Electronic Supplementary Information

for

Chiroptical and catalytic properties of doubly binaphthyl-strapped chiral porphyrins

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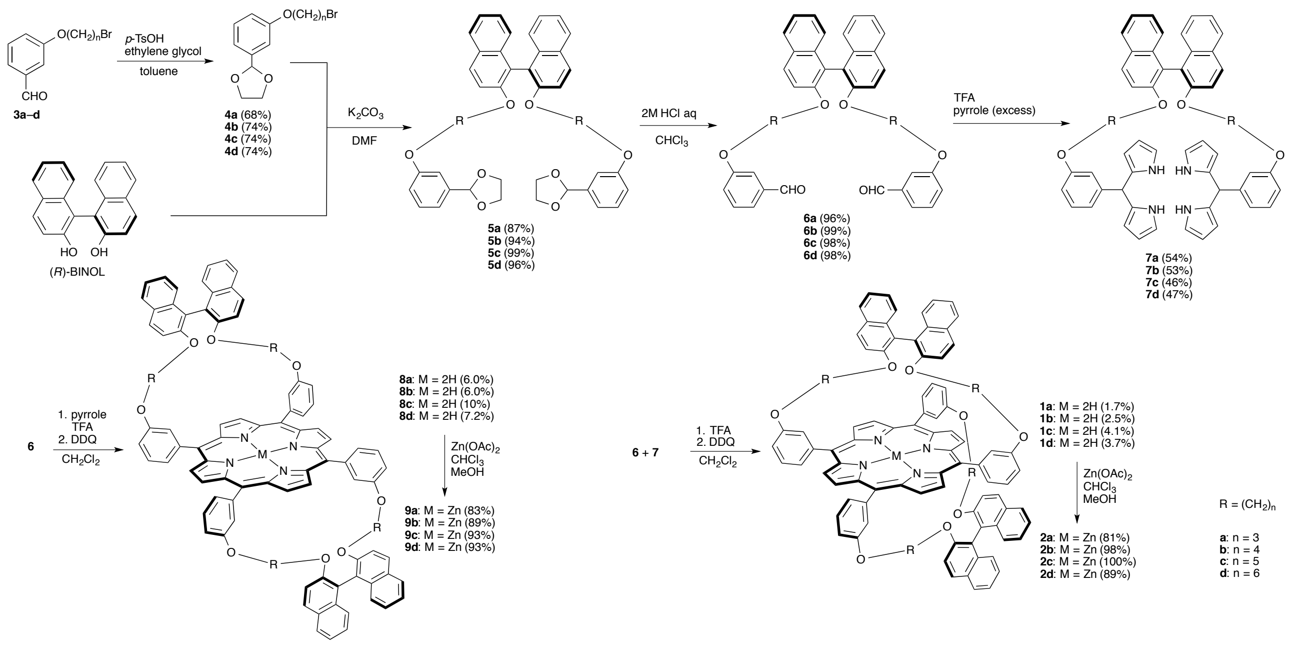
Table of Contents

[A] Instrumentation and Materials

NMR spectroscopy was performed on a JEOL 400 MHz spectrometer and chemical shifts were reported as the delta scale in ppm as internal reference $\delta = 7.26$ ($CDCl_3$) for ^{1}H NMR, and $\delta = 77.16$ ($CDCl_3$) for ^{13}C NMR. MS spectra were recorded on a Bruker micrOTOF. IR spectra were recorded on a Shimadzu IRAffinity-1 spectrophotometer. UV/Vis spectra were recorded on a Shimadzu UV-2600 spectrophotometer. Fluorescence spectra were measured on a HITACHI F-2700 spectrophotometer. Absolute fluorescence quantum yields were recorded on a Hamamatsu Photonics C9920-02 spectrometer by the photon-counting method using an integration sphere. CD spectra were recorded on a JASCO J-720 or J-1500 spectropolarimeter. CPL spectra were measured on a JASCO CPL-200. Commercial reagents were used without further purification. Compounds **3a**,[S1] **3b**,[S2] **3c**,[S3] and **3d**[S2] were prepared by the literature method. Dry CH_2Cl_2 was distilled from CaH_2.

Single crystals of **1d** were obtained by slow diffusion of CH_3CN vapor into a solution of **1d** in CH_2Cl_2. X-ray data at 93 K were taken on a Rigaku XtaLAB P200 with Cu-K_α radiation (λ = 1.54187 Å). The structures were solved by direct methods (SHELXS-97) and refined with full-matrix least square technique (SHELXL-97). All non-hydrogen atoms were refined anisotropically and the hydrogen atoms were calculated in ideal positions.

[B] Experimental Procedures and Compound Data



Scheme S1 Synthesis of doubly binaphthyl strapped porphyrins **1**, **2**, **8**, and **9**.

Synthesis of 4a

p-Toluenesulfonic acid monohydrate (687 mg, 3.61 mmol) was dissolved in dry toluene (51.5 mL) under Ar. **3a** (8.78 g, 36.1 mmol) and ethylene glycol (10.1 mL, 180 mmol) were added via syringe, and the mixture was heated at reflux for 12 h. After cooling to room temperature, water was added, and the organic products were extracted with EtOAc. The organic layer was washed with saturated $NaHCO_3$ solution and brine, dried over Na_2SO_4, and concentrated. Purification by silica gel column chromatography (hexane/EtOAc (7:1)) gave **4a** as a pale yellow oil (7.05 g, 24.5 mmol, 68%).

Synthesis of 5a

To a flask containing (*R*)-(+)-1,1'-bi-2-naphthol (1.03 g, 3.60 mmol) and K_2CO_3 (4.98 g, 36.0 mmol) was added a solution of **4a** (2.17 g, 7.57 mmol) in dry DMF (10.0 mL) under Ar. The mixture was heated at 100 °C for 6 h. After cooling to room temperature, the mixture was diluted with $CHCl_3$ and filtered. The solution was washed with water, dried over Na_2SO_4, and concentrated. Purification by silica gel column chromatography (hexane/EtOAc (2:1)) gave **5a** as a pale yellow oil (2.19 g, 3.13 mmol, 87%).

Synthesis of 6a

2M HCl (2.70 mL) was added to a solution of **5a** (1.90 g, 2.70 mmol) in $CHCl_3$ (40.0 mL) under Ar. The mixture was heated at 50 °C for 3 h. The organic layer was separated, washed with saturated $NaHCO_3$ solution and brine, dried over Na_2SO_4, and concentrated to give **6a** as a pale yellow oil (1.58 g, 2.59 mmol, 96%).

Synthesis of 7a

6a (973 mg, 1.59 mmol) was dissolved in pyrrole (11.0 mL, 159 mmol), and TFA (243 µL, 3.18 mmol) was added. The mixture was heated at 50 °C for 12 h under Ar. After cooling to room temperature, the reaction was quenched by addition of aqueous 10% NaOH solution. Organic products were extracted with $CHCl_3$, and the organic layer was washed with saturated $NaHCO_3$ solution, dried over Na_2SO_4, and concentrated. Purification by silica gel column chromatography (hexane/EtOAc (3:1)) gave **7a** as a brownish solid (728 mg, 864 µmol, 54%).

Synthesis of 1a

A solution of **7a** (1.03 g, 1.22 mmol) and **6a** (747 mg, 1.22 mmol) in dry CH_2Cl_2 (245 mL) was bubbled with Ar for 20 min, and TFA (93.0 µL, 1.22 mmol) was added. The mixture was stirred at room temperature for 1 h in the dark. Et_3N (510 µL, 3.67 mmol) and DDQ (1.67 g, 7.34 mmol) were added, and the mixture was stirred for 12 h. After the solvents were evaporated, purification by silica gel column chromatography ($CHCl_3$) and recrystallization from $CHCl_3$/MeOH gave **1a** as a purple solid (29.5 mg, 20.9 µmol, 1.7%).

Synthesis of 2a

To a solution of **1a** (10.5 mg, 7.44 µmol) in $CHCl_3$ (1.04 mL) was added a solution of $Zn(OAc)_2{\cdot}2H_2O$ (16.3 mg, 74.4 µmol) in MeOH (149 µL), and the mixture was stirred at 60 °C for 2 h. $CHCl_3$ was added, and the mixture was washed with water, dried over Na_2SO_4, and concentrated. Purification by silica gel column chromatography ($CHCl_3$) and recrystallization from $CHCl_3$/MeOH gave **2a** as a purple solid (8.89 mg, 6.03 µmol, 81%).

Compounds **2b−d** were synthesized according to a method similar to the synthesis of **2a**.

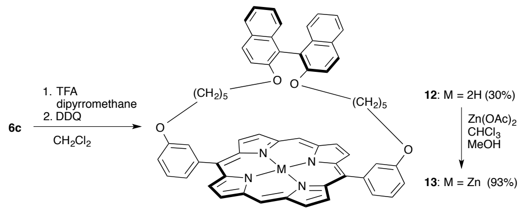
Synthesis of 8a

A solution of **6a** (287 mg, 470 µmol) and pyrrole (65.0 µL, 940 µmol) in dry CH_2Cl_2 (94.0 mL) was bubbled with Ar for 20 min, and TFA (36.0 µL, 470 µmol) was added. The mixture was stirred at room temperature for 1 h in the dark. Et_3N (130 µL, 940 µmol) and DDQ (320 mg, 1.41 mmol) were added, and the mixture was stirred for 1 h. After the solvents were evaporated, purification by silica gel column chromatography ($CHCl_3$) and recrystallization from $CHCl_3$/MeOH gave **8a** as a purple solid (20.0 mg, 14.2 µmol, 6.0%).

Synthesis of 9a

To a solution of **8a** (9.30 mg, 6.59 µmol) in $CHCl_3$ (920 µL) was added a solution of $Zn(OAc)_2·2H_2O$ (14.5 mg, 65.9 µmol) in MeOH (130 µL), and the mixture was stirred at 60 °C for 3 h. $CHCl_3$ was added, and the mixture was washed with water, dried over Na_2SO_4, and concentrated. Purification by silica gel column chromatography ($CHCl_3$) and recrystallization from $CHCl_3$/MeOH gave **9a** as a purple solid (8.08 mg, 5.48 µmol, 83%).

Compounds **9b−d** were synthesized according to a method similar to the synthesis of **9a**.



Scheme S2 Synthesis of singly strapped porphyrins **12** and **13**

Synthesis of 12

A solution of **6c** (279 mg, 418 µmol) and dipyrromethane (122 mg, 837 µmol) in dry CH_2Cl_2 (84.0 mL) was bubbled with Ar for 20 min, and TFA (32.0 µL, 418 µmol) was added. The mixture was stirred at room temperature for 7.5 h in the dark. DDQ (380 mg, 1.67 mmol) was added, and the mixture was stirred for 12 h. Et_3N (116 µL, 837 µmol) was added, and the mixture was stirred for 1 h. After the solvents were evaporated, purification by silica gel column chromatography ($CHCl_3$) and recrystallization from $CHCl_3$/MeOH gave **12** as purple solid (113 mg, 124 µmol, 30%).

Synthesis of 13

To a solution of **12** (56.6 mg, 61.7 µmol) in $CHCl_3$ (8.60 mL) was added a solution of $Zn(OAc)_2·2H_2O$ (136 mg, 617 µmol) in MeOH (1.30 mL), and the mixture was stirred at room temperature for 24 h. $CHCl_3$ was added, and the mixture was washed with water, dried over Na_2SO_4, and concentrated. Purification by silica gel column chromatography ($CHCl_3$) and recrystallization from $CHCl_3$/MeOH gave **13** as a purple solid (56.3 mg, 57.4 µmol, 93%).

Compound data for 4a

Pale yellow oil, 7.05 g, 68% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 2.32 (quin, J = 6.2 Hz, 2H, CH_2), 3.60 (t, J = 6.5 Hz, 2H, CH_2), 4.03 (t, J = 6.9 Hz, 2H, CH_2), 4.08−4.17 (m, 4H, CH_2), 5.79 (s, 1H, CH), 6.91 (dd, J = 2.6, 8.2 Hz, 1H, Ph), 7.04 (d, J = 2.3 Hz, 1H, Ph), 7.07 (d, J = 7.6 Hz, 1H, Ph), 7.29 ppm (t, J = 7.9 Hz, 1H, Ph); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 30.1, 32.5, 65.41, 65.42, 103.6, 112.3, 115.7, 119.2, 129.7, 139.7, 158.9 ppm; IR (neat) 2953, 2884, 1605, 1491, 1458, 1389, 1319, 1267, 1213, 1182, 1099, 1034, 945, 870, 783, 721, 694, 654, 602, 561 cm^{-1}; HRMS (APCI) calcd for $C_{12}H_{16}O_3Br$ 287.0277, found 287.0268 ($[M+H]^+$).

Compound data for 5a

Pale yellow oil, 2.19 g, 87% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 1.75−1.86 (m, 4H, CH_2), 3.37−3.46 (m, 4H, CH_2), 4.01−4.08 (m, 8H, CH_2), 4.11–4.14 (m, 4H, CH_2), 5.77 (s, 2H, CH), 6.50 (dd, J = 2.5, 8.2 Hz, 2H, Ph), 6.77

(s, 2H, Ph), 7.03 (d, J = 7.6 Hz, 2H, Ph), 7.15 (d, J = 3.6 Hz, 4H, Np), 7.21 (t, J = 7.9 Hz, 2H, Ph), 7.27−7.31 (m, 2H, Np), 7.39 (d, J = 9.0 Hz, 2H, Np), 7.84 (d, J = 8.2 Hz, 2H, Np), 7.90 ppm (d, J = 9.0 Hz, 2H, Np); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 29.3, 64.1, 65.4, 66.1, 103.8, 112.6, 115.2, 115.8, 118.6, 120.7, 123.8, 125.4, 126.4, 128.0, 129.39, 129.43, 134.2, 139.3, 154.1, 158.9 ppm; IR (neat) 3055, 2926, 2886, 1732, 1593, 1506, 1456, 1395, 1269, 1182, 1086, 945, 864, 810, 775, 750, 723, 694 cm^{-1}; HRMS (ESI) calcd for $C_{44}H_{42}O_8Na$ 721.2772, found 721.2779 ($[M+Na]^+$).

Compound data for 6a

Pale yellow oil, 1.58 g, 96% yield; ^1H NMR ($CDCl_3$, 400 MHz) δ = 1.80−1.86 (m, 4H, CH_2), 3.32−3.46 (m, 4H, CH_2), 4.02−4.12 (m, 4H, CH_2), 6.78−6.81 (m, 2H, Ph), 7.01−7.02 (m, 2H, Ph), 7.10−7.13 (m, 4H, Np), 7.21−7.26 (m, 2H, Np), 7.35 (t, J = 7.8 Hz, 2H, Ph), 7.39−7.43 (m, 2H for Np and 2H for Ph), 7.81 (d, J = 8.2 Hz, 2H, Np), 7.91 (d, J = 9.0 Hz, 2H, Np), 9.95 ppm (s, 2H, CHO); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 29.2, 64.3, 66.0, 113.2, 115.8, 120.8, 121.8, 123.1, 123.9, 125.4, 126.5, 128.0, 129.5, 129.6, 129.9, 134.1, 137.7, 154.1, 159.4, 192.4 ppm; IR (neat) 3057, 2957, 2880, 2729, 1682, 1622, 1593, 1506, 1456, 1387, 1260, 1169, 1148, 1061, 1015, 866, 783, 754, 683, 648 cm^{-1}; HRMS (ESI) calcd for $C_{40}H_{34}O_6Na$ 633.2248, found 633.2238 ($[M+Na]^+$).

Compound data for 7a

Brownish solid, 728 mg, 54% yield; ^1H NMR ($CDCl_3$, 400 MHz) δ = 1.71−1.76 (m, 4H, CH_2), 3.32−3.41 (m, 4H, CH_2), 3.93−4.02 (m, 4H, CH_2), 5.36 (s, 2H, CH), 5.93 (s, 4H, pyrrole-β), 6.14−6.16 (m, 4H, pyrrole-β), 6.39 (dd, J = 2.2, 8.2 Hz, 2H, Ph), 6.54 (t, J = 1.9 Hz, 2H, Ph), 6.64−6.66 (m, 4H, pyrrole-α), 6.76 (d, J = 7.7 Hz, 2H, Ph), 7.10−7.17 (m, 4H for Np and 2H for Ph), 7.25−7.31 (m, 4H, Np), 7.81 (d, J = 8.1 Hz, 2H, Np), 7.84 (d, J = 9.1 Hz, 2H, Np), 7.90 ppm (s, 4H, NH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 29.3, 44.1, 64.1, 66.1, 107.28, 107.30, 108.6, 112.5, 115.1, 115.8, 117.31, 117.33, 120.72, 120.73, 123.8, 125.5, 126.4, 128.0, 129.4, 129.5, 129.6, 132.4, 132.5, 134.2, 143.6, 154.1, 159.1 ppm; IR (KBr) 3406, 3100, 3055, 2934, 2878, 1697, 1647, 1593, 1506, 1489, 1458, 1400, 1354, 1331, 1261, 1148, 1088, 1061, 1028, 883, 810, 756, 721 cm^{-1}; HRMS (ESI) calcd for $C_{56}H_{50}N_4O_4Na$ 865.3724, found 865.3758 ($[M+Na]^+$).

Compound data for 1a

Purple solid, 29.5 mg, 1.7% yield; ^1H NMR ($CDCl_3$, 400 MHz) δ = 0.01 (s, 2H, NH), 1.31−1.39 (m, 4H, CH_2), 1.54 (m, 4H, CH_2), 3.16 (m, 4H, CH_2), 3.32−3.38 (m, 8H, CH_2), 3.41−3.49 (m, 4H, CH_2), 5.06 (d, J = 9.0 Hz, 4H, Np), 5.53 (d, J = 9.1 Hz, 4H, Np), 5.61 (s, 4H, Ph), 6.22 (d, J = 8.0 Hz, 4H, Np), 6.55 (d, J = 8.3 Hz, 4H, Np), 6.83 (t, J = 7.6 Hz, 4H, Np), 6.89 (t, J = 7.3 Hz, 4H, Np), 7.05 (dd, J = 2.4, 8.2 Hz, 4H, Ph), 7.77 (t, J = 7.9 Hz, 4H, Ph), 8.63 (d, J = 7.3 Hz, 4H, Ph), 8.98 (s, 4H, β), 9.00 ppm (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 27.8, 65.1, 65.5, 112.7, 116.8, 118.6, 118.8, 120.1, 122.1, 123.1, 125.0, 125.7, 127.4, 128.0, 128.2, 128.8, 130.3, 133.2, 134.0, 142.1, 152.2, 156.6 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (5.08), 430 (4.97), 529 (3.73), 568 (3.52), 601 (3.57), 654 nm (3.46); IR (KBr) 3283, 3057, 2957, 2930, 1595, 1506, 1491, 1427, 1339, 1229, 1146, 1045, 989, 924, 791, 748, 716 cm^{-1}; HRMS (APCl) calcd for $C_{96}H_{75}N_4O_8$ 1412.5612, found 1412.5656 ($[M+H]^+$).

Compound data for 2a

Purple solid, 8.89 mg, 81% yield; ^1H NMR ($CDCl_3$, 400 MHz) δ = 1.21−1.26 (m, 4H, CH_2), 1.44−1.48 (m, 4H,

CH_2), 3.21−3.32 (m, 12H, CH_2), 3.44 (m, 4H, CH_2), 5.56 (d, J = 9.1 Hz, 4H, Np), 5.60 (d, J = 9.1 Hz, 4H, Np), 5.65 (s, 4H, Ph), 6.61 (d, J = 8.5 Hz, 4H, Np), 6.75 (d, J = 8.1 Hz, 4H, Np), 6.87 (t, J = 7.5 Hz, 4H, Np), 6.97 (t, J = 7.3 Hz, 4H, Np), 7.06 (dd, J = 2.2, 8.0 Hz, 4H, Ph), 7.79 (t, J = 7.9 Hz, 4H, Ph), 8.64 (d, J = 7.4 Hz, 4H, Ph), 9.05 (s, 4H, β), 9.08 ppm (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 27.8, 65.4, 65.6, 112.5, 116.5, 118.0, 120.2, 120.6, 121.9, 123.1, 125.1, 125.7, 127.4, 128.0, 128.7, 132.6, 132.88, 132.93, 143.0, 147.6, 147.9, 152.3, 156.1 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (4.77), 439 (4.60), 573 (3.38), 618 nm (3.20); IR (KBr) 3057, 2928, 2855, 1622, 1595, 1506, 1489, 1472, 1458, 1319, 1263, 1148, 1130, 1059, 1011, 806, 789, 748 cm^{-1}; HRMS (APCI) calcd for $C_{96}H_{72}N_4O_8Zn$ 1474.4624, found 1474.4658 ($[M]^-$).

Compound data for 8a

Purple solid, 20.0 mg, 6.0% yield; ^1H NMR ($CDCl_3$, 400 MHz) δ = −2.38 (s, 2H, NH), 1.84 (s, 4H, CH_2), 2.05 (s, 4H, CH_2), 3.22 (s, 2H, CH_2), 3.76−4.08 (m, 12H, CH_2), 4.32 (s, 2H, CH_2), 5.59 (s, 2H, Np or Ph), 6.26 (s, 2H, Np or Ph), 6.56 (s, 2H, Np or Ph), 6.90−7.34 (m, 18H, Np or Ph), 7.52−8.18 (m, 16H, Np or Ph), 8.77 (s, 4H, β), 9.06−9.20 (m, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 30.1, 64.9, 66.6, 68.4, 68.7, 117.1, 117.6, 117.9, 118.2, 120.6, 120.7, 121.7, 122.4, 122.6, 123.8, 124.2, 125.4, 125.7, 126.0, 126.4, 127.6, 128.0, 129.0, 129.8, 130.2, 132.6, 134.2, 143.7, 154.9, 157.4 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 229 (5.40), 421 (5.63), 516 (4.26), 550 (3.93), 592 (3.75), 647 nm (3.57); IR (KBr) 3314, 3055, 2953, 2878, 1595, 1470, 1429, 1352, 1261, 1238, 1211, 1182, 1159, 1082, 1053, 804, 750 cm^{-1}; HRMS (APCI) calcd for $C_{96}H_{74}N_4O_8$ 1411.5545, found 1411.5501 ($[M]^-$).

Compound data for 9a

Purple solid, 8.08 mg, 83% yield; ^1H NMR ($CDCl_3$, 400 MHz) δ = 1.41−1.64 (m, 8H, CH_2), 3.66−4.07 (m, 16H, CH_2), 6.63−7.10 (m, 14H, Np or Ph), 7.29−7.43 (m, 10H, Np or Ph), 7.62−8.03 (m, 16H, Np or Ph), 9.06−9.18 (m, 8H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 22.4, 22.5, 22.6, 28.5, 28.7, 29.1, 29.2, 67.9, 68.7, 70.2, 70.6, 114.9, 115.9, 116.3, 116.4, 117.2, 121.2, 121.5, 121.6, 122.2, 123.4, 123.7, 125.6, 125.7, 125.9, 126.2, 127.2, 127.4, 127.5, 127.68, 127.73, 128.0, 128.9, 129.4, 129.7, 132.2, 132.36, 132.41, 134.3, 134.5, 144.3, 144.4, 150.7, 150.8, 154.9, 157.4, 154.8, 157.7 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 229 (5.43), 427 (5.73), 557 (4.34), 597 nm (3.92); IR (KBr) 3055, 2953, 2926, 2878, 1595, 1506, 1473, 1458, 1337, 1260, 1209, 1184, 1159, 1082, 1053, 1001, 799, 748, 721 cm^{-1}; HRMS (APCI) calcd for $C_{96}H_{72}N_4O_8Zn$ 1474.4664, found 1474.4631 ($[M]^-$).

Compound data for 4b

Yellow oil, 3.49 g, 74% yield; ^1H NMR ($CDCl_3$, 400 MHz) δ = 1.94 (m, 2H, CH_2), 2.07 (m, 2H, CH_2), 3.49 (t, J = 6.6 Hz, 2H, CH_2), 4.01 (t, J = 6.2 Hz, 2H, CH_2), 4.03−4.16 (m, 4H, CH_2), 5.79 (s, 1H, CH), 6.89 (dd, J = 2.6, 8.2 Hz, 1H, Ph), 7.02 (s, 1H, Ph), 7.06 (d, J = 7.6 Hz, 1H, Ph), 7.29 ppm (t, J = 7.9 Hz, 1H, Ph); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 28.0, 29.6, 33.6, 65.4, 66.9, 103.7, 112.1, 115.7, 119.0, 129.6, 139.6, 159.1 ppm; IR (neat) 3042, 2953, 2884, 2754, 1605, 1489, 1456, 1395, 1317, 1254, 1182, 1159, 1072, 961, 874, 781, 721, 694, 646, 559 cm^{-1}; HRMS (APCI) calcd for $C_{13}H_{18}O_3Br$ 301.0434, found 301.0447 ($[M+H]^+$).

Compound data for 5b

Yellow oil, 6.34 g, 94% yield; ^1H NMR ($CDCl_3$, 400 MHz) δ = 1.24–1.40 (m, 4H, CH_2), 1.50−1.64 (m, 4H, CH_2), 3.52 (t, J = 6.3 Hz, 4H, CH_2), 3.91−3.99 (m, 2H, CH_2), 4.01−4.08 (m, 6H, CH_2), 4.10−4.16 (m, 4H, CH_2), 5.78 (s, 2H, CH), 6.72 (dd, J = 2.5, 8.2 Hz, 2H, Ph), 6.89 (s, 2H, Ph), 7.03 (d, J = 7.6 Hz, 2H, Np), 7.18−7.25 (m, 2H for Np and 4H for Ph), 7.27−7.34 (m, 2H, Np), 7.41 (d, J = 9.0 Hz, 2H, Np), 7.85 (d, J = 8.1 Hz, 2H, Np), 7.92 ppm (d, J = 9.1 Hz, 2H, Np); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.4, 25.9, 65.4, 67.1, 69.4, 103.7, 112.3, 115.5, 116.2, 118.6, 120.9, 123.7, 125.6, 126.3, 128.0, 129.4, 129.46, 129.49, 134.2, 139.4, 154.5, 159.2 ppm; IR (neat) 3055, 2953, 2878, 2758, 1738, 1732, 1614, 1593, 1504, 1393, 1227, 1180, 1148, 1036, 945, 864, 808, 779, 750, 721, 694, 608 cm^{-1}; HRMS (ESI) calcd for $C_{46}H_{47}O_8$ 727.3265, found 727.3293 ($[M+H]^+$).

Compound data for 6b

Yellow oil, 5.53 g, 99% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 1.24–1.38 (m, 4H, CH_2), 1.50−1.64 (m, 4H, CH_2), 3.49 (t, J = 6.3 Hz, 4H, CH_2), 3.94 (m, 2H, CH_2), 4.06 (m, 2H, CH_2), 6.98 (m, 2H, Ph), 7.16−7.24 (m, 4H for Np and 2H for Ph), 7.31 (m, 2H, Ph), 7.36−7.43 (m, 4H for Np and 2H for Ph), 7.83 (d, J = 8.2 Hz, 2H, Np), 7.91 (d, J = 8.9 Hz, 2H, Np), 9.95 ppm (s, 2H, CHO); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.3, 25.8, 67.3, 69.4, 112.8, 116.1, 120.9, 121.9, 123.3, 123.8, 125.5, 126.3, 128.0, 129.4, 129.5, 130.0, 134.2, 137.8, 154.5, 159.6, 192.3 ppm; IR (neat) 3057, 2947, 2874, 2729, 1699, 1593, 1504, 1485, 1454, 1387, 1331, 1219, 1169, 1148, 1086, 1018, 864, 808, 746, 683, 648, 592 cm^{-1}; HRMS (ESI) calcd for $C_{42}H_{38}O_6Na$ 661.2561, found 661.2591 ($[M+Na]^+$).

Compound data for 7b

Brownish solid, 731 mg, 53% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 1.27 (m, 4H, CH_2), 1.48−1.53 (m, 4H, CH_2), 3.43 (t, J = 6.3 Hz, 4H, CH_2), 3.87−4.02 (m, 4H, CH_2), 5.38 (s, 2H, CH), 5.92 (s, 4H, pyrrole-β), 6.13−6.15 (m, 4H, pyrrole-β), 6.57−6.66 (m, 4H for pyrrole-α and 4H for Ph), 6.76 (d, J = 7.7 Hz, 2H, Ph), 7.13−7.20 (m, 4H for Np and 2H for Ph), 7.28−7.29 (m, 2H, Np), 7.36 (d, J = 9.0 Hz, 2H, Np), 7.81 (d, J = 8.2 Hz, 2H, Np), 7.88 (d, J = 8.9 Hz, 2H, Np), 7.89 (s, 4H, NH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.4, 25.9, 44.1, 67.1, 69.4, 107.3, 108.6, 112.8, 115.0, 116.1, 117.3, 120.7, 120.9, 123.7, 125.6, 126.3, 128.0, 129.4, 129.5, 129.7, 132.5, 134.3, 143.6, 154.5, 159.4 ppm; IR (KBr) 3395, 3100, 3055, 2936, 2874, 1701, 1593, 1508, 1489, 1472, 1431, 1398, 1354, 1331, 1261, 1148, 1115, 1088, 1028, 883, 810, 756, 721 cm^{-1}; HRMS (ESI) calcd for $C_{58}H_{54}N_4O_4Na$ 893.4037, found 893.4033 ($[M+Na]^+$).

Compound data for 1b

Purple solid, 18.7 mg, 2.5% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = −1.41 (s, 2H, NH), 0.67−0.81 (m, 8H, CH_2), 1.12 (m, 8H, CH_2), 3.13 (m, 4H, CH_2), 3.22 (m, 4H, CH_2), 3.53 (m, 8H, CH_2), 6.09 (d, J = 9.1 Hz, 4H, Np), 6.18 (s, 4H, Ph), 6.45 (d, J = 9.1 Hz, 4H, Np), 6.69 (d, J = 8.4 Hz, 4H Np), 6.90 (t, J = 7.2 Hz, 4H, Np), 6.97 (t, J = 7.4 Hz, 4H, Np), 7.09 (d, J = 7.8 Hz, 4H, Np), 7.15 (dd, J = 2.2, 8.5 Hz, 4H, Ph), 7.77 (t, J = 7.9 Hz, 4H, Ph), 8.50 (d, J = 7.3 Hz, 4H, Ph), 8.84 (s, 4H, β), 8.89 ppm (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 24.4, 25.0, 68.3, 68.4, 113.8, 117.2, 119.19, 119.20, 120.4, 123.1, 123.9, 125.3, 125.7, 127.6, 128.5, 128.7, 130.7, 132.9, 133.7, 142.8, 153.3, 156.8 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 231 (5.32), 423 (5.48), 520 (4.12), 555 (3.75), 595 (3.66), 648 nm (3.35); IR (KBr) 3300, 3057, 2953, 2876, 1620, 1595, 1506, 1491, 1472, 1458, 1427, 1352, 1337, 1260, 1252, 1219, 1078, 1047, 1016, 995, 795, 748, 716 cm^{-1}; HRMS (ESI) calcd for $C_{100}H_{82}N_4O_8Na$ 1490.6058, found 1490.6009 ($[M+Na]^+$).

Compound data for 2b

Purple solid, 5.8 mg, 98% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.53 (m, 4H, CH_2), 0.74 (m, 4H, CH_2), 1.13–1.23 (m, 8H, CH_2), 3.02 (m, 4H, CH_2), 3.24 (m, 4H, CH_2), 3.55 (m, 4H, CH_2), 3.69 (m, 4H, CH_2), 6.29 (s, 4H, Ph), 6.31 (d, J = 9.2 Hz, 4H, Np), 6.73 (d, J = 8.5 Hz, 4H, Np), 6.88 (d, J = 9.0 Hz, 4H, Np), 6.93 (t, J = 7.6 Hz, 4H, Np), 7.03 (t, J = 7.3 Hz, 4H, Np), 7.16 (dd, J = 2.1, 8.4 Hz, 4H, Np), 7.33 (d, J = 8.1 Hz, 4H, Ph), 7.76 (t, J = 7.9 Hz, 4H, Ph), 8.45 (d, J = 7.4 Hz, 4H, Ph), 8.87 (s, 4H, β), 8.97 ppm (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 23.9, 24.7, 68.1, 113.2, 116.9, 118.5, 119.9, 120.6, 123.3, 124.2, 125.3, 125.9, 127.8, 128.5, 128.7, 128.9, 132.3, 132.6, 133.5, 143.9, 149.0, 149.1, 153.1, 156.2 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (5.14), 430 (5.17), 562 (3.86), 603 nm (3.47); IR (KBr) 3057, 2953, 2874, 1653, 1622, 1595, 1506, 1476, 1427, 1323, 1261, 1240, 1215, 1148, 1057, 1003, 866, 793, 748, 719 cm^{-1}; HRMS (ESI) calcd for $C_{100}H_{80}N_4O_8ZnCl$ 1565.5019, found 1565.5023 ([M+Cl]$^-$).

Compound data for 8b

Purple solid, 21.0 mg, 6.0% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = −2.38 (s, 2H, NH), 1.39–1.86 (m, 16H, CH_2), 3.40–3.65 (m, 4H, CH_2), 3.84–4.20 (m, 12H, CH_2), 6.31–7.23 (m, 12H, Np or Ph), 7.29–7.65 (m, 12H, Np or Ph), 7.76–8.10 (m, 16H, Np or Ph), 8.91 (s, 4H, β), 9.10 (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.3, 25.9, 26.5, 67.9, 68.1, 69.4, 70.0, 116.0, 116.3, 120.8, 121.1, 121.4, 122.8, 123.4, 123.7, 125.6, 126.1, 127.5, 127.8, 128.0, 129.0, 129.4, 129.5, 129.7, 130.4, 132.4, 134.2, 134.4, 143.7, 154.2, 154.7, 157.4, 157.5 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 231 (5.41), 420 (5.64), 515 (4.30), 551 (3.93), 592 (3.75), 647 nm (3.56); IR (KBr) 3314, 3057, 2943, 2874, 1595, 1508, 1472, 1429, 1352, 1317, 1261, 1242, 1207, 1180, 1148, 1084, 1045, 1018, 997, 804, 777, 748 cm^{-1}; HRMS (APCI) calcd for $C_{100}H_{82}N_4O_8$ 1467.6171, found 1467.6118 ([M]$^-$).

Compound data for 9b

Purple solid, 8.3 mg, 89% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 1.30–1.71 (m, 16H, CH_2), 3.42–3.51 (m, 4H, CH_2), 3.84–4.13 (m, 12H, CH_2), 5.73–6.72 (m, 4H, Np or Ph), 6.92–7.10 (m, 8H, Np or Ph), 7.23–7.50 (m, 12H, Np or Ph), 7.60–8.09 (m, 16H, Np or Ph), 9.04–9.21 (m, 8H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.2, 25.6, 25.9, 26.0, 29.9, 67.8, 68.0, 69.4, 70.1, 115.6, 115.8, 116.2, 121.1, 121.8, 122.5, 123.4, 123.7, 125.5, 125.6, 126.0, 126.2, 127.5, 127.6, 128.0, 128.9, 129.5, 129.7, 132.1, 132.4, 132.5, 134.4, 144.2, 144.4, 150.7, 150.8, 154.7, 157.1, 157.4 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 232 (5.31), 426 (5.63), 556 (4.21), 596 nm (3.75); IR (KBr) 3055, 2943, 2874, 1595, 1506, 1474, 1458, 1431, 1354, 1337, 1261, 1209, 1182, 1159, 1148, 1082, 1069, 1045, 999, 799, 748 cm^{-1}; HRMS (APCI) calcd for $C_{100}H_{80}N_4O_8Zn$ 1530.5292, found 1530.5278 ([M]$^-$).

Compound data for 4c

Yellow oil, 3.76 g, 74% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 1.61 (m, 2H, CH_2), 1.81 (m, 2H, CH_2), 1.93 (m, 2H, CH_2), 3.43 (t, J = 6.7 Hz, 2H, CH_2), 3.98 (t, J = 6.3 Hz, 2H, CH_2), 4.00−4.15 (m, 4H, CH_2), 5.78 (s, 1H, CH), 6.89 (dd, J = 2.3, 7.9 Hz, 1H, Ph), 7.02 (s, 1H, Ph), 7.03 (d, J = 6.5 Hz, 1H, Ph), 7.28 ppm (t, J = 7.9 Hz, 1H, Ph); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 24.9, 28.5, 32.5, 33.7, 65.3, 67.6, 103.6, 112.1, 115.6, 118.8, 129.5, 139.5, 159.1 ppm; IR (neat) 3040, 2943, 2884, 2754, 1605, 1587 1491, 1456, 1389, 1319, 1273, 1182, 1159, 1070, 964, 874, 783, 721, 694, 642, 559 cm^{-1}; HRMS (APCI) calcd for $C_{14}H_{20}O_3Br$ 315.0590, found 315.0582 ([M+H]$^+$).

Compound data for 5c

Yellow oil, 1.11 g, 99% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.95−1.02 (m, 4H, CH_2), 1.38−1.49 (m, 8H, CH_2), 3.56 (t, J = 6.5 Hz, 4H, CH_2), 3.88−3.94 (m, 2H, CH_2), 3.99−4.09 (m, 6H, CH_2), 4.11−4.17 (m, 4H, CH_2), 5.82 (s, 2H, CH), 6.82 (dd, J = 2.5, 8.2 Hz, 2H, Ph), 6.97 (s, 2H, Ph), 7.06 (d, J = 7.6 Hz, 2H, Ph), 7.16−7.22 (m, 4H, Np), 7.27−7.31 (m, 2H for Ph and 2H for Np), 7.40 (d, J = 9.0 Hz, 2H, Np), 7.82 (d, J = 8.2 Hz, 2H, Np), 7.90 ppm (d, J = 8.9 Hz, 2H, Np); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 22.3, 28.6, 29.1, 65.4, 67.7, 69.7, 103.7, 112.2, 115.6, 116.0, 118.6, 120.9, 123.6, 125.6, 126.2, 127.9, 129.2, 129.4, 129.5, 134.3, 139.4, 154.6, 159.3 ppm; IR (neat) 3055, 2945, 2874, 1695, 1591, 1504, 1456, 1354, 1329, 1260, 1182, 1148, 1078, 962, 876, 810, 777, 750, 721, 694 cm^{-1}; HRMS (ESI) calcd for $C_{48}H_{50}O_8Na$ 777.3398, found 777.3362 ([M+Na]$^+$).

Compound data for 6c

Yellow oil, 242 mg, 98% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.94−1.02 (m, 4H, CH_2), 1.36−1.53 (m, 8H, CH_2), 3.55 (t, J = 6.5 Hz, 4H, CH_2), 3.88−3.94 (m, 2H, CH_2), 4.02−4.07 (m, 2H, CH_2), 7.06−7.09 (m, 2H, Ph), 7.15−7.21 (m, 2H for Ph and 2H for Np), 7.25−7.30 (m, 2H, Np), 7.40 (d, J = 9.0 Hz, 2H, Np), 7.43–7.45 (m, 4H for Ph and 2H for Np), 7.81 (d, J = 8.1 Hz, 2H, Np), 7.90 (d, J = 8.9 Hz, 2H, Np), 9.99 ppm (s, 2H, CHO); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 22.3, 28.5, 29.0, 68.0, 69.7, 112.6, 115.9, 120.9, 122.1, 123.6, 123.7, 125.6, 126.3, 127.9, 129.3, 129.4, 130.1, 134.3, 137.9, 154.6, 159.8, 192.4 ppm; IR (neat) 3057, 2922, 2870, 2729, 1705, 1593, 1506, 1456, 1387, 1319, 1261, 1169, 1148, 1084, 1043, 883, 777, 748, 685, 648 cm^{-1}; HRMS (ESI) calcd for $C_{44}H_{42}O_6Na$ 689.2874, found 689.2907 ([M+Na]$^+$).

Compound data for 7c

Brownish solid, 205 mg, 46% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.92−0.98 (m, 4H, CH_2), 1.31−1.47 (m, 8H, CH_2), 3.48 (t, J = 6.5 Hz, 4H, CH_2), 3.85−3.90 (m, 2H, CH_2), 3.97–4.01 (m, 2H, CH_2), 5.43 (s, 2H, CH), 5.96 (s, 4H, pyrrole-β), 6.16−6.18 (m, 4H, pyrrole-β), 6.68−6.70 (m, 4H for pyrrole-α and 4H for Ph), 6.80 (d, J = 7.7 Hz, 2H, Ph), 7.13−7.25 (m, 6H for Np and 2H for Ph), 7.35 (d, J = 9.0 Hz, 2H, Np), 7.76 (d, J = 7.9 Hz, 2H, Np), 7.84 (d, J = 9.0 Hz, 2H, Np), 7.94 ppm (s, 4H, NH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 22.4, 28.6, 29.1, 44.2, 67.7, 69.7, 107.3, 108.6, 112.9, 114.9, 116.0, 117.3, 120.7, 120.8, 123.6, 125.6, 126.3, 127.9, 129.3, 129.4, 129.7, 132.5, 134.3, 143.7, 154.6, 159.5 ppm; IR (KBr) 3374, 3098, 3055, 2934, 2868, 1724, 1593, 1508, 1489, 1468, 1458, 1431, 1398, 1354, 1317, 1261, 1148, 1088, 1028, 883, 810, 760, 719 cm^{-1}; HRMS (APCl) calcd for $C_{60}H_{59}N_4O_4$ 899.4531, found 899.4553 ([M+H]$^+$).

Compound data for 1c

Purple solid, 8.1 mg, 4.1% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = −1.54 (s, 2H, NH), 0.30 (m, 4H, CH_2), 0.42 (m, 4H, CH_2), 0.87 (m, 8H, CH_2), 1.28 (m, 8H, CH_2), 2.87 (m, 4H, CH_2), 3.09 (m, 4H, CH_2), 3.54 (m, 8H, CH_2), 5.08 (s, 8H, Np), 6.48 (d, J = 9.1 Hz, 8H, Np), 6.63 (s, 4H, Ph), 6.76 (t, J = 7.6 Hz, 4H, Np), 6.84 (t, J = 7.5 Hz, 4H Np), 7.22 (d, J = 8.4 Hz, 4H, Ph), 7.76 (t, J = 7.9 Hz, 4H, Ph), 8.45 (d, J = 7.4 Hz, 4H, Ph), 9.02 (s, 4H, β), 9.05 ppm (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 20.8, 26.9, 27.9, 67.5, 67.9, 112.8, 117.0, 118.4, 119.9, 120.1, 122.8, 125.1, 125.4, 127.2, 127.9, 128.0, 128.3, 133.1, 143.0, 153.0, 156.8 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (5.46), 422 (5.48), 518 (4.25), 553 (3.96), 592 (3.96), 647 nm (3.88); IR (KBr) 3310, 3055, 2926, 2868, 1734, 1595, 1506, 1472, 1427, 1335, 1263, 1242, 1219, 1146, 1134, 1078, 1047, 918, 864, 800, 748, 721, 698 cm^{-1}; HRMS (APCl) calcd for $C_{104}H_{91}N_4O_8$ 1524.6864, found 1524.6833 ($[M+H]^+$).

Compound data for 2c

Purple solid, 4.6 mg, 100% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.30 (m, 4H, CH_2), 0.54 (m, 4H, CH_2), 0.67 (m, 4H, CH_2), 0.77 (m, 4H, CH_2), 1.26–1.37 (m, 8H, CH_2), 2.91 (m, 4H, CH_2), 3.06 (m, 4H, CH_2), 3.60 (m, 4H, CH_2), 3.65 (m, 4H, CH_2), 5.38 (d, J = 9.0 Hz, 4H, Np), 5.76 (d, J = 9.0 Hz, 4H, Np), 6.62 (d, J = 8.4 Hz, 4H, Np), 6.70 (s, 4H, Ph), 6.87 (t, J = 7.6 Hz, 4H, Np), 6.92 (d, J = 7.9 Hz, 4H, Np), 6.99 (t, J = 7.5 Hz, 4H, Np), 7.24 (dd, J = 2.4, 8.5 Hz, 4H, Ph), 7.75 (t, J = 7.9 Hz, 4H, Ph), 8.42 (d, J = 7.7 Hz, 4H, Ph), 9.04 (s, 4H, β), 9.19 ppm (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 21.3, 27.3, 28.2, 68.1, 68.6, 113.8, 117.1, 119.1, 120.0, 121.3, 123.3, 125.4, 125.8, 127.6, 128.3, 128.4, 128.6, 132.6, 132.8, 133.4, 144.0, 149.9, 153.4, 156.7 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (5.26), 429 (5.30), 559 (4.00), 596 nm (3.66); IR (KBr) 3055, 2936, 2870, 1620, 1593, 1543, 1508, 1474, 1458, 1427, 1319, 1265, 1242, 1211, 1169, 1146, 1061, 1007, 934, 868, 795, 748, 718, 702 cm^{-1}; HRMS (APCI) calcd for $C_{100}H_{88}N_4O_8Zn$ 1586.5958, found 1586.5897 ($[M]^-$).

Compound data for 8c

Purple solid, 35.8 mg, 10% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = −2.60 (s, 2H, NH), 1.11–1.18 (m, 8H, CH_2), 1.42–1.52 (m, 12H, CH_2), 1.57–1.64 (m, 4H, CH_2), 3.68–3.72 (m, 8H, CH_2), 3.84–3.92 (m, 4H, CH_2), 3.98–4.03 (m, 4H, CH_2), 6.70–7.14 (m, 16H, Np or Ph), 7.26–7.45 (m, 8H, Np or Ph), 7.64–8.03 (m, 16H, Np or Ph), 8.94–9.06 (m, 8H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 22.1, 22.4, 22.5, 28.2, 28.4, 28.5, 28.8, 29.0, 29.1, 67.6, 68.5, 70.0, 70.5, 114.5, 115.7, 116.2, 117.3, 120.4, 120.5, 120.8, 121.6, 122.1, 123.5, 123.6, 125.4, 125.5, 125.9, 126.2, 127.5, 127.8, 128.0, 129.0, 129.3, 129.4, 134.0, 134.3, 143.5, 143.6, 154.6, 154.7, 157.2, 157.6 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (5.36), 419 (5.62), 514 (4.26), 550 (3.82), 591 (3.71), 647 nm (3.48); IR (KBr) 3314, 3055, 2941, 1595, 1576, 1558, 1541, 1506, 1489, 1472, 1458, 1429, 1352, 1339, 1317, 1263, 1242, 1180, 1163, 1084, 997, 804 cm^{-1}; HRMS (APCI) calcd for $C_{100}H_{90}N_4O_8$ 1523.6797, found 1523.6777 ($[M]^-$).

Compound data for 9c

Purple solid, 10.4 mg, 93% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 1.09–1.63 (m, 24H, CH_2), 3.70–4.05 (m, 16H, CH_2), 6.62–7.09 (m, 16H, Np or Ph), 7.24–7.42 (m, 8H, Np or Ph), 7.62–8.03 (m, 16H, Np or Ph), 9.06–9.16 (m, 8H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 22.4, 22.6, 28.4, 28.5, 28.6, 28.7, 29.1, 29.17, 29.24, 67.9, 68.7, 70.2, 70.6, 114.9, 115.1, 115.9, 116.0, 116.3, 116.4, 117.2, 121.2, 123.4, 123.7, 125.6, 125.7, 125.9, 126.2, 127.5, 127.68, 127.73, 128.0, 128.9, 129.4, 129.7, 132.17, 132.00, 132.3, 132.35, 132.40, 144.3, 144.4, 150.7, 150.8, 154.9, 157.4 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (5.42), 425 (5.73), 555 (4.33), 596 nm (3.84); IR (KBr) 3055, 2940, 2868, 1595, 1576, 1558, 1506, 1474, 1458, 1431, 1354, 1337, 1261, 1180, 1148, 1084, 1069, 1001, 934, 799, 748, 719, 700 cm^{-1}; HRMS (APCI) $C_{104}H_{88}N_4O_8Zn$ 1586.5920, found 1586.5920, found 1586.5931 ($[M]^-$).

Compound data for 4d

Pale orange oil, 4.95 g, 74% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 1.48−1.54 (m, 4H, CH_2), 1.79 (m, 2H, CH_2), 1.89 (m, 2H, CH_2), 3.42 (t, J = 6.8 Hz, 2H, CH_2), 3.97 (t, J = 6.4 Hz, 2H, CH_2), 4.00−4.15 (m, 4H, CH_2), 5.79 (s, 1H, CH), 6.89 (dd, J = 2.4 Hz, 8.2 Hz, 1H, Ph), 7.02 (d, J = 2.3 Hz, 1H, Ph), 7.05 (d, J = 7.7 Hz, 1H, Ph), 7.28 ppm (t, J = 8.0 Hz, 1H, Ph); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.4, 28.0, 29.1, 32.7, 33.9, 65.3, 67.8, 103.6, 112.1, 115.6, 118.7, 129.5, 139.5, 159.2 ppm; IR (neat) 2938, 2886, 1605, 1587, 1495, 1454, 1385, 1317, 1260, 1182, 1159, 1072, 945, 874, 781, 721, 694, 644, 606, 561 cm^{-1}; HRMS (APCI) calcd for $C_{15}H_{22}O_3Br$ 329.0747, found 329.0755 ($[M+H]^+$).

Compound data for 5d

Pale orange oil, 7.00 g, 96% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.91−0.96 (m, 4H, CH_2), 1.10–1.14 (m, 4H, CH_2), 1.40−1.51 (m, 8H, CH_2), 3.77 (t, J = 6.6 Hz, 4H, CH_2), 3.90−4.05 (m, 4H, CH_2), 4.05−4.15 (m, 8H, CH_2), 5.81 (s, 2H, CH), 6.86−6.89 (m, 2H, Ph), 7.02−7.03 (m, 2H, Ph), 7.07 (d, J = 7.6 Hz, 2H, Ph), 7.17−7.23 (m, 4H, Np), 7.28−7.35 (m, 2H for Ph and 2H for Np), 7.41 (d, J = 9.0 Hz, 2H, Np), 7.84 (d, J = 8.2 Hz, 2H, Np), 7.92 ppm (d, J = 9.0 Hz, 2H, Np); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.51, 25.53, 29.1, 29.4, 65.4, 67.8, 69.8, 103.7, 112.2, 115.7, 116.1, 118.7, 120.9, 123.6, 125.6, 126.2, 127.9, 129.2, 129.4, 129.5, 134.3, 139.5, 154.6, 159.3 ppm; IR (neat) 3055, 2941, 2872, 2758, 1732, 1591, 1506, 1456, 1387, 1354, 1275, 1180, 1065, 1018, 962, 862, 808, 779, 750, 721, 694, 608 cm^{-1}; HRMS (APCI) calcd for $C_{50}H_{55}O_8$ 783.3891, found 783.3860 ($[M+H]^+$).

