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

Supporting Information

Porphyrins with intense absorptivity: highly efficient sensitizers with photovoltaic efficiency of up to 10.7% without a cosensitizer and a coabsorbate

Chengming Li,[a] Liang Luo,[a] Di Wu,[a,] Ruyong Jiang,[a] Jingbo Lan,[a] Ruilin Wang,[b,*] Luyi Huang,[c] Shengyong Yang[c] and Jingsong You[a,*]*

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I. General remark

^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectra were recorded on Bruker AV II-400 MHz spectrometer. The ^{1}H NMR chemical shifts were measured relative to $CDCl_3$, TMS or DMSO-d_6 as internal reference ($CDCl_3$: δ = 7.26 ppm; TMS: δ = 0.00 ppm; DMSO-d_6: δ = 2.50 ppm). The ^{13}C NMR chemical shifts were given using $CDCl_3$ or DMSO-d_6 as internal standard ($CDCl_3$: δ = 77.16 ppm; DMSO-d_6: δ = 39.52 ppm). High-resolution mass spectra (HRMS) were obtained with Waters-Q-TOF-Premier (ESI$^+$). IR spectra was obtained with NEXUS670FT-IR. Absorption and transimitance spectra were detected on HITACHI U-2910 absorption spectrophotometer. Fluorescence spectra were collected on Horiba Jobin Yvon-Edison Fluoromax-4 fluorescence spectrometer. Cyclic voltammetry (CV) were performed on LK2005A. The measurements were performed at a scan rate of 50 mV·s^{-1} in dry CH_3CN/THF (7/3, v/v) solution of dye containing 0.10 M of *tetra*-*n*-butylammonium hexafluorophosphate ($TBAPF_6$) as supporting electrolyte, using Ag/Ag$^+$ (0.01 M of $AgNO_3$ in acetonitrile) as a reference electrode, a platinum wire as a counter electrode and a platinum plate as a working electrode. Energy levels were calculated with respect to a standard ferrocene/ferrocenium (Fc/Fc$^+$) redox couple as an external reference.

Photoelectro-chemical characterizations on the solar cells were performed by employing an Oriel Class AAA solar simulator (Oriel 94023A, Newport Corp.). Photo-current-voltage characteristics of the DSSCs were recorded by a potentiostat/galvanostat (Keithley Series 2400 SourceMeter, Keithley Instruments, Inc.) at a light intensity of 100 mW cm^{-2} calibrated by an Oriel reference solar cell (Oriel 91150V, Newport Corp.). IPCE test was performed by using a Qtest Station 1000AD (Crowntech, Inc.) which has a xenon light source and a monochromator (Czerny-Turner). The system is equipped with a NIST traceable Si detector as a reference. Short circuit photocurrent spectrum was recorded with a Keithley 2000 multimeter. Electrochemical impedance spectroscopy (EIS) was recorded using an Autolab PGSTAT 30/302 electrochemical workstation (Eco Chemie B.V., Amsterdam, the Netherlands) under dark conditions over a frequency range of 0.1–10^5 Hz with an alternate current amplitude of 10 mV. Parameters were fitted by Z-View software (v3.1, Scribner Associates, Inc.).

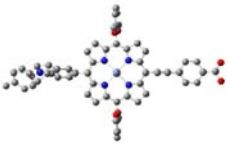
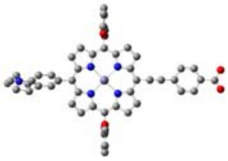
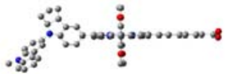
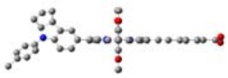
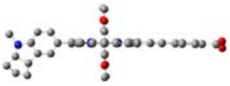
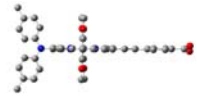
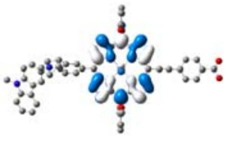
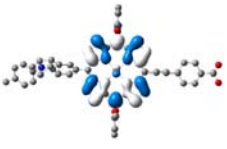
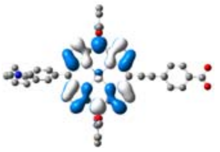
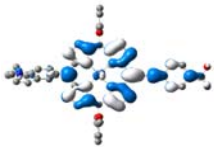
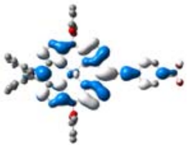
Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Anhydrous solvents were freshly distilled from CaH_2 (diisopropylamine ($^iPr_2NH$), triethylamine (Et_3N), acetonitrile (CH_3CN)) or sodium/benzophenone (toluene, and tetrahydrofuran (THF)) before use. $TBAPF_6$ was recrystallized from absolute ethanol and further dried under vacuum for 48 h.

Pt-counter electrode and two types of TiO_2 films were purchased from OPV Tech (China) Co., Ltd.. A 7 μm-thick film of 20 nm TiO_2 particles as the absorbing layer coated on a FTO glass substrate with dimensions of 1.0 × 1.0 cm^2 was used to determine *LHE*. A 13 μm-thick film of 20 nm TiO_2 particles as the absorbing layer covered by a 5 μm-thick film of 400 nm TiO_2 particles as the scattering layer coated on a FTO glass substrate with dimensions of 0.4 × 0.4 cm^2 was used to assemble DSSCs.

II. DFT Calculation detail

The calculations were performed at TDDFT/B3LYP/6–31G(d,p) level using Gaussian 03 package.[S1] Ground state geometries of porphyrins were fully optimized in gas phase at DFT/B3LYP/6–31G(d,p) level using the default convergence criteria without any constraints and confirmed by frequency calculations.

Table S1. (TD)DFT optimized structure, parameter and frontier orbital profile of porphyrins.

	CM-a1	**CM-b1**	**CM-c1**	**YD2-*o*-C8-1**
Face view				
Side view				
$\angle_{\textbf{D-Por}}$/° [a]	63.8	64.55	65.18	71.12
$\angle_{\textbf{Por-A}}$/° [b]	0.02	1.44	1.04	2.40
$\angle_{\textbf{mesoph-porph}}$/° [c]	87.23	89.02	87.96	87.82
$\boldsymbol{E}_{\textbf{L+1}}$**/eV**	-1.88	-1.92	-1.90	-2.03
L+1				
$\boldsymbol{E}_{\textbf{L}}$**/eV**	-2.20	-2.24	-2.22	-2.37
L				
$\boldsymbol{E}_{\textbf{H}}$**/eV**	-4.55	-4.66	-4.68	-4.68
H				
$\boldsymbol{E}_{\textbf{H-1}}$**/eV**	-4.86	-4.96	-4.94	-5.07

H-1				
Selected Excitation energy/nm (f)[d] **Assignment** (coefficient)[e]	609 (0.4586) **H->L** (0.67476) **H-2->L+1**(-0.19577) 427 (1.2927) **H->L+2** (0.42556) **H-2->L+1** (0.42092) **H-1->L+2** (0.20163) 419 (0.4723) **H-1->L+1**(0.42755) **H-2->L** (-0.41863) **H-2->L+2**(-0.29849) **H ->L+1** (-0.29849) 403 (0.6482) **H->L+2** (0.53671) **H-2->L+1** (-0.30556)	591 (0.4731) **H->L** (0.65216) **H-1->L+1** (0.25406) 424 (1.4619) **H-1->L+1**(0.42642) **H->L+2** (-0.40548) **H-2->L** (0.23208) 417 (0.4731) **H-1->L** (0.39138) **H-2->L+1** (-0.38280) **H-1->L+2** (0.28785) **H->L+1** (0.27138) 392 (0.5506) **H->L+2** (0.52011) **H-1->L+1** (0.27532)	582 (0.4157) **H->L** (0.63395) **H-1->L+1** (0.30444) 424 (1.3808) **H-1->L+1** (0.44206) **H->L+2** (-0.41929) **H->L** (-0.25555) 415 (0.4114) **H-2->L+1** (0.41896) **H-1->L** (-0.37449) **H-1->L+2**(-0.29700) **H->L+1** (-0.29137) 388 (0.4543) **H->L+2** (0.50125) **H-1->L+1** (0.29321)	639(0.3293) **H->L** (0.66657) **H-1->L+1**(0.18562) 427 (1.0511) **H->L+2** (0.52230) **H-1->L+1**(-0.36821) **H-2->L** (-0.20932) 413 (0.4671) **H-2->L+1** (0.46163) **H-1->L** (-0.37943) **H-1->L+2**(-0.27897) **H->L+1** (-0.21798) 404 (0.7432) **H->L+2** (0.43483) **H-1->L+1** (0.38086)

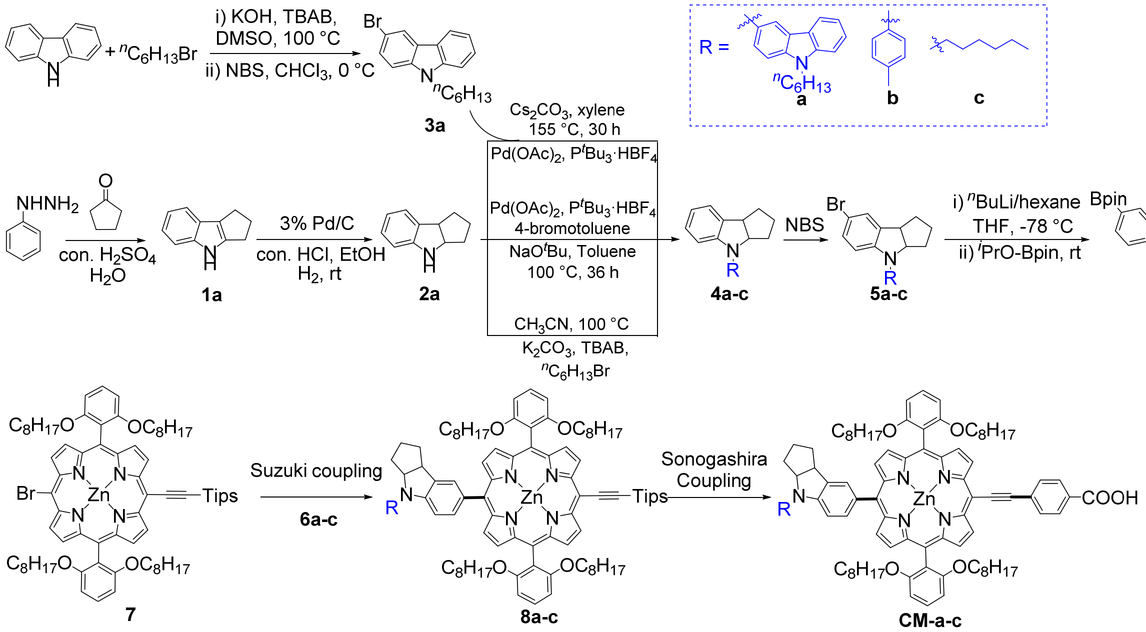
Dihedral angles between porphyrin plane and [a] 10-donor; [b] 20-acceptor and [c] 5,15-Bis(2,6-dioctoxyphenyl). [d] Excited energies with *f* over 0.4 are listed. [e] Assignment with coefficient over 0.18 are listed. L: LUMO; H: HOMO.

Table S2. TDDFT calculated parameters of porphyrins.

	f_B	λ_B/nm	λ_{Qx}/nm
XW1	0.7401	394	536
WW3	1.9640	438	601
IDB	1.7866	421	572
YD2-o-C8-1	1.0511	427	639
A1	1.3426	423	578
A2	1.6319	423	584
CM-a1	1.2927	427	609
CM-b1	1.4619	424	591
CM-c1	1.3808	424	582

f_B: oscillator strength of B band; λ_B and λ_{Qx}: wavelength of the peak of B and Q_x bands, respectively.

III. Synthesis and characterization



Scheme S1 Synthetic routes toward **CM-a–c.** Intermediate **7** was prepared according to the literatures.[S2]

Compound 2a:[S3] Concentrated sulfuric acid (3.5 mL) was added dropwise to a mixture of phenyl hydrazine (51 mmol, 5 mL), cyclopentanone (4.5 mL, 51 mmol) and water (30 mL). The mixture was heated to reflux for 30 min and then allowed to cool to room temperature. The liquid was decanted from the reaction mixture, leaving a red and gummy solid. *n*-Hexane (50–60 mL) was added to the flask and the mixture was heated to reflux. The yellow hexane solution was decanted while the mixture was hot and placed in the freezer (crystallization begins immediately). *n*-Hexane was added again and the recrystallization procedure was repeated twice. After 1 h in the freezer, the white solid was collected from the flask and dried, providing the known indole **1a** (4.11 g, 51%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.54-2.61 (m, 2H), 2.86-2.89 (m, 4H), 7.10-7.14 (m, 2H), 7.28-7.31 (m, 1H), 7.46-7.49 (m, 1H), 7.45 (brs, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 24.6, 25.9, 28.8, 111.5, 118.6, 119.6, 119.8, 120.6, 124.8, 141.1, 143.9 ppm.

A mixture of 1,2,3,4-tetrahydrocyclopenta[*b*]indole (6.25 g, 39.8 mmol), 3% Pd/C (3.30 g), and concentrated hydrochloric acid (4.2 mL) in ethanol (EtOH) (70 mL) was hydrogenated at 10 atm on a Parr shaker. After 3 h, the mixture was removed from the shaker and filtered through Celite. The solid was washed with methanol (MeOH). The filtrate was concentrated. The crude oil was dissolved in 1 N HCl and washed with ether. The aqueous phase was treated with 2.5 N NaOH to pH >10 and then extracted with chloroform. The combined chloroform extracts were dried over Na_2SO_4, filtered and concentrated to give the crude indoline. The material was purified by flash column chromatography (silica gel) using ethyl acetate (EtOAc)/petroleum ether (PE) (1/15, *v*:*v*) as eluent to give **2a** (4.93 g, 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.51-1.82 (m, 5H), 1.91-2.01 (m, 1H), 3.78 (m, 2H), 4.34-4.39 (m, 1H), 6.53 (d, J = 7.6 Hz, 1H), 6.68 (td, J = 7.2 Hz, 0.8 Hz, 1H), 6.99 (t, J = 7.6 Hz, 1H), 7.04 (d, J = 7.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 24.5, 35.0, 37.1, 47.3, 63.5, 108.5, 118.4, 124.6, 127.5, 133.5, 151.5 ppm.

Compound 3a was prepared according to the literature.[S4] 50% KOH (aq) (35 g) was added to a stirred solution of carbazole (10 g, 60 mmol) and tetrabutylammonium bromide (TBAB; 0.40 g, 1.2 mmol) in dimethylsulfoxide (DMSO; 50 mL). Then *n*-hexylbromide (11.6 g, 70.3 mmol) was added dropwise. After complete addition, the reaction mixture was heated at 100 ^{o}C for 30 h. The organic layer was separated, washed with water, dried over Na_2SO_4 and concentrated. Pure product was obtained as a white solid (13.51 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.88-0.91 (m, 3H), 1.33-1.43 (m, 6H), 1.85-1.93 (m, 2H), 4.32 (t, J = 7.6 Hz, 2H), 7.24-7.28 (m, 2H), 7.42-7.52 (m, 4H), 8.14 (d, J = 7.6 Hz, 2H) ppm.

In a flask, covered with aluminum foil, a stirred solution of 9-hexylcarbazole (5 g, 20 mmol) in chloroform ($CHCl_3$; 100 mL) was cooled to 0 ^{o}C. *N*-bromosuccinimide (NBS; 3.56 g, 20.0 mmol) was added in small portions. The mixture was allowed to warm to room temperature overnight. $CHCl_3$ was evaporated and the crude product was purified by column chromatography (silica gel) using petroleum ether (PE) as eluent. The final product was obtained as white crystals (5.8 g, 88%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.93 (t, J = 7.2 Hz, 3H), 1.29-1.41 (m, 6H), 1.84-1.91 (m, 2H), 4.28 (t, J = 7.2 Hz, 2H), 7.28-7.31 (m, 2H), 7.44 (d, J = 8.0 Hz, 1H), 7.52-7.60 (m, 2H), 8.09 (d, J = 8.0 Hz, 1H), 8.25 (d, J = 2.0 Hz, 1H) ppm.

Compound 4a: A flame-dried Schlenk flask was charged with **2a** (1.6 g, 10 mmol), 3-bromo-9-hexylcarbazole **3a** (3.63 g, 11 mmol), $Pd(OAc)_2$ (112 mg, 0.5 mmol), tri-*tert*-butylphosphine tetrafluoroborate ($P^tBu_3\cdot HBF_4$; 290.1 mg, 1 mmol), Cs_2CO_3 (0.46 g, 1.4 mmol) and xylene (25 mL). The mixture was stirred at 155 ºC for 30 h in an oil bath. After being cooling down, the reaction mixture was filtered through a Celite pad and then washed with 10-20 mL of dichloromethane (CH_2Cl_2). The solvent of the filtrate was removed under reduced pressure. The residue was purified by column chromatography (silica gel, CH_2Cl_2/PE = 1/10 to 1/5 to 1/3 (*v:v*)) to give **4a** as yellow oil (2.70 g, 66%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.91 (t, J = 7.2 Hz, 3H), 1.30-1.48 (m, 6H), 1.66-1.80 (m, 3H), 1.87-1.96 (m, 3H), 2.01-2.13 (m, 2H), 3.91 (s, 1H), 4.31 (t, J = 6.8 Hz, 2H), 4.89 (s, 1H), 6.71-6.76 (m, 2H), 7.04 (t, J = 7.6 Hz, 1H), 7.16 (d, J = 7.2 Hz, 1H), 7.23 (t, J = 7.6 Hz, 1H), 7.39-7.53 (m, 4H), 8.04 (s, 1H), 8.08 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.7, 24.6, 27.2, 29.2, 31.7, 33.9, 35.5, 43.3, 45.8, 70.6, 106.6, 108.9, 109.3, 114.7, 117.5, 118.7, 120.5, 121.9, 122.6, 123.5, 124.7, 125.8, 127.4, 134.4, 135.5, 137.3, 141.0 ppm. IR (KBr): 2953, 2929, 2860, 1603, 1487, 1462, 1377, 1259, 1153, 1024, 849, 802, 742 cm^{-1}. HRMS (ESI$^+$): calcd for $C_{29}H_{32}NaN_2$ [M+Na]$^+$ 431.2463, found 431.2466.

Compound 4b:[S5] The mixture of **2a** (1.43 g, 9 mmol), 4-bromotoluene (1.65 g, 9.3 mmol), $Pd(OAc)_2$ (101.1 mg, 0.45 mmol) , $P^tBu_3\cdot HBF_4$ (261.9 mg, 0.9 mmol) and sodium *tert*-butoxide (NaO^tBu; 1.21 g, 12.6 mmol) in toluene (10 mL) was heated at 100 ºC under N_2 for 36 h. After being cooling down, the reaction mixture was filtered through a Celite pad, and then washed with 30 mL of CH_2Cl_2. The solvent of the filtrate was removed under reduced pressure. The residue was purified by column chromatography (silica gel) using CH_2Cl_2/PE = 1/15 (*v:v*) as eluent to give **4b** as yellow oil (2.10 g, 93%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.56-1.67 (m, 2H), 1.79-1.98 (m, 3H), 2.01-2.08 (m, 1H), 2.36 (s, 3H), 3.85 (td, J = 8.4 Hz, 2.4 Hz, 1H), 4.75-4.80 (m, 1H), 6.73 (td, J = 7.2 Hz, 0.8 Hz, 1H), 6.95 (d, J = 8.0 Hz, 1H), 7.06 (t, J = 7.6 Hz, 1H), 7.13-7.18 (m, 3H), 7.21-7.23 (m, 2H) ppm.

Compound 4c:[S6] The mixture of **2a** (1.43 g, 9 mmol), TBAB (60 mg, 0.19 mmol), 1-bromohexane ($^nC_6H_{13}Br$; 3 mL) and K_2CO_3 (4.14 g, 30 mmol) in CH_3CN (10 mL) was heated at 100 ºC under N_2 for 36 h. The organic layer was separated and concentrated. The residue was purified by column chromatography (silica gel) using PE as eluent to give **4c** as colorless oil (2.02 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.90 (t, J = 6.4 Hz, 3H), 1.32-1.36 (m, 6H), 1.50-1.69 (m, 5H), 1.72-1.78 (m, 1H), 1.82-1.86 (m, 1H), 1.92-2.01 (m, 1H), 3.04-3.18 (m, 2H), 3.70 (td, J = 8.8 Hz, 2.8 Hz, 1H), 4.14-4.17 (m, 1H), 6.28 (d, J = 8.8 Hz, 2H), 6.54 (t, J = 7.2 Hz, 1H), 6.98-7.03 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 24.7, 27.2, 27.4, 31.9, 33.6, 35.2, 45.9, 47.0, 69.2, 105.1, 116.0, 124.2, 127.5,133.7, 152.3 ppm.

