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

Supporting Information

β-Functionalized Push-Pull *Opp*-Dibenzoporphyrins as Sensitizers for Dye-Sensitized Solar Cells: The Role of the Phenylethynyl Bridge

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1. Experimental Section

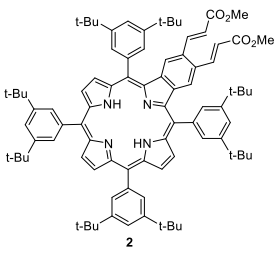
1.1 Material and synthetic procedures

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).

Dibromoporphyrin **1** was synthesized according previous published procedure. [1]

Procedure for the synthesis of monobenzoporphyrins 2: Dibromoporphyrin **1** (100 mg, 0.08 mmol) and N, N-dicyclohexylmethylamine (76 µL, 0.18 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 (10 mL). The mixture was then degassed by three freeze-pump-thaw cycles before the addition of bis(tri-tert-butylphosphine)palladium (8.4 mg, 0.016 mmol), tris(dibenzyldeneacetone)dipalladium (8.5 mg, 0.008 mmol) and the methyl 2,4-pentadienoate (cis/trans mixture, 15-fold excess). The Schlenk flask was then sealed and heated at 45 °C for 12 h. The mixture was passed through a short silica plug using THF as the eluent. The solvent was removed under vacuum, and the residue was recrystallized using CH_2Cl_2/MeOH to give the crude product. The Crude product (97 mg) and *p*-chloranil (48 mg) were dissolved in toluene (10 mL). The mixture was heated at reflux for 12 h. Then the mixture was diluted with EtOAc and washed with 10% NaOH (aq) and water. The organic layer was separated and the solvent was removed under vacuum. Product **2** was obtained after recrystallization using CH_2Cl_2/MeOH.

Monobenzoporphyrin 2

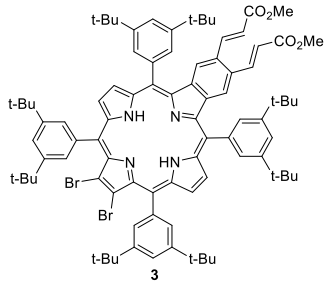


2

$C_{88}H_{104}N_4O_4$; purple crystalline solid; m.p. > 300 °C; yield: 82 mg (0.06 mmol, 78%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.96 (d, J = 4.9 Hz, 2H), 8.91 (d, J = 4.9 Hz, 2H), 8.77 (s, 2H), 8.16 (d, J = 15.7 Hz, 2H), 8.08 (d, J = 1.8 Hz, 4H), 8.06 (d, J = 1.8 Hz, 4H), 8.04 (t, 2H), 7.79 (t, 2H), 7.31 (s, 2H), 6.10 (d, J = 15.6 Hz, 2H), 3.91 (s, 6H), 1.52 (s, 36H), 1.49 (s, 36H), -2.54 (s, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.26, 150.58, 148.93, 141.78, 141.52, 141.15, 130.96, 129.70, 128.54, 128.04, 123.79, 122.60, 121.22, 120.21, 118.44, 51.81, 35.33, 35.20, 31.89, 31.79 ppm; UV/Vis ($CHCl_3$): λ_{max} = 446, 529, 602, 667 nm; HRMS (MALDI): m/z: calcd for $C_{88}H_{104}N_4O_4$: 1280.8058; found: 1280.8058; FTIR (ATR) ν_{max}/cm^{-1} 3064 (sp^2 CH), 2955–2870 (sp^3 CH), 1723 (CO), 1634 and 1592 (aromatic CC).

Procedure for the synthesis of monobenzoporphyrins 3: Monobenzoporphyrin **2** (100 mg, 0.08 mmol) and N-bromosuccinimide (2.2 equiv.) were dissolved in dry dichloroethane. The mixture was heated at reflux for 12 h. The progress of the reaction was monitored by UV/Vis spectroscopy. Upon completion of the reaction, the mixture was washed with 10% NaOH (aq) and water. The organic layer was separated, and the solvent was removed under reduced pressure. The resulting residue was recrystallized using CH_2Cl_2/MeOH to afford pure compound **3**.

Dibromomonobenzoporphyrin 3

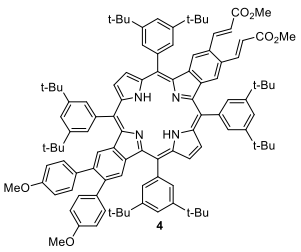


3

$C_{88}H_{102}Br_2N_4O_4$; purple crystalline solid; m.p. > 300 °C; yield: 99 mg (0.07 mmol, 88%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.90 (d, J = 4.4 Hz, 2H), 8.84 (d, J = 4.3 Hz, 2H), 8.13 (d, J = 15.7 Hz, 2H), 8.03 (s, 6H), 7.95 (d, J = 1.6 Hz, 4H), 7.80 (s, 2H), 7.24 (s, 2H), 6.07 (d, J = 15.7 Hz, 2H), 3.90 (s, 6H), 1.51 (s, 36H), 1.48 (s, 36H), -2.72 (s, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.17, 150.77, 150.46, 149.48, 146.33, 143.17, 141.33, 141.16, 140.61, 140.29, 138.77, 131.35, 129.97, 129.71, 128.48, 127.71, 125.79, 123.73, 122.77, 122.34, 121.73, 120.42, 118.74, 51.85, 35.34, 35.25, 31.86, 31.78 ppm; UV/Vis ($CHCl_3$): λ_{max} = 450, 534, 569, 606 nm; HRMS (MALDI): m/z: calcd for $C_{88}H_{102}Br_2N_4O_4$: 1436.6268; found: 1436.6265; FTIR (ATR) ν_{max}/cm^{-1} 3066 (sp^2 CH), 2952–2868 (sp^3 CH), 1722 (CO), 1631 and 1592 (aromatic CC), 710 (CBr).

Procedure for the synthesis of dibenzoporphyrins 4: Dibromoporphyrin **3** (100mg, 0.07 mmol) and N, N-dicyclohexylmethylamine (32 µL, 0.15 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 (10 mL). The mixture was then degassed by three freeze-pump-thaw cycles before the addition of bis(tri-tert-butylphosphine)palladium (7.1 mg, 0.014 mmol), tris(dibenzyldeneacetone)dipalladium (7.2 mg, 0.007 mmol) and the 4-methoxy styrene (15-fold excess). The Schlenk flask was then sealed and heated at 45 °C for 12 h. Then the mixture was passed through a short silica plug using THF as the eluent. The solvent was removed under vacuum, and the residue was recrystallized using CH_2Cl_2/MeOH to give the crude product. The Crude product (90 mg) and *p*-chloranil (45 mg) were dissolved in toluene (10 mL). The mixture was heated at reflux for 12 h. Then the mixture was diluted with EtOAc and washed with 10% NaOH (aq) and water. The organic layer was separated and the solvent was removed under vacuum. The resulting residue was subjected to silica column chromatography (CH_2Cl_2/cyclohexane). The band containing desired product **4** was collected and recrystallized using CH_2Cl_2/MeOH.

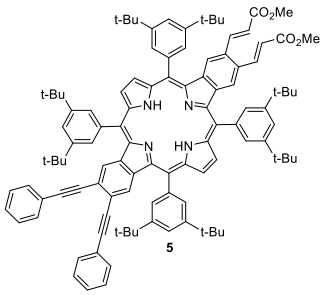
Dibenzoporphyrin 4



$C_{106}H_{118}N_4O_6$; purple crystalline solid; m.p. > 300 °C; yield: 53 mg (0.03 mmol, 49%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.90 (d, J = 6.1 Hz, 2H), 8.88 (d, J = 4.6 Hz, 2H), 8.17 (d, J = 15.7 Hz, 2H), 8.07 (d, J = 1.7 Hz, 4H), 8.03 (d, J = 1.7 Hz, H), 8.01 (d, J = 1.7 Hz, 4H), 7.82 (s, 2H), 7.30 (s, 2H), 6.97 (d, J = 8.4 Hz, 6H), 6.74 (d, J = 8.6 Hz, 4H), 6.10 (d, J = 15.6 Hz, 2H), 3.90 (s, 6H), 3.83 (s, 6H), 1.49 (s, 36H), 1.37 (s, 36H), -2.56 (s, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.30, 158.25, 150.57, 150.26, 148.58, 142.93, 141.68, 141.64, 141.60, 141.16, 139.21, 138.56, 137.81, 134.91, 131.28, 130.73, 128.38, 127.78, 127.69, 127.60, 123.61, 122.59, 122.35, 120.04, 119.56, 119.33, 113.21, 55.48, 51.80, 35.33, 35.22, 31.79, 31.73 ppm; UV/Vis ($CHCl_3$): λ_{max} = 460, 534, 573, 615, 672 nm; HRMS (MALDI): m/z: calcd for $C_{106}H_{118}N_4O_6$: 1542.9051; found: 1542.9052; FTIR (ATR) ν_{max}/cm^{-1} 3067 (sp^2 CH), 2954–2866 (sp^3 CH), 1724 and 1706 (CO), 1631, 1609 and 1594 (aromatic CC), 1244, 1220, 1173 (CO).

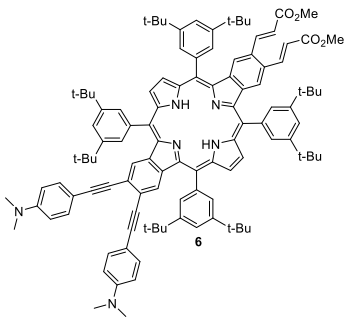
General procedure for the synthesis of dibenzoporphyrins 5 and **6:** Dibromoporphyrin **3** (100mg, 0.07 mmol) and K_2CO_3 (21 mg, 0.15 mmol) were added to a Schlenk flask and dried under vacuum. The vacuum was released under an argon atmosphere to allow the addition of dry THF (10 mL). The mixture was then degassed by three freeze-pump-thaw cycles before the addition of bis(tri-tert-butylphosphine)palladium (14 mg, 0.028 mmol) and the enyne (10-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/cyclohexane). The band containing desired product was collected and the product was recrystallized using CH_2Cl_2/MeOH.

Dibenzoporphyrin 5



$C_{108}H_{114}N_4O_4$; purple crystalline solid; m.p. > 300 °C; yield: 48 mg (0.031 mmol, 45%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.99 (d, J = 4.9 Hz, 2H), 8.92 (d, J = 4.8 Hz, 2H), 8.17 (d, J = 15.6 Hz, 2H), 8.05 (dt, 12H), 7.61 – 7.56 (m, 4H), 7.44 – 7.36 (m, 6H), 7.30 (s, 2H), 6.84 (s, 2H), 6.11 (d, J = 15.6 Hz, 2H), 3.91 (s, 6H), 1.52 (s, 36H), 1.50 (s, 36H), -2.57 (s, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.26, 150.82, 150.65, 149.52, 149.08, 142.97, 141.51, 141.37, 141.16, 138.99, 138.93, 131.67, 130.92, 129.16, 128.53, 128.41, 128.27, 128.02, 127.95, 127.77, 124.04, 123.66, 122.67, 122.63, 122.30, 120.18, 119.90, 119.48, 92.78, 89.94, 51.82, 35.37, 35.35, 31.90, 31.80 ppm; UV/Vis ($CHCl_3$): λ_{max} = 463, 538, 579, 616, 673 nm; HRMS (MALDI): m/z: calcd for $C_{108}H_{114}N_4O_4$: 1530.8840; found: 1530.8847; FTIR (ATR) ν_{max}/cm^{-1} 3067 (sp^2 CH), 2956–2870 (sp^3 CH), 2352 (alkyne CC), 1722 (CO), 1631 and 1594 (aromatic CC).

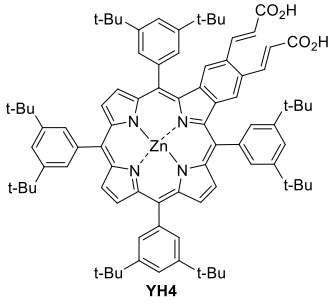
Dibenzoporphyrin 6



$C_{112}H_{124}N_6O_4$; purple crystalline solid; m.p. > 300 °C; yield: 26 mg (0.016 mmol, 23%); ^{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).. ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.29, 150.78, 150.59, 150.09, 148.79, 142.93, 141.59, 141.45, 140.58, 139.00, 138.78, 132.88, 130.78, 128.57, 128.42, 127.99, 127.77, 127.64, 123.61, 123.34, 122.61, 122.20, 120.08, 119.75, 119.35, 112.05, 111.28, 94.78, 94.08, 88.30, 51.80, 40.47, 35.37, 35.34, 31.93, 31.80 ppm; UV/Vis ($CHCl_3$): λ_{max} = 469, 539, 583, 617, 676 nm; HRMS (MALDI): m/z: calcd for $C_{112}H_{124}N_6O_4$: 1616.9684; found: 1616.9688; FTIR (ATR) ν_{max}/cm^{-1} 3069 (sp^2 CH), 2954–2868 (sp^3 CH), 2355 (alkyne CC), 1724 (CO), 1634 and 1592 (aromatic CC).

General procedure for the synthesis of porphyrin dye YH4 – **YH7:** dibenzoporphyrin (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 intermediate. The zinc inserted intermediate was dissolved in THF (3 mL). A solution of 20% NaOH (aq) (1 mL) and MeOH was added. The mixture was heated at reflux for 12 h. the progress of the reaction was monitored by TLC. The mixture was washed with 10% citric acid solution the water and then extracted with ethyl acetate. The organic layer was separated and the solvent was removed under reduced pressure. Pure product **YH4** – **YH7** were obtained after recrystallization using CH_2Cl_2/MeOH.

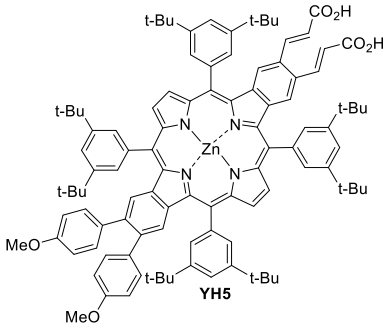
Porphyrin Dye YH4



$C_{86}H_{98}N_4O_4Zn$; purple crystalline solid; m.p. > 300 °C; yield: 43 mg (0.046 mmol, 94%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.89 (d, J = 4.6 Hz, 2H), 8.82 (d, J = 1.4 Hz, 4H), 8.17 (d, J = 15.8 Hz, 2H), 8.06 – 7.97 (m, 10H), 7.73 (s, 2H), 7.47 (s, 2H), 6.09 (d, J = 15.6 Hz, 2H), 1.46 (d, J = 15.4 Hz, 72H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 168.86, 151.57, 150.18, 149.95, 149.12, 148.46, 147.52, 144.93, 142.76, 142.49, 142.14, 141.29, 134.84, 132.04, 131.46, 131.11, 130.38, 129.60, 128.38, 128.24, 124.02, 123.70, 122.21, 121.54, 120.69, 120.35, 119.58, 118.63, 35.21, 35.08, 31.80, 31.72 ppm; UV/Vis (THF): λ_{max} (log ε) = 455 (5.33), 574 (4.56) nm; HRMS (MALDI): m/z: calcd for $C_{86}H_{98}N_4O_4Zn$: 1314.6880; found: 1314.6873; FTIR (ATR) ν_{max}/cm^{-1} 3300–2500 (OH) 3064 (sp^2 CH), 2956–2870 (sp^3 CH), 1693 (CO), 1623 and 1592 (aromatic CC).

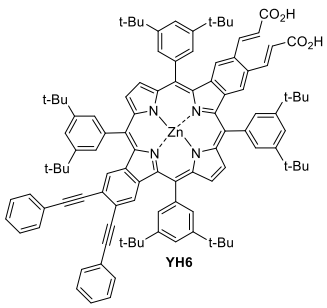
Porphyrin Dye YH5

$C_{104}H_{116}N_4O_6Zn$; purple crystalline solid; m.p. > 300 °C; yield: 43 mg, (0.027 mmol, 84%); ^{1}H NMR (500 MHz, $CDCl_3$):



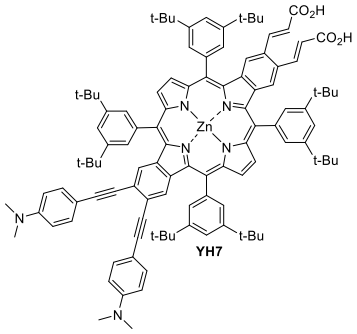
δ 8.86 (d, J = 4.6 Hz, 1H), 8.83 (d, J = 4.6 Hz, 1H), 8.17 (d, J = 15.8 Hz, 1H), 8.03 (d, J = 1.8 Hz, 2H), 8.01 – 7.96 (m, 3H), 7.77 (t, J = 1.8 Hz, 1H), 7.45 (s, 1H), 7.12 (s, 1H), 6.96 (d, J = 8.7 Hz, 2H), 6.71 (d, J = 8.7 Hz, 2H), 6.09 (d, J = 15.6 Hz, 1H), 3.80 (s, 3H), 1.45 (s, 16H), 1.32 (s, 17H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 168.91, 158.12, 150.42, 150.12, 149.77, 145.62, 143.97, 142.76, 142.69, 142.22, 140.86, 139.28, 137.43, 134.99, 131.27, 130.92, 130.07, 128.15, 127.70, 127.62, 123.81, 122.19, 121.91, 120.18, 120.07, 113.15, 55.42, 35.20, 35.08, 31.71, 31.63.ppm; UV/Vis (THF): λ_{max} (log ε) = 470 (5.51), 562 (4.16), 594 (4.61), 638 (4.28) nm; HRMS (MALDI): m/z: calcd for $C_{104}H_{116}N_4O_6Zn$: 1576.7873; found: 1576.7864; FTIR (ATR) ν_{max}/cm^{-1} 3300–2500 (OH) 3069 (sp^2 CH), 2961–2833 (sp^3 CH), 1696 (CO), 1623 and 1592 (aromatic CC), 1246 and 1224 (CO).

Porphyrin Dye YH6



$C_{106}H_{118}N_4O_4Zn$; purple crystalline solid; m.p. > 300 °C; yield: 36 mg (0.023 mmol, 70%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.90 (d, J = 4.6 Hz, 1=2H), 8.84 (d, J = 4.6 Hz, 2H), 8.14 (d, J = 15.7 Hz, 2H), 8.00 (d, J = 1.8 Hz, 4H), 7.98 – 7.95 (m, 8H), 7.54 (m, 5H), 7.42 (s, 2H), 7.38 – 7.31 (m, 5H), 6.92 (s, 2H), 6.07 (d, J = 15.6 Hz, 2H), 1.44 (d, J = 9.9 Hz, 72H) ppm ^{13}C NMR (126 MHz, $CDCl_3$): δ 168.86, 150.27, 150.22, 150.13, 144.57, 144.34, 142.57, 142.48, 142.04, 140.91, 139.14, 131.50, 131.17, 131.05, 130.20, 129.20, 128.41, 128.10, 127.79, 123.92, 123.78, 122.20, 121.72, 120.37, 120.34, 120.06, 92.36, 89.93, 35.18, 35.15, 31.73, 31.64; UV/Vis (THF): λ_{max} (log ε) = 475 (5.66), 596 (4.65), 616 (4.39), 638 (4.13) nm; HRMS (MALDI): m/z: calcd for $C_{106}H_{118}N_4O_4Zn$: 1564.7662; found: 1564.7655; FTIR (ATR) ν_{max}/cm^{-1} 3300–2500 (OH) 3058 (sp^2 CH), 2956–2868 (sp^3 CH), 2356 (alkyne CC), 1696 (CO), 1623 and 1590 (aromatic CC).

