12782400
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H	9.16977900	2.94534900	3.36147300
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H	9.77258000	4.19769400	4.44887300
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H	11.47451900	4.87637500	2.77177200
H	9.40773600	7.13338900	2.20473300
H	9.88121900	6.57180500	3.81134100
H	8.16994100	6.59797300	3.34861600
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H	-3.70773800	-5.35871500	-1.90674300
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H	-1.81627600	-8.60876500	-1.64166900
H	-2.13923300	-8.21357000	0.05127700
H	-0.51215900	-8.00074200	-0.60649600
H	-1.40224700	-6.85121700	-3.33300200
H	-0.05387500	-6.21078000	-2.38963700
H	-1.35898400	-5.13415800	-2.92289100
H	-2.73183200	-7.20647800	3.38530300
H	-2.97111300	-6.59608800	5.02691300
H	-1.36162000	-6.54427300	4.28568000
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H	10.54939700	2.63264100	-1.44160500

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H	-10.49581000	10.19458600	-2.24486800
H	-9.05474600	8.51751100	-3.38907400
H	-9.15670600	6.13410700	-2.73521900
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H	-11.34374500	3.42343900	1.18561500
H	-13.54269000	2.35569500	1.55600900
H	-12.87318400	5.35702700	-2.33387400
H	-15.08260400	4.31633700	-1.94694200
H	-15.43222000	2.79987400	-0.00327400
H	-9.89977100	-5.82080600	1.66134900
H	-10.06869500	-8.12462700	2.54626100
H	-11.18150200	-9.90395700	1.20675700
H	-11.91195400	-7.04922600	-1.93030000
H	-12.10984000	-9.34710700	-1.03513000
H	-10.77063900	-3.50293300	-2.95344200
H	-12.72765000	-2.46059300	-4.04803100
H	-15.00416400	-2.74157700	-3.08034600
H	-13.32701400	-5.08260000	0.11774200
H	-15.29033600	-4.06867800	-0.99316100

Atom coordinates for optimized structure **YH10**

	X	Y	Z
C	0.85860500	0.74958100	0.34935200
C	0.84884200	-0.66588400	0.34498100
C	-0.55373000	-1.06693400	0.45825600

N	-1.34649000	0.05676300	0.46348200
C	-0.53874600	1.16902700	0.46333000
C	-4.15409800	4.24226800	0.54550200
C	-2.80708800	4.23316400	0.73214400
C	-2.36283800	2.87063900	0.56740500
N	-3.45116800	2.05754300	0.32349300
C	-4.55497700	2.88486600	0.27070100
C	-1.00921900	2.48666900	0.59853300
C	-7.69345600	-0.62339100	-0.56959800
C	-7.65584200	0.78620700	-0.66835300
C	-6.31849400	1.19658500	-0.24485900
N	-5.56146900	0.07667600	-0.00163600
C	-6.36068000	-1.03619000	-0.12733400
C	-5.87462200	2.51491000	-0.04357500
C	-2.85770200	-4.09228600	0.82434200
C	-4.21249800	-4.08089100	0.71039500
C	-4.60561500	-2.72216200	0.42778600
N	-3.48580600	-1.91400500	0.40587800
C	-2.40091800	-2.74010200	0.61725000
C	-1.04107200	-2.37664500	0.60147600
C	-5.93353000	-2.34424900	0.15717600
C	-0.01876800	3.59265000	0.81982400
C	-6.87281300	3.63362300	-0.11838900
C	-6.94275600	-3.45607400	0.22496300
C	-0.06462600	-3.50167600	0.79174100
C	0.60197500	3.73181900	2.06681500
C	1.53719200	4.74667500	2.30170000
C	1.82087400	5.62492900	1.24529300
C	1.21118900	5.52727500	-0.01388900
C	0.28436500	4.49446000	-0.20744000

C	0.22365200	-4.37821600	-0.26112600
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C	1.73574200	-5.57914900	1.16003900
C	1.46689200	-4.72653100	2.24114400
C	0.55239500	-3.68672100	2.03437900
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C	-8.06904300	-5.36176100	-0.79311800
C	-8.74898000	-5.55523200	0.42351000
C	-8.54765900	-4.74118900	1.54290000
C	-7.63716700	-3.67967000	1.41379100
C	-7.77978600	3.82775700	0.93012500
C	-8.73263100	4.85226400	0.88305800
C	-8.74443000	5.67631800	-0.25198300
C	-7.84522800	5.52280500	-1.31756600
C	-6.90375400	4.48843000	-1.22709500
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C	-9.94126300	-0.63595600	-1.48999300
C	-9.90416600	0.79114000	-1.59031800
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C	2.04425100	-1.37797300	0.19709000
C	3.25752500	-0.69127700	0.07282500
C	3.26814100	0.74242400	0.08299200
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C	4.49315000	1.45658600	-0.02136000
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C	6.77840800	2.77032800	-0.16595300
C	7.98622900	2.11491300	0.14916400
C	6.82622600	4.12502300	-0.55354600
C	8.04245600	4.79594400	-0.62714800
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C	2.17730500	-4.95296400	3.58964200
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C	-10.37747600	-6.03134100	2.78074700
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O	-12.04480600	-4.31071100	-0.14366900
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