Compound 5a was prepared according to the reported procedure. To a solution of **4a** (8.8 g, 21.6 mmol) in $CHCl_3$ (90 mL) was added dropwise a solution of NBS (4.24 g, 24 mmol) in $CHCl_3$ (260 mL) under N_2. After be stirring at room temperature overnight, the reaction mixture was quenched with acetone. $CHCl_3$ was evaporated under reduced pressure and the residue was purified by column chromatography (silica gel, sequential PE, CH_2Cl_2/PE = 1/10 (*v:v*)) to give **5a** as a yellow thick oil (8.03 g, 76%). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 0.78-0.84 (m, 3H), 1.21-1.27 (m, 6H), 1.45-1.52 (m, 1H), 1.62-1.75 (m, 6H), 1.95-1.90 (m, 1H), 3.81 (t, J = 8.4 Hz, 1H), 4.34 (t, J = 6.8 Hz, 2H), 4.89 (t, J = 6.8 Hz, 1H), 6.50 (d, J = 8.4 Hz, 1H), 7.04 (d, J = 8.0 Hz, 1H), 7.15 (t, J = 7.2 Hz, 1H), 7.20 (s, 1H), 7.35 (d, J = 8.4 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.54-7.58 (m, 2H), 8.05 (s, 1H), 8.13 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.9, 22.1, 24.0, 26.2, 28.6, 31.0, 33.0, 35.1, 42.3, 44.7, 69.8, 107.2, 109.3, 110.0, 114.3, 118.5, 120.6, 121.4, 121.7, 122.7, 125.9, 127.1, 129.7, 134.0, 136.8, 140.5, 148.9 ppm. IR (KBr): 2953, 2927, 2860, 1595, 1487, 1375, 1255, 1155, 1020, 876, 802, 744 cm^{-1}. HRMS (ESI$^+$): calcd for $C_{29}H_{32}BrN_2$ [M+H]$^+$ 487.1749, found 487.1736.

Compound 5b:[S5] The procedure was similar to that described for **5a. 4b** (4 g, 16 mmol) in $CHCl_3$ (90 mL) and NBS (3.14 g, 17.6 mmol) in $CHCl_3$ (160 mL) were used. Purification via column chromatography was performed using PE and CH_2Cl_2/PE = 1/10 to 1/5 (*v:v*) sequentially to give **5b** as a white solid (2.97 g, 56%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.49-1.59 (m, 1H), 1.63-1.68 (m,1H), 1.74-1.89 (m, 3H), 1.98-2.06 (m, 1H), 2.34 (s, 3H), 3.80 (td, *J* = 8.4 Hz, 2.4 Hz, 1H), 4.74-4.78 (m, 1H), 6.75 (d, *J* = 8.4 Hz, 1H), 7.10 (dd, *J* = 8.4 Hz, 2.0 Hz, 1H), 7.16 (m, 4H), 7.18 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.9, 24.5, 33.9, 35.1, 45.4, 69.4, 108.9, 109.3, 120.1, 127.6, 129.8, 129.9, 131.7, 137.3, 140.4, 147.3 ppm.

Compound 5c: [S6] The procedure was similar to that described for **5a. 4c** (2 g, 8.2 mmol) in $CHCl_3$ (90 mL) and NBS (1.8 g, 10 mmol) in $CHCl_3$ (100 mL) were used. PE was used as eluent to perform column chromatography to give **5c** as yellow oil (1.74 g, 64%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.89 (t, *J* = 6.8 Hz, 3H), 1.30 (s, 6H), 1.45-1.56 (m, 3H), 1.58-1.67 (m, 2H), 1.69-1.75 (m, 1H), 1.80-1.84 (m,1H), 1.90-1.99 (m,1H), 2.99-3.11 (m, 2H), 3.66 (td, *J* = 8.8 Hz, 2.4 Hz, 1H), 4.15-4.19 (m, 1H), 6.11 (d, *J* = 8.0 Hz, 1H), 7.03-7.07 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 24.6, 27.10, 27.12, 31.8, 33.5, 35.2, 45.7, 46.6, 69.2, 106.1, 107.0, 127.1, 130.0, 36.0, 151.3 ppm.

Compound 6a: *n*-Butyllithium (^{n}BuLi; 2.5 M hexane solution, 2.4 mL) was added dropwise to a soluion of **5a** (2.44 g, 5 mmol) in THF (30 mL) at -78 ºC under N_2. The mixture was stirred at -78 ºC for 1 h and 2-isopropoxy-4,4,5,5-tetramethyl[1,3,2]dioxaborolane (1.5 mL, 7.5 mmol) was added subsequently. The mixture was allowed to warm to room temperature and stirred for 3 h. Thereafter, water was added carefully to quench the reaction. The organic layer was separated and the aqueous phase was extracted with EtOAc. The combined organic phases were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. Purification via column chromatography was performed with PE and EtOAc/PE = 1/30 (*v:v*) as eluent sequentially to give **6a** as a colorless solid (1.33 g, 59%). Mp: 138−140 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.87-0.90 (m, 3H), 1.25-1.34 (m, 16H), 1.39-1.44 (m, 2H), 1.60-1.73 (m, 3H), 1.85-2.06 (m, 5H), 3.87 (t, *J* = 8.4 Hz, 1H), 4.29 (t, *J* = 7.2 Hz, 2H), 4.88-4.91 (m, 1H), 6.66 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.19-7.23 (m, 1H), 7.39-7.41 (m, 3H), 7.45-7.53 (m, 2H), 7.59 (s, 1H), 7.99 (s, 1H), 8.04 (d, *J* = 7.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.7, 24.5, 24.9, 25.1, 27.2, 29.2, 31.7, 33.6, 35.6, 43.4, 45.5, 70.7, 83.2, 105.8, 108.9, 109.4, 115.4, 118.8, 120.5, 122.4, 122.6, 123.6, 125.9, 131.1, 133.7, 134.5, 135.5, 137.6, 141.1, 153.1 ppm. IR (KBr): 2929, 2858, 1605, 1487, 1439, 1377, 1350, 1269, 1144, 964, 860, 806, 746 cm^{-1}. HRMS (ESI^{+}): calcd for $C_{35}H_{43}BN_2NaO_2$ [M+Na]$^{+}$ 557.3315, found 557.3317.

Compound 6b:[S5] **5b** (1.32 g, 4 mmol) in THF (20 mL) was used in the similar synthesis procedue to that of **6a**. Column chromatography purification was employed with EtOAc/PE = 1/100 to 1/40 (*v:v*)) as eluent to give **6b** as a white solid (1.45 g, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.33 (s, 6H), 1.34 (s, 6H), 1.46-1.55 (m, 1H), 1.61-1.66 (m, 1H), 1.70-1.79 (m, 1H), 1.86-1.93 (m, 2H), 1.96-2.02 (m, 1H), 2.33 (s, 3H), 3.80 (td, *J* = 8.4, 2.4 Hz, 1H), 4.77-4.82 (m, 1H), 6.84 (d, *J* = 8.0 Hz, 1H), 7.14-7.20 (m, 4H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.55 (s, 1H) ppm.

Compound 6c: 5c (1.29 g, 4 mmol) in THF (20 mL) was used in the similar synthesis procedue to that of **6a**. Column chromatography purification was employed with EtOAc/PE = 1/100 to 1/40 (*v:v*) as eluent to give **6c** as colorless oil (670 mg, 45%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.88-0.91 (m, 3H), 1.32-1.38 (m, 17H), 1.45-1.68 (m, 6H), 1.78-1.86 (m, 2H), 1.90-1.99 (m, 1H), 3.06-3.25 (m, 2H), 3.68-3.72 (m, 1H), 4.20-4.23 (m, 1H), 6.25 (d, *J* = 8.0 Hz, 1H), 7.43 (s, 1H), 7.53 (d, *J* = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 24.5, 24.9, 25.0, 27.0, 27.2, 31.8, 33.3, 35.3, 45.4, 45.7, 104.0, 130.4, 132.9, 135.7, 154.8 ppm. IR (KBr): 2927, 2858, 1459, 1451, 1376, 1350, 1265, 1124, 973, 861, 806, 744 cm^{-1}. HRMS (ESI^{+}): calcd for $C_{23}H_{36}BNNaO_2$ [M+Na]$^{+}$ 392.2737, found 392.2741.

Compound 8a: Following the general procedure, the mixture of **7** (260 mg, 0.2 mmol), **6a** (134.8 mg, 0.3 mmol), $Pd(PPh_3)_4$ (46.4 mg, 0.04 mmol), Cs_2CO_3 (0.33 g, 1 mol) and toluene (10 mL) was stirred at 110 ºC for 48 h. The residue was purified by column chromatography (silica gel, CH_2Cl_2/PE = 1/3 to 1/2 (*v:v*)) to give **8a** as a fuchsia solid (270 mg, 58%). Mp: 92–94 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.34-0.64 (m, 42H), 0.69-0.82 (m, 8H), 0.88-0.98 (m, 11H), 1.32-1.39 (m, 5H), 1.42-1.50 (m, 24H), 1.83-1.97 (m, 5H), 2.14-2.21 (m, 3H), 3.79-3.85 (m, 8H), 4.11-4.16 (m, 1H), 4.35 (t, *J* = 7.2 Hz, 2H), 5.14-5.18 (m, 1H), 6.97-7.01 (m, 4H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.22-7.26 (m, 1H), 7.42-7.51 (m, 3H), 7.64-7.70 (m, 3H), 7.79 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.94 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.25 (d, *J* = 2.0 Hz, 1H), 8.80 (d, *J* = 4.8 Hz, 1H), 8.84 (d, *J* = 4.8 Hz, 1H), 8.90-8.92 (m, 2H), 9.00 (d, *J* = 4.8 Hz, 1H), 9.03 (d, *J* = 4.4 Hz, 1H), 9.70 (dd, *J* = 4.8, 0.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.1, 13.9, 13.95, 13.97, 13.99, 14.2, 19.2, 19.3, 22.29, 22.31, 22.34, 22.7, 24.9, 25.3, 27.2, 28.7, 29.2, 31.40, 31.43, 31.45, 31.8, 34.2, 35.9, 43.4, 46.0, 68.8, 68.9, 70.9, 95.7, 98.4, 104.6, 105.5, 105.6, 108.8, 109.4, 110.4, 114.3, 114.5, 118.6, 120.6, 121.62, 121.64, 121.8, 122.7, 123.3, 123.6, 125.8, 129.8, 130.6, 130.68, 130.72, 131.4, 132.1, 132.35, 132.41, 132.5, 132.8, 134.6, 135.5, 137.3, 141.0, 149.3, 150.2, 150.4, 150.95, 150.98, 152.6, 160.1, 160.2 ppm. IR (KBr): 2926, 2858, 2137, 1587, 1489, 1458, 1377, 1248, 1097, 999, 883, 796, 714 cm^{-1}. HRMS (ESI$^+$): calcd for $C_{104}H_{135}N_6O_4SiZn$ [M+H]$^+$ 1623.9606, found 1623.9613.

Compound 8b: Following the general procedure, the mixture of **7** (360 mg, 0.28 mmol), **6b** (168.9 mg, 0.45 mmol), $Pd(PPh_3)_4$ (69.3 mg, 0.06 mmol), Cs_2CO_3 (490 mg, 1.5 mol) and toluene (10 mL) was stirred at 110 ºC for 48 h. The residue was purified by column chromatography (silica gel) using CH_2Cl_2/PE = 1/4 (*v:v*) as eluent to give **8b** as a fuchsia solid (290 mg, 71%). Mp: 82−84 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.36-0.62 (m, 43H), 0.72-0.80 (m, 8H), 0.91-0.99 (m, 8H), 1.42-1.50 (m, 22H), 1.80-1.85 (m, 2H), 1.92-2.01 (m, 1H), 2.08-2.19 (m, 3H), 2.40 (s, 3H), 3.80-3.83 (m, 8H), 4.06-4.11 (m, 1H), 5.00-5.04 (m, 1H), 6.99 (dd, *J* = 8.4, 1.6 Hz, 4H), 7.25-7.27 (m, 3H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.67 (t, *J* = 8.4 Hz, 2H), 7.82 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.92 (s, 1H), 8.79-8.83 (m, 2H), 8.91 (dd, *J* = 4.8, 1.6 Hz, 2H), 8.96 (d, *J* = 8.8 Hz, 2H), 9.70 (d, *J* = 4.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.1, 14.0, 19.3, 21.0, 22.30, 22.33, 24.9, 25.3, 28.70, 28.72, 31.41, 31.44, 34.3, 35.5, 45.8, 68.81, 68.84, 68.9, 69.4, 95.9, 98.5, 105.49, 105.54, 105.9, 110.4, 114.4, 119.8, 121.6, 122.9, 129.9, 130.0, 130.6, 130.75, 130.77, 131.1, 131.4, 132.1, 132.2, 132.3, 133.3, 133.4, 134.3, 141.0, 147.1, 150.2, 150.3, 150.96, 151.00, 152.6, 160.1, 160.2 ppm. IR (KBr): 2926, 2860, 2139, 1587, 1514, 1485, 1456, 1375, 1250, 1097, 999, 881, 798, 714 cm^{-1}. HRMS (ESI$^+$): calcd for $C_{93}H_{122}N_5O_4SiZn$ [M+H]$^+$ 1464.8558, found 1464.8571.

Compound 8c: Following the general procedure, the mixture of **7** (390 mg, 0.3 mmol), **6c** (166.2 mg, 0.45 mmol), $Pd(PPh_3)_4$ (69.3 mg, 0.06 mmol), Cs_2CO_3 (490 mg, 1.5 mol) and toluene (10 mL) was stirred at 110 ºC for 48 h. The residue was purified by column chromatography (silica gel) using CH_2Cl_2/PE = 1/3 (*v:v*) as eluent to give **8c** as a fuchsia solid (330 mg, 75%). Mp: 43−45 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.37-0.60 (m, 42H), 0.75-0.78 (m, 8H), 0.92-0.97 (m, 11H), 1.37-1.50 (m, 29H), 1.80 (s, 5H), 1.97-2.10 (m, 3H), 3.31-3.40 (m, 2H), 3.80-3.98 (m, 9H), 4.42-4.44 (m, 1H), 6.60 (d, *J* = 8.0 Hz, 1H), 6.98 (d, *J* = 8.4 Hz, 4H), 7.67 (t, *J* = 8.0 Hz, 2H), 7.77-7.80 (m, 2H), 8.78-8.80 (m, 2H), 8.90-8.98 (m, 4H), 9.69 (d, *J* = 4.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.1, 13.9, 14.3, 19.3, 22.28, 22.31, 22.9, 25.0, 25.3, 27.4, 27.8, 28.7, 31.1, 31.39, 31.43, 32.0, 33.8, 35.5, 46.0, 47.3, 68.8, 68.9, 69.6, 95.7, 98.3, 103.2, 105.5, 110.4, 114.2, 121.7, 123.6, 129.7, 130.5, 130.6, 131.0, 131.1, 131.9, 132.0, 132.4, 134.8, 150.2, 150.4, 150.5, 150.90, 150.92, 151.6, 152.6, 160.1, 160.2 ppm. IR (KBr): 2926, 2860, 2139, 1587, 1495, 1456, 1379, 1248, 1099, 999, 881, 796, 714 cm^{-1}. HRMS (ESI$^+$): calcd for $C_{92}H_{128}N_5O_4SiZn$ [M+H]$^+$ 1458.9027, found 1458.9019.

Compound CM-a: To a solution of **8a** (230 mg, 0.15 mmol) in THF (20 mL) was added dropwise a solution of 1 M TBAF in THF (1 mL) under N_2. After being stirring at 30 °C for 3 h, the reaction mixture was quenched with water. The organic layer was separated and the aqueous phase was extracted with CH_2Cl_2. The combined organic phases were dried over anhydrous $MgSO_4$ and concentrated under reduced pressure.The crude product was dried under vacuum. Then the mixture of crude product, 4-iodobenzoic acid (248 mg, 1 mmol), $Pd_2(dba)_3$ (63 mg, 0.069 mmol), $AsPh_3$ (138 mg, 0.45 mmol), Et_3N (10 mL), and THF (30 mL) was stirred at 80 ºC under N_2 for 8 h. After being cooling down, the reaction mixture was concentrated under reduced pressure. The residue was purified by column chromatography (silica gel) using CH_2Cl_2/MeOH = 50/1 (*v:v*) as eluent to give **CM-a** as a deep green solid (130 mg, 54%). Mp: 132−134 ºC. ^{1}H NMR (400 MHz, $CDCl_3$/*d*$_5$-pyridine = 99/1 (*v:v*)): δ = 0.42-0.98 (m, 62H), 1.29-1.46 (m, 7H), 1.81-1.93 (m, 5H), 2.12-2.19 (m, 3H), 3.82-3.87 (m, 8H), 4.07-4.12 (m, 1H), 4.33 (t, *J* = 7.2 Hz, 2H), 5.11-5.14 (m, 1H), 6.98-7.05 (m, 5H), 7.21-7.25 (t, *J* = 8.0 Hz, 1H), 7.41-7.49 (m, 3H), 7.65-7.72 (m, 4H), 7.88 (s, 1H), 8.03 (d, *J* = 8.0 Hz, 2H), 8.14 (d, *J* = 8.0 Hz, 1H), 8.22 (d, *J* = 1.6 Hz, 1H), 8.28 (d, *J* = 8.0 Hz, 2H), 8.71 (d, *J* = 4.4 Hz, 1H), 8.75 (d, *J* = 4.4 Hz, 1H), 9.85-8.91 (m, 4H), 9.62 (dd, *J* = 4.0, 0.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$/*d*$_5$-pyridine = 99/1(*v:v*)): δ = 14.0, 14.07, 14.10, 14.2, 22.5, 22.7, 24.9, 25.4, 27.2, 28.8, 28.9, 29.2, 31.6, 31.8, 34.2, 35.8, 43.4, 45.9, 68.7, 68.8, 70.8, 94.0, 95.8, 98.4, 104.5, 105.3, 108.9, 109.4, 114.0, 114.3, 118.6, 120.6, 121.6, 122.1, 122.7, 123.6, 125.8, 129.5, 129.8, 130.1, 130.3, 131.0, 131.5, 131.9, 132.06, 132.12, 132.5, 133.2, 134.6, 135.7 137.2, 141.1, 148.9, 150.0, 150.1, 150.98, 151.02, 152.1, 160.15, 160.19 ppm. IR (KBr): 2924, 2854, 2189, 1689, 1601, 1489, 1456, 1416, 1377, 1248, 1097, 999, 856, 796, 719 cm^{-1}. HRMS (ESI$^+$): calcd for $C_{102}H_{119}N_6O_6Zn$ $[M+H]^+$ 1587.8483, found 1587.8480.

Compound CM-b: The synthesis procedure is similar to that of **CM-a** using **8b** (290 mg, 0.2 mmol), 1 M TBAF in THF (1.5 mL), THF (20 mL); 4-iodobenzoic acid (372 mg, 1.5 mmol), $Pd_2(dba)_3$ (119 mg, 0.13 mmol), $AsPh_3$ (245 mg, 0.8 mmol), Et_3N (10 mL), and THF (40 mL) were used. The residue was purified by column chromatography (silica gel, CH_2Cl_2/MeOH = 50/1 to 40/1 (*v:v*)) to give **CM-b** as a deep green solid (170 mg, 60%). Mp: 194−196 ºC. ^{1}H NMR (400 MHz, $CDCl_3$/*d*$_5$-pyridine = 99/1(*v:v*)): δ = 0.42-0.92 (m, 59H), 1.78-1.98 (m, 3H), 2.08-2.16 (m, 4H), 2.38 (s, 3H), 3.83 (s, 8H), 4.04 (t, *J* = 7.6 Hz, 1H), 4.98 (t, *J* = 7.6 Hz, 1H), 6.99 (d, *J* = 7.6 Hz, 4H), 7.19-7.24 (m, 3H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.65-7.74 (m, 3H), 7.85 (s, 1H), 8.03 (d, *J* = 7.2 Hz, 2H), 8.28 (d, *J* = 7.2 Hz, 2H), 8.70-8.74 (m, 2H), 8.82-8.86 (m, 4H), 9.61 (d, *J* = 8.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$/*d*$_5$-pyridine = 99/1(*v:v*)): δ = 14.05, 14.07, 20.9, 22.5, 24.8, 25.4, 28.8, 28.9, 31.1, 31.59, 31.62, 34.3, 35.4, 45.7, 68.7, 68.8, 69.3, 94.1, 96.1, 98.0, 105.3, 105.4, 105.6, 114.0, 119.6, 122.1, 122.8, 123.1, 123.3, 129.5, 129.6, 129.8, 129.9, 130.1, 130.3, 130.8, 131.0, 131.4, 131.9, 132.0, 132.9, 134.0, 134.3, 135.5, 135.7, 136.0, 141.1, 146.8, 147.8, 148.1, 148.4, 149.9, 150.1, 150.95, 150.99, 152.1, 160.2 ppm. IR (KBr): 2924, 2854, 2189, 1687, 1601, 1514, 1485, 1456, 1373, 1250, 1414, 1097, 999, 856, 796, 717 cm^{-1}. HRMS (ESI^{+}): calcd for $C_{91}H_{106}N_5O_6Zn$ [M+H]$^{+}$ 1428.7435, found 1428.7433.