Porphyrin Dye YH7



$C_{110}H_{118}N_6O_4Zn$; purple crystalline solid; m.p. > 300 °C; yield: 47 mg (0.028 mmol, 91%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.96 (d, J = 4.9 Hz, 1H), 8.91 (d, J = 4.9 Hz, 1H), 8.77 (s, 1H), 8.16 (d, J = 15.7 Hz, 1H), 8.08 (d, J = 1.8 Hz, 2H), 8.06 (d, J = 1.8 Hz, 2H), 8.04 (t, 1H), 7.79 (t, 1H), 7.31 (s, 1H), 6.10 (d, J = 15.6 Hz, 1H), 3.91 (s, 3H), 1.52 (s, 16H), 1.49 (s, 16H), -2.54 (s, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 168.86, 150.27, 150.22, 150.13, 144.57, 144.34, 142.57, 142.48, 142.04, 140.91, 139.14, 131.50, 131.17, 131.05, 130.20, 129.20, 128.41, 128.10, 127.79, 123.92, 123.78, 122.20, 121.72, 120.37, 120.34, 120.06, 92.36, 89.93, 35.18, 35.15, 31.73, 31.64 pm; UV/Vis (THF): λ_{max} (log ε) = 458 (4.91), 480 (5.32), 598 (4.42), 618 (4.15), 641 (3.87) nm; HRMS (MALDI): m/z: calcd for $C_{110}H_{118}N_6O_4Zn$: 1650.8506; found: 1650.8504; FTIR (ATR) ν_{max}/cm^{-1} 3300–2500 (OH) 3062 (sp^2 CH), 2959–2870 (sp^3 CH), 2205 (alkyne CC), 1698 (CO), 1623, 1610, 1594 and 1522 (aromatic CC).

1.2 Instruments and measurements

1.2.1 Spectra measurement

The UV/Vis spectra were recorded with an Agilent Carry 5000 UV/Vis/NIR spectrometer with samples in *o*-DCB or THF. 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. All NMR spectra were recorded on a 500 MHz (^{1}H NMR)/126 MHz (^{13}C NMR) spectrometer. All samples were prepared in $CDCl_3$ or $CDCl_3$ and MeOD. $CDCl_3$ was used as internal standard for ^{1}H NMR and ^{13}C NMR (δ = 7.26 and 77.0 ppm, respectively). IR spectra were obtained using PerkinElmer Spectrum Two FT-IR Spectrometer using solid compounds. Mass spectra were obtained with a Thermoscientific MALDI-LTQ-XL-Orbitrap mass spectrometer. 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.

1.2.2 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 TiO_2 as the working electrode and Pt-ized FTO as the counter electrode. The thin film TiO_2 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 I_2, 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).

1.2.3 Spectroelectrochemical Measurement

Spectroelectrochemical study was performed by using a cell assembly (SEC-C) supplied by ALS Co., Ltd. (Tokyo, Japan). This assembly comprised of a Pt counter electrode, a 6 mm Pt Gauze working electrode, and an Ag/AgCl reference electrode in a 1.0 mm path length quartz cell. The optical transmission was limited to 6 mm covering the Pt Gauze working electrode.

1.2.4 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 (V_{OC}). 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.

1.2.5 Femtosecond Transient Absorption Spectral Measurement

Femtosecond transient absorption spectroscopy experiments were performed using an Ultrafast Femtosecond Laser Source (Libra) by Coherent incorporating diode-pumped, mode locked Ti: Sapphire laser (Vitesse) and diode-pumped intra cavity doubled Nd: YLF laser (Evolution) to generate a compressed laser output of 1.45 W. For optical detection, a Helios transient absorption spectrometer coupled with femtosecond harmonics generator both provided by Ultrafast Systems LLC was used. The source for the pump and probe pulses were derived from the fundamental output of Libra (Compressed output 1.45 W, pulse width 100 fs) at a repetition rate of 1 kHz. 95% of the fundamental output of the laser was introduced into a TOPAS-Prime-OPA System with 290-2600 nm Tuning Range from Altos Photonics Inc., (Bozeman, MT), while the rest of the output was used for generation of white light continuum. Kinetic traces at appropriate wavelengths were assembled from the time-resolved spectral data. All measurements were conducted at 298 K.

1.2.6 Preparation of Electrodes for Photoelectrochemical and Transient Studies

Electrodes were prepared by cleaning FTO by sonicating individually in ethanol solutions of 0.1 M HCl, acetone, and isopropanol. Next, the FTO was allowed to soak in 20 mM solution of $TiCl_4$ at 70 °C for 30 minutes. Then, a layer of 20 nm anatase TiO_2 (18 NRT, Dyesol) was applied on the surface of the FTO using the doctor blade technique and allowed to dry in air for 15 minutes. The FTO/TiO_2 was then annealed in a heat cycle of 130 °C, 230 °C, 330 °C, 395 °C, 430 °C, and 515 °C for 10 minutes each. After cooling, a second layer of 20 nm opaque anatase TiO_2 was applied and annealed in a similar fashion. Next, the electrodes were allowed to soak in a fresh $TiCl_4$ solution for an additional 30 minutes at 70 °C before immersing in 0.2mM-0.3 mM sensitizer solution ($CHCl_3$/MeOH, v: v, 1:1-1:3) for 3 hours. The counter electrodes were made using chloroplatinic acid and Ethanol. They were then annealed at 500 °C for 30 minutes and then cooled to room temperature.

2. Supplementary Figures and Tables

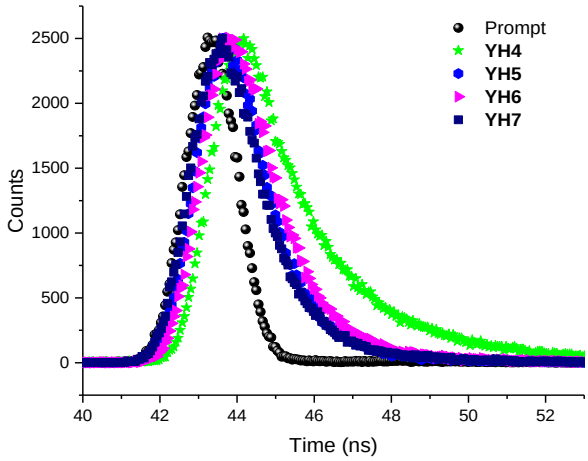


Figure S1 Fluorescence decay profile of **YH4** – **YH7** in *o*-DCB

Table S1 Fluorescence lifetimes of **YH4** – **YH7** in *o*-DCB.

Compound	**Average Lifetime (ns)**	**Chi^2**
YH4	2.14	1.21
YH5	1.01	1.02
YH6	1.12	1.00
YH7	1.06	1.03

Table S2 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	2nd Reduction	3rd Reduction
YH4	0.83	1.09	-1.34	-1.70	
YH5	0.74	0.97	-1.27	-1.63	
YH6	0.79	0.98	-1.25	-1.59	-1.80
YH7	0.78	0.96	-1.28	-1.62	-1.84

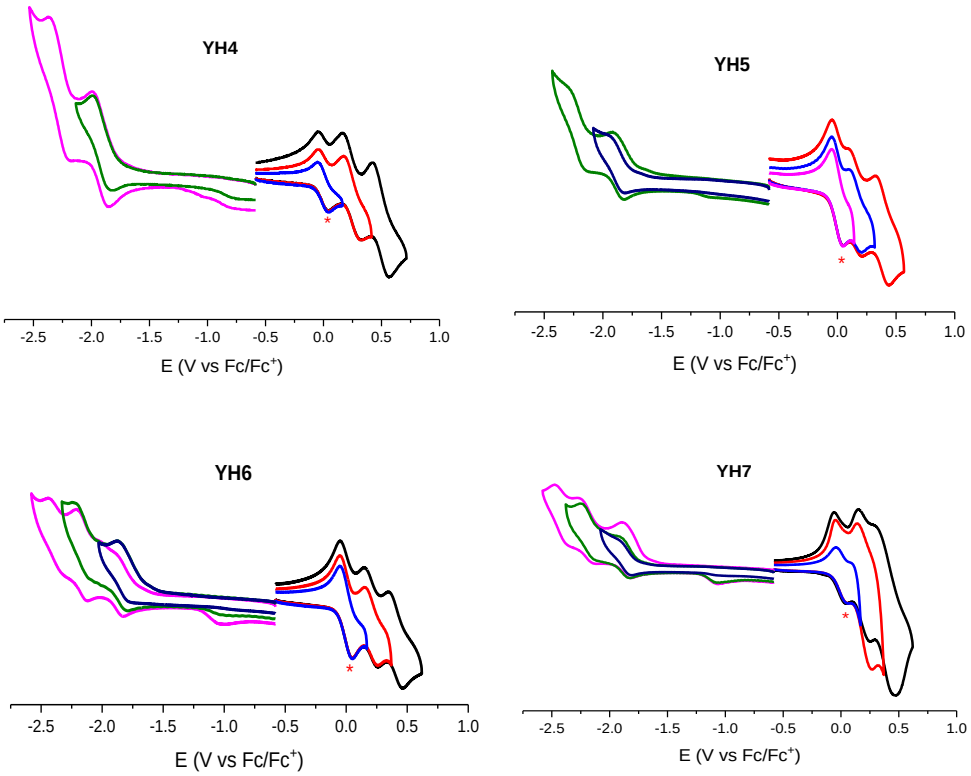


Figure S2 Cyclic voltammograms of compounds **YH4** – **YH7**. Ferrocene/ferrocenium redox couple was used as an internal standard

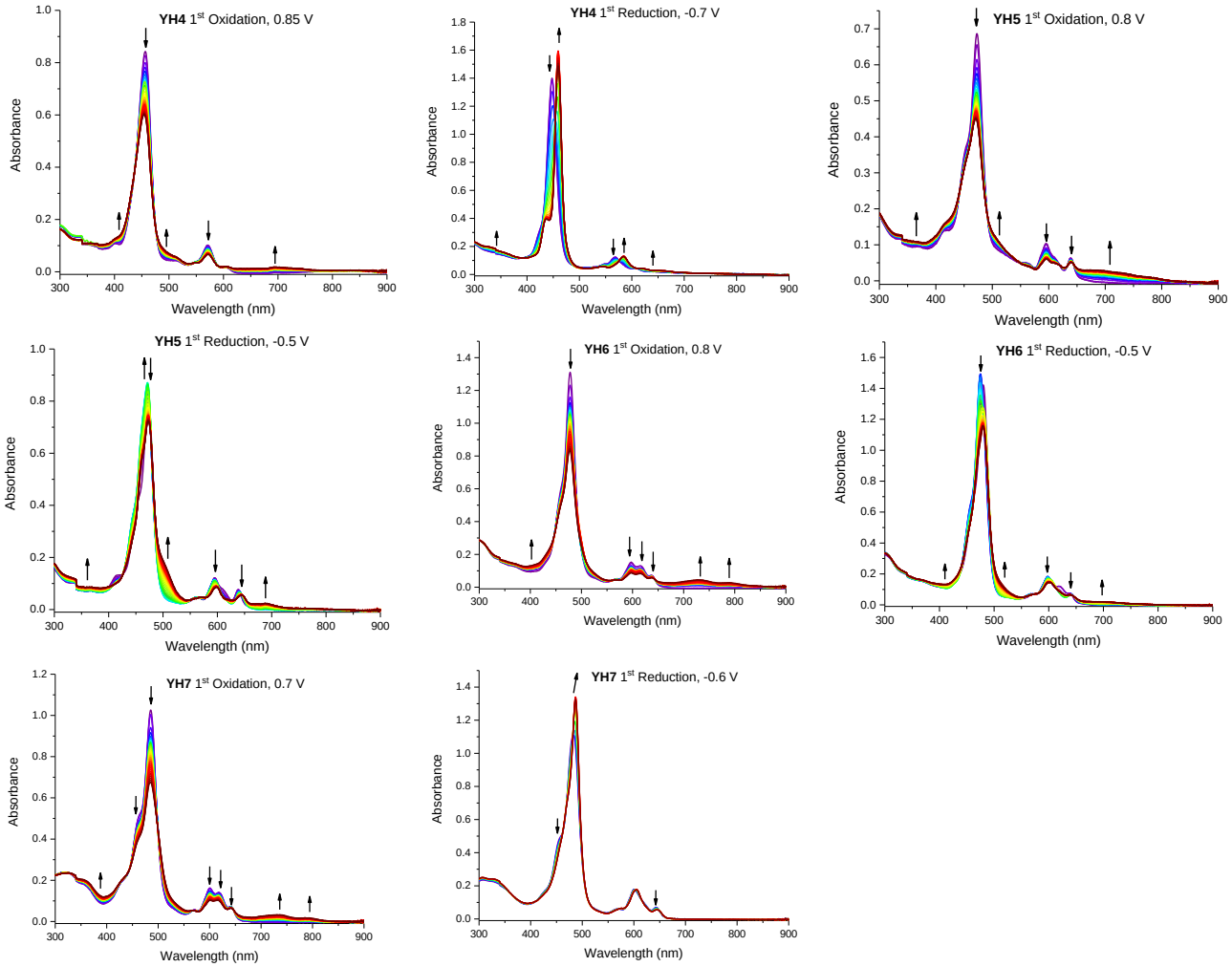


Figure S3 Spectroelectrocchemical studies of **YH4** – **YH7** in *o*-DCB containing 0.2 M $(TBA)ClO_4$

Computational Information

All calculations were carried out using Gaussian 09 program. The calculations were performed by density functional theory (DFT) with B3LYP level employing a basis sets 6-31G(d,p) for all atoms.[2]

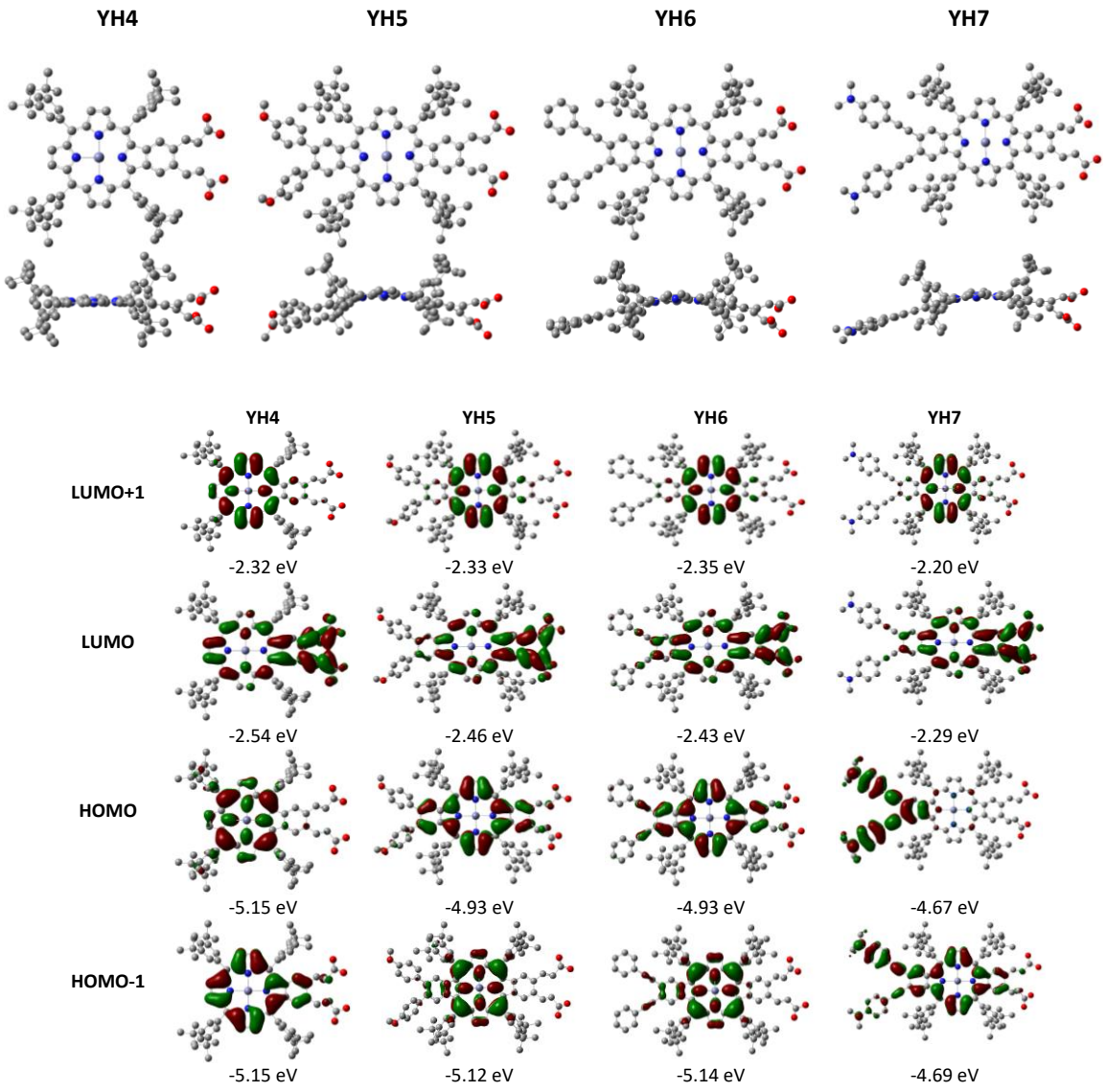


Figure S4 Geometry-optimized molecule structures of **YH4** – **YH7** (Top); Isodensity surface of LUMO+1, LUMO, HOMO, HOMO-1 for **YH4** – **YH7** calculated by Gaussian09 DFT B3LYP/6-31G(d,p). Hydrogen atoms were omitted for clarity

Table S3 Photovoltaic performance of **YH4** with different soaking time

Soaking time (h)	J_{sc} **(mA/cm^2)**	V_{oc} **(V)**	**FF (%)**	η **(%)**
3	13.05	0.56	68	4.9
4	10.55	0.58	64	3.9
6	9.30	0.56	64	3.3
8	8.17	0.57	64	3.0
9	6.31	0.53	53	1.8
The photovoltaic measurements were conducted under AM 1.5G illumination (power 100 mW cm^{-2}) in the presence of a mask and with a cell active area of 0.16 cm^2 and a TiO_2 thickness of 25 μm. The TiO_2 film was soaked in 0.3 mM dye solution in MeOH/$CHCl_3$ (v/v = 3/1) containing 0.6 mM 3α,7α-dihydroxy-5β-cholic acid (CDCA) at different soaking time.				

Table S4 Photovoltaic performance of **YH4** with different CDCA concentration

CDCA concentration (mM)	J_{sc} **(mA/cm^2)**	V_{oc} **(V)**	**FF (%)**	η **(%)**
0.0	4.83	0.56	58	1.6
0.2	5.01	0.54	59	1.6
0.4	7.65	0.60	64	3.0
0.6	8.07	0.61	63	3.1
0.8	6.86	0.60	66	2.7
1.0	5.88	0.58	59	2.0
The photovoltaic measurements were conducted under AM 1.5G illumination (power 100 mW cm^{-2}) in the presence of a mask and with a cell active area of 0.16 cm^2 and a TiO_2 thickness of 25 μm. The TiO_2 film was soaked in 0.3 mM dye solution in MeOH/$CHCl_3$ (v/v = 4/1) containing different concentration of 3α,7α-dihydroxy-5β-cholic acid (CDCA) for 3 h.				

