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Systematic Optimization of the Substituents on the Phenothiazine Donor of Doubly Strapped Porphyrin Sensitizers: An Efficiency over 11% Unassisted by any Cosensitizer or Coadsorbent

Kaiwen Zeng,[a] Weiqiang Tang,[b] Chengjie Li,[a] Yingying Chen,[a] Shuangliang Zhao,[b] Qingyun Liu[c] and Yongshu Xie[a]*

[a]*Key Laboratory for Advanced Materials and Institute of Fine Chemicals, Shanghai Key Laboratory of Functional Materials Chemistry, School of Chemistry and Molecular Engineering, East China University of Science &Technology, 130 Meilong Rd, Shanghai 200237, China. E-mail: yshxie@ecust.edu.cn*

[b]*School of Chemical Engineering and State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai, 200237, China*

[c]*College of Chemical and Environmental Engineering, Shandong University of Science and Technology, Qingdao, China*

Contents

1. Experimental Section

1.1 Materials and Reagents

All the reagents and solvents were purchased from commercial sources and used without further purification unless otherwise noted. THF was dried over 4 Å molecular sieves, and distilled under nitrogen from sodium benzophenone prior to use. Tetrabutylammonium hexafluorophosphate ($TBAPF_6$) was vacuum-dried for 48 h. The transparent FTO conducting glass (fluorine-doped SnO_2, transmission >90% in the visible range, sheet resistance 15 Ω/square) and the TiO_2 paste were purchased from Geao Science and Educational Co. Ltd. The FTO conducting glass was washed with a detergent solution, deionized water, ethanol, and acetone successively under ultrasonication for 20 min before use. Compounds ***2b*** and **3b** were synthesized according to a literature procedure.[1]

1.2 Equipment and Apparatus

^1H NMR and ^{13}C NMR spectra were obtained using a Bruker AM 400 spectrometer. FT-IR spectra were recorded in the region of 400−4000 cm^{-1} on a Thermo Electron Avatar 380 FT-IR instrument (KBr Discs). HRMS measurements were performed using a Waters LCT Premier XE spectrometer. Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) was measured using a Shimadzu-Kratos model Axima CFR+ mass spectrometer using dithranol as the matrix. UV-Vis absorption spectra were recorded on a Varian Cary 100 spectrophotometer and fluorescence spectra were recorded on a Varian Cray Eclipse fluorescence spectrophotometer. The cyclic voltammograms of the dyes were obtained in acetonitrile with a Versastat II electrochemical workstation (Princeton Applied Research) using 0.1 M $TBAPF_6$ (Aldrich) as the supporting electrolyte, the sensitizer attached to a nanocrystalline TiO_2 film deposited on the conducting FTO glass as the working electrode, a platinum wire as the counter electrode, and a regular calomel electrode in saturated KCl solution as the reference electrode. The scan rate was 100 mV s^{-1}.