Compound CM-c: The synthesis procedure is similar to that of **CM-a** using **8c** (220 mg, 0.15 mmol), 1M TBAF in THF (1 mL), THF (20 mL); 4-iodobenzoic acid (186 mg, 0.75 mmol), $Pd_2(dba)_3$ (61.8 mg, 0.067 mmol), $AsPh_3$ (138 mg, 0.45 mmol), Et_3N (6 mL), and THF (30 mL) were used. The residue was purified by column chromatography (silica gel) using CH_2Cl_2/MeOH = 50/1 (*v:v*) as eluent to give **CM-c** as a deep green solid (140 mg, 67%). Mp: 212−214 °C. ^{1}H NMR (400 MHz, $CDCl_3$/*d*$_5$-pyridine = 99/1 (*v:v*)): δ = 0.43-0.92 (m, 64H), 1.41-1.48 (m, 6H), 1.76 (s, 4H), 1.97-2.01 (m, 3H), 3.30-3.36 (m, 2H), 3.82-3.93 (m, 9H), 4.38-4.40 (m, 1H), 6.54 (d, *J* = 8.0 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 4H), 7.65-7.73 (m, 4H), 8.02 (d, *J* = 7.6 Hz, 2H), 8.27-8.29 (m, 2H), 8.70 (s, 2H), 8.81-8.90 (m, 4H), 9.60 (d, *J* = 4.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$/*d*$_5$-pyridine =99/1(*v:v*)): δ = 14.1, 14.3, 22.5, 22.9, 24.9, 25.4, 27.3, 27.8, 28.8, 31.0, 31.59, 31.62, 32.0, 33.8, 35.4, 46.0, 47.4, 68.7, 68.8, 69.6, 94.0, 95.8, 98.2, 103.0, 105.3, 113.9, 122.2, 122.5, 122.7, 123.0, 124.0, 129.4, 129.7, 129.9, 130.07, 130.10, 130.2, 131.0, 131.1, 131.6, 131.76, 131.83, 132.1, 134.9, 135.7, 146.5, 146.8, 147.0, 150.0, 150.1, 150.2, 150.91, 150.94, 151.3, 152.1, 160.2 ppm. IR (KBr): 2926, 2854, 2189, 1689, 1603, 1495, 1456, 1413, 1379, 1248, 1097, 999, 856, 795, 717 cm^{-1}. HRMS (ESI^{+}): calcd for $C_{90}H_{112}N_5O_6Zn$ [M+H]$^{+}$ 1422.7904, found 1422.7911.

IV. UV-*vis*-NIR absorption and fluorescence spectra

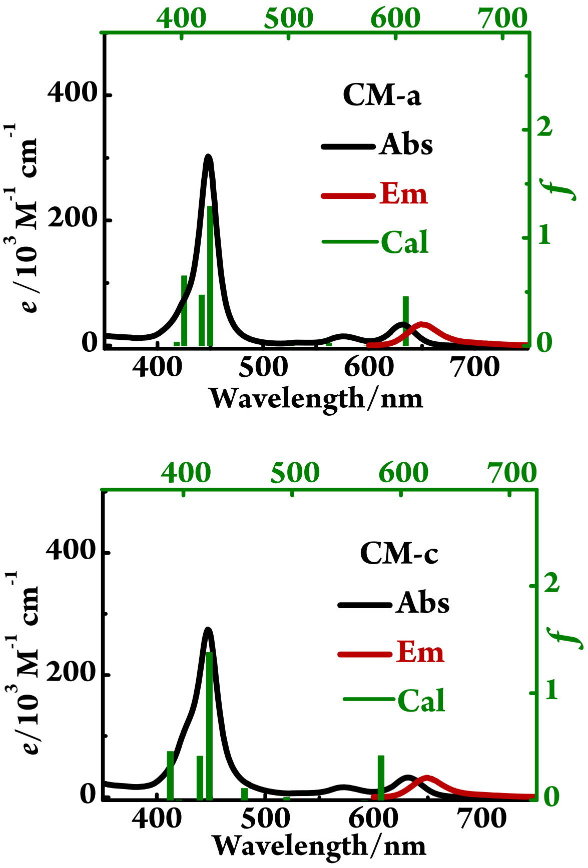


Fig. S1 Electronic spectra of **CM-a** and **CM-c**. UV-*vis*-NIR (black line and axes), and normalized emission (red line, bottom x-axis) measured in THF solution (c = 4.0 × 10^{-6} M) as well as excited energy calculated by TDDFT/B3LYP/6-31(d,p) (green line and axes). Due to a systematic underestimation of the TDDFT/B3LYP calculation, a 25 nm bias of wavelengths (x-axes) exists between the calculated data (top x-axis) and the measured data (bottom x-axis).

V. Electrochemical data

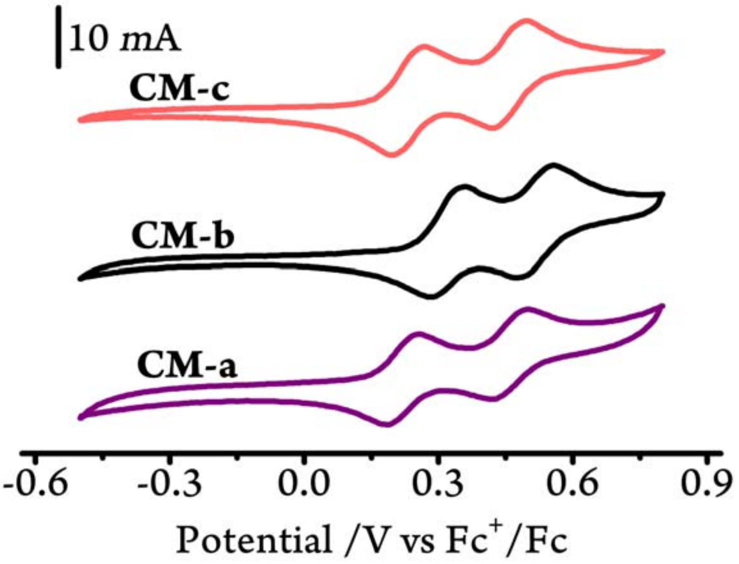


Fig. S2 Cyclic voltammograms of **CM-a–c**

Table S3. Absorption, emission and electrochemical data of **CM-a–c** and **YD2-*o*-C8**.

Dye	λ_{em}/nm [a]	$E^{ox}_{1/2}$/V *vs*. NHE [b]	$E_{0\text{-}0}$/eV [c]	$E^{ox*}_{1/2}$/V *vs*. NHE [d]
CM-a	648	0.74, 0.98	1.93	-1.19
CM-b	645	0.80, 0.99	1.94	-1.14
CM-c	650	0.75, 0.98	1.93	-1.18
YD2-*o*-C8[S2]	663	0.82, -[e]	1.89	-1.07

[a] Emission maxima measured in THF solution (4.0×10^{-6} M); [b] Measured by cyclic voltammetry; [c] Optical band gap estimated from the equation of $E_{0\text{–}0} = 1240/\lambda_{\mathrm{inter}}$, where λ_{inter} is the intersection wavelengths between normalized Q_x absorption and emission band; [d] $E^{ox*}_{1/2} = E^{ox}_{1/2} - E_{0\text{–}0}$; [e] irreversible.

VI. DSSC fabrication and photovoltaic performance

Cell fabrication: Porphyrin dye was dissolved in a mixed solvent of $CHCl_3$ and EtOH (4/6, *v:v*) to give the colorizing solution (0.10 mM). After 10-minute ultrasound, TiO_2 anode was immersed into this solution at 35 °C overnight. The dye-loaded TiO_2 anode was then rinsed with CH_2Cl_2/EtOH (1/1, *v:v*) and dried in air. Then dye-loaded TiO_2 anode and Pt-counter electrode were assembled into a sandwich type cell and sealed by a hot-melt parafilm with a small gap. A drop of electrolyte solution was injected into cell via syringe.

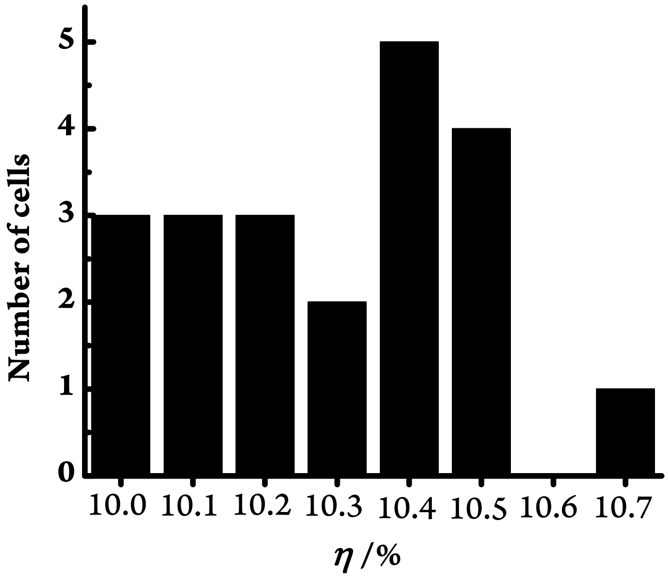


Fig. S3 Histogram of overall efficiency η for devices parallelly made with **CM-b** as sensitizer and LCM2 as electrolyte. Measured under standard photovoltaic conditions (global AM1.5 sunlight with irradiance of 100 mW cm^{-2} at 298 K).

Table S4. Photovoltaic parameters of **CM** and **YD2-*o*-C8** cells under the optimized condition.

Sensitizer	J_{sc}/mA cm^{-2}	V_{oc}/mV	*FF*/%	η/%
CM-a	19.02	693	61.4	8.2
	19.32	703	61.6	8.4
	19.56	668	65.1	**8.5**
	19.34	705	61.2	8.3
	19.19	691	60.6	8.1
	19.12	693	61.6	8.2
Average	19.26±0.17	692±12	61.9±1.5	8.3±0.1
CM-b	22.58	734	64.5	**10.7**
	21.00	733	65.7	10.1
	21.78	738	65.0	10.5
	21.85	733	65.1	10.4
	22.30	725	63.4	10.3
	21.88	726	65.8	10.5
Average	21.90±0.49	732±5	64.9±0.8	10.4±0.2

CM-c	20.88	726	64.1	**9.7**
	20.84	723	63.4	9.6
	20.76	720	62.4	9.3
	20.49	723	62.3	9.2
	20.73	729	61.0	9.1
	21.00	720	63.8	9.6
Average	20.78±0.16	724±3	62.8±1.1	8.4±0.1
YD2-*o*-C8	18.76	701	64.0	8.4
	18.61	703	63.8	8.3
	18.66	707	64.4	8.5
	18.46	706	63.2	8.2
	18.81	701	64.6	**8.5**
	18.57	709	62.8	8.3
Average	18.65±0.12	705±3	63.8±0.6	8.4±0.1

***LHE* spectra:** 7 μm-thick TiO_2 film (area: 1.0×1.0 cm^2) was immersed into a 0.10 mM solution of the porphyrin dye in a mixture of $CHCl_3$/EtOH (4/6, v/v) at 35 ^{o}C for 24 h. Then the film was washed with CH_2Cl_2/EtOH (1/1, v/v), dried in air, and the transmittance (T%) spectrum was collected by HITACHI U-2910 absorption spectrophotometer. $LHE = 100\% - \mathrm{T}\,\%$.

Dye loading amount testing: Dye was loaded on 13 μm-thick nanocrystalline TiO_2 film anode (0.40 cm × 0.40 cm) by immersing TiO_2 anode in $CHCl_3$/EtOH (4/6, *v:v*) solution of dye (0.10 mM if not otherwise noted) following the same procedure as fabricating cell. Dye adsorbed on TiO_2 film was then detached by NaOH (0.10 M) solution in THF/H_2O (1:1, v/v, 6 mL). Dye loading amount was obtained by comparing absorbance of desorbed solution and reference solution at the same wavelength according to the Beers' law. The reference solution of alkalized dye (with specific concentration noted in **Fig. S4**) was prepared by dissolving dye in NaOH (0.10 M) in THF/H_2O (1:1, v/v).

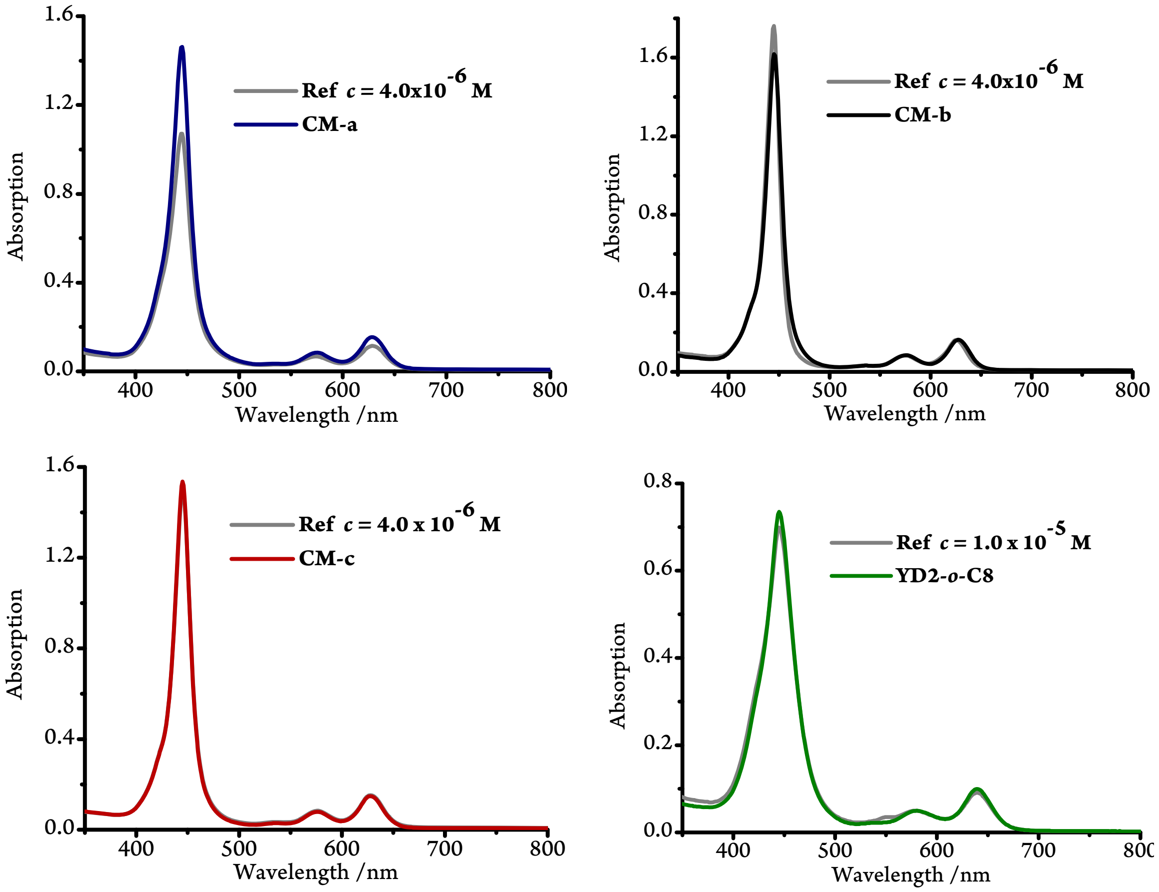


Fig. S4 The absorption spectra of alkalized **CM** and **YD2-*o*-C8** dyes in THF/H_2O (1:1, v/v, 6 mL) detached from TiO_2 anode by comparing with the corresponding reference (grey lines).

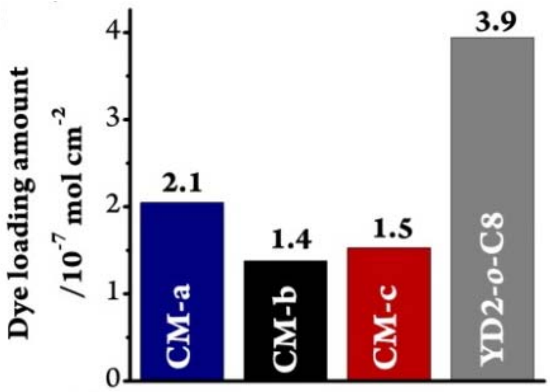


Fig. S5 Dye loading amount (Γ) of dyes.

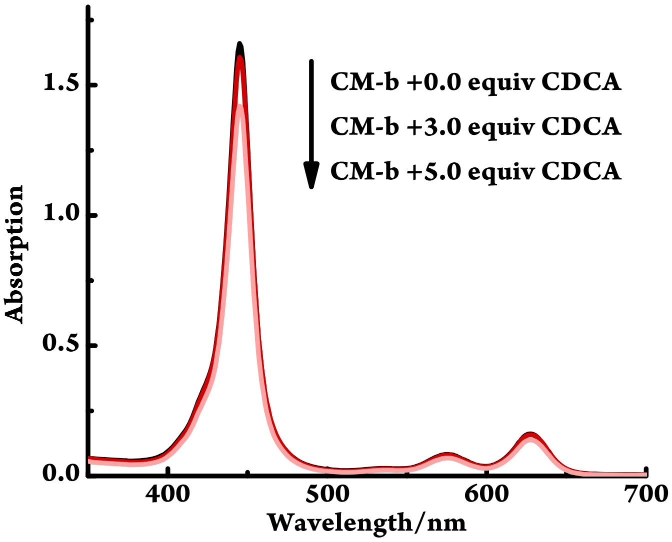


Fig. S6 The absorption spectra of alkalized dyes in THF/H_2O (1:1, v/v, 6 mL) detached from TiO_2 anode. Various equivalents of CDCA were presented in **CM-b** solution (c = 0.1 mM) during colorizing TiO_2 anode.

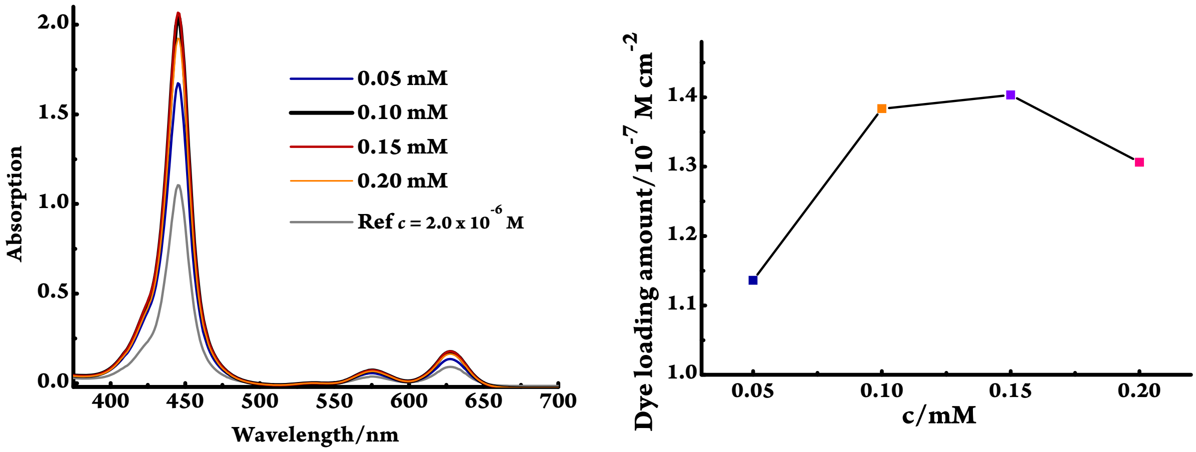


Fig. S7 Left: The absorption of THF/H_2O (1:1, v/v, 6.0 mL) solution of alkalized **CM-b** detached from TiO_2 film, which was colorized by **CM-b** solutions with different concentrations as marked. For reference solution (grey line): $c = 2.0 \times 10^{-6}$ M, $\varepsilon_{max} = 552000$ M^{-1} cm^{-1}. Right: Dye loading amount *vs* concentration (c) of colorizing solution.

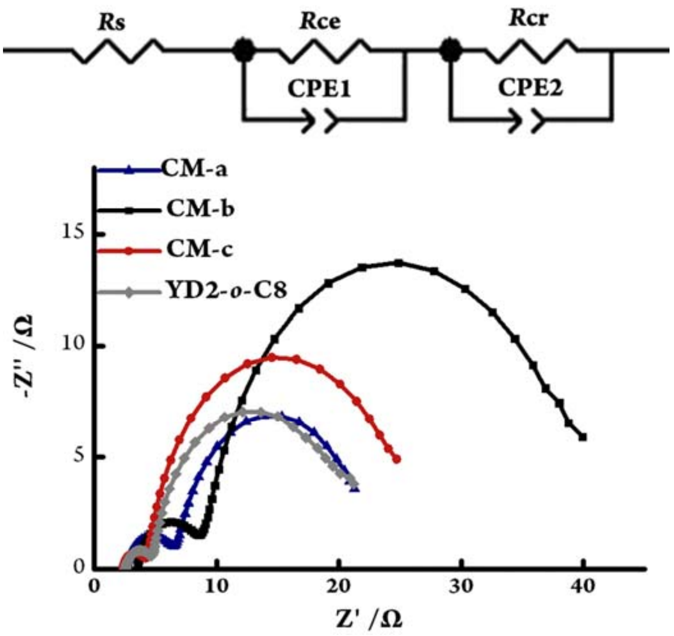


Fig. S8 Nyquist plot of EIS spectra measured at a forward bias of -0.70 V for the DSSCs under dark condition. Inserted is an equivalent electrical circuit with a constant phase element (CPE) as component modeling the behaviour of a double layer.

R_s: Series resistance from reference electrode to working electrode.

R_{ce}: The resistance of charge transfer at counter electrode/electrolyte interface.

R_{cr}: The resistance of electron recombination at TiO_2/dye/electrolyte interface.

Table S5. EIS data of CPE2. [a] [S7]

	α	Q /10^{-4} Ω^{-1} cm^{-2} s^{α}	C_μ/μF cm^{-2}	R_{cr}/Ω cm^2	τ /ms
CM-a	0.897	9.073	312	101	31.5
CM-b	0.895	9.439	346	204	70.6
CM-c	0.904	9.544	370	140	51.8
YD2-o-C8	0.878	11.65	335	109	36.5

[a] Constant Phase Element (CPE) has two parameters: magnitude (Q) and exponent (α).