Compound data for 6d

Pale orange oil, 4.91 g, 98% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.91 (m, 4H, CH_2), 1.11 (m, 4H, CH_2), 1.40−1.49 (m, 8H, CH_2), 3.78 (t, J = 6.6 Hz, 4H, CH_2), 3.90 (m, 2H, CH_2), 4.01 (m, 2H, CH_2), 7.11−7.15 (m, 2H, Ph), 7.17−7.22 (m, 2H for Ph and 2H for Np), 7.26−7.30 (m, 4H, Np), 7.34 (d, J = 9.2 Hz, 2H, Np), 7.42–7.46 (m, 4H, Ph), 7.82 (d, J = 8.1 Hz, 2H, Np), 7.90 (d, J = 9.0 Hz, 2H, Np), 9.98 ppm (s, 2H, CHO); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.46, 25.52, 29.0, 29.4, 68.1, 69.8, 112.7, 116.1, 120.9, 122.1, 123.5, 123.6, 125.6, 126.2, 127.9, 129.2, 129.4, 130.1, 134.3, 137.9, 154.6, 159.8, 192.4 ppm; IR (neat) 3057, 2938, 2866, 2729, 1694, 1593, 1504, 1456, 1387, 1325, 1260, 1169, 1148, 1086, 1047, 864, 808, 787, 750, 683, 648 cm^{-1}; HRMS (ESI) calcd for $C_{46}H_{46}O_6Na$ 717.3198, found 717.3168 ($[M+Na]^+$).

Compound data for 7d

Brownish solid, 761 mg, 47% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.89−0.92 (m, 4H, CH_2), 1.07–1.08 (m, 4H, CH_2), 1.36−1.43 (m, 8H, CH_2), 3.67 (t, J = 6.6 Hz, 4H, CH_2), 3.86–3.88 (m, 2H, CH_2), 3.90–3.99 (m, 2H, CH_2), 5.42 (s, 2H, CH), 5.94 (s, 4H, pyrrole-β), 6.14−6.16 (m, 4H, pyrrole-β), 6.67 (m, 4H, pyrrole-α), 6.73 (d, J = 6.4 Hz, 4H, Ph), 6.79 (d, J = 7.5 Hz, 2H, Ph), 7.13−7.28 (m, 2H for Ph and 6H for Np), 7.37 (d, J = 9.0 Hz, 2H, Np), 7.80 (d, J = 8.1 Hz, 2H, Np), 7.87 (d, J = 9.0 Hz, 2H, Np), 7.93 ppm (s, 4H, NH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.52, 25.54, 29.1, 29.4, 44.1, 67.8, 69.8, 107.3, 108.5, 112.9, 115.0, 116.1, 117.3, 120.7, 120.9, 123.6, 125.6, 126.2, 127.9, 129.2, 129.4, 129.7, 132.5, 134.3, 143.7, 154.6, 159.5 ppm; IR (KBr) 3375, 3098, 3055, 2936, 2860, 1724, 1593, 1506, 1489, 1468, 1429, 1398, 1354, 1317, 1261, 1148, 1115, 1088, 1028, 883, 810, 758, 719 cm^{-1}; HRMS (APCl) calcd for $C_{62}H_{63}N_4O_4$ 927.4844, found 927.4831 ($[M+H]^+$).

Compound data for 1d

Purple solid, 23.1 mg, 3.7% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = −1.92 (s, 2H, NH), 0.01 (m, 8H, CH_2), 0.59–0.67 (m, 12H, CH_2), 0.76 (m, 4H, CH_2), 1.41 (m, 8H, CH_2), 2.29 (m, 4H, CH_2), 2.57 (m, 4H, CH_2), 3.50–3.55 (m, 4H, CH_2), 3.58–3.64 (m, 4H, CH_2), 4.89 (d, J = 8.8 Hz, 4H, Np), 5.73 (d, J = 8.8 Hz, 4H, Np), 6.42 (d, J = 8.4 Hz, 4H, Np), 6.77 (t, J = 7.3 Hz, 4H, Np), 6.88–6.95 (m, 4H for Ph and 8H for Np), 7.28 (dd, J = 2.0, 9.2 Hz, 4H, Ph), 7.74 (t, J = 7.9 Hz, 4H, Ph), 8.31 (d, J = 7.3 Hz, 4H, Ph), 8.95 (s, 4H, β), 9.05 ppm (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 24.5, 24.8, 27.7, 28.9, 68.3, 68.4, 114.4, 117.2, 119.7, 120.2, 120.6, 123.0, 125.3, 125.56, 125.63, 127.4, 128.1, 128.2, 128.6, 130.8, 132.5, 133.6, 143.2, 153.7, 157.2 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (5.52), 420 (5.68), 515 (4.36), 550 (3.93), 590 (3.82), 645 nm (3.60); IR (KBr) 3308, 3057, 2936, 2860, 1595, 1508, 1474, 1458, 1429, 1333, 1261, 1159, 1047, 1016, 918, 802, 748, 727 cm^{-1}; HRMS (ESI) calcd for $C_{108}H_{98}N_4O_8Na$ 1602.7310, found 1602.7351 ([M+Na]$^+$).

Compound data for 2d

Purple solid, 23.5 mg, 89% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.03 (m, 8H, CH_2), 0.58–0.64 (m, 12H, CH_2), 0.74 (m, 4H, CH_2), 1.43 (m, 8H, CH_2), 2.33 (m, 4H, CH_2), 2.65 (m, 4H, CH_2), 3.52–3.59 (m, 4H, CH_2), 3.62–3.69 (m, 4H, CH_2), 5.01 (d, J = 9.0 Hz, 4H, Np), 5.89 (d, J = 8.9 Hz, 4H, Np), 6.47 (d, J = 8.5 Hz, 4H, Np), 6.80 (t, J = 7.6 Hz, 4H, Np), 6.95 (t, J = 7.3 Hz, 4H, Np), 7.04−7.06 (m, 4H for Ph and 4H for Np), 7.29 (dd, J = 2.0, 8.4 Hz, 4H, Ph), 7.76 (t, J = 7.9 Hz, 4H, Ph), 8.32 (d, J = 7.4 Hz, 4H, Ph), 9.06 (s, 4H, β), 9.21 ppm (s, 4H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 24.4, 24.8, 27.5, 29.0, 68.1, 68.6, 114.4, 117.1, 119.6, 120.3, 121.6, 123.3, 125.3, 125.7, 125.8, 127.6, 128.1, 128.4, 128.5, 132.7, 132.8, 133.4, 143.9, 150.4, 153.5, 156.9 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 230 (5.31), 426 (5.47), 555 (4.17), 593 nm (3.71); IR (KBr) 3055, 2936, 2862, 1697, 1620, 1593, 1508, 1474, 1427, 1265, 1238, 1211, 1173, 1080, 1057, 1003, 934, 868, 799, 748, 721, 702 cm^{-1}; HRMS (APCI) calcd for $C_{108}H_{96}N_4O_8Zn$ 1642.6585, found 1642.6598 ([M]$^-$).

Compound data for 8d

Purple solid, 46.7 mg, 7.2% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = −2.50 (s, 2H, NH), 1.07 (m, 8H, CH_2), 1.17–1.44 (m, 16H, CH_2), 1.61–1.76 (m, 8H, CH_2), 3.69–4.08 (m, 16H, CH_2), 6.97–7.21 (m, 16H, Np or Ph), 7.31–7.43 (m, 8H, Np or Ph), 7.68–7.96 (m, 16H, Np or Ph), 8.97–9.03 (m, 8H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.4, 25.5, 29.0, 29.3, 29.5, 68.3, 69.6, 69.9, 115.1, 115.6, 116.0, 116.2, 120.4, 121.0, 121.2, 121.6, 122.1, 123.3, 123.6, 125.7, 126.0, 126.1, 127.7, 127.8, 127.9, 128.9, 129.2, 129.6, 130.8, 131.8, 134.4, 134.5, 143.7, 154.8, 157.7; UV/Vis (1,4-dioxane): λ_{max} (logε) = 232 (5.40), 419 (5.66), 514 (4.31), 549 (3.89), 590 (3.75), 646 nm (353); IR (KBr) 3314, 3055, 2936, 2862, 1593, 1576, 1506, 1472, 1458, 1429, 1350, 1317, 1261, 1240, 1180, 1163, 1148, 1084, 1045, 1018, 997, 976, 804, 775, 746, 735 cm^{-1}; HRMS (APCI) calcd for $C_{108}H_{98}N_4O_8$ 1579.7423, found 1579.7415 ([M]$^-$).

Compound data for 9d

Purple solid, 18.6 mg, 93% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.99 (m, 8H, CH_2), 1.15–1.43 (m, 16H, CH_2), 1.58–1.75 (m, 8H, CH_2), 3.61–3.78 (m, 4H, CH_2), 3.88–4.07 (m, 12H, CH_2), 6.79–7.17 (m, 16H, Np or Ph), 7.30–7.40 (m, 8H, Np or Ph), 7.63–8.00 (m, 16H, Np or Ph), 8.95–9.19 (m, 8H, β); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 25.2, 25.26, 25.34, 25.4, 25.5, 28.8, 28.9, 29.1, 29.2, 29.6, 68.2, 68.4, 69.6, 69.9, 115.0, 115.1, 115.5, 115.6, 115.9, 116.2, 121.0, 121.1, 121.3, 121.4, 121.8, 121.9, 123.3, 123.6, 125.6, 125.7, 126.0, 126.1, 127.35, 127.44, 127.5, 127.7, 127.9, 128.8, 129.2, 129.6, 132.2, 132.3, 134.3, 134.5, 144.3, 144.4, 150.6, 150.7, 154.6, 154.7, 157.6 ppm ; UV/Vis (1,4-dioxane): λ_{max} (logε) = 231 (5.42), 425 (5.71), 555 (4.32), 595 nm (3.82); IR (KBr) 3055, 2936, 2864, 1653, 1593, 1576, 1558, 1506, 1489, 1474, 1458, 1431, 1337, 1261, 1182, 1084, 1047, 999, 799, 750 cm^{-1}; HRMS (APCI) calcd for $C_{108}H_{96}N_4O_8Zn$ 1642.6548, found 1642.6535 ($[M]^-$).

Compound data for 12

Purple solid, 113 mg, 30% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = −2.62 (s, 2H, NH), 0.27–0.47 (m, 4H, CH_2), 0.64–0.84 (m, 4H, CH_2), 1.26–1.43 (m, 4H, CH_2), 2.73 (m, 2H, CH_2), 2.94 (m, 2H, CH_2), 3.54–3.69 (m, 4H, CH_2), 4.62 (d, J = 9.0 Hz, 2H, Np), 4.68 (d, J = 9.1 Hz, 2H, Np), 6.19 (d, J = 8.1 Hz, 2H, Np), 6.37 (d, J = 8.4 Hz, 2H, Np), 6.66–6.69 (m, 2H for Ph and 2H for Np), 6.75 (t, J = 7.1 Hz, 2H, Np), 7.29 (dd, J = 2.3, 8.3 Hz, 2H, Ph), 7.83 (t, J = 7.9 Hz, 2H, Ph), 8.48 (d, J = 7.4 Hz, 2H, Ph), 9.09 (d, J = 4.6 Hz, 2H, β), 9.18 (d, J = 4.4 Hz, 2H, β), 9.36 (d, J = 4.4 Hz, 2H, β), 9.43 (d, J = 4.5 Hz, 2H, β), 10.29 ppm (s, 2H, meso); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 21.1, 27.3, 28.1, 67.7, 68.1, 105.5, 112.7, 117.3, 118.5, 119.1, 121.0, 122.6, 124.9, 125.1, 125.2, 127.0, 127.5, 128.0, 128.4, 130.0, 130.7, 132.7, 133.2, 133.3, 142.5, 142.9, 144.0, 148.8, 150.5, 153.0, 157.1 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 231 (5.13), 408 (5.51), 502 (4.21), 537 (3.67), 576 (3.72), 630 nm (3.16); IR (KBr) 3289, 3055, 2949, 2868, 1595, 1506, 1489, 1474, 1458, 1429, 1321, 1261, 1240, 1223, 1204, 1144, 1076, 1047, 1013, 961, 918, 851, 791, 750, 735, 692 cm^{-1}; HRMS (APCI) calcd for $C_{62}H_{52}N_4O_4$ 916.3994, found 916.4025 ($[M]^-$).

Compound data for 13

Purple solid, 56.3 mg, 93% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 0.23 (m, 2H, CH_2), 0.41 (m, 2H, CH_2), 0.51 (m, 2H, CH_2), 0.61 (m, 2H, CH_2), 1.23–1.30 (m, 4H, CH_2), 2.65 (m, 2H, CH_2), 2.79 (m, 2H, CH_2), 3.47–3.62 (m, 4H, CH_2), 4.91 (d, J = 9.0 Hz, 2H, Np), 5.23 (d, J = 9.0 Hz, 2H, Np), 6.42 (d, J = 8.5 Hz, 2H, Np), 6.55 (s, 2H, Ph), 6.61 (d, J = 8.2 Hz, 2H, Np), 6.72 (t, J = 7.6 Hz, 2H, Np), 6.85 (t, J = 7.5 Hz, 2H, Np), 7.24 (dd, J = 2.4, 8.3 Hz, 2H, Ph), 7.83 (t, J = 7.9 Hz, 2H, Ph), 8.46 (d, J = 7.3 Hz, 2H, Ph), 9.02 (d, J = 4.5 Hz, 2H, β), 9.13 (d, J = 4.4 Hz, 2H, β), 9.25 (d, J = 4.4 Hz, 2H, β), 9.35 (d, J = 4.2 Hz, 2H, β), 10.07 ppm (s, 2H, meso); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 21.2, 27.4, 28.2, 68.1, 68.4, 106.2, 106.4, 113.4, 117.1, 119.0, 119.9, 120.8, 123.0, 125.0, 125.1, 125.4, 127.2, 127.6, 128.1, 128.3, 132.1, 132.6, 133.3, 144.0, 149.5, 150.2, 153.1, 156.8 ppm; UV/Vis (1,4-dioxane): λ_{max} (logε) = 231 (4.98), 413 (5.47), 543 (4.14), 578 nm (3.32); IR (KBr) 3057, 2947, 2868, 1595, 1506, 1491, 1474, 1458, 1429, 1393, 1319, 1285, 1263, 1240, 1211, 1059, 993, 806, 783, 750, 727, 700 cm^{-1}; HRMS (APCI) calcd for $C_{62}H_{50}N_4O_4Zn$ 978.3129, found 978.3146 ($[M]^-$).

[C] Kinetic Resolution of Styrene Oxide

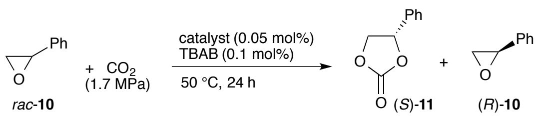
General procedure

A 30 mL stainless autoclave was charged with styrene oxide (**10**, 0.50 mmol), catalyst (0.05 mol%), TBAB (0.10 mol%), and then CO_2 (1.7 MPa). The mixture was heated with stirring at 50 °C for 24 h. The reaction mixture was cooled in ice water, and excess CO_2 was released carefully. **10** and styrene carbonate (**11**) were separated by silica gel column chromatography (hexane/EtOAc = 3/1). The enantiomeric purity of **11** was determined by HPLC using chiral columns (Daicel Chemical Industries), and that of **10** was determined by GC with a CP-cyclodextrin-β-2,3,6-M-19 column (Varian, ϕ 0.25 mm × 25 m). The absolute configurations of **10** and **11** were determined by comparison with the reported literature.[S4]

Kinetic resolution of 10

50 °C, 6 h. (*R*)-**10**: Pale yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 2.81 (dd, *J* = 2.8, 5.6 Hz, 1H), 3.15 (dd, *J* = 4.4, 5.8 Hz, 1H), 3.86 (dd, *J* = 2.4, 3.8 Hz, 1H), 7.27–7.38 (m, 5H); GC for **10**: Inj. 250 °C, Col. 75 °C, Det. 220 °C, (*R*) 38.1 min, (*S*) 40.3 min. (*S*)-**11**: White solid; $[\alpha]^{25}_D$ +26.1 (*c* 0.54, $CHCl_3$), 54% ee, lit.[S4] $[\alpha]^{23}_D$ –18.2 (*c* 1.00, $CHCl_3$) for (*R*)-**11** with 42% ee; ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 4.35 (t, *J* = 8.4 Hz, 1H), 4.80 (t, *J* = 8.0 Hz, 1H), 5.68 (t, *J* = 7.6 Hz, 1H), 7.36–7.38 (m, 2H), 7.42–7.47 (m, 3H); HPLC for **11**: Chiralcel OD-H, hexane/*i*-PrOH = 4/1, 0.5 mL/min, 220 nm, (*R*) 25.8 min, (*S*) 30.9 min.

Table S1 Kinetic resolution of styrene oxide with CO_2.[a]



			% Yield[c] (% ee)[d]		
Entry	Cat.	*c* %[b]	(*S*)-**11**	(*R*)-**10**	*s* value[e]
1	**9a**	24	15 (4.8)	56 (1.5)	1.1
2	**9b**	41	42 (5.2)	31 (3.6)	1.1
3	**9c**	50	40 (0.5)	26 (0.5)	1.0
4	**9d**	50	40 (0.5)	32 (0.5)	1.0

[a]Reaction conditions: styrene oxide (0.3 mmol), Zn(II) porphyrin (0.05 mol%), TBAB (0.1 mol%), CO_2 (1.7 MPa) in a 30 mL autoclave. [b]Conversion calculated from *c* = ee(**10**)/(ee(**10**) + ee(**11**)). [c]Isolated yield. [d]Determined by HPLC or GC analyses. [e]Calculated from *s* = ln[1 – *c*(1 + ee(**11**))]/ln[1 – *c*(1 – ee(**11**)).

[D] References

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[S3] S. Muthusamy, T. Karikalan and E. Suresh, *Tetrahedron Lett.*, 2011, **52**, 1934–1937.

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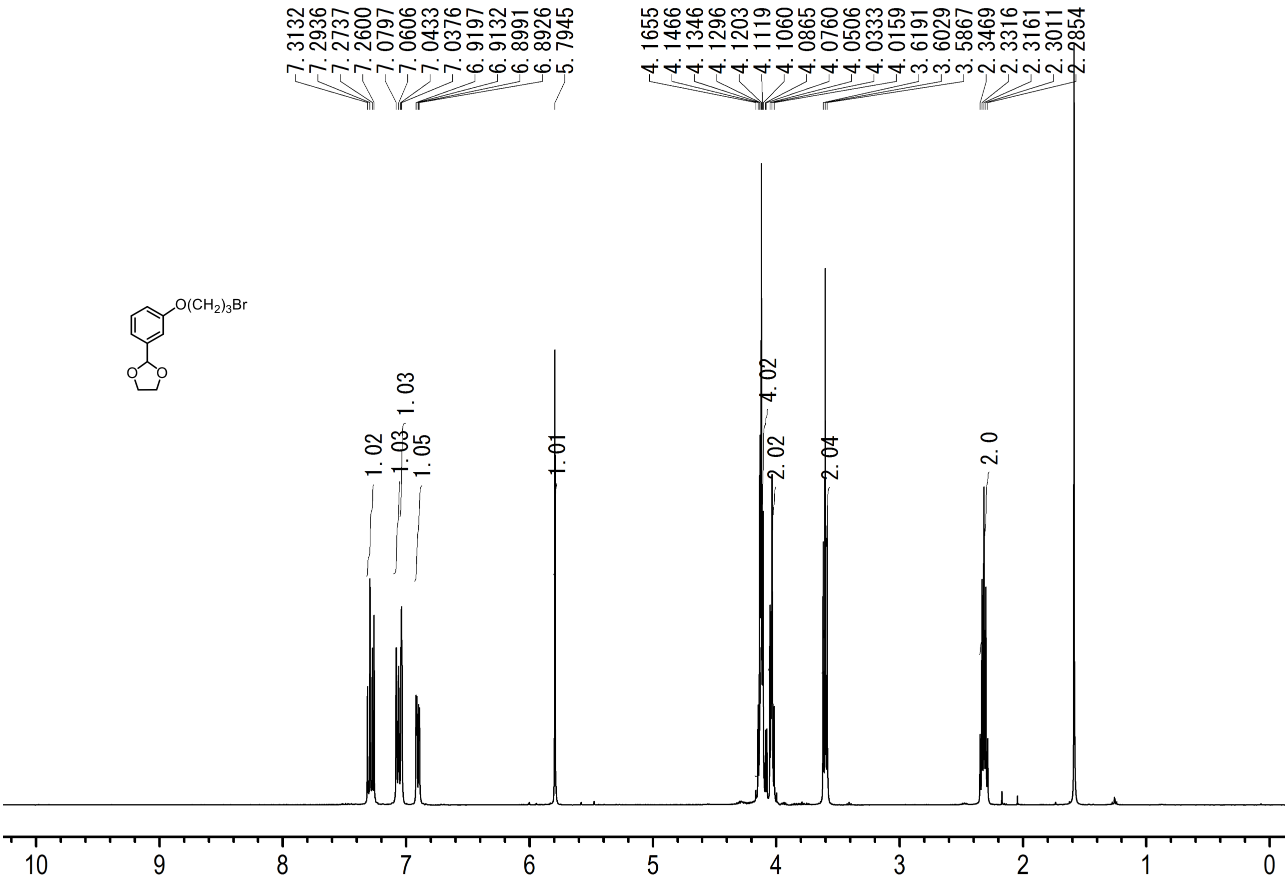
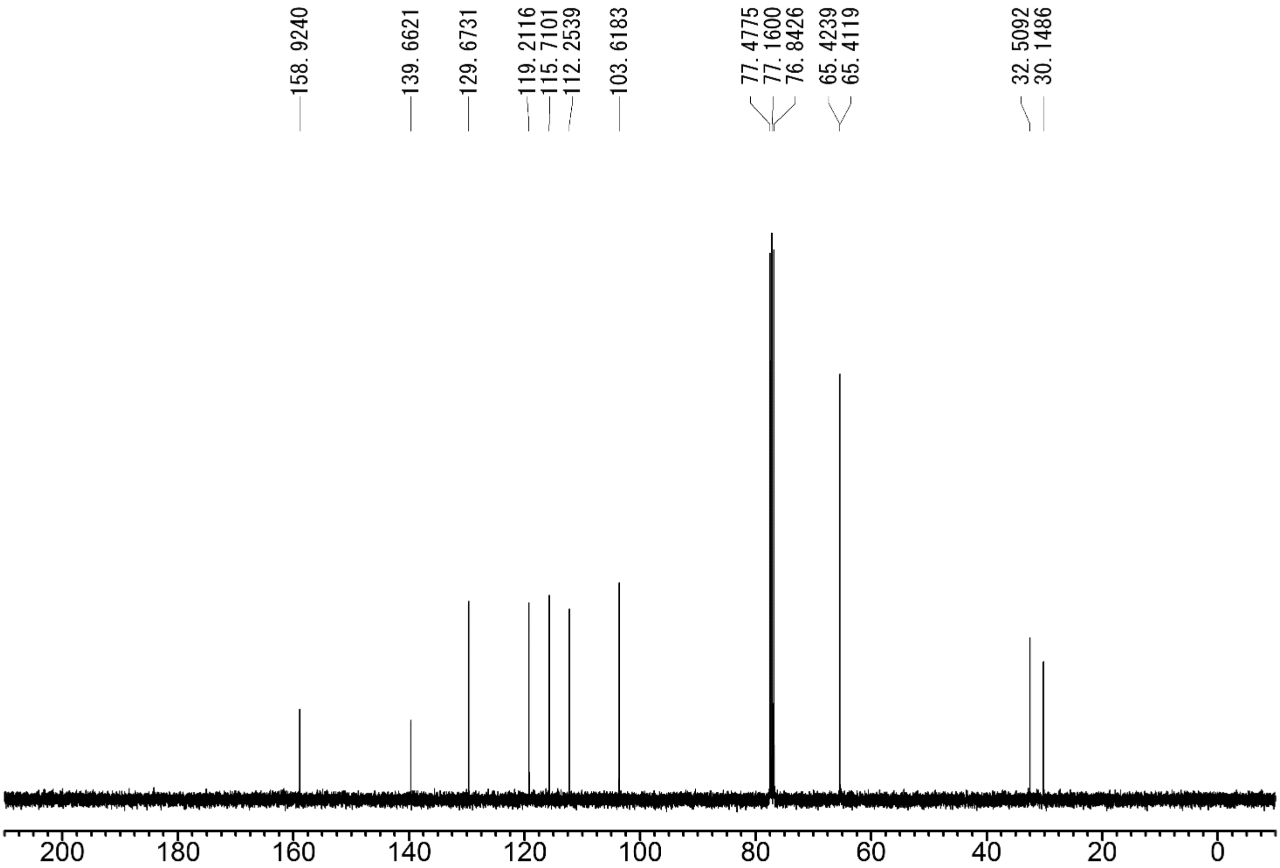
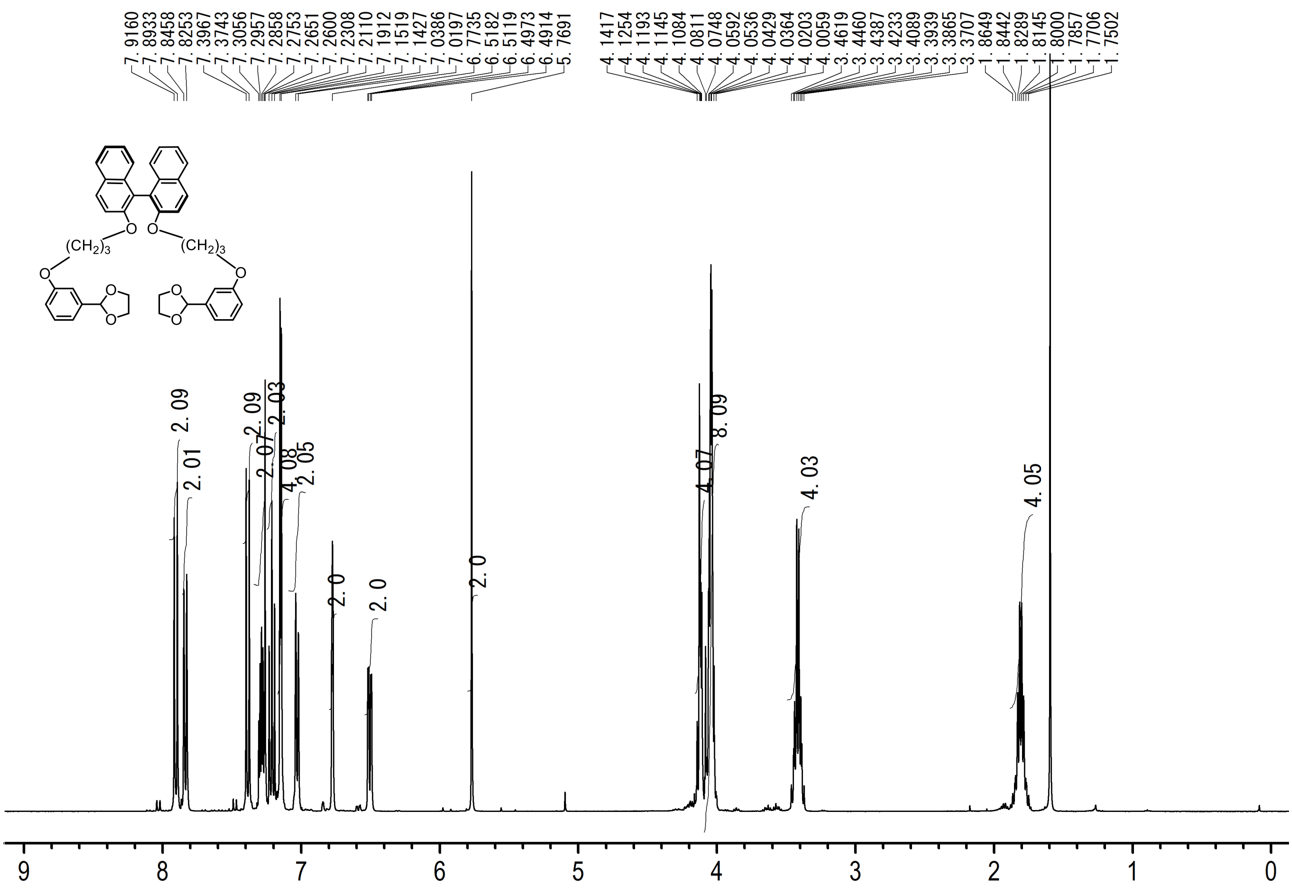
[E] NMR Spectra



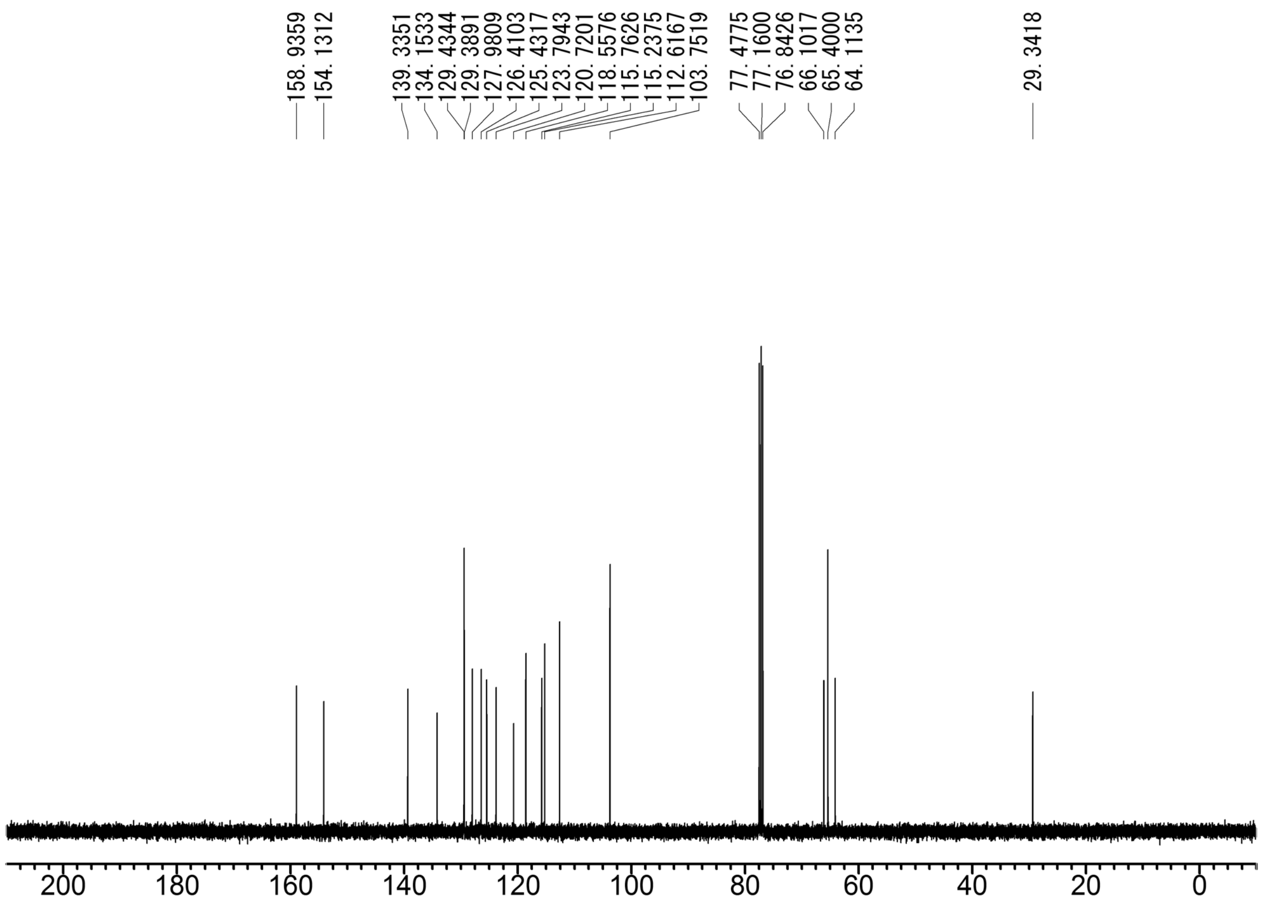
400 MHz ^{1}H NMR spectrum of **4a** in $CDCl_3$



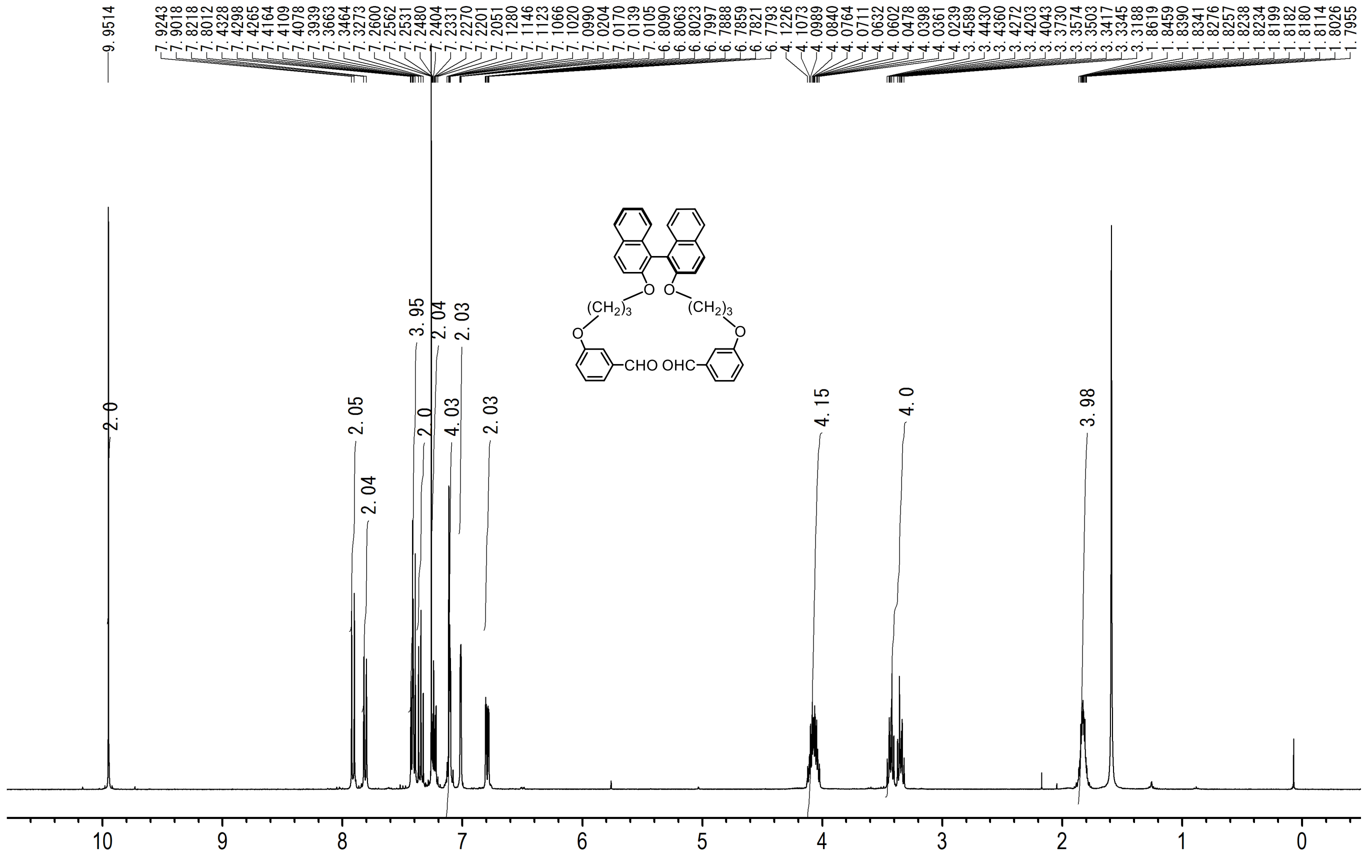
100 MHz ^{13}C NMR spectrum of **4a** in $CDCl_3$



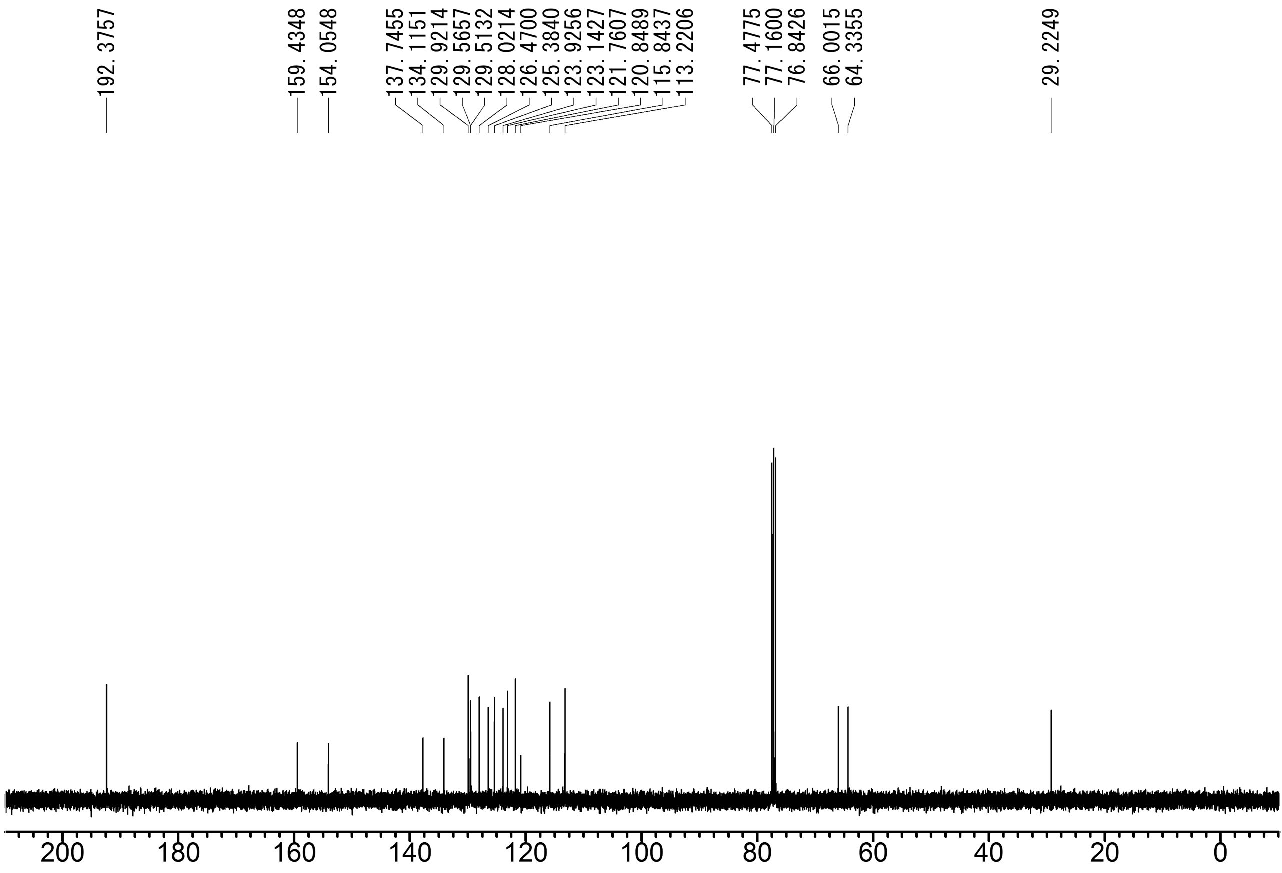
400 MHz ^{1}H NMR spectrum of **5a** in $CDCl_3$



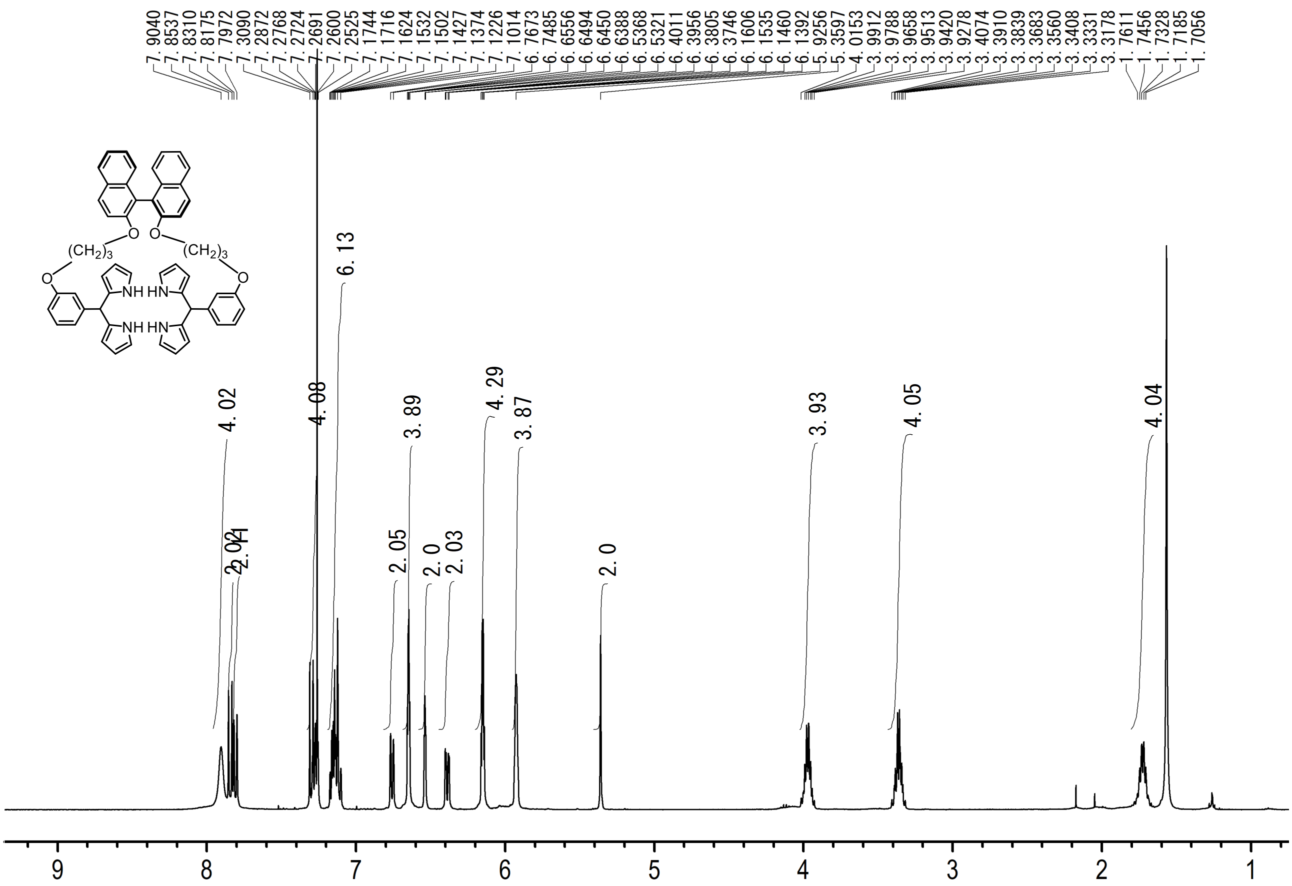
100 MHz ^{13}C NMR spectrum of **5a** in $CDCl_3$



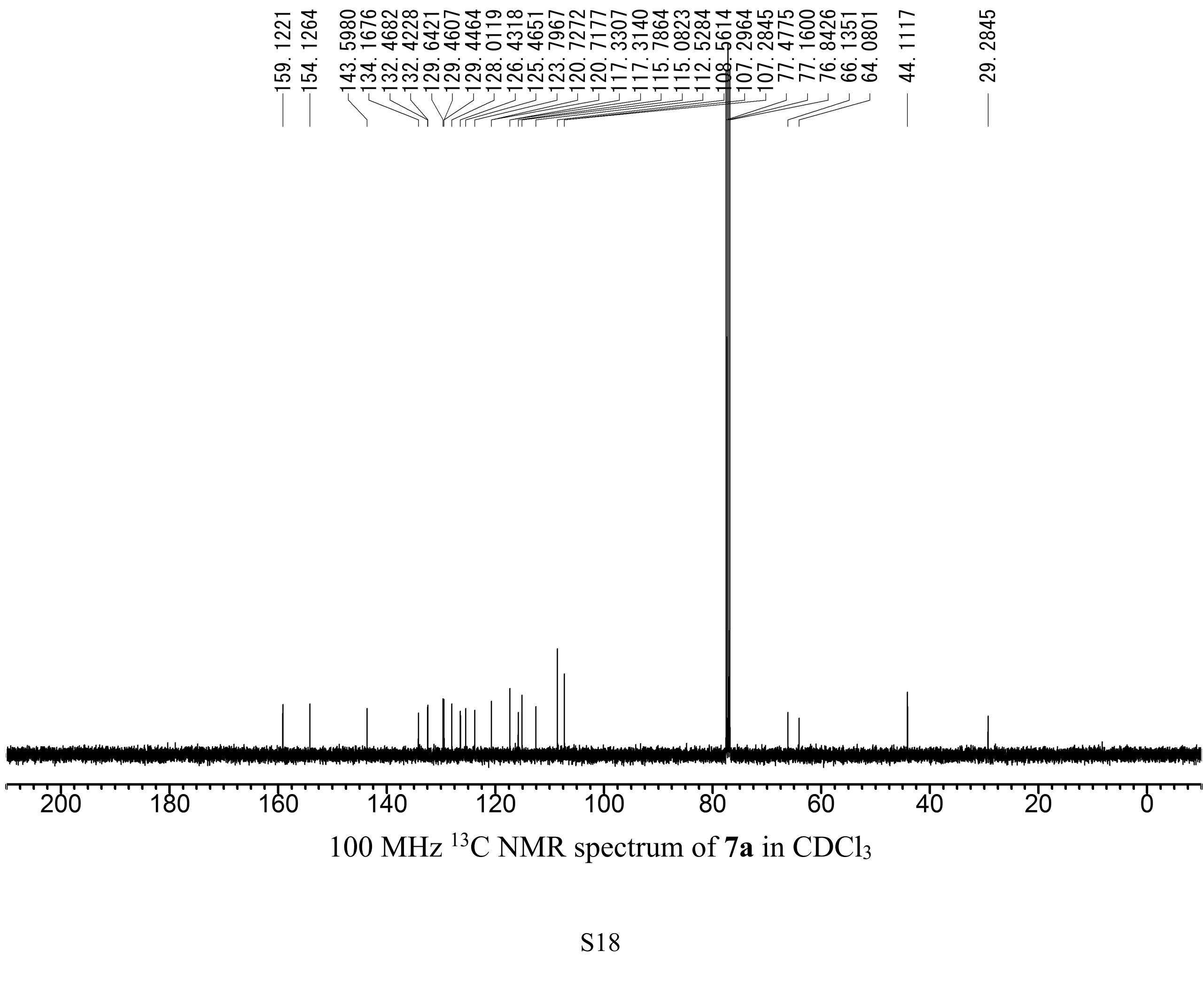
400 MHz ^{1}H NMR spectrum of **6a** in $CDCl_3$



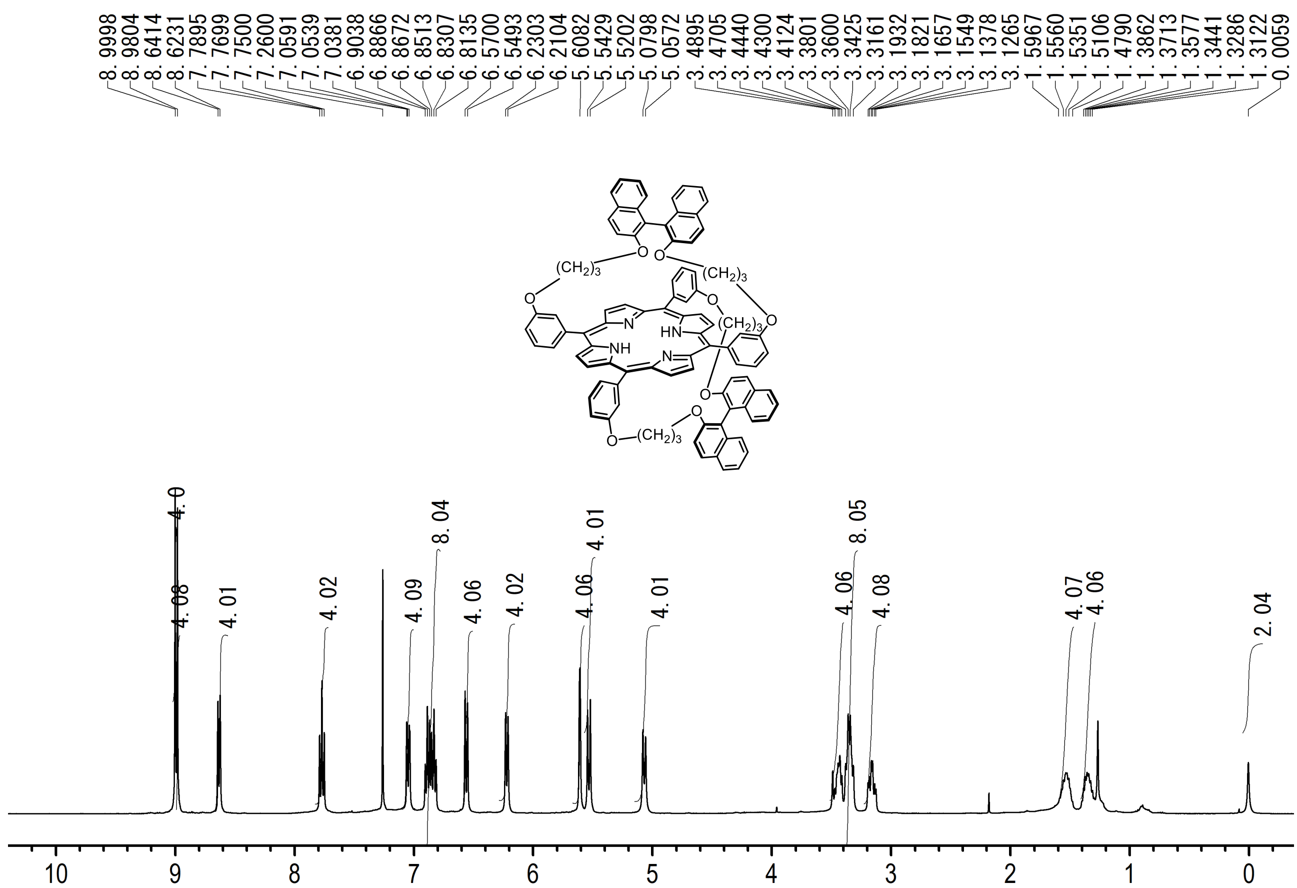
100 MHz ^{13}C NMR spectrum of **6a** in $CDCl_3$