1.3 Fabrication of DSSCs

The procedures for preparation of TiO_2 electrodes and fabrication of the sealed cells for photovoltaic measurements were adapted from that reported by Grätzel and co-workers.[2] A screen-printed double layer of TiO_2 particles was used as the photoelectrod.[3] The FTO conducting glass was washed with a detergent solution, deionized water, acetone and ethanol successively for 20 min under ultrasonication before use. The FTO conducting glass was further pre-treated with a 40 mM aqueous $TiCl_4$ solution at 70°C for 30 min for cobalt electrolyte-based DSSCs. A 2-μm thick film of 30-nm-sized TiO_2 particles (for cobalt electrolyte-based DSSCs) or 10-μm thick film of 13-nm-sized TiO_2 particles (for iodine electrolyte-based DSSCs) was first printed on the FTO conducting glass, kept in a clean box for 10 minutes, dried at 130°C over 5 min, and then coated by a 4-μm thick second layer of 400-nm light-scattering anatase particles. Finally, the electrodes coated with the TiO_2 pastes were gradually sintered in a muffle furnace at 275°C for 5 min, at 325°C for 5 min, at 375°C for 5 min, at 450°C for 15 min and at 500°C for 15 min, respectively. The size of the TiO_2 film was 0.12 cm^2. These films were immersed into a 40 mM aqueous $TiCl_4$ solution at 70°C for 30 min, washed with water and ethanol, and then heated again at 450°C for 30 min. The films were then immersed into a 0.2 mM solution of the porphyrin dyes in a mixture of chloroform and ethanol (volume ratio of 3 : 2) at 25^{o}C for the indicated time. The counter electrode was also prepared according to the procedure reported in our previous work.[4-5] The iodine electrolyte solution contains 0.1 M LiI, 0.05 M I_2, 0.6 M 1-methyl-3-propyl-imidazolium iodide (PMII) and 0.5 M 4-tert-butylpyridine (TBP) in acetonitrile. The cobalt electrolyte is composed of 0.1 M lithium bis(trifluoromethanesulfonyl)imide (LiTFSI), 0.5 M 4-tert-butylpyridine (TBP), 0.06 M tris(2,2'bipyridine) cobalt(II) di[bis(trifluoromethanesulfonyl)imide] and 0.25 M cobalt(III) tris(2,2'bipyridine) tris[bis(trifluoromethanesulfonyl)imide] in CH_3CN.

1.4 Photovoltaic Behavior Measurements

Photovoltaic measurements were performed by employing an AM 1.5 solar simulator equipped with a 300 W xenon lamp (model no. 91160, Oriel). The power of the simulated light was calibrated to 100 mW cm^{-2} using a Newport Oriel PV reference cell system (model 91150 V). *J–V* curves were obtained by applying an external bias to the cell and measuring the generated photocurrent with a model 2400 source meter (Keithley Instruments, Inc. USA). The voltage step and delay time of the photocurrent were 10 mV and 40 ms, respectively. Action spectra of the incident monochromatic photon-to-electron conversion efficiency (IPCE) for the solar cells were obtained with a Newport-74125 system (Newport Instruments). The intensity of monochromatic light was measured with a Si detector (Newport-71640). The electrochemical impedance spectroscopy (EIS) measurements of all the DSSCs were performed using a Zahner IM6e Impedance Analyzer (ZAHNER-Elektrik GmbH & CoKG, Kronach, Germany), with the frequency range of 0.1 Hz–100 kHz and the alternative signal of 10 mV. The ZSimpWin software was used to fit the experimental EIS data of the DSSCs.

1.5 Theoretical Calculations

We employed density functional theory (DFT) calculations to optimize the ground state geometries of the sensitizers, using the hybrid B3LYP functional[6-7] and the 6-31G* basis set.[8] For zinc atoms, the Los Alamos effective core potential basis set (LANL2DZ) was used.[9] All calculations were carried out using the Gaussian09 program package.[10]

1.6 Measurement of the Amounts of Dye Adsorption

The amounts of dye adsorption on the TiO_2 films were measured by a Varian Cary 100 spectrophotometer. The sensitized electrodes were immersed into a 0.1 M NaOH solution in a mixed solvent (H_2O : THF = 1 : 1), which resulted in desorption of each dyes.

1.7 Syntheses of the Dyes

Synthesis of compound 2a. To a 250 mL three-neck flask was added **1a**[11] (4.55 g, 10.31 mmol), 2-(2,6-bis(hexyloxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane[12] (5.42 g, 13.41 mmol), and THF (100 mL). The flask was flushed with N_2, and then $Pd(PPh_3)_4$ (238 mg, 0.21 mmol) and aqueous 2M K_2CO_3 (12.89 mL, 25.78 mmol) were quickly added under nitrogen. After refluxing for 12 h, the mixture was cooled to room temperature, and then poured into water. The resulting mixture was extracted with CH_2Cl_2. The combined organic extracts were dried using anhydrous