$C_\mu = Q^{1/\alpha} \cdot R_{cr}{}^{1-\alpha/\alpha}$; $\tau = C_\mu \cdot R_{cr}$

VII. References

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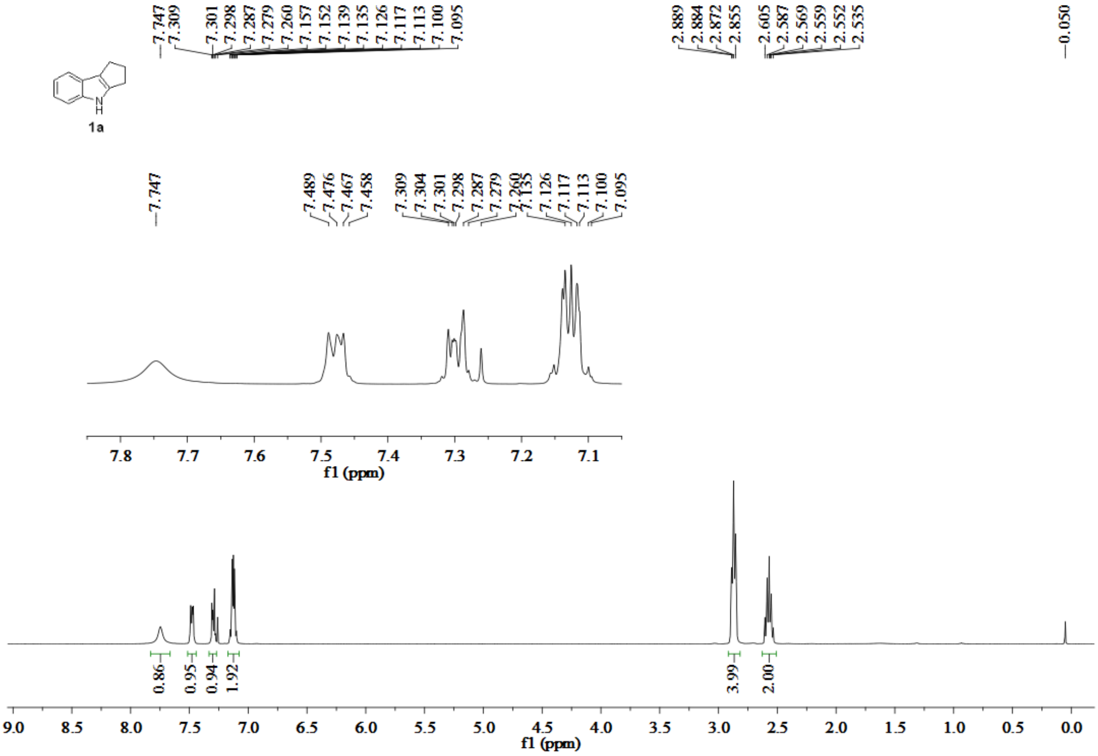
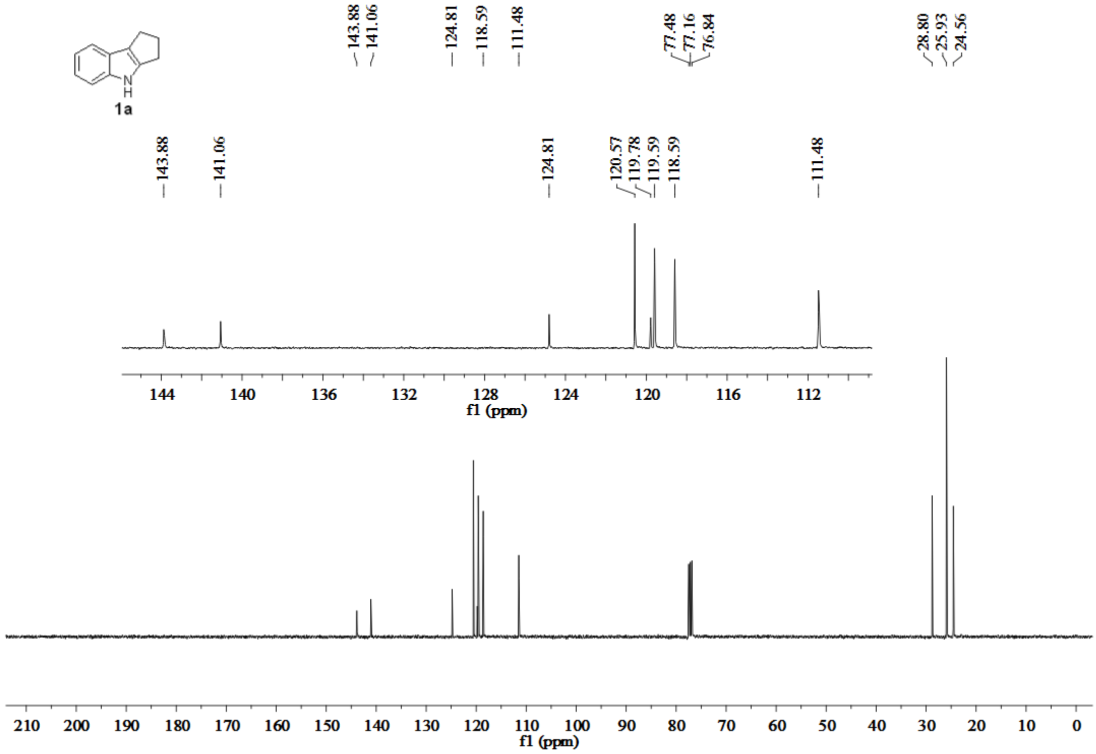
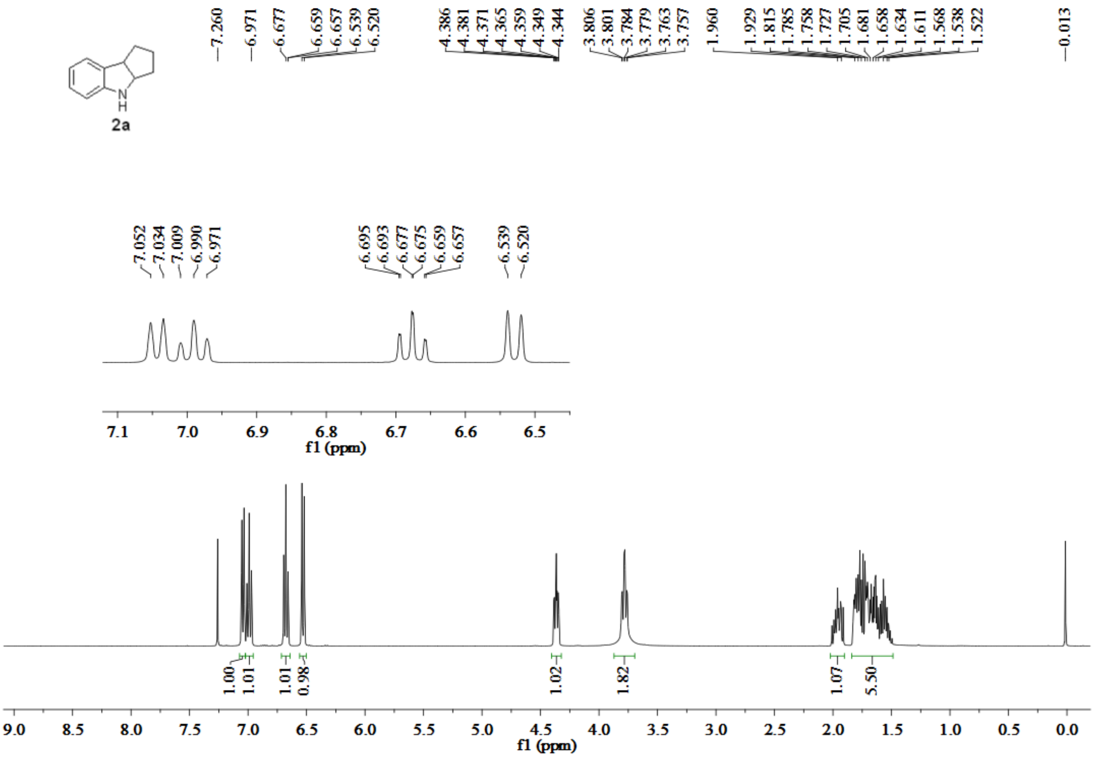
VIII. Copies of ^{1}H and ^{13}C NMR spectra



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4.365
4.359
4.349
4.344
3.806
3.801
3.784
3.779
3.763
3.757
1.960
1.929
1.815
1.785
1.758
1.727
1.705
1.681
1.658
1.634
1.611
1.568
1.538
1.522
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7.052
7.034
7.009
6.990
6.971
6.695
6.693
6.677
6.675
6.659
6.657
6.539
6.520
7.1
7.0
6.9
6.8
6.7
6.6
6.5
f1 (ppm)
1.00
1.01
1.01
0.98
1.02
1.82
1.07
5.50
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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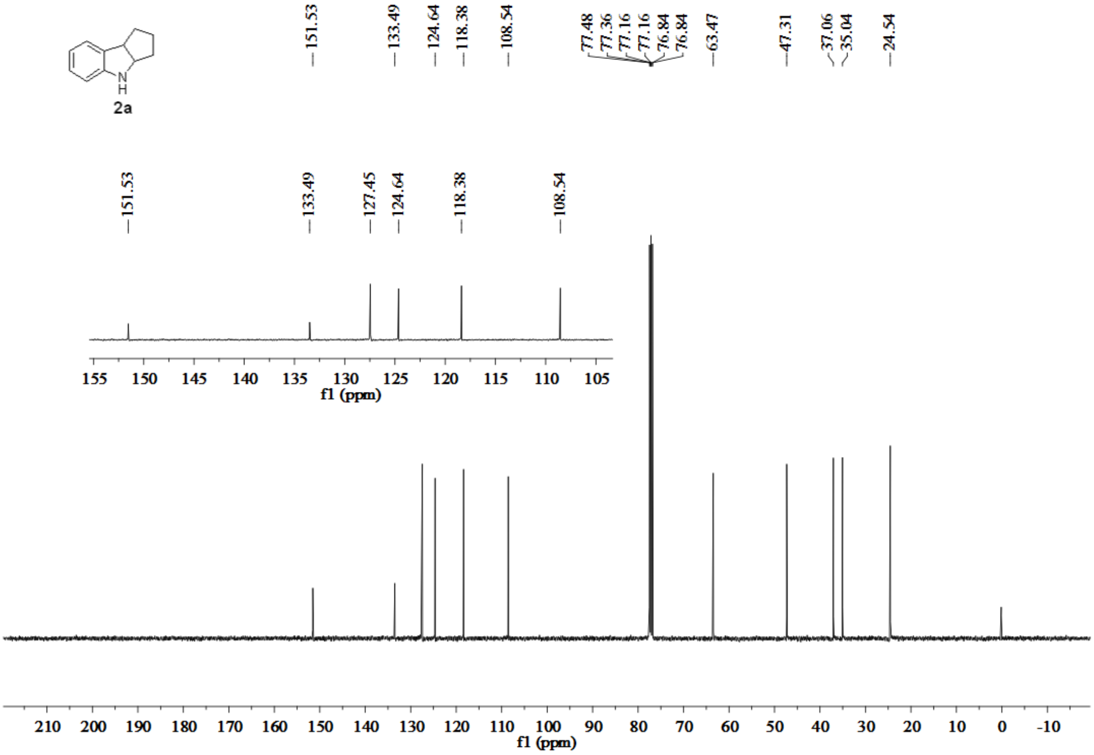
1.0
0.5
0.0
f1 (ppm)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H
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76.84
63.47
47.31
37.06
35.04
24.54
151.53
133.49
127.45
124.64
118.38
108.54
155
150
145
140
135
130
125
120
115
110
105
f1 (ppm)
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200
190
180
170
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140
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120
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100
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80
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60
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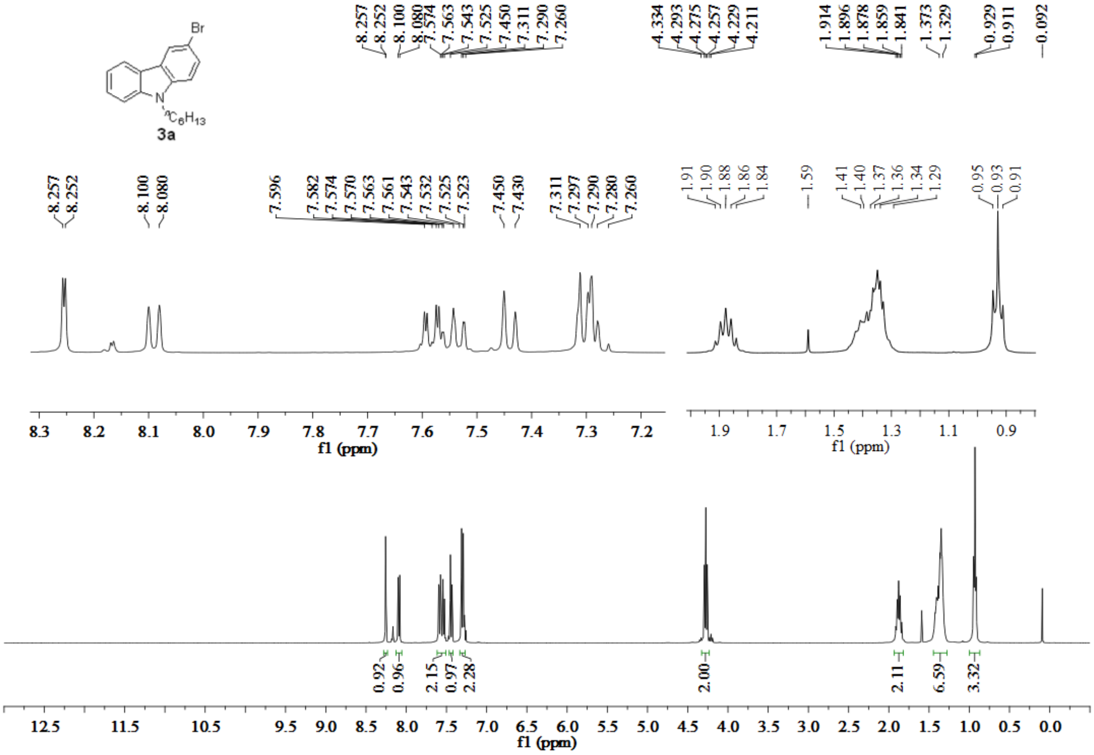
40
30
20
10
0
-10
f1 (ppm)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7.525
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7.311
7.290
7.260
4.334
4.293
4.275
4.257
4.229
4.211
1.914
1.896
1.878
1.859
1.841
1.373
1.329
0.929
0.911
-0.092
8.257
8.252
8.100
8.080
7.596
7.582
7.574
7.570
7.563
7.561
7.543
7.532
7.525
7.523
7.450
7.430
7.311
7.297
7.290
7.280
7.260
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1.90
1.88
1.86
1.84
1.59
1.41
1.40
1.37
1.36
1.34
1.29
0.95
0.93
0.91
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
1.9 1.7 1.5 1.3 1.1 0.9
f1 (ppm)
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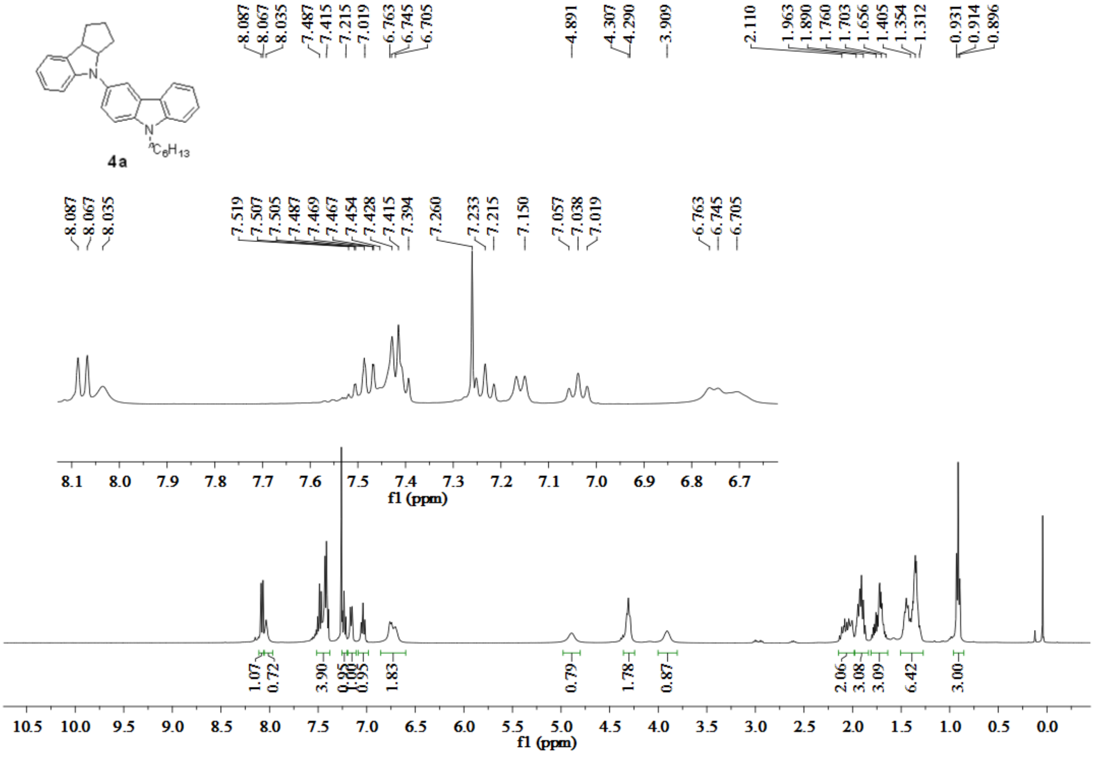
0.96
2.15
0.97
2.28
2.00
2.11
6.59
3.32
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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4.307
4.290
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2.110
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1.656
1.405
1.354
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0.914
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8.067
8.035
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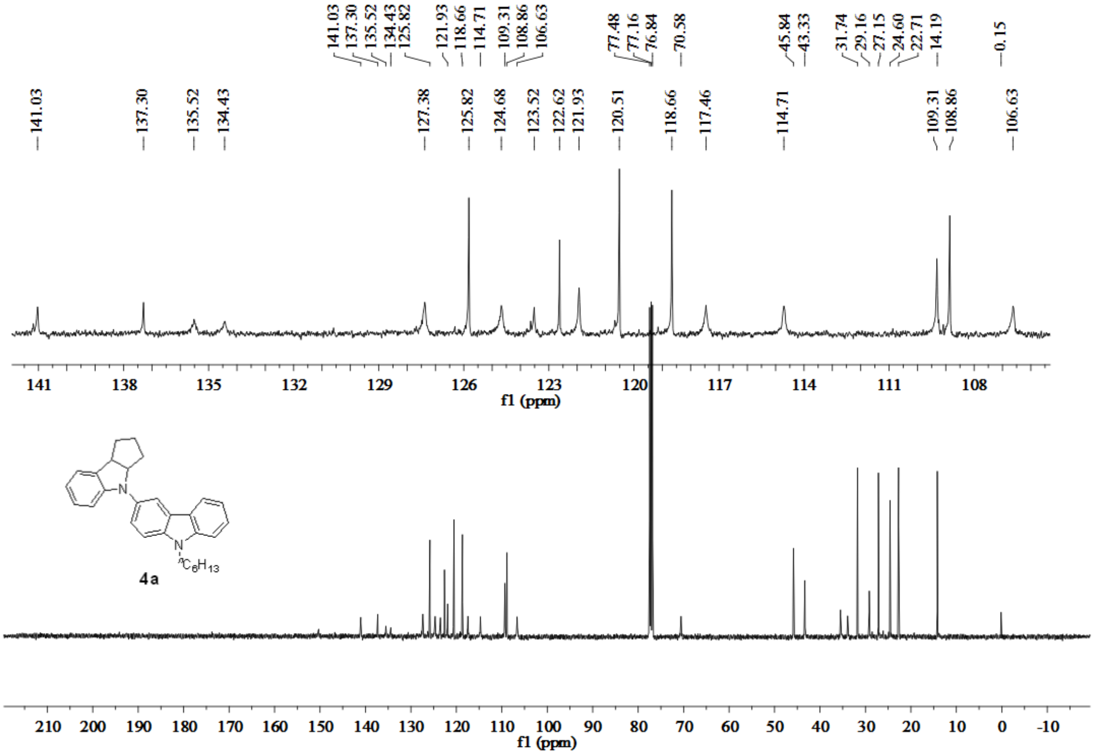
3.09
6.42
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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76.84
70.58
45.84
43.33
31.74
29.16
27.15
24.60
22.71
14.19
0.15
141.03
137.30
135.52
134.43
127.38
125.82
124.68
123.52
122.62
121.93
120.51
118.66
117.46
114.71
109.31
108.86
106.63
141 138 135 132 129 126 123 120 117 114 111 108
f1 (ppm)
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N
^{n}C$_6$H$_{13}$
4a
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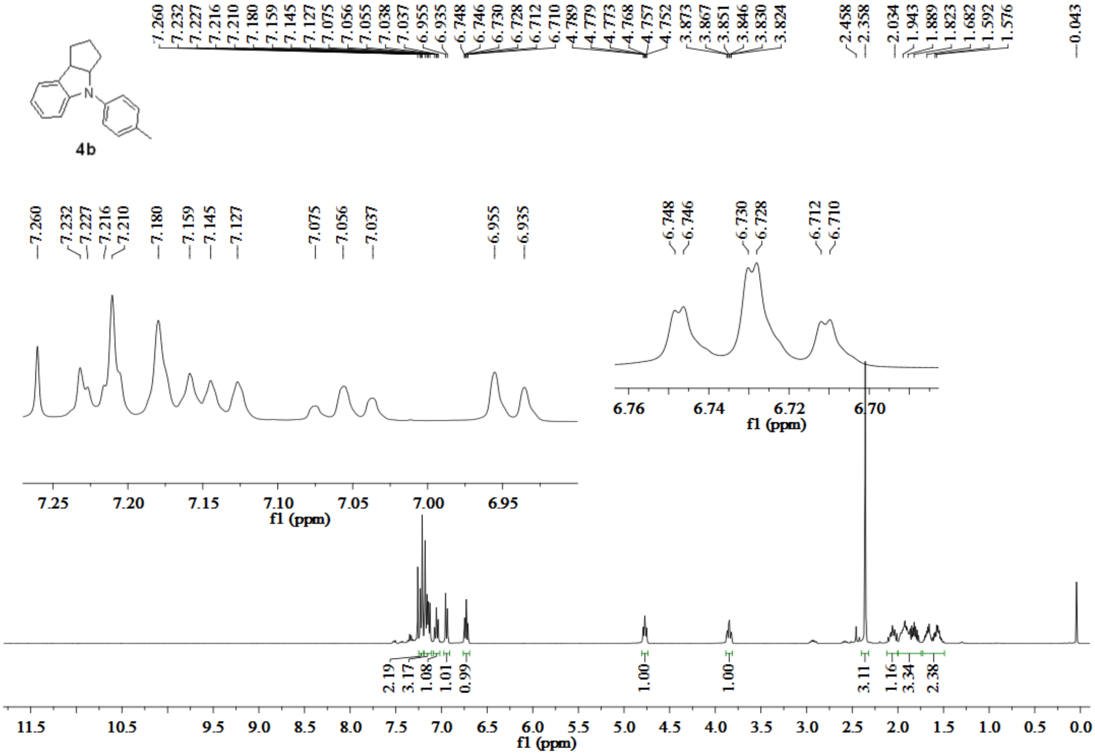
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N
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7.227
7.216
7.210
7.180
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7.075
7.056
7.037
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6.935
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6.710
6.76 6.74 6.72 6.70
f1 (ppm)
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1.01
0.99
1.00
1.00
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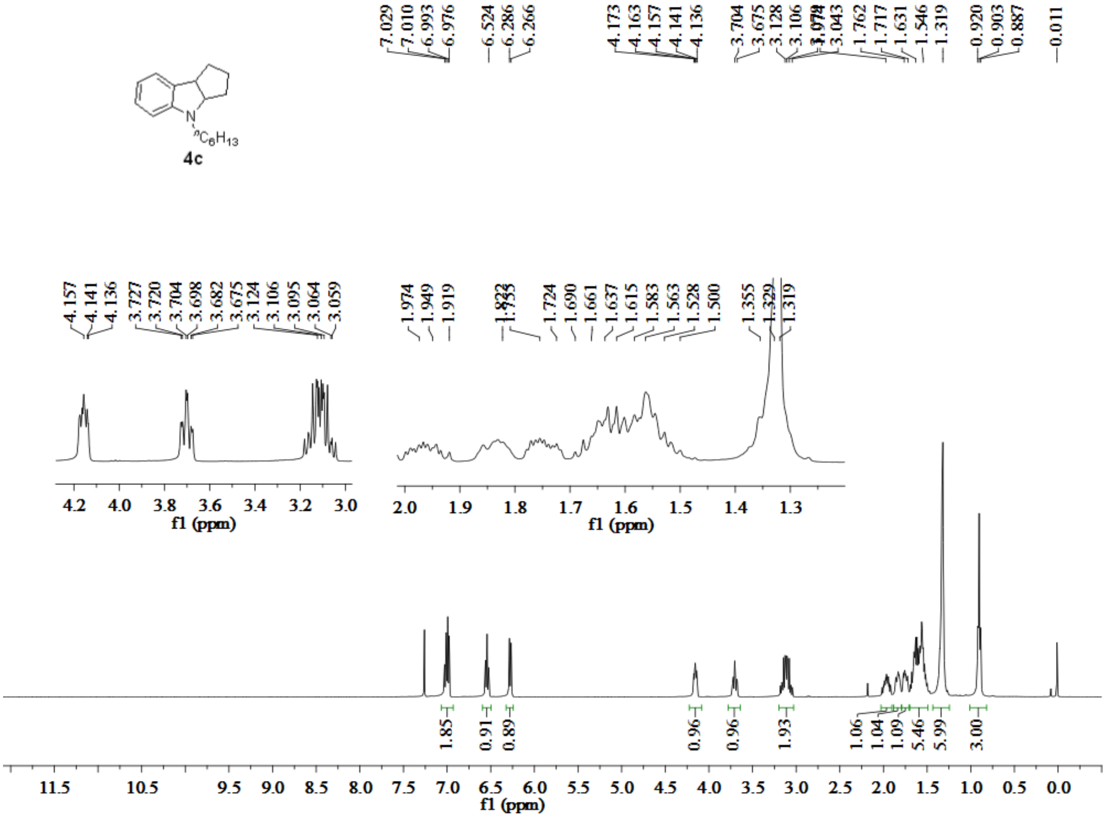
3.34
2.38
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