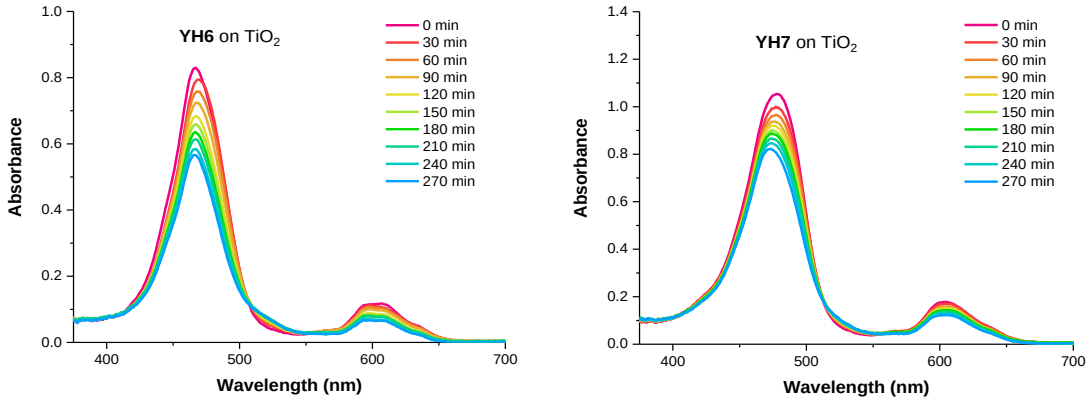


Figure S5 Stability studies of **YH6** and **YH7** on TiO_2 surface under ambient conditions. TiO_2 films were soaked in a 0.05 mM MeOH/$CHCl_3$ (v/v = 2/1) dye solution for 10 min

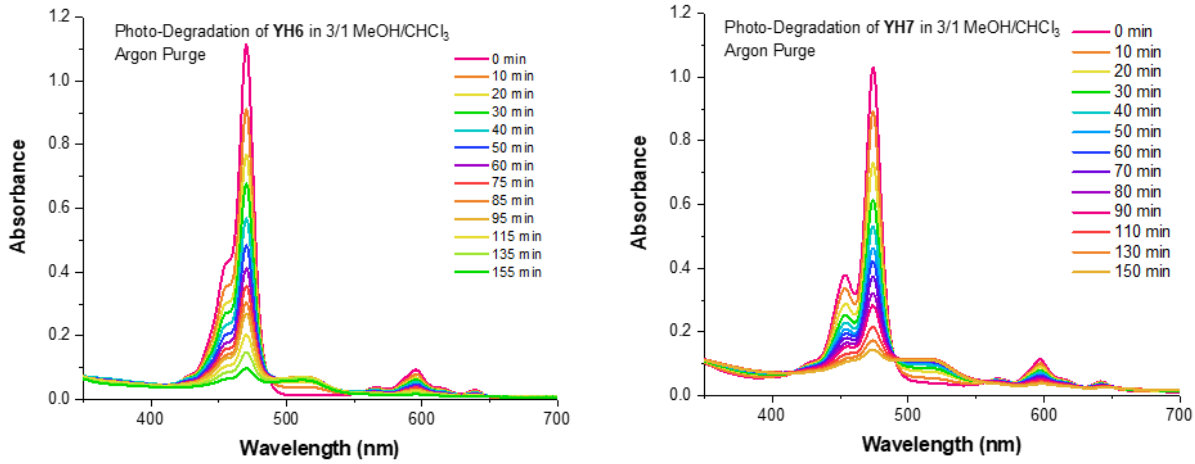
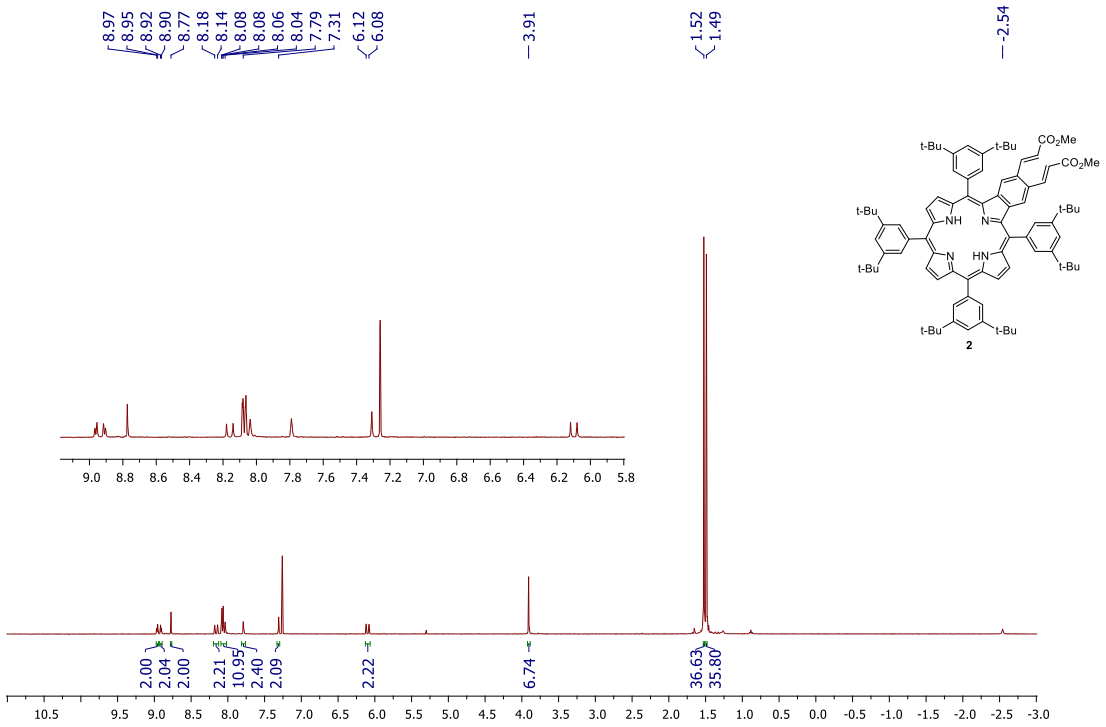
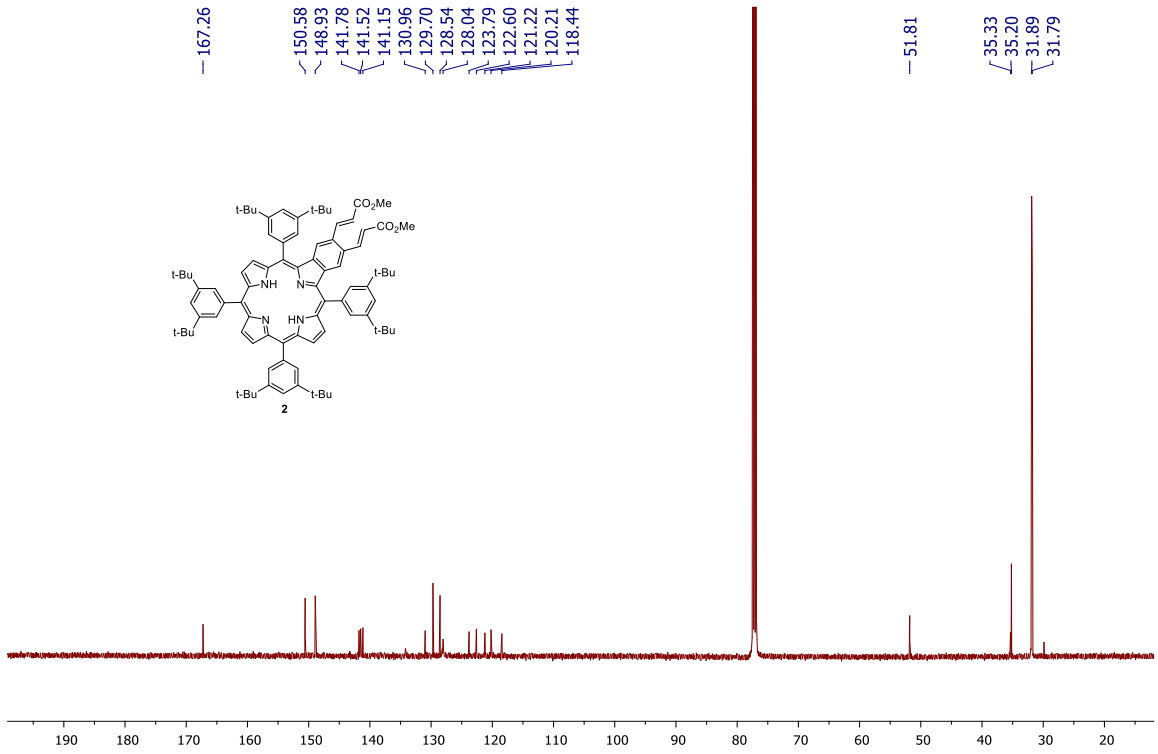
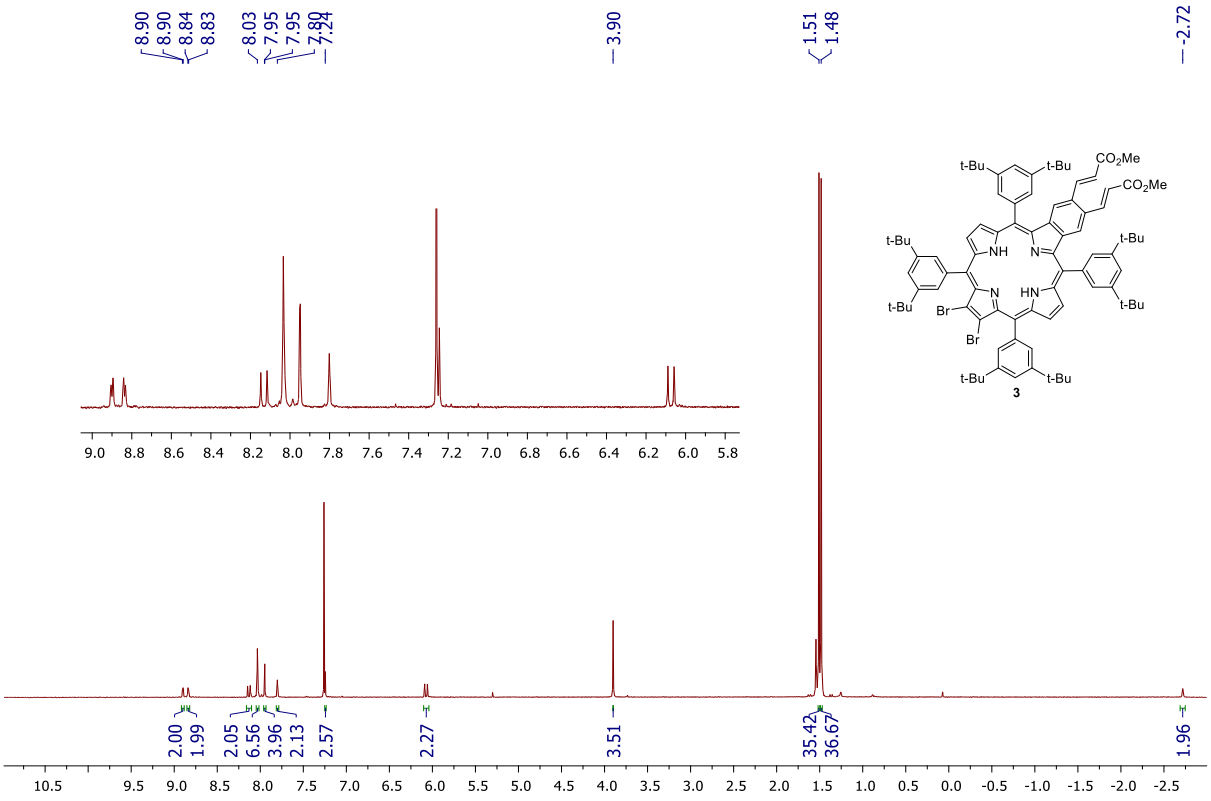


Figure S6 Stability studies of 0.002 mM **YH6** and **YH7** in MeOH/$CHCl_3$ (v/v = 3/1) solution under AM 1.5G illumination