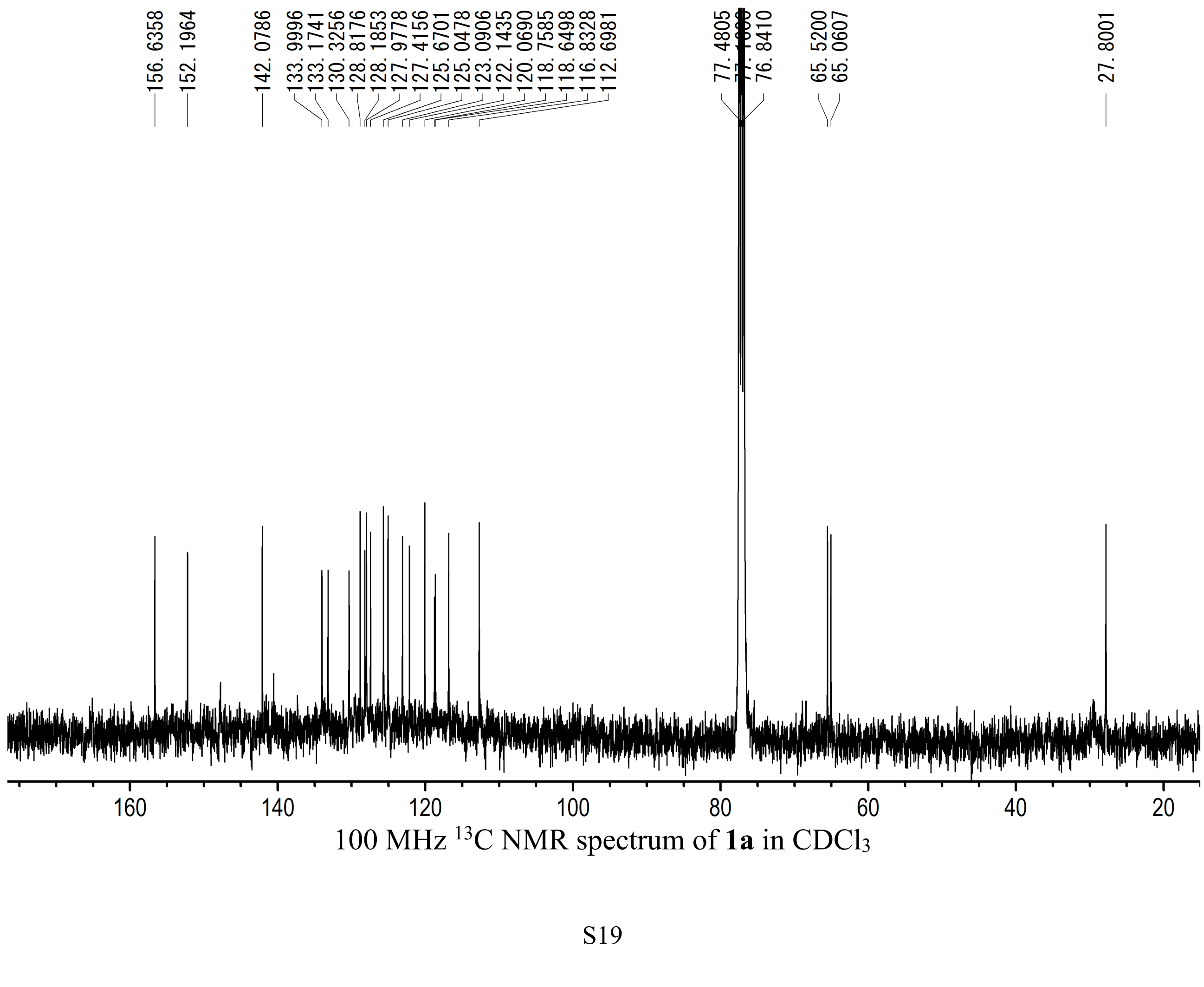
400 MHz ^{1}H NMR spectrum of **7a** in $CDCl_3$



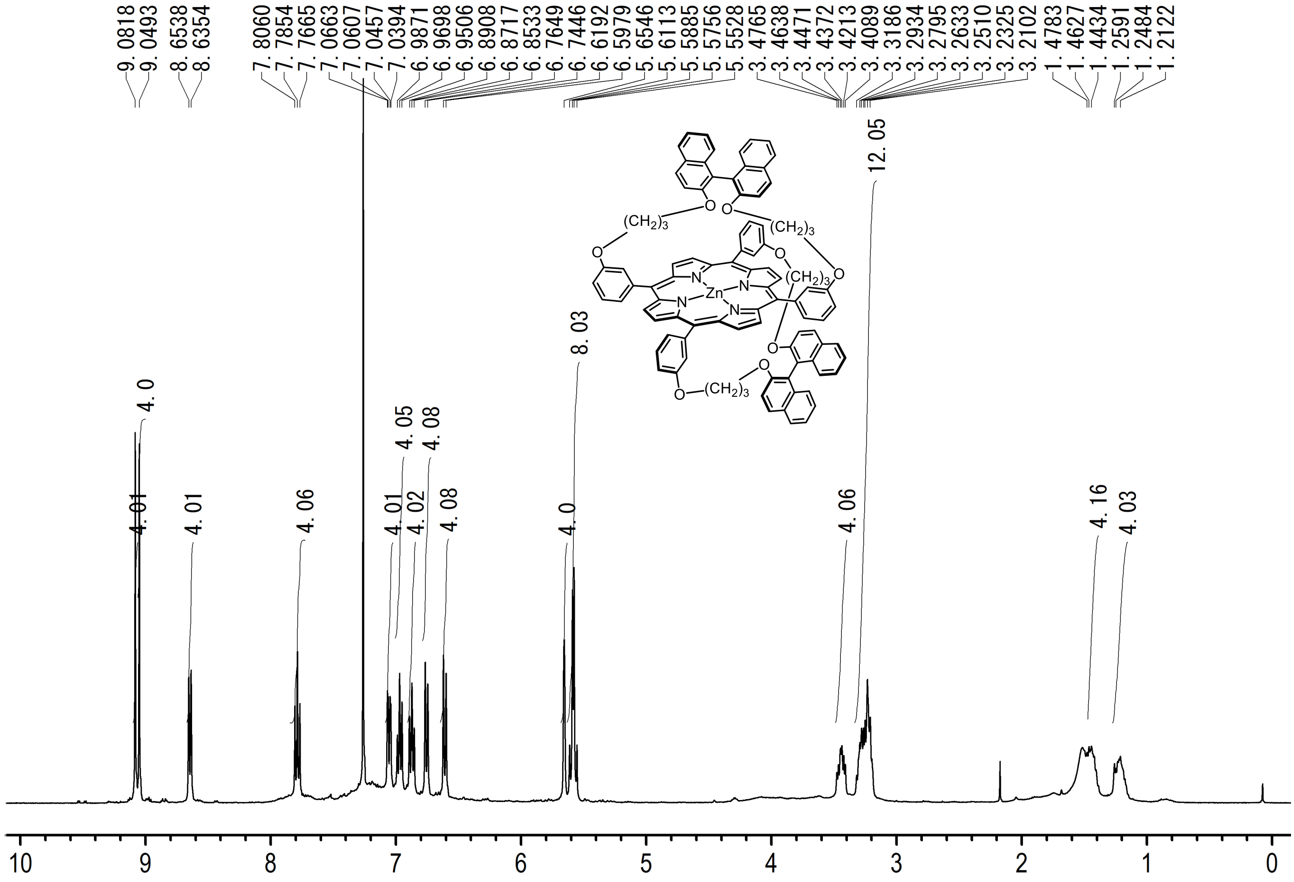
100 MHz ^{13}C NMR spectrum of **7a** in $CDCl_3$



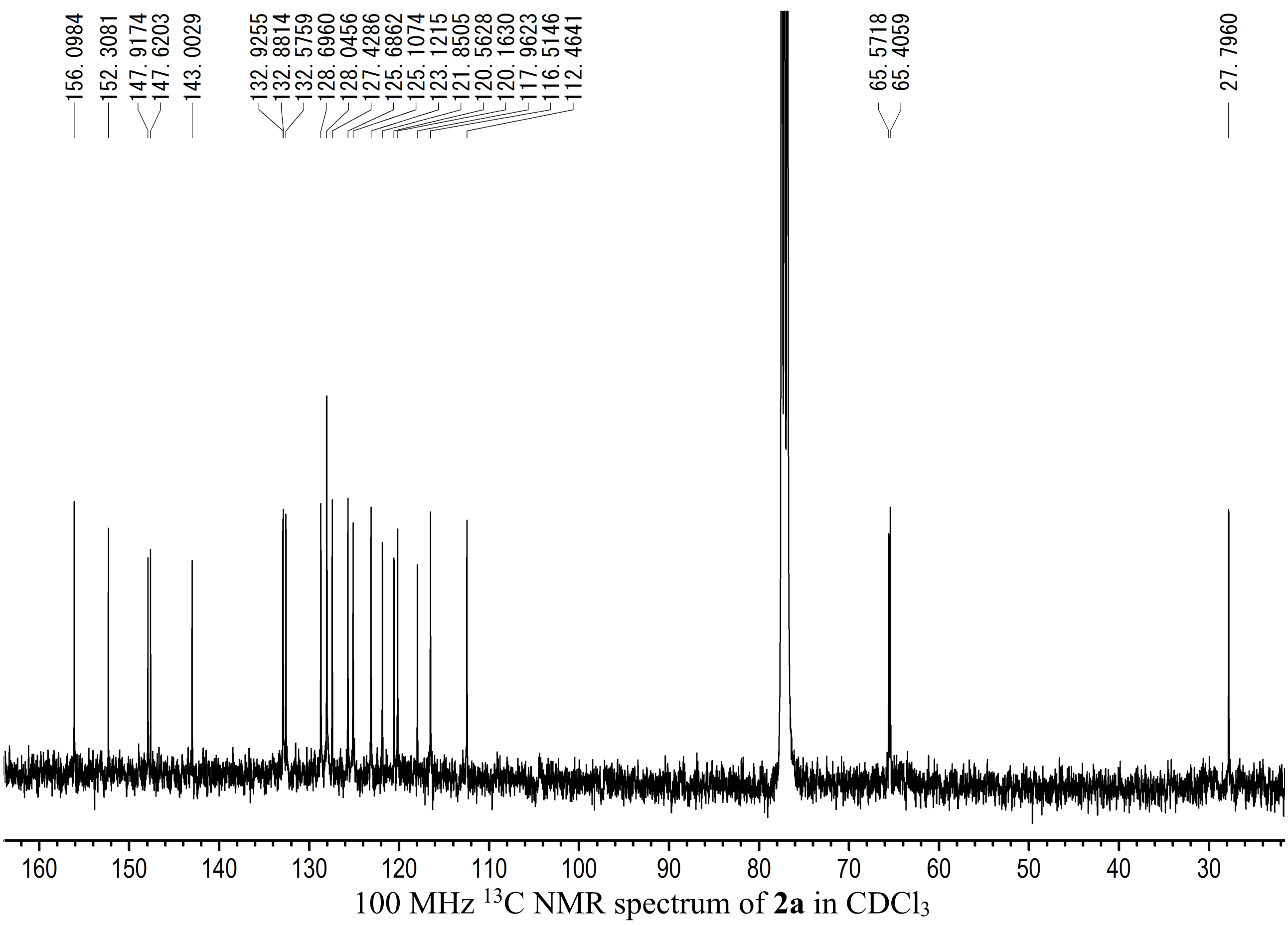
400 MHz ^{1}H NMR spectrum of **1a** in $CDCl_3$



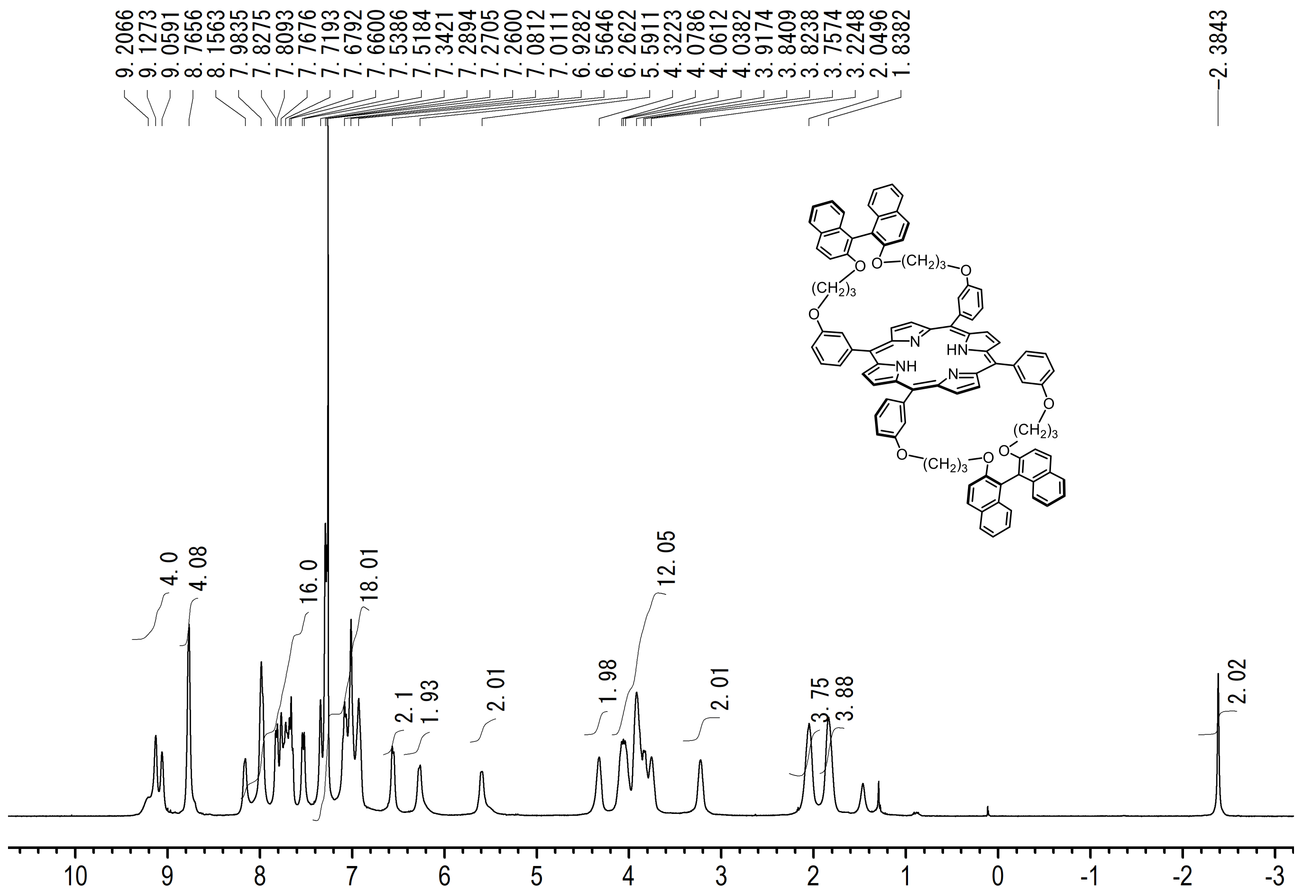
100 MHz ^{13}C NMR spectrum of **1a** in $CDCl_3$



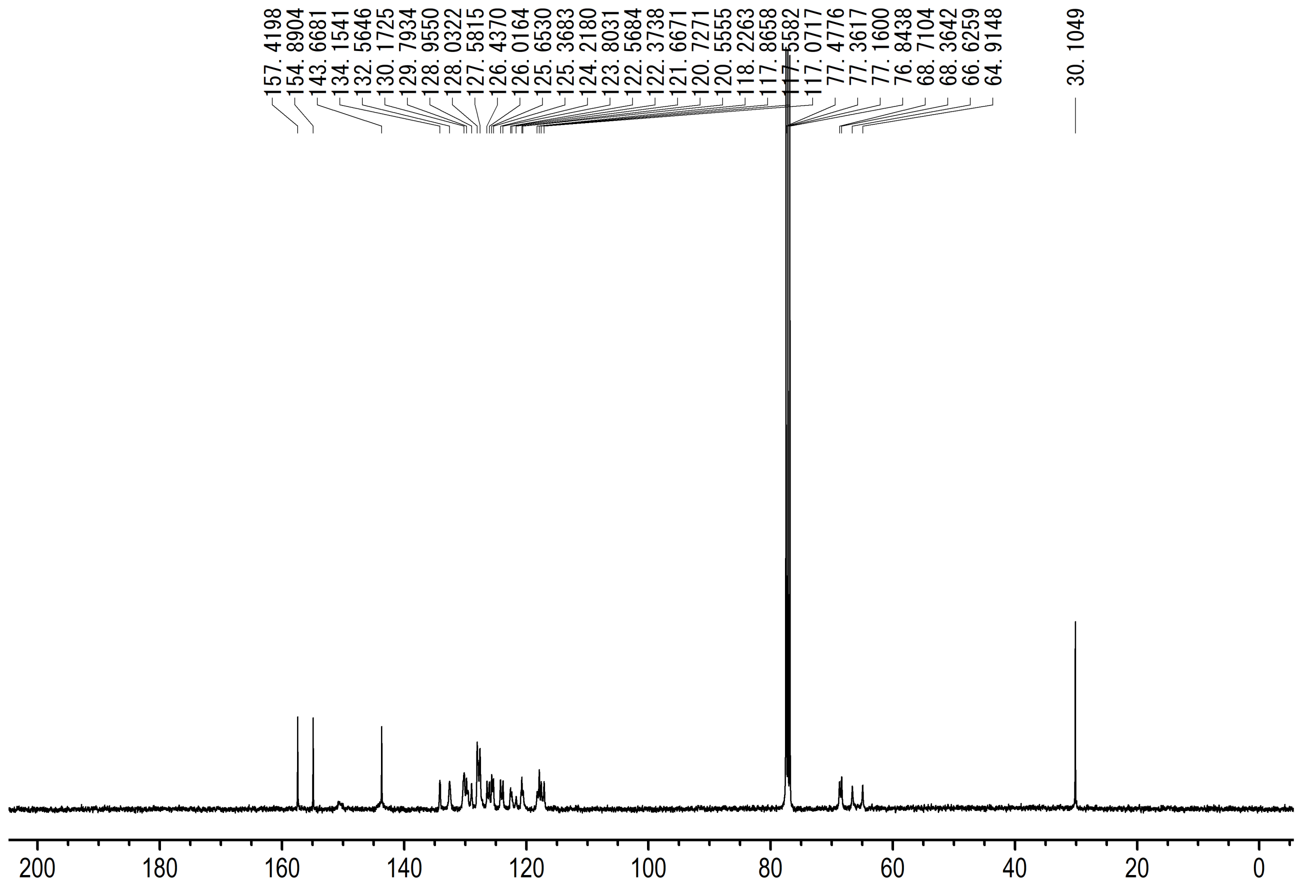
400 MHz ^{1}H NMR spectrum of **2a** in $CDCl_3$



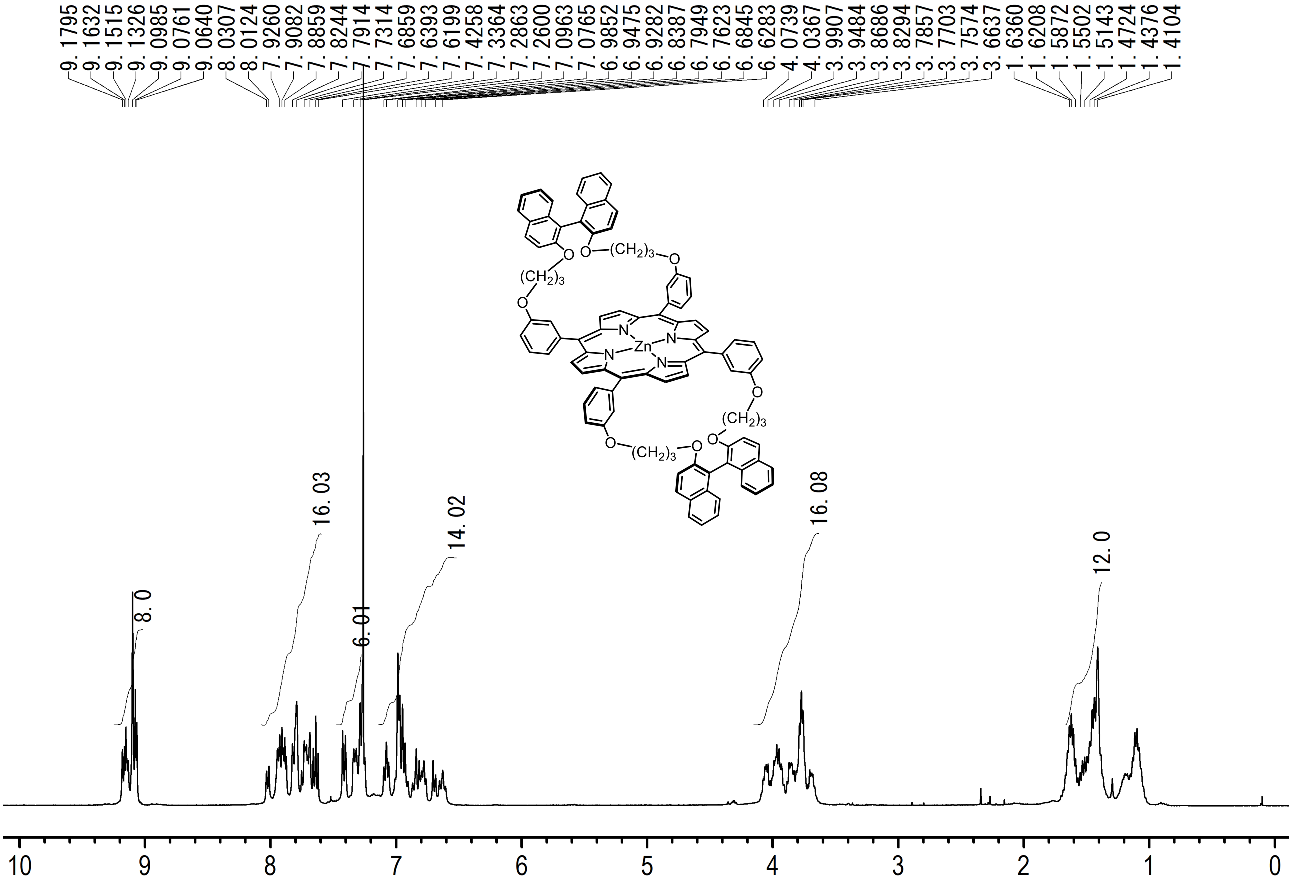
100 MHz ^{13}C NMR spectrum of **2a** in $CDCl_3$



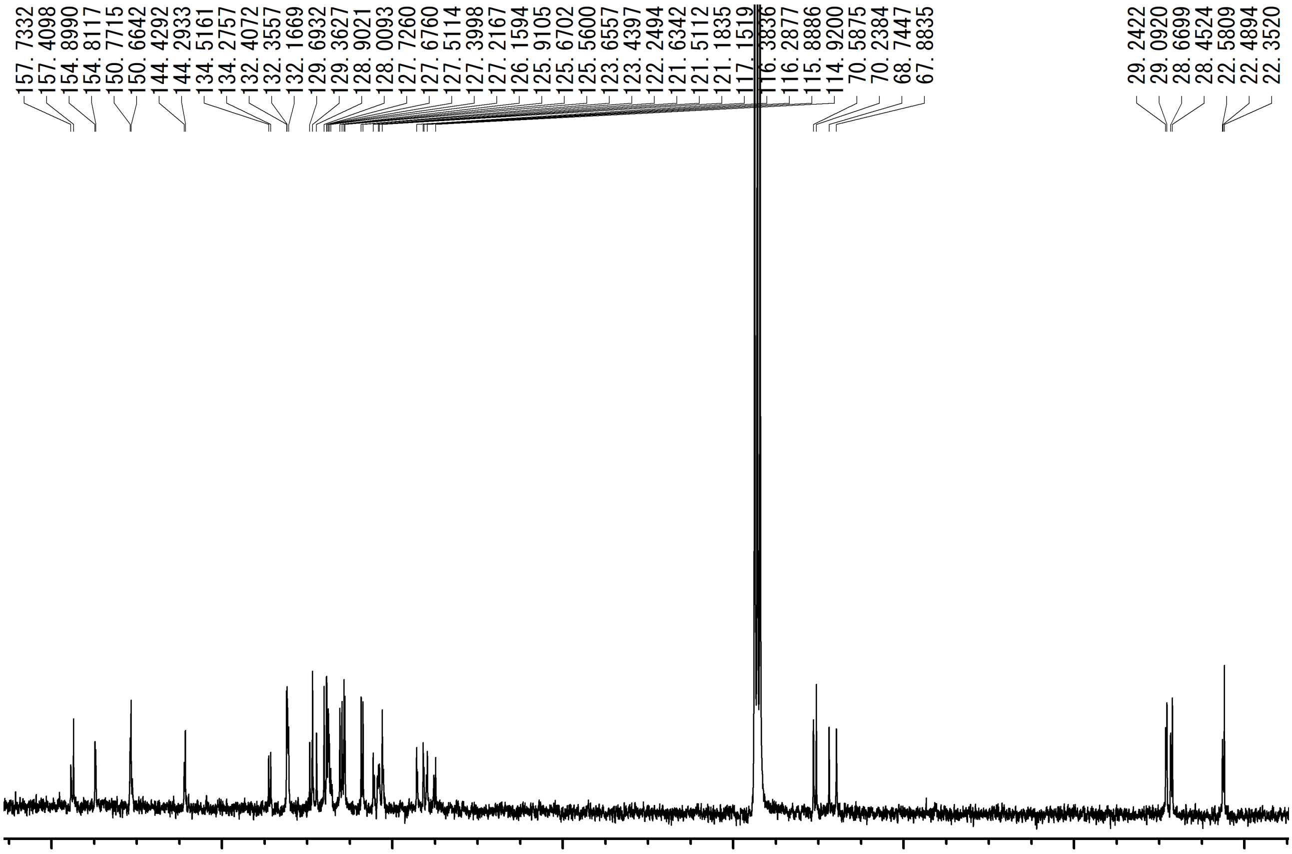
400 MHz ^{1}H NMR spectrum of **8a** in $CDCl_3$



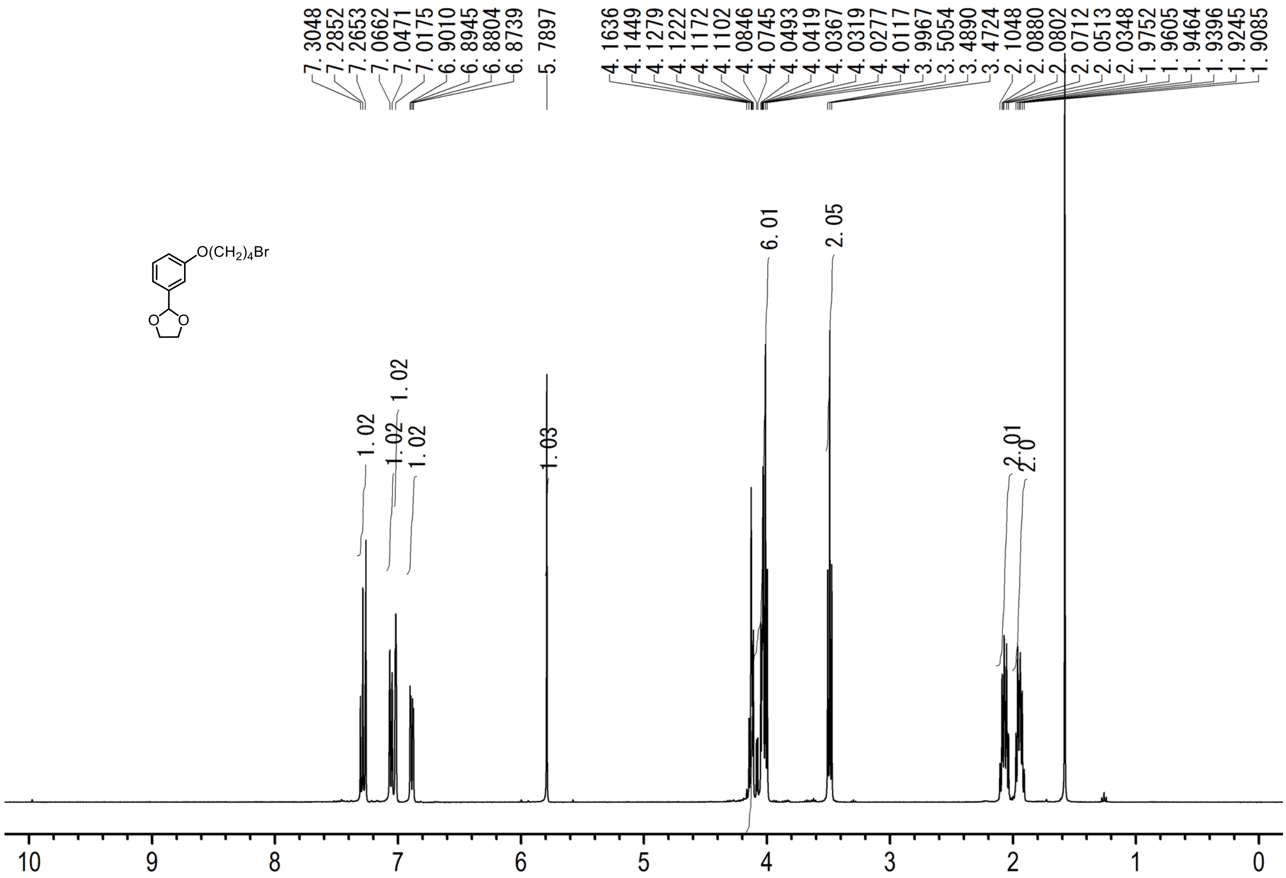
100 MHz ^{13}C NMR spectrum of **8a** in $CDCl_3$



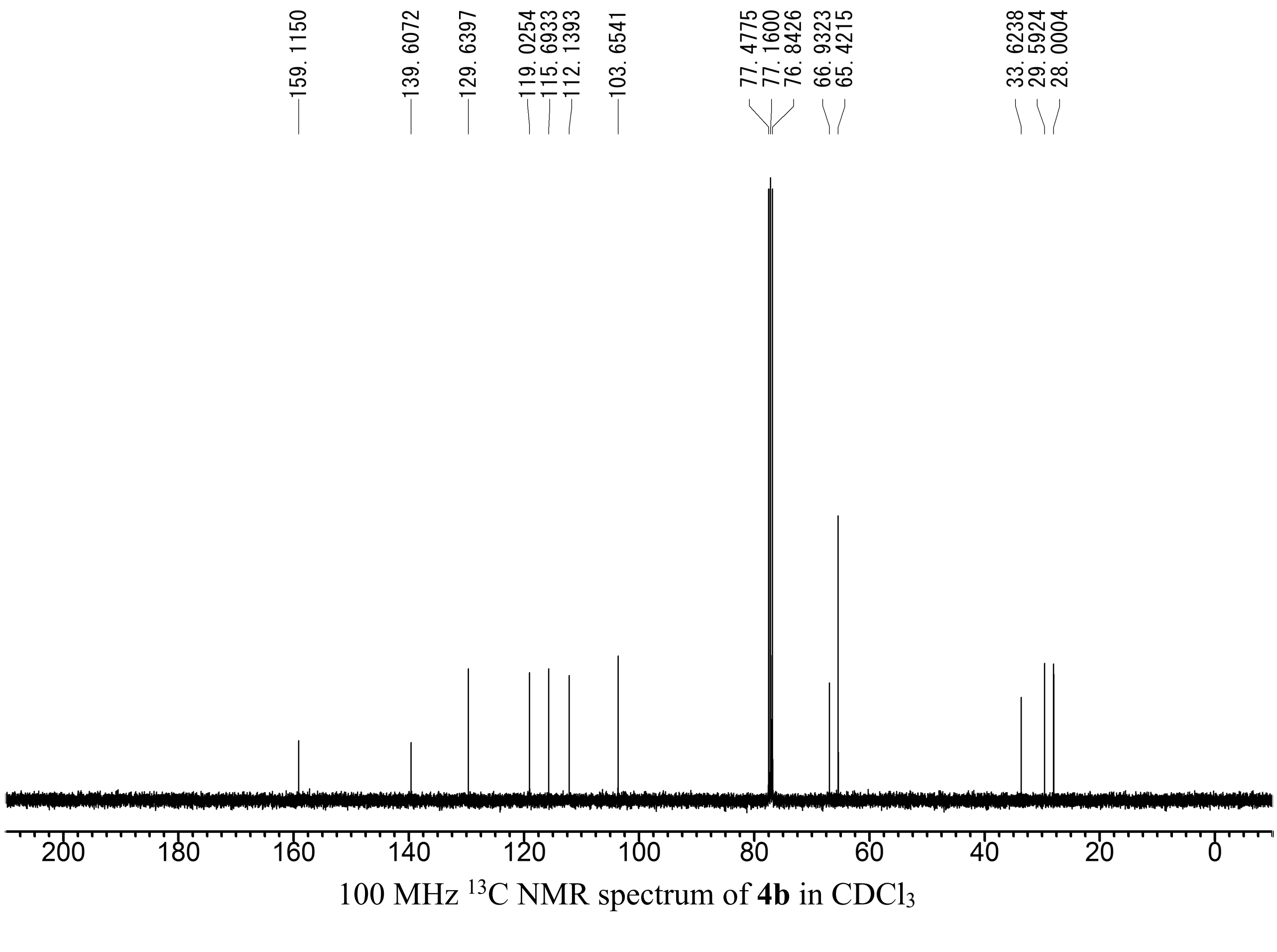
400 MHz ^{1}H NMR spectrum of **9a** in $CDCl_3$



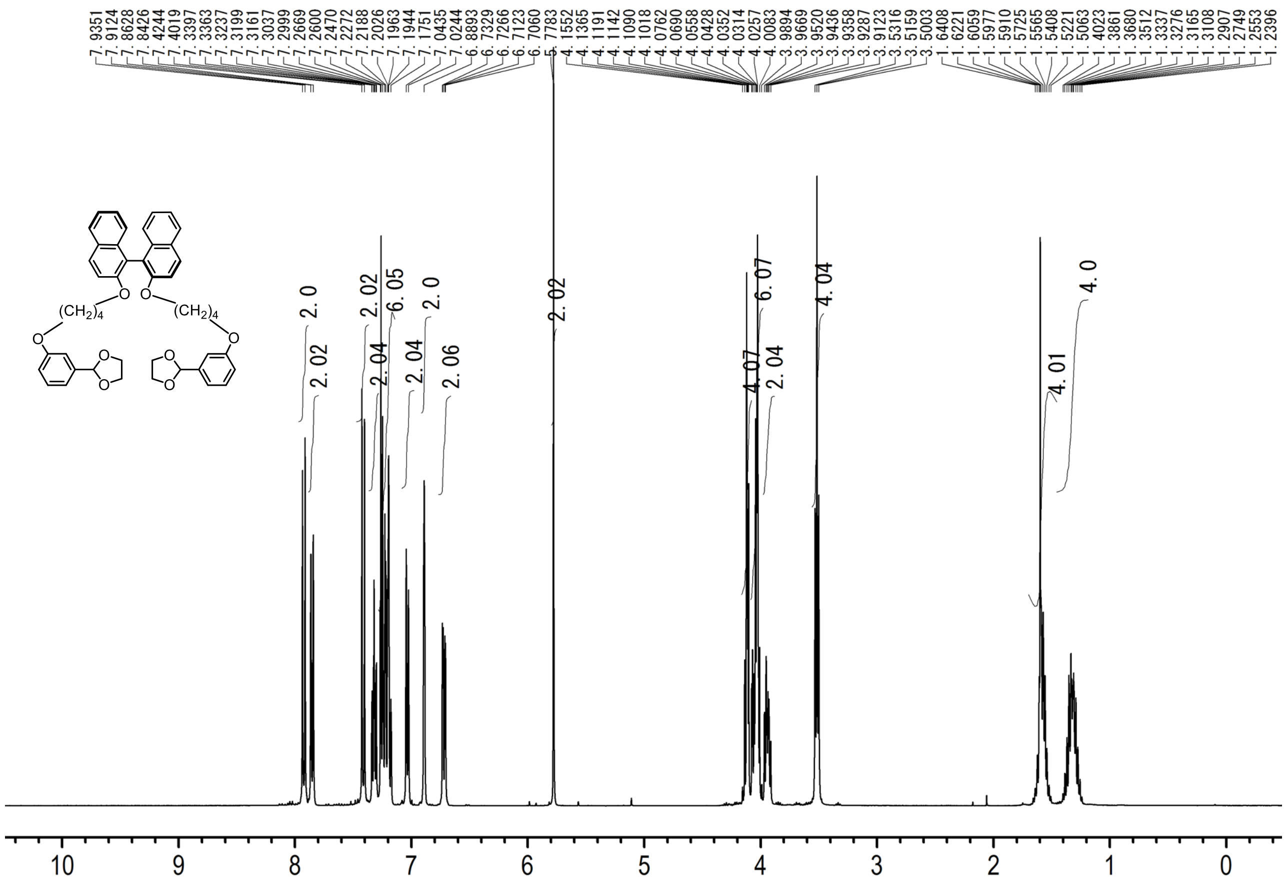
100 MHz ^{13}C NMR spectrum of **9a** in $CDCl_3$



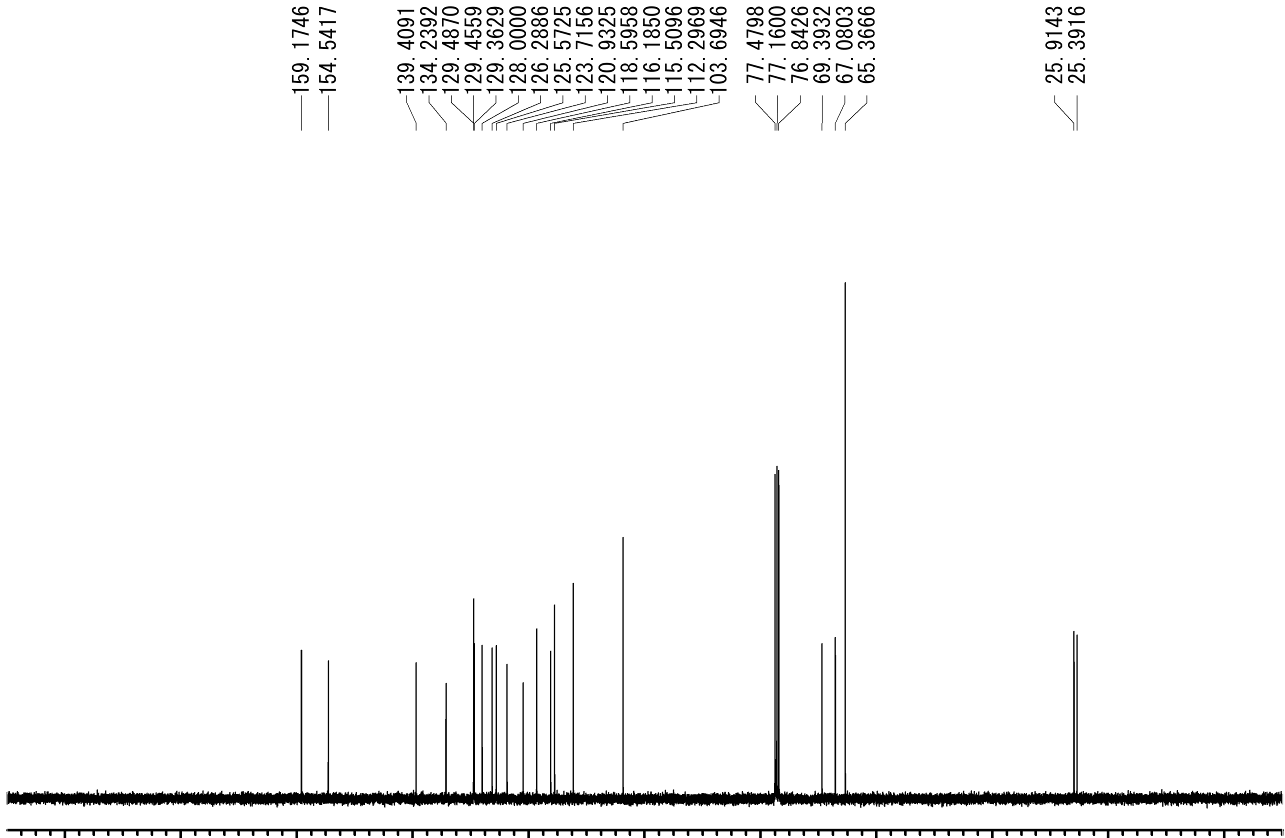
400 MHz ^{1}H NMR spectrum of **4b** in $CDCl_3$



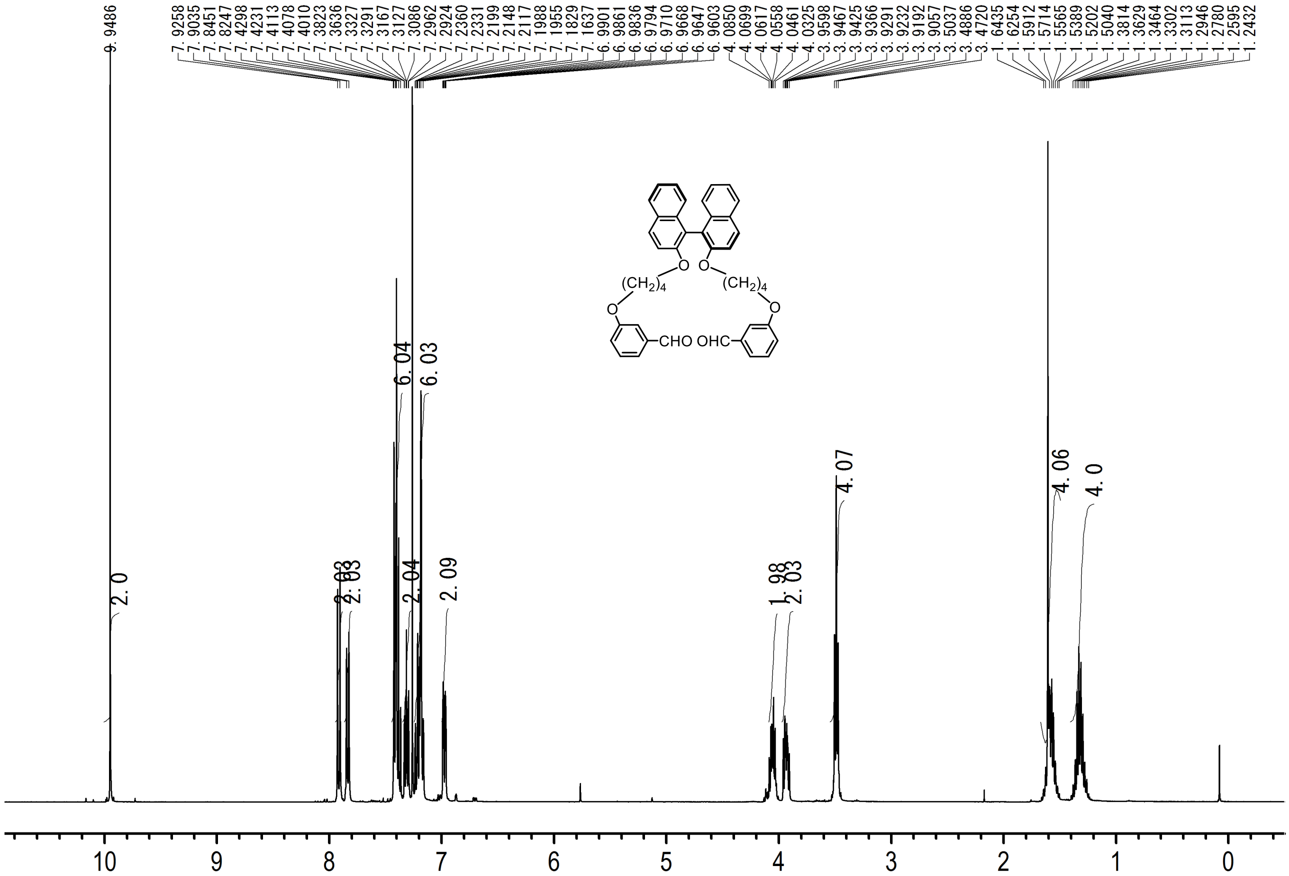
100 MHz ^{13}C NMR spectrum of **4b** in $CDCl_3$



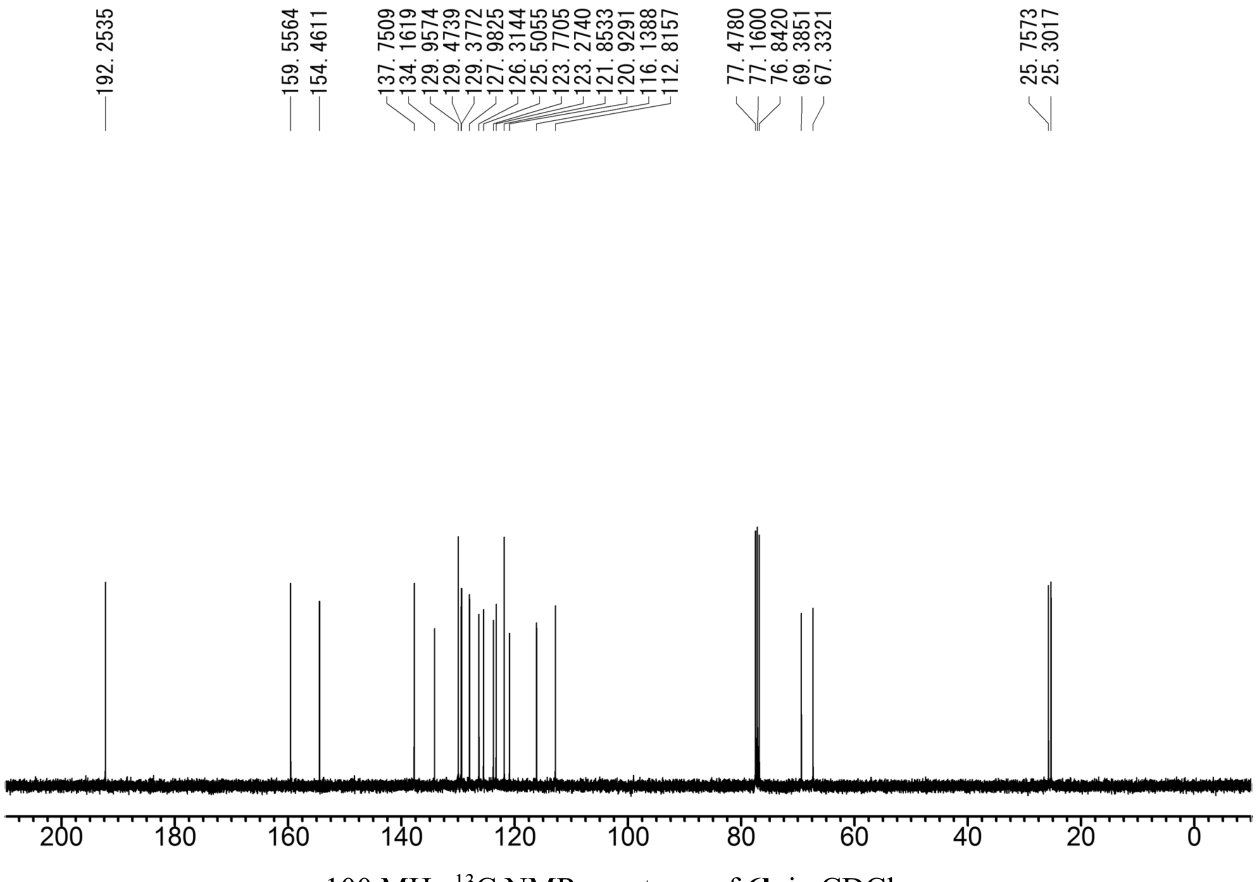
400 MHz ^{1}H NMR spectrum of **5b** in $CDCl_3$