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3.106
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1.637
1.615
1.583
1.563
1.528
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1.329
1.319
4.2 4.0 3.8 3.6 3.4 3.2 3.0
f1 (ppm)
2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3
f1 (ppm)
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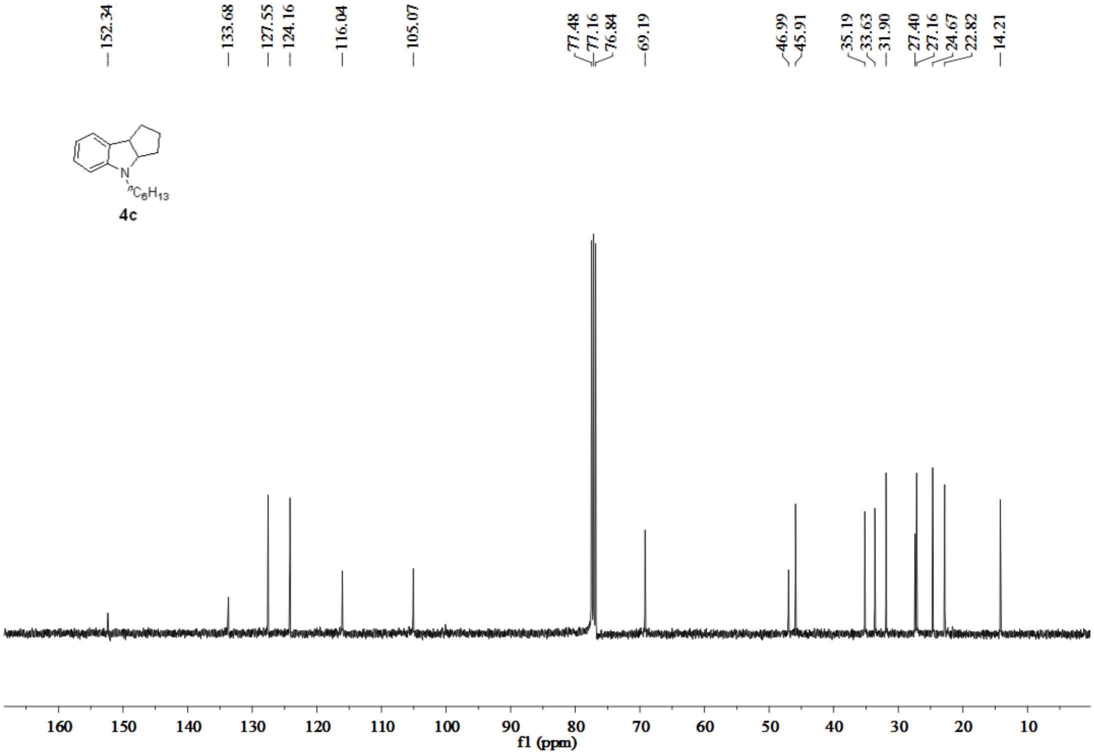
0.96
0.96
1.93
1.06
1.04
1.09
5.46
5.99
3.00
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



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31.90
27.40
27.16
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14.21
4c
^{n}C$_6$H$_{13}$
N
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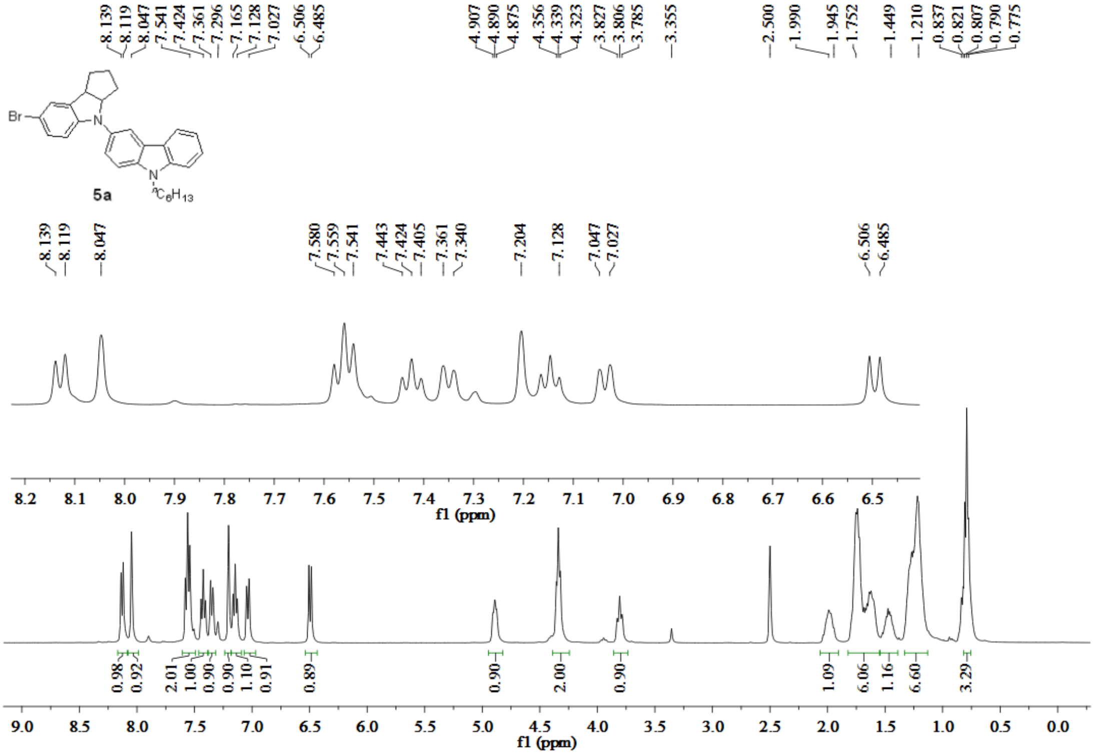
f1 (ppm)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4.890
4.875
4.356
4.339
4.323
3.827
3.806
3.785
3.355
2.500
1.990
1.945
1.752
1.449
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0.837
0.821
0.807
0.790
0.775
Br
N
N
5a
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8.119
8.047
7.580
7.559
7.541
7.443
7.424
7.405
7.361
7.340
7.204
7.128
7.047
7.027
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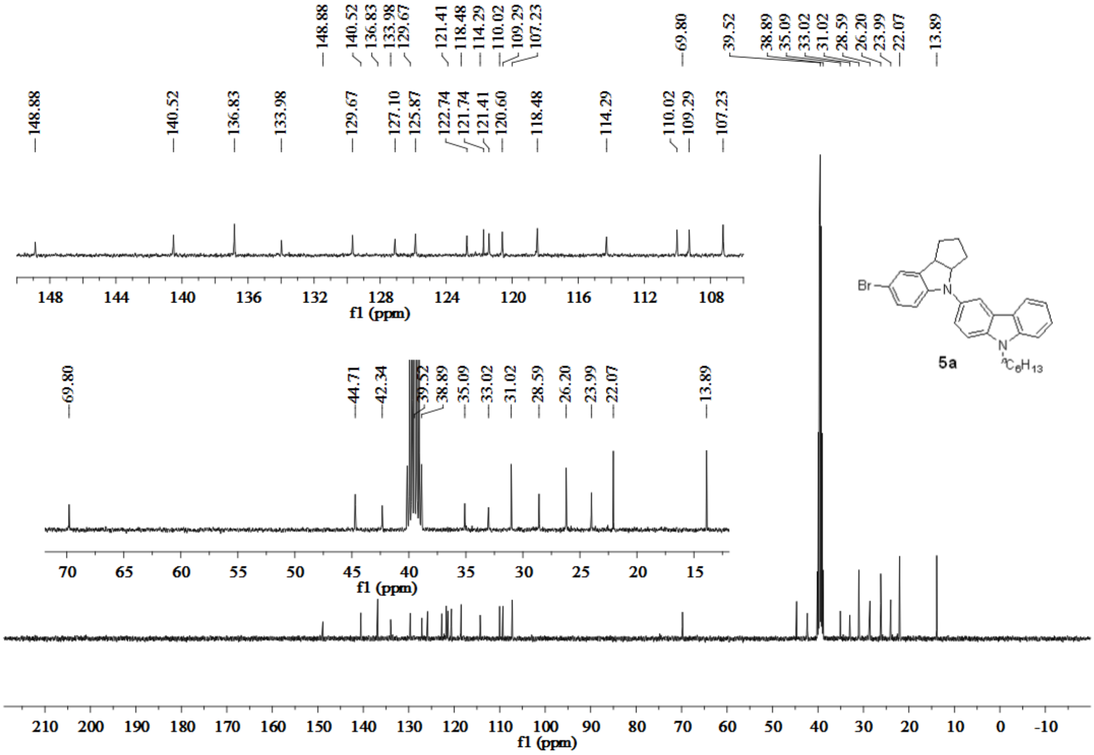
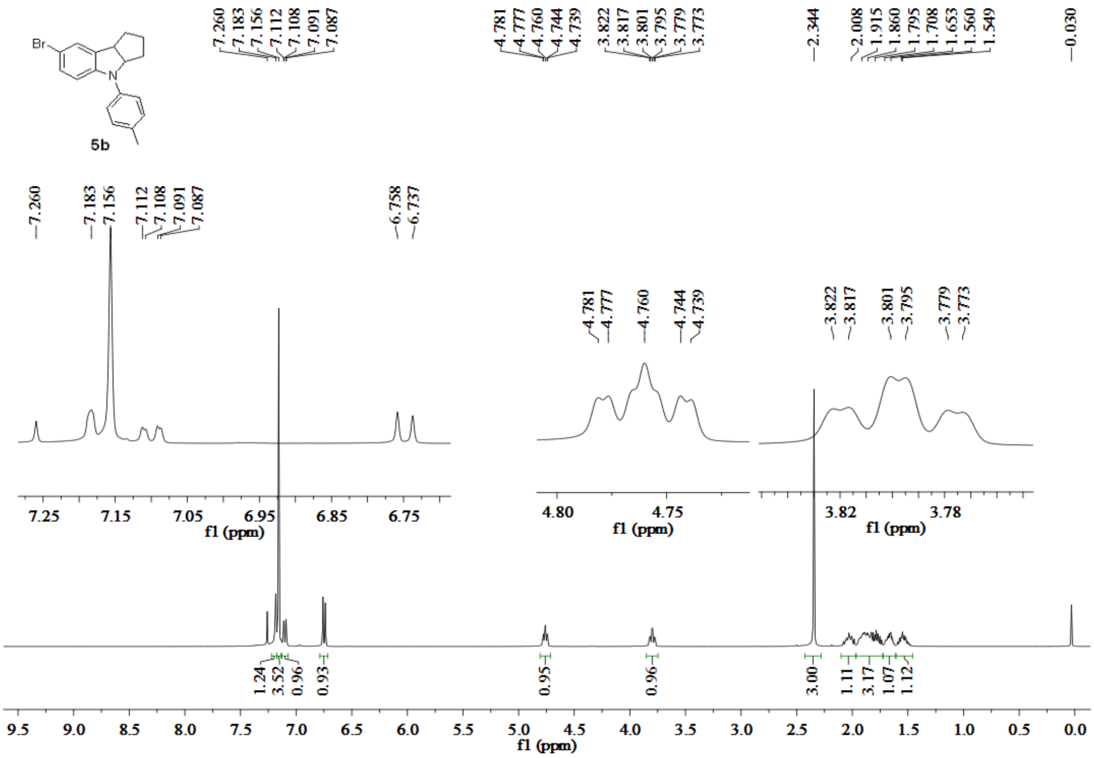
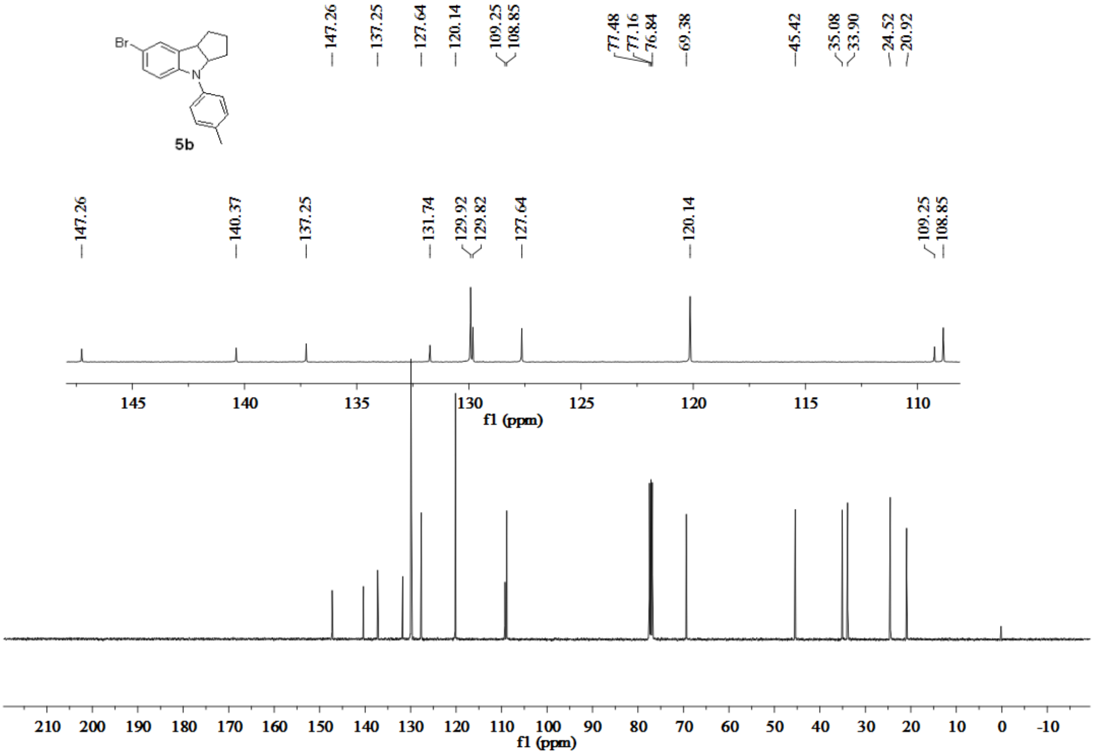
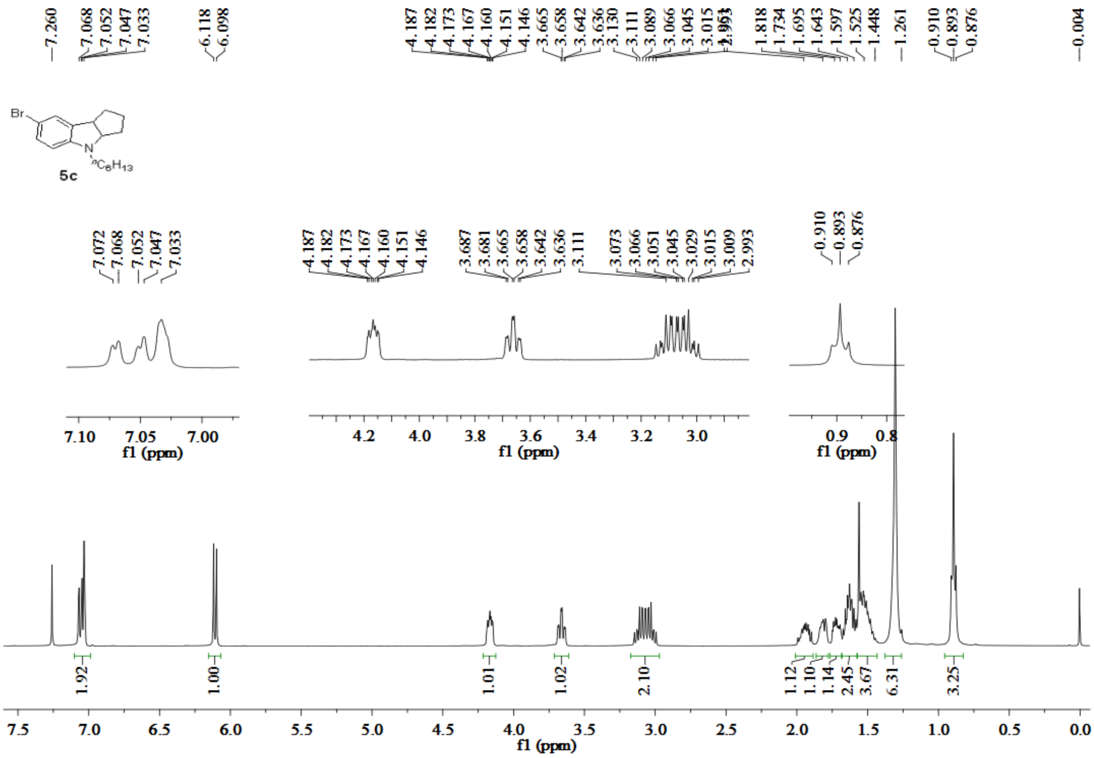
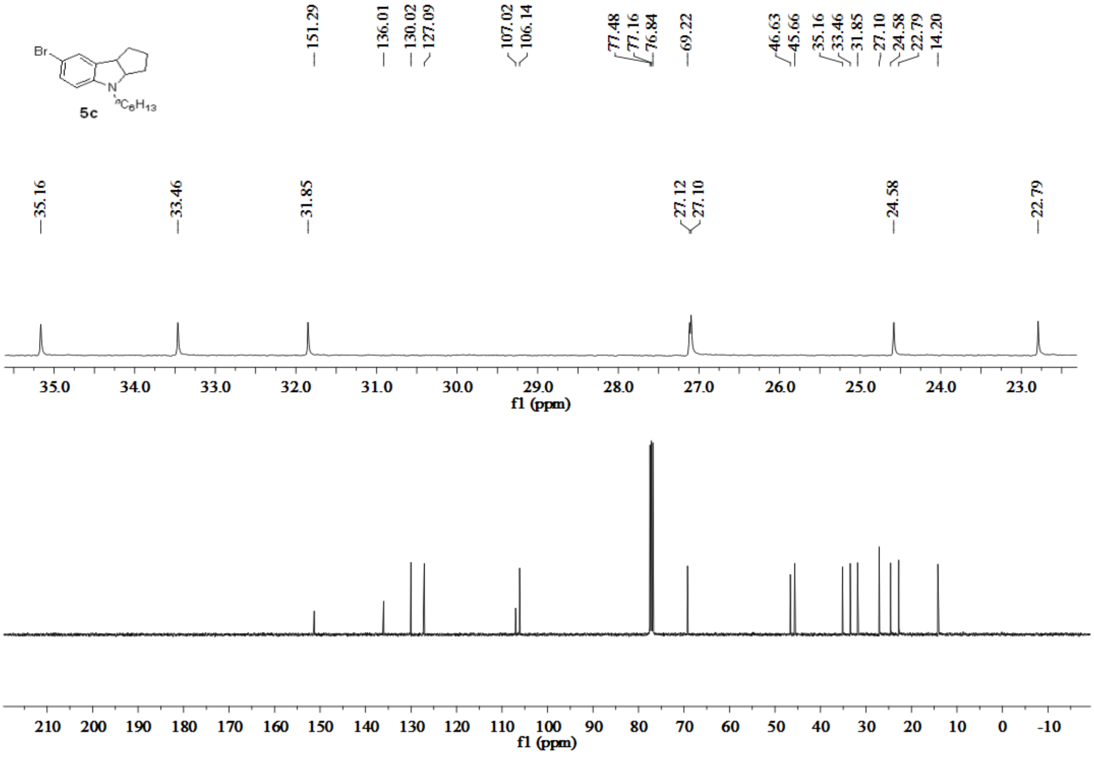
0.90
0.90
1.10
0.91
0.89
0.90
2.00
0.90
1.09
6.06
1.16
6.60
3.29
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