3. NMR Characterization of Compounds



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2.05
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1.96
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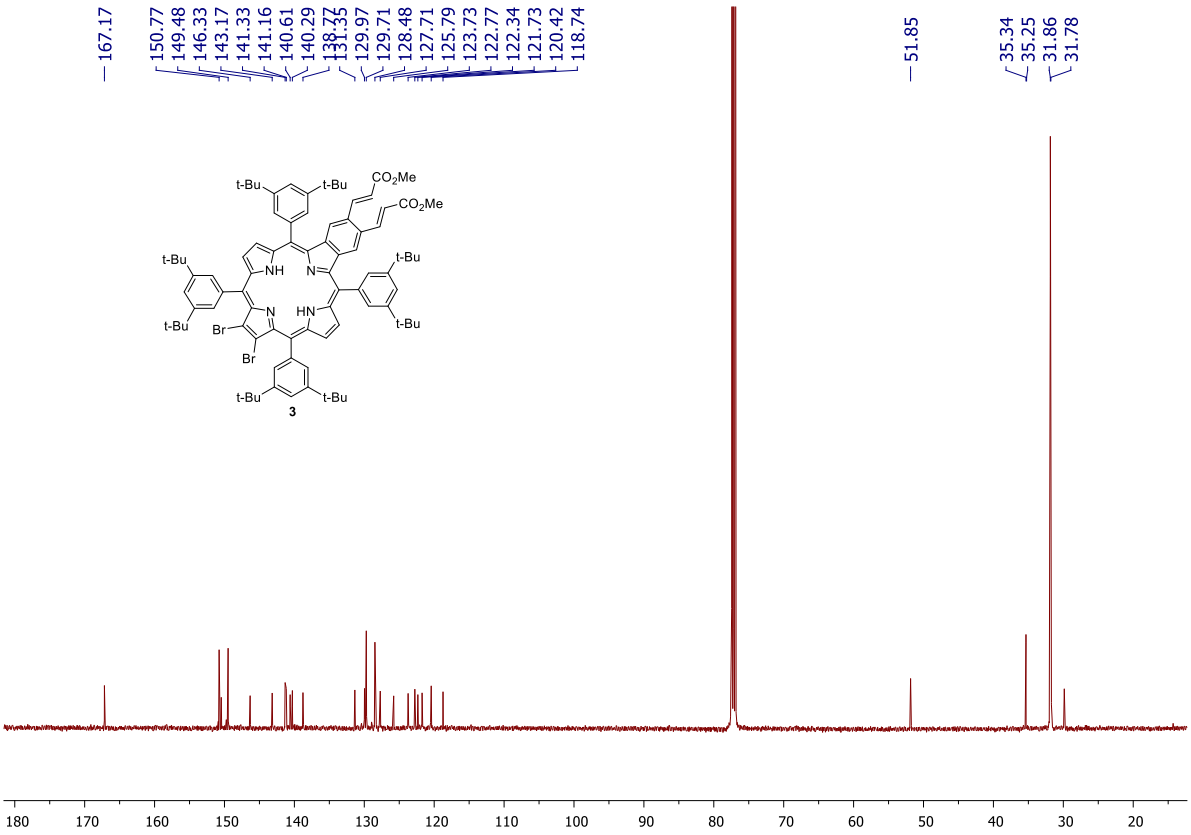
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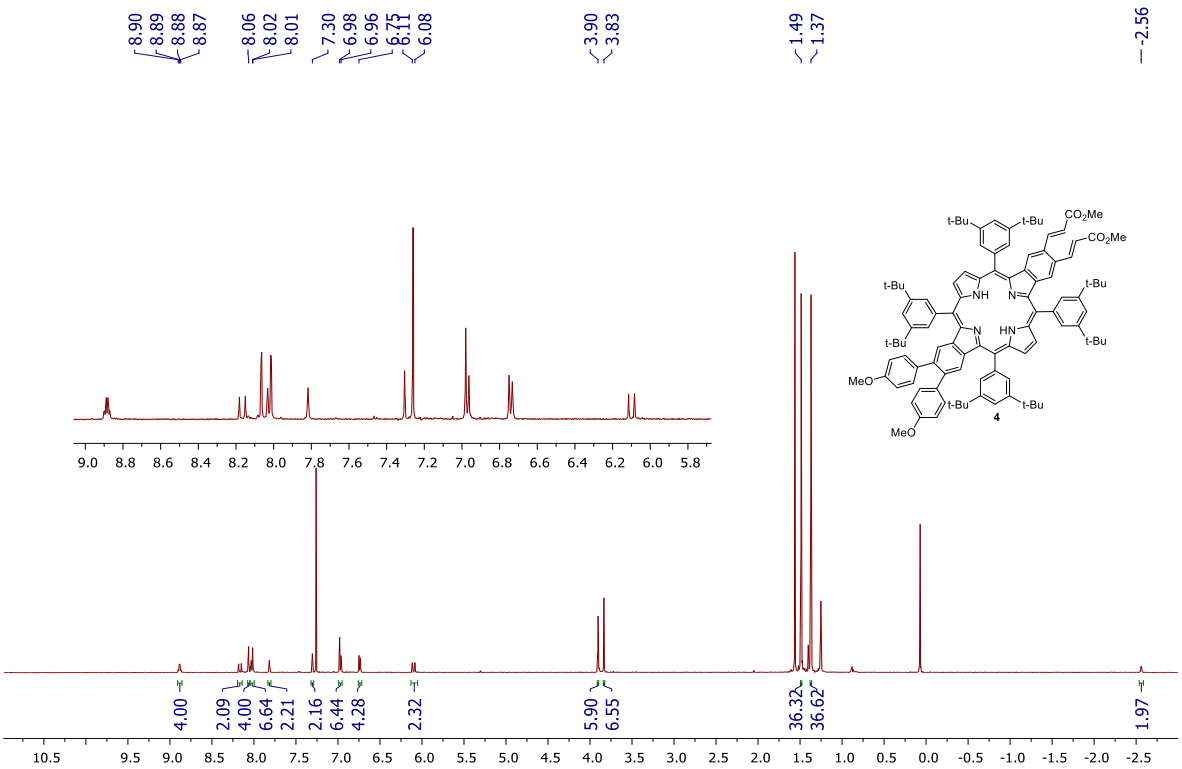
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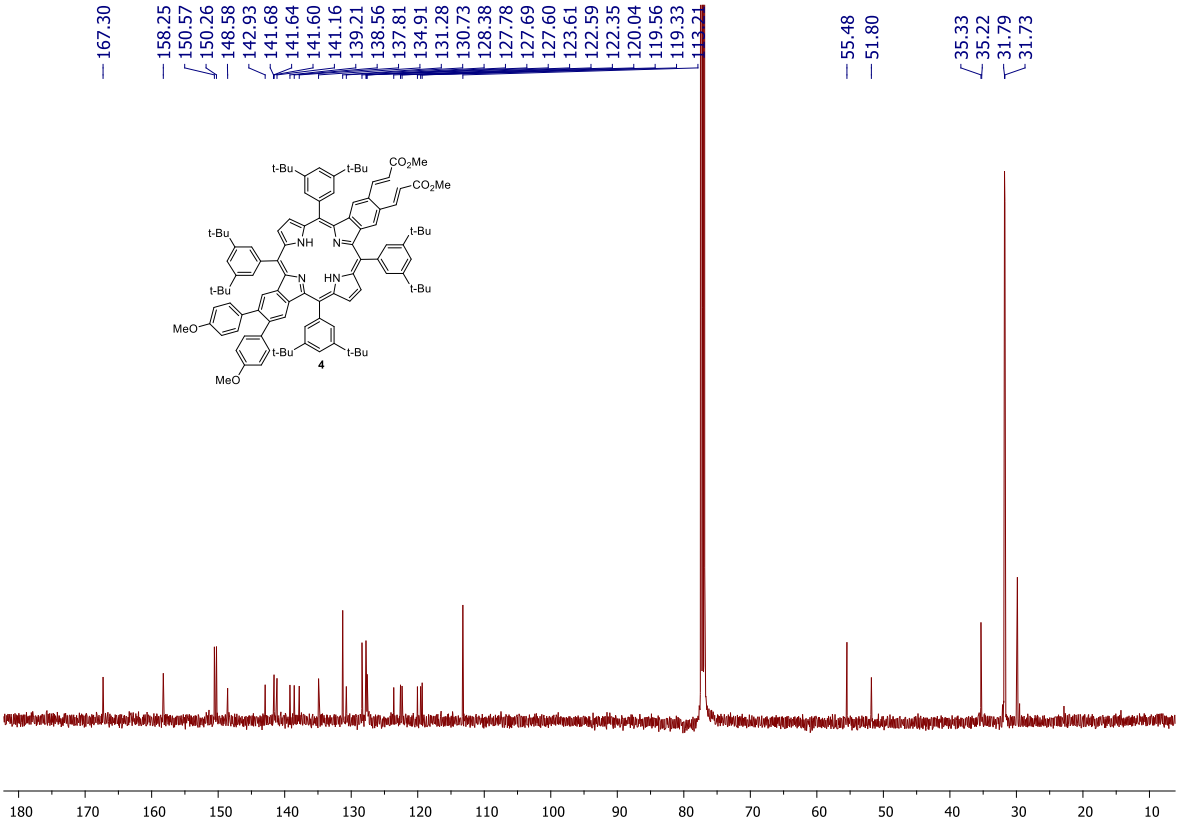
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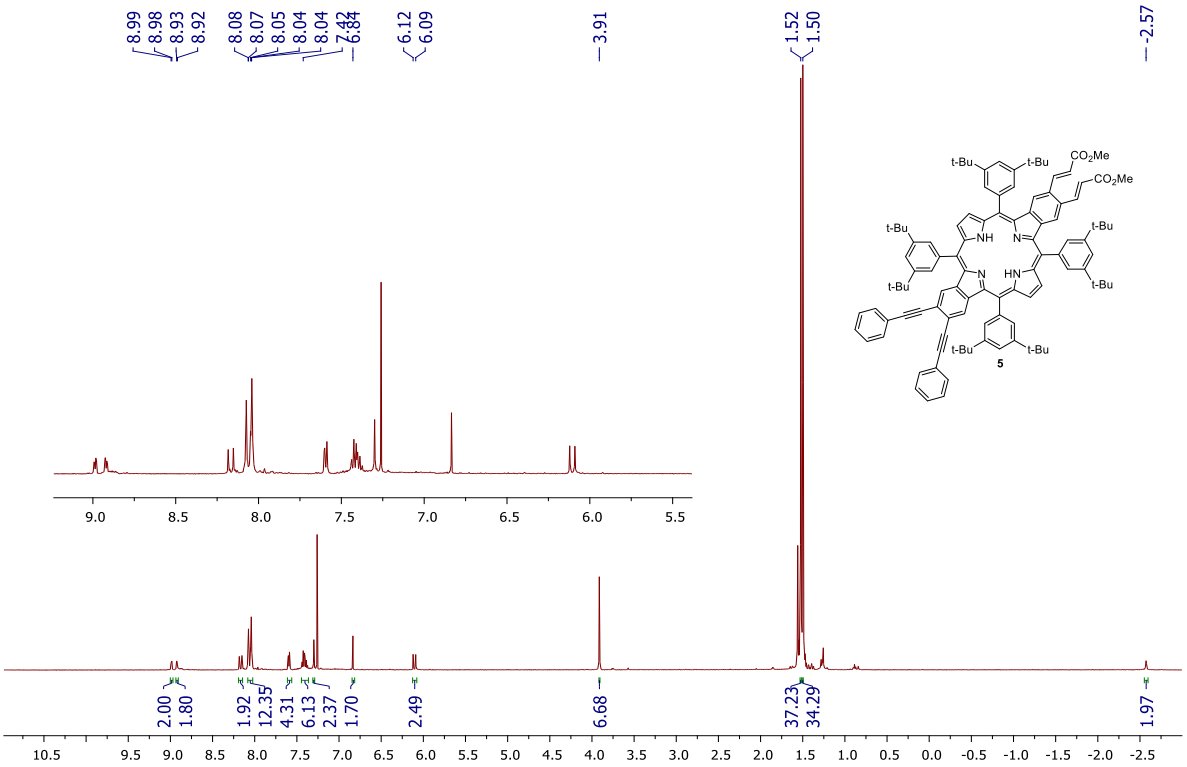
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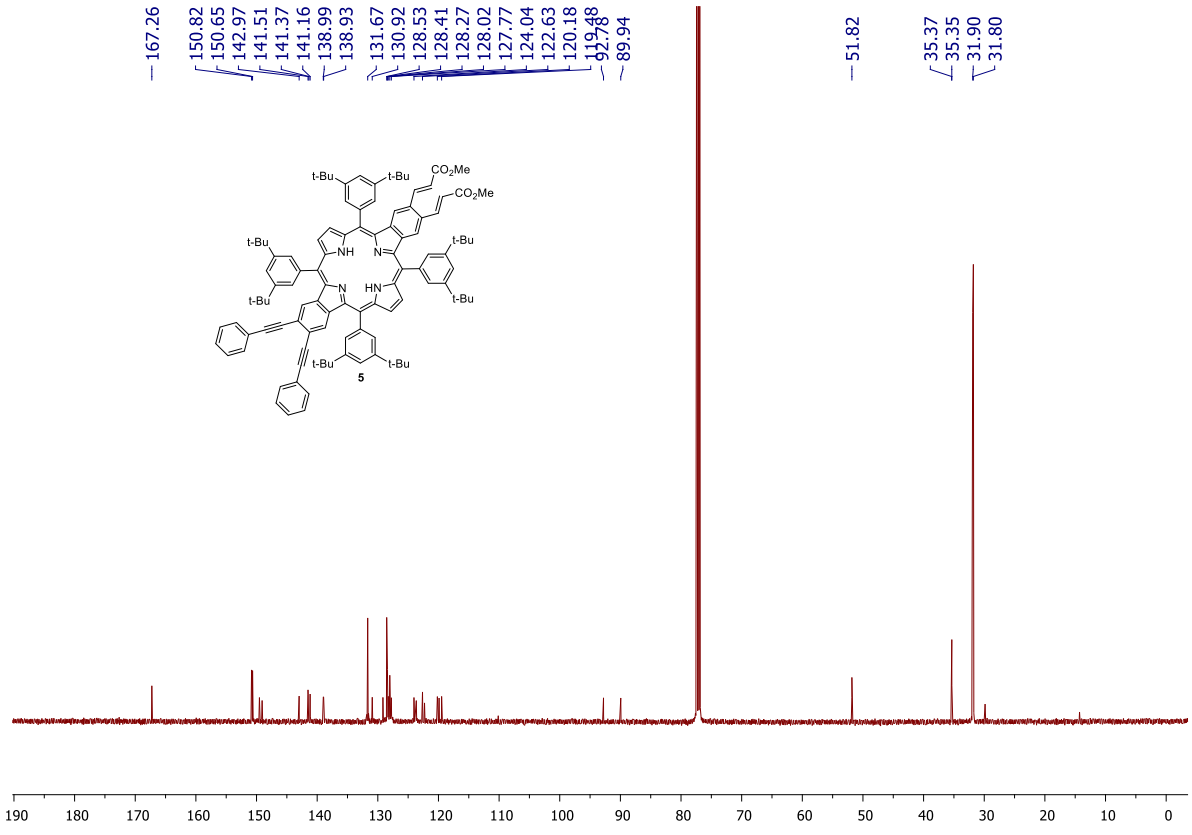
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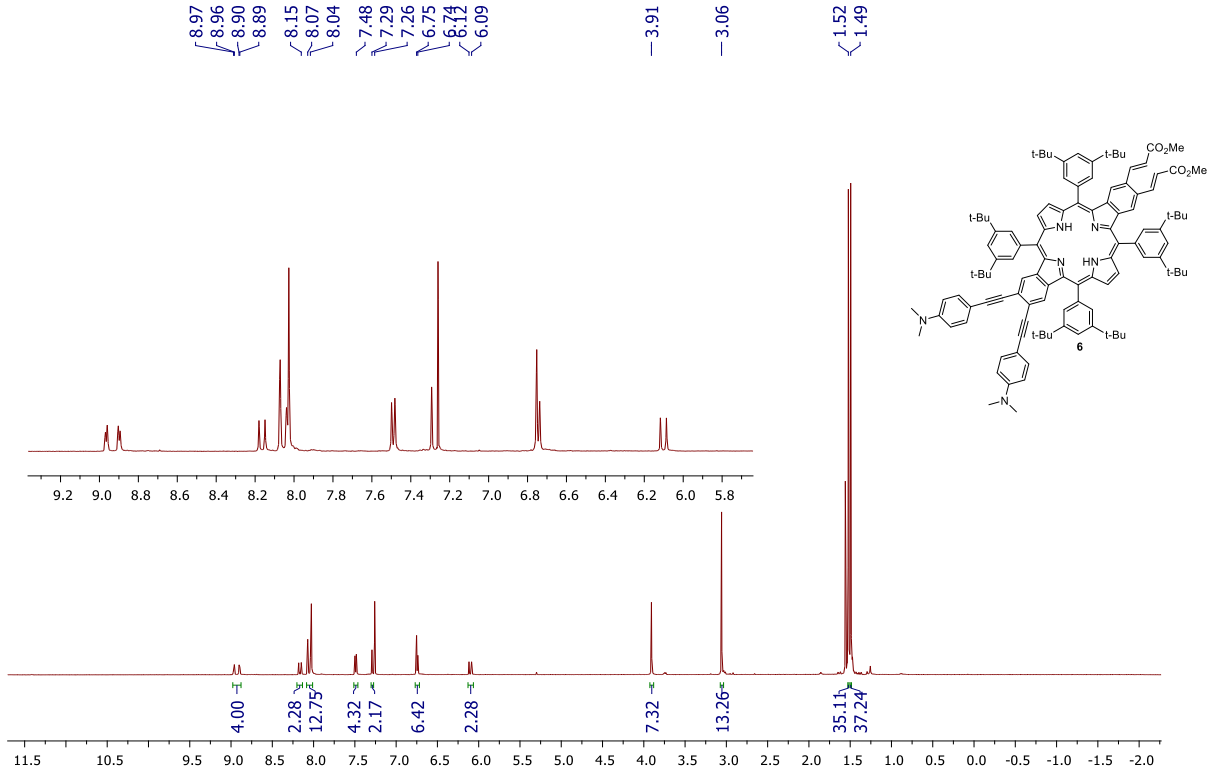
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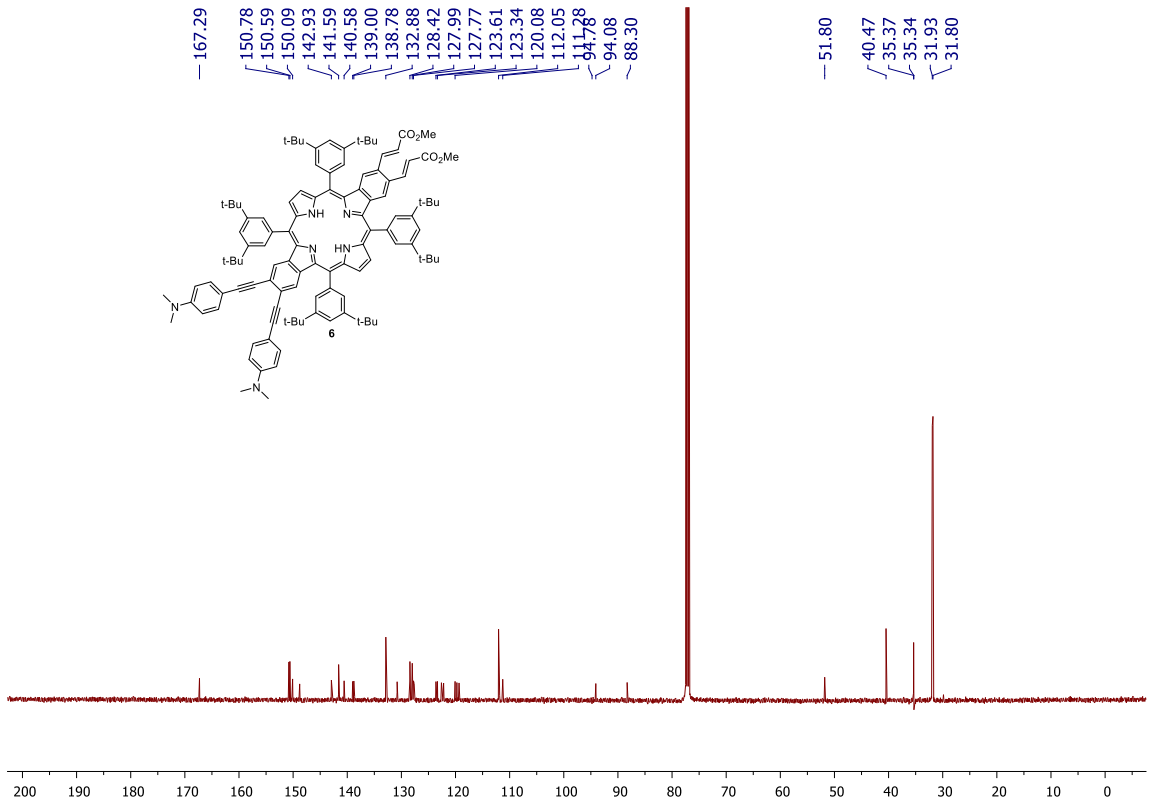
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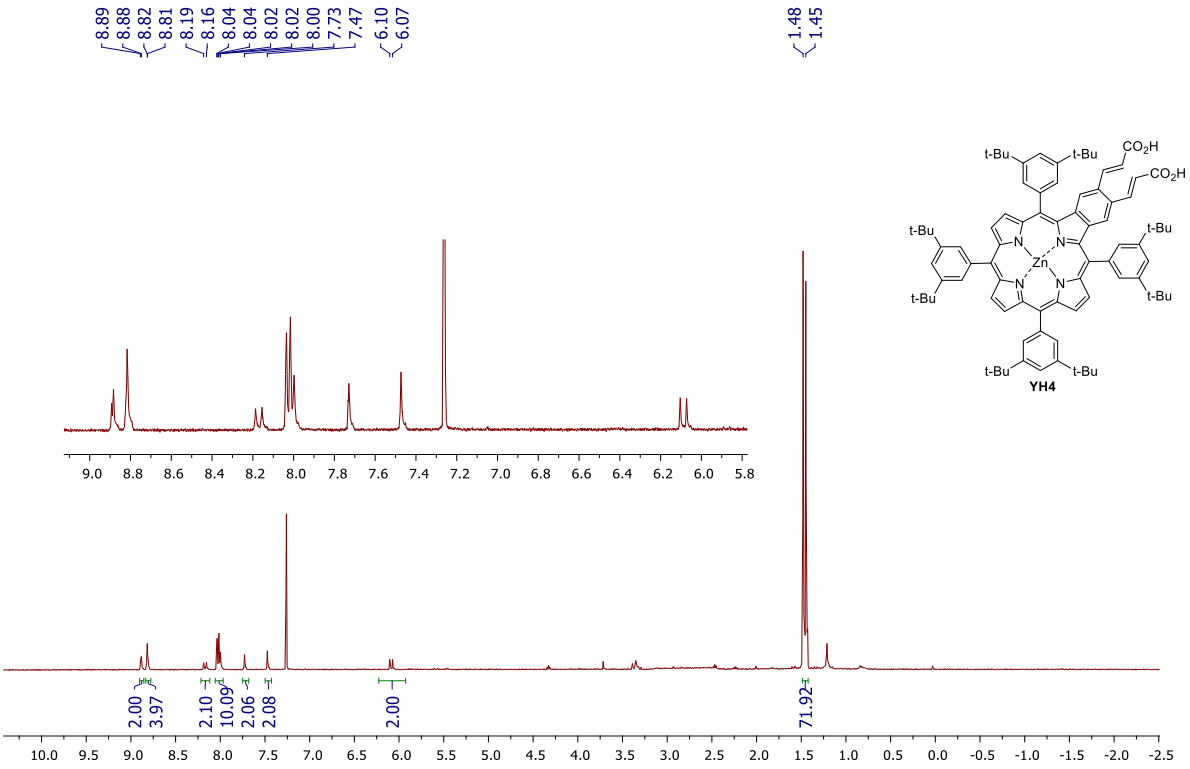