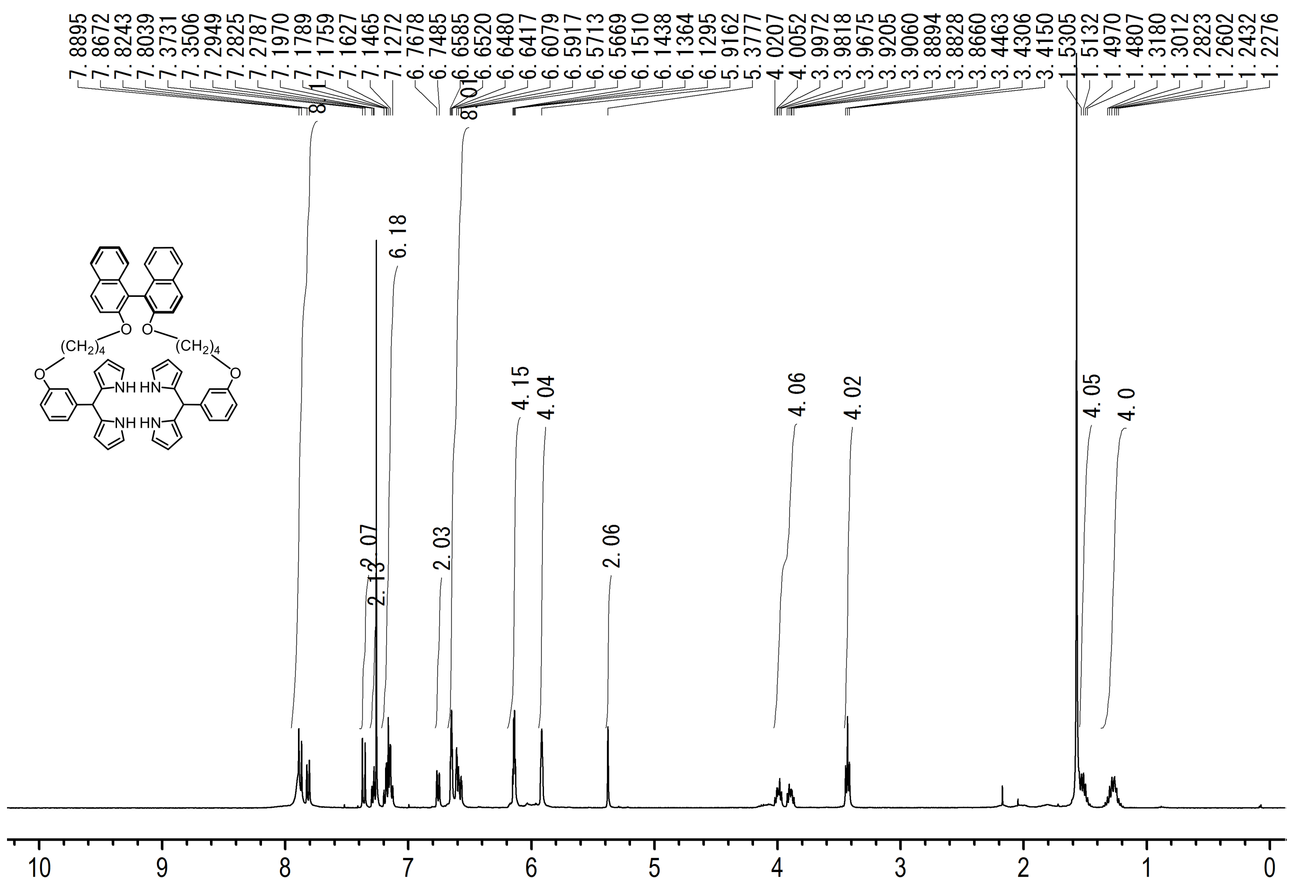
100 MHz ^{13}C NMR spectrum of **5b** in $CDCl_3$



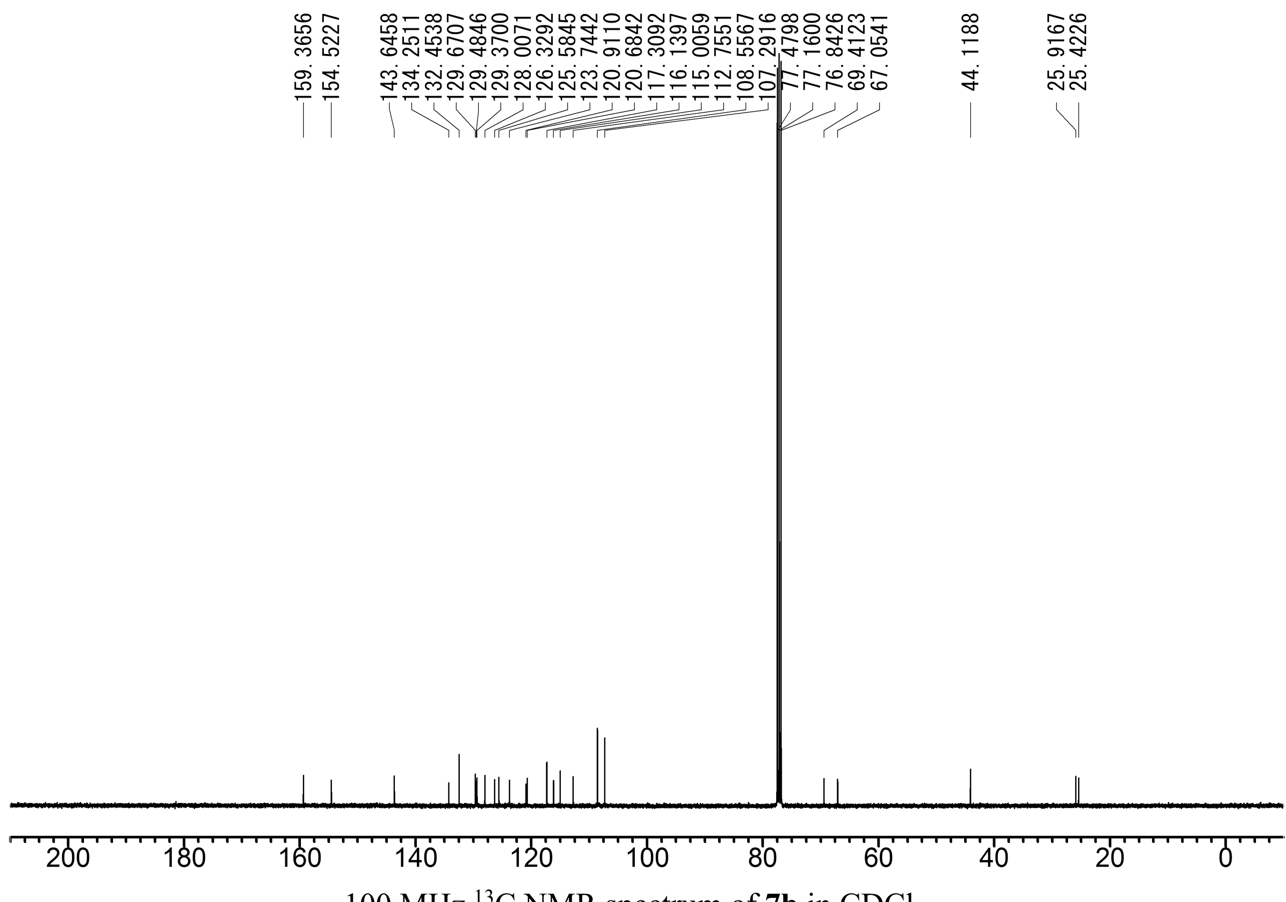
400 MHz ^{1}H NMR spectrum of **6b** in $CDCl_3$



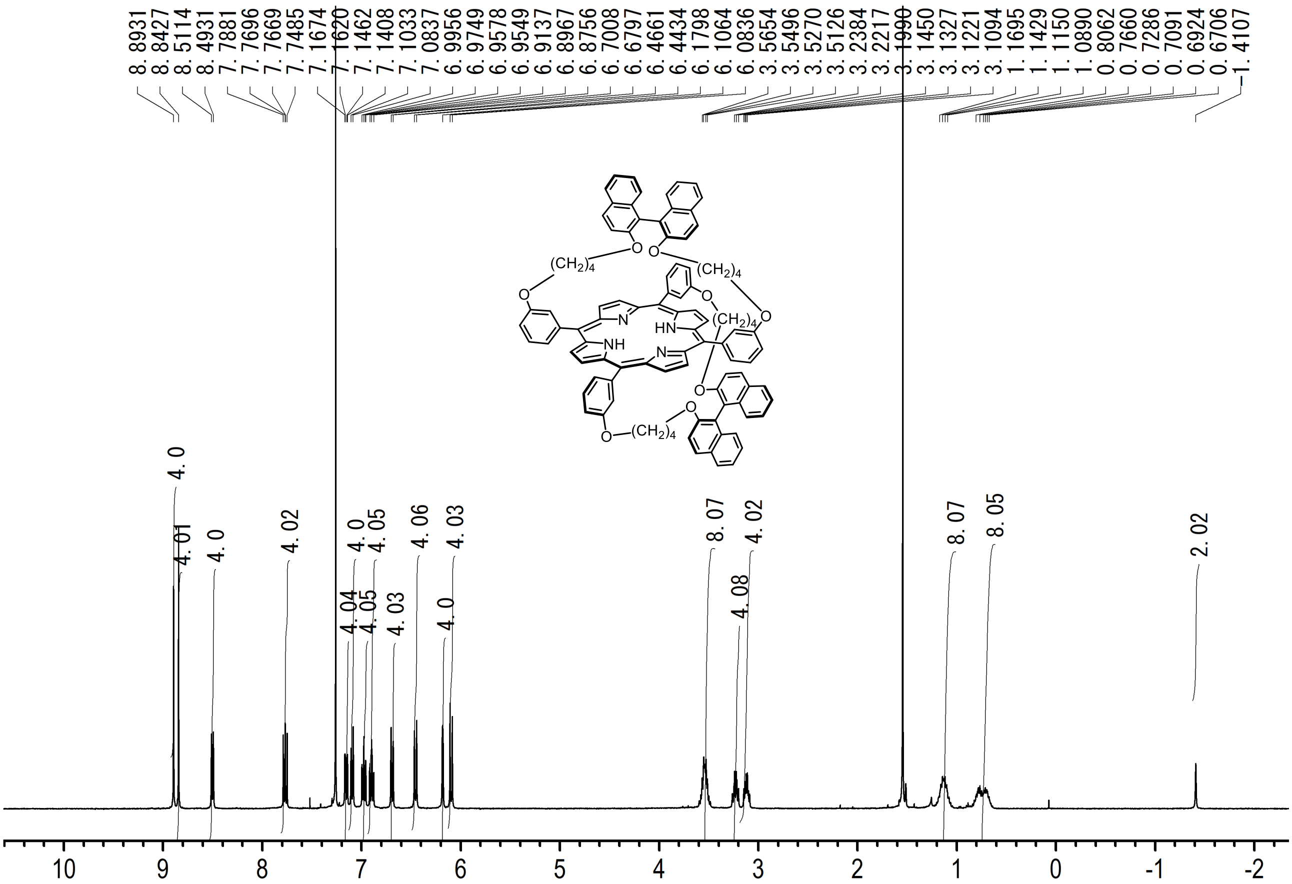
100 MHz ^{13}C NMR spectrum of **6b** in $CDCl_3$



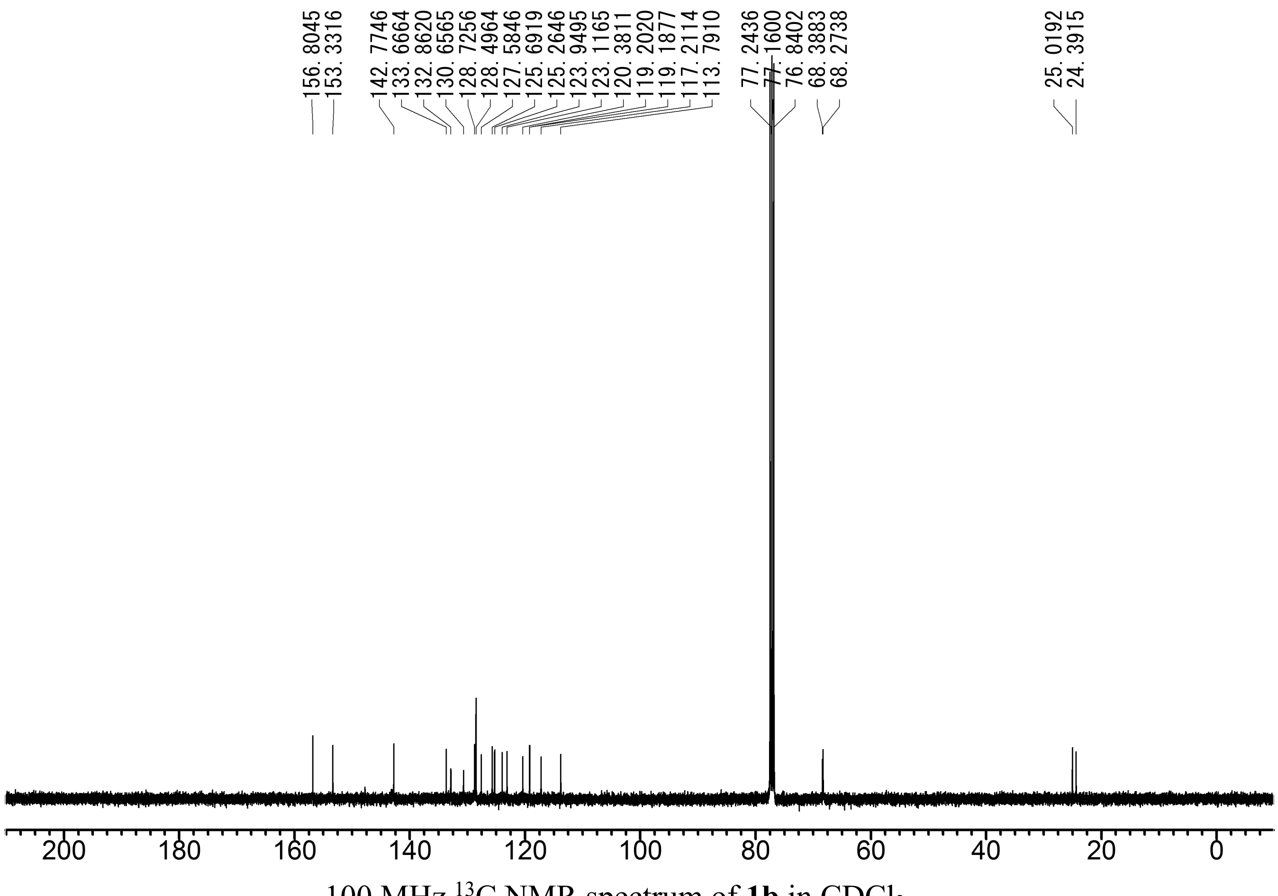
400 MHz ^{1}H NMR spectrum of **7b** in $CDCl_3$



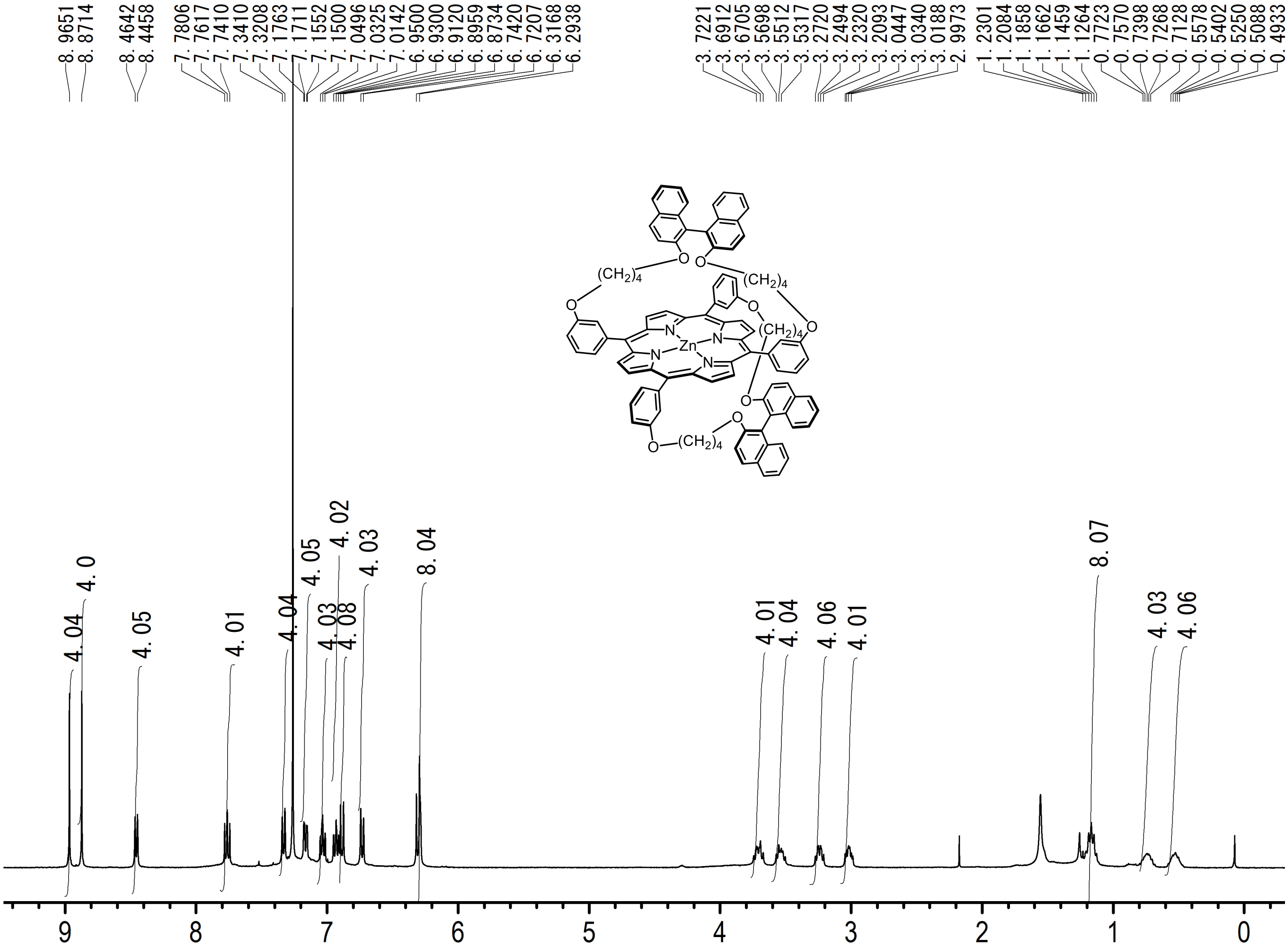
100 MHz ^{13}C NMR spectrum of **7b** in $CDCl_3$



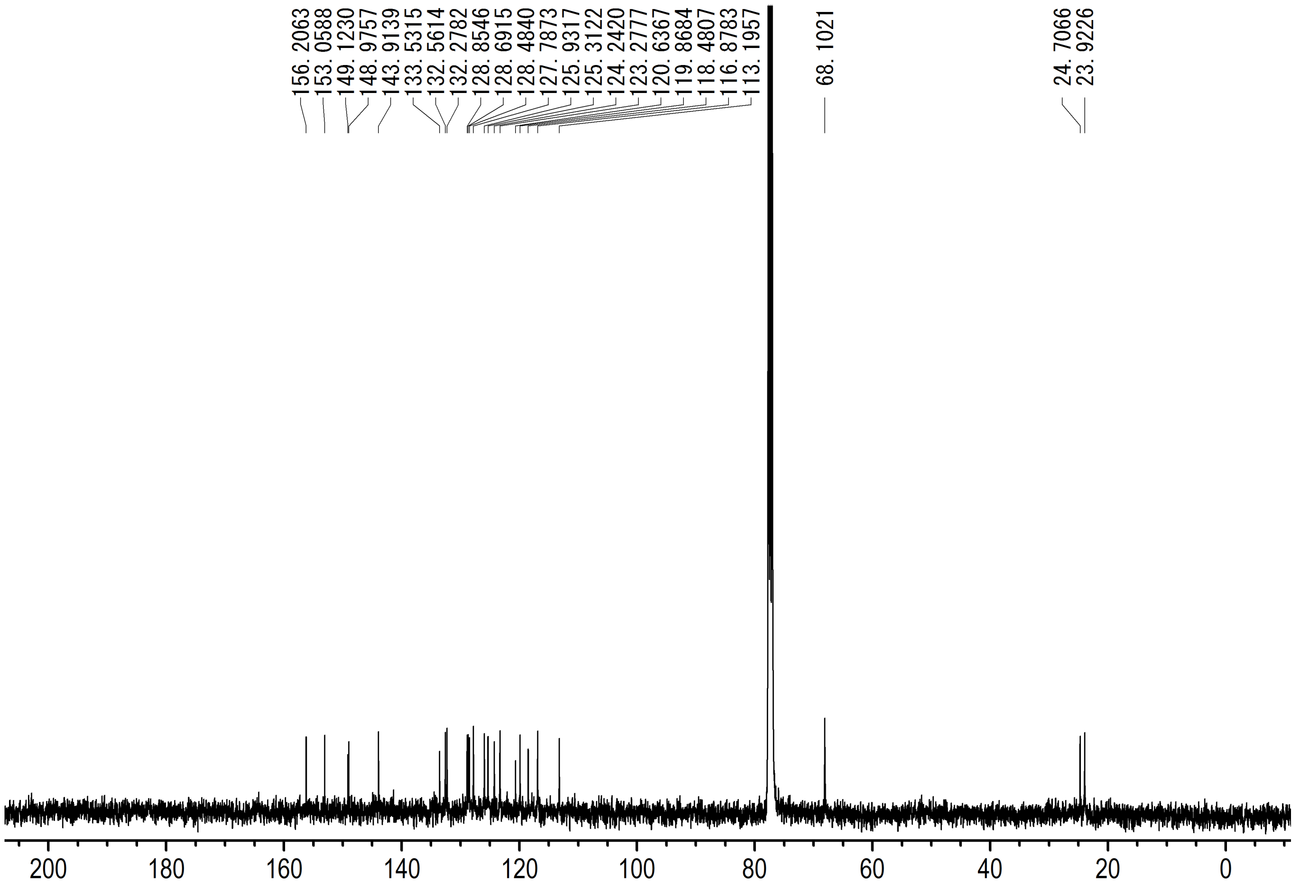
400 MHz ^{1}H NMR spectrum of **1b** in $CDCl_3$



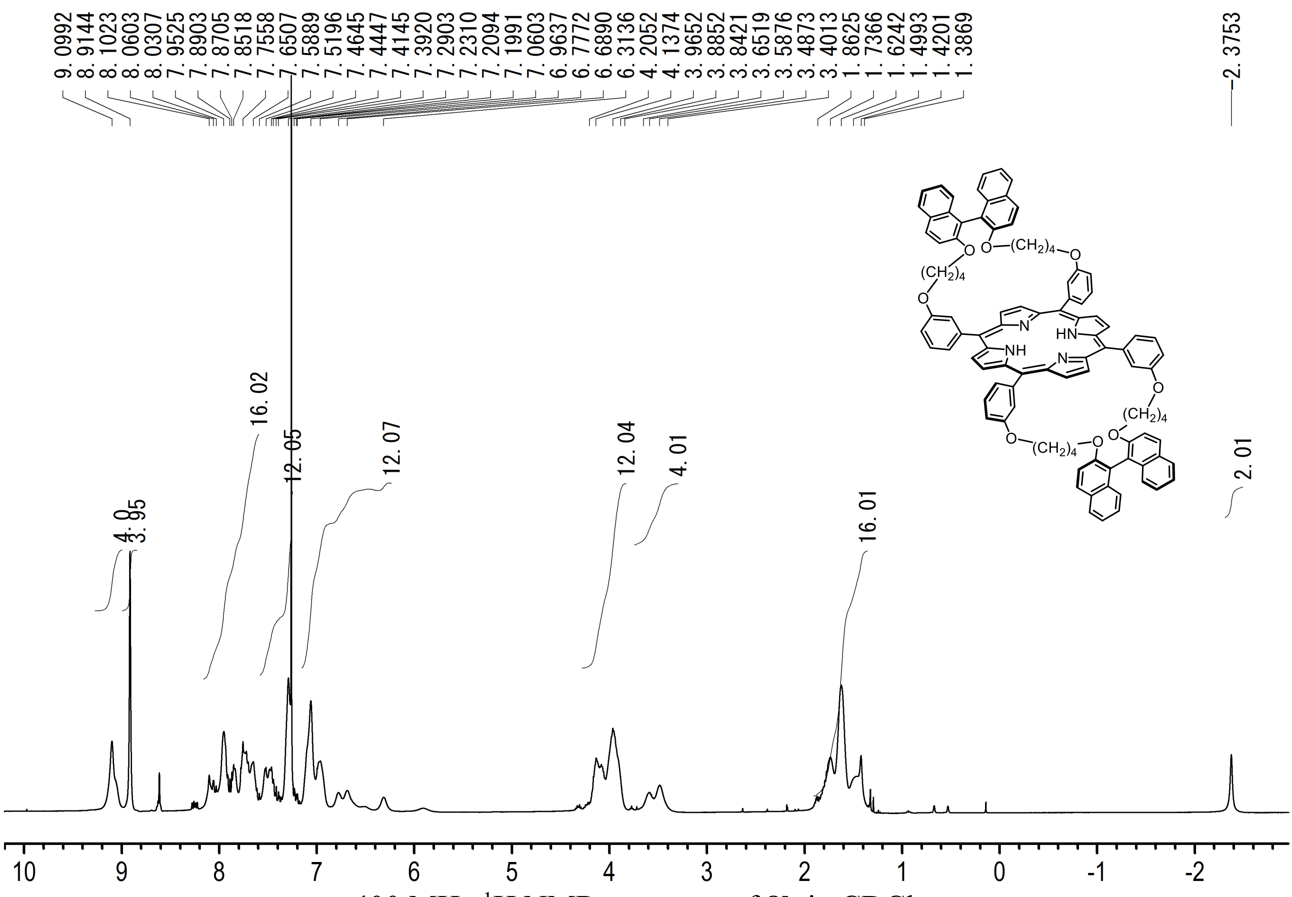
100 MHz ^{13}C NMR spectrum of **1b** in $CDCl_3$



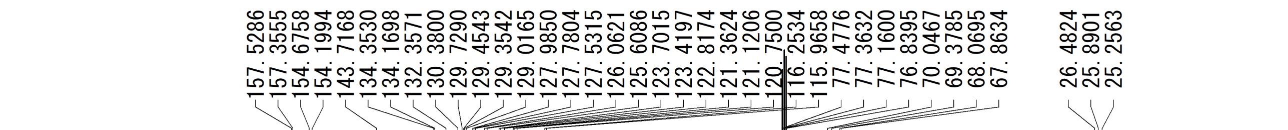
400 MHz ^{1}H NMR spectrum of **2b** in $CDCl_3$



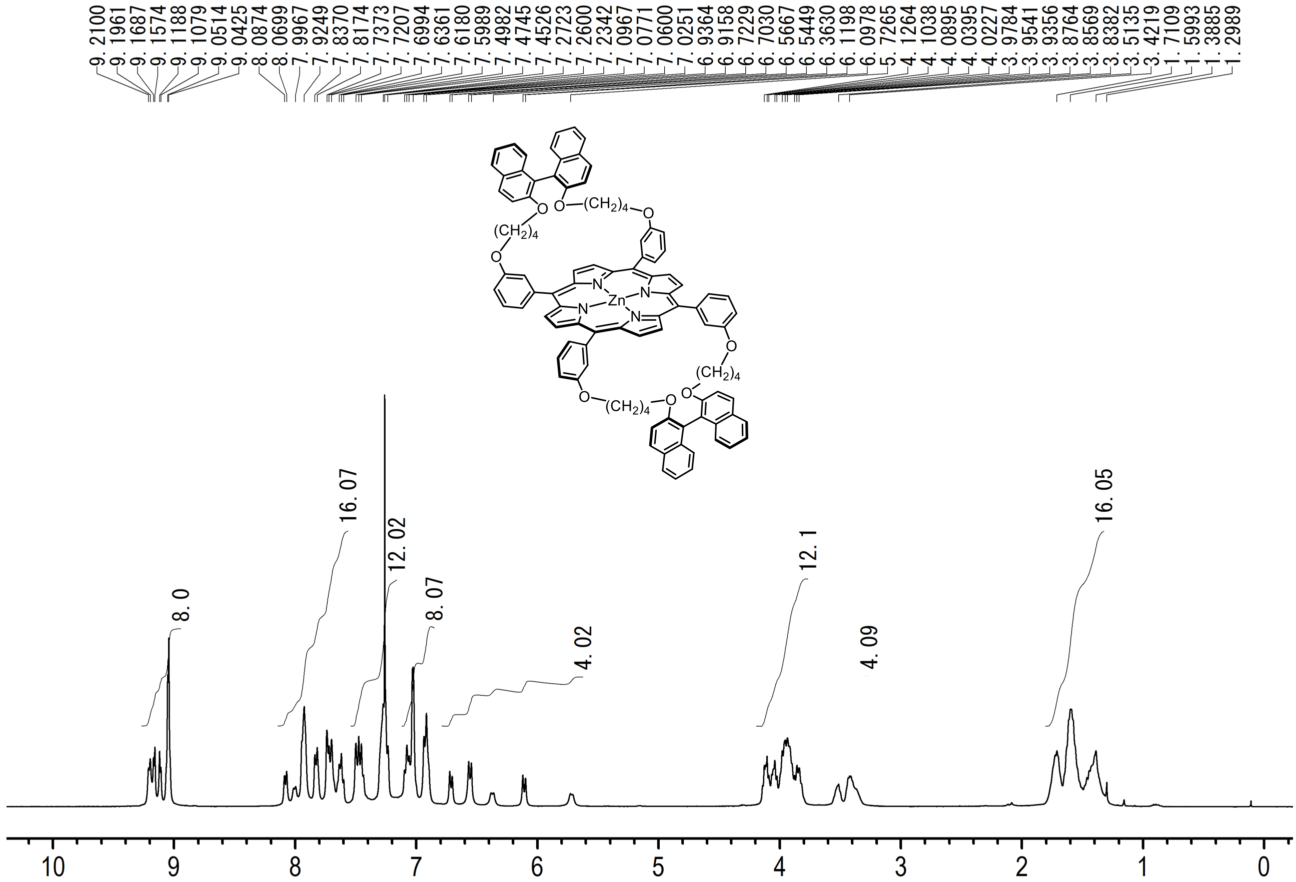
100 MHz ^{13}C NMR spectrum of **2b** in $CDCl_3$



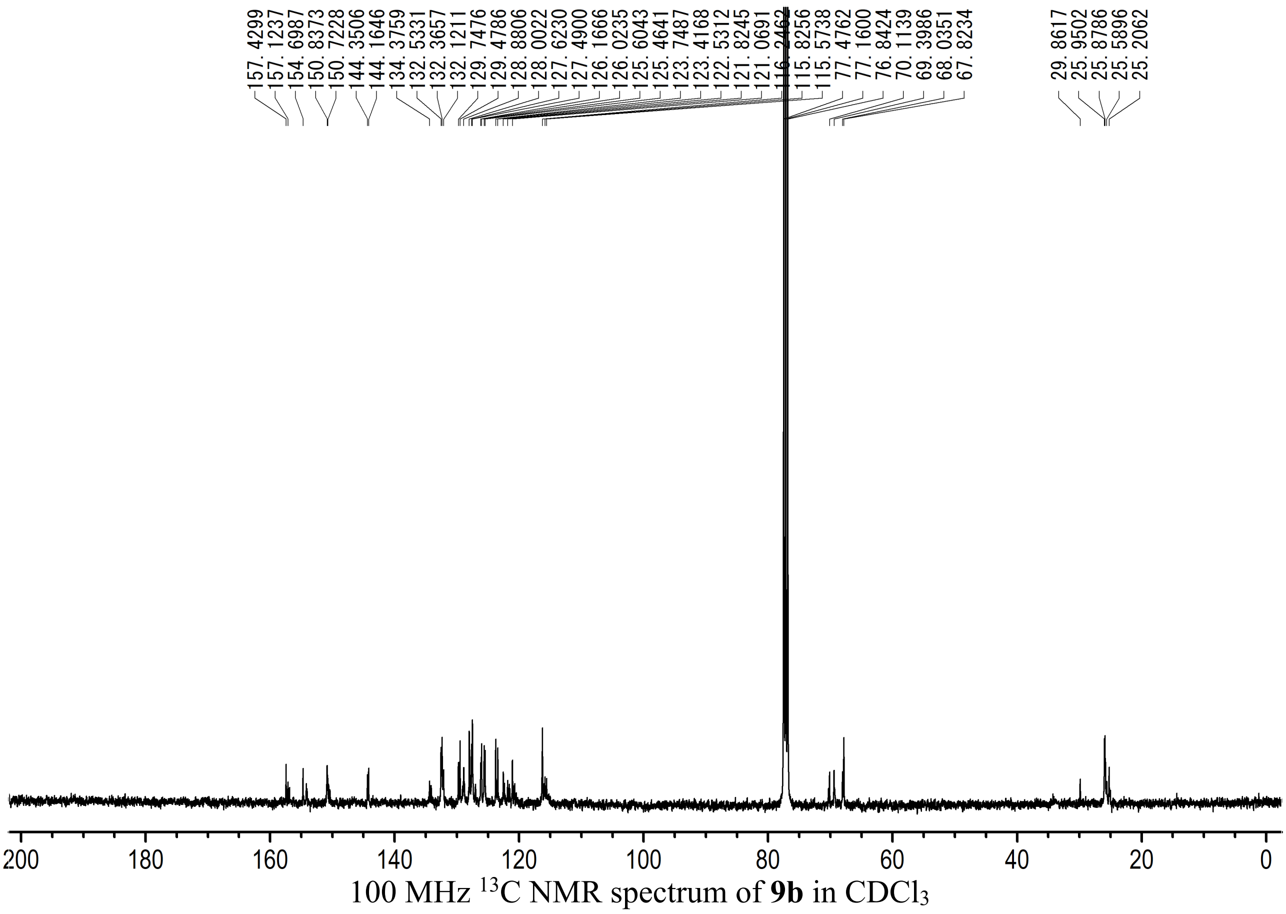
400 MHz ^{1}H NMR spectrum of **8b** in $CDCl_3$



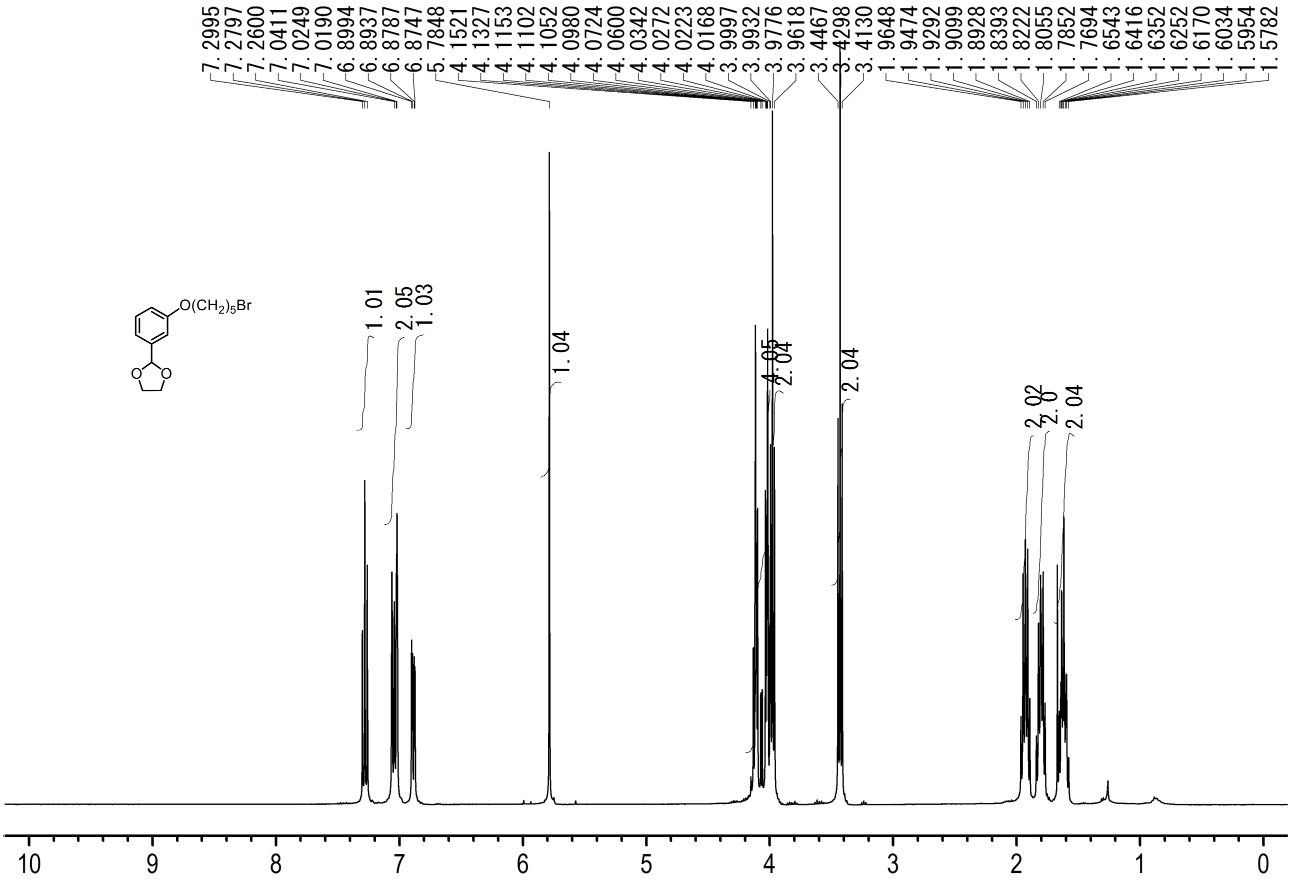
100 MHz ^{13}C NMR spectrum of **8b** in $CDCl_3$



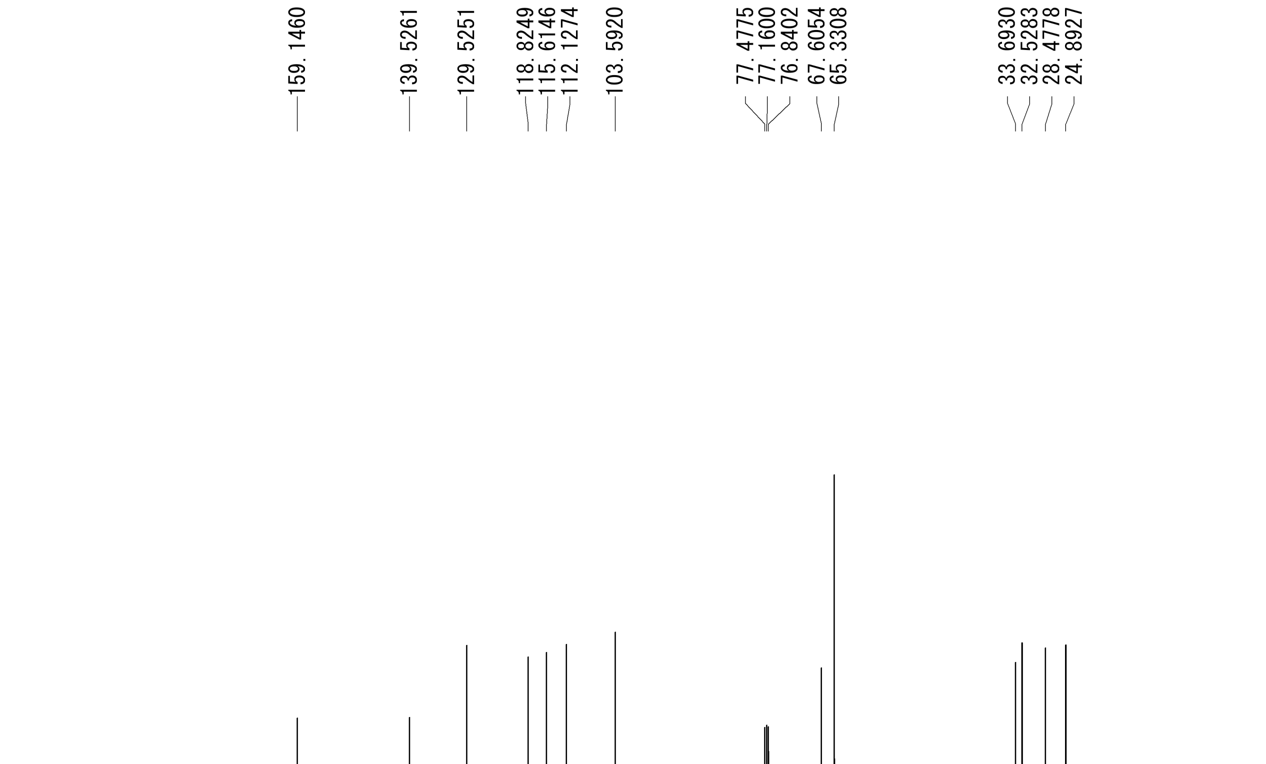
400 MHz ^1H NMR spectrum of **9b** in $CDCl_3$



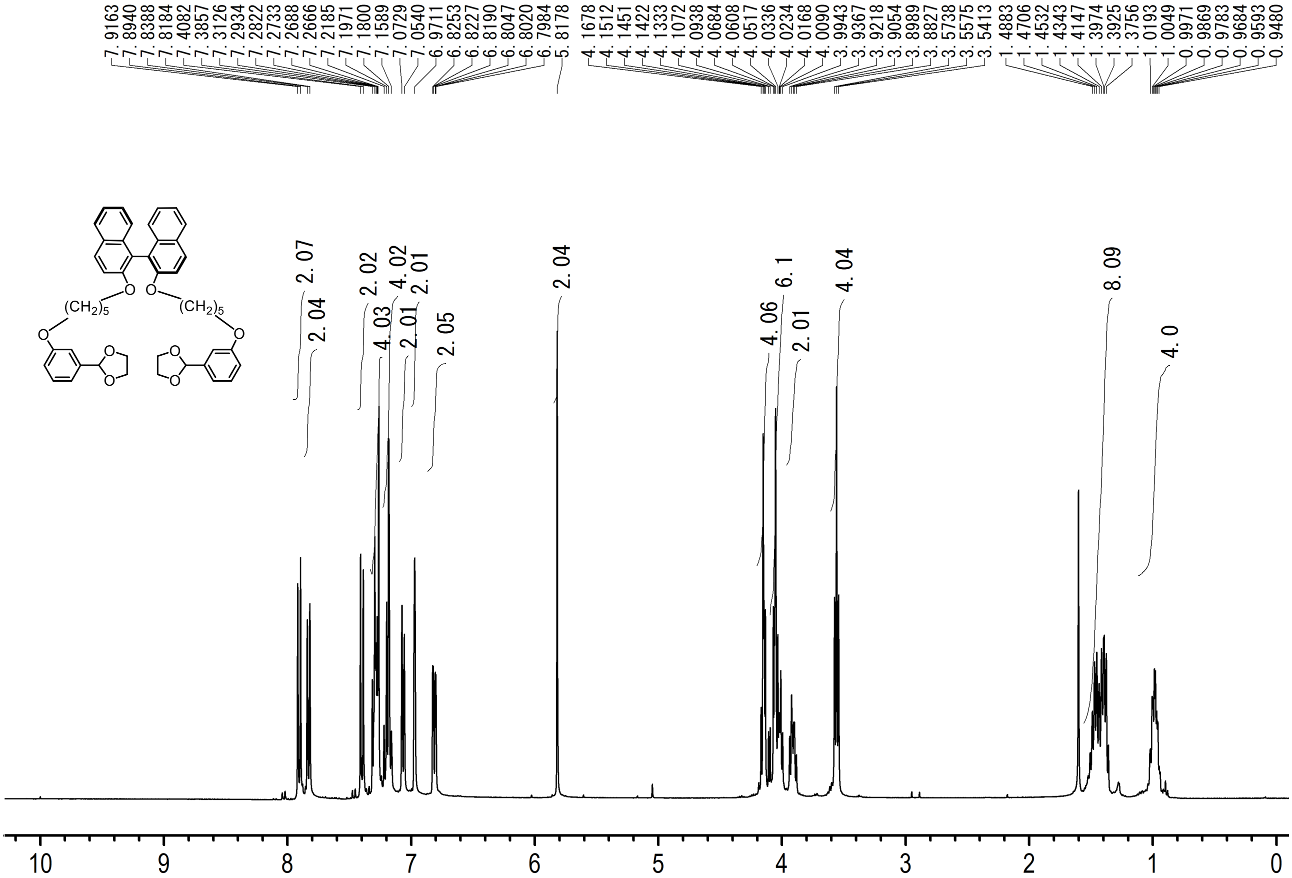
100 MHz ^{13}C NMR spectrum of **9b** in $CDCl_3$



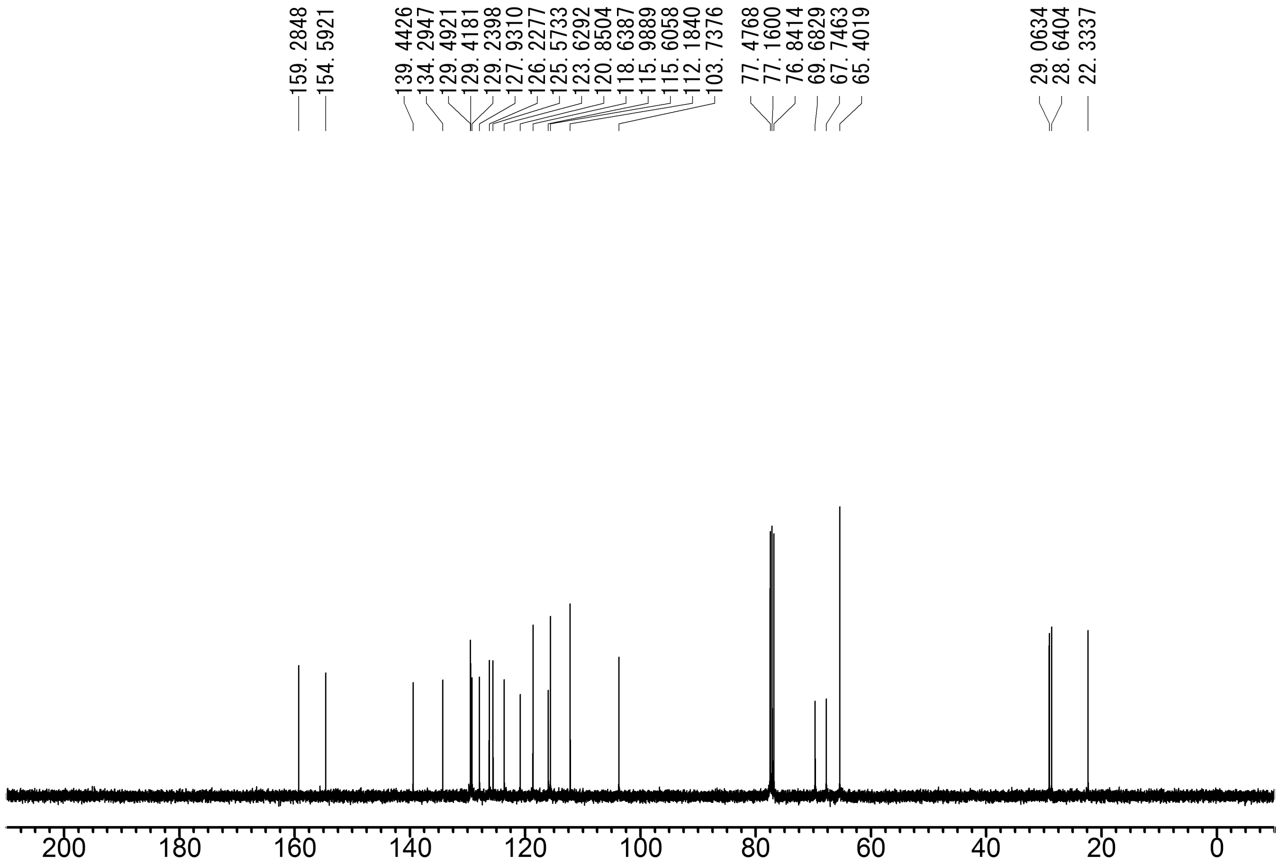
400 MHz ^{1}H NMR spectrum of **4c** in $CDCl_3$



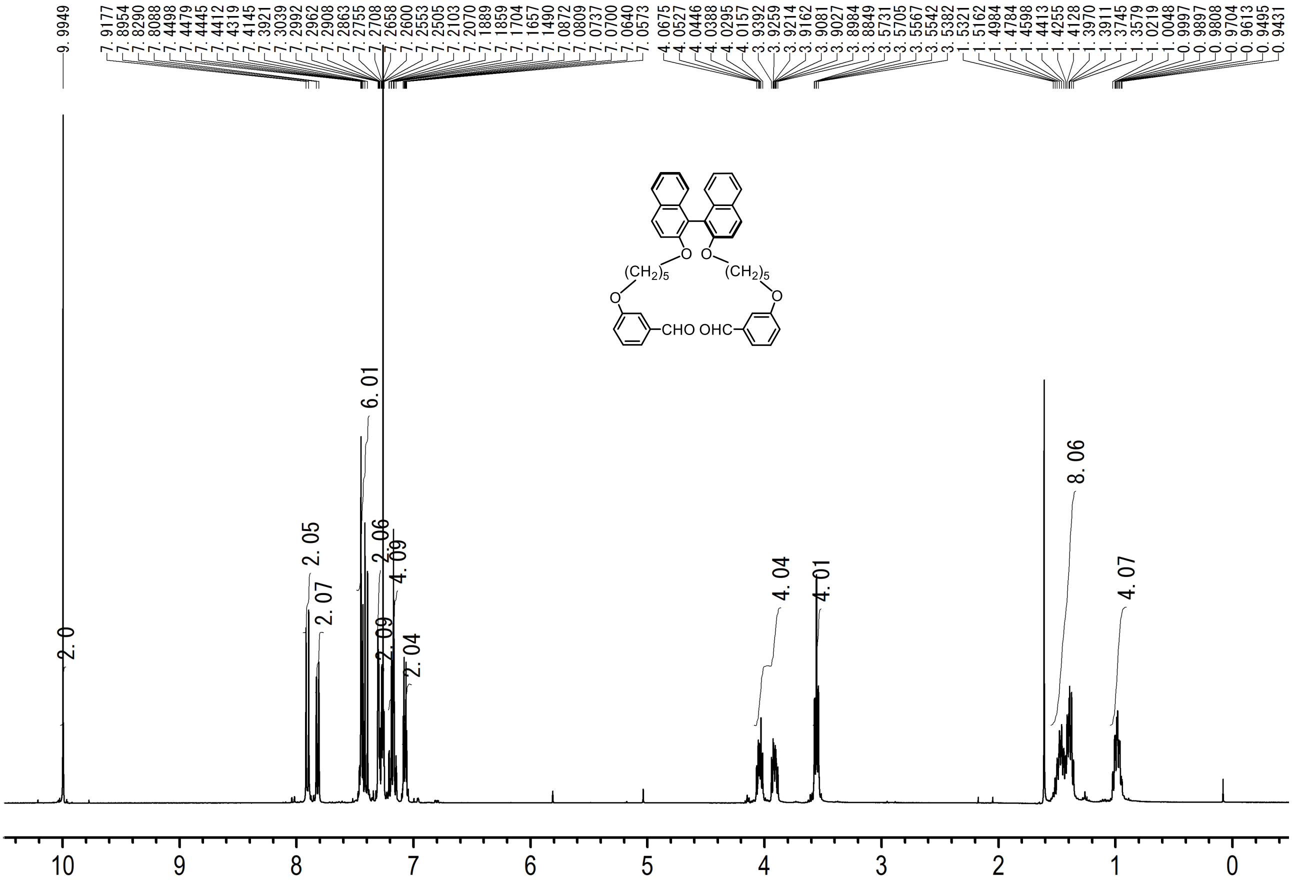
100 MHz ^{13}C NMR spectrum of **4c** in $CDCl_3$