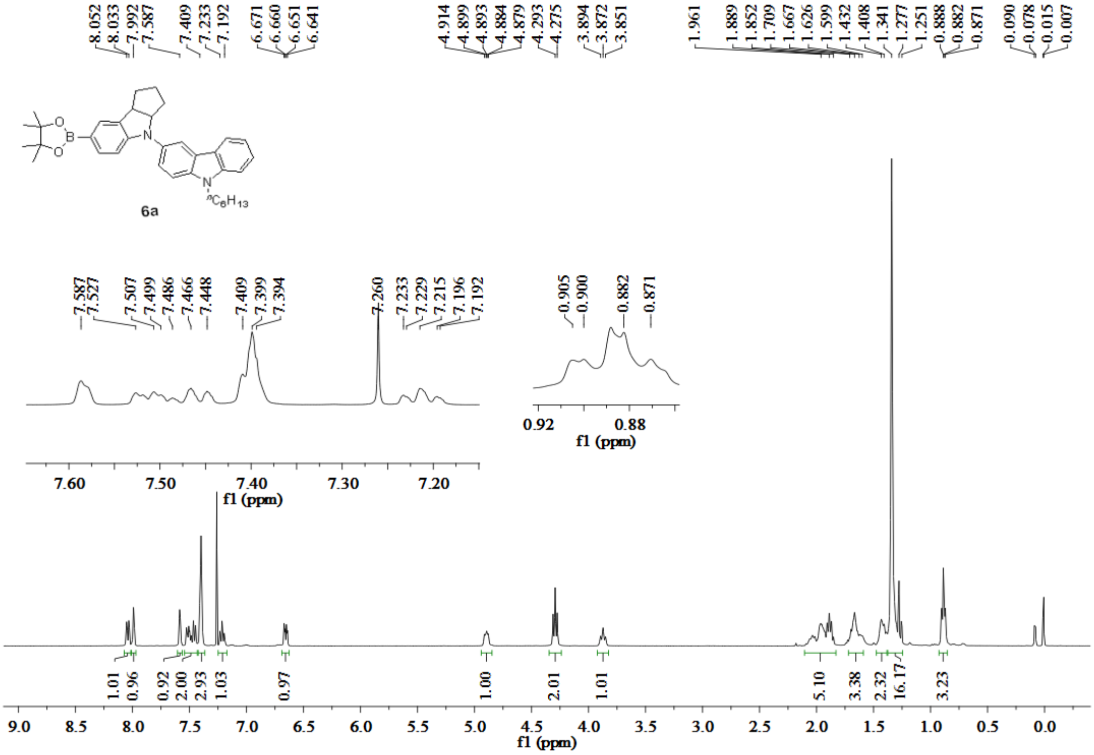

148.88
140.52
136.83
133.98
129.67
121.41
118.48
114.29
110.02
109.29
107.23
69.80
39.52
38.89
35.09
33.02
31.02
28.59
26.20
23.99
22.07
13.89
148.88
140.52
136.83
133.98
129.67
127.10
125.87
122.74
121.74
121.41
120.60
118.48
114.29
110.02
109.29
107.23
148 144 140 136 132 128 124 120 116 112 108
f1 (ppm)
Br
N
N
5a
nC6H13
69.80
44.71
42.34
39.52
38.89
35.09
33.02
31.02
28.59
26.20
23.99
22.07
13.89
70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

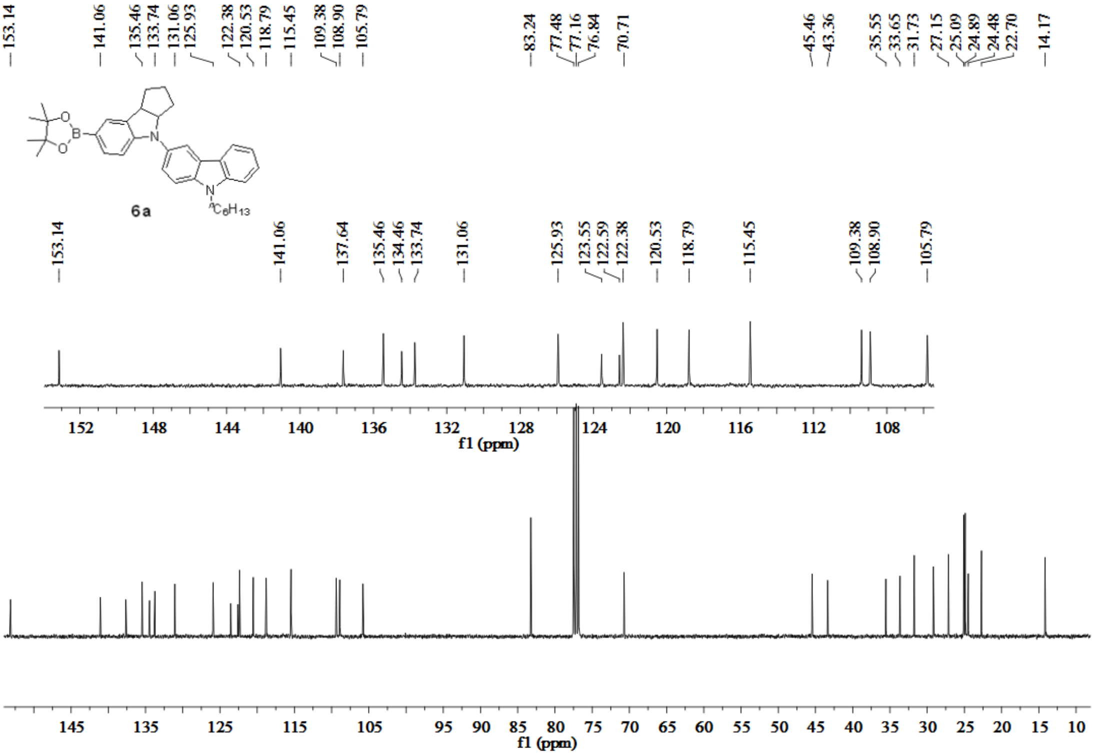

Br
N
5b
7.260
7.183
7.156
7.112
7.108
7.091
7.087
4.781
4.777
4.760
4.744
4.739
3.822
3.817
3.801
3.795
3.779
3.773
2.344
2.008
1.915
1.860
1.795
1.708
1.653
1.560
1.549
0.030
6.758
6.737
7.25
7.15
7.05
6.95
6.85
6.75
f1 (ppm)
4.80
4.75
f1 (ppm)
3.82
3.78
f1 (ppm)
1.24
3.52
0.96
0.93
0.95
0.96
3.00
1.11
3.17
1.07
1.12
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

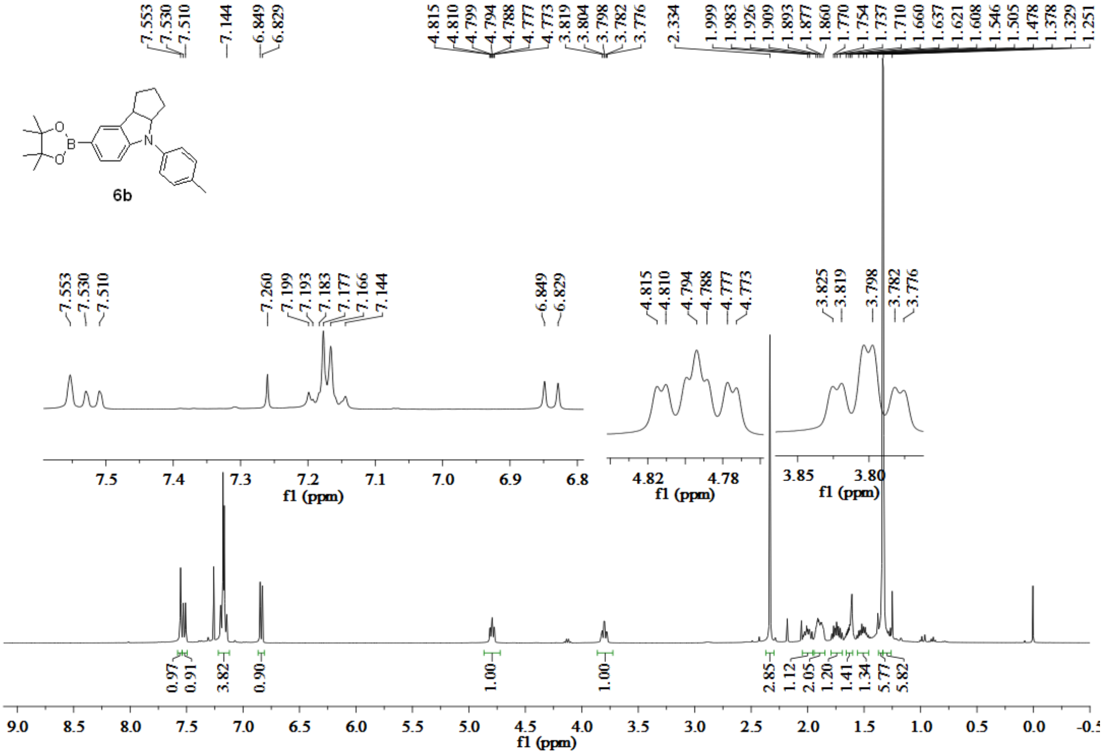

Br
N
5b
147.26
137.25
127.64
120.14
109.25
108.85
77.48
77.16
76.84
69.38
45.42
35.08
33.90
24.52
20.92
147.26
140.37
137.25
131.74
129.92
129.82
127.64
120.14
109.25
108.85
145
140
135
130
125
120
115
110
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

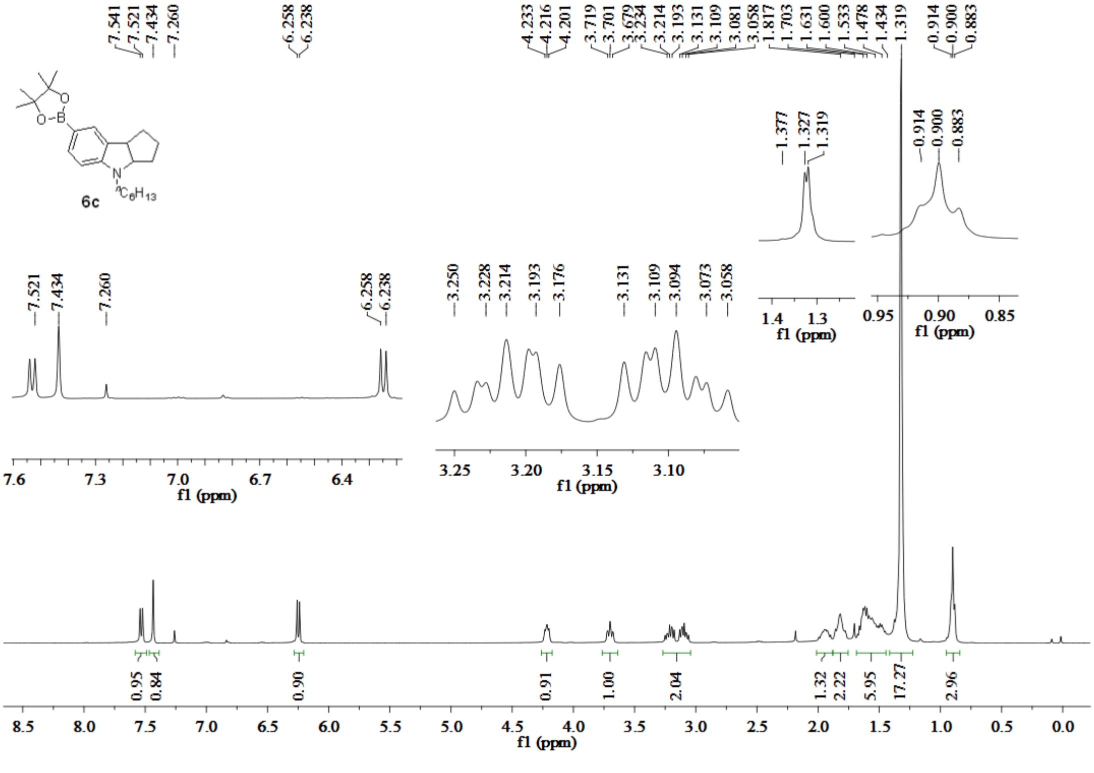

7.260
7.068
7.052
7.047
7.033
6.118
6.098
4.187
4.182
4.173
4.167
4.160
4.151
4.146
3.665
3.658
3.642
3.636
3.130
3.111
3.089
3.066
3.045
3.015
1.961
1.953
1.818
1.734
1.695
1.643
1.597
1.525
1.448
1.261
0.910
0.893
0.876
-0.004
Br
N
$^{n}C_6H_{13}$
5c
7.072
7.068
7.052
7.047
7.033
7.10
7.05
7.00
f1 (ppm)
4.187
4.182
4.173
4.167
4.160
4.151
4.146
3.687
3.681
3.665
3.658
3.642
3.636
3.111
3.073
3.066
3.051
3.045
3.029
3.015
3.009
2.993
4.2
4.0
3.8
3.6
3.4
3.2
3.0
f1 (ppm)
0.910
0.893
0.876
0.9
0.8
f1 (ppm)
1.92
1.00
1.01
1.02
2.10
1.12
1.10
1.14
2.45
3.67
6.31
3.25
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

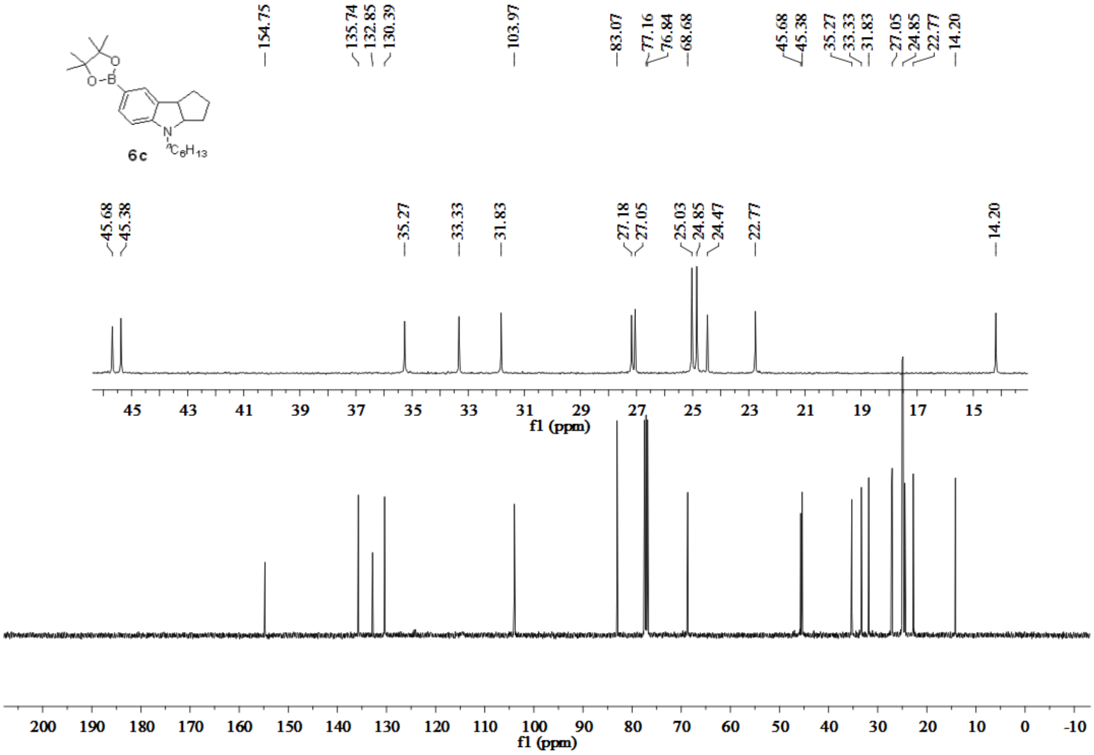

Br
N
$^{n}C_6H_{13}$
5c
151.29
136.01
130.02
127.09
107.02
106.14
77.48
77.16
76.84
69.22
46.63
45.66
35.16
33.46
31.85
27.10
24.58
22.79
14.20
35.16
33.46
31.85
27.12
27.10
24.58
22.79
35.0
34.0
33.0
32.0
31.0
30.0
29.0
28.0
27.0
26.0
25.0
24.0
23.0
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