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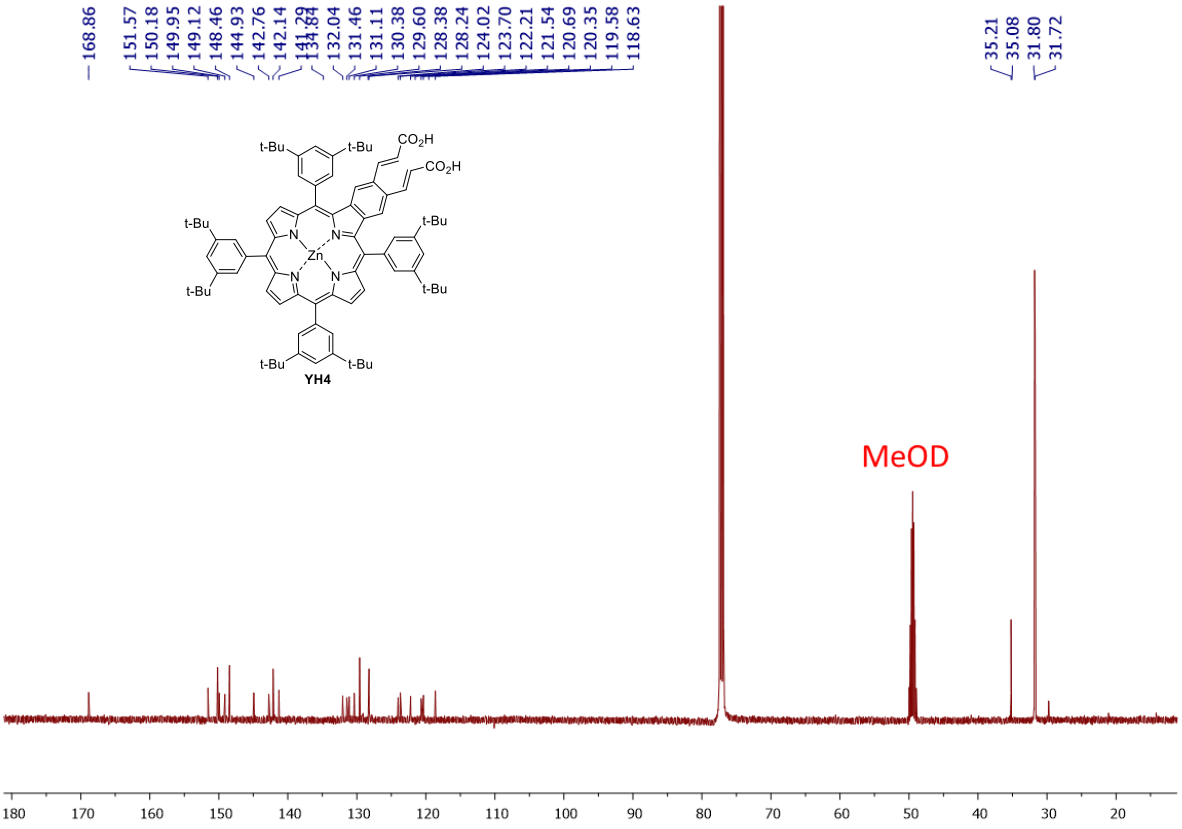
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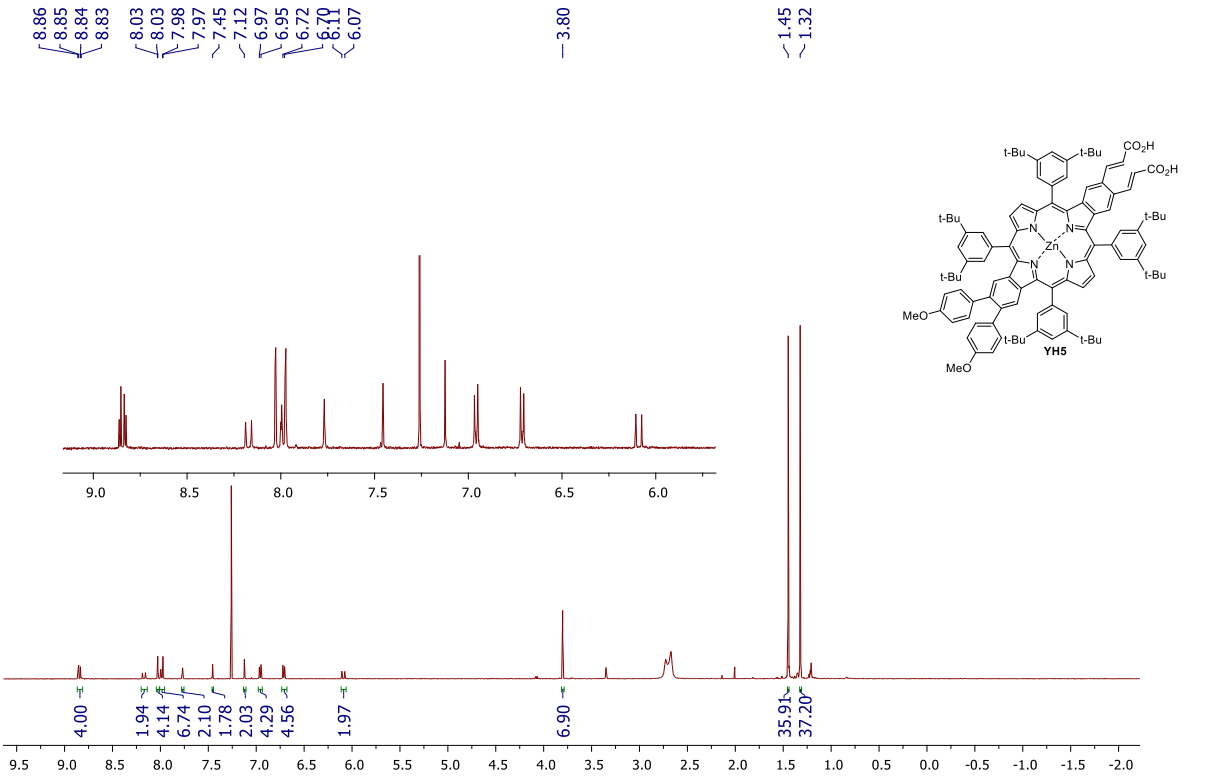
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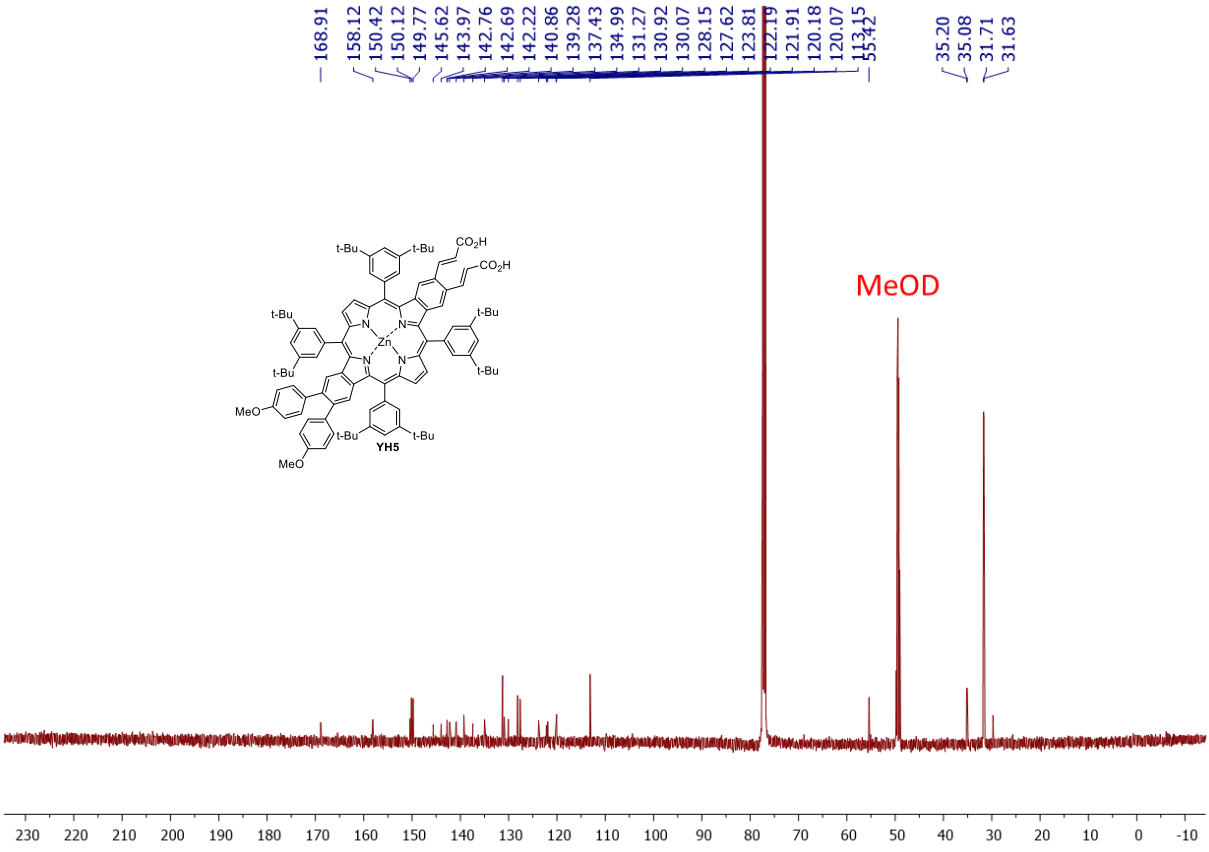
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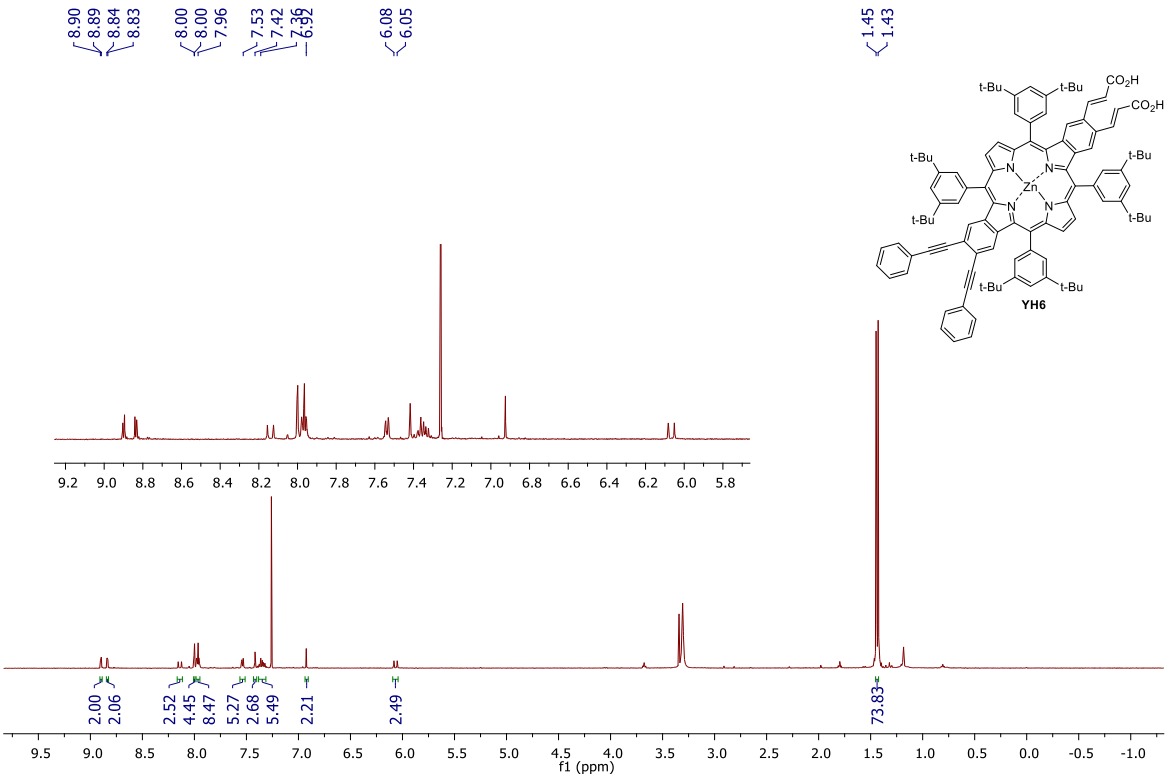
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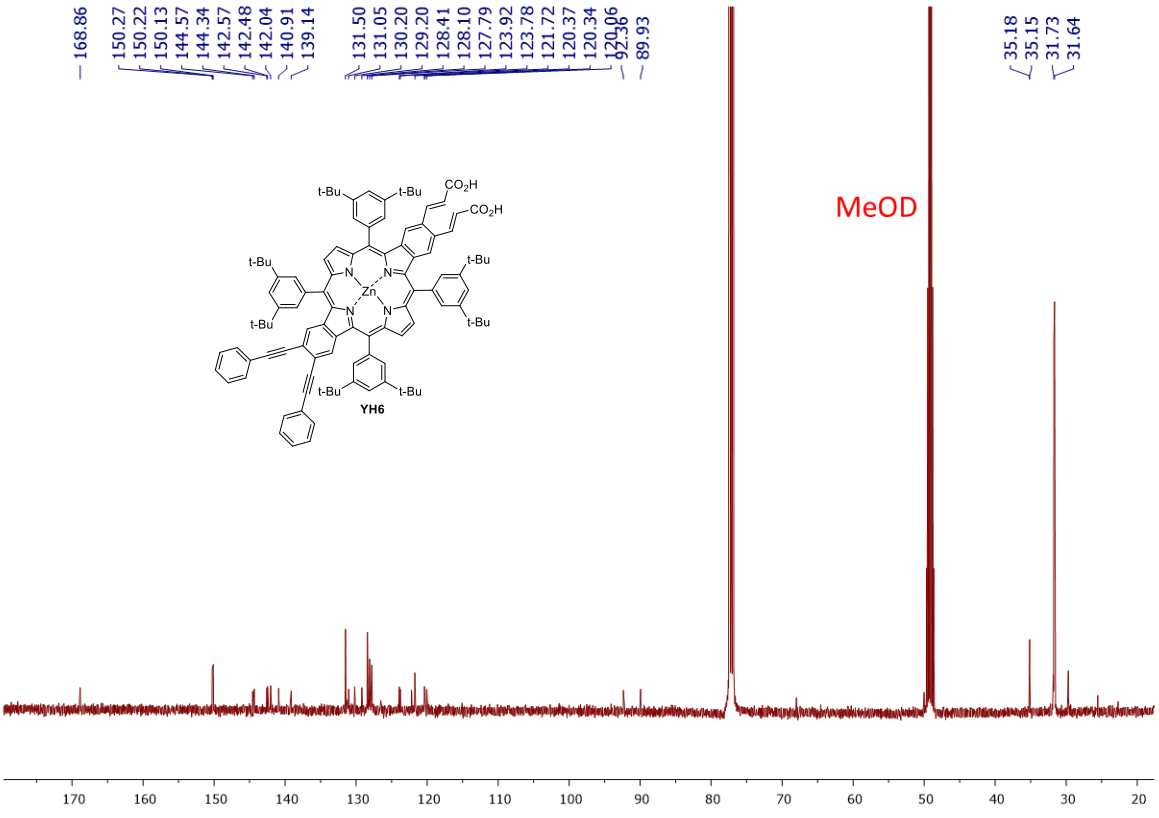
f1 (ppm)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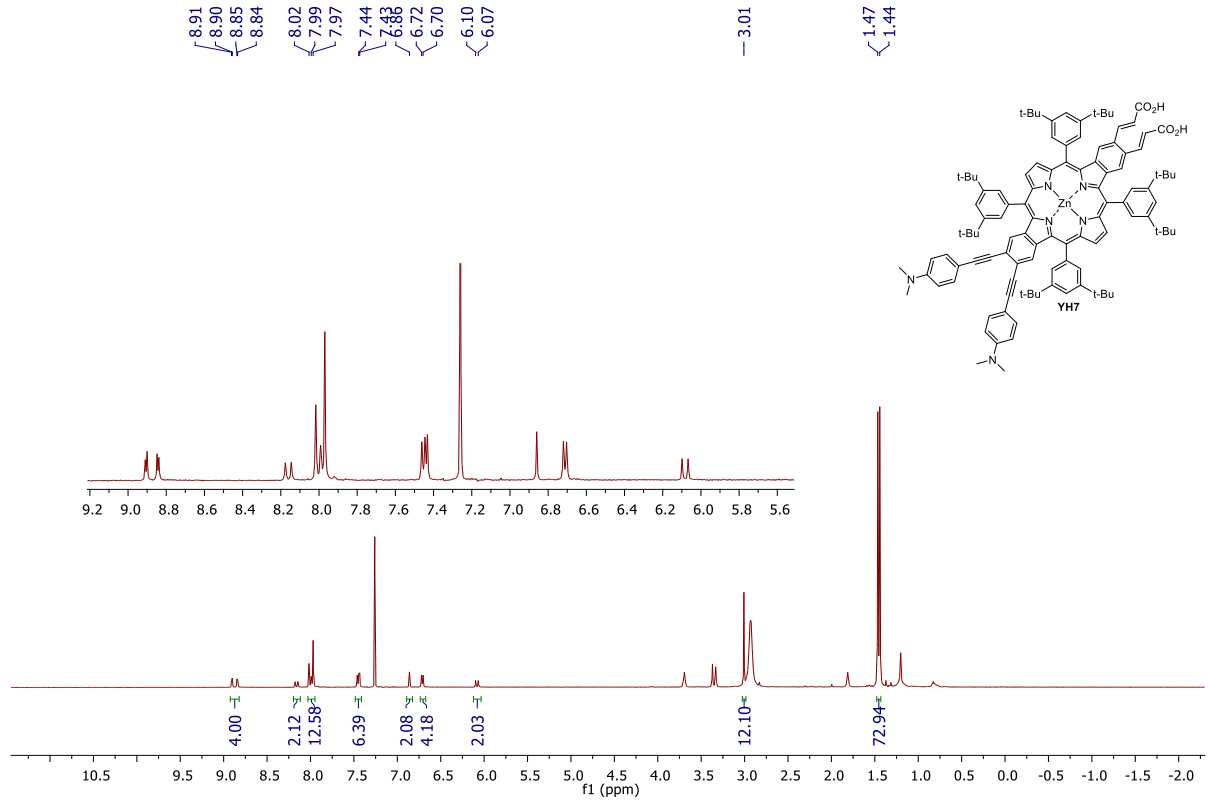
YH6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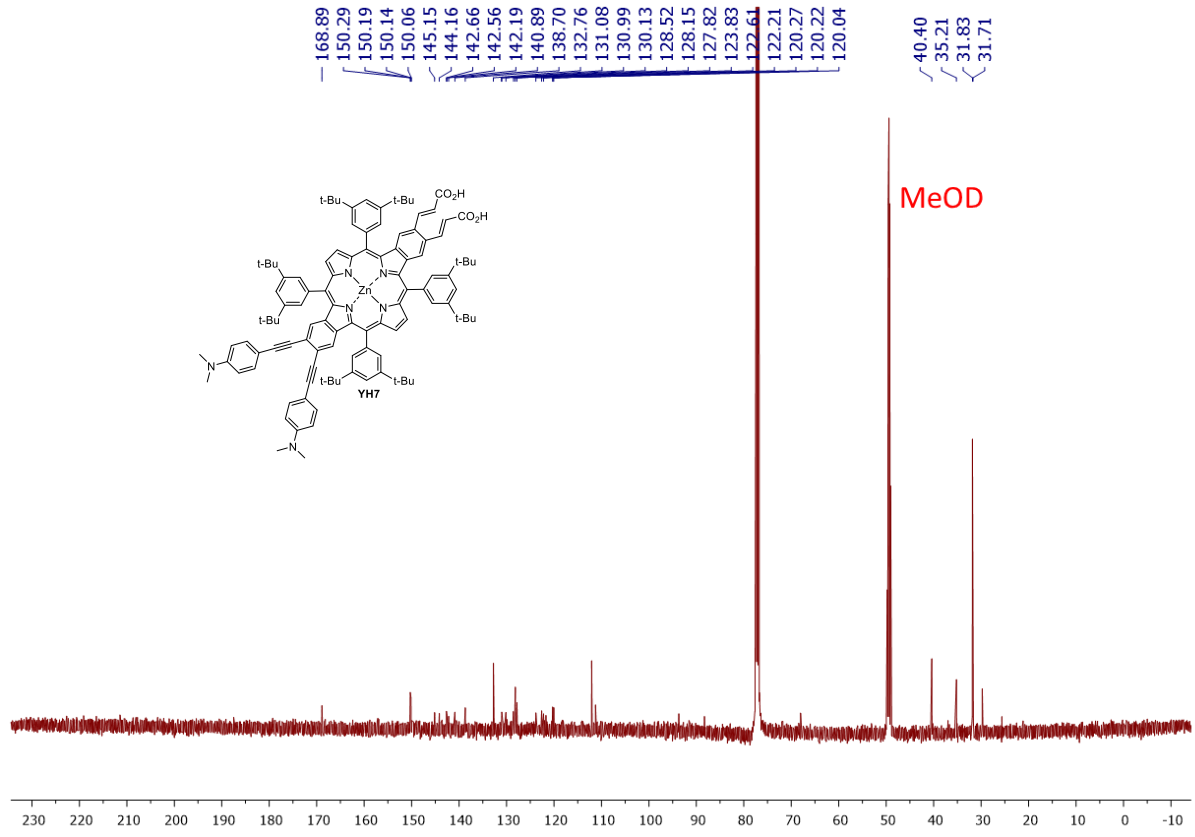
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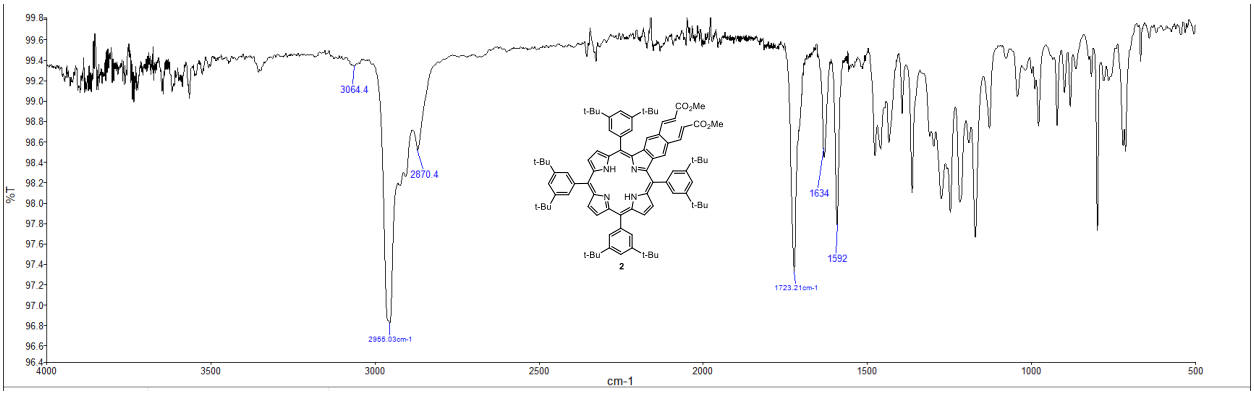
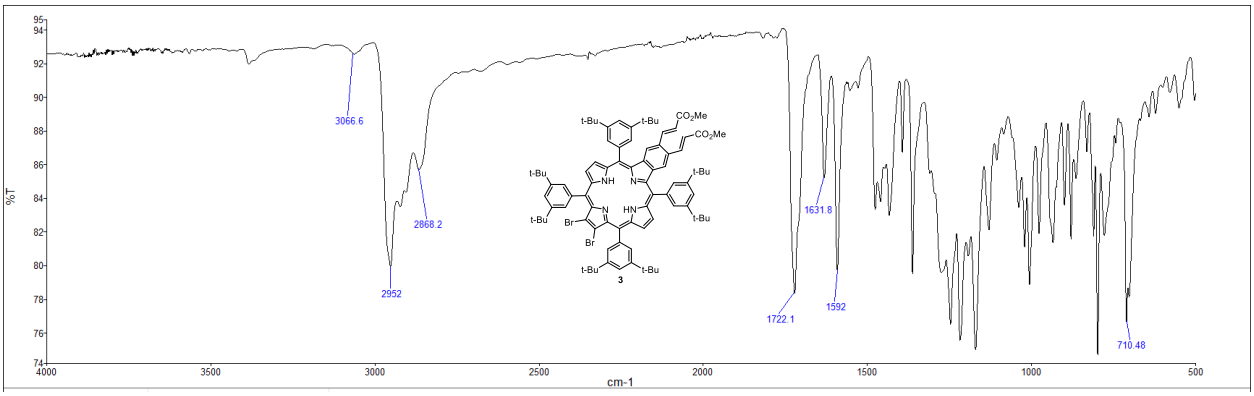
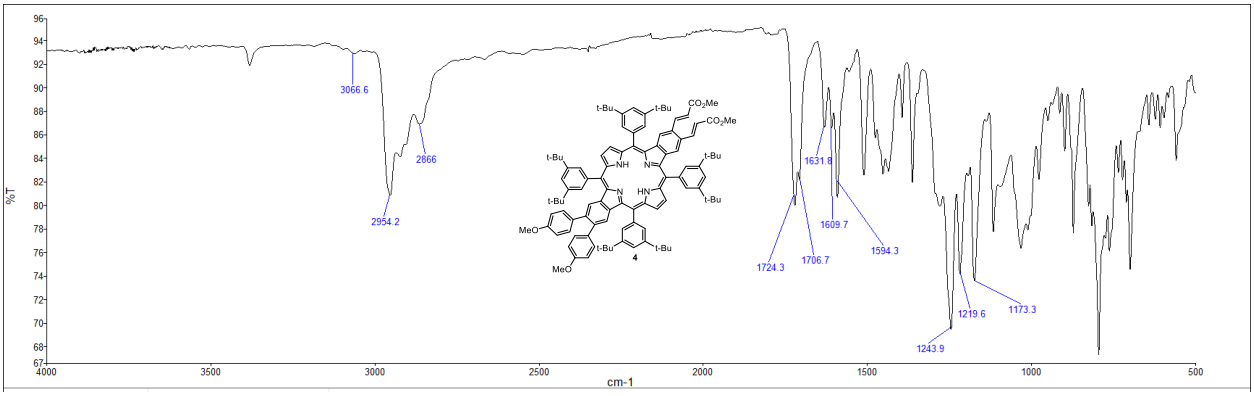
YH7