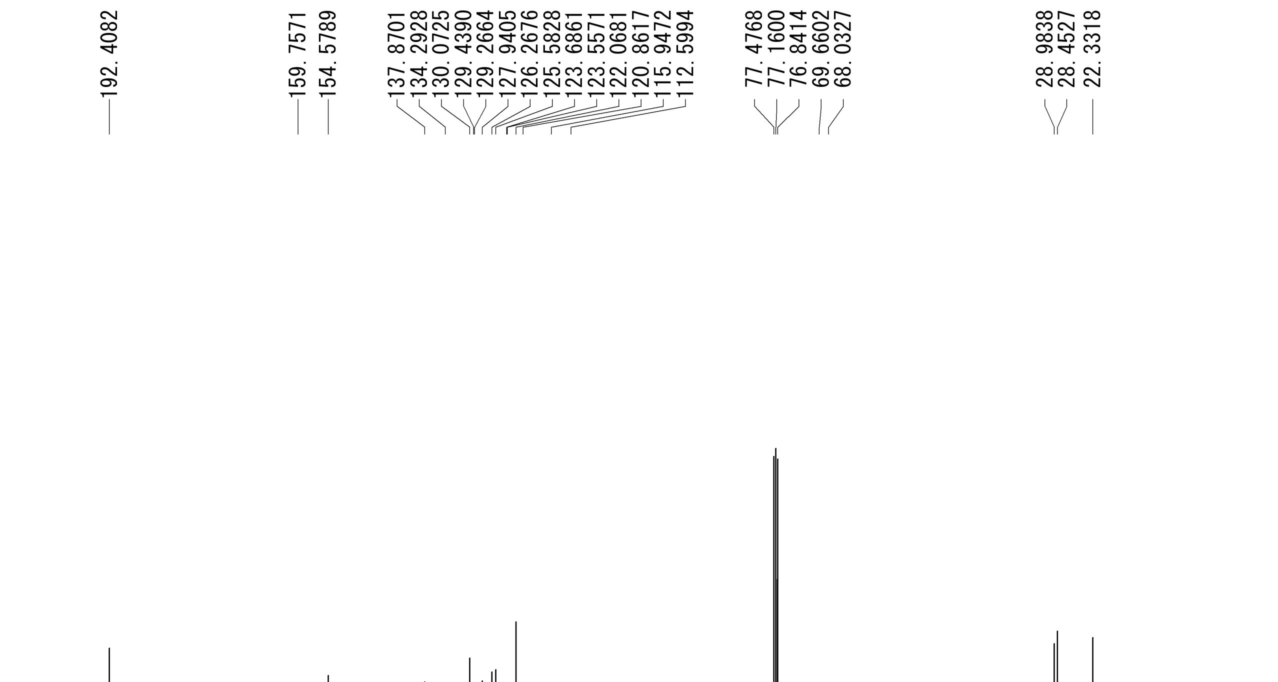
400 MHz ^{1}H NMR spectrum of **5c** in $CDCl_3$



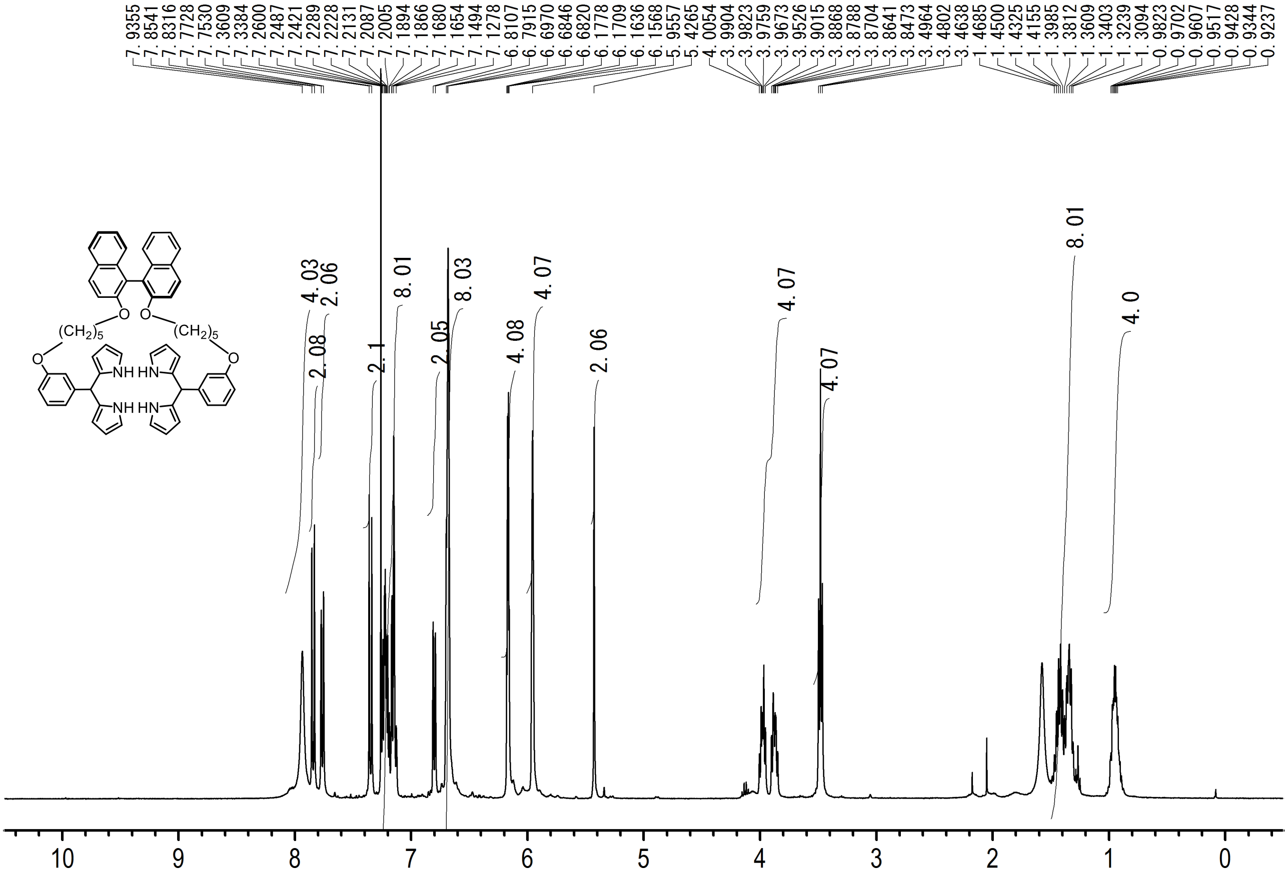
100 MHz ^{13}C NMR spectrum of **5c** in $CDCl_3$



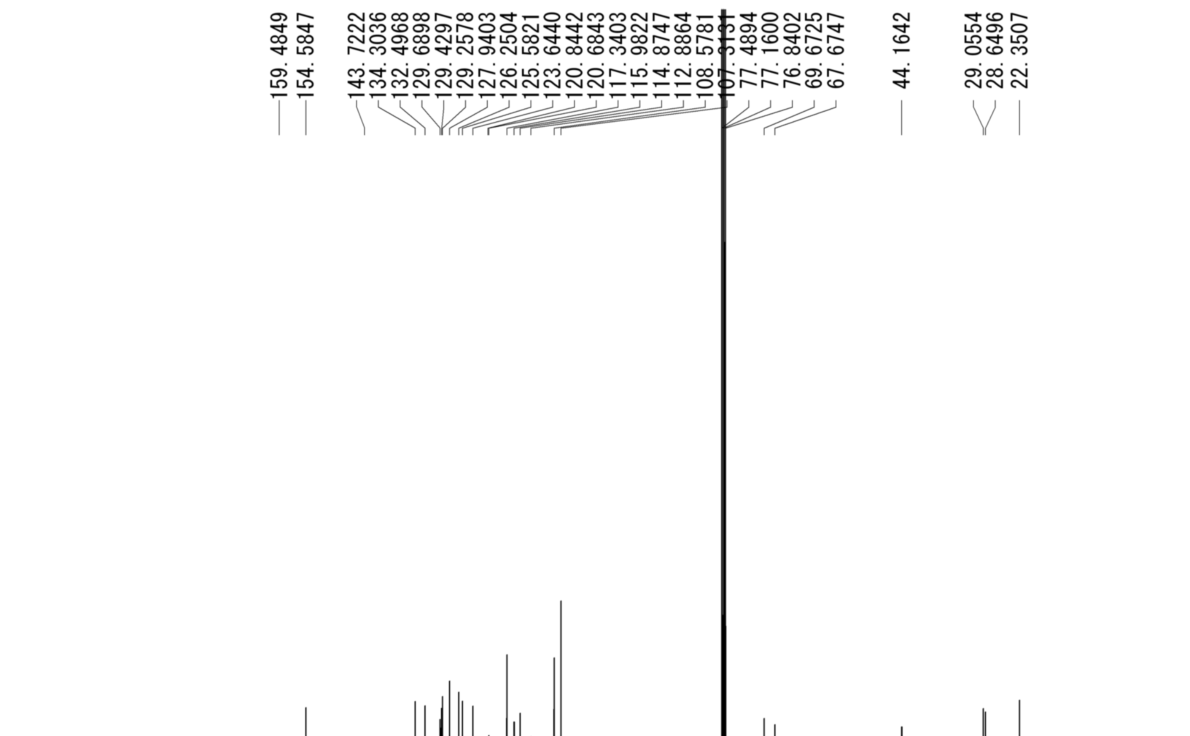
400 MHz ^{1}H NMR spectrum of **6c** in $CDCl_3$



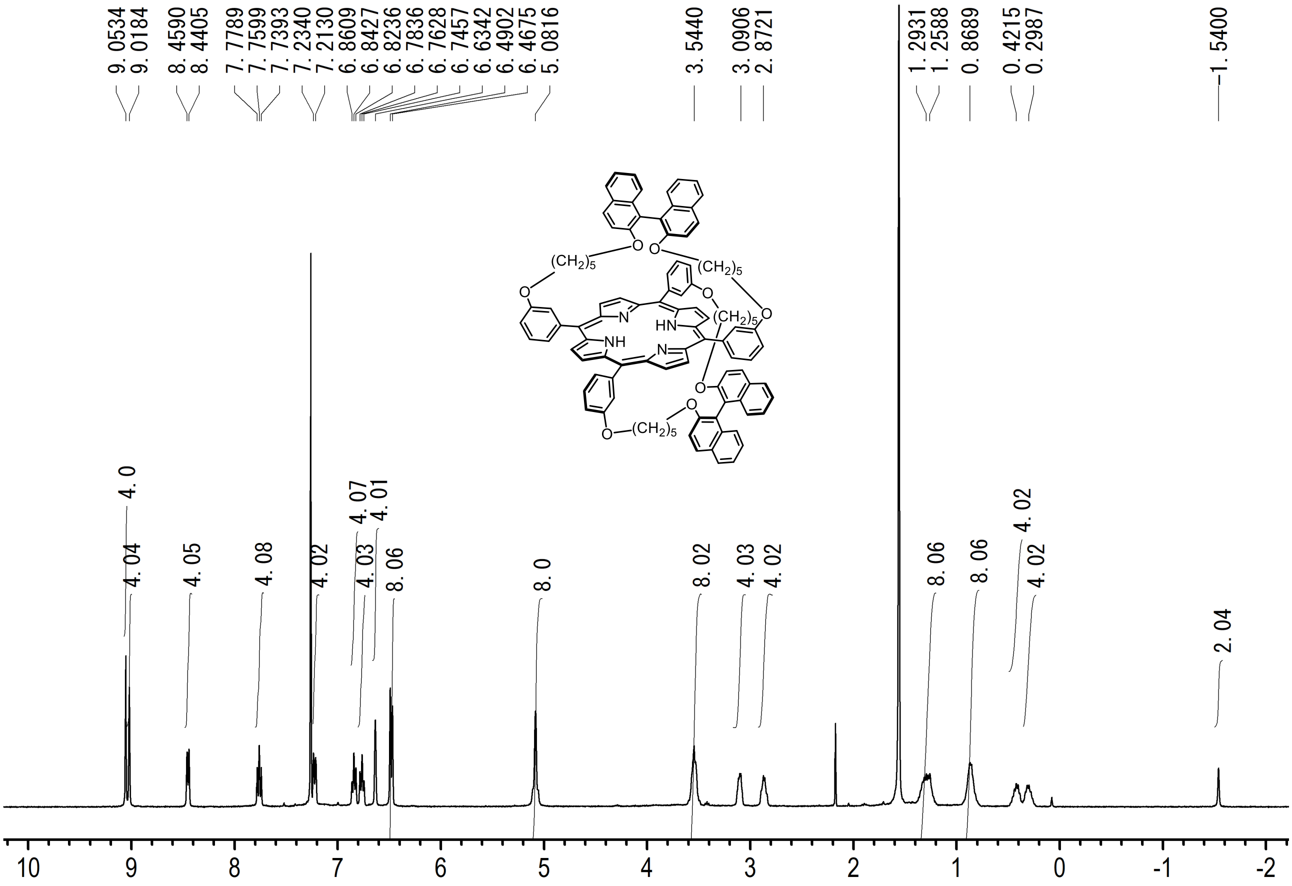
100 MHz ^{13}C NMR spectrum of **6c** in $CDCl_3$



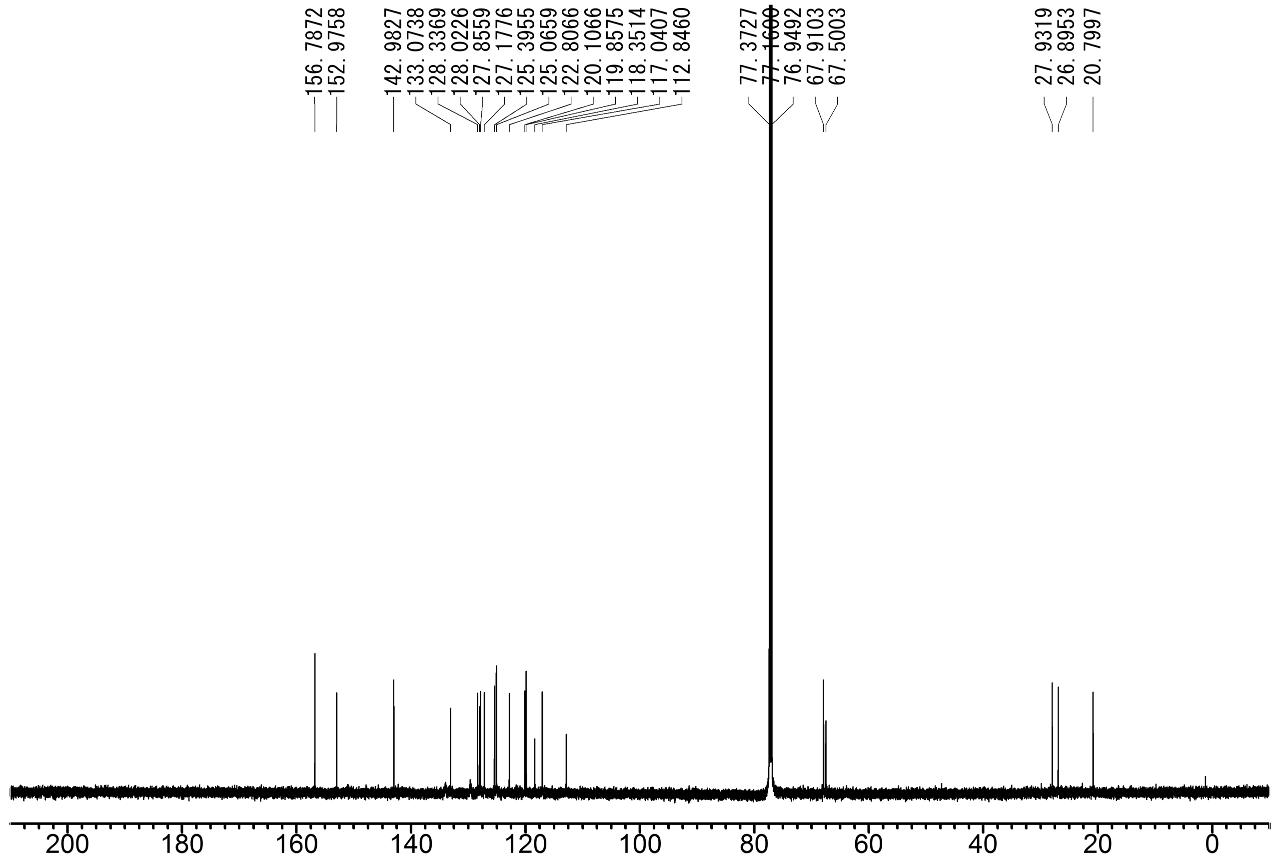
400 MHz ^{1}H NMR spectrum of **7c** in $CDCl_3$



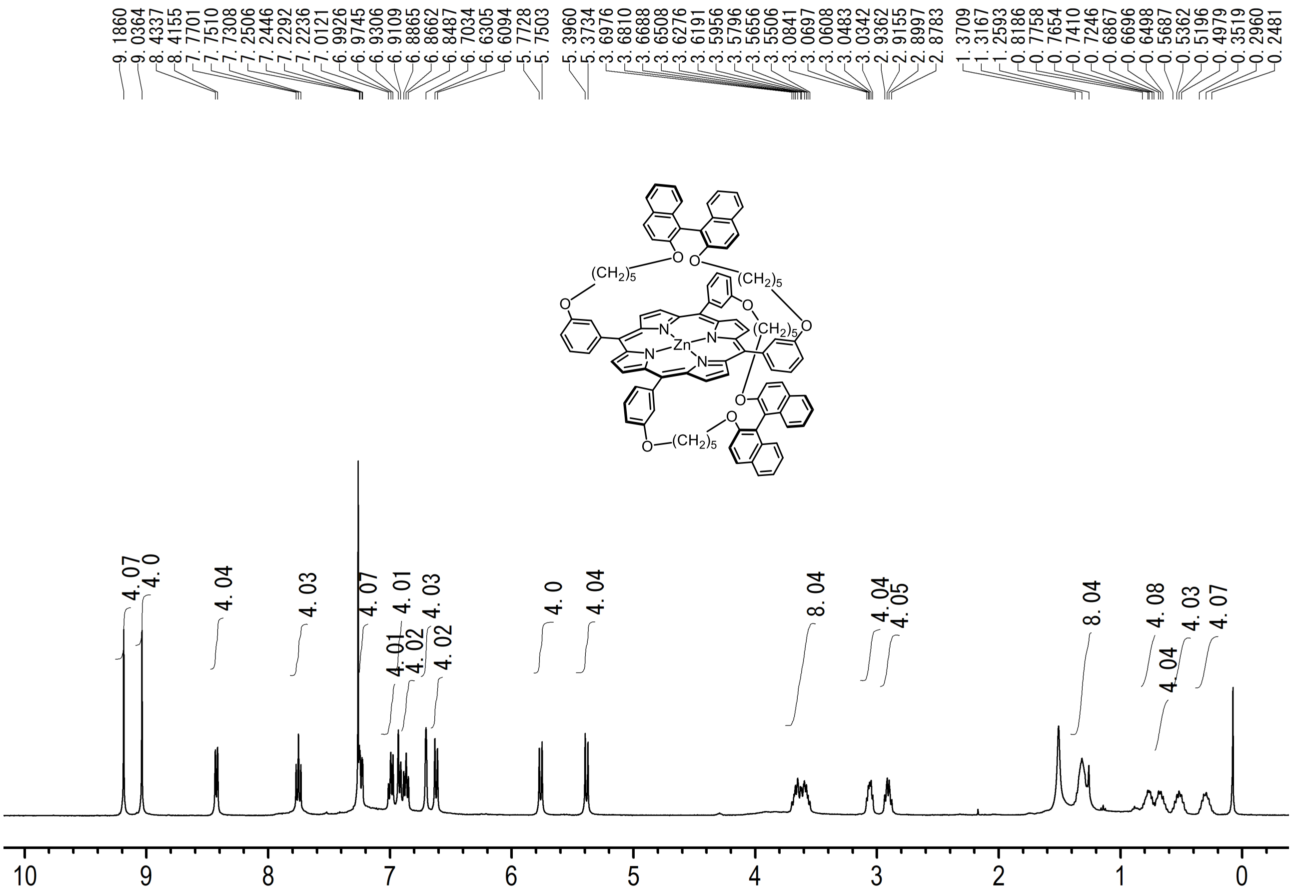
100 MHz ^{13}C NMR spectrum of **7c** in $CDCl_3$



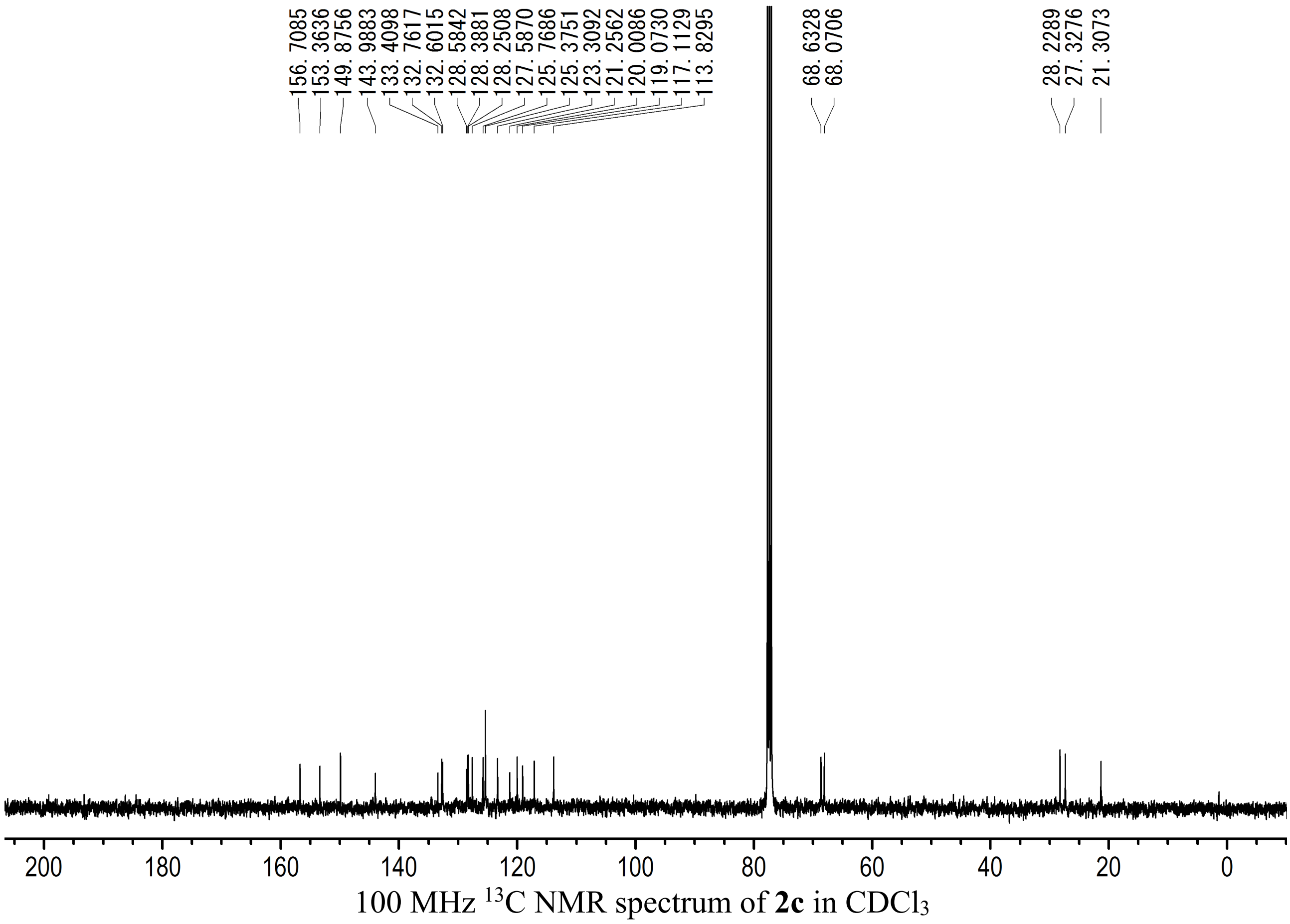
400 MHz ^{1}H NMR spectrum of **1c** in $CDCl_3$



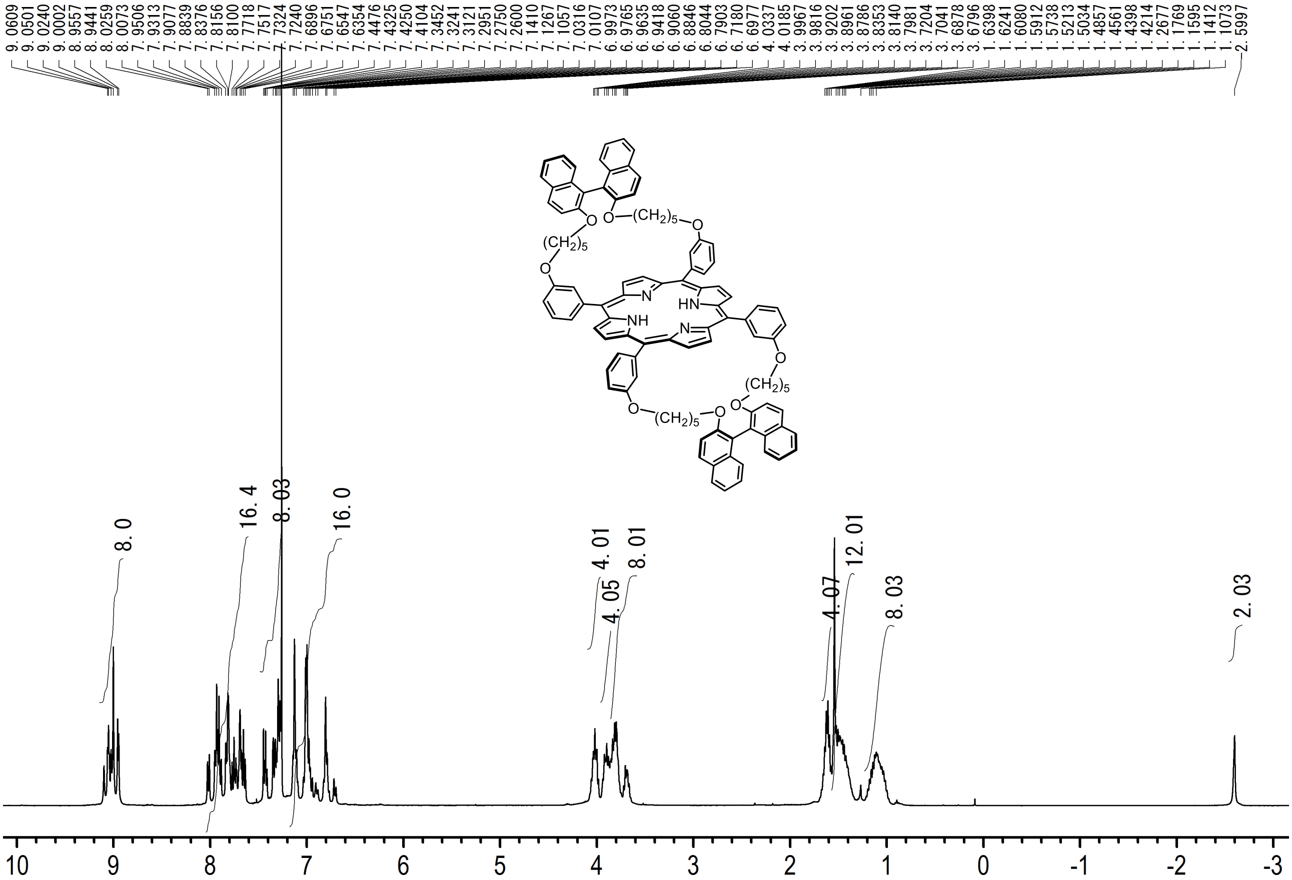
100 MHz ^{13}C NMR spectrum of **1c** in $CDCl_3$



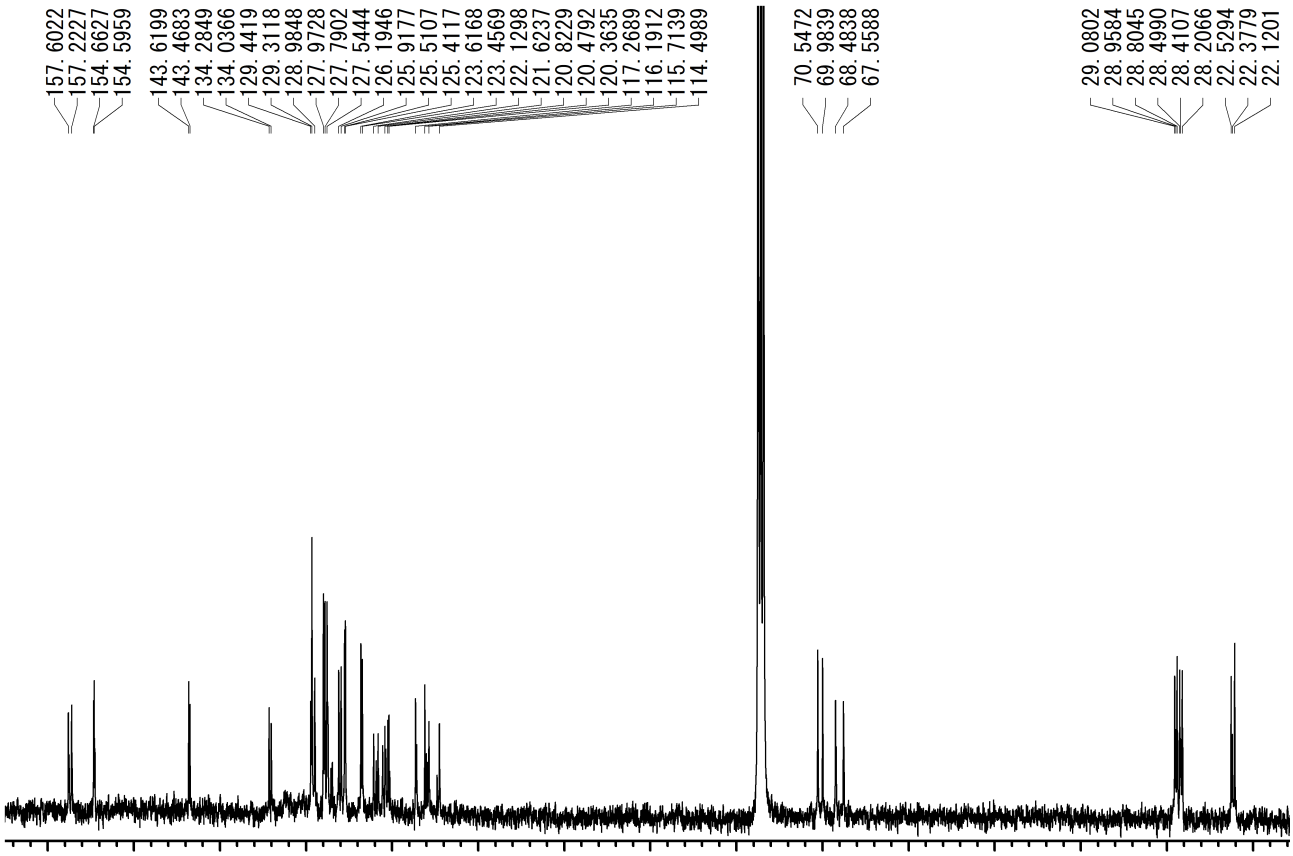
400 MHz ^{1}H NMR spectrum of **2c** in $CDCl_3$



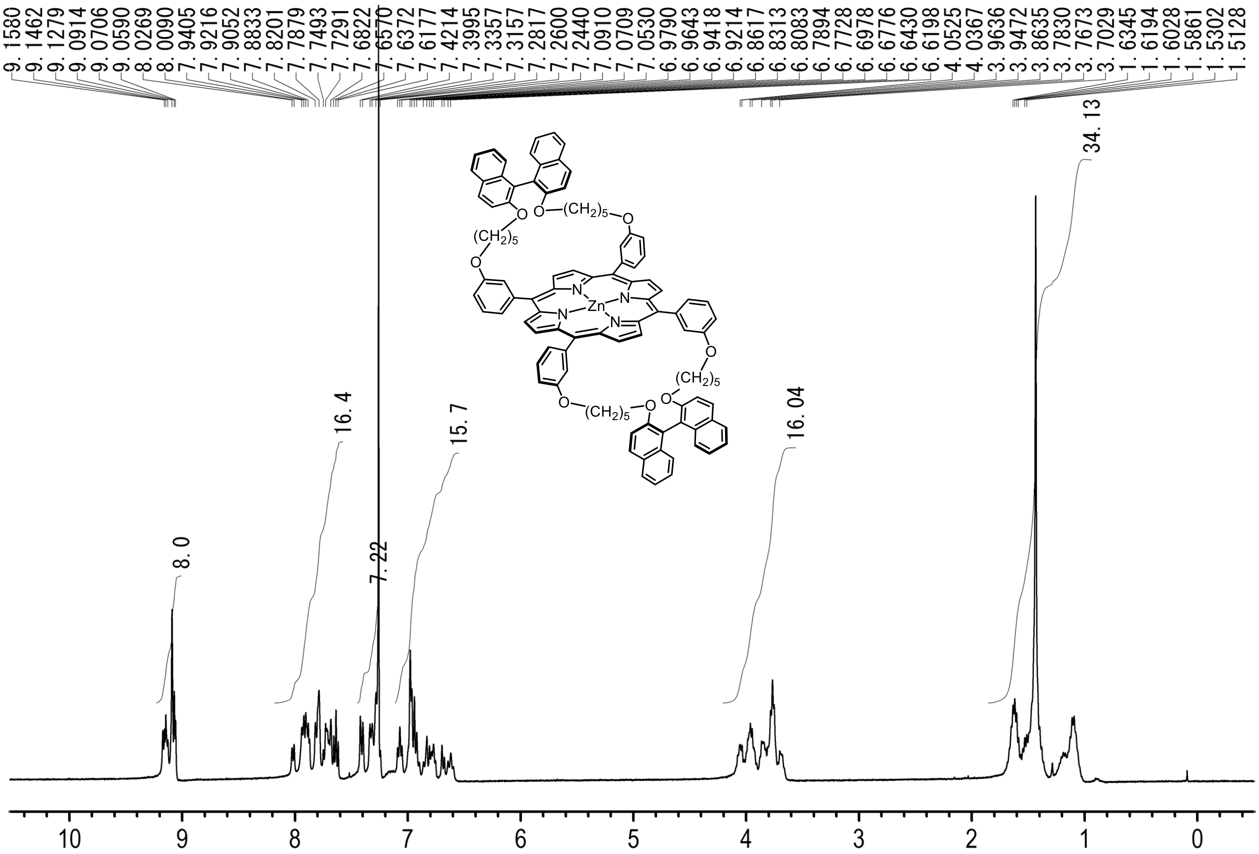
100 MHz ^{13}C NMR spectrum of **2c** in $CDCl_3$



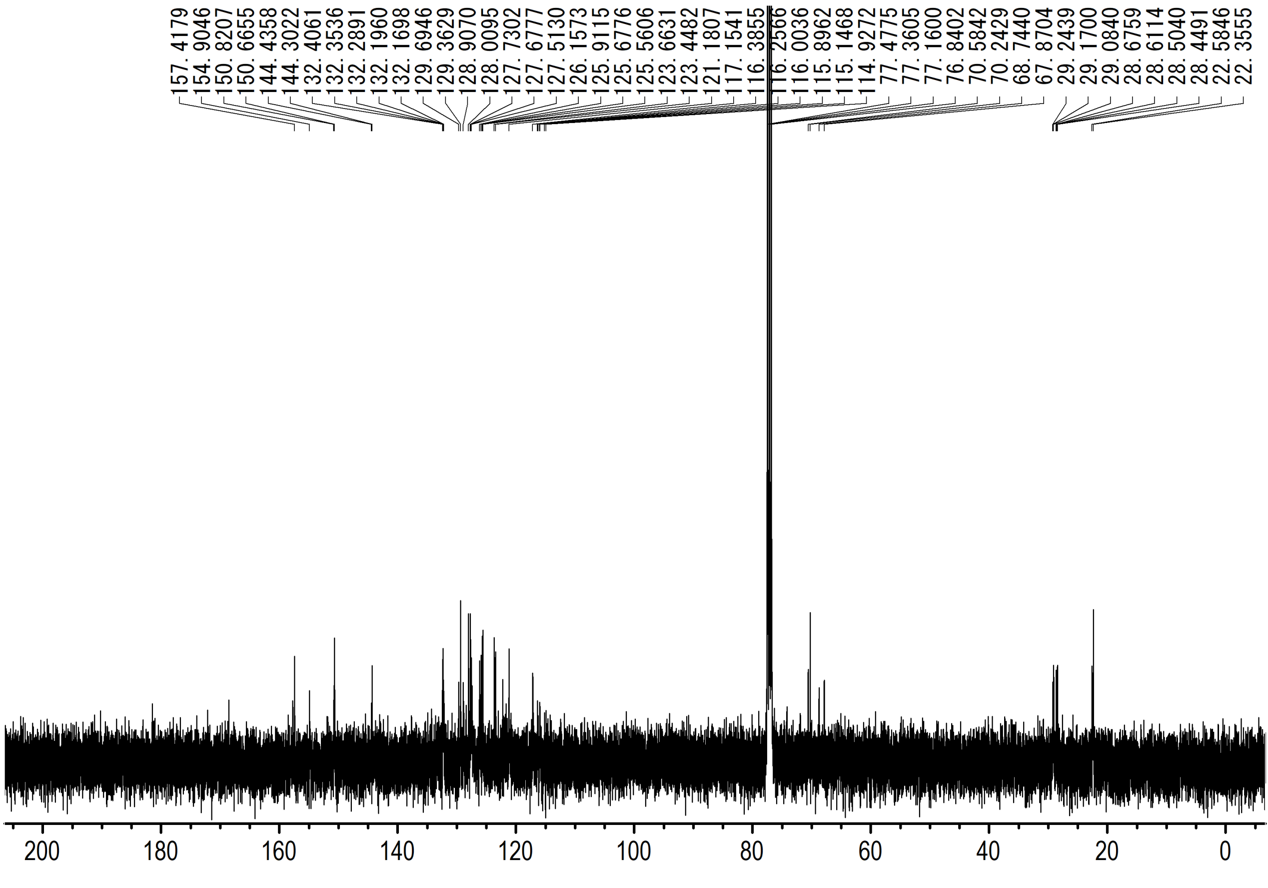
400 MHz ^{1}H NMR spectrum of **8c** in $CDCl_3$



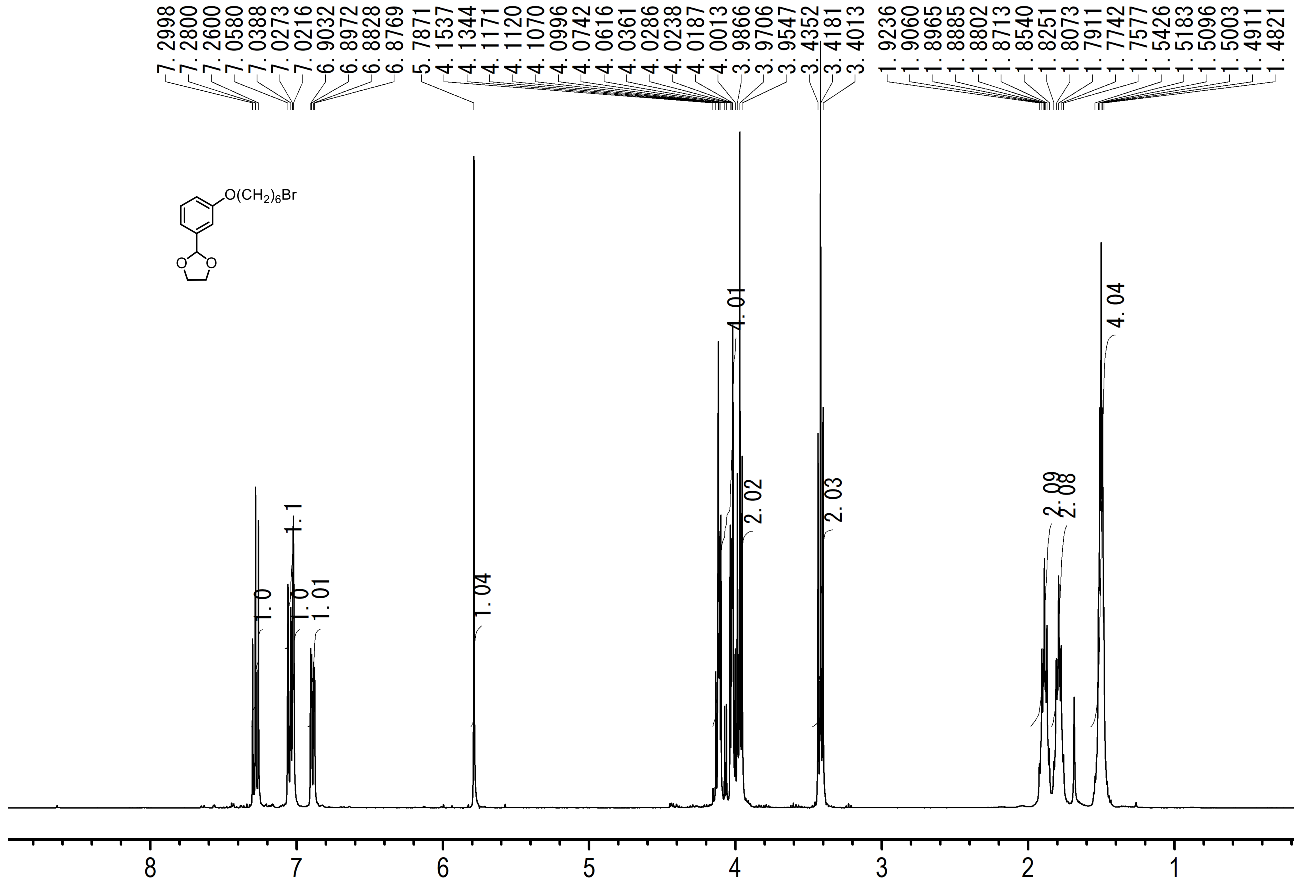
100 MHz ^{13}C NMR spectrum of **8c** in $CDCl_3$



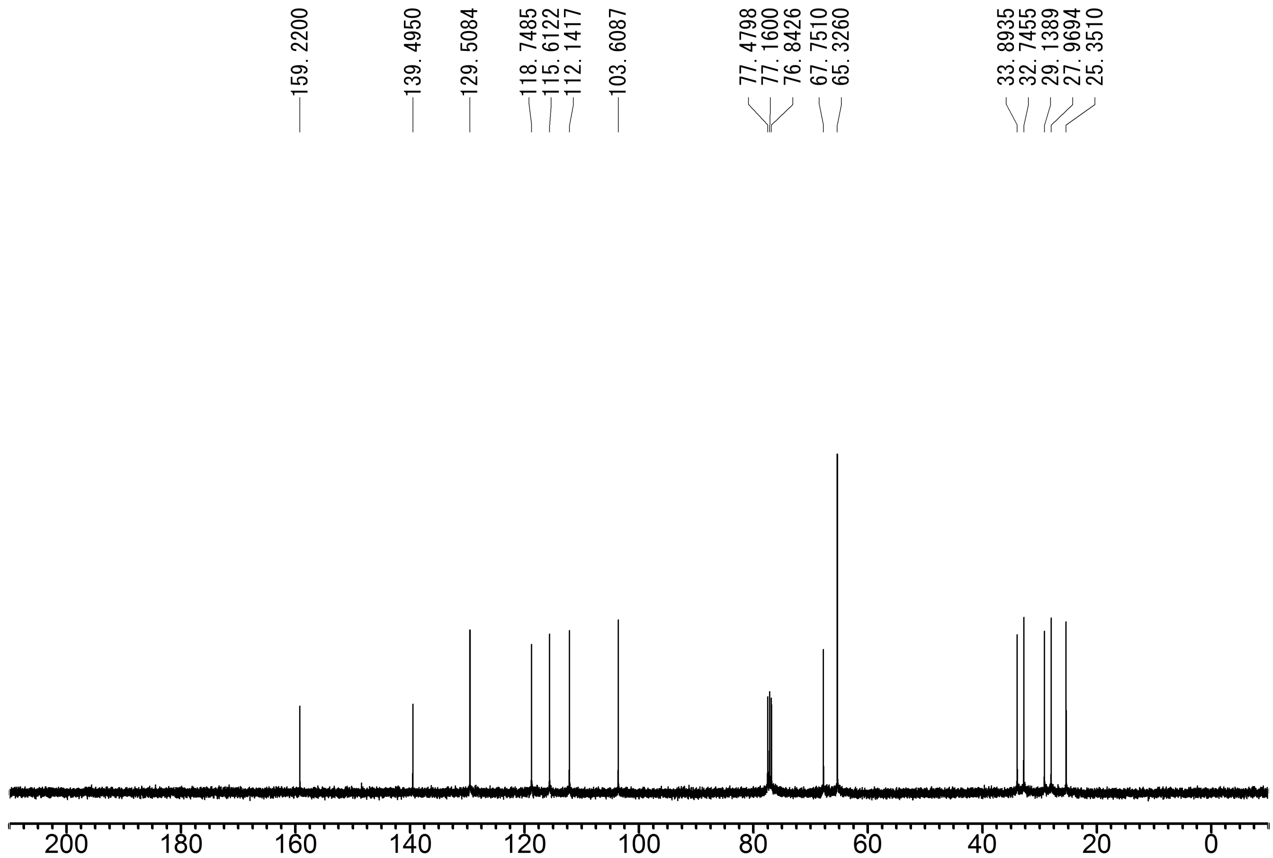
400 MHz ^{1}H NMR spectrum of **9c** in $CDCl_3$



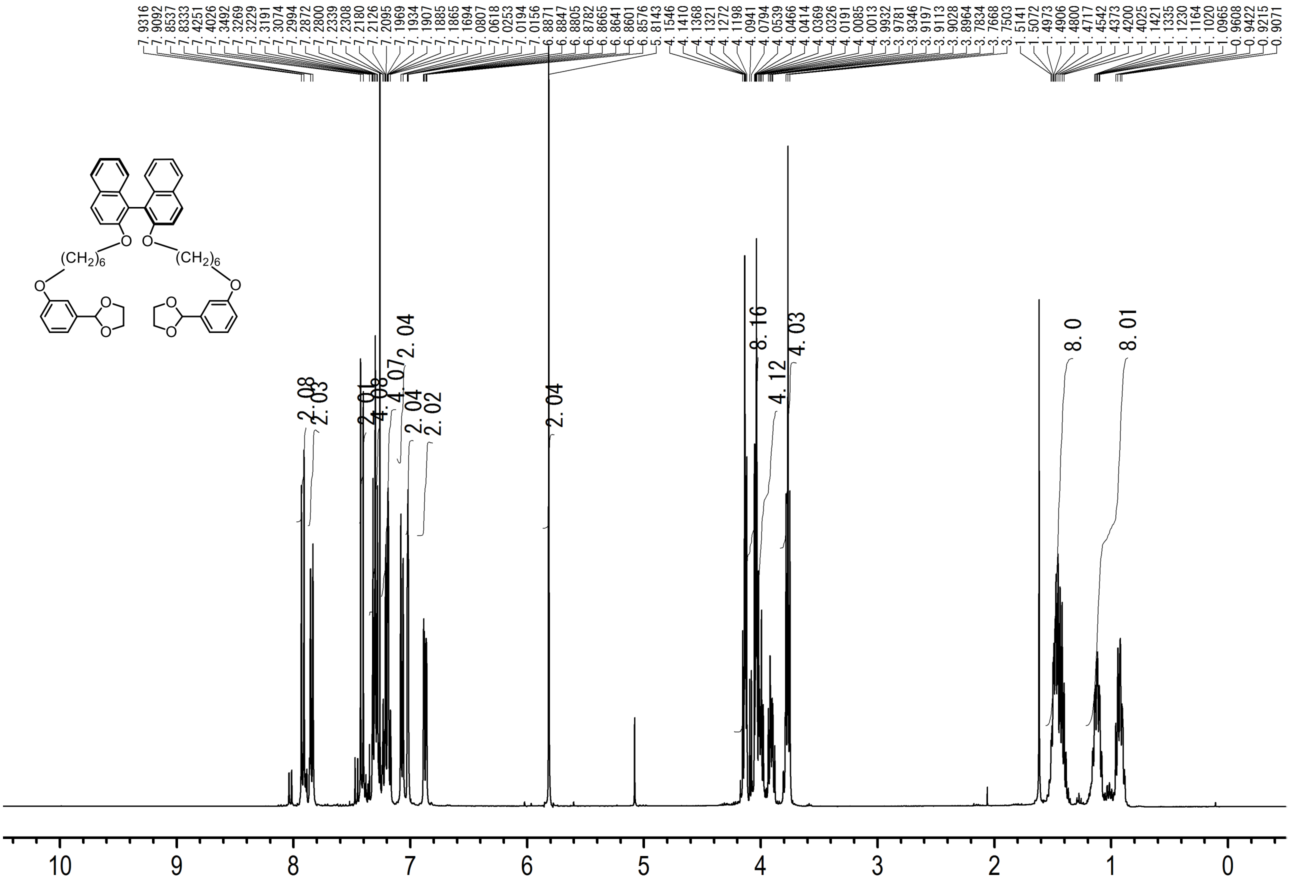
100 MHz ^{13}C NMR spectrum of **9c** in $CDCl_3$