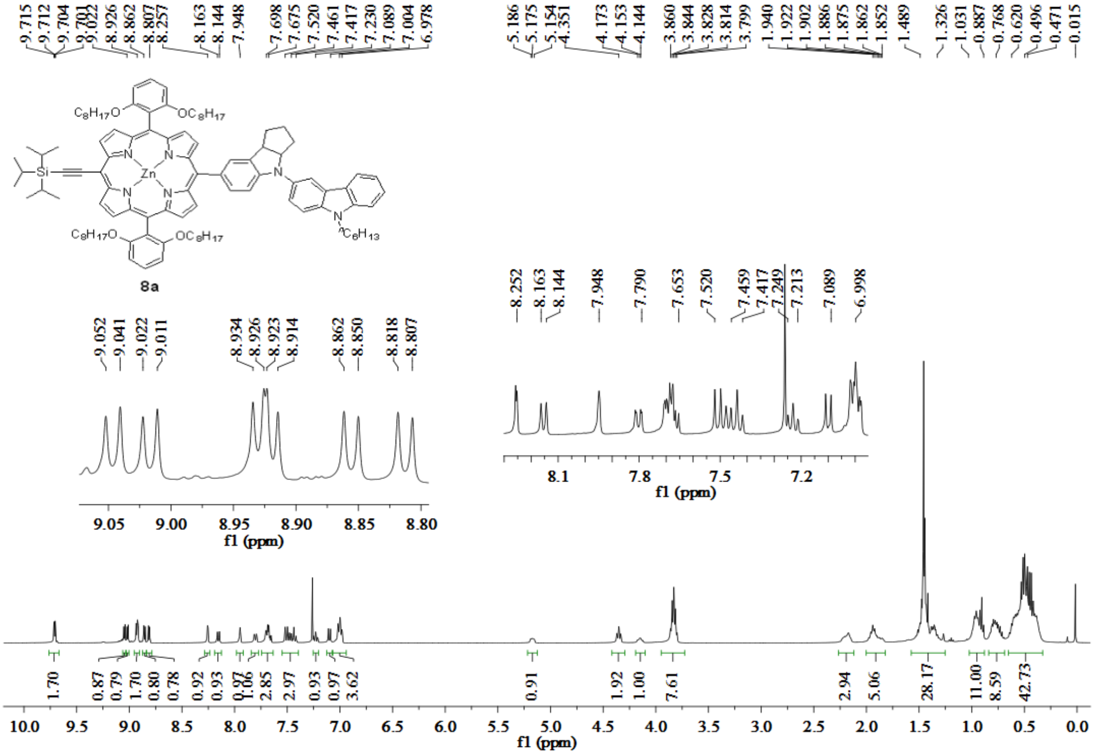

8.052
8.033
7.992
7.587
7.409
7.233
7.192
6.671
6.660
6.651
6.641
4.914
4.899
4.893
4.884
4.879
4.293
4.275
3.894
3.872
3.851
1.961
1.889
1.852
1.709
1.667
1.626
1.599
1.432
1.408
1.341
1.277
1.251
0.888
0.882
0.871
0.090
0.078
0.015
0.007
O
B
O
N
N
^{n}C$_6$H$_{13}$
6a
7.587
7.527
7.507
7.499
7.486
7.466
7.448
7.409
7.399
7.394
7.260
7.233
7.229
7.215
7.196
7.192
7.60
7.50
7.40
7.30
7.20
f1 (ppm)
0.905
0.900
0.882
0.871
0.92
0.88
f1 (ppm)
1.01
0.96
0.92
2.00
2.93
1.03
0.97
1.00
2.01
1.01
5.10
3.38
2.32
16.17
3.23
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

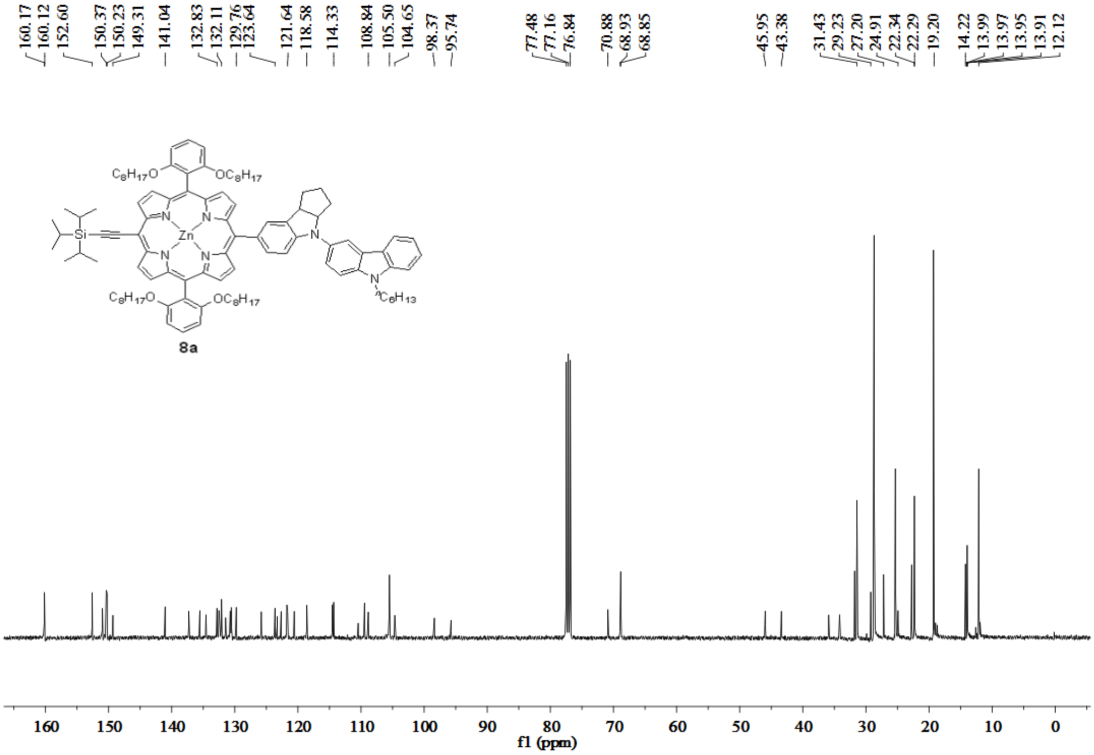

153.14
141.06
135.46
133.74
131.06
125.93
122.38
120.53
118.79
115.45
109.38
108.90
105.79
83.24
77.48
77.16
76.84
70.71
45.46
43.36
35.55
33.65
31.73
27.15
25.09
24.89
24.48
22.70
14.17
O
B
O
N
N
^{n}C$_6$H$_{13}$
6a
153.14
141.06
137.64
135.46
134.46
133.74
131.06
125.93
123.55
122.59
122.38
120.53
118.79
115.45
109.38
108.90
105.79
152
148
144
140
136
132
128
124
120
116
112
108
f1 (ppm)
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)


6b
7.553 7.530 7.510 7.144 6.849 6.829
4.815 4.810 4.799 4.794 4.788 4.777 4.773 3.819 3.804 3.798 3.782 3.776 2.334 1.999 1.983 1.926 1.909 1.893 1.877 1.860 1.770 1.754 1.737 1.710 1.660 1.637 1.621 1.608 1.546 1.505 1.478 1.378 1.329 1.251
7.553 7.530 7.510 7.260 7.199 7.193 7.183 7.177 7.166 7.144 6.849 6.829
4.815 4.810 4.794 4.788 4.777 4.773
3.825 3.819 3.798 3.782 3.776
0.97 0.91 3.82 0.90 1.00 1.00 2.85 1.12 2.05 1.20 1.41 1.34 5.77 5.82
f1 (ppm)

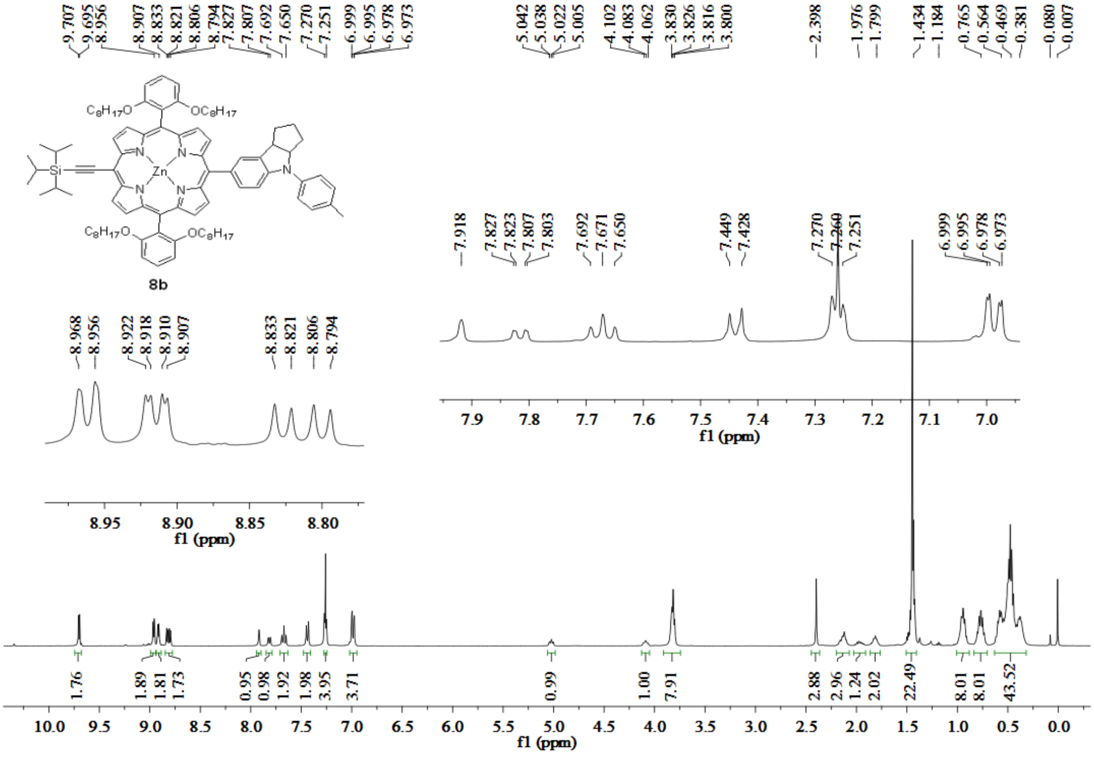

6c
7.541 7.521 7.434 7.260 6.258 6.238
4.233 4.216 4.201 3.719 3.701 3.679 3.234 3.214 3.193 3.131 3.109 3.081 3.058 1.817 1.703 1.631 1.600 1.533 1.478 1.434 1.319 0.914 0.900 0.883
7.521 7.434 7.260 6.258 6.238
3.250 3.228 3.214 3.193 3.176 3.131 3.109 3.094 3.073 3.058
1.377 1.327 1.319
0.914 0.900 0.883
0.95 0.84 0.90 0.91 1.00 2.04 1.32 2.22 5.95 17.27 2.96
f1 (ppm)


6c
O
O
B
N
^{n}C$_6$H$_{13}$
154.75
135.74
132.85
130.39
103.97
83.07
77.16
76.84
68.68
45.68
45.38
35.27
33.33
31.83
27.05
24.85
22.77
14.20
45.68
45.38
35.27
33.33
31.83
27.18
27.05
25.03
24.85
24.47
22.77
14.20
45 43 41 39 37 35 33 31 29 27 25 23 21 19 17 15
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

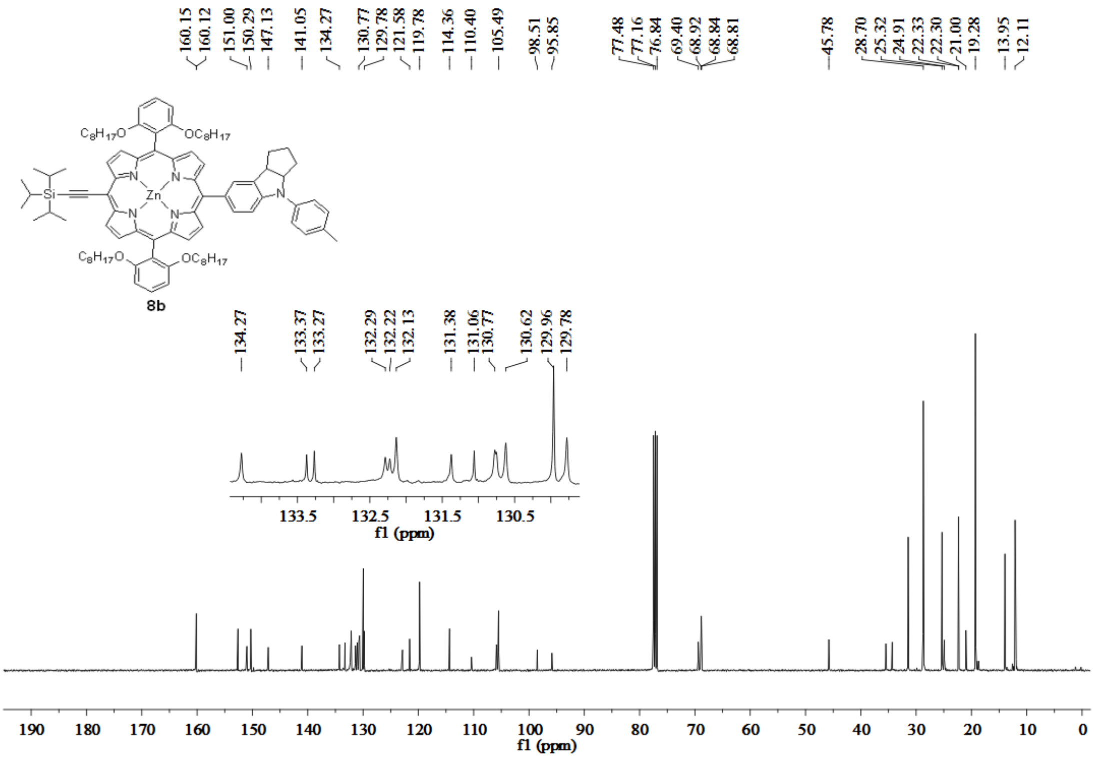

8a
C$_8$H$_{17}$O
OC$_8$H$_{17}$
Si
Zn
N
N
N
N
N
N
^{n}C$_6$H$_{13}$
C$_8$H$_{17}$O
OC$_8$H$_{17}$
9.715
9.712
9.704
9.701
9.022
8.926
8.862
8.807
8.257
8.163
8.144
7.948
7.698
7.675
7.520
7.461
7.417
7.230
7.089
7.004
6.978
5.186
5.175
5.154
4.351
4.173
4.153
4.144
3.860
3.844
3.828
3.814
3.799
1.940
1.922
1.902
1.886
1.875
1.862
1.852
1.489
1.326
1.031
0.887
0.768
0.620
0.496
0.471
-0.015
9.052
9.041
9.022
9.011
8.934
8.926
8.923
8.914
8.862
8.850
8.818
8.807
9.05 9.00 8.95 8.90 8.85 8.80
f1 (ppm)
8.252
8.163
8.144
7.948
7.790
7.653
7.520
7.459
7.417
7.249
7.213
7.089
6.998
8.1 7.8 7.5 7.2
f1 (ppm)
1.70
0.87
0.79
1.70
0.80
0.78
0.92
0.93
0.97
1.06
2.85
2.97
0.93
0.97
3.62
0.91
1.92
1.00
7.61
2.94
5.06
28.17
11.00
8.59
42.73
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.17
160.12
152.60
150.37
150.23
149.31
141.04
132.83
132.11
129.76
123.64
121.64
118.58
114.33
108.84
105.50
104.65
98.37
95.74
77.48
77.16
76.84
70.88
68.93
68.85
45.95
43.38
31.43
29.23
27.20
24.91
22.34
22.29
19.20
14.22
13.99
13.97
13.95
13.91
12.12
C8H17O
OC8H17
Si
N
Zn
C8H17O
OC8H17
N
N
C6H13
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

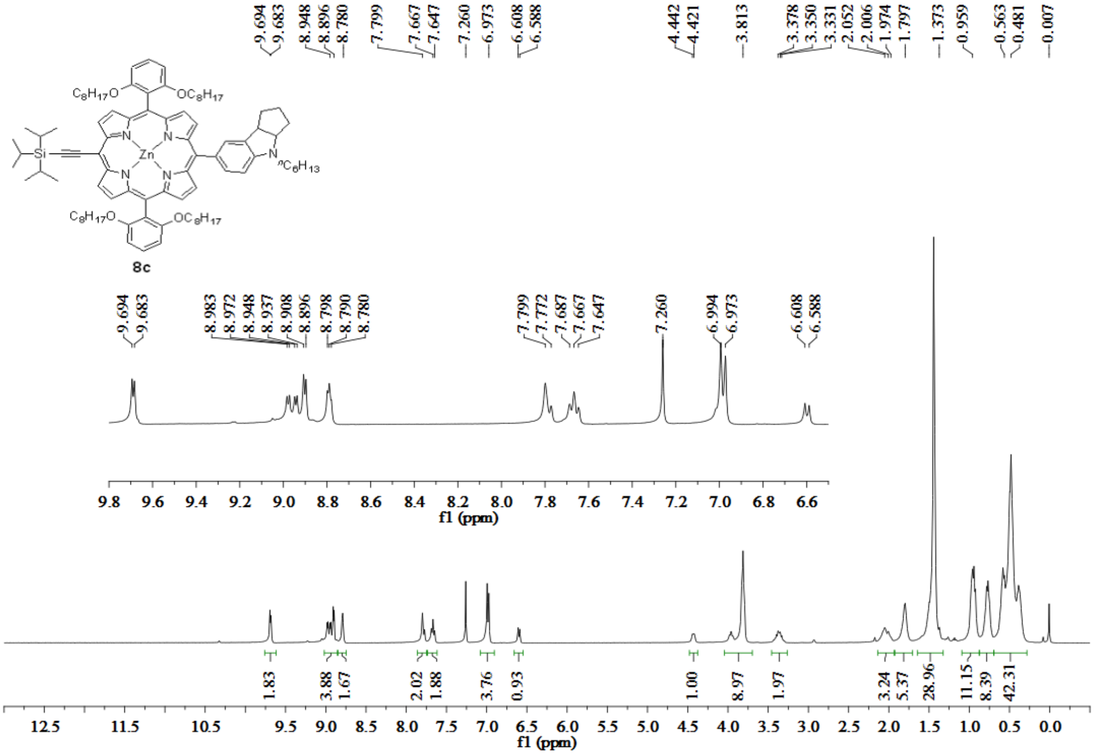
8a


9.707
9.695
8.956
8.907
8.833
8.821
8.806
8.794
7.827
7.807
7.692
7.650
7.270
7.251
6.999
6.995
6.978
6.973
5.042
5.038
5.022
5.005
4.102
4.083
4.062
3.830
3.826
3.816
3.800
2.398
1.976
1.799
1.434
1.184
0.765
0.564
0.469
0.381
0.080
0.007
C8H17O
OC8H17
Si
N
Zn
C8H17O
OC8H17
N
8.968
8.956
8.922
8.918
8.910
8.907
8.833
8.821
8.806
8.794
8.95 8.90 8.85 8.80
f1 (ppm)
7.918
7.827
7.823
7.807
7.803
7.692
7.671
7.650
7.449
7.428
7.270
7.260
7.251
6.999
6.995
6.978
6.973
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
1.76
1.89
1.81
1.73
0.95
0.98
1.92
1.98
3.95
3.71
0.99
1.00
7.91
2.88
2.96
1.24
2.02
22.49
8.01
8.01
43.52
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

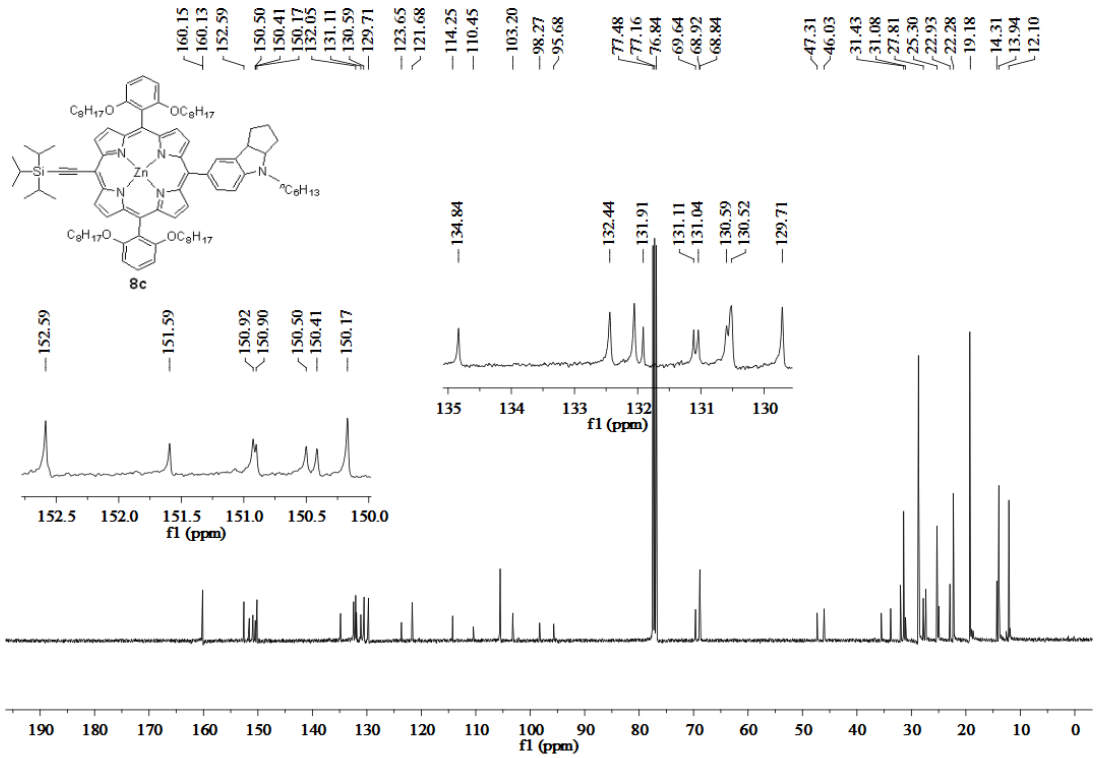
8b

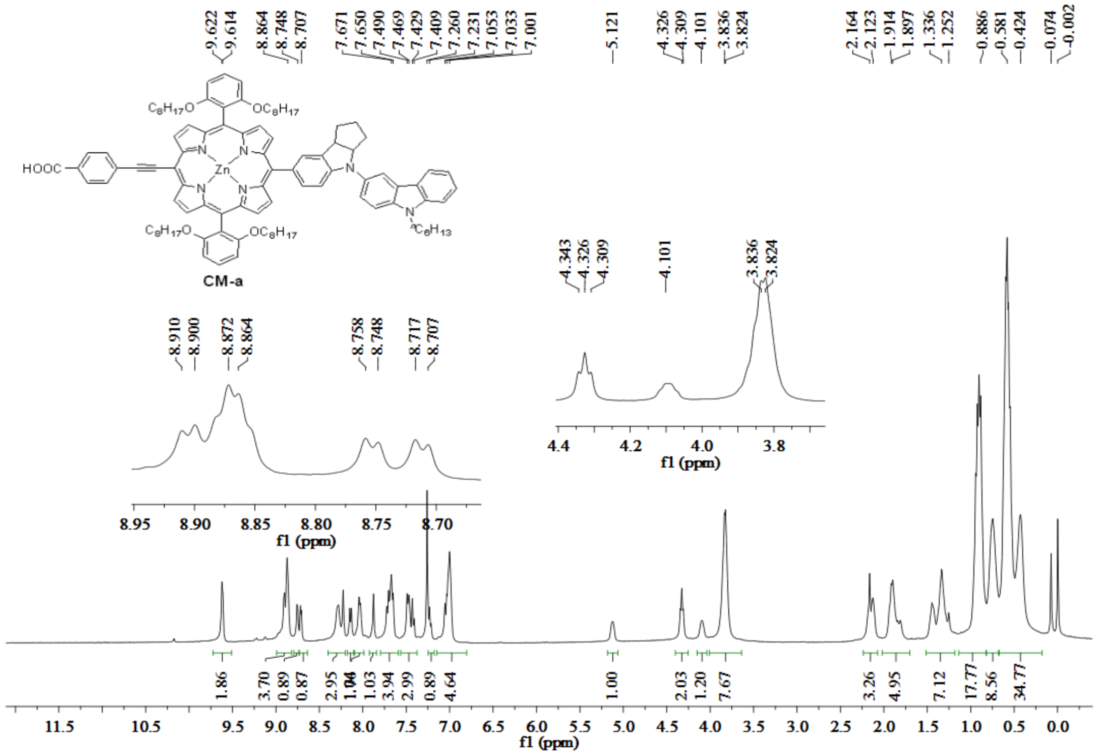

160.15
160.12
151.00
150.29
147.13
141.05
134.27
130.77
129.78
121.58
119.78
114.36
110.40
105.49
98.51
95.85
77.48
77.16
76.84
69.40
68.92
68.84
68.81
45.78
28.70
25.32
24.91
22.33
22.30
21.00
19.28
13.95
12.11
C8H17O
OC8H17
Si
Zn
N
134.27
133.37
133.27
132.29
132.22
132.13
131.38
131.06
130.77
130.62
129.96
129.78
133.5
132.5
131.5
130.5
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