Na_2SO_4, filtered, and concentrated under reduced pressure. Purification via column chromatography (silica gel, DCM : PE = 1 : 9) afforded **2a** as a yellow oil (4.31 g, yield 65%). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 0.84-0.90 (m, 8H), 1.25-1.27 (m,8H), 1.32-1.33 (m, 8H), 1.43-1.46 (m, 2H), 1.59-1.65 (m, 5H), 1.80-1.84 (m, 2H), 3.80-3.84 (t, *J*=7.2 Hz, 2H), 3.88-3.91 (t, *J*=6.2 Hz, 4H), 6.59-6.62 (d, *J*=8.4 Hz, 2H), 6.68-6.70 (d, *J*=9.2 Hz, 1H), 6.84-6.86 (d, *J*=8.0 Hz, 1H), 7.16-7.23 (m, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 14.02, 14.08, 22.65, 22.83, 26.68, 26.77, 29.15, 31.50, 31.53, 47.56, 68.69, 105.44, 114.00, 114.24, 116.22, 118.95, 122.26, 127.44, 128.40, 128.53, 129.53, 129.57, 130.25, 130.39, 143.10, 144.65, 157.19. HRMS (ESI, *m/z*): $[M+H]^+$ calcd for $C_{36}H_{49}NO_2SBr$, 638.2667; Found, 638.2668. FT-IR (neat, cm^{-1}): 2954 (s), 2928 (s), 2857 (m), 1590 (m), 1501 (w), 1458 (s), 1391 (m), 1330 (w), 1244 (m), 1197 (w), 1148 (w), 1098 (s), 1033 (w), 891 (w), 874 (w), 815 (m), 779 (m), 725 (m), 547 (w), 469 (w).

Synthesis of compound 2c. To a 500 mL three-neck flask was added **1b** (9.12 g, 14.4 mmol), 2-(2,6-bis(hexyloxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (7.45 g, 18.60 mmol), and dry toluene (300 mL). The flask was flushed with N_2. 2-Dicyclohexylphosphino-2',6'-dimethoxybiphenyl (600 mg, 1.44 mmol), $Pd_2(dba)_3$ (660 mg, 0.72 mmol) and K_3PO_4 (20.16 g, 86.4 mmol) were then quickly added under nitrogen. After refluxing for 12 h the mixture was cooled to room temperature, and then poured into water. The resulting mixture was extracted with DCM for three times. The combined organic extracts were dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography (silica gel, DCM : PE = 1 : 5) to afford **2c** as a yellow oil (2.95 g, yield 25%). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 0.78-0.82 (t, *J*=6.8 Hz, 6H), 0.83-0.87 (t, *J*=6.8 Hz, 6H), 1.17-1.19 (m, 8H), 1.26-1.29 (m, 12H), 1.33-1.38 (m, 4H), 1.60-1.69 (m, 8H), 3.85-3.88 (t, *J*=6.2 Hz, 4H), 3.94-3.98 (m, 4H), 5.93-5.95 (d, *J*=8.8 Hz, 1H), 6.08-6.10 (d, *J*=8.4 Hz, 1H), 6.56-6.59 (d, *J*=8.4 Hz, 2H), 6.67-6.69 (d, *J*=8.4 Hz, 2H), 6.82-6.83 (t, *J*=2.2 Hz, 1H), 6.84-6.85 (t, *J*=2.2 Hz, 1H), 6.96 (d, *J*=2.2 Hz, 1H), 7.00-7.01 (d, *J*=2.2 Hz, 1H), 7.13-7.17 (t, *J*=8.2 Hz, 1H), 7.31-7.36 (t, *J*=8.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.0, 157.2, 142.6, 140.8, 129.9, 129.6, 128.9, 128.9, 128.0, 128.0, 127.7, 123.0, 119.3, 118.4, 117.7, 116.4, 114.4, 113.1, 105.8, 105.5, 68.7, 68.7, 31.6, 31.4, 29.2, 29.1, 25.8, 25.5, 22.6, 22.5, 14.1, 14.0. HRMS (ESI, *m/z*): $[M+H]^+$ calcd for $C_{48}H_{65}NO_4SBr$, 830.3818; Found, 830.3816. FT-IR (neat, cm^{-1}): 2955 (s), 2929 (s), 2858 (s), 1608 (s), 1579 (m), 1512 (w), 1492 (s), 1461 (s), 1433 (w), 1381 (m), 1298 (s), 1275 (m), 1245 (m), 1182 (s), 1135 (m), 1047 (m), 1022 (m), 1005 (w), 921 (w), 835 (m), 819 (m), 802 (m),726 (w), 596 (w).