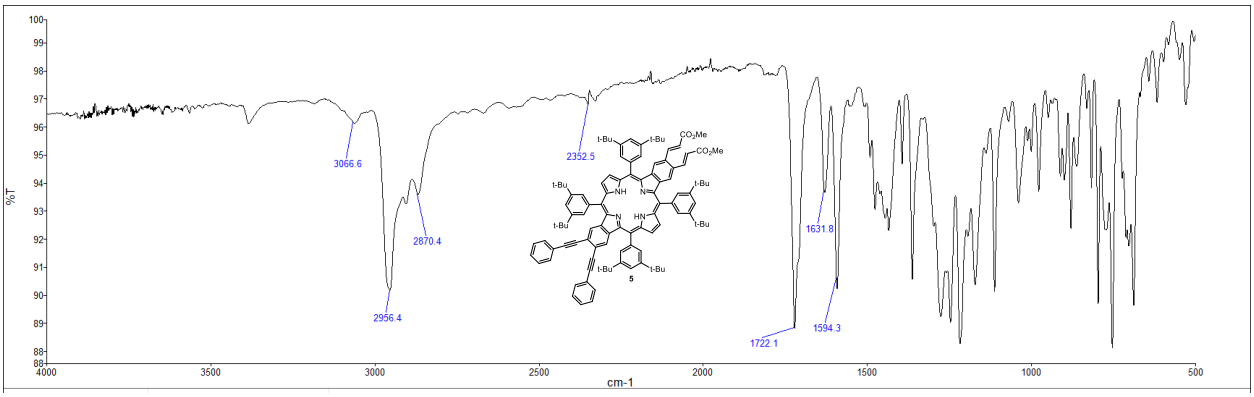
4. IR Characterization of Compounds

All FT-IR spectra were obtained using solid compounds.





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cm-1
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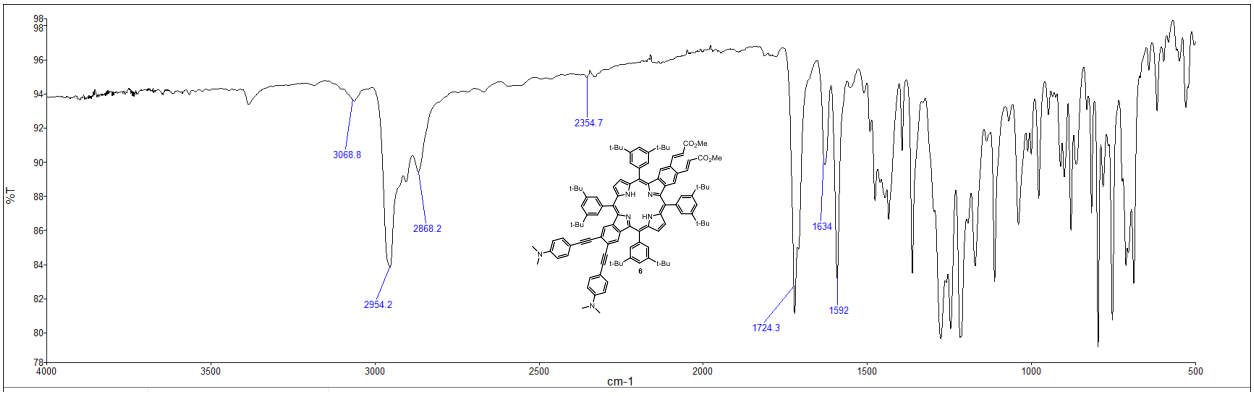
2956.4
2870.4
2352.5
1722.1
1631.8
1594.3
5


%T
cm-1
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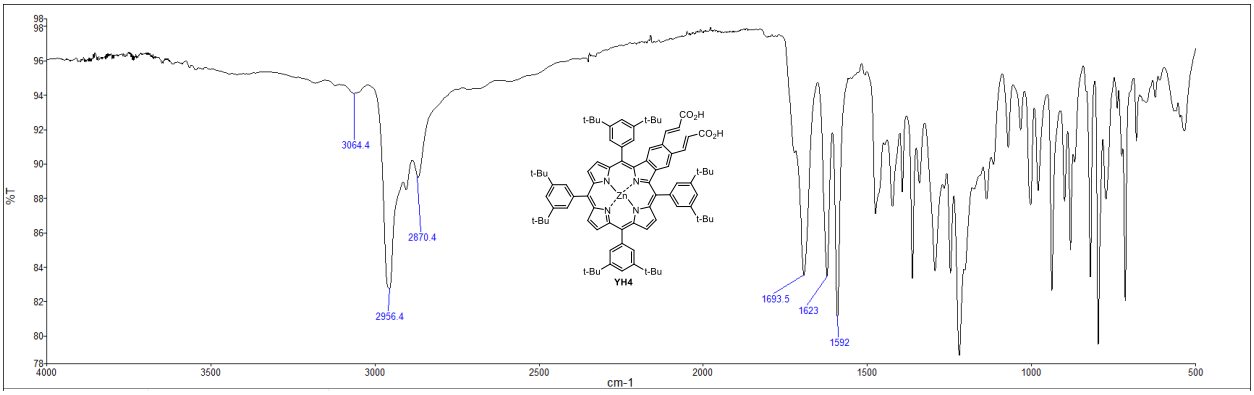
2954.2
2868.2
2354.7
1724.3
1634
1592
6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cm-1
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2870.4
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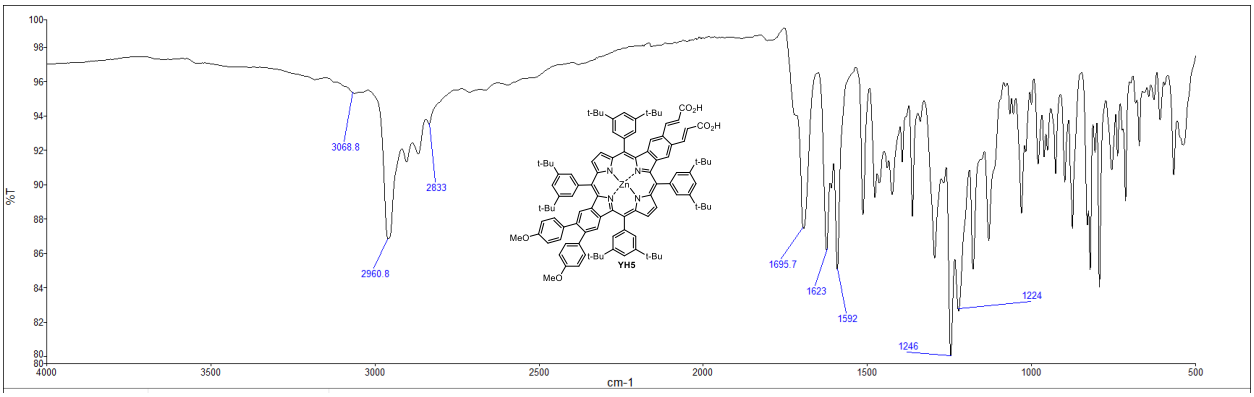
1623
1592
YH4


%T
cm-1
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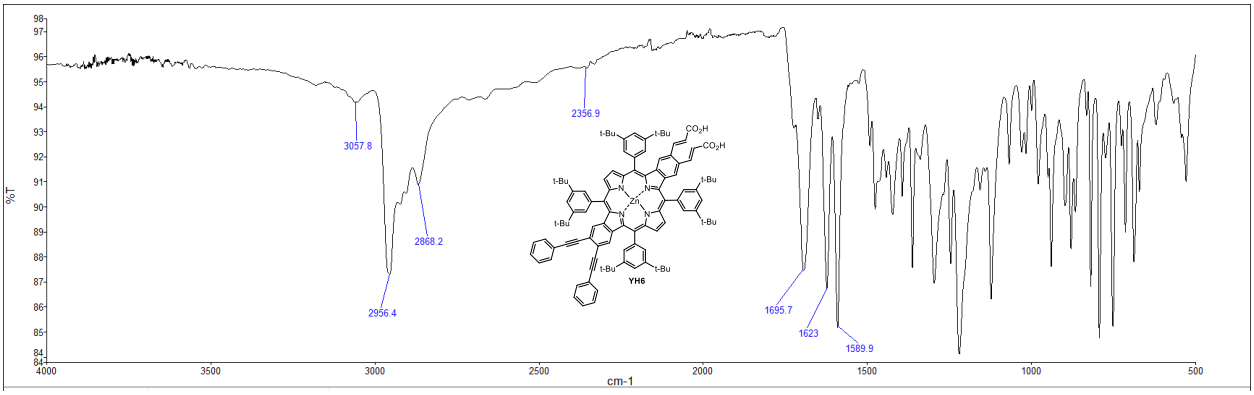
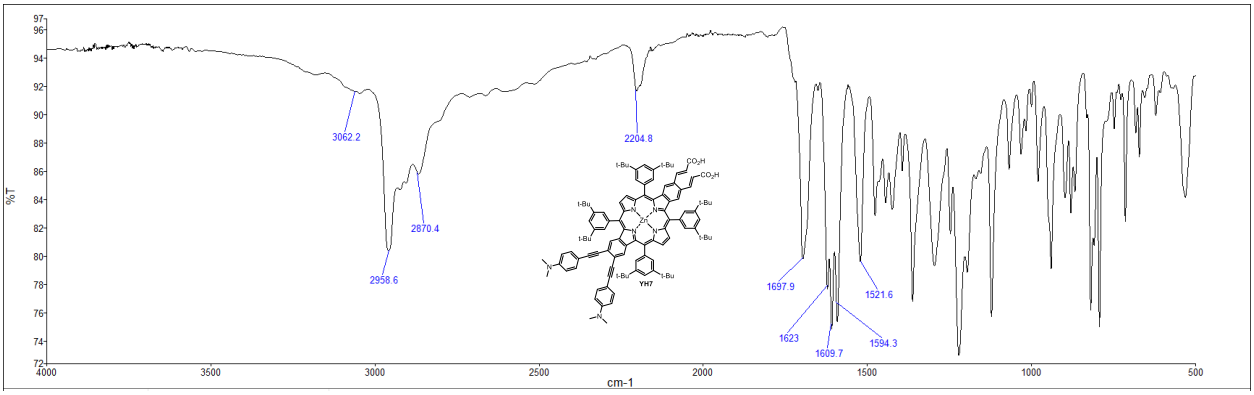
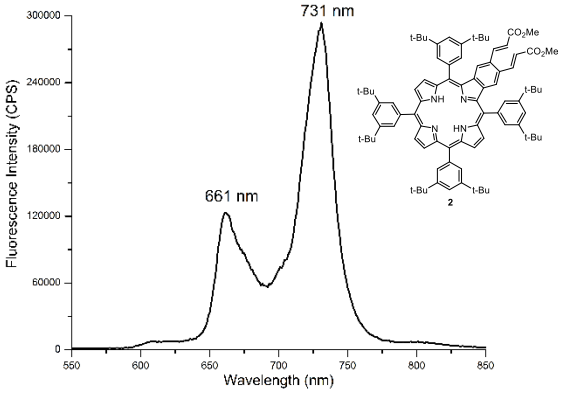
2960.8
2833
1695.7
1623
1592
1246
1224
YH5

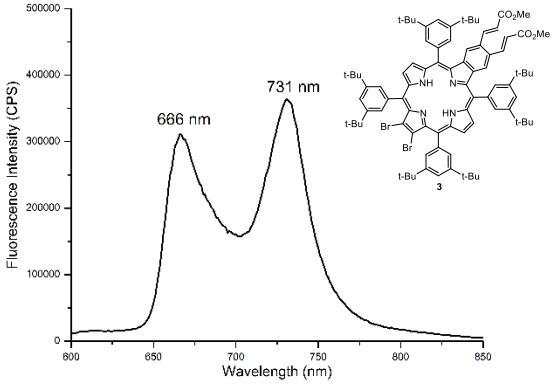

%T
cm-1
3057.8
2956.4
2868.2
2356.9
1695.7
1623
1589.9
YH6


%T
cm-1
3062.2
2958.6
2870.4
2204.8
1697.9
1623
1609.7
1594.3
1521.6
YH7

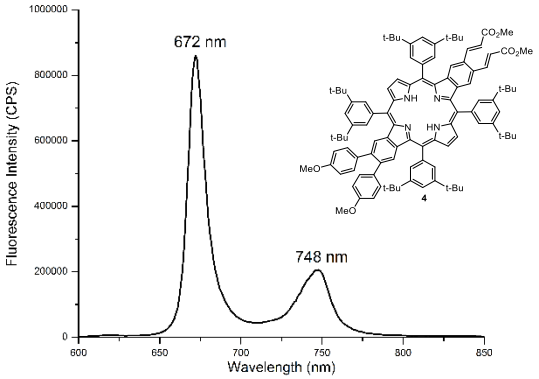
5. Steady-State Fluorescence Spectra in THF



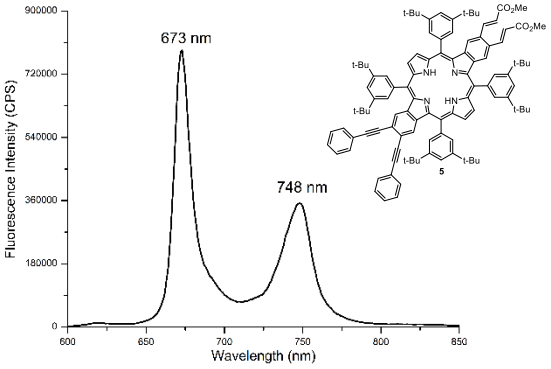
The sample was excited at 443 nm.



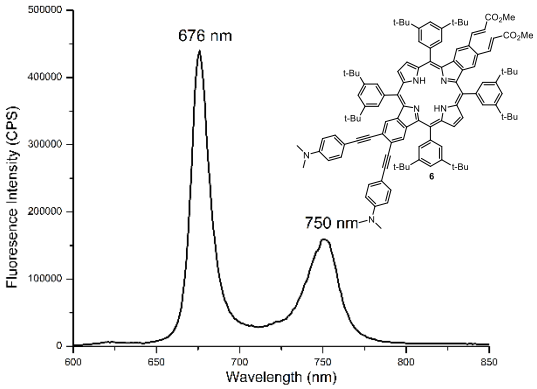
The sample was excited at 446 nm.



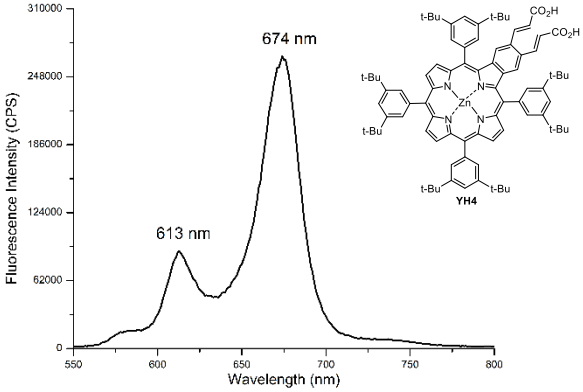
The sample was excited at 455 nm.



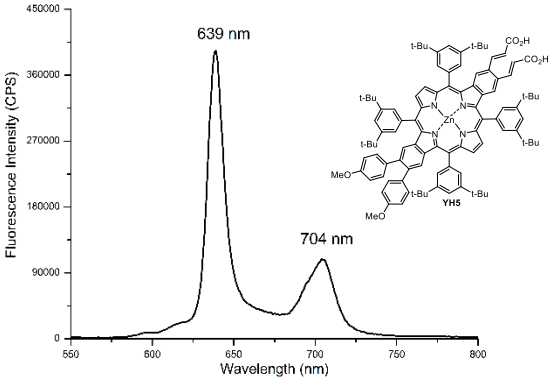
The sample was excited at 459 nm.



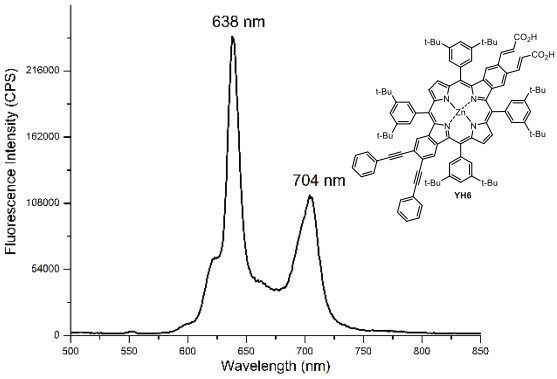
The sample was excited at 464 nm.