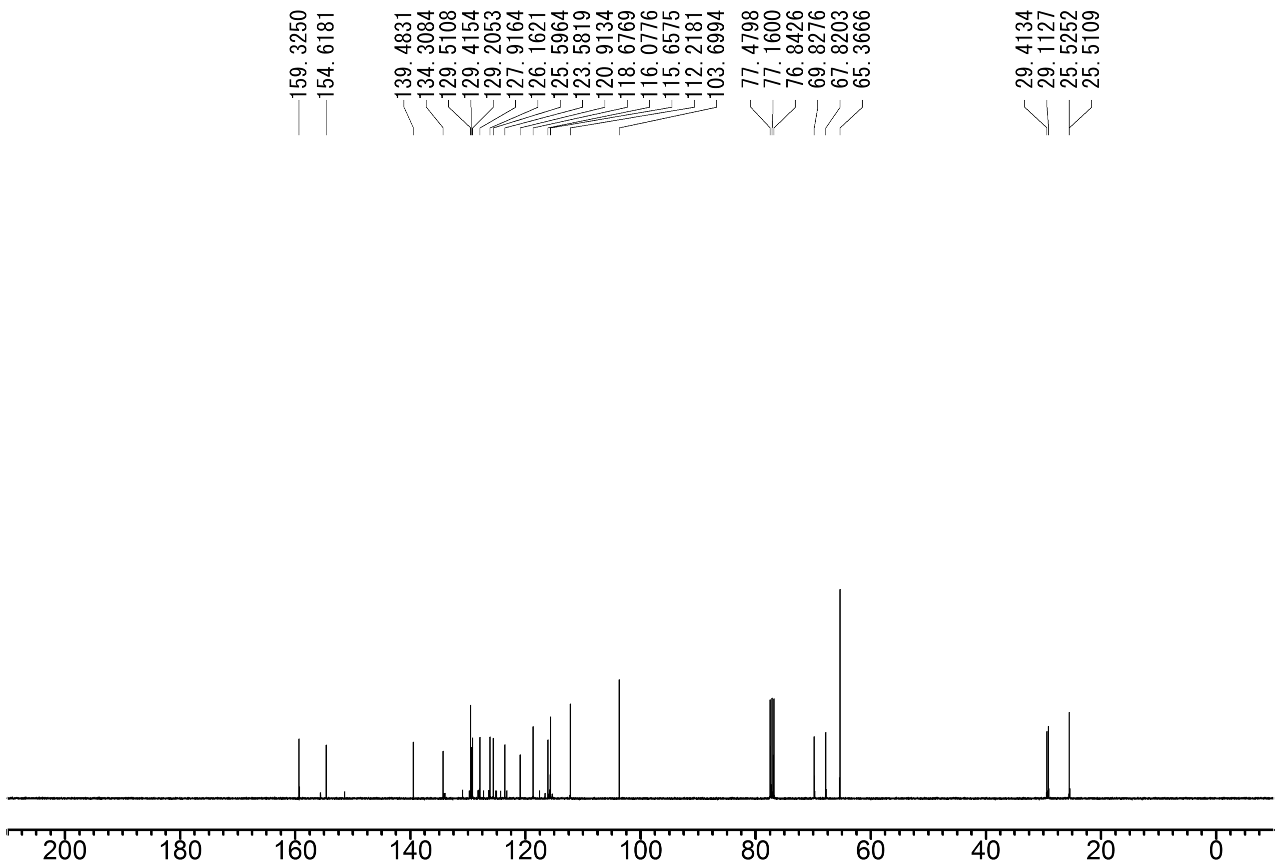
400 MHz ^{1}H NMR spectrum of **4d** in $CDCl_3$



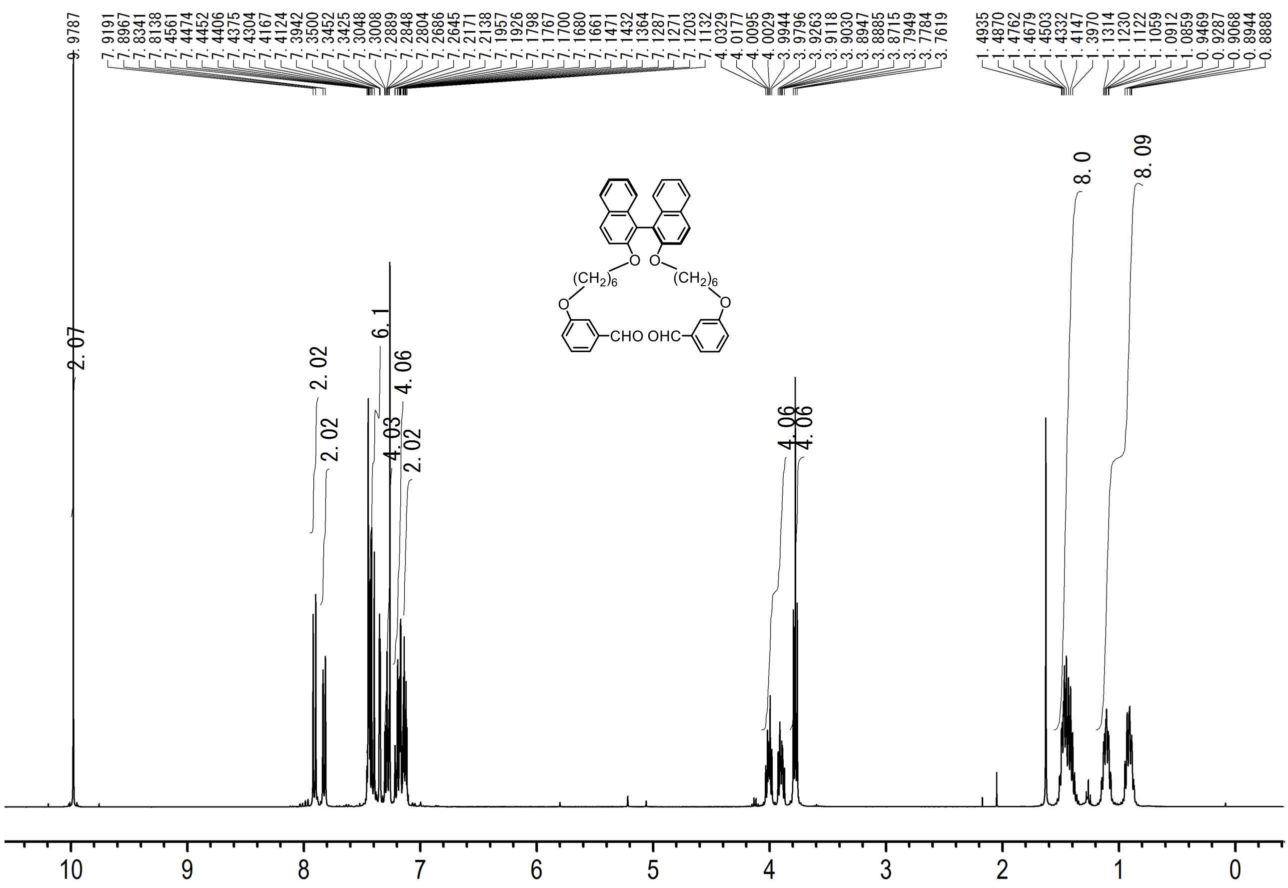
100 MHz ^{13}C NMR spectrum of **4d** in $CDCl_3$



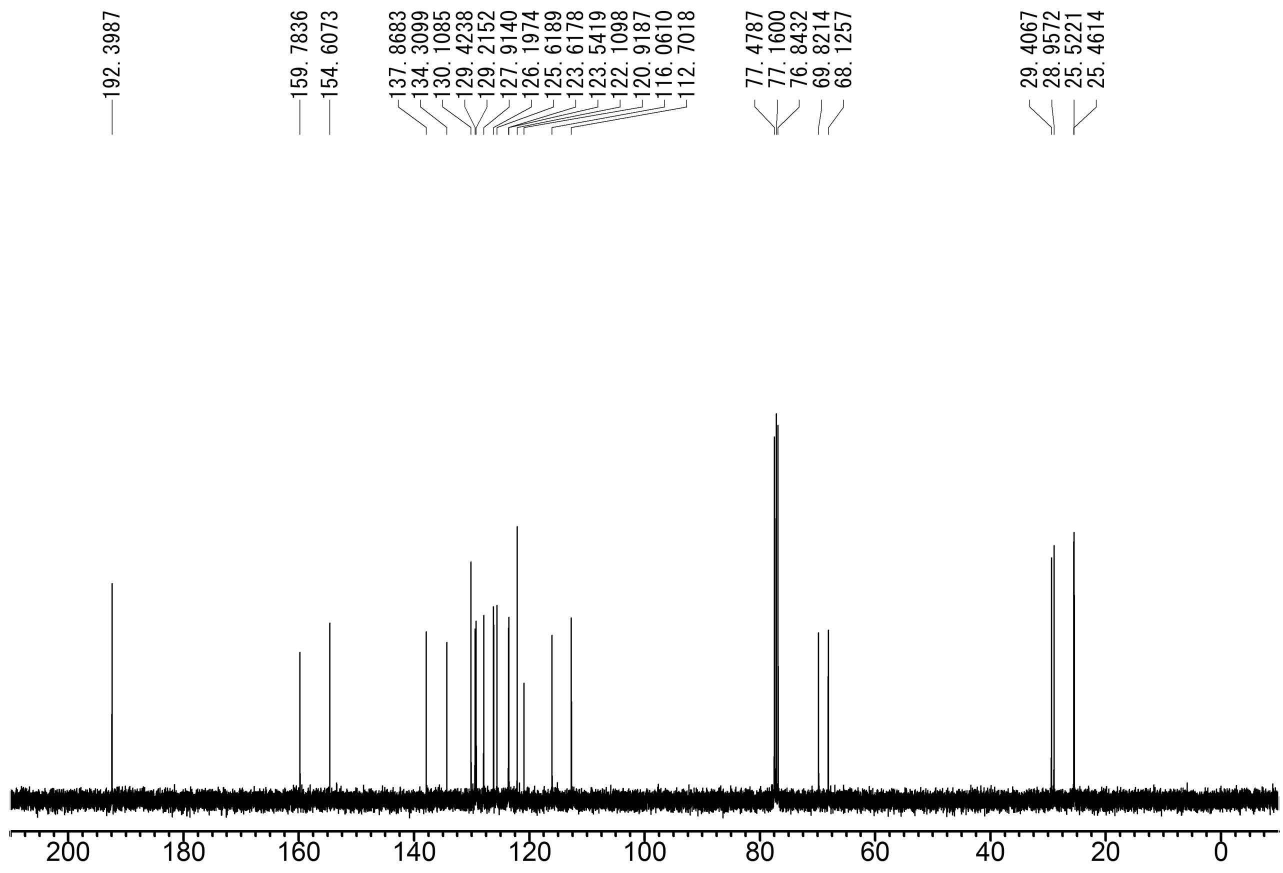
400 MHz ^{1}H NMR spectrum of **5d** in $CDCl_3$



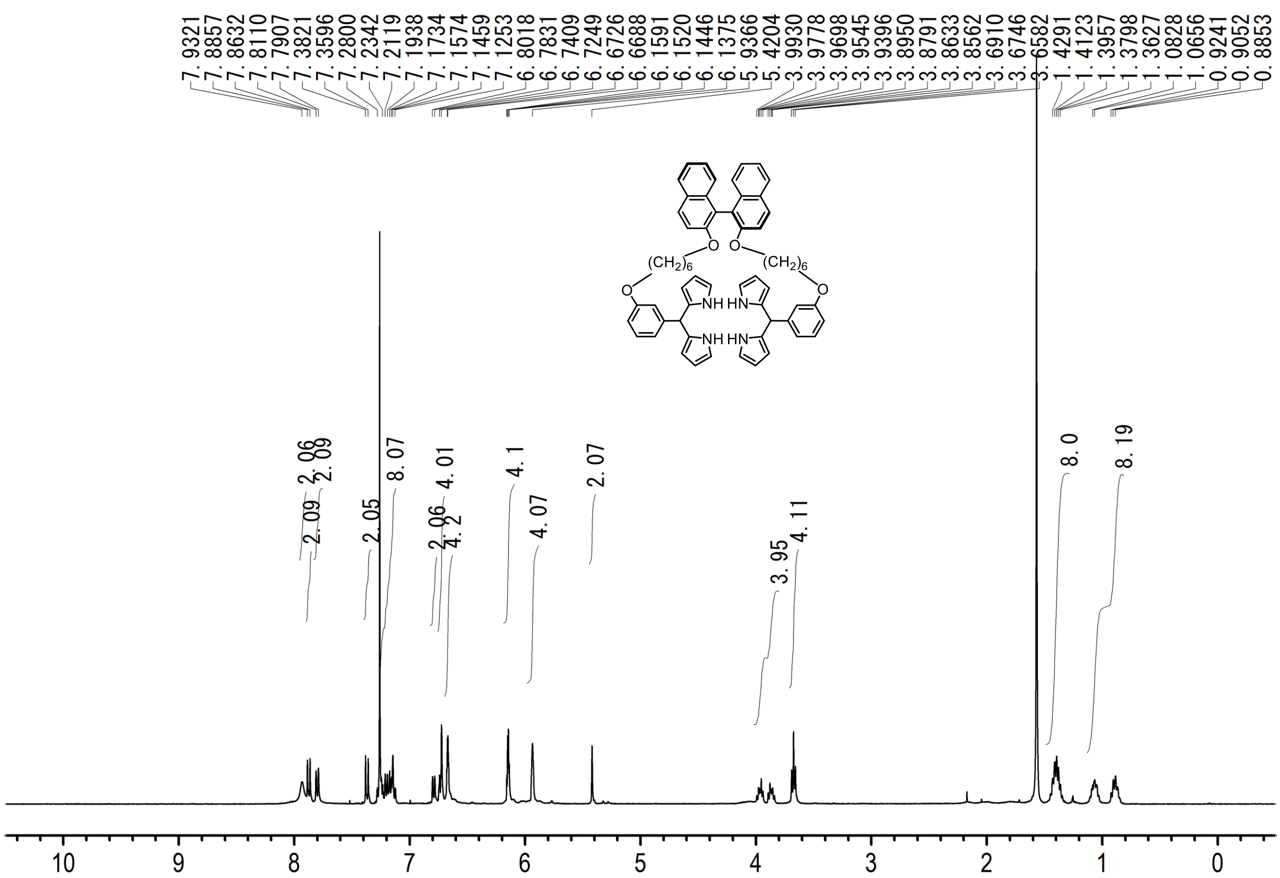
100 MHz ^{13}C NMR spectrum of **5d** in $CDCl_3$



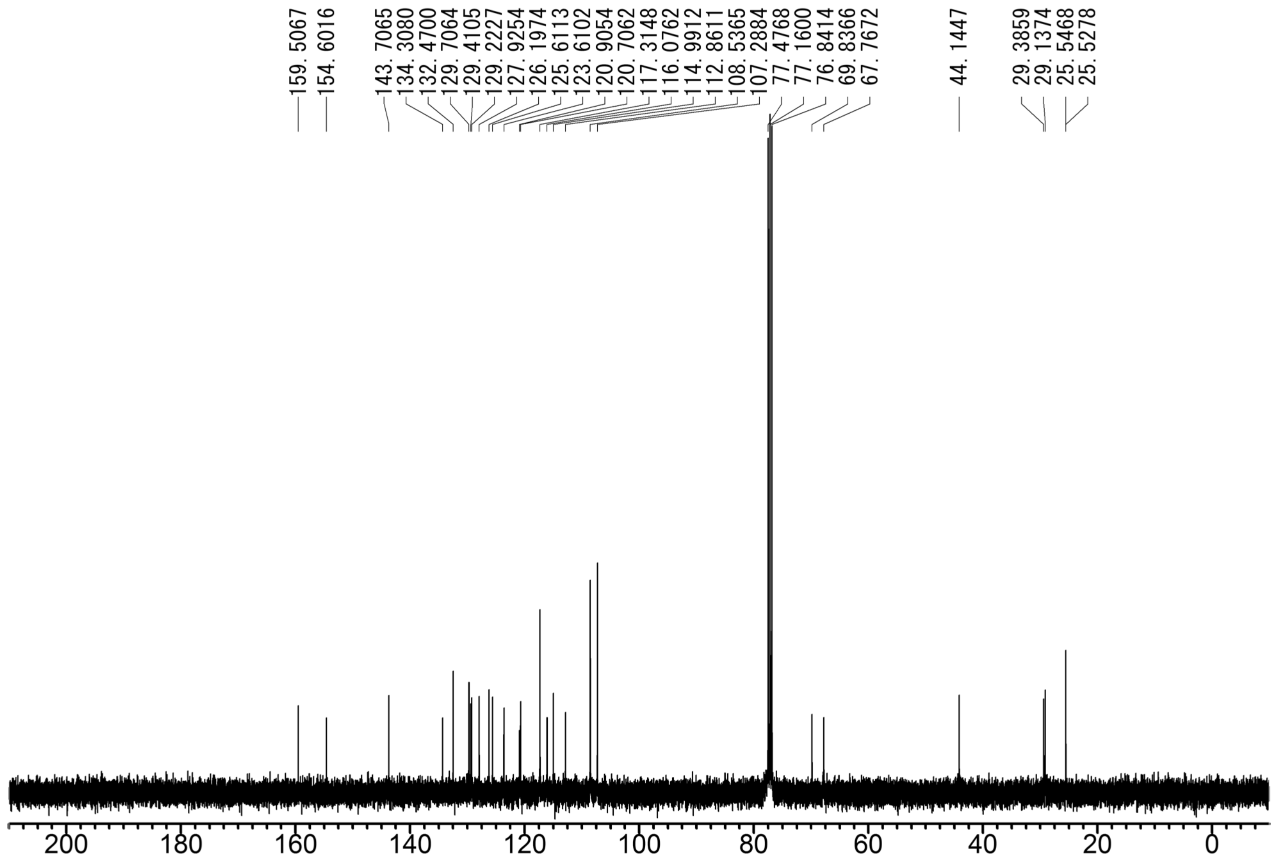
400 MHz ^{1}H NMR spectrum of **6d** in $CDCl_3$



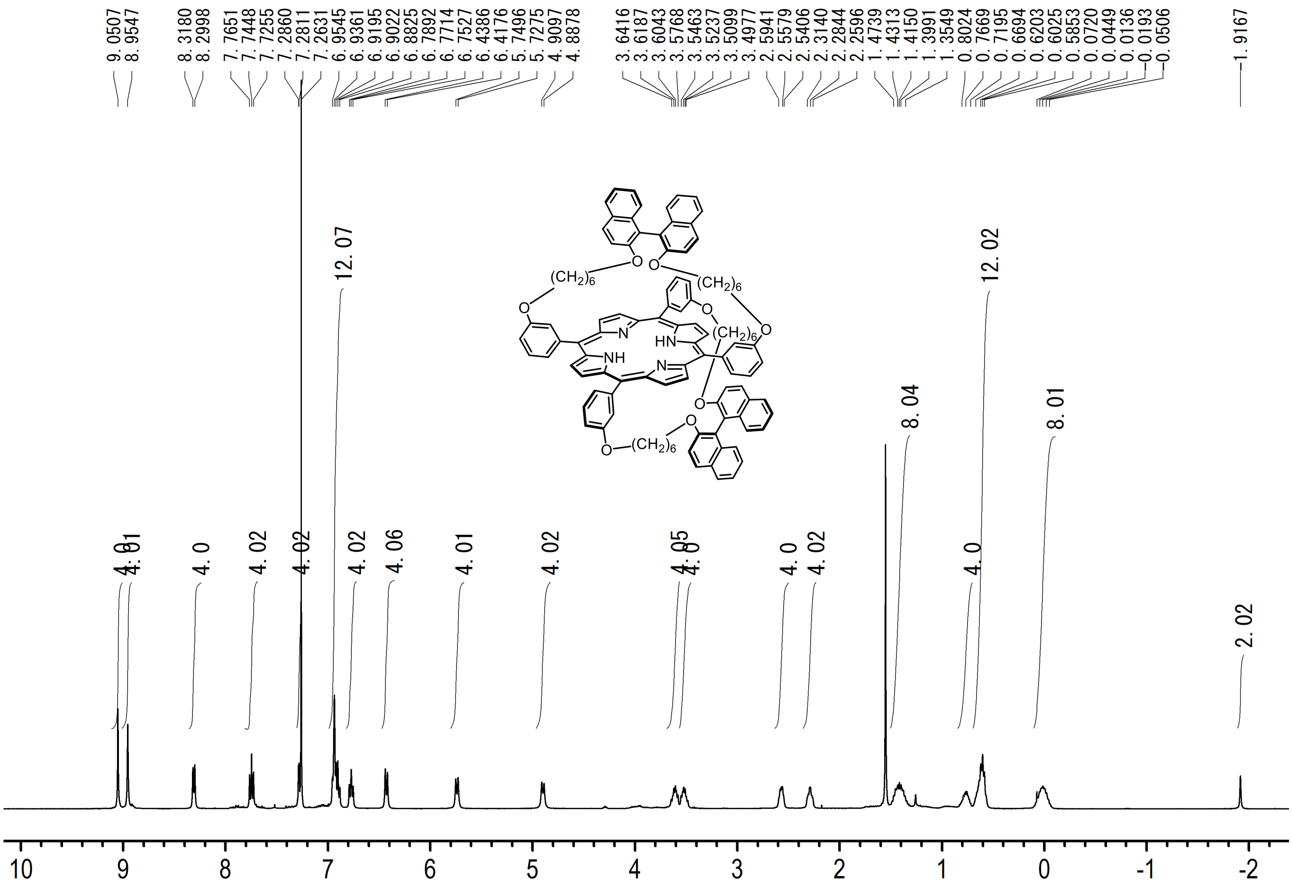
100 MHz ^{13}C NMR spectrum of **6d** in $CDCl_3$



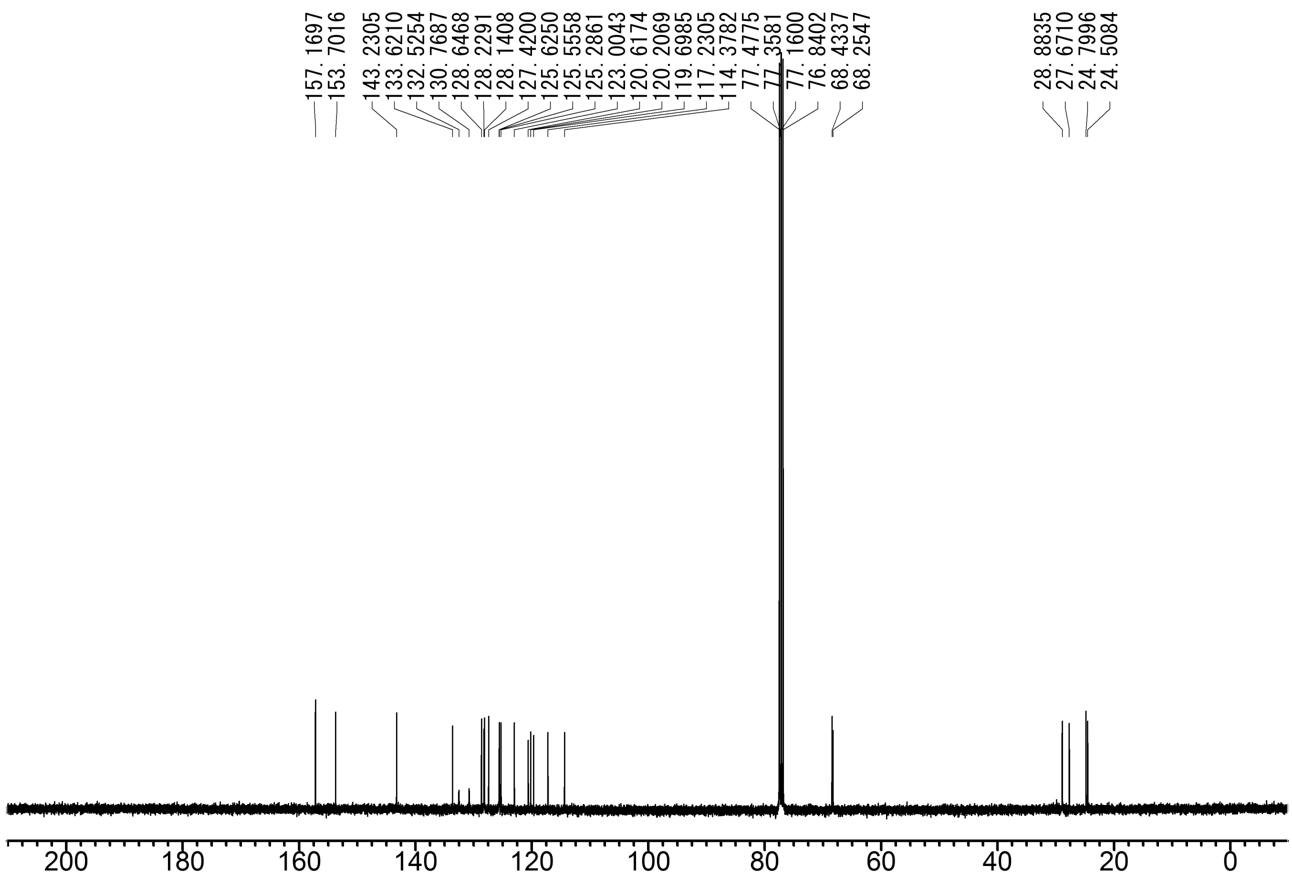
400 MHz ^{1}H NMR spectrum of **7d** in $CDCl_3$



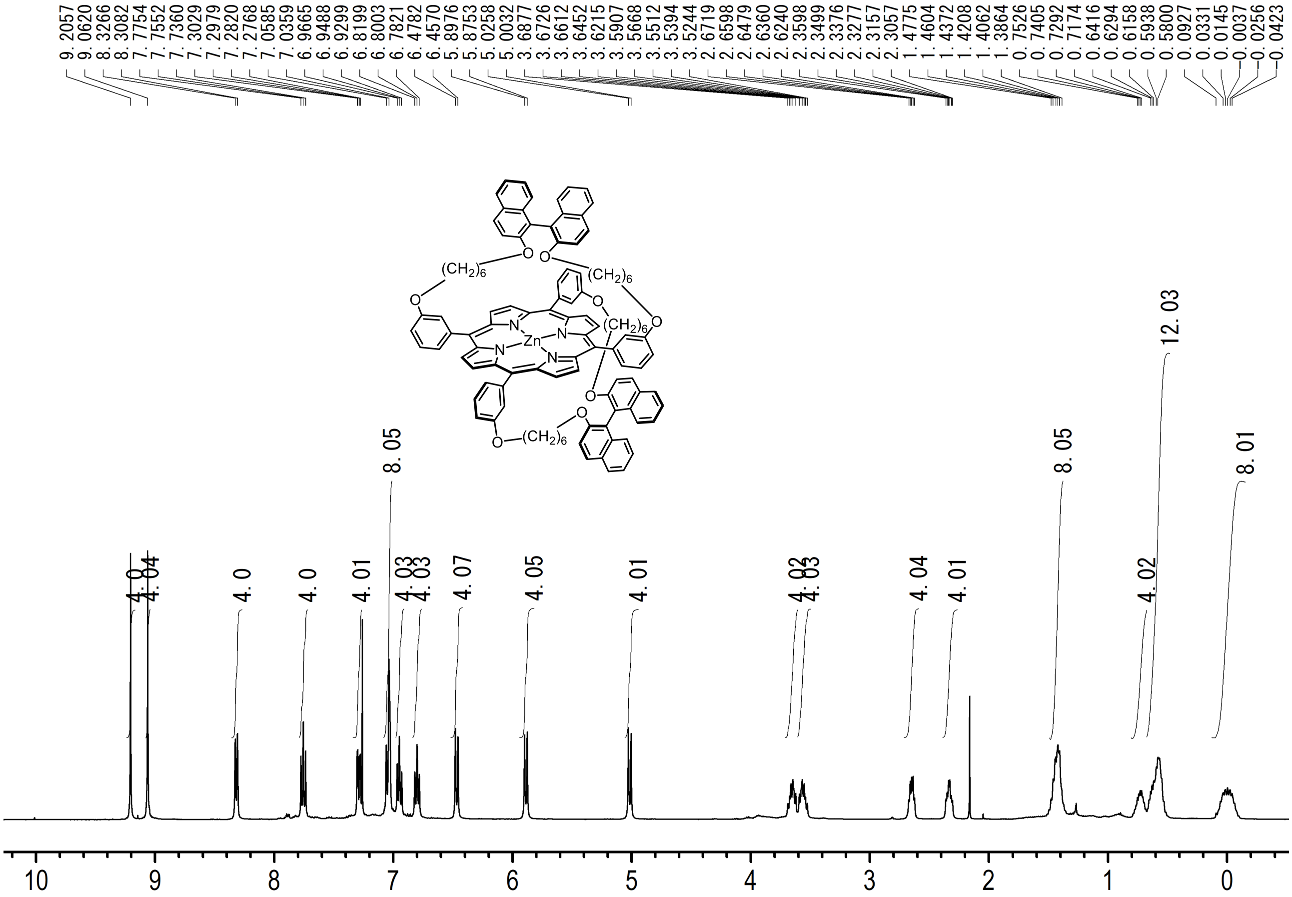
100 MHz ^{13}C NMR spectrum of **7d** in $CDCl_3$



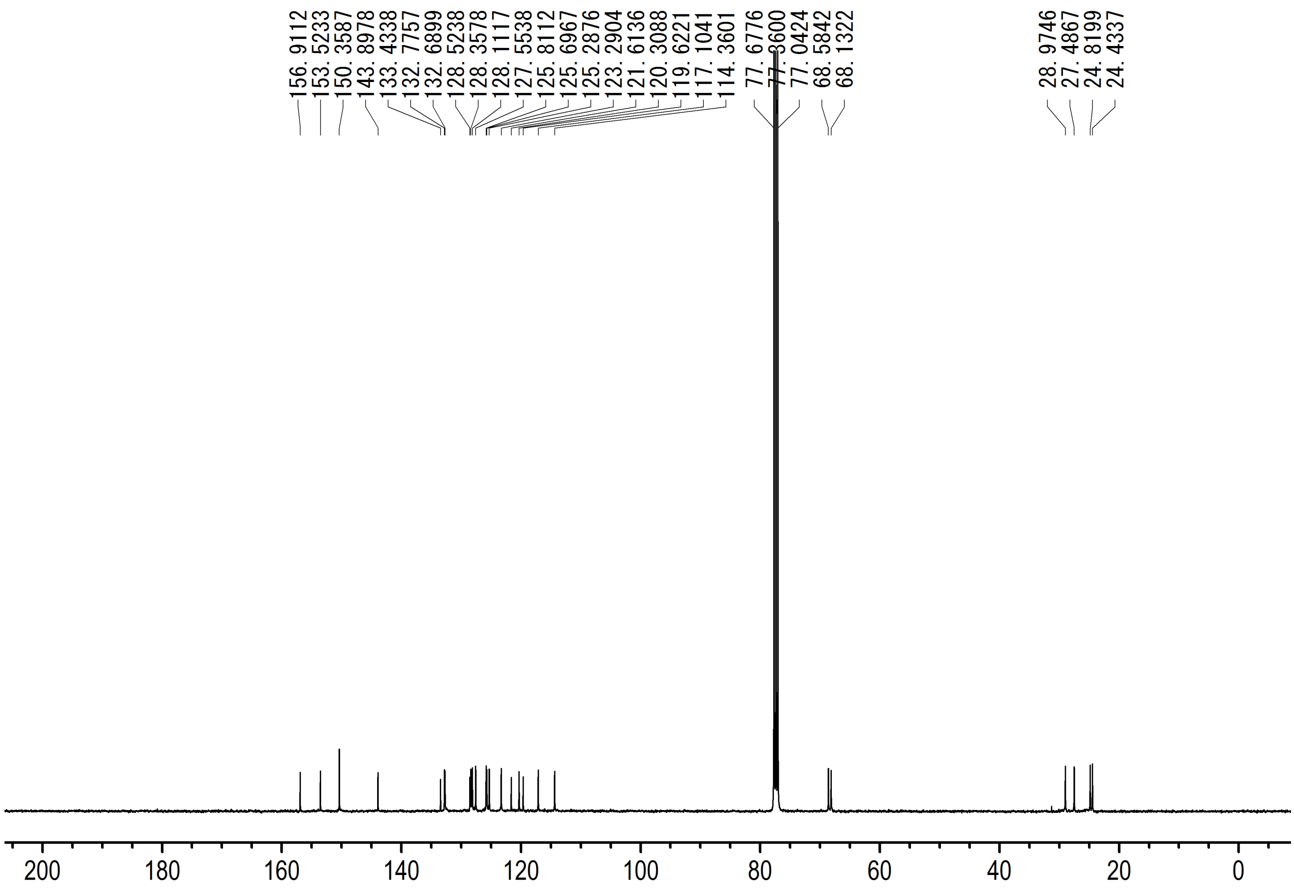
400 MHz ^{1}H NMR spectrum of **1d** in $CDCl_3$



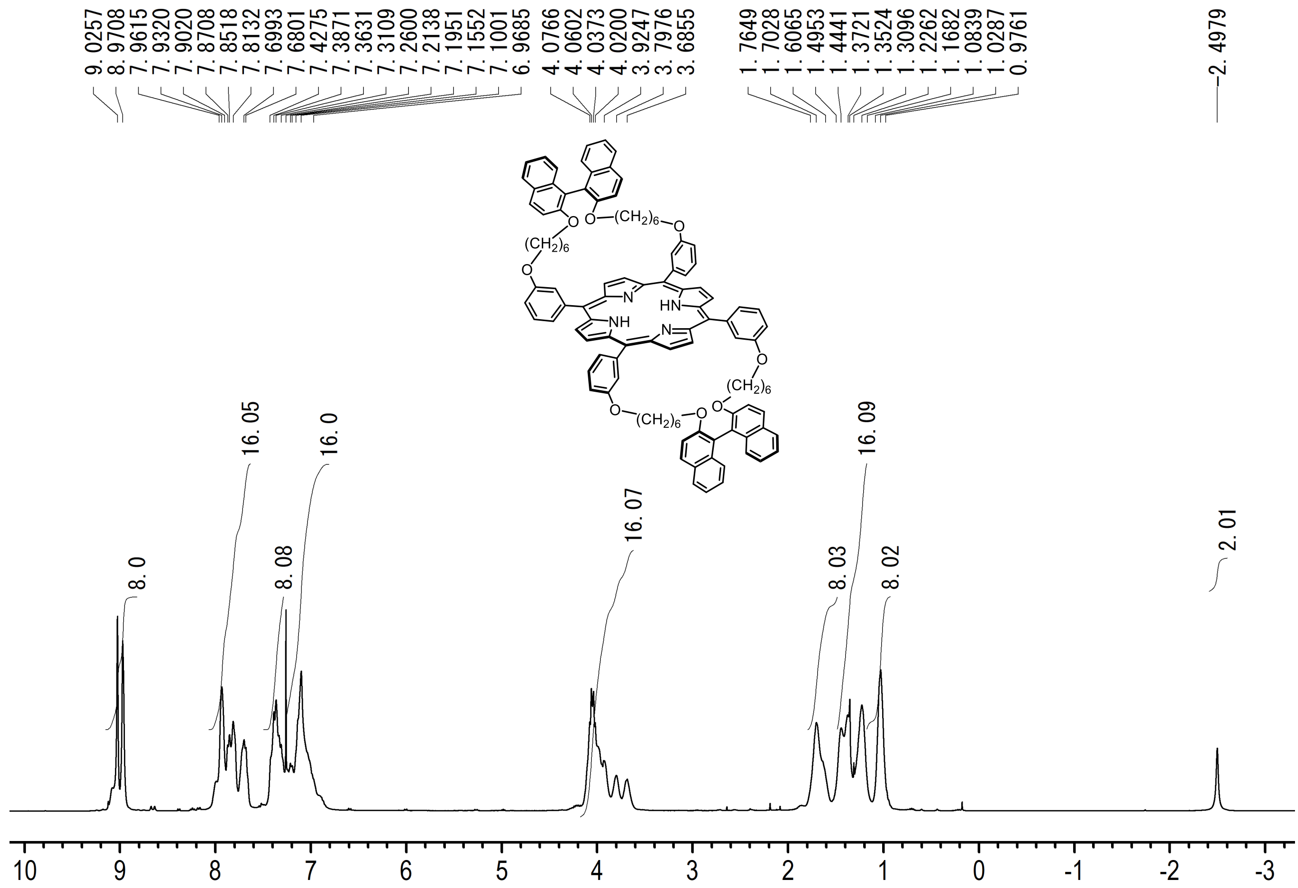
100 MHz ^{13}C NMR spectrum of **1d** in $CDCl_3$



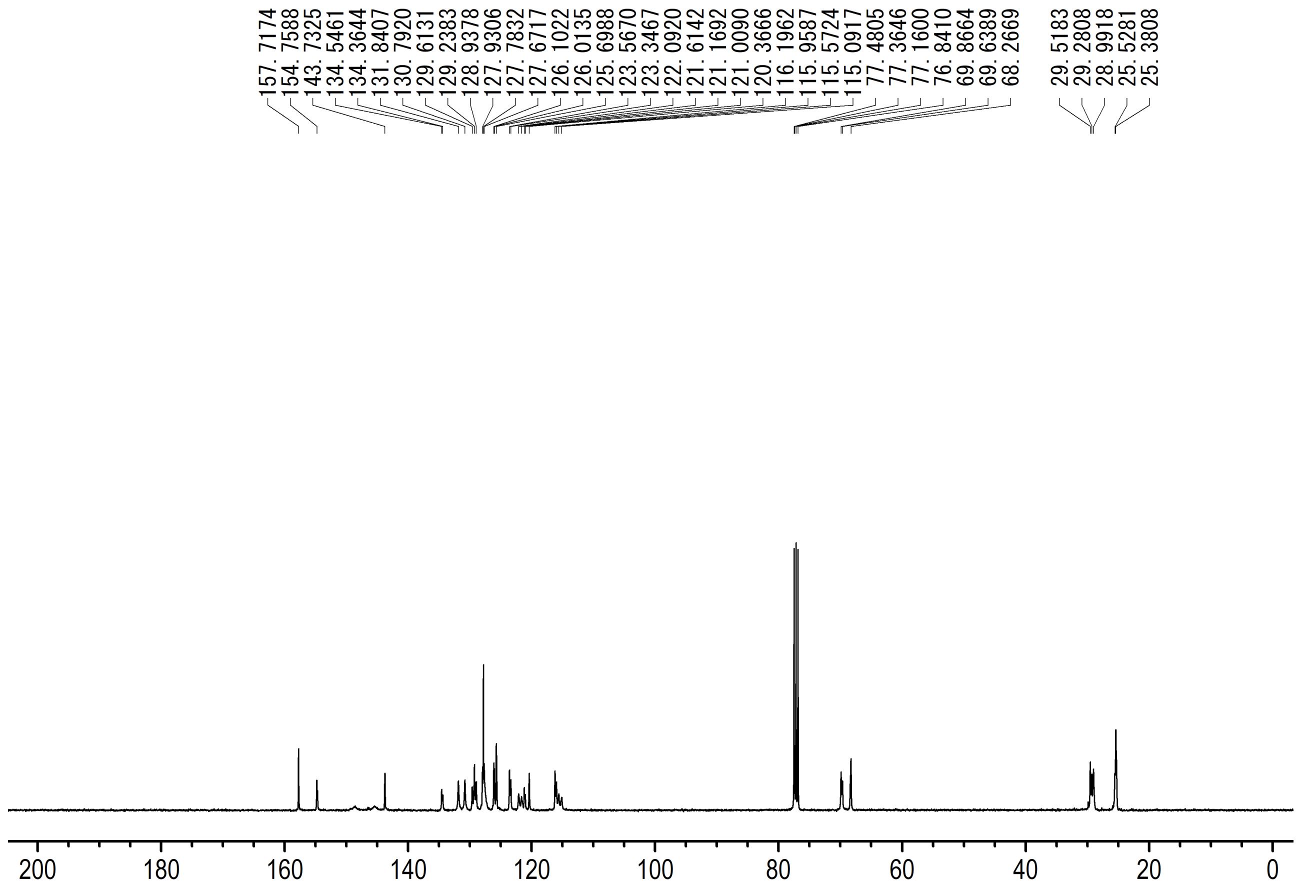
400 MHz ^{1}H NMR spectrum of **2d** in $CDCl_3$



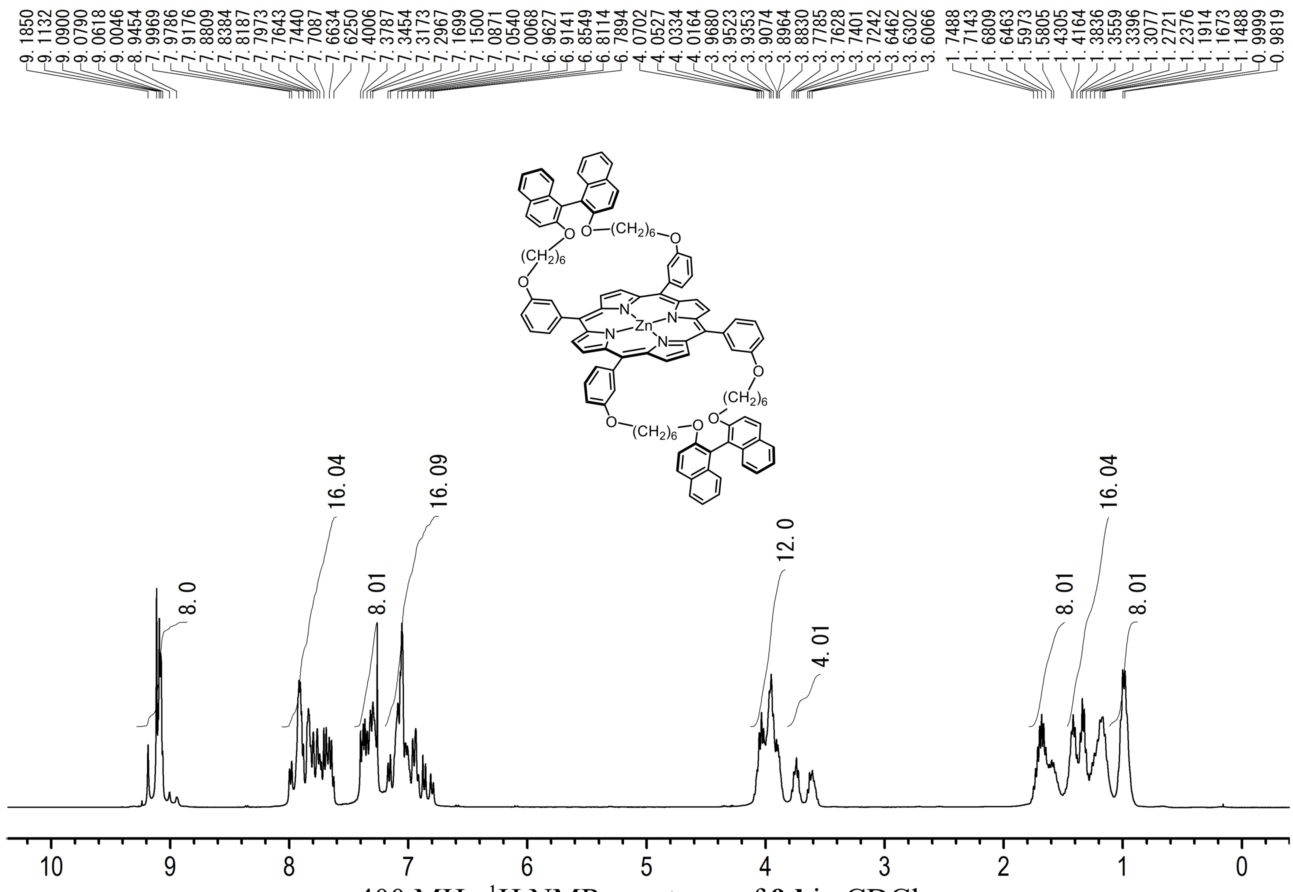
100 MHz ^{13}C NMR spectrum of **2d** in $CDCl_3$



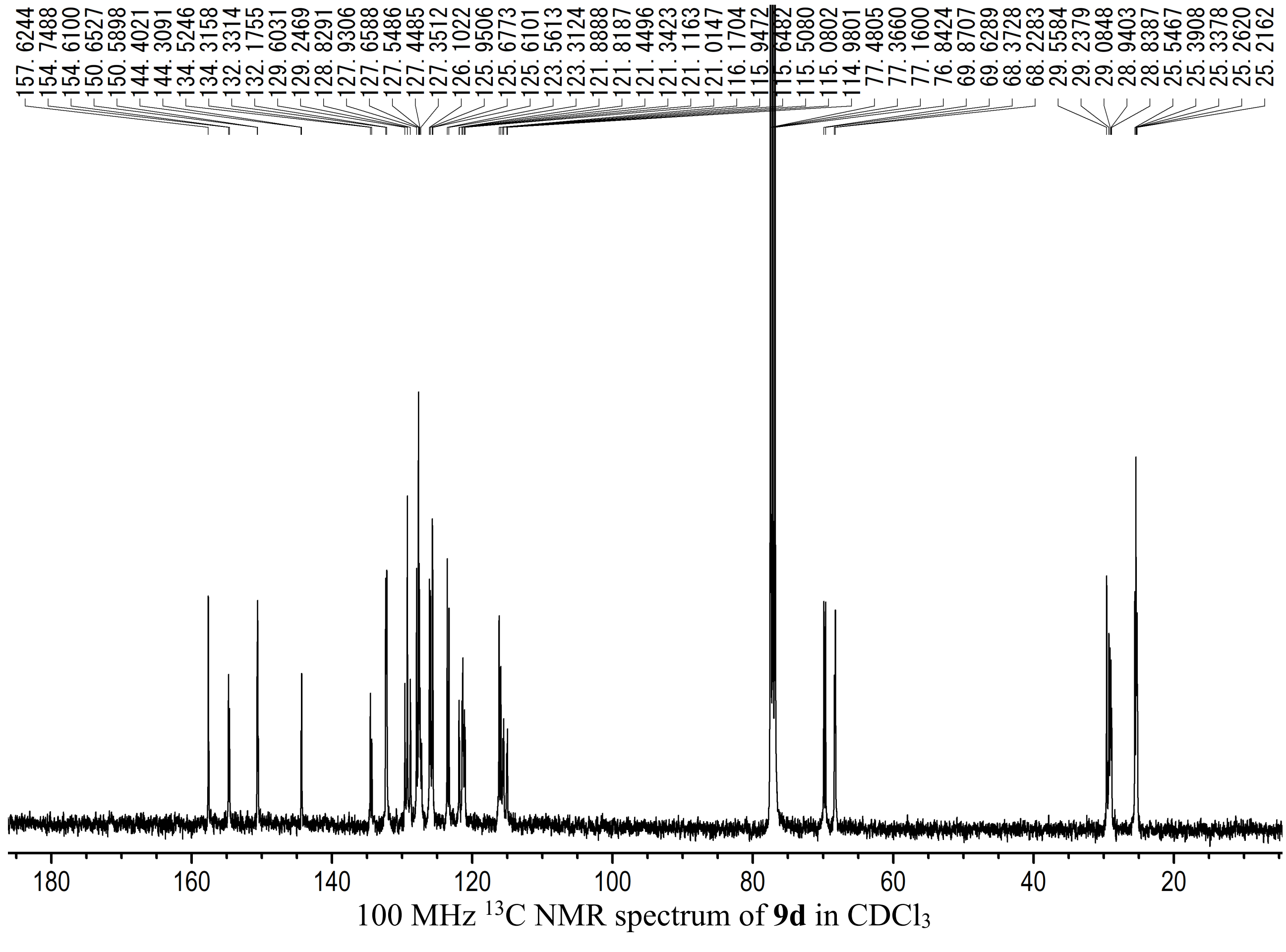
400 MHz ^{1}H NMR spectrum of **8d** in $CDCl_3$



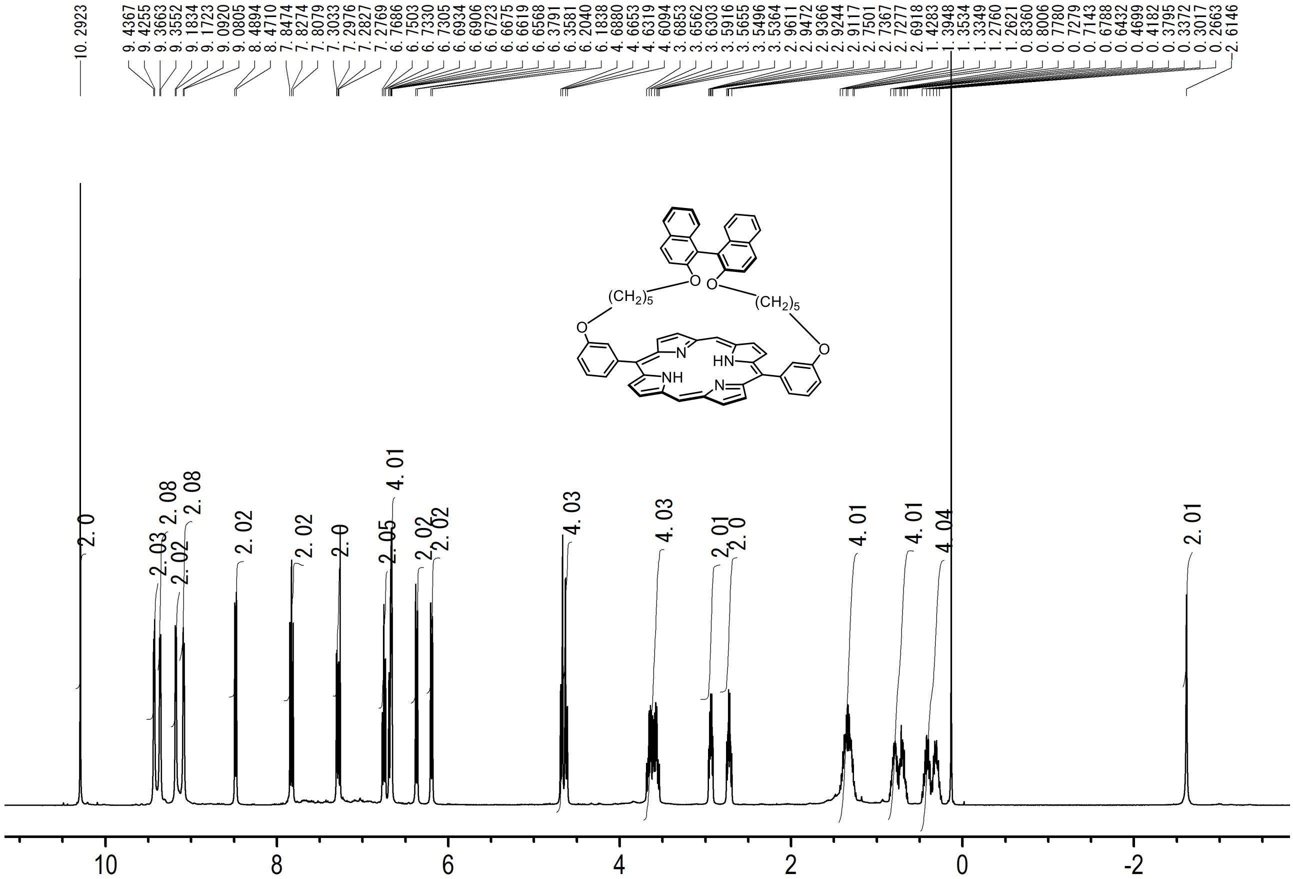
100 MHz ^{13}C NMR spectrum of **8d** in $CDCl_3$