Synthesis of compound 2d. In a 250 mL three-neck flask, 2,4-bis(hexyloxy)-4'-iodo-1,1'-biphenyle[13] (5.55 g, 11.57 mmol), 3,7-dibromo-10H-phenothiazine (4.12 g, 11.57 mmol), sodium *tert*-butoxide (1.66 g,17.27 mmol), tri-*tert*-butylphosphine tetrafluoroborate (338 mg, 1.16 mmol) and $Pd_2(dba)_3$ (528 mg, 0.58 mmol) were mixed in dry toluene (100 mL) under nitrogen. After heating at 45^{o}C for 6 h, the mixture was poured into water and extracted with DCM for three times. The combined organic extracts were dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography (silica gel, DCM : PE = 1 : 9) to afford **1c** as a colorless oil (5.86 g, yield 71%). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.30 – 7.34 (m, 3H), 7.09 (d, *J* = 2.4 Hz, 2H), 6.92 (dd, *J* = 8.8, 2.4 Hz, 2H), 6.62 – 6.57 (m, 2H), 6.12 (d, *J* = 8.8 Hz, 2H), 3.99 – 4.03 (m, 3H), 1.73 – 1.86 (m, 4H), 1.46 – 1.1.53 (m, 2H), 1.36 – 1.43 (m, 6H), 1.28 – 1.32 (m, 4H), 0.92 – 0.95 (m, 3H), 0.85 – 0.89 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.3, 157.0, 143.3, 139.2, 137.9, 132.0, 131.1, 129.8, 129.7, 128.7, 121.9, 121.2, 117.2, 114.6, 105.4, 100.3, 68.4, 68.2, 31.6, 31.4, 29.3, 29.1, 25.8, 22.7, 22.6. HRMS (ESI, *m/z*): $[M+Na]^+$ calcd for $C_{36}H_{39}Br_2NO_2SNa$, 730.0966; Found, 730.0992. FT-IR (neat, cm^{-1}): 3034 (w), 2955 (s), 2927 (s), 2861 (s), 2550 (w), 1923 (w), 1859 (w), 1731 (w), 1675 (w), 1607 (s), 1581 (s), 1490 (s), 1458 (s), 1383 (s), 1301 (s), 1262 (s), 1181 (s), 1132 (m), 1094 (m), 1028 (m), 927 (w), 865 (w), 839 (m), 803 (s), 729 (m), 593 (m), 547 (m), 582 (w), 449 (w).

Compound **2d** was synthesized according to a procedure similar to that described for **2a** except that the **1c** and (2,4-bis(hexyloxy)phenyl)boronic acid were used instead of **1a** and (2,6-bis(hexyloxy)phenyl)boronic acid, respectively. Yellow oil, 58%. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.76 (d, *J* = 8.2 Hz, 2H), 7.35 (t, *J* = 9.0 Hz, 3H), 7.21 (d, *J* = 2.0 Hz, 1H), 7.17 – 7.08 (m, 2H), 7.01 (d, *J* = 9.4 Hz, 1H), 6.91 (dd, *J* = 8.9, 2.3 Hz, 1H), 6.59 (m, 2H), 6.49 (m, 2H), 6.28 (d, *J* = 8.6 Hz, 1H), 6.12 (d, *J* = 8.6 Hz, 1H), 4.01 (m, 4H), 4.00 – 3.92 (t, *J* = 6.5 Hz, 2H), 3.92 (t, *J* = 6.5 Hz, 2H), 1.88 – 1.68 (m, 8H), 1.54 – 1.38 (m, 8H), 1.40 – 1.26 (m, 16H), 0.97 – 0.83 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 160.2, 159.6, 157.0, 156.9, 143.7, 142.2, 138.8, 138.5, 133.1, 131.8, 131.1, 130.4, 130.0, 129.3, 128.7, 127.9, 127.6, 122.3, 122.2, 122.0, 118.3, 117.0, 115.6, 114.0, 105.4, 105.2, 100.3, 68.4, 68.2, 68.1, 31.6, 31.6, 31.6, 31.4, 29.3, 29.3, 29.1, 29.1, 25.9, 25.8, 25.8, 22.6, 22.6, 22.6, 14.1, 14.1, 14.0. HRMS (ESI, *m/z*): $[M+H]^+$ calcd for $C_{54}H_{69}BrNO_4S$, 906.4131; Found, 906.4128. FT-IR (neat, cm^{-1}): 2957 (s), 2927 (s), 2858 (s), 1589 (s), 1501 (m), 1460 (s), 1381 (m), 1307 (m), 1250 (s), 1186 (w), 1099 (s), 1033 (w), 861 (w), 803 (m), 771 (m), 730 (m), 675 (w).