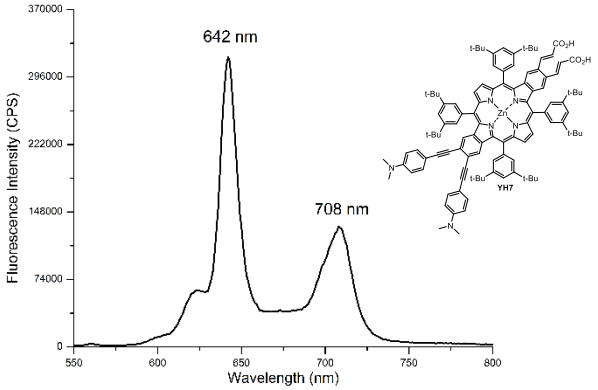
The sample was excited at 455 nm.



The sample was excited at 471 nm.



The sample was excited at 475 nm.



The sample was excited at 481 nm.

6. Table of Atom Coordinates for Optimized (in Vacuo) Structures YH4 – YH7

Atom coordinates for optimized structure **YH4**

	X	Y	Z
N	-3.25262	-0.01812	-0.03257
N	-1.20291	2.00522	0.00942
N	-1.18981	-2.02751	-0.00604
N	0.91957	-0.00487	0.05309
C	-4.07702	1.07973	-0.10842
C	-3.65436	2.42054	-0.06448
C	-2.31367	2.82893	0.0153
C	-4.0698	-1.12117	-0.11116
C	-3.63827	-2.45934	-0.07399
C	-2.29459	-2.85925	-0.00258
C	-0.08737	-2.84627	0.06923
C	1.26339	-2.44918	0.06844
C	1.72568	-1.12307	0.02979
C	-0.1072	2.8303	0.11219
C	1.24613	2.44179	0.12102
C	1.71627	1.11977	0.05252
C	-1.89609	4.20398	0.14059
C	-0.53805	4.20606	0.20179
C	3.11809	0.70982	-0.01996
C	3.12516	-0.69991	-0.02864
C	-0.50733	-4.22637	0.14068
C	-5.44438	-0.7057	-0.25884
C	-5.44882	0.65563	-0.2575
C	-4.70977	3.48479	-0.10016
C	-4.68689	-3.53012	-0.11566
C	2.26733	-3.56642	0.11441
C	2.23898	3.56304	0.25088
C	-5.57904	3.65328	0.9855
C	-6.57047	4.64183	0.97435
C	-6.66643	5.45368	-0.16463
C	-5.8187	5.31551	-1.2728
C	-4.83728	4.31813	-1.21911
C	-5.55166	-3.71388	0.97104
C	-6.53739	-4.70808	0.95354
C	-6.63229	-5.50969	-0.19277
C	-5.78891	-5.35611	-1.30225
C	-4.81322	-4.3535	-1.24209
C	2.66187	4.28019	-0.87468
C	3.60588	5.31071	-0.76341
C	4.08903	5.61159	0.51881
C	3.67263	4.93106	1.67233
C	2.74026	3.89813	1.51384
C	2.65937	-4.20714	-1.06652
C	3.62909	-5.21831	-1.0532
C	4.1859	-5.5674	0.18608
C	2.82319	-3.96425	1.33598
C	3.79882	-4.968	1.3942

C	4.32824	1.40768	-0.13532
C	5.55071	0.73657	-0.24847
C	4.34871	-1.38152	-0.08979
C	5.56657	-0.6946	-0.14863
C	-1.86614	-4.23295	0.09855
C	6.67872	1.60692	-0.59427
C	7.77624	1.33886	-1.32687
C	8.71061	2.44072	-1.66487
O	9.78686	2.08937	-2.42428
O	8.57637	3.59464	-1.31873
C	6.74474	-1.55119	0.01618
C	7.94044	-1.26849	0.56772
C	8.93647	-2.35472	0.74141
O	10.10504	-1.99191	1.34357
O	8.77719	-3.5041	0.39202
Zn	-1.18928	-0.01124	0.00648
C	4.10259	-5.93401	-2.33367
C	5.61338	-5.67147	-2.53981
C	3.86114	-7.45593	-2.19482
C	3.35425	-5.44468	-3.58795
C	4.46278	-5.40977	2.71305
C	4.2405	-6.92642	2.92273
C	5.98062	-5.11641	2.64424
C	3.88421	-4.67048	3.93426
C	-7.49724	-4.94647	2.13608
C	-7.30769	-6.38612	2.66988
C	-8.95825	-4.76487	1.66061
C	-7.24886	-3.96811	3.29975
C	-5.9632	-6.27468	-2.52813
C	-4.94692	-5.96345	-3.64281
C	-5.76969	-7.74873	-2.09995
C	-7.38523	-6.09309	-3.10987
C	4.10813	6.11495	-1.97873
C	5.65425	6.08525	-2.03251
C	3.57206	5.55369	-3.30947
C	3.63131	7.5813	-1.84404
C	4.25149	5.32492	3.04522
C	3.64715	4.49594	4.19444
C	5.7821	5.09898	3.03944
C	3.95494	6.81753	3.32466
C	-7.53514	4.86385	2.15623
C	-7.28564	3.8752	3.31087
C	-8.99384	4.68	1.67456
C	-7.35399	6.29902	2.70481
C	-5.99483	6.24467	-2.49043
C	-4.9731	5.9507	-3.60484
C	-5.81212	7.71577	-2.04758
C	-7.41386	6.05948	-3.07838
H	-2.56225	5.05189	0.18644
H	0.11837	5.0565	0.30201
H	0.15661	-5.07334	0.21891
H	-6.28778	-1.37128	-0.36338
H	-6.29651	1.3159	-0.36084
H	-5.45995	3.0016	1.84237

H	-7.43086	6.22384	-0.18922
H	-4.15834	4.16667	-2.04936
H	-5.43372	-3.06967	1.83373
H	-7.39249	-6.28389	-0.22216
H	-4.13796	-4.18982	-2.07304
H	2.25706	4.00342	-1.84085
H	4.81731	6.40902	0.62206
H	2.3926	3.33115	2.36906
H	2.20634	-3.88834	-1.99763
H	4.95031	-6.33741	0.21179
H	2.49693	-3.45828	2.23682
H	4.3376	2.48537	-0.19722
H	4.38265	-2.45936	-0.0543
H	-2.52591	-5.08607	0.14004
H	6.55851	2.65178	-0.31013
H	7.98199	0.33883	-1.69736
H	9.75662	1.14461	-2.6314
H	6.59593	-2.59739	-0.24902
H	8.18669	-0.26603	0.90592
H	10.08337	-1.05356	1.57886
H	5.81111	-4.60162	-2.66329
H	5.97042	-6.18676	-3.43857
H	6.2106	-6.02366	-1.69428
H	4.40403	-7.88063	-1.34564
H	4.19765	-7.97704	-3.09796
H	2.79714	-7.673	-2.0542
H	3.51777	-4.37781	-3.77121
H	2.27568	-5.61773	-3.51347
H	3.71586	-5.98769	-4.46694
H	3.1727	-7.16263	2.97917
H	4.71044	-7.25264	3.85712
H	4.67215	-7.51943	2.11145
H	6.46584	-5.63509	1.81317
H	6.47159	-5.43743	3.56974
H	6.16899	-4.04604	2.51476
H	2.81044	-4.85116	4.05059
H	4.04505	-3.58948	3.87134
H	4.37903	-5.02281	4.84489
H	-6.28149	-6.54224	3.01801
H	-7.51713	-7.13636	1.90188
H	-7.98423	-6.5732	3.51132
H	-9.21731	-5.46214	0.85855
H	-9.12495	-3.74928	1.28688
H	-9.65284	-4.9393	2.48999
H	-6.2386	-4.0687	3.70929
H	-7.95488	-4.17427	4.11056
H	-7.39207	-2.9263	2.99517
H	-5.05186	-4.9399	-4.0167
H	-5.10844	-6.64075	-4.48752
H	-3.91482	-6.0995	-3.30397
H	-4.7669	-7.90922	-1.69073
H	-5.89557	-8.41502	-2.96076
H	-6.49341	-8.05155	-1.33762
H	-7.54932	-5.05779	-3.42594

H	-8.16017	-6.34622	-2.38034
H	-7.52541	-6.74111	-3.98236
H	6.04003	5.06359	-2.10104
H	6.10739	6.54627	-1.15056
H	6.00942	6.63934	-2.90832
H	3.87766	4.51372	-3.46373
H	3.96919	6.14198	-4.14269
H	2.47975	5.60236	-3.36547
H	4.00921	8.04593	-0.92835
H	2.53789	7.63944	-1.82202
H	3.98619	8.17712	-2.69247
H	2.56195	4.62422	4.26273
H	4.07849	4.81956	5.14708
H	3.85885	3.42751	4.08399
H	6.02079	4.04604	2.85697
H	6.21255	5.38173	4.00673
H	6.28041	5.69167	2.26701
H	2.8766	7.00688	3.33905
H	4.39947	7.47195	2.56937
H	4.36391	7.10976	4.29822
H	-6.27724	3.97666	3.72475
H	-7.4227	2.8358	2.99539
H	-7.9953	4.06974	4.12139
H	-9.15449	3.66746	1.29009
H	-9.254	5.38409	0.87883
H	-9.69172	4.84268	2.50356
H	-6.3294	6.4566	3.057
H	-8.03343	6.4743	3.54647
H	-7.56527	7.05597	1.9439
H	-5.07027	4.93017	-3.98891
H	-3.94295	6.09022	-3.26151
H	-5.13643	6.63509	-4.44347
H	-4.81152	7.87881	-1.63401
H	-6.5399	8.00662	-1.28444
H	-5.93984	8.38943	-2.90234
H	-7.57025	5.02614	-3.40459
H	-7.55544	6.71466	-3.94527
H	-8.19271	6.3008	-2.34902

Atom coordinates for optimized structure **YH5**

	X	Y	Z
N	1.66245	-0.01031	0.30365
N	-0.46484	-1.98929	0.37994
N	-0.4421	1.99127	0.36412
N	-2.56323	0.01286	0.16789
C	2.45552	-1.13184	0.22319
C	1.98794	-2.44113	0.41337
C	0.63244	-2.8115	0.52038
C	2.46883	1.10252	0.23384
C	2.01455	2.41669	0.42965
C	0.66166	2.80138	0.52485
C	-1.54832	2.81734	0.42136
C	-2.88852	2.45007	0.21888
C	-3.34799	1.13398	0.02749
C	-1.57885	-2.80317	0.46028
C	-2.91751	-2.42018	0.28254
C	-3.36052	-1.1022	0.06525
C	0.19365	-4.16784	0.74555
C	-1.1657	-4.16215	0.70828
C	-4.72171	-0.68716	-0.25546
C	-4.71445	0.72383	-0.28211
C	-1.12544	4.1709	0.68032
C	3.84832	0.6826	-0.02545
C	3.84001	-0.7266	-0.02956
C	2.97708	-3.56152	0.57201
C	3.02057	3.51868	0.5943
C	-3.8916	3.5671	0.23242
C	-3.94104	-3.51564	0.37422
C	3.61121	-3.74885	1.80575
C	4.49358	-4.81659	2.01286
C	4.73357	-5.67864	0.93258
C	4.1275	-5.51807	-0.322
C	3.2347	-4.44954	-0.47919
C	3.7529	3.61339	1.78375
C	4.68658	4.63704	1.98205
C	4.85562	5.56978	0.94845
C	4.13962	5.51281	-0.25576
C	3.21735	4.4701	-0.41428
C	-4.16923	-4.37954	-0.70416
C	-5.15195	-5.37684	-0.63644
C	-5.8771	-5.49315	0.55874
C	-5.66245	-4.66152	1.66752
C	-4.68346	-3.6672	1.5512
C	-4.04023	4.39661	-0.8855
C	-5.00592	5.41169	-0.91036
C	-5.81024	5.56999	0.2277
C	-4.6967	3.77348	1.35915
C	-5.67418	4.77594	1.37622
C	-5.89244	-1.38061	-0.59054
C	-7.06359	-0.70339	-0.94643
C	-5.89344	1.41343	-0.59854

C	-7.08265	0.73192	-0.88113
C	0.23277	4.16078	0.75028
C	5.01092	-1.43041	-0.33261
C	6.20032	-0.75284	-0.62394
C	6.21586	0.6736	-0.58777
C	5.03662	1.36935	-0.30202
C	-8.11385	-1.57422	-1.48199
C	-9.05999	-1.31986	-2.40606
C	-9.9213	-2.42905	-2.88408
O	-10.83952	-2.09498	-3.83527
O	-9.85863	-3.57479	-2.49311
C	-8.26207	1.59773	-0.96725
C	-9.54306	1.33557	-0.64329
C	-10.54549	2.42813	-0.69378
O	-11.80818	2.08758	-0.30579
O	-10.31624	3.56448	-1.04665
C	7.38289	-1.57113	-1.01539
C	8.79978	-3.52544	-0.6557
C	7.73425	-2.71821	-0.27894
C	9.55129	-3.21205	-1.79663
C	9.21403	-2.08232	-2.55104
C	8.14348	-1.27967	-2.15599
C	7.45134	1.47898	-0.81105
C	8.62412	1.25384	-0.06512
C	9.75064	2.04452	-0.23735
C	9.74544	3.08971	-1.17345
C	7.4634	2.53032	-1.73509
C	8.59331	3.33075	-1.92818
O	10.58085	-4.06199	-2.085
C	11.38079	-3.78285	-3.22295
O	10.90555	3.80481	-1.271
C	10.95312	4.87966	-2.19484
Zn	-0.44507	0.0007	0.30362
C	-5.21481	6.33308	-2.12846
C	-6.64928	6.14398	-2.6763
C	-5.02012	7.80699	-1.69983
C	-4.22192	6.03245	-3.26694
C	-6.60063	5.01579	2.58439
C	-6.43998	6.47253	3.07978
C	-8.06872	4.77634	2.15741
C	-6.28291	4.07408	3.76122
C	4.38018	6.58222	-1.33947
C	3.54519	6.32752	-2.60865
C	3.99576	7.97299	-0.78063
C	5.8744	6.58862	-1.74034
C	5.51901	4.76505	3.27233
C	5.21533	6.1217	3.95119
C	7.02428	4.69235	2.92128
C	5.20794	3.64347	4.28145
C	5.16959	-5.0856	3.37219
C	4.69809	-6.45858	3.90831
C	4.82053	-4.01363	4.42172
C	6.70692	-5.10681	3.20291
C	4.44485	-6.50968	-1.45838

C	3.75353	-6.12413	-2.78014
C	5.97127	-6.5439	-1.70822
C	3.96036	-7.92232	-1.05384
C	-5.45013	-6.33416	-1.8072
C	-6.95163	-6.26362	-2.1757
C	-4.63124	-5.98986	-3.06587
C	-5.0975	-7.77951	-1.38095
C	-6.50072	-4.85747	2.94587
C	-6.11184	-3.86453	4.05723
C	-7.99774	-4.64925	2.61532
C	-6.29038	-6.29114	3.48812
H	0.84565	-5.01271	0.90387
H	-1.83417	-5.00049	0.83035
H	-1.78708	5.01595	0.79309
H	3.39087	-3.05057	2.60423
H	5.41424	-6.5121	1.07514
H	2.73055	-4.28445	-1.42375
H	3.58159	2.86631	2.54927
H	5.57212	6.37315	1.08763
H	2.63825	4.37727	-1.32514
H	-3.58236	-4.24271	-1.60447
H	-6.63893	-6.26276	0.62677
H	-4.48527	-2.98773	2.37139
H	-3.39981	4.22207	-1.74164
H	-6.57289	6.34191	0.21974
H	-4.55871	3.12304	2.21439
H	-5.89503	-2.4601	-0.63888
H	-5.91677	2.49331	-0.59957
H	0.88948	4.99712	0.93175
H	5.00401	-2.50856	-0.40241
H	5.07318	2.44875	-0.28144
H	-8.05368	-2.61413	-1.16302
H	-9.19387	-0.32759	-2.82689
H	-10.76697	-1.15542	-4.05512
H	-8.05697	2.63508	-1.22966
H	-9.85658	0.34482	-0.32721
H	-11.83687	1.15803	-0.03855
H	9.07344	-4.40179	-0.07744
H	7.165	-2.9746	0.60939
H	9.7689	-1.82023	-3.44393
H	7.89393	-0.41194	-2.7569
H	8.64672	0.44892	0.66232
H	10.6509	1.87487	0.34412
H	6.57521	2.72199	-2.33046
H	8.56129	4.12598	-2.66352
H	12.13714	-4.56825	-3.25965
H	11.87727	-2.80753	-3.14033
H	10.7923	-3.80655	-4.1492
H	11.95148	5.31052	-2.10587
H	10.20605	5.64918	-1.96107
H	10.79997	4.53602	-3.22611
H	-6.81005	5.11253	-3.00666
H	-6.81889	6.80374	-3.53458
H	-7.40992	6.37295	-1.92482

H	-5.73014	8.10464	-0.92296
H	-5.16755	8.47386	-2.55662
H	-4.00989	7.97233	-1.31106
H	-4.33337	5.01201	-3.64752
H	-3.18281	6.16763	-2.94936
H	-4.40326	6.71588	-4.1026
H	-5.40885	6.66995	3.39111
H	-7.09516	6.65547	3.93862
H	-6.7003	7.19925	2.30496
H	-8.37485	5.43548	1.34054
H	-8.74379	4.9559	3.00172
H	-8.21575	3.74579	1.81909
H	-5.25835	4.20524	4.12481
H	-6.41821	3.02202	3.49048
H	-6.95919	4.28748	4.59513
H	3.78361	5.36187	-3.06627
H	3.75466	7.10553	-3.34979
H	2.47042	6.35117	-2.40228
H	2.93766	8.00363	-0.50069
H	4.16962	8.74942	-1.53428
H	4.58242	8.23144	0.10587
H	6.18006	5.61046	-2.12525
H	6.52431	6.82739	-0.89358
H	6.05579	7.33657	-2.52053
H	4.15762	6.19536	4.22453
H	5.45072	6.9668	3.29755
H	5.81082	6.23147	4.86442
H	7.32508	5.49882	2.24613
H	7.27	3.74336	2.43436
H	7.63037	4.77722	3.83037
H	4.15932	3.65599	4.59595
H	5.82213	3.7753	5.17799
H	5.43083	2.65348	3.87096
H	3.61216	-6.4723	4.04694
H	5.16689	-6.67242	4.87546
H	4.95745	-7.27215	3.22444
H	3.74645	-3.98034	4.63025
H	5.13854	-3.01521	4.10456
H	5.33131	-4.24018	5.36318
H	7.03036	-5.86693	2.48601
H	7.19097	-5.32715	4.16093
H	7.07777	-4.13701	2.85485
H	4.06366	-5.13345	-3.12793
H	2.6625	-6.12928	-2.68946
H	4.02061	-6.84635	-3.55824
H	6.35291	-5.5511	-1.96591
H	6.20426	-7.22557	-2.53385
H	6.52187	-6.89219	-0.82954
H	2.87858	-7.93206	-0.88449
H	4.44527	-8.27036	-0.13687
H	4.18645	-8.64484	-1.84612
H	-7.2513	-5.2531	-2.47003
H	-7.59431	-6.56517	-1.34393
H	-7.1651	-6.9357	-3.01413