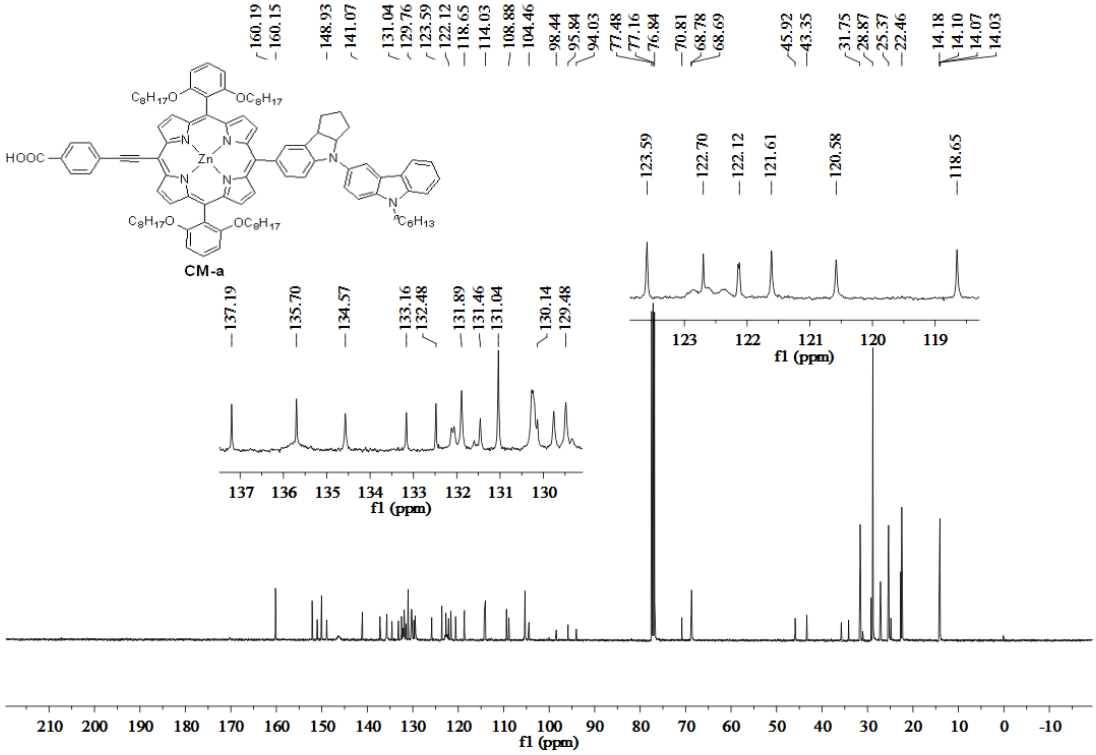
8b


9.694
9.683
8.948
8.896
8.780
7.799
7.667
7.647
7.260
6.973
6.608
6.588
4.442
4.421
3.813
3.378
3.350
3.331
2.052
2.006
1.974
1.797
1.373
0.959
0.563
0.481
0.007
C8H17O
OC8H17
Si
Zn
N
nC6H13
9.694
9.683
8.983
8.972
8.948
8.937
8.908
8.896
8.798
8.790
8.780
7.799
7.772
7.687
7.667
7.647
7.260
6.994
6.973
6.608
6.588
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
f1 (ppm)
1.83
3.88
1.67
2.02
1.88
3.76
0.93
1.00
8.97
1.97
3.24
5.37
28.96
11.15
8.39
42.31
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

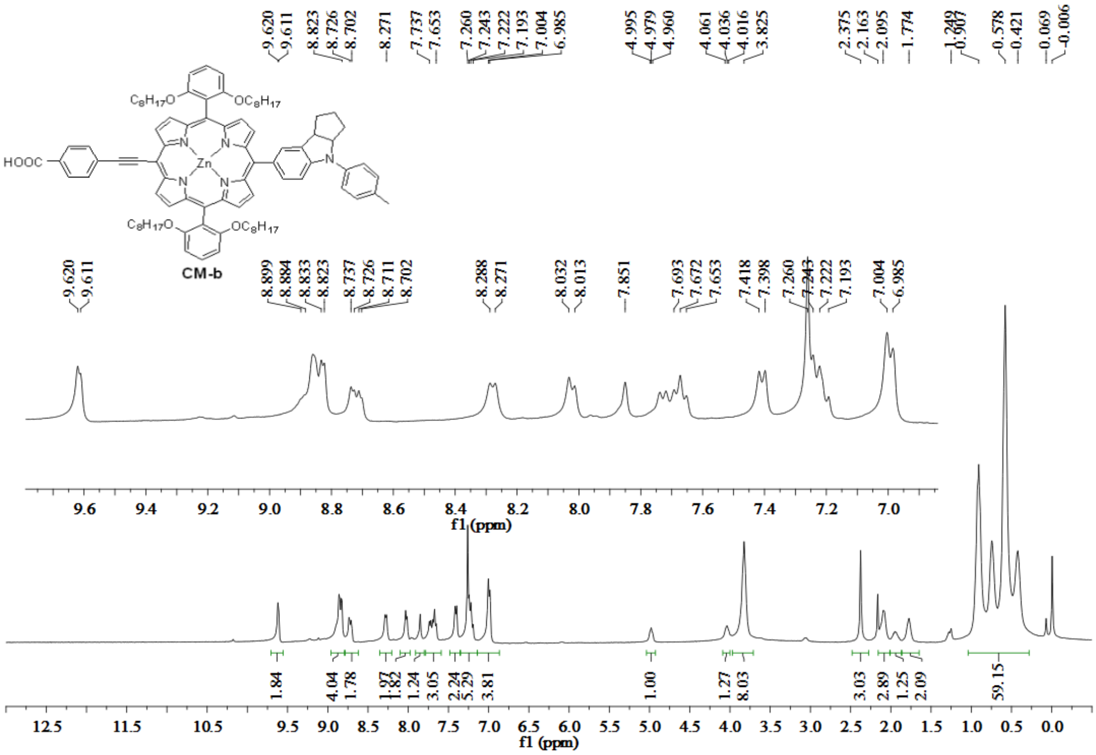
8c


160.15
160.13
152.59
150.50
150.41
150.17
132.05
131.11
130.59
129.71
123.65
121.68
114.25
110.45
103.20
98.27
95.68
77.48
77.16
76.84
69.64
68.92
68.84
47.31
46.03
31.43
31.08
27.81
25.30
22.93
22.28
19.18
14.31
13.94
12.10
C8H17O
OC8H17
Si
N
Zn
nC6H13
8c
134.84
132.44
131.91
131.11
131.04
130.59
130.52
129.71
135
134
133
132
131
130
f1 (ppm)
152.59
151.59
150.92
150.90
150.50
150.41
150.17
152.5
152.0
151.5
151.0
150.5
150.0
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

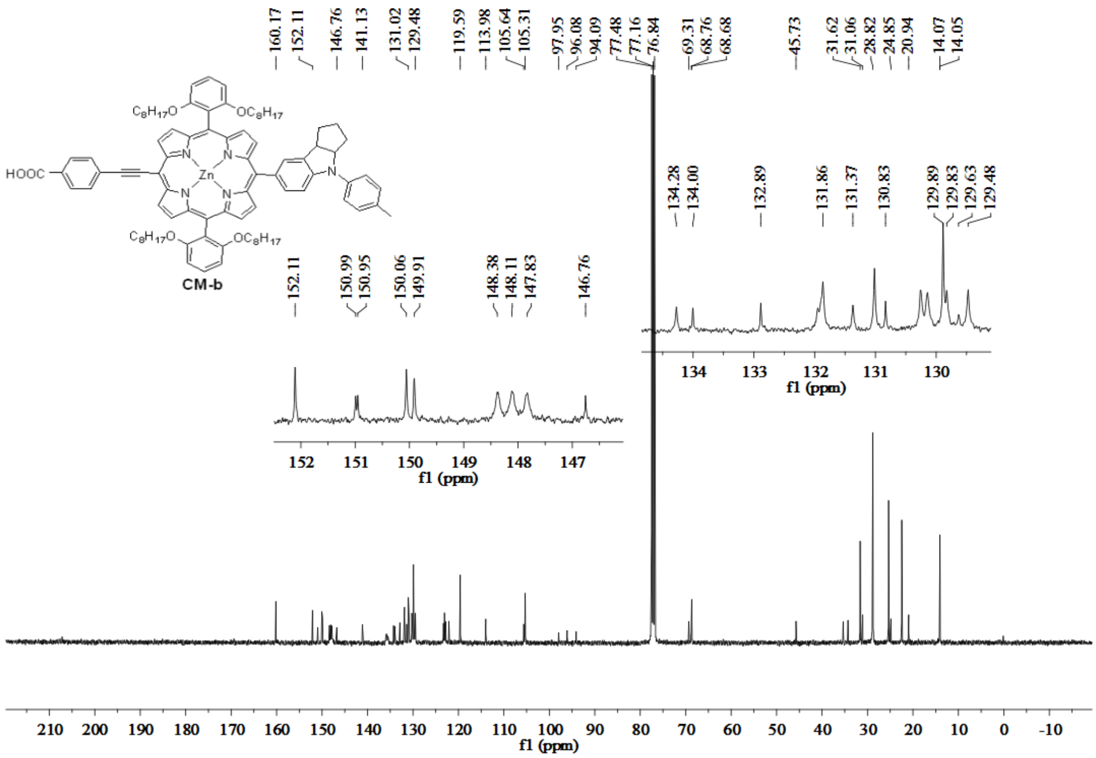

9.622
9.614
8.864
8.748
8.707
7.671
7.650
7.490
7.469
7.429
7.409
7.260
7.231
7.053
7.033
7.001
5.121
4.326
4.309
4.101
3.836
3.824
2.164
2.123
1.914
1.897
1.336
1.252
0.886
0.581
0.424
0.074
-0.002
HOOC
C8H17O
OC8H17
N
Zn
nC6H13
CM-a
4.343
4.326
4.309
4.101
3.836
3.824
4.4
4.2
4.0
3.8
f1 (ppm)
8.910
8.900
8.872
8.864
8.758
8.748
8.717
8.707
8.95
8.90
8.85
8.80
8.75
8.70
f1 (ppm)
1.86
3.70
0.89
0.87
2.95
1.04
1.03
3.94
2.99
0.89
4.64
1.00
2.03
1.20
7.67
3.26
4.95
7.12
17.77
8.56
34.77
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

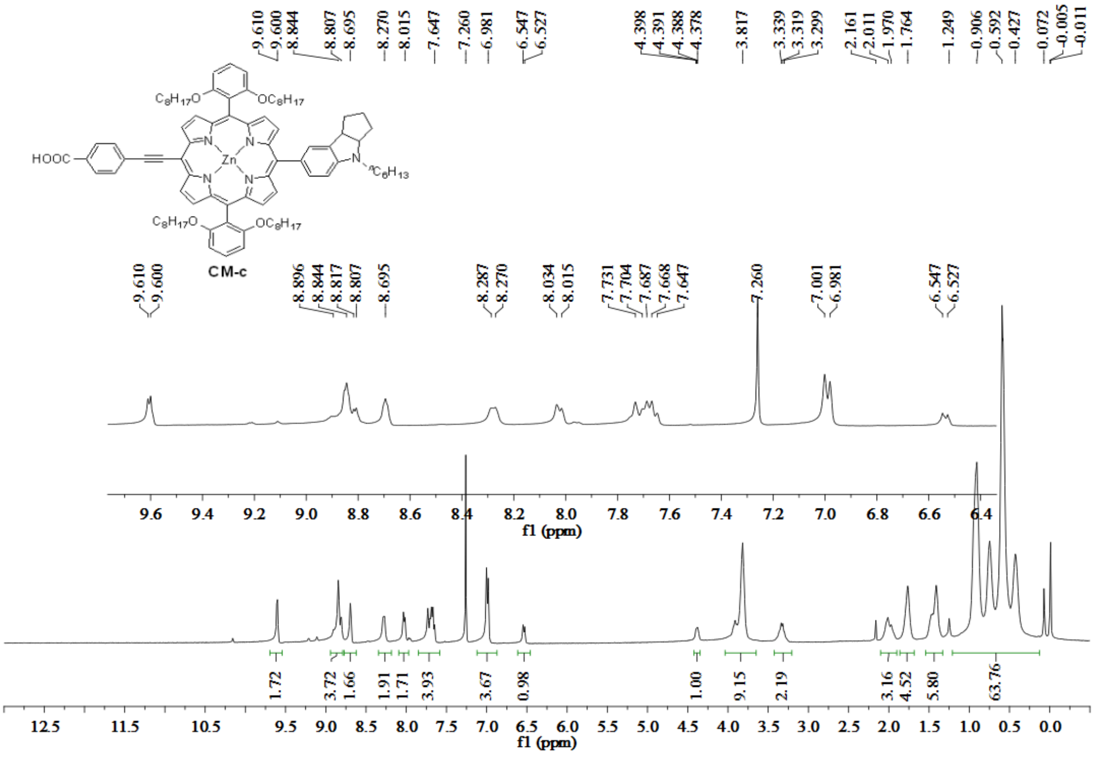

160.19
160.15
148.93
141.07
131.04
129.76
123.59
122.12
118.65
114.03
108.88
104.46
98.44
95.84
94.03
77.48
77.16
76.84
70.81
68.78
68.69
45.92
43.35
31.75
28.87
25.37
22.46
14.18
14.10
14.07
14.03
HOOC
C8H17O
OC8H17
Zn
N
C6H13
123.59
122.70
122.12
121.61
120.58
118.65
123 122 121 120 119
f1 (ppm)
137.19
135.70
134.57
133.16
132.48
131.89
131.46
131.04
130.14
129.48
137 136 135 134 133 132 131 130
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

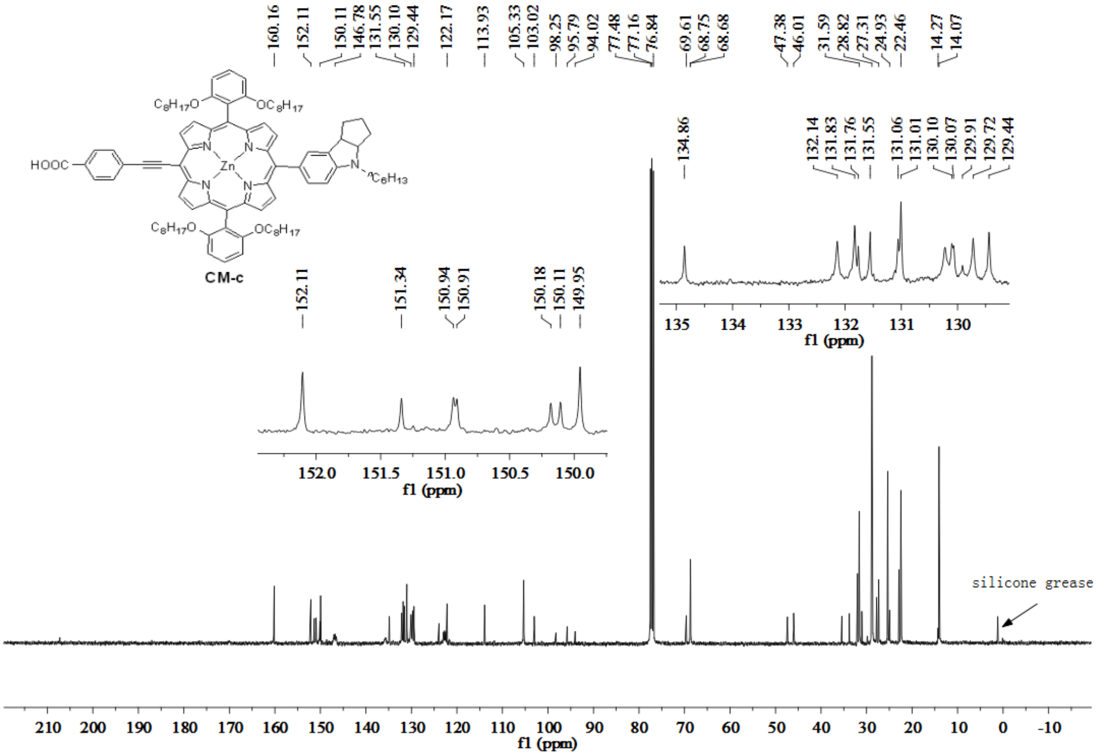
CM-a


9.620
9.611
8.823
8.726
8.702
8.271
7.737
7.653
7.260
7.243
7.222
7.193
7.004
6.985
4.995
4.979
4.960
4.061
4.036
4.016
3.825
2.375
2.163
2.095
1.774
1.249
0.907
0.578
0.421
0.069
-0.006
HOOC
C8H17O
OC8H17
Zn
N
9.620
9.611
8.899
8.884
8.833
8.823
8.737
8.726
8.711
8.702
8.288
8.271
8.032
8.013
7.851
7.693
7.672
7.653
7.418
7.398
7.260
7.243
7.222
7.193
7.004
6.985
9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
1.84
4.04
1.78
1.97
1.82
1.24
3.05
2.24
5.29
3.81
1.00
1.27
8.03
3.03
2.89
1.25
2.09
59.15
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

CM-b


CM-b
160.17
152.11
146.76
141.13
131.02
129.48
119.59
113.98
105.64
105.31
97.95
96.08
94.09
77.48
77.16
76.84
69.31
68.76
68.68
45.73
31.62
31.06
28.82
24.85
20.94
14.07
14.05
C8H17O
OC8H17
HOOC
Zn
N
134.28
134.00
132.89
131.86
131.37
130.83
129.89
129.83
129.63
129.48
134 133 132 131 130
f1 (ppm)
152.11
150.99
150.95
150.06
149.91
148.38
148.11
147.83
146.76
152 151 150 149 148 147
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


CM-c
9.610
9.600
8.844
8.807
8.695
8.270
8.015
7.647
7.260
6.981
6.547
6.527
4.398
4.391
4.388
4.378
3.817
3.339
3.319
3.299
2.161
2.011
1.970
1.764
1.249
0.906
0.592
0.427
0.072
0.005
-0.011
C8H17O
OC8H17
HOOC
Zn
N
nC6H13
9.610
9.600
8.896
8.844
8.817
8.807
8.695
8.287
8.270
8.034
8.015
7.731
7.704
7.687
7.668
7.647
7.260
7.001
6.981
6.547
6.527
9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4
f1 (ppm)
1.72
3.72
1.66
1.91
1.71
3.93
3.67
0.98
1.00
9.15
2.19
3.16
4.52
5.80
63.76
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.16
152.11
150.11
146.78
131.55
130.10
129.44
122.17
113.93
105.33
103.02
98.25
95.79
94.02
77.48
77.16
76.84
69.61
68.75
68.68
47.38
46.01
31.59
28.82
27.31
24.93
22.46
14.27
14.07
C8H17O
OC8H17
HOOC
Zn
N
C6H13
CM-c
134.86
132.14
131.83
131.76
131.55
131.06
131.01
130.10
130.07
129.91
129.72
129.44
135
134
133
132
131
130
f1 (ppm)
152.11
151.34
150.94
150.91
150.18
150.11
149.95
152.0
151.5
151.0
150.5
150.0
f1 (ppm)
silicone grease
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)