Synthesis of compound 3a. To a solution of **2a** (4.31 g, 6.75 mmol) in THF/Piperidine (20 mL/80 mL) were added $Pd(PPh_3)_2Cl_2$ (237 mg, 0.34 mmol), CuI (65 mg, 0.34 mmol) and PPh_3 (90 mg, 0.34 mmol) under nitrogen. The mixture was stirred at 50^oC under N_2 before trimethylsilylacetylene (2.65 g, 27.00 mmol) was added *via* a syringe over 20 min. Then the mixture was heated at 90^oC for 3 h. The solvents were removed under reduced pressure and the residue was purified by column chromatography (silica gel, DCM : PE = 1 : 9) to afford a yellow oil as the intermediate product of 3-(2,6-bis(hexyloxy)phenyl)-10-hexyl-7-((trimethylsilyl)ethynyl)-10H-phenothiazine (3.01 g, yield 69%), which was then added to a 100 mL flask with THF/methanol (30 mL/30 mL). After adding dropwise an aqueous TBAF solution (1M, 5.05 mL), the reaction mixture was stirred at room temperature for 30 min. Then water was added, extracted with DCM, dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography (silica gel, DCM : PE = 1 : 9) to afford **3a** as a yellow oil (2.52, 94%). ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 0.82-0.90 (m, 9H), 1.21-1.26 (m, 8H), 1.30-1.33 (m, 8H), 1.42-1.46 (m, 2H), 1.60-1.64 (m,4H), 1.80-1.84 (m, 2H), 3.01 (s, 1H), 3.82-3.85 (t, *J*=7.2 Hz, 2H), 3.87-3.90 (t, *J*=6.4 Hz, 4H), 6.58-6.60 (d, *J*=6.54 Hz, 2H), 6.73-6.75 (d, *J*=8.4 Hz, 1H), 6.82-6.84 (d, *J*=8.4 Hz, 1H), 7.14-7.14 (m, 1H), 7.16-7.17 (m, 1H), 7.18-7.21 (m, 2H) 7.24-7.26 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 14.02, 14.07, 22.65, 25.82, 26.67, 26.77, 29.14, 31.50, 31.52, 47.60, 68.68, 83.33, 105.43,114.25, 114.60, 115.31, 118.94, 122.20, 124.95, 128.40, 128.66, 130.22, 131.10, 142.70, 145.94, 157.19. HRMS (ESI, *m/z*): $[M+H]^+$ calcd for $C_{38}H_{50}NO_2S$, 584.3562; Found, 584.3558. FT-IR (neat, cm^{-1}): 3308 (m), 2953 (s), 2928 (s), 2860 (s), 2106 (w), 1586 (s), 1503 (w), 1460 (s), 1395 (m), 1335 (m), 1244 (s), 1195 (w), 1145 (w), 1098 (s), 1030 (w), 885 (m), 816 (m), 781 (m), 728 (m), 649 (m), 603 (w), 580 (w).