H	-4.84302	-4.97713	-3.42384
H	-4.88784	-6.68494	-3.87152
H	-3.55365	-6.07392	-2.89104
H	-5.67567	-8.09642	-0.50785
H	-4.03549	-7.86747	-1.12849
H	-5.31211	-8.47987	-2.19588
H	-5.06445	-3.97623	4.35592
H	-6.72859	-4.04425	4.94361
H	-6.27119	-2.82576	3.75067
H	-8.17733	-3.63793	2.2361
H	-8.60904	-4.78838	3.51413
H	-8.35223	-5.3558	1.85948
H	-5.23811	-6.4663	3.73493
H	-6.59469	-7.05152	2.76304
H	-6.88261	-6.44408	4.39725

Atom coordinates for optimized structure **YH6**

	X	Y	Z
C	3.79922	0.71337	-0.02409
C	3.80332	-0.7014	0.00005
C	2.41844	-1.11231	0.23752
N	1.61783	0.00433	0.29574
C	2.413	1.12351	0.20868
C	-1.1988	4.16209	0.72399
C	0.161	4.16615	0.73348
C	0.59338	2.8094	0.50104
N	-0.50815	1.9883	0.38153
C	-1.61852	2.80413	0.48143
C	1.94584	2.43743	0.37822
C	-4.7736	-0.70441	-0.26738
C	-4.77713	0.70509	-0.22078
C	-3.4112	1.11245	0.09541
N	-2.61578	-0.00557	0.17829
C	-3.40488	-1.12242	0.02761
C	-2.96169	2.42597	0.31993
C	0.17027	-4.16884	0.69816
C	-1.18769	-4.17393	0.62573
C	-1.60675	-2.81428	0.3923
N	-0.49922	-1.99008	0.35222
C	0.6025	-2.8065	0.50119
C	1.9556	-2.42643	0.4184
C	-2.94741	-2.44116	0.19666
C	2.94158	3.55748	0.46799
C	-3.97957	3.52466	0.43421
C	-3.95032	-3.55845	0.18949
C	2.95674	-3.53641	0.55978
C	3.68415	3.74058	1.64039
C	4.63143	4.7662	1.74493
C	4.8018	5.60811	0.636
C	4.06753	5.46642	-0.55022
C	3.13107	4.42657	-0.61314
C	3.19139	-4.42596	-0.49579
C	4.13052	-5.45863	-0.3766
C	4.8177	-5.57387	0.84054
C	4.60349	-4.70908	1.92387
C	3.65817	-3.68922	1.76132
C	-4.09845	-4.36559	-0.94468
C	-5.06073	-5.38323	-0.98831
C	-5.86315	-5.56596	0.1474
C	-5.72895	-4.79328	1.31057
C	-4.75357	-3.7887	1.31278
C	-4.70452	3.66914	1.62278
C	-5.6748	4.66887	1.76285
C	-5.89885	5.51319	0.66558
C	-5.19283	5.40272	-0.5415
C	-4.218	4.39958	-0.63293
C	-5.95597	-1.38581	-0.58589
C	-7.14625	-0.69836	-0.85225

C	-7.12394	0.73705	-0.89721
C	-5.94782	1.40542	-0.53841
C	4.98725	-1.40629	-0.24228
C	6.17656	-0.71291	-0.49703
C	6.17399	0.72059	-0.51548
C	4.97991	1.41597	-0.28923
C	7.37477	1.4432	-0.75453
C	8.4005	2.07039	-0.94204
C	9.61473	2.78259	-1.15864
C	10.85779	2.12937	-1.03006
C	9.59728	4.14928	-1.50271
C	10.78884	4.83664	-1.71495
C	12.04374	2.8258	-1.24365
C	12.01502	4.17968	-1.58719
C	7.37078	-1.44027	-0.75349
C	8.38093	-2.07924	-0.98127
C	9.57061	-2.81224	-1.25619
C	9.6575	-4.18426	-0.94489
C	10.68222	-2.17714	-1.84703
C	11.84376	-2.89632	-2.11303
C	10.82362	-4.89457	-1.2147
C	11.9202	-4.25529	-1.79808
C	-5.49944	6.374	-1.69854
C	-4.71596	6.02304	-2.97782
C	-5.10929	7.80892	-1.26969
C	-7.00969	6.33592	-2.03462
C	-6.49359	4.85729	3.05476
C	-6.26556	6.2838	3.60869
C	-7.99651	4.66251	2.74327
C	-6.0958	3.8501	4.15008
C	4.42772	-6.4477	-1.5207
C	5.92562	-6.36332	-1.89983
C	4.09752	-7.88628	-1.05676
C	3.59769	-6.14853	-2.78353
C	5.40699	-4.89818	3.22495
C	5.04263	-3.85055	4.29367
C	6.91784	-4.76616	2.91715
C	5.12292	-6.3019	3.80992
C	-5.26702	-6.28209	-2.22347
C	-4.27841	-5.95348	-3.35785
C	-5.06278	-7.76272	-1.82346
C	-6.70372	-6.09115	-2.76486
C	-6.65534	-5.05751	2.51358
C	-6.34264	-4.13481	3.70676
C	-8.12396	-4.81632	2.08916
C	-6.48948	-6.52208	2.98358
C	4.31566	6.4332	-1.72482
C	5.7912	6.32279	-2.17801
C	4.02757	7.88372	-1.27017
C	3.41803	6.12484	-2.93812
C	5.48706	4.98357	3.00805
C	5.22653	6.39983	3.5734
C	6.98384	4.84372	2.64086
C	5.16739	3.96017	4.11374

Zn	-0.49872	-0.00047	0.30014
C	-8.32569	-1.56484	-0.9502
C	-9.60795	-1.30661	-0.63025
C	-10.60016	-2.39533	-0.68652
O	-11.8373	-1.96	-0.32763
O	-10.38943	-3.55314	-1.00135
H	-12.41761	-2.73667	-0.39093
C	-8.17532	1.62244	-1.40939
C	-9.13467	1.38533	-2.32363
C	-9.98174	2.50094	-2.78194
O	-10.89761	2.0879	-3.69738
O	-9.90742	3.66344	-2.4235
H	-11.39988	2.88223	-3.94398
H	-1.86368	5.00087	0.86113
H	0.8176	5.00932	0.88167
H	0.82564	-5.00999	0.86212
H	-1.85179	-5.01922	0.72005
H	3.51813	3.05637	2.46355
H	5.53643	6.40455	0.69884
H	2.54238	4.26689	-1.50829
H	2.63598	-4.28728	-1.41537
H	5.54826	-6.36918	0.94892
H	3.45755	-2.98855	2.56275
H	-3.45992	-4.17175	-1.7981
H	-6.62323	-6.34022	0.12588
H	-4.61674	-3.15467	2.18042
H	-4.49927	2.98036	2.43341
H	-6.65306	6.28826	0.75305
H	-3.64539	4.26652	-1.54295
H	-5.98176	-2.46536	-0.60387
H	-5.9484	2.48544	-0.5694
H	5.01439	-2.48501	-0.25522
H	5.00296	2.49399	-0.3329
H	10.87524	1.07974	-0.75497
H	8.64295	4.65609	-1.60217
H	10.76134	5.8892	-1.98153
H	12.99463	2.31127	-1.13994
H	12.94246	4.71951	-1.75348
H	8.80345	-4.67615	-0.49079
H	10.61564	-1.12343	-2.09785
H	12.69234	-2.39562	-2.57003
H	10.87784	-5.95121	-0.96924
H	12.82823	-4.81293	-2.00721
H	-4.97935	6.72681	-3.77375
H	-4.95286	5.01582	-3.33551
H	-3.63336	6.08847	-2.82806
H	-5.32918	8.52029	-2.07369
H	-4.0402	7.87434	-1.0415
H	-5.66072	8.1288	-0.38049
H	-7.22562	7.01373	-2.86796
H	-7.62757	6.65185	-1.18942
H	-7.33788	5.33243	-2.32251
H	-6.57391	7.0538	2.8955
H	-5.20885	6.44898	3.84325

H	-6.84453	6.4316	4.52716
H	-8.35676	5.38044	2.00091
H	-8.59386	4.79517	3.65234
H	-8.18866	3.65707	2.35501
H	-6.26695	2.81582	3.83499
H	-6.69872	4.02483	5.0469
H	-5.0435	3.9516	4.43495
H	6.15106	-7.05628	-2.71812
H	6.57423	-6.62406	-1.05806
H	6.19195	-5.35315	-2.22691
H	4.31373	-8.60308	-1.85688
H	3.03862	-7.98052	-0.79448
H	4.68501	-8.17773	-0.18116
H	3.84457	-6.87343	-3.56573
H	3.80645	-5.15025	-3.18121
H	2.52223	-6.22336	-2.59288
H	5.25233	-2.8315	3.95345
H	5.63572	-4.02533	5.19702
H	3.98655	-3.90699	4.57689
H	7.25755	-5.53079	2.212
H	7.50474	-4.87889	3.83563
H	7.14651	-3.78713	2.48413
H	5.39819	-7.09841	3.11223
H	4.06081	-6.41933	4.0487
H	5.69681	-6.45378	4.73097
H	-4.45751	-6.62133	-4.20649
H	-3.23791	-6.0889	-3.04509
H	-4.39664	-4.92644	-3.71796
H	-5.20772	-8.4141	-2.69254
H	-5.76968	-8.07921	-1.05115
H	-4.05096	-7.92948	-1.43948
H	-6.87061	-6.73501	-3.63568
H	-6.87188	-5.05444	-3.07421
H	-7.46117	-6.34021	-2.01643
H	-6.48194	-3.07891	3.45381
H	-5.31796	-4.26823	4.06917
H	-7.01888	-4.36519	4.53619
H	-8.42651	-5.46405	1.26181
H	-8.27472	-3.78144	1.7664
H	-8.79853	-5.01149	2.93054
H	-6.74328	-7.23592	2.19468
H	-7.14658	-6.72364	3.83682
H	-5.45848	-6.72023	3.29486
H	5.98596	7.00407	-3.01382
H	6.02271	5.30468	-2.50814
H	6.4835	6.58015	-1.37071
H	4.20772	8.58338	-2.09401
H	4.66489	8.18429	-0.4335
H	2.98557	7.99499	-0.9529
H	3.62832	6.83773	-3.74183
H	2.35489	6.21074	-2.69132
H	3.59727	5.11998	-3.33374
H	5.47611	7.18118	2.84942
H	5.83567	6.56994	4.46821

H	4.17449	6.5243	3.85041
H	7.29397	5.58843	1.90191
H	7.19589	3.85414	2.22398
H	7.60805	4.98054	3.53108
H	5.36523	2.93388	3.78852
H	4.12352	4.0222	4.43833
H	5.7964	4.15548	4.98812
H	-8.11188	-2.59896	-1.21778
H	-9.95817	-0.33229	-0.31342
H	-8.09615	2.65709	-1.07827
H	-9.31305	0.41309	-2.76534

Atom coordinates for optimized structure **YH7**

	X	Y	Z
C	3.05659	0.71518	0.20592
C	3.05618	-0.69962	0.21376
C	1.66389	-1.10884	0.40802
N	0.86234	0.00875	0.44624
C	1.66356	1.12626	0.39487
C	-1.9624	4.17435	0.72767
C	-0.60499	4.17457	0.81176
C	-0.16458	2.81541	0.60987
N	-1.26062	1.99645	0.43938
C	-2.37276	2.81569	0.47457
C	1.19192	2.43983	0.5524
C	-5.5067	-0.70164	-0.32166
C	-5.50477	0.70906	-0.32076
C	-4.15067	1.12098	0.03531
N	-3.36322	0.00313	0.1783
C	-4.15073	-1.11509	0.03059
C	-3.70677	2.43815	0.25119
C	-0.60134	-4.15717	0.84195
C	-1.95775	-4.16043	0.74267
C	-2.36865	-2.80379	0.47972
N	-1.25804	-1.98242	0.45207
C	-0.16192	-2.79848	0.63562
C	1.19411	-2.42115	0.5804
C	-3.70226	-2.43116	0.24371
C	2.18535	3.55527	0.70257
C	-4.72395	3.54272	0.28554
C	-4.7097	-3.54436	0.23775
C	2.18878	-3.53267	0.75126
C	2.87557	3.71471	1.90975
C	3.81718	4.73699	2.07688
C	4.03542	5.6015	0.99409
C	3.35634	5.48233	-0.22696
C	2.42431	4.44411	-0.35243
C	2.43681	-4.43613	-0.28923
C	3.36758	-5.47271	-0.14128
C	4.03377	-5.57655	1.08835
C	3.80706	-4.69631	2.15658
C	2.86939	-3.67459	1.96601
C	-4.83636	-4.37655	-0.88086
C	-5.80388	-5.38916	-0.92407
C	-6.63374	-5.54169	0.19629
C	-6.52158	-4.74368	1.34454
C	-5.54034	-3.74485	1.3467
C	-5.51207	3.72152	1.42853
C	-6.48637	4.72533	1.48701
C	-6.6485	5.53935	0.35649
C	-5.8761	5.39586	-0.80554
C	-4.90051	4.3896	-0.8157
C	-6.68247	-1.388	-0.65465
C	-7.85969	-0.70531	-0.98348

C	-7.82685	0.72781	-1.08054
C	-6.65969	1.40264	-0.70513
Zn	-1.24877	0.00672	0.3769
C	4.2434	-1.40494	-0.00638
C	5.44372	-0.71382	-0.21814
C	5.44727	0.72098	-0.21133
C	4.24711	1.41637	-0.01137
C	6.65591	1.44253	-0.40094
C	7.68963	2.07048	-0.54469
C	8.90886	2.7807	-0.71037
C	10.1531	2.12652	-0.60891
C	8.92533	4.16461	-0.97344
C	10.11494	4.85832	-1.13584
C	11.34781	2.81192	-0.76839
C	11.36472	4.19953	-1.04836
C	6.63925	-1.44231	-0.45781
C	7.64984	-2.08514	-0.67907
C	8.83566	-2.81915	-0.95
C	8.91563	-4.20368	-0.70208
C	9.97596	-2.19195	-1.49073
C	11.13409	-2.90378	-1.76398
C	10.0696	-4.92384	-0.97134
C	11.21969	-4.2925	-1.50271
N	12.55556	4.88342	-1.23624
N	12.38346	-5.0035	-1.7514
C	13.81757	4.21728	-0.96437
C	12.54227	6.33163	-1.34932
C	12.37463	-6.45264	-1.64818
C	13.47645	-4.36415	-2.46354
C	-6.11906	6.33351	-2.00482
C	-5.24905	5.96387	-3.22115
C	-5.77888	7.78507	-1.5899
C	-7.60381	6.26121	-2.43527
C	-7.37516	4.95137	2.72586
C	-7.16461	6.38927	3.25664
C	-8.86	4.76152	2.33473
C	-7.05064	3.96851	3.86641
C	3.67697	-6.47847	-1.26747
C	5.18198	-6.412	-1.62097
C	3.32559	-7.90818	-0.79185
C	2.87252	-6.18775	-2.54864
C	4.59133	-4.86968	3.47138
C	4.21229	-3.80822	4.52131
C	6.10635	-4.74167	3.18289
C	4.29837	-6.26563	4.07021
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C	-4.97163	-6.0176	-3.26192
C	-5.80412	-7.78668	-1.70643
C	-7.41077	-6.12495	-2.72206
C	-7.47656	-4.9754	2.53189
C	-7.18581	-4.02705	3.71041
C	-8.93395	-4.73626	2.06911
C	-7.32927	-6.42939	3.0391
C	3.65635	6.47164	-1.37011

C	5.15348	6.3798	-1.75118
C	3.33446	7.91163	-0.90494
C	2.82328	6.17858	-2.63236
C	4.61721	4.92559	3.38005
C	4.33906	6.33186	3.96154
C	6.12791	4.78419	3.07551
C	4.24391	3.88229	4.44993
C	-9.04018	-1.56919	-1.08448
C	-10.33168	-1.29227	-0.82079
C	-11.32696	-2.37812	-0.86351
O	-12.57307	-1.92343	-0.56273
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C	-8.85355	1.59904	-1.66107
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C	-10.61125	2.4352	-3.12045
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O	-10.53852	3.61066	-2.80646
H	-11.98975	2.78136	-4.33935
H	-13.15425	-2.7004	-0.61222
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H	0.04862	-4.99718	1.03139
H	-2.62549	-5.003	0.83589
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H	1.877	4.30077	-1.27613
H	1.89777	-4.30517	-1.21963
H	4.75813	-6.37431	1.21903
H	2.6594	-2.96262	2.75495
H	-4.17668	-4.20591	-1.72304
H	-7.39798	-6.31177	0.17399
H	-5.41972	-3.09182	2.20254
H	-5.35508	3.05474	2.2677
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H	-6.71458	-2.46728	-0.63394
H	-6.65304	2.48081	-0.77593
H	4.26665	-2.48349	-0.03716
H	4.27565	2.49486	-0.03743
H	10.17203	1.0638	-0.38823
H	7.98282	4.69784	-1.04862
H	10.07031	5.92226	-1.33181
H	12.27576	2.26256	-0.67108
H	8.05008	-4.71569	-0.2934
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H	11.9773	-2.37413	-2.18946
H	10.07409	-5.98737	-0.76804
H	14.63795	4.90066	-1.18738
H	13.94331	3.33313	-1.60018
H	13.91362	3.89649	0.08421
H	11.93589	6.65592	-2.20302
H	13.55994	6.68696	-1.51632
H	12.14993	6.82679	-0.44783
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H	11.67084	-6.92615	-2.34974
H	12.10922	-6.77542	-0.63481
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H	13.8401	-3.48402	-1.92078
H	13.19552	-4.04382	-3.47854
H	-5.46637	6.64652	-4.04883
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H	-7.79264	6.56528	4.13716
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H	-6.01584	4.06885	4.20974
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H	5.81331	-6.66945	-0.76513
H	5.46337	-5.40792	-1.9539
H	3.55038	-8.63729	-1.57851
H	2.26116	-7.9899	-0.54829
H	3.89389	-8.19299	0.09852
H	3.12708	-6.92408	-3.31771
H	3.09723	-5.19605	-2.95386
H	1.79321	-6.25099	-2.37652
H	4.42866	-2.79398	4.17128
H	4.79139	-3.97249	5.43573
H	3.15186	-3.85965	4.7889
H	6.45557	-5.51583	2.49297
H	6.68033	-4.84147	4.11109
H	6.34108	-3.76914	2.73887
H	4.58107	-7.07095	3.38571
H	3.23321	-6.37906	4.29728
H	4.86068	-6.4068	5.00014
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H	-3.93964	-6.15396	-2.92245
H	-5.07336	-4.99782	-3.64675
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H	-7.56353	-5.09413	-3.05787
H	-8.18736	-6.35173	-1.98622
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H	-7.88241	-4.23447	4.52902
H	-9.22132	-5.39993	1.24897

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H	-7.57225	-7.1601	2.26235
H	-8.00393	-6.60708	3.88395
H	-6.3057	-6.62605	3.37488
H	5.38349	7.07653	-2.56519
H	5.40971	5.36918	-2.08568
H	5.80356	6.62881	-0.90691
H	3.55212	8.62785	-1.70531
H	3.92505	8.20008	-0.03048
H	2.27658	8.01055	-0.64035
H	3.07031	6.9053	-3.41296
H	1.74849	6.25521	-2.43878
H	3.02838	5.181	-3.03355
H	4.62065	7.12567	3.26327
H	4.91152	6.48234	4.88377
H	3.27695	6.45575	4.19748
H	6.47383	5.54434	2.36883
H	6.35228	3.80383	2.64373
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H	4.45144	2.86175	4.11315
H	3.1867	3.94339	4.72824
H	4.83387	4.0572	5.35539
H	-8.82313	-2.61506	-1.29861
H	-10.68728	-0.30394	-0.55814
H	-8.77431	2.64592	-1.37084
H	-9.96382	0.34464	-2.99925

7. Reference

1. Li, K.-L.; Guo, C.-C.; Chen, Q.-Y. *Synlett,* 2009, 2867−2871

2. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009