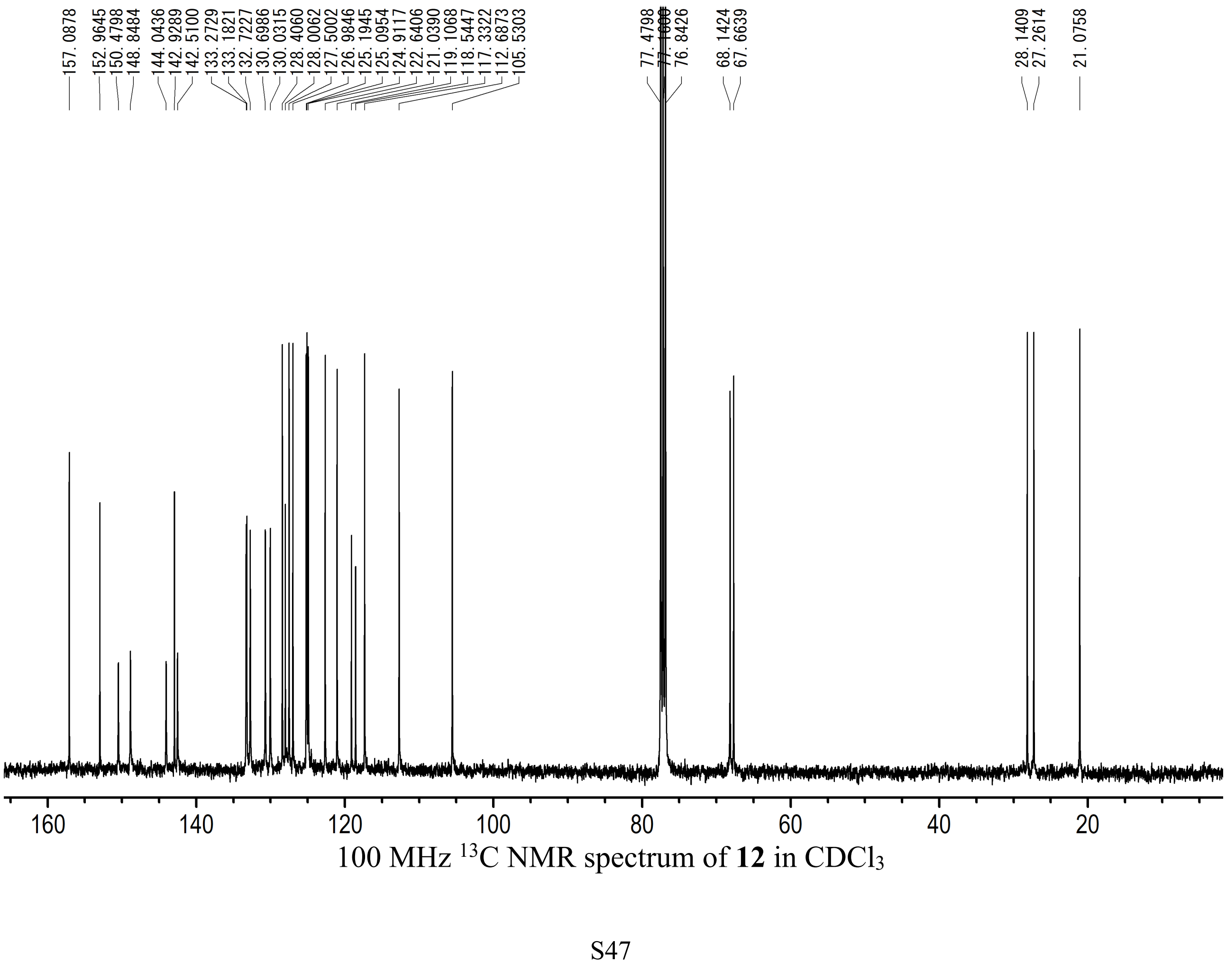
400 MHz ^{1}H NMR spectrum of **9d** in $CDCl_3$



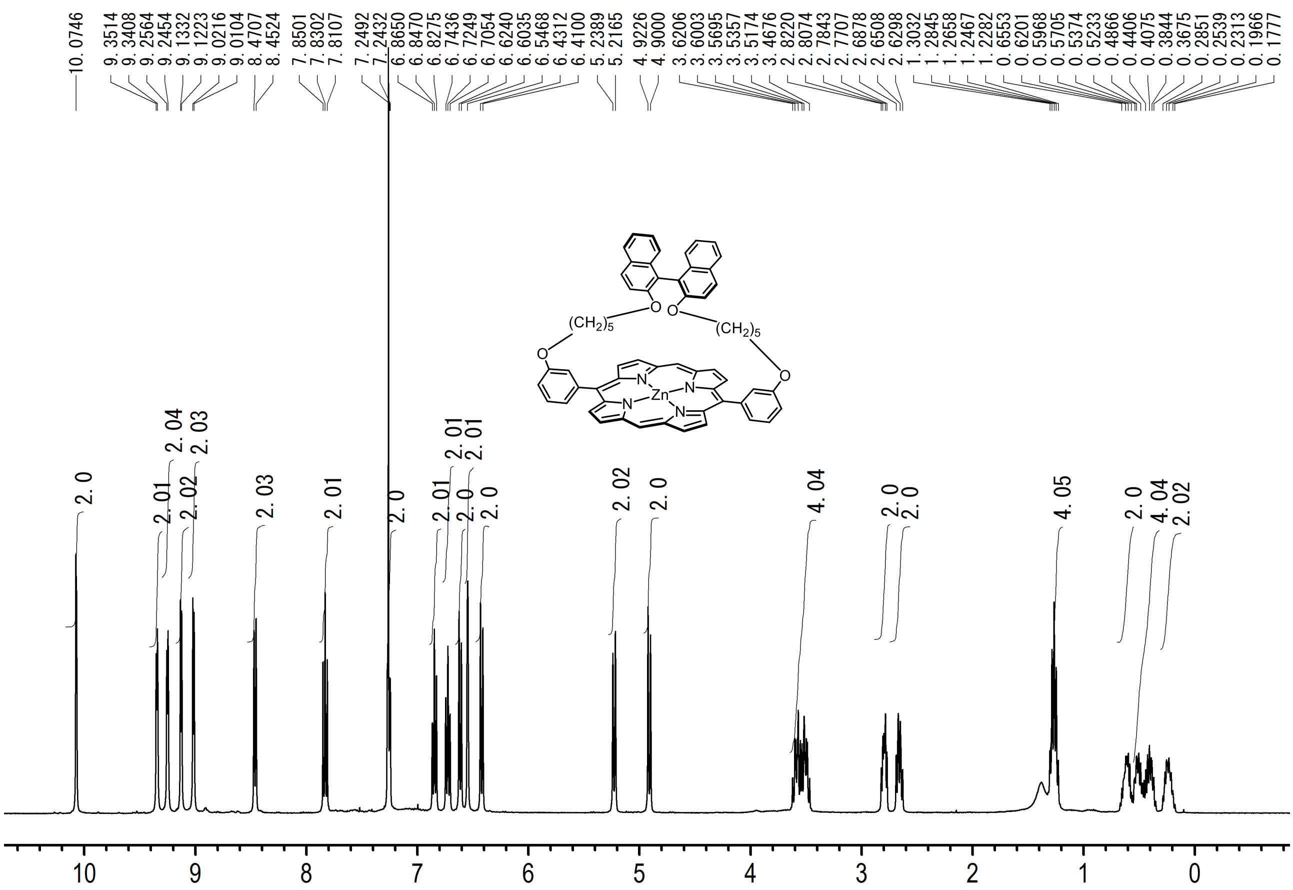
100 MHz ^{13}C NMR spectrum of **9d** in $CDCl_3$



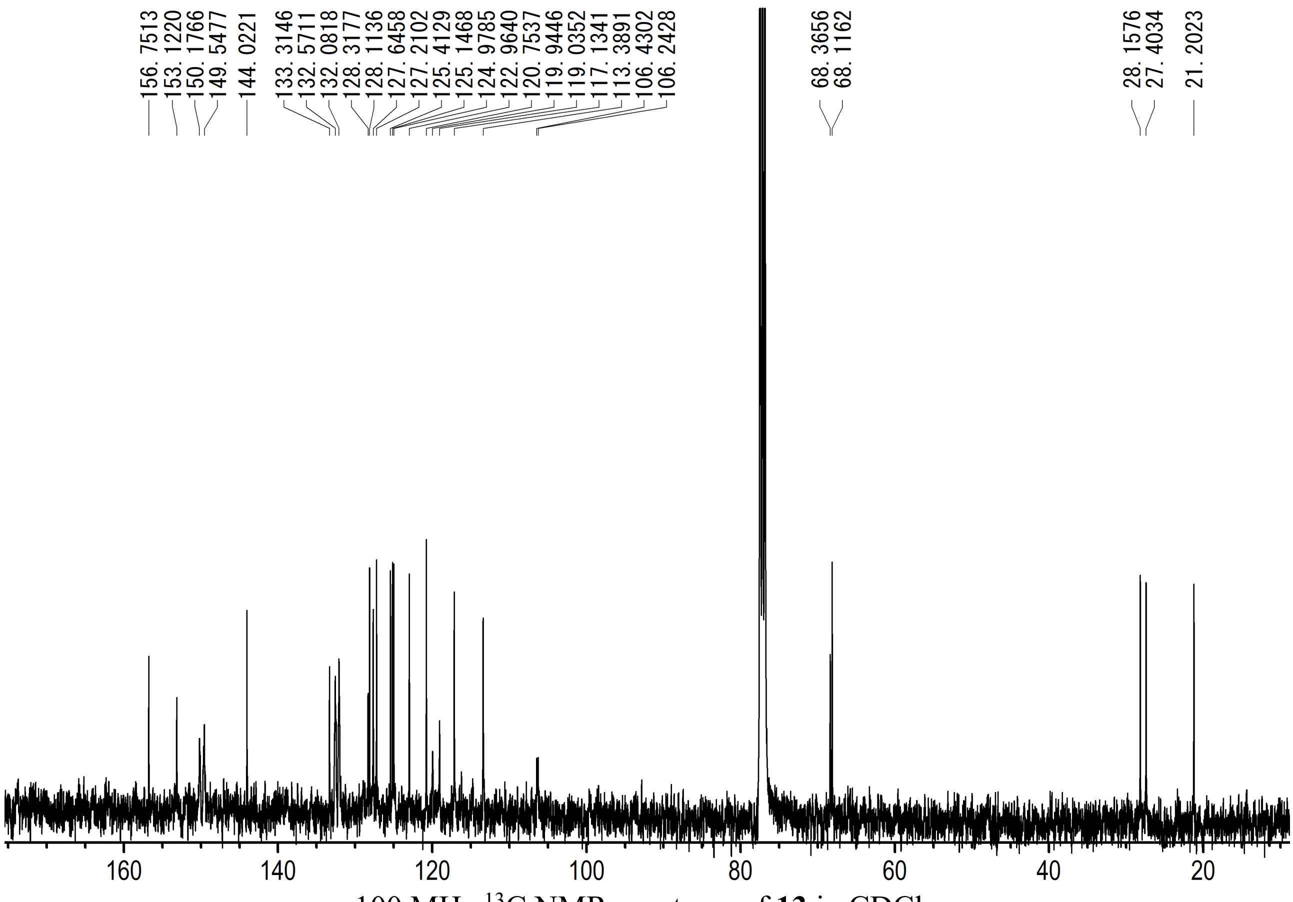
400 MHz ^{1}H NMR spectrum of **12** in $CDCl_3$



100 MHz ^{13}C NMR spectrum of **12** in $CDCl_3$



400 MHz ^{1}H NMR spectrum of **13** in $CDCl_3$



100 MHz ^{13}C NMR spectrum of **13** in $CDCl_3$

[F] Photophysical Properties

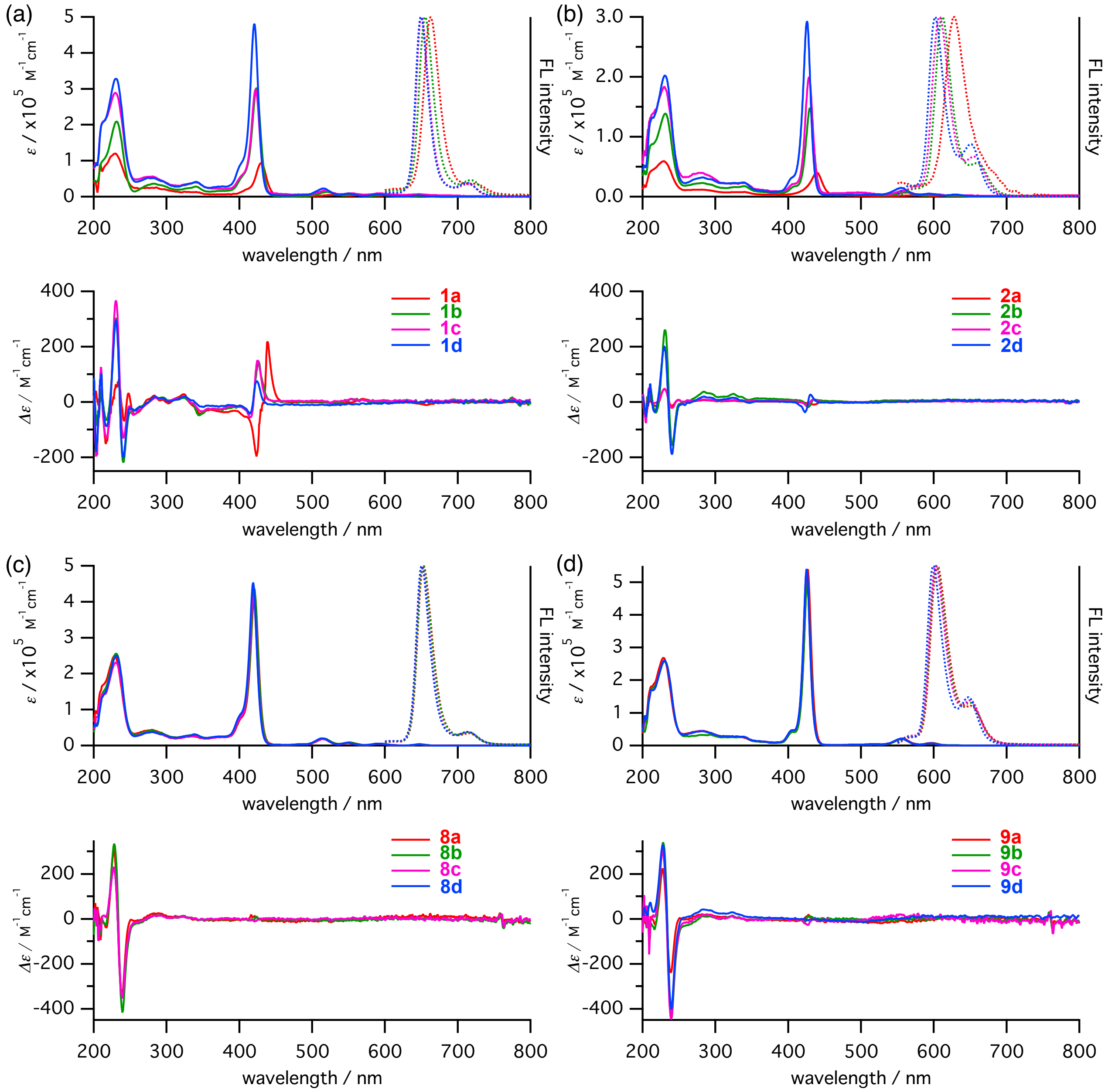


Fig. S1 UV, FL, CD spectra of (a) **1a–d**, (b) **2a–d**, (c) **8a–d**, and (d) **9a–d** in 1,4-dioxane.

[G] DFT calculations

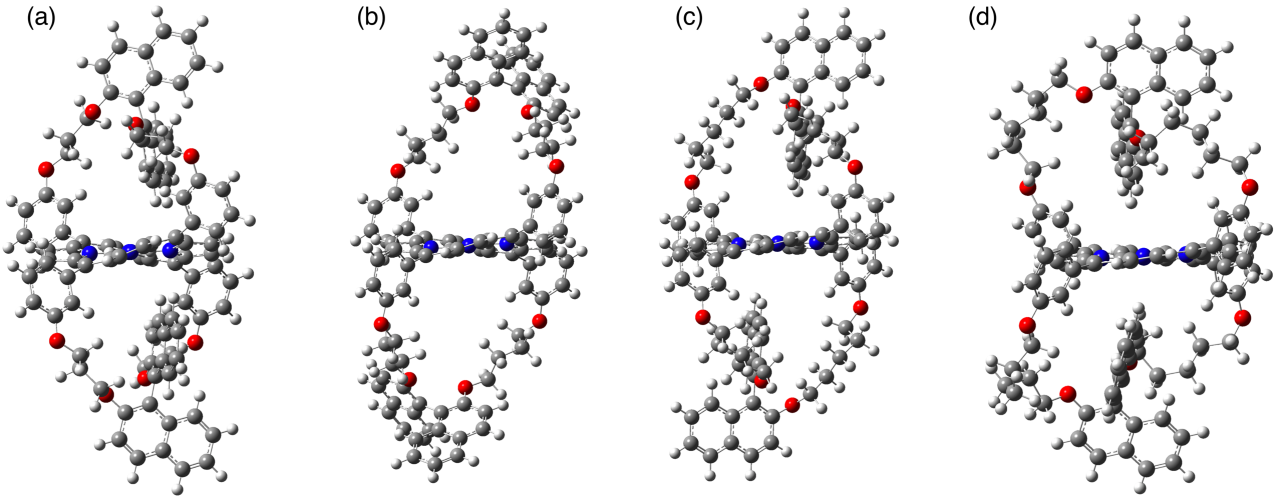


Fig. S2 Optimized structures of (a) **1a**, (b) **1b**, (c) **1c**, and (d) **1d** calculated at the B3LYP/6-31G* level.

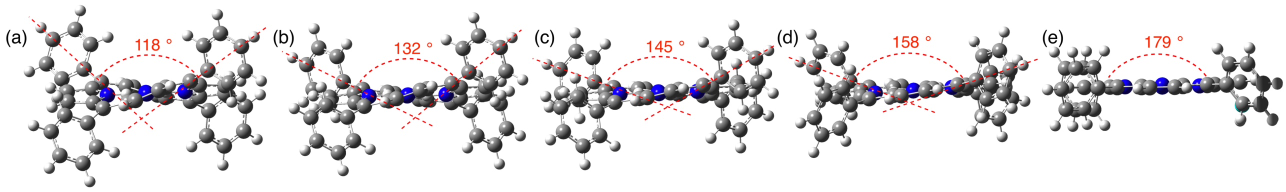


Fig. S3 Structures of TPP based on (a) **1a**, (b) **1b**, (c) **1c**, (d) **1d**, and (e) optimized structure. Dihedral angles between the trans-phenyl rings are shown.

Table S2 MPD and strain energy in **1a**–**d**.[a]

	MPD (Å)	Total energy (a.u.)	Strain energy (a.u.)	Strain energy (kcal/mol)
TPP	0.039	–1913.75073235	0	0
1a	0.301	–1913.73081422	0.01991813	12.5
1b	0.241	–1913.73786911	0.01286324	8.1
1c	0.170	–1913.74258572	0.00814663	5.1
1d	0.119	–1913.74487267	0.00585968	3.7

[a] The total energy was calculated for the optimized structure of TPP and the TPP moieties of **1a**–**d**, and the strain energy was calculated by comparing the energy of the TPP moieties of **1a**–**d** with that of the optimized structure of TPP.

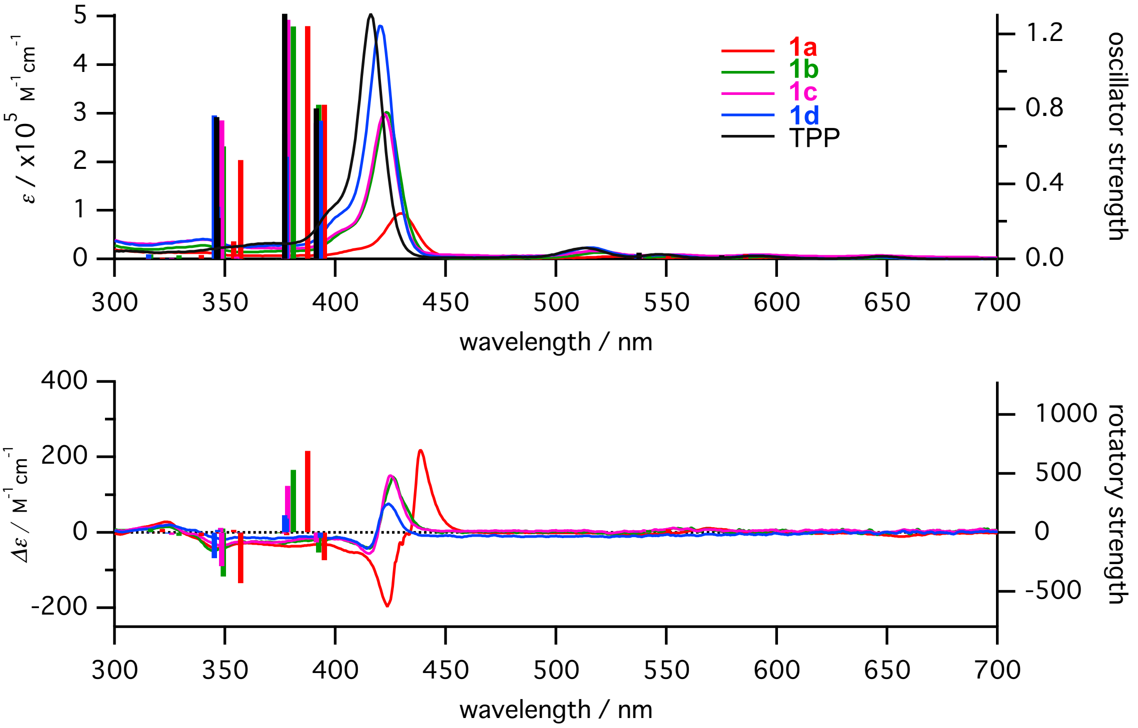


Fig. S4 UV/vis absorption (top) and CD (bottom) spectra of **1a–d** in 1,4-dioxane. Calculated oscillator strengths and rotatory strengths of TPP based on **1a–d** and the optimized structure are inserted.

Table S3 Oscillator strengths (*f*) and rotatory strengths (*R*) of TPP based on **1a–d** and the optimized structure calculated at the B3LYP/6-31G(d) level.

1a			**1b**			**1c**			**1d**			TPP		
λ (nm)	*f*	*R*	λ (nm)	*f*	*R*	λ (nm)	*f*	*R*	λ (nm)	*f*	*R*	λ (nm)	*f*	*R*
586	0.0267	–5.5295	578	0.016	–3.2815	575	0.0192	0.9238	575	0.0127	–2.2218	575	0.0188	–1.7424
551	0.0277	28.8398	542	0.024	18.5276	538	0.0209	15.6371	537	0.0257	6.4939	538	0.0344	–3.4737
395	0.8225	–235.793	392	0.823	–170.406	391	0.7252	–84.7388	393	0.7384	–46.6777	391	0.8026	6.4071
387	1.2422	692.325	381	1.2414	531.094	378	1.2769	394.461	378	0.5463	119.614	377	1.3082	1.4768
378	0.0024	–23.1235	374	0.0003	–6.5145	377	0.0096	–9.4321	377	0.6668	147.908	375	0.0001	1.8253
358	0.0022	–2.1332	355	0	0.0416	355	0.0116	2.7777	356	0.0005	0.1162	355	0.0004	0.0605
357	0.5281	–430.449	349	0.6007	–373.973	348	0.7395	–285.037	347	0.2783	21.1971	347	0.2183	–9.9921
354	0.0941	22.3395	349	0.1543	34.2321	348	0.1714	39.8536	345	0.7652	–217.452	346	0.758	–5.8096

The oscillator strengths slightly decrease and the rotatory strengths increase with increasing distortion.

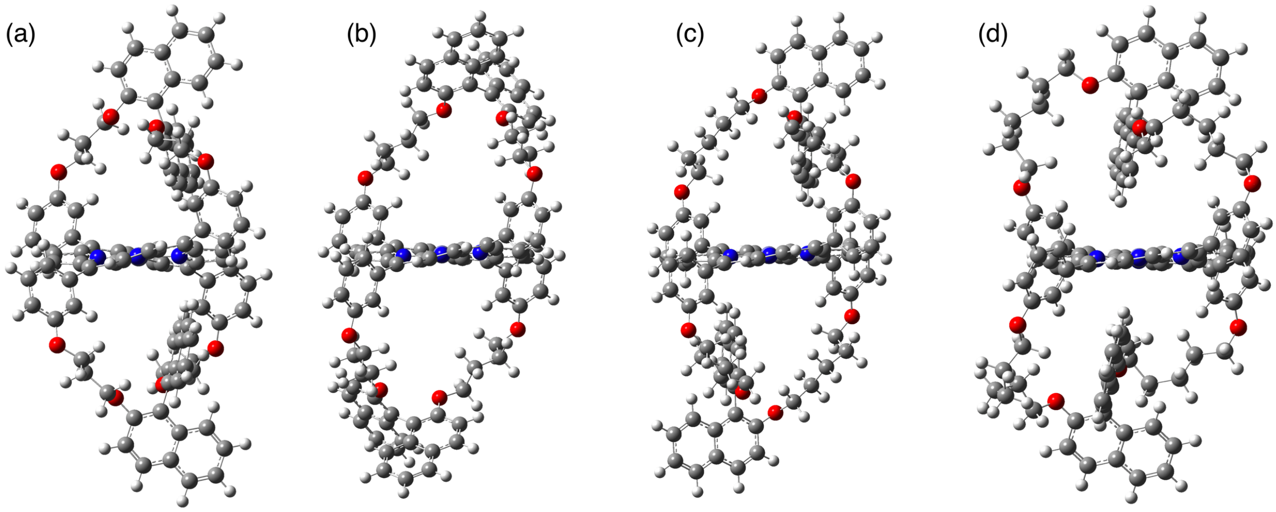


Fig. S5 Optimized structures of (a) **2a**, (b) **2b**, (c) **2c**, and (d) **2d** calculated at the B3LYP/6-31G* level.

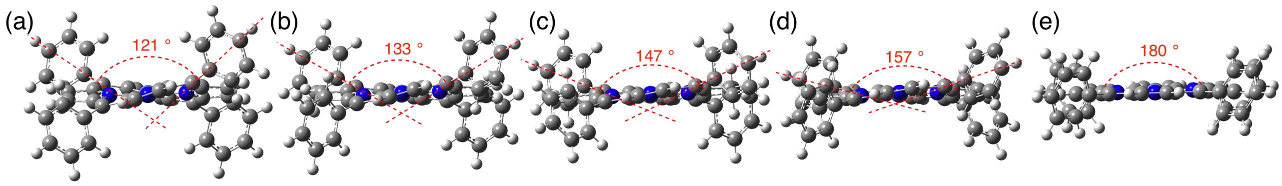


Fig. S6 Structures of ZnTPP based on (a) **2a**, (b) **2b**, (c) **2c**, (d) **2d**, and (e) optimized structure. Dihedral angles between the trans-phenyl rings are shown.

Table S4 MPD and strain energy in **2a–d**.[a]

	MPD (Å)	Total energy (a.u.)	Strain energy (a.u.)[a]	Strain energy (kcal/mol)
ZnTPP	0.032	–3691.78565550	0	0
2a	0.243	–3691.76595291	0.01970259	12.4
2b	0.206	–3691.77272566	0.01292984	8.1
2c	0.141	–3691.77788263	0.00777287	4.9
2d	0.128	–3691.77975724	0.00589826	3.7

[a] The total energy was calculated for the optimized structure of ZnTPP and the ZnTPP moieties of **2a–d**, and the strain energy was calculated by comparing the energy of the ZnTPP moieties of **2a–d** with that of the optimized structure of ZnTPP

Optimized structure of 1a

H	3.54313	-1.7486	-0.61416
C	4.24479	-0.9315	-0.73151
H	2.69234	0.49004	-1.07845
C	3.7634	0.3283	-1.00188
C	6.53594	-0.08907	-0.68039
C	4.64145	1.42473	-1.18177
C	5.63861	-1.14961	-0.5847
C	6.05113	1.20822	-1.03049
C	4.16202	2.72315	-1.50499
H	7.99462	2.1615	-1.16817
C	5.03236	3.77128	-1.6968
H	3.08931	2.87137	-1.59779
H	4.65486	4.75918	-1.94602
C	6.42735	3.55767	-1.57609
H	7.11422	4.38265	-1.74793
C	6.92316	2.31513	-1.24843
C	8.4223	-0.04744	0.93861
C	7.97886	-0.30497	-0.35064
C	10.68878	-0.6894	0.38169
C	8.91785	-0.77803	-1.32346
C	9.77772	-0.23896	1.3052
C	10.29033	-0.96879	-0.9523
C	8.53718	-1.06314	-2.66382
H	10.068	-0.0429	2.33342
H	12.25124	-1.57799	-1.63079
H	11.72752	-0.84357	0.66449
C	9.4583	-1.5123	-3.58383
H	7.50167	-0.91641	-2.95429
H	9.14517	-1.72245	-4.60321
C	10.81124	-1.7031	-3.21394
H	11.5281	-2.05921	-3.94892
C	11.21384	-1.43583	-1.92545
O	6.18804	-2.37634	-0.32016
C	7.52723	1.75484	2.20615
C	6.46252	2.03018	3.26745
H	6.81758	1.7239	4.2577
H	5.58047	1.42459	3.03572
C	6.11249	3.52289	3.29358

H	5.55096	3.81097	2.39547
H	7.0306	4.12053	3.31444
O	5.40851	3.93114	4.46983
C	4.04865	3.83005	4.54056
C	1.27042	3.70475	4.91755
C	3.24607	3.13279	3.63171
C	3.4545	4.47498	5.63653
C	2.07718	4.41425	5.81287
C	1.85536	3.0518	3.82656
H	3.6816	2.61106	2.78782
H	4.09259	5.01546	6.32856
H	1.62407	4.9261	6.65786
H	0.19517	3.6613	5.0609
N	-0.43809	-1.88287	0.47832
N	0.40446	1.92284	0.50711
C	0.22663	2.80929	-0.51655
C	0.89803	2.65697	1.5499
C	0.54754	0.98756	3.35964
C	-0.54407	-0.99627	3.34681
C	-0.91986	-2.63372	1.51348
C	-0.27315	-2.75024	-0.56242
C	0.08552	-1.0836	-2.37717
C	-0.13943	1.17385	-2.35877
C	-0.13428	0.73638	-3.72364
C	-0.13641	2.48622	-1.84517
C	0.60437	4.15686	-0.10564
C	1.07166	2.202	2.87566
C	0.06482	-0.62336	-3.73471
C	0.08288	-2.40507	-1.88788
C	-0.65019	-4.10517	-0.17207
C	0.36767	0.5694	4.72041
C	-1.0751	-2.20211	2.84976
C	-1.09844	-4.02239	1.10548
C	1.06854	4.05208	1.16456
C	-0.34222	-0.60516	4.71293
H	0.7116	1.11861	5.58349
H	1.45392	4.8359	1.8022
H	-0.60826	-4.97752	-0.80994
H	0.55358	5.04017	-0.72772
H	-0.67224	-1.17398	5.5688

H	0.15227	-1.26202	-4.60067
H	-1.47755	-4.81713	1.73323
H	-0.23208	1.38717	-4.57928
C	0.57223	-3.49881	-2.78328
C	1.77371	-5.45876	-4.39658
C	-0.04511	-3.90069	-3.97229
C	1.77903	-4.10636	-2.39518
C	2.3918	-5.07114	-3.19793
C	0.56308	-4.88114	-4.76567
H	-0.99253	-3.46231	-4.27004
H	2.23307	-3.78092	-1.4685
H	0.08244	-5.19943	-5.68697
H	2.254	-6.21242	-5.0126
O	3.57645	-5.68531	-2.89903
C	4.23419	-5.36272	-1.66936
H	3.50495	-5.37146	-0.84764
H	4.92235	-6.19577	-1.50049
C	5.00119	-4.03299	-1.72115
H	4.38812	-3.2734	-2.21526
H	5.9087	-4.15038	-2.32315
C	5.38338	-3.55291	-0.3144
O	7.52649	0.35203	1.91366
H	7.30944	2.31723	1.28863
H	8.52077	2.06838	2.56089
H	4.49063	-3.40881	0.31006
H	6.00984	-4.2981	0.18613
H	-3.5505	1.79126	-0.53126
C	-4.23294	0.96015	-0.66201
H	-2.64546	-0.4277	-0.98474
C	-3.72076	-0.28872	-0.92625
C	-6.50645	0.06985	-0.6509
C	-4.57233	-1.40296	-1.12275
C	-5.6332	1.1485	-0.5369
C	-5.9888	-1.21612	-0.99626
C	-4.05992	-2.69069	-1.43825
H	-7.90902	-2.20983	-1.16986
C	-4.90458	-3.75636	-1.64745
H	-2.9826	-2.81653	-1.51001
H	-4.5022	-4.73588	-1.89075
C	-6.30572	-3.57191	-1.55216

H	-6.97195	-4.4108	-1.73738
C	-6.83334	-2.34068	-1.23145
C	-8.4198	-0.02149	0.93419
C	-7.95875	0.25584	-0.34467
C	-10.68707	0.58673	0.34409
C	-8.88898	0.72172	-1.32939
C	-9.78447	0.14297	1.27905
C	-10.27066	0.88562	-0.98019
C	-8.49042	1.02622	-2.66025
H	-10.08908	-0.06857	2.30003
H	-12.22981	1.46818	-1.6866
H	-11.73308	0.72008	0.61019
C	-9.40323	1.46873	-3.5917
H	-7.44784	0.8997	-2.93443
H	-9.07636	1.69407	-4.6035
C	-10.76534	1.63304	-3.24342
H	-11.47552	1.98415	-3.98724
C	-11.18526	1.34644	-1.96466
O	-6.21297	2.36218	-0.2765
C	-7.52027	-1.82341	2.19742
C	-6.46527	-2.09751	3.26833
H	-6.83485	-1.80639	4.25786
H	-5.58795	-1.47911	3.05299
C	-6.0977	-3.58609	3.28061
H	-5.53633	-3.85997	2.37797
H	-7.00861	-4.19469	3.29959
O	-5.38365	-3.99657	4.4499
C	-4.02469	-3.88005	4.51463
C	-1.2455	-3.7329	4.87437
C	-3.23497	-3.16378	3.6092
C	-3.41722	-4.53204	5.59897
C	-2.03931	-4.46084	5.76629
C	-1.84383	-3.07071	3.79608
H	-3.68097	-2.63627	2.77445
H	-4.04532	-5.08742	6.28833
H	-1.57544	-4.97937	6.60131
H	-0.16959	-3.6828	5.0101
C	-0.63343	3.59316	-2.71936
C	-1.84961	5.56993	-4.29968
C	-0.01948	4.01829	-3.90176

C	-1.84461	4.18463	-2.32089
C	-2.46494	5.15746	-3.10783
C	-0.63482	5.00762	-4.67856
H	0.92969	3.58946	-4.20789
H	-2.29629	3.8399	-1.40001
H	-0.15732	5.34393	-5.59508
H	-2.33617	6.32942	-4.90349
O	-3.65646	5.75394	-2.80099
C	-4.31205	5.40407	-1.57768
H	-3.58556	5.41494	-0.75352
H	-5.01549	6.22241	-1.40025
C	-5.05418	4.06097	-1.64964
H	-4.42452	3.31963	-2.15049
H	-5.96087	4.16874	-2.25468
C	-5.43473	3.55611	-0.25118
O	-7.534	-0.41778	1.91948
H	-7.28252	-2.37229	1.27666
H	-8.51425	-2.15423	2.53474
H	-4.54358	3.42463	0.37831
H	-6.08101	4.28183	0.25283
H	-0.01512	0.03286	-0.57151
H	-0.01637	0.01857	1.55895
N	-0.02431	0.03826	-1.59222
N	-0.00296	0.00241	2.57859

Optimized structure of 1b

H	-7.8953	-0.67848	4.13526
C	-8.51569	-0.45751	3.27474
H	-9.58541	1.08258	4.29517
C	-9.46416	0.53409	3.36396
C	-9.13172	-0.89223	0.94752
C	-10.29102	0.86061	2.26232
C	-8.34398	-1.17499	2.06239
C	-10.12317	0.13377	1.03694
C	-11.27858	1.87928	2.34464
H	-10.87704	-0.0901	-0.98149
C	-12.08185	2.17482	1.26848
H	-11.38852	2.42062	3.28188
H	-12.83541	2.9542	1.34236
C	-11.92812	1.45231	0.05966

H	-12.57057	1.68109	-0.78693
C	-10.97863	0.46241	-0.05344
C	-8.27842	-1.08997	-1.39699
C	-8.93546	-1.6714	-0.31428
C	-8.50427	-3.11496	-2.70635
C	-9.41067	-3.01494	-0.43018
C	-8.06062	-1.81824	-2.59509
C	-9.19047	-3.74903	-1.64316
C	-10.11945	-3.66502	0.62058
H	-7.53543	-1.35964	-3.42458
H	-9.48751	-5.62446	-2.67855
H	-8.33016	-3.66845	-3.62615
C	-10.57126	-4.95741	0.48226
H	-10.3099	-3.11843	1.53807
H	-11.11316	-5.42842	1.29849
C	-10.3416	-5.68139	-0.71358
H	-10.70272	-6.70193	-0.8076
C	-9.66663	-5.0838	-1.75163
O	-7.42033	-2.17279	1.90773
C	-7.30688	0.90216	-2.34834
C	-7.08657	2.34777	-1.91956
H	-6.45234	2.34964	-1.02377
H	-8.05229	2.77556	-1.62186
C	-6.43853	3.18931	-3.02858
H	-7.0648	3.18887	-3.93012
H	-5.47706	2.74721	-3.3165
C	-6.22416	4.63941	-2.58523
H	-5.69201	4.68568	-1.62599
H	-7.18924	5.13754	-2.45014
O	-5.54144	5.43225	-3.56106
C	-4.17584	5.40538	-3.61087
C	-1.37758	5.51982	-3.83314
C	-3.36961	4.54434	-2.8601
C	-3.57471	6.32463	-4.48447
C	-2.18884	6.37598	-4.58744
C	-1.97039	4.59541	-2.96865
H	-3.80278	3.81926	-2.18227
H	-4.21175	6.98722	-5.06192
H	-1.73169	7.09201	-5.2654
H	-0.29657	5.55769	-3.92819

N	0.00016	-0.84045	-0.00037
N	-0.00024	3.31052	-0.00014
C	0.592	4.08924	0.9643
C	-0.59255	4.08919	-0.96456
C	-1.11633	2.28154	-2.59836
C	-0.61107	0.17189	-2.77401
C	-0.07155	-1.61837	-1.12911
C	0.07191	-1.61843	1.12833
C	0.61125	0.17179	2.77333
C	1.11619	2.28153	2.59787
C	1.40393	1.90394	3.97807
C	1.18959	3.61722	2.14161
C	0.37806	5.45376	0.57156
C	-1.18999	3.61716	-2.14195
C	1.03913	0.60352	4.10032
C	0.26762	-1.15651	2.44427
C	0.02796	-2.98129	0.6851
C	-1.40396	1.90405	-3.97861
C	-0.26728	-1.1564	-2.44504
C	-0.02755	-2.98126	-0.68596
C	-0.37875	5.45372	-0.57182
C	-1.03898	0.60369	-4.10097
H	-1.77667	2.56639	-4.74763
H	-0.73606	6.31013	-1.12504
H	0.06804	-3.83862	1.34081
H	0.73531	6.3102	1.12476
H	-1.06568	-0.01176	-4.98866
H	1.06594	-0.01201	4.98796
H	-0.06762	-3.83856	-1.3417
H	1.77656	2.56627	4.74715
C	0.05263	-2.16091	3.53298
C	-0.53537	-4.00247	5.57057
C	1.06509	-2.6085	4.38832
C	-1.25393	-2.65436	3.69579
C	-1.55487	-3.56787	4.71021
C	0.76005	-3.52559	5.40013
H	2.08155	-2.25056	4.25833
H	-2.02275	-2.29032	3.02609
H	1.54742	-3.87733	6.06161
H	-0.7805	-4.7139	6.35287

O	-2.79716	-4.09242	4.93817
C	-3.86994	-3.75126	4.05482
H	-3.52474	-3.79021	3.0127
H	-4.59545	-4.55837	4.18953
C	-4.49379	-2.38562	4.37841
H	-3.6884	-1.66506	4.55579
H	-5.04989	-2.46137	5.32205
C	-5.39605	-1.83686	3.25876
H	-4.83648	-1.79202	2.31507
H	-5.67392	-0.80403	3.49791
O	-7.85978	0.20247	-1.23681
C	-6.66494	-2.659	3.01677
H	-7.99335	0.85529	-3.20619
H	-6.35477	0.442	-2.65154
H	-6.41192	-3.68615	2.73578
H	-7.28798	-2.71142	3.92004
H	7.8955	-0.6778	-4.1348
C	8.51585	-0.45692	-3.27423
H	9.58565	1.08326	-4.29444
C	9.46434	0.53468	-3.36329
C	9.13177	-0.89189	-0.94702
C	10.29114	0.86107	-2.26158
C	8.34408	-1.17453	-2.06196
C	10.12322	0.13412	-1.03628
C	11.27871	1.87975	-2.34374
H	10.87698	-0.08996	0.98217
C	12.08193	2.17517	-1.2675
H	11.38871	2.42118	-3.28092
H	12.8355	2.95455	-1.34126
C	11.92813	1.45255	-0.05876
H	12.57052	1.68124	0.78788
C	10.97862	0.46264	0.05418
C	8.27837	-1.08991	1.39743
C	8.93545	-1.67121	0.31468
C	8.50416	-3.11505	2.70656
C	9.41064	-3.01477	0.43044
C	8.06051	-1.81832	2.59544
C	9.1904	-3.749	1.64332
C	10.11947	-3.66473	-0.62038
H	7.5353	-1.35982	3.42496

H	9.48738	-5.62457	2.6785
H	8.33001	-3.66865	3.62629
C	10.57126	-4.95714	-0.48219
H	10.30996	-3.11803	-1.53779
H	11.11318	-5.42806	-1.29846
C	10.34154	-5.68126	0.71356
H	10.70265	-6.70181	0.80747
C	9.66654	-5.08379	1.75165
O	7.4204	-2.17233	-1.90746
C	7.30666	0.90208	2.34893
C	7.08633	2.34772	1.92027
H	6.45225	2.34964	1.02437
H	8.05207	2.77561	1.62277
C	6.43804	3.18911	3.02926
H	7.06414	3.18862	3.93092
H	5.47653	2.74694	3.31695
C	6.2237	4.63924	2.586
H	5.69169	4.68557	1.62668
H	7.1888	5.1374	2.45108
O	5.54082	5.43201	3.56176
C	4.17519	5.4053	3.61118
C	1.37688	5.52012	3.83256
C	3.3691	4.54423	2.86031
C	3.57391	6.32475	4.48446
C	2.18801	6.37628	4.587
C	1.96985	4.59549	2.9684
H	3.8024	3.81899	2.18272
H	4.21084	6.98735	5.06201
H	1.73074	7.09246	5.26471
H	0.29585	5.55813	3.92727
C	-0.05215	-2.16071	-3.53379
C	0.53613	-4.00211	-5.57146
C	-1.06452	-2.60828	-4.38928
C	1.25444	-2.65411	-3.69651
C	1.55551	-3.56753	-4.71096
C	-0.75934	-3.52528	-5.40112
H	-2.081	-2.25039	-4.25936
H	2.02318	-2.29009	-3.0267
H	-1.54663	-3.87701	-6.06271
H	0.78136	-4.71347	-6.35378

O	2.79785	-4.09202	-4.93882
C	3.8705	-3.75091	-4.05531
H	3.52519	-3.79	-3.01323
H	4.59608	-4.55796	-4.19002
C	4.4943	-2.38519	-4.37865
H	3.68888	-1.66467	-4.55609
H	5.05056	-2.46079	-5.3222
C	5.39633	-1.83646	-3.25879
H	4.83658	-1.79174	-2.3152
H	5.67416	-0.80359	-3.4978
O	7.85975	0.20256	1.23739
C	6.66522	-2.65853	-3.01665
H	7.99303	0.85516	3.20686
H	6.35454	0.44182	2.65195
H	6.41223	-3.68572	-2.73577
H	7.28841	-2.71084	-3.91982
H	-0.41044	1.20234	-0.97857
H	0.40596	1.2011	0.97921
N	0.65113	1.21439	1.88823
N	-0.65109	1.21441	-1.88882

Optimized structure of 1c

H	-11.01825	-2.7832	2.52912
C	-10.64198	-2.30072	1.63448
H	-12.55897	-1.96134	0.74191
C	-11.48297	-1.85026	0.64414
C	-8.66185	-1.55778	0.38712
C	-10.9566	-1.23524	-0.5258
C	-9.2374	-2.15241	1.50707
C	-9.53182	-1.09241	-0.66154
C	-11.8078	-0.7725	-1.56925
H	-7.95837	-0.41133	-1.98513
C	-11.28735	-0.19952	-2.71108
H	-12.88188	-0.88499	-1.44888
H	-11.94631	0.14717	-3.50079
C	-9.88244	-0.07146	-2.85632
H	-9.47517	0.36753	-3.76202
C	-9.03038	-0.50549	-1.85997
C	-6.58001	-0.16518	0.38897
C	-7.17601	-1.42051	0.25675

C	-4.36272	-1.08871	0.06346
C	-6.33996	-2.55994	0.01022
C	-5.17476	0.0032	0.28969
C	-4.91259	-2.39055	-0.08111
C	-6.87128	-3.87421	-0.1543
H	-4.72988	0.98431	0.39713
H	-3.00975	-3.38222	-0.38137
H	-3.28661	-0.95672	-0.00888
C	-6.04196	-4.95245	-0.3872
H	-7.94301	-4.01578	-0.09123
H	-6.46896	-5.94295	-0.50961
C	-4.63487	-4.78243	-0.4676
H	-3.99723	-5.64178	-0.64881
C	-4.08478	-3.52631	-0.31853
O	-8.47296	-2.72469	2.53619
C	-6.80506	2.83241	-0.73428
H	-7.75262	2.73509	-1.27787
H	-6.06578	2.22544	-1.27359
C	-6.33757	4.30076	-0.71418
H	-5.45518	4.3855	-0.05978
H	-7.11617	4.9341	-0.26399
C	-5.96814	4.83115	-2.11367
H	-6.85226	4.85737	-2.76247
H	-5.25934	4.13625	-2.58043
C	-5.3384	6.23003	-2.0518
H	-4.62004	6.30426	-1.22419
H	-6.09696	7.00326	-1.91257
O	-4.67742	6.61031	-3.30264
C	-3.42926	6.06931	-3.60315
C	-0.93184	5.05549	-4.38758
C	-2.75046	5.15973	-2.78469
C	-2.85502	6.48597	-4.8144
C	-1.61038	5.98337	-5.19257
C	-1.50487	4.63297	-3.17858
H	-3.17478	4.82256	-1.84887
H	-3.39576	7.19431	-5.43073
H	-1.16249	6.31468	-6.12403
H	0.03444	4.6685	-4.692
N	-0.00044	-0.84664	0.00056
N	0.00041	3.16339	0.00071

C	0.4362	3.9977	1.01424
C	-0.43513	3.99796	-1.01274
C	-0.82339	2.28113	-2.78066
C	-0.44431	0.03646	-2.86382
C	-0.04243	-1.6818	-1.10294
C	0.04158	-1.6819	1.10397
C	0.44396	0.03607	2.86502
C	0.82393	2.28062	2.78203
C	1.0953	1.82476	4.12082
C	0.88155	3.59676	2.29173
C	0.28051	5.3991	0.62122
C	-0.88053	3.59727	-2.29027
C	0.82881	0.47652	4.1796
C	0.19362	-1.28027	2.44717
C	0.01335	-3.08273	0.68187
C	-1.09491	1.8255	-4.11949
C	-0.19438	-1.28	-2.44608
C	-0.01431	-3.08266	-0.68098
C	-0.27909	5.39926	-0.61953
C	-0.82895	0.47715	-4.17837
H	-1.43237	2.45763	-4.9239
H	-0.54203	6.25068	-1.22746
H	0.02978	-3.93381	1.34438
H	0.54369	6.25037	1.22926
H	-0.91587	-0.16925	-5.03629
H	0.91545	-0.16998	5.03747
H	-0.03071	-3.93367	-1.34359
H	1.43304	2.45667	4.92528
C	0.08685	-2.33831	3.50822
C	-0.22208	-4.35114	5.44656
C	1.20827	-2.84182	4.18358
C	-1.19268	-2.84236	3.81061
C	-1.34682	-3.84967	4.77082
C	1.04267	-3.84553	5.15033
H	2.19753	-2.46724	3.94401
H	-2.04464	-2.43291	3.28369
H	1.91065	-4.24039	5.66866
H	-0.3662	-5.1312	6.18471
O	-2.563	-4.43418	5.10877
C	-3.80852	-3.91653	4.53113