Synthesis of compound 3c. It was prepared in a similar way with that of **3a** using **2c** (6.17 g, 7.42 mmol) as the starting material and the product was obtained as a yellow oil (3.72 g, 65%). ^1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.33-

7.37 (t, J = 8.4 Hz, 1H), 6.14-7.18 (t, J = 8.3 Hz, 1H), 7.04 (s, 1H), 6.97 (s, 1H), 6.89-6.92 (d, J = 8.4 Hz, 1H), 6.83-6.85 (d, J = 8.0 Hz, 1H), 6.69-6.71 (d, J = 8.4 Hz, 2H), 6.57-6.60 (d, J = 8.4 Hz, 2H), 6.09-6.11 (d, J = 8.4 Hz, 1H), 5.99-6.01 (d, J = 8.4 Hz, 1H), 3.95-3.98 (m, 4H), 3.86-3.89 (t, J = 6.4 Hz, 4H), 2.98 (s, 1H), 1.61-1.68 (m, 8H), 1.32-1.40 (m, 4H), 1.24-1.29 (m, 12H), 1.17-1.20 (m, 8H), 0.85-0.88 (t, J = 6.8 Hz, 6H), 0.79-0.83 (t, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.0, 157.2, 143.8, 140.5, 130.6, 129.8, 129.6, 129.4, 128.9, 128.0, 128.0, 120.7, 119.3, 118.3, 118.0, 114.6, 114.5, 105.8, 105.5, 83.8, 75.9, 68.7, 68.7, 53.4, 31.6, 31.4, 29.2, 29.1, 25.8, 25.5, 22.6, 22.5, 14.1, 14.0. HRMS (ESI, *m/z*): $[M+H]^+$ calcd for $C_{50}H_{66}NO_4S$, 776.4713; Found, 776.4707. FT-IR (neat, cm^{-1}): 3313 (m), 2955 (s), 2929 (s), 2104 (w), 1589 (s), 1504 (m), 1460 (s), 1385 (s), 1315 (s), 1248 (s), 1193 (w), 1099 (s), 880 (w), 812 (m), 776 (m), 729 (m), 647 (w), 598 (w), 577 (w).

Synthesis of compound 3d. It was prepared in a similar way with that of **3a** using **2d** (600 mg, 0.66mmol) as the starting material. Yellow oil, 460 mg, yield 76%. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.77 (d, J = 8.4 Hz, 2H), 7.33 – 7.38 (m, 3H), 7.20 (d, J = 1.8 Hz, 1H), 7.14 (d, J = 8.8 Hz, 1H), 7.11 (d, J = 1.8 Hz, 1H), 6.99 (dd, J = 8.4, 1.8 Hz, 1H), 6.95 (dd, J = 8.4, 1.8 Hz, 1H), 6.58 – 6.61 (m, 2H), 6.48 – 6.50 (m, 2H), 6.25 (d, J = 8.4 Hz, 1H), 6.17 (d, J = 8.4 Hz, 1H), 3.99 – 4.03 (m, 4H), 3.96 (t, J = 6.6 Hz, 2H), 3.92 (t, J = 6.6 Hz, 2H), 3.01 (s, 1H), 1.69 – 1.86 (m, 8H), 1.40 – 1.52 (m, 8H), 1.26 – 1.38 (m, 16H), 0.84 – 0.94 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.2, 159.7, 157.0, 156.9, 144.9, 141.9, 138.9, 138.3, 133.2, 131.9, 131.2, 130.8, 130.4, 130.2, 129.9, 127.8, 127.6, 122.2, 122.0, 119.9, 118.4, 115.7, 115.4, 115.3, 105.5, 105.3, 100.4, 100.4, 83.2, 68.4, 68.2, 68.1, 31.7, 31.7, 31.6, 31.4, 29.4, 29.3, 29.2, 29.1, 25.8, 25.8, 22.7, 22.6, 14.1, 14.1. HRMS (ESI, *m/z*): $[M+H]^+$ calcd for $C_{56}H_{70}NO_4S$, 852.5026; Found, 852.5029. FT-IR (neat, cm^{-1}): 3290 (w), 3034 (w), 2957 (s), 2929 (s), 2862 (s), 2105 (w), 1606 (s), 1581 (m), 1492 (s), 1467 (s), 1436 (w), 1386 (m), 1303 (s), 1250 (s), 1183 (s), 1135 (m), 1047 (m), 928 (w), 882 (w), 816 (m), 726 (w), 648 (w), 601 (w), 583 (w).