H	-3.66381	-3.68314	3.46932
H	-4.49424	-4.76293	4.5957
C	-4.3279	-2.70613	5.31965
H	-3.48233	-2.04406	5.54652
H	-4.71845	-3.05646	6.28375
C	-5.40324	-1.89564	4.56706
H	-4.93735	-1.39125	3.70707
H	-5.76516	-1.09843	5.23222
O	-7.44919	0.88801	0.68444
C	-6.59422	-2.72812	4.05349
H	-6.25445	-3.44214	3.29411
H	-7.03955	-3.31438	4.86827
C	-7.65859	-1.85085	3.39731
C	-6.98881	2.27416	0.68002
H	-6.06737	2.37157	1.26968
H	-7.78421	2.80574	1.20827
H	-8.31494	-1.37637	4.13911
H	-7.19821	-1.06582	2.7918
H	11.01733	-2.78483	-2.53046
C	10.64131	-2.30212	-1.63582
H	12.55854	-1.96278	-0.74376
C	11.48257	-1.85158	-0.64575
C	8.66155	-1.55879	-0.38809
C	10.95654	-1.23631	0.52421
C	9.23678	-2.15366	-1.50808
C	9.53181	-1.09333	0.66027
C	11.80803	-0.77344	1.56736
H	7.95872	-0.41192	1.98414
C	11.2879	-0.2002	2.70921
H	12.88207	-0.88603	1.44676
H	11.94709	0.1466	3.49868
C	9.88303	-0.07202	2.85479
H	9.47603	0.36716	3.76051
C	9.0307	-0.50617	1.85873
C	6.57993	-0.16589	-0.39001
C	7.17575	-1.42129	-0.25757
C	4.36254	-1.08895	-0.06392
C	6.33953	-2.56051	-0.01063
C	5.17473	0.00276	-0.29057
C	4.91221	-2.39085	0.08089

C	6.87066	-3.87482	0.15418
H	4.73002	0.98393	-0.39817
H	3.00926	-3.3821	0.38173
H	3.28647	-0.95675	0.00859
C	6.0412	-4.95285	0.38751
H	7.94235	-4.01659	0.091
H	6.46805	-5.94339	0.51013
C	4.63414	-4.78258	0.46807
H	3.99639	-5.64176	0.6496
C	4.08425	-3.5264	0.31875
O	8.47183	-2.7259	-2.53686
C	6.80565	2.8313	0.73335
H	7.75329	2.73379	1.27675
H	6.06641	2.22427	1.27267
C	6.33826	4.29969	0.71365
H	5.45574	4.38462	0.05944
H	7.11682	4.93307	0.26343
C	5.96917	4.82985	2.11332
H	6.85341	4.85578	2.76197
H	5.26033	4.13498	2.58007
C	5.33969	6.22885	2.05183
H	4.62109	6.30333	1.22444
H	6.09838	7.00193	1.91241
O	4.67921	6.60918	3.30291
C	3.43118	6.06818	3.60397
C	0.93402	5.0545	4.38938
C	2.75185	5.15889	2.78562
C	2.85761	6.48461	4.81561
C	1.61309	5.98207	5.19427
C	1.50639	4.63218	3.18
H	3.17567	4.82189	1.84952
H	3.39875	7.19272	5.43185
H	1.1657	6.31322	6.12603
H	-0.03219	4.66761	4.69418
C	-0.0879	-2.33793	-3.50727
C	0.22038	-4.35059	-5.44587
C	-1.20959	-2.84162	-4.18204
C	1.19157	-2.84167	-3.8104
C	1.3454	-3.8489	-4.77074
C	-1.04432	-3.84526	-5.14893

H	-2.19879	-2.46725	-3.94188
H	2.04372	-2.43207	-3.2839
H	-1.91249	-4.24029	-5.66679
H	0.36427	-5.13059	-6.18413
O	2.56151	-4.43305	-5.10948
C	3.80716	-3.91577	-4.53178
H	3.6625	-3.68242	-3.46995
H	4.49268	-4.76233	-4.59642
C	4.32682	-2.70542	-5.32021
H	3.48144	-2.04302	-5.54684
H	4.71707	-3.05574	-6.28444
C	5.40258	-1.89541	-4.56767
H	4.93704	-1.39113	-3.70743
H	5.76458	-1.09813	-5.23269
O	7.44922	0.88711	-0.68587
C	6.59345	-2.72837	-4.05461
H	6.25361	-3.44253	-3.2954
H	7.03845	-3.3145	-4.86967
C	7.6582	-1.85165	-3.39827
C	6.9891	2.27333	-0.6811
H	6.06759	2.37104	-1.2706
H	7.78453	2.80488	-1.20934
H	8.315	-1.37759	-4.13994
H	7.19815	-1.06629	-2.7929
H	0.20345	1.16923	1.07332
H	-0.20339	1.16938	-1.07202
N	0.44228	1.16275	2.05946
N	-0.44222	1.16307	-2.05816

Optimized structure of 1d

C	0.3759	-2.30944	2.18606
C	0.49163	-2.19807	3.6389
H	0.53695	-3.02833	4.32593
C	0.47703	-0.86845	3.93595
H	0.51667	-0.40934	4.91085
C	0.39558	-0.15122	2.66382
N	0.33128	-1.05093	1.61009
C	0.37807	1.25349	2.54772
C	0.39336	1.962	1.33306
C	0.54258	3.3837	1.16909

H	0.63041	4.084	1.98314
C	0.57072	3.6624	-0.17678
H	0.6714	4.62905	-0.6416
C	0.41865	2.426	-0.89651
N	0.32139	1.42683	0.05758
H	0.20816	0.44205	-0.15277
C	0.31294	2.26755	-2.28999
C	-0.01127	1.05939	-2.93949
C	-0.21399	0.93424	-4.38296
H	-0.11071	1.73266	-5.10026
C	-0.56085	-0.36052	-4.62182
H	-0.79301	-0.81853	-5.57019
C	-0.52847	-1.05303	-3.33449
N	-0.19944	-0.16813	-2.32129
C	-0.75533	-2.43705	-3.19053
C	-0.58548	-3.1672	-2.00488
C	-0.65342	-4.59813	-1.85508
H	-0.89626	-5.28105	-2.65283
C	-0.33102	-4.91178	-0.55616
H	-0.27396	-5.89299	-0.11379
C	-0.08004	-3.685	0.15461
N	-0.24385	-2.65919	-0.76264
H	-0.11904	-1.67573	-0.55255
C	0.23703	-3.54096	1.51233
C	0.26836	2.07911	3.79634
C	-0.93786	2.77306	4.01548
H	-1.72963	2.68063	3.28425
C	-1.11159	3.54434	5.17012
C	-0.08286	3.62686	6.1224
H	-0.24025	4.22967	7.00899
C	1.11169	2.94216	5.90209
H	1.91071	3.01429	6.63315
C	1.29794	2.1704	4.74472
H	2.23653	1.654	4.57541
C	0.56778	3.49077	-3.12143
C	-0.45452	4.1126	-3.85507
H	-1.46261	3.71477	-3.81637
C	-0.17018	5.25107	-4.62327
H	-0.96357	5.73156	-5.18697
C	1.11865	5.77971	-4.66426

H	1.357	6.66017	-5.24921
C	2.14282	5.16372	-3.92692
C	1.87216	4.02356	-3.16049
H	2.65706	3.52312	-2.60772
C	-1.22234	-3.20492	-4.39688
C	-2.5957	-3.48755	-4.51829
H	-3.26185	-3.15934	-3.7311
C	-3.08202	-4.15852	-5.64772
C	-2.19477	-4.56764	-6.65611
H	-2.59438	-5.088	-7.51846
C	-0.83301	-4.29878	-6.5266
H	-0.14867	-4.62001	-7.30536
C	-0.33834	-3.61665	-5.4046
H	0.72092	-3.4028	-5.31309
C	0.44445	-4.79692	2.31213
C	-0.62934	-5.55401	2.80224
H	-1.64767	-5.2476	2.58927
C	-0.37657	-6.68973	3.58687
H	-1.20711	-7.27269	3.97201
C	0.92924	-7.07656	3.88486
H	1.14138	-7.94917	4.49124
C	2.0066	-6.32614	3.38681
C	1.76372	-5.19319	2.59999
H	2.57712	-4.59808	2.2064
O	-2.26824	4.26219	5.44506
C	-3.32055	4.30435	4.42438
H	-3.72689	3.29628	4.28221
H	-2.88196	4.6424	3.47486
C	-4.38218	5.29189	4.89748
H	-4.92638	4.87015	5.75209
H	-3.86432	6.18838	5.26016
C	-5.36103	5.68702	3.77208
H	-4.78018	6.06519	2.91613
H	-5.97269	6.53195	4.11941
C	-6.2999	4.56238	3.28812
H	-6.97532	4.27616	4.10865
H	-5.73568	3.66061	3.02475
C	-7.12446	5.00164	2.06472
H	-7.61941	5.96165	2.27721
H	-6.45325	5.17406	1.21305

C	-8.20875	4.01873	1.64142
H	-8.9165	3.8372	2.46289
H	-8.76611	4.41326	0.7814
O	-7.56118	2.76255	1.27269
C	-7.19487	-0.68471	-3.88237
H	-7.86187	-0.50085	-3.03313
H	-7.78721	-0.52563	-4.79501
C	-5.80628	-2.58584	-4.97928
H	-6.2918	-2.41042	-5.94819
H	-4.89381	-1.97738	-4.97294
C	4.457	-6.14586	3.14676
H	4.28329	-5.96509	2.07743
H	5.23792	-6.9043	3.23987
C	4.8588	-4.85401	3.86746
H	3.97801	-4.21056	3.97617
H	5.19424	-5.09714	4.88397
C	5.96785	-4.1083	3.09884
H	5.62955	-3.91065	2.0711
H	6.84561	-4.76346	3.00165
C	7.69045	3.72196	-0.17048
H	8.25682	3.59378	-1.1029
H	8.35587	4.16834	0.5807
C	6.45568	4.5964	-0.37389
H	5.72879	4.018	-0.95509
H	5.99845	4.7829	0.60534
C	6.78578	5.93143	-1.0801
H	6.00048	6.6652	-0.85237
H	7.7078	6.34292	-0.64393
C	6.94381	5.82458	-2.62137
H	7.27428	4.81124	-2.89307
H	7.74126	6.50172	-2.9531
C	4.49311	5.24829	-3.19305
H	4.73363	4.21833	-3.48832
H	4.17528	5.24587	-2.14302
C	5.67374	6.18531	-3.42425
H	5.35871	7.20636	-3.17173
H	5.90475	6.18321	-4.49684
C	-8.34672	1.67704	0.88474
C	-9.74863	1.79347	0.69185
H	-10.2439	2.74394	0.84232

C	-10.48793	0.69698	0.3036
H	-11.55967	0.79115	0.15359
C	-9.87276	-0.56514	0.10001
C	-10.62468	-1.71175	-0.28647
H	-11.69548	-1.6026	-0.43652
C	-10.01386	-2.93539	-0.46201
H	-10.59634	-3.80372	-0.75312
C	-8.61516	-3.06054	-0.2524
H	-8.14008	-4.0286	-0.3793
C	-7.85696	-1.96805	0.11738
H	-6.79168	-2.07619	0.28343
C	-8.45284	-0.68372	0.30199
C	-7.68781	0.46429	0.69191
C	-6.21184	0.3538	0.90347
C	-5.35086	0.31047	-0.19233
C	-3.95054	0.14546	-0.02806
H	-3.29152	0.10891	-0.88689
C	-3.41466	0.0256	1.23687
H	-2.34604	-0.12462	1.35656
C	-4.24211	0.07699	2.38998
C	-3.70246	-0.04165	3.704
H	-2.63042	-0.17675	3.81485
C	-4.52119	0.00448	4.81403
H	-4.09995	-0.08771	5.81001
C	-5.92273	0.16394	4.65134
H	-6.56324	0.19174	5.52771
C	-6.47719	0.27767	3.3926
H	-7.54876	0.39068	3.27806
C	-5.66186	0.24414	2.22138
O	-5.94446	0.42502	-1.44839
C	-5.13044	0.27678	-2.65112
H	-4.60588	-0.68741	-2.6218
H	-4.37607	1.07336	-2.68918
C	-6.06698	0.36955	-3.85205
H	-6.52136	1.36826	-3.85912
H	-5.44851	0.30057	-4.75804
C	-6.73737	-2.15738	-3.82788
H	-7.63373	-2.79431	-3.82917
H	-6.24214	-2.34745	-2.86475
C	-5.42675	-4.06651	-4.87341

H	-5.07218	-4.31664	-3.86448
H	-6.28234	-4.70716	-5.09909
O	-4.42122	-4.4692	-5.86069
O	3.2739	-6.78874	3.72592
C	6.42512	-2.78231	3.74263
H	6.86252	-2.99185	4.72946
H	7.2233	-2.35947	3.12305
C	5.32699	-1.71093	3.91887
H	5.78633	-0.80377	4.33103
H	4.57603	-2.04232	4.6495
C	4.58415	-1.33689	2.63957
H	4.06295	-2.20281	2.21153
H	3.8378	-0.55659	2.83591
O	5.57479	-0.84267	1.68747
C	5.18295	-0.49302	0.39687
C	3.83504	-0.58412	-0.03889
H	3.05418	-0.91576	0.63442
C	3.50203	-0.22537	-1.32779
H	2.46952	-0.29605	-1.65688
C	4.48968	0.23886	-2.23666
C	4.15844	0.62181	-3.56877
H	3.12238	0.5472	-3.88702
C	5.12848	1.07533	-4.43992
H	4.86589	1.36063	-5.45374
C	6.47986	1.15471	-4.01037
H	7.24275	1.49586	-4.70403
C	6.8333	0.79134	-2.72594
H	7.86983	0.84329	-2.41277
C	5.85593	0.3296	-1.79306
C	6.19233	-0.04221	-0.45137
C	7.5958	0.08757	0.04665
C	8.45686	-1.05105	0.17671
C	8.02726	-2.3705	-0.15407
H	7.0145	-2.51172	-0.51303
C	8.87959	-3.44965	-0.03087
H	8.5328	-4.44466	-0.29261
C	10.21034	-3.27164	0.42988
H	10.86849	-4.12969	0.52305
C	10.66179	-2.00846	0.75125
H	11.68029	-1.85874	1.09943

C	9.81047	-0.87293	0.63202
C	10.26529	0.43726	0.94209
H	11.28702	0.57135	1.28577
C	9.4299	1.52537	0.81424
H	9.78508	2.51737	1.06769
C	8.09399	1.34557	0.37237
O	7.20466	2.41855	0.27982
O	3.3956	5.7557	-4.02055

Optimized structure of 2a

H	3.56375	-1.707	-0.45622
C	4.26073	-0.89369	-0.62035
H	2.7004	0.50118	-1.03527
C	3.77213	0.34831	-0.95132
C	6.54695	-0.03591	-0.60536
C	4.64379	1.44066	-1.18107
C	5.65585	-1.0959	-0.46186
C	6.05452	1.24141	-1.01506
C	4.15617	2.719	-1.56618
H	7.99156	2.20186	-1.18934
C	5.01988	3.76338	-1.8035
H	3.08261	2.85468	-1.67015
H	4.63645	4.73589	-2.09978
C	6.41584	3.56577	-1.66774
H	7.09738	4.38712	-1.87453
C	6.91938	2.3434	-1.2811
C	8.42711	0.04821	1.02191
C	7.99062	-0.2311	-0.2653
C	10.70052	-0.58494	0.48392
C	8.93707	-0.71266	-1.22674
C	9.78239	-0.12724	1.39674
C	10.30922	-0.88794	-0.84705
C	8.56394	-1.02074	-2.56418
H	10.066	0.08671	2.42323
H	12.27697	-1.49416	-1.50821
H	11.73923	-0.72718	0.77292
C	9.49175	-1.47818	-3.47336
H	7.52897	-0.88383	-2.86111
H	9.18448	-1.7057	-4.49079
C	10.84433	-1.65412	-3.09489

H	11.56666	-2.01665	-3.82132
C	11.23981	-1.36387	-1.80915
O	6.20889	-2.3039	-0.1265
C	7.49482	1.85915	2.25131
C	6.41689	2.13481	3.29876
H	6.76728	1.84737	4.29637
H	5.54607	1.51324	3.0675
C	6.04617	3.62259	3.29947
H	5.50122	3.89296	2.38571
H	6.95573	4.23237	3.33357
O	5.31085	4.03785	4.45377
C	3.95276	3.90598	4.49994
C	1.17007	3.73084	4.81966
C	3.18257	3.18903	3.57845
C	3.32394	4.54452	5.5804
C	1.9447	4.45908	5.72849
C	1.78984	3.08434	3.74474
H	3.64456	2.67387	2.74498
H	3.93724	5.10092	6.28214
H	1.46458	4.96654	6.56109
H	0.09315	3.66616	4.94156
N	-0.37834	-1.90943	0.41702
N	0.37852	1.9097	0.41738
C	0.17981	2.78381	-0.6117
C	0.86392	2.66037	1.45257
C	0.53237	0.9985	3.26936
C	-0.53232	-0.99858	3.26915
C	-0.86362	-2.66028	1.45213
C	-0.17953	-2.78342	-0.61216
C	0.14843	-1.1242	-2.43715
C	-0.14842	1.12488	-2.43693
C	-0.12428	0.67605	-3.79859
C	-0.18457	2.43984	-1.93638
C	0.53794	4.14171	-0.21449
C	1.04007	2.2163	2.7817
C	0.12438	-0.67511	-3.79872
C	0.18475	-2.43922	-1.93681
C	-0.53748	-4.14141	-0.21508
C	0.34822	0.59087	4.63334
C	-1.03987	-2.21636	2.78129

C	-1.01239	-4.05435	1.05411
C	1.01285	4.05447	1.05468
C	-0.3481	-0.59129	4.63321
H	0.67704	1.15666	5.49209
H	1.38842	4.85027	1.68289
H	-0.47134	-5.01885	-0.84349
H	0.47191	5.01924	-0.84279
H	-0.67682	-1.15732	5.49184
H	0.23968	-1.31614	-4.6599
H	-1.38785	-4.85024	1.68227
H	-0.23957	1.31727	-4.65964
C	0.719	-3.52155	-2.8192
C	2.00831	-5.45556	-4.39711
C	0.14372	-3.93824	-4.02384
C	1.93059	-4.09928	-2.40032
C	2.58602	-5.05087	-3.18406
C	0.79501	-4.90562	-4.79884
H	-0.80619	-3.52381	-4.34712
H	2.35534	-3.75997	-1.46511
H	0.34575	-5.23613	-5.7316
H	2.52122	-6.19887	-4.9992
O	3.77951	-5.63053	-2.85454
C	4.37897	-5.31376	-1.59401
H	3.61569	-5.34684	-0.80431
H	5.07499	-6.13667	-1.40837
C	5.12344	-3.96947	-1.59561
H	4.52129	-3.21508	-2.11093
H	6.06156	-4.06251	-2.15342
C	5.43017	-3.49742	-0.16815
O	7.52539	0.45045	1.99043
H	7.27127	2.39667	1.32063
H	8.47929	2.2011	2.6055
H	4.50678	-3.37905	0.41584
H	6.04858	-4.23431	0.35406
H	-3.56416	1.70709	-0.45809
C	-4.26112	0.89363	-0.62155
H	-2.70077	-0.50128	-1.03629
C	-3.77249	-0.34849	-0.95209
C	-6.54725	0.03563	-0.60561
C	-4.6441	-1.44101	-1.18115

C	-5.65621	1.09576	-0.46274
C	-6.05481	-1.24181	-1.01492
C	-4.15645	-2.71948	-1.56582
H	-7.99181	-2.20244	-1.18858
C	-5.02012	-3.76402	-1.80255
H	-3.0829	-2.85511	-1.66996
H	-4.63667	-4.73662	-2.09849
C	-6.41608	-3.56644	-1.66665
H	-7.0976	-4.38792	-1.87303
C	-6.91963	-2.34396	-1.28042
C	-8.42717	-0.04841	1.02196
C	-7.99087	0.2308	-0.26534
C	-10.7007	0.5845	0.48422
C	-8.9375	0.71219	-1.22669
C	-9.7824	0.12698	1.39697
C	-10.30961	0.88738	-0.84684
C	-8.56459	1.02013	-2.56422
H	-10.06587	-0.08684	2.42352
H	-12.27751	1.49333	-1.50778
H	-11.73938	0.7267	0.77335
C	-9.49258	1.47737	-3.47332
H	-7.52965	0.88328	-2.86129
H	-9.18547	1.7048	-4.49083
C	-10.84511	1.65324	-3.09469
H	-11.56758	2.0156	-3.82107
C	-11.24038	1.36311	-1.80886
O	-6.20934	2.30384	-0.12783
C	-7.49509	-1.85907	2.25193
C	-6.41672	-2.13468	3.29896
H	-6.76666	-1.84725	4.29672
H	-5.54599	-1.51313	3.0673
C	-6.04601	-3.62248	3.29953
H	-5.50118	-3.89278	2.38568
H	-6.95557	-4.23226	3.3337
O	-5.31055	-4.03781	4.45372
C	-3.95243	-3.90616	4.49964
C	-1.16965	-3.7315	4.81882
C	-3.18234	-3.18901	3.57822
C	-3.32347	-4.54514	5.57975
C	-1.94418	-4.45993	5.72759

C	-1.78957	-3.08459	3.74425
H	-3.64444	-2.67355	2.74499
H	-3.93669	-5.1017	6.28143
H	-1.46395	-4.96772	6.55993
H	-0.0927	-3.66695	4.94053
C	-0.71874	3.52236	-2.81859
C	-2.0079	5.45672	-4.3962
C	-0.14344	3.9392	-4.02318
C	-1.93027	4.10015	-2.39961
C	-2.58564	5.0519	-3.18321
C	-0.79464	4.90675	-4.79801
H	0.80643	3.52472	-4.34652
H	-2.35501	3.76079	-1.46441
H	-0.34536	5.23738	-5.73073
H	-2.52076	6.20015	-4.99818
O	-3.77906	5.63164	-2.85358
C	-4.37887	5.31427	-1.59336
H	-3.61582	5.34701	-0.80343
H	-5.07496	6.13708	-1.40755
C	-5.12332	3.96997	-1.59579
H	-4.52105	3.21583	-2.11132
H	-6.06131	4.0633	-2.15377
C	-5.43041	3.49724	-0.16863
O	-7.52523	-0.45047	1.99037
H	-7.27224	-2.39712	1.32138
H	-8.4795	-2.20046	2.60681
H	-4.50718	3.37839	0.41549
H	-6.04881	4.23398	0.35383
N	-0.00003	0.00027	-1.66049
N	0.00001	0.00005	2.49347
Zn	0.00004	0.00015	0.41685

Optimized structure of 2b

H	7.96825	-0.67056	-4.09554
C	8.58818	-0.41361	-3.24476
H	9.60079	1.13861	-4.30429
C	9.50453	0.60499	-3.3616
C	9.2373	-0.78339	-0.91551
C	10.33036	0.97833	-2.27421
C	8.44915	-1.11233	-2.01728

C	10.19576	0.27054	-1.03368
C	11.28514	2.02518	-2.38498
H	10.97345	0.10875	0.9815
C	12.08817	2.36597	-1.3221
H	11.37025	2.55151	-3.3333
H	12.8165	3.16668	-1.41778
C	11.9674	1.66255	-0.09835
H	12.60984	1.92726	0.7377
C	11.04999	0.6463	0.04233
C	8.40323	-0.96243	1.43718
C	9.07494	-1.54271	0.36301
C	8.70379	-2.95217	2.78511
C	9.59681	-2.86645	0.50322
C	8.21542	-1.67384	2.6504
C	9.40702	-3.58338	1.73145
C	10.323	-3.51249	-0.53812
H	7.67834	-1.21733	3.47337
H	9.77283	-5.42666	2.80211
H	8.55249	-3.49289	3.71646
C	10.81955	-4.78564	-0.37656
H	10.49048	-2.97813	-1.46723
H	11.37378	-5.25398	-1.186
C	10.61994	-5.49315	0.83445
H	11.01625	-6.49868	0.94674
C	9.92927	-4.89863	1.86388
O	7.55908	-2.13556	-1.83483
C	7.36335	1.0105	2.35343
C	7.08856	2.4401	1.9025
H	6.45542	2.40542	1.00667
H	8.03737	2.90075	1.59963
C	6.40794	3.26943	3.0011
H	7.0306	3.29795	3.90472
H	5.46126	2.79648	3.28936
C	6.14376	4.70841	2.54867
H	5.60906	4.73229	1.59006
H	7.09061	5.23915	2.40955
O	5.43719	5.48104	3.52362
C	4.0754	5.38856	3.59624
C	1.28004	5.36073	3.87721
C	3.29562	4.5098	2.83777

C	3.44903	6.25548	4.5048
C	2.06477	6.23704	4.63642
C	1.89822	4.49067	2.97526
H	3.74897	3.8251	2.13148
H	4.0655	6.93309	5.08715
H	1.58809	6.91385	5.34069
H	0.20027	5.34663	3.99048
N	0.00002	-0.89425	-0.00007
N	-0.00003	3.0807	-0.00002
C	-0.55565	3.90687	-0.934
C	0.55556	3.90687	0.93398
C	1.09155	2.18235	2.65062
C	0.56904	-0.0134	2.82159
C	0.03795	-1.71971	1.08747
C	-0.03789	-1.71969	-1.08762
C	-0.56901	-0.01336	-2.8217
C	-1.09158	2.18238	-2.65069
C	-1.33819	1.76912	-4.00222
C	-1.14617	3.49231	-2.14461
C	-0.36742	5.30882	-0.56967
C	1.14611	3.4923	2.14458
C	-0.97626	0.45092	-4.1171
C	-0.21019	-1.31497	-2.43155
C	-0.0043	-3.11915	-0.67832
C	1.33818	1.76906	4.00214
C	0.21024	-1.31501	2.43141
C	0.0044	-3.11917	0.67814
C	0.36731	5.30882	0.56967
C	0.97628	0.45085	4.11699
H	1.69267	2.42414	4.78475
H	0.72363	6.15898	1.13467
H	-0.02382	-3.97073	-1.34376
H	-0.72376	6.15898	-1.13466
H	0.9983	-0.15937	5.00759
H	-0.99826	-0.15928	-5.00771
H	0.02393	-3.97075	1.34356
H	-1.6927	2.42421	-4.78481
C	0.04926	-2.32336	-3.50567
C	0.72735	-4.1535	-5.52475
C	-0.92951	-2.78448	-4.39264

C	1.36783	-2.79556	-3.62857
C	1.71372	-3.70234	-4.63443
C	-0.58006	-3.69772	-5.39368
H	-1.95561	-2.44442	-4.29246
H	2.1086	-2.42095	-2.93377
H	-1.34152	-4.06236	-6.07815
H	1.00758	-4.86022	-6.29949
O	2.97068	-4.20466	-4.82797
C	4.02053	-3.82261	-3.93365
H	3.6629	-3.85865	-2.89573
H	4.77035	-4.61032	-4.04869
C	4.60918	-2.44426	-4.26755
H	3.78542	-1.74418	-4.44255
H	5.16007	-2.51218	-5.21491
C	5.50662	-1.86803	-3.1579
H	4.95442	-1.83215	-2.20959
H	5.7567	-0.82995	-3.40486
O	7.94015	0.312	1.25375
C	6.79829	-2.65623	-2.92438
H	8.05198	1.00374	3.21081
H	6.42937	0.52054	2.66661
H	6.57458	-3.68476	-2.6245
H	7.40824	-2.70728	-3.83665
H	-7.96815	-0.6707	4.0956
C	-8.5881	-0.41373	3.24484
H	-9.60067	1.13848	4.30444
C	-9.50443	0.60488	3.36173
C	-9.23728	-0.78344	0.9156
C	-10.33029	0.97826	2.27437
C	-8.4491	-1.11242	2.01734
C	-10.19574	0.27049	1.03382
C	-11.28506	2.02511	2.38519
H	-10.97348	0.10876	-0.98135
C	-12.08812	2.36593	1.32234
H	-11.37014	2.55141	3.33352
H	-12.81643	3.16664	1.41806
C	-11.96739	1.66254	0.09857
H	-12.60984	1.92728	-0.73745
C	-11.04998	0.64628	-0.04215
C	-8.40327	-0.96242	-1.43712

C	-9.07496	-1.54273	-0.36295
C	-8.70388	-2.95214	-2.78509
C	-9.59684	-2.86646	-0.50317
C	-8.2155	-1.6738	-2.65036
C	-9.40709	-3.58337	-1.73143
C	-10.32301	-3.51253	0.53817
H	-7.67844	-1.21728	-3.47333
H	-9.77294	-5.42662	-2.80213
H	-8.55261	-3.49284	-3.71646
C	-10.81956	-4.78568	0.37659
H	-10.49046	-2.97819	1.4673
H	-11.37378	-5.25403	1.18604
C	-10.61999	-5.49315	-0.83444
H	-11.01631	-6.49867	-0.94675
C	-9.92935	-4.89861	-1.86388
O	-7.55905	-2.13565	1.83484
C	-7.36341	1.01052	-2.35335
C	-7.08861	2.44012	-1.9024
H	-6.45545	2.40541	-1.00658
H	-8.03741	2.90076	-1.59948
C	-6.40803	3.26946	-3.001
H	-7.03071	3.298	-3.9046
H	-5.46135	2.79653	-3.28929
C	-6.14384	4.70844	-2.54855
H	-5.60911	4.7323	-1.58994
H	-7.09068	5.23917	-2.40939
O	-5.43729	5.48109	-3.5235
C	-4.07551	5.38859	-3.59618
C	-1.28016	5.36074	-3.87725
C	-3.2957	4.50983	-2.83772
C	-3.44916	6.25549	-4.50476
C	-2.0649	6.23704	-4.63644
C	-1.89831	4.49068	-2.97527
H	-3.74903	3.82514	-2.13141
H	-4.06565	6.93311	-5.08709
H	-1.58825	6.91385	-5.34073
H	-0.2004	5.34662	-3.99056
C	-0.04918	-2.32343	3.50551
C	-0.72722	-4.15362	5.52456
C	0.92961	-2.78455	4.39246

C	-1.36774	-2.79566	3.62841
C	-1.7136	-3.70246	4.63426
C	0.58018	-3.69782	5.39349
H	1.95569	-2.44447	4.29228
H	-2.10852	-2.42106	2.93362
H	1.34165	-4.06245	6.07795
H	-1.00743	-4.86036	6.29929
O	-2.97056	-4.20481	4.82779
C	-4.02043	-3.82273	3.93352
H	-3.66282	-3.85874	2.89558
H	-4.77024	-4.61045	4.04854
C	-4.60908	-2.4444	4.26747
H	-3.78532	-1.74432	4.44247
H	-5.15995	-2.51236	5.21484
C	-5.50656	-1.86814	3.15786
H	-4.95438	-1.83223	2.20954
H	-5.75664	-0.83007	3.40485
O	-7.94019	0.31199	-1.25367
C	-6.79822	-2.65634	2.92435
H	-8.05207	1.00378	-3.21071
H	-6.42944	0.52057	-2.66657
H	-6.57452	-3.68486	2.62444
H	-7.40815	-2.70742	3.83664
N	-0.65059	1.06985	-1.97909
N	0.65059	1.06982	1.979
Zn	0.	1.08153	-0.00004

Optimized structure of 2c

H	-10.87226	-2.86707	2.72483
C	-10.55019	-2.38242	1.80822
H	-12.52013	-2.01777	1.05748
C	-11.45127	-1.91718	0.88417
C	-8.65859	-1.65087	0.43489
C	-11.0025	-1.30316	-0.31413
C	-9.15679	-2.25003	1.58674
C	-9.59296	-1.1741	-0.54652
C	-11.9179	-0.82825	-1.29152
H	-8.10922	-0.50569	-1.97391
C	-11.47436	-0.25683	-2.46154
H	-12.98309	-0.93119	-1.09639

H	-12.18496	0.09989	-3.20228
C	-10.08458	-0.14301	-2.70316
H	-9.73504	0.2954	-3.63446
C	-9.17192	-0.58807	-1.7727
C	-6.58987	-0.25284	0.31993
C	-7.18308	-1.51213	0.2197
C	-4.38865	-1.18249	-0.08116
C	-6.35862	-2.64902	-0.05554
C	-5.1889	-0.09075	0.16528
C	-4.93992	-2.4822	-0.19987
C	-6.89279	-3.96162	-0.19891
H	-4.73669	0.89026	0.24953
H	-3.04803	-3.46915	-0.55821
H	-3.31475	-1.04933	-0.19034
C	-6.07404	-5.03702	-0.45855
H	-7.96331	-4.10467	-0.10266
H	-6.50732	-6.02814	-0.56554
C	-4.67331	-4.86885	-0.58686
H	-4.04056	-5.72919	-0.78734
C	-4.12143	-3.61537	-0.46103
O	-8.33422	-2.82182	2.53396
C	-6.815	2.72346	-0.76456
H	-7.77206	2.63303	-1.29266
H	-6.08604	2.13019	-1.33094
C	-6.35487	4.18775	-0.72006
H	-5.46524	4.26255	-0.07589
H	-7.12747	4.80715	-0.24194
C	-6.00744	4.75299	-2.10513
H	-6.89428	4.76916	-2.7508
H	-5.28413	4.08753	-2.59017
C	-5.41367	6.16546	-2.02301
H	-4.70169	6.24489	-1.19019
H	-6.19931	6.90726	-1.8527
O	-4.7828	6.58312	-3.23818
C	-3.54041	6.09779	-3.53566
C	-1.00574	5.18321	-4.32962
C	-2.82883	5.19628	-2.73742
C	-2.97073	6.55314	-4.73445
C	-1.71225	6.10054	-5.11611
C	-1.56803	4.72185	-3.13518

H	-3.24285	4.82321	-1.80955
H	-3.52987	7.2566	-5.3433
H	-1.27382	6.46515	-6.04135
H	-0.02614	4.83182	-4.63914
N	0.00006	-0.74288	0.00009
N	0.00012	3.2645	-0.00014
C	0.44813	4.09194	0.99112
C	-0.44789	4.09183	-0.99149
C	-0.87035	2.377	-2.75565
C	-0.49805	0.14545	-2.84624
C	-0.06476	-1.57063	-1.0872
C	0.06486	-1.5705	1.08748
C	0.49817	0.14578	2.84633
C	0.87053	2.37731	2.75548
C	1.1656	1.92756	4.08609
C	0.91823	3.69177	2.26107
C	0.29206	5.49251	0.61132
C	-0.91801	3.69152	-2.2614
C	0.90212	0.58414	4.15083
C	0.24282	-1.16985	2.42985
C	0.02699	-2.97067	0.67826
C	-1.16546	1.9271	-4.0862
C	-0.24272	-1.17014	-2.42961
C	-0.02692	-2.97075	-0.67781
C	-0.2918	5.49244	-0.61186
C	-0.90201	0.58367	-4.15078
H	-1.51338	2.5655	-4.88439
H	-0.56893	6.343	-1.21869
H	0.05664	-3.8217	1.34383
H	0.56919	6.34313	1.21806
H	-1.00399	-0.0658	-5.00758
H	1.00407	-0.06523	5.0077
H	-0.0566	-3.82185	-1.34328
H	1.51351	2.56605	4.88421
C	0.16185	-2.2269	3.49133
C	-0.10175	-4.23367	5.42935
C	1.29574	-2.72413	4.14112
C	-1.1068	-2.73286	3.81869
C	-1.24456	-3.74247	4.77801
C	1.15141	-3.72447	5.10925

H	2.27977	-2.34606	3.88105
H	-1.9696	-2.32278	3.30848
H	2.03112	-4.11743	5.61208
H	-0.22388	-5.01618	6.1717
O	-2.42618	-4.32494	5.13382
C	-3.64919	-3.85685	4.55104
H	-3.50886	-3.64698	3.48342
H	-4.32873	-4.70983	4.62429
C	-4.2115	-2.64296	5.30142
H	-3.39003	-1.94673	5.51026
H	-4.588	-2.97987	6.27585
C	-5.31105	-1.8929	4.5317
H	-4.86211	-1.39109	3.66242
H	-5.70061	-1.0929	5.17668
O	-7.43444	0.78072	0.62963
C	-6.46841	-2.77103	4.03419
H	-6.10332	-3.48271	3.28472
H	-6.89176	-3.36355	4.85632
C	-7.56488	-1.94303	3.36789
C	-6.97226	2.13145	0.63785
H	-6.03855	2.21744	1.21047
H	-7.74428	2.67336	1.19304
H	-8.22486	-1.47458	4.11359
H	-7.1251	-1.1439	2.76319
H	10.87219	-2.86767	-2.72443
C	10.55009	-2.38287	-1.80791
H	12.52001	-2.01821	-1.05712
C	11.45115	-1.91755	-0.88388
C	8.65846	-1.65102	-0.43478
C	11.00236	-1.30333	0.31431
C	9.15669	-2.25037	-1.58652
C	9.59281	-1.17417	0.54661
C	11.91773	-0.82833	1.29167
H	8.10903	-0.50546	1.97382
C	11.47416	-0.25672	2.46159
H	12.98292	-0.93135	1.09661
H	12.18474	0.10007	3.20232
C	10.08437	-0.14279	2.70312
H	9.73481	0.29578	3.63434
C	9.17173	-0.58794	1.77268

C	6.58982	-0.25287	-0.32
C	7.18295	-1.51218	-0.21967
C	4.38853	-1.18237	0.08106
C	6.35841	-2.64901	0.0556
C	5.18884	-0.09069	-0.16541
C	4.93972	-2.4821	0.19986
C	6.8925	-3.96163	0.19905
H	4.7367	0.89035	-0.24973
H	3.04776	-3.46892	0.55819
H	3.31463	-1.04914	0.19019
C	6.07369	-5.03698	0.45872
H	7.96302	-4.10475	0.10285
H	6.50691	-6.02811	0.56578
C	4.67296	-4.86871	0.58697
H	4.04016	-5.72901	0.78747
C	4.12115	-3.61522	0.46106
O	8.33415	-2.82228	-2.53369
C	6.81504	2.72348	0.76432
H	7.77205	2.63302	1.29249
H	6.086	2.13029	1.33069
C	6.355	4.1878	0.71971
H	5.46542	4.26263	0.07548
H	7.12767	4.80712	0.24161
C	6.00753	4.75314	2.10473
H	6.89433	4.76926	2.75047
H	5.28411	4.08777	2.58975
C	5.4139	6.16567	2.02251
H	4.70196	6.24512	1.18965
H	6.19962	6.90738	1.85218
O	4.78302	6.58345	3.23762
C	3.54061	6.09817	3.53512
C	1.00591	5.1837	4.32912
C	2.82905	5.19656	2.73698
C	2.9709	6.55367	4.73384
C	1.7124	6.10113	5.11551
C	1.56824	4.72219	3.13476
H	3.2431	4.82337	1.80917
H	3.53003	7.2572	5.34262
H	1.27395	6.46586	6.04069
H	0.02629	4.83237	4.63865

C	-0.16182	-2.22731	-3.49096
C	0.10166	-4.23433	-5.42876
C	-1.29574	-2.72459	-4.14065
C	1.10682	-2.73334	-3.81832
C	1.24451	-3.74307	-4.77752
C	-1.15147	-3.72506	-5.10867
H	-2.27975	-2.34647	-3.88059
H	1.96964	-2.32323	-3.30818
H	-2.03121	-4.11806	-5.61142
H	0.22375	-5.01693	-6.17102
O	2.4261	-4.32561	-5.1333
C	3.64914	-3.85746	-4.55063
H	3.50884	-3.6474	-3.48305
H	4.32865	-4.71048	-4.62375
C	4.21148	-2.64373	-5.30124
H	3.39004	-1.9475	-5.51019
H	4.58796	-2.98083	-6.27561
C	5.31107	-1.89358	-4.53167
H	4.86216	-1.39157	-3.66248
H	5.70068	-1.09372	-5.1768
O	7.43446	0.78063	-0.62972
C	6.46839	-2.77167	-4.03399
H	6.10325	-3.4832	-3.28439
H	6.89171	-3.36436	-4.856
C	7.56488	-1.94361	-3.36781
C	6.97235	2.13138	-0.63805
H	6.03869	2.21739	-1.21072
H	7.74443	2.67322	-1.19322
H	8.22491	-1.47534	-4.11358
H	7.12514	-1.14432	-2.76328
N	0.48015	1.26521	2.04756
N	-0.47997	1.26498	-2.04761
Zn	0.00009	1.26295	-0.00003

Optimized structure of 2d

C	0.38915	2.31183	-2.18333
C	0.50081	2.22174	-3.63369
H	0.54974	3.06026	-4.31378
C	0.47486	0.90014	-3.93889
H	0.50948	0.44363	-4.91752

C	0.39329	0.18627	-2.66975
N	0.33845	1.0657	-1.62007
C	0.37111	-1.22114	-2.56559
C	0.38318	-1.94107	-1.35797
C	0.52553	-3.36004	-1.20624
H	0.61203	-4.05471	-2.02826
C	0.55013	-3.6464	0.13298
H	0.64551	-4.61719	0.59564
C	0.40148	-2.41665	0.85535
N	0.31284	-1.41922	-0.08737
C	0.29125	-2.26318	2.24863
C	-0.02963	-1.05548	2.90418
C	-0.22857	-0.94983	4.34552
H	-0.1283	-1.75722	5.05641
C	-0.56946	0.33916	4.59137
H	-0.79947	0.7966	5.54302
C	-0.53061	1.02779	3.307
N	-0.2111	0.16033	2.29795
C	-0.74615	2.41637	3.17471
C	-0.56661	3.15708	1.99778
C	-0.62168	4.58514	1.86198
H	-0.86071	5.26331	2.66803
C	-0.2937	4.9043	0.57118
H	-0.22598	5.88899	0.13246
C	-0.05551	3.68282	-0.14377
N	-0.23022	2.66045	0.76036
C	0.26168	3.54203	-1.50142
C	0.25906	-2.03621	-3.81874
C	-0.95	-2.71528	-4.04622
H	-1.74392	-2.61803	-3.31665
C	-1.13123	-3.47996	-5.20326
C	-0.09606	-3.56284	-6.14747
H	-0.25121	-4.15966	-7.04084
C	1.10081	-2.89322	-5.91801
H	1.90286	-2.97017	-6.64744
C	1.29032	-2.13238	-4.75865
H	2.23381	-1.62496	-4.58191
C	0.53668	-3.49168	3.07205
C	-0.49352	-4.12212	3.77843
H	-1.50301	-3.72597	3.72729

C	-0.21745	-5.26441	4.53699
H	-1.01866	-5.75527	5.08329
C	1.06876	-5.78783	4.59388
H	1.29648	-6.67581	5.17524
C	2.10649	-5.16557	3.8825
C	1.83897	-4.01882	3.12626
H	2.63044	-3.50874	2.59019
C	-1.2096	3.17701	4.38474
C	-2.58317	3.43081	4.52299
H	-3.25094	3.08513	3.74343
C	-3.0738	4.09499	5.65373
C	-2.17659	4.52194	6.64499
H	-2.57123	5.03871	7.5142
C	-0.81528	4.28115	6.49789
H	-0.12757	4.61954	7.26845
C	-0.32163	3.60867	5.37432
H	0.74143	3.4149	5.26884
C	0.48337	4.80007	-2.29034
C	-0.57771	5.56587	-2.78211
H	-1.6014	5.26595	-2.57974
C	-0.30764	6.70115	-3.55473
H	-1.12995	7.29566	-3.94407
C	1.00018	7.0781	-3.83842
H	1.22054	7.95556	-4.43828
C	2.07089	6.32004	-3.33926
C	1.80511	5.18599	-2.56276
H	2.60858	4.57917	-2.1642
O	-2.26994	-4.173	-5.48695
C	-3.28928	-4.22826	-4.482
H	-3.69495	-3.22303	-4.3114
H	-2.84881	-4.58213	-3.53815
C	-4.36669	-5.20008	-4.94941
H	-4.9086	-4.76936	-5.80118
H	-3.86302	-6.10202	-5.3184
C	-5.34235	-5.59027	-3.82679
H	-4.76292	-5.98366	-2.97789
H	-5.9616	-6.42687	-4.17866
C	-6.26822	-4.46821	-3.32924
H	-6.93318	-4.15695	-4.14832
H	-5.69447	-3.57848	-3.04732

C	-7.10586	-4.91985	-2.12533
H	-7.61632	-5.86499	-2.36113
H	-6.44488	-5.12672	-1.27338
C	-8.1787	-3.93361	-1.68319
H	-8.88455	-3.7368	-2.50427
H	-8.74659	-4.35585	-0.84176
O	-7.54845	-2.71684	-1.28695
C	-7.16011	0.63156	3.89783
H	-7.84912	0.47104	3.06167
H	-7.73655	0.45711	4.81695
C	-5.75248	2.50663	5.00285
H	-6.22224	2.31811	5.97722
H	-4.84081	1.89885	4.9768
C	4.4629	6.12212	-3.09054
H	4.28526	5.93247	-2.02328
H	5.26224	6.86612	-3.16179
C	4.86691	4.83545	-3.81642
H	3.98554	4.19491	-3.92973
H	5.19886	5.0863	-4.8324
C	5.97382	4.08773	-3.05828
H	5.64016	3.88993	-2.0299
H	6.85193	4.74113	-2.96064
C	7.62307	-3.69676	0.16639
H	8.17994	-3.56104	1.10452
H	8.30018	-4.16851	-0.56094
C	6.39207	-4.57445	0.37118
H	5.65793	-3.99578	0.943
H	5.94142	-4.76885	-0.60966
C	6.7226	-5.89993	1.0834
H	5.94659	-6.64023	0.84829
H	7.64995	-6.30617	0.65585
C	6.86744	-5.79258	2.62146
H	7.19038	-4.77888	2.89753
H	7.66782	-6.4627	2.95795
C	4.40939	-5.24402	3.19003
H	4.64651	-4.2106	3.48032
H	4.10273	-5.2387	2.13558
C	5.60301	-6.16392	3.41762
H	5.30012	-7.18895	3.16614
H	5.8336	-6.16114	4.49033

C	-8.32737	-1.66197	-0.89628
C	-9.72968	-1.77997	-0.70849
H	-10.22521	-2.72854	-0.87643
C	-10.46934	-0.69373	-0.30393
H	-11.54243	-0.79471	-0.15886
C	-9.86071	0.56344	-0.07596
C	-10.61506	1.69773	0.32995
H	-11.68687	1.58199	0.47629
C	-10.01018	2.9163	0.52943
H	-10.59694	3.77774	0.83676
C	-8.61451	3.04791	0.32397
H	-8.13993	4.01507	0.4694
C	-7.85472	1.96773	-0.06445
H	-6.78879	2.08398	-0.22902
C	-8.44476	0.68733	-0.27317
C	-7.67773	-0.4486	-0.68105
C	-6.20144	-0.33203	-0.88983
C	-5.34436	-0.31357	0.20897
C	-3.94426	-0.15083	0.04085
H	-3.28167	-0.1323	0.89868
C	-3.41231	-0.01107	-1.22005
H	-2.34175	0.13457	-1.33833
C	-4.23765	-0.03656	-2.37115
C	-3.69886	0.10303	-3.68
H	-2.62488	0.23343	-3.78868
C	-4.51586	0.08243	-4.78724
H	-4.0934	0.19118	-5.78246
C	-5.91502	-0.07108	-4.6255
H	-6.55894	-0.07786	-5.50147
C	-6.4679	-0.20506	-3.37209
H	-7.54173	-0.31131	-3.26007
C	-5.65362	-0.19899	-2.20291
O	-5.92882	-0.45104	1.43775
C	-5.12862	-0.32821	2.61226
H	-4.59184	0.63073	2.5996
H	-4.37545	-1.12804	2.6427
C	-6.0461	-0.42886	3.82626
H	-6.50859	-1.42379	3.82827
H	-5.40844	-0.38275	4.71923
C	-6.69835	2.09848	3.86377

H	-7.59213	2.73736	3.88762
H	-6.21848	2.30586	2.8973
C	-5.37124	3.98664	4.91628
H	-5.02671	4.24866	3.9067
H	-6.23794	4.61655	5.13843
O	-4.38937	4.37693	5.88292
O	3.31911	6.76847	-3.66097
C	6.42839	2.76682	-3.70336
H	6.85948	2.9769	-4.69203
H	7.23599	2.3503	-3.09203
C	5.33862	1.69219	-3.87437
H	5.79826	0.79095	-4.29884
H	4.57829	2.02106	-4.59492
C	4.60668	1.30348	-2.59418
H	4.08315	2.16766	-2.16317
H	3.85119	0.53378	-2.80435
O	5.56945	0.80527	-1.66612
C	5.17475	0.47016	-0.40084
C	3.82694	0.56679	0.03407
H	3.04812	0.90041	-0.64216
C	3.49003	0.21274	1.31972
H	2.45545	0.28886	1.64473
C	4.46823	-0.25264	2.23278
C	4.12971	-0.62927	3.56146
H	3.09129	-0.54958	3.87459
C	5.09089	-1.08324	4.43611
H	4.82141	-1.36461	5.45058
C	6.44039	-1.16952	4.01241
H	7.20113	-1.51237	4.70962
C	6.80016	-0.81306	2.7317
H	7.83938	-0.87074	2.42444
C	5.83123	-0.35035	1.7946
C	6.17379	0.01568	0.45655
C	7.57831	-0.1263	-0.03585
C	8.45339	0.9995	-0.14979
C	8.0407	2.31908	0.18975
H	7.02757	2.47148	0.54714
C	8.90565	3.38512	0.0811
H	8.5684	4.38281	0.3505
C	10.23369	3.19492	-0.37275

H	10.9052	4.04531	-0.45513
C	10.66852	1.93193	-0.70166
H	11.68792	1.77115	-1.04589
C	9.80336	0.80962	-0.59764
C	10.24023	-0.50098	-0.91707
H	11.26309	-0.6468	-1.25666
C	9.39229	-1.57668	-0.80687
H	9.737	-2.57123	-1.06974
C	8.05553	-1.38803	-0.37168
O	7.166	-2.4289	-0.30486
O	3.33479	-5.74602	3.99152
Zn	0.05249	0.61682	0.33772