Synthesis of compound 4a. To a 250 mL three-neck flask was added **ZnPBr$_2$**[14] (200 mg, 0.197 mmol), **3a** (126 mg, 0.217 mmol), dry THF (120mL) and Et_3N (40 mL). The flask was flushed with N_2. $Pd_2(dba)_3$ (90 mg, 0.10 mmol), and $AsPh_3$ (121 mg, 0.39 mmol) were then quickly added under nitrogen. After the mixture was refluxed for 12 h, the solvent was removed under reduced pressure and the residue was purified by column chromatography (silica gel, DCM : PE = 3 : 2) to afford **4a** as a dark green powder (153 mg, yield 51%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.71 (d, J = 4.8 Hz, 2H), 9.63 (d, J = 4.8 Hz, 2H), 8.89 (d, J = 4.4 Hz, 2H), 8.86 (d, J = 4.8 Hz, 2H), 7.79 (d, J = 8.4 Hz, 1H), 7.70-7.76 (m, 3H), 7.19-7.24 (m, 3H), 7.12 (d, J = 8.4 Hz, 4H), 7.00 (d, J = 8.4 Hz, 1H), 6.92 (d, J = 8.8 Hz, 1H), 6.62 (d, J = 8.4 Hz, 2H), 3.97 (t, J = 7.4 Hz, 2H), 3.92 (t, J = 6.4 Hz, 4H), 3.85 (t, J = 5.4 Hz, 8H), 1.92-1.96 (m, 6H), 1.64-1.71 (m, 4H), 1.50-1.57 (m, 2H), 1.35-1.41 (m, 8H), 1.27-1.32 (m, 8H), 0.84-0.93 (m, 17H), (-0.80)-(-0.76) (m, 8H), (-0.99)-(-0.91) (m, 8H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.34, 157.24, 152.27, 151.36, 150.57, 149.11, 145.55, 142.84, 132.64, 132.46, 132.39, 130.94, 130.61, 130.34, 130.29, 130.23, 130.04, 128.66, 128.40, 127.54, 125.26, 125.13, 122.28, 119.05, 117.67, 115.11, 115.03, 114.29, 109.72, 105.49, 104.86, 100.39, 95.60, 92.55, 71.31, 68.74, 47.78, 31.57, 30.64, 29.43, 29.19, 26.91, 26.77, 25.87, 25.29, 22.70, 14.16, 14.08. MS (MALDI-TOF): [M] calcd for $C_{90}H_{98}BrN_5O_6SZn$, 1521.57; Found, 1521.58. FT-IR (neat, cm^{-1}): 3754 (w), 3447 (br), 2924 (s), 2857 (m), 1628 (w), 1585 (m), 1458 (s), 1386 (w), 1332 (w), 1243 (m), 1095 (s), 1001 (m), 966 (w), 891 (w), 793 (m), 725 (m), 600 (w), 478 (w). m.p.: 244–246^{o}C.

Synthesis of compound 4b. It was prepared in a similar way with that of **4a** using **3b** (147 mg, 0.217 mmol) as the starting material. Dark green powder, 155 mg, yield 49%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.66 (d, J = 4.8 Hz, 2H), 9.61 (d, J = 4.8 Hz, 2H), 8.85 (m, 4H), 7.71 (t, J = 8.4 Hz, 2H), 7.57 (s, 1H), 7.42 (d, J = 8.8 Hz, 4H), 7.17 (s, 1H), 7.11 (d, J = 8.4 Hz, 4H), 7.00 (d, J = 8.4 Hz, 1H), 6.92 (d, J = 8.8 Hz, 2H), 6.76 (d, J = 8.4 Hz, 2H), 6.22 (d, J = 8.4 Hz, 1H), 6.18 (d, J = 8.4 Hz, 1H), 4.04 (t, J = 6.4 Hz, 4H), 3.98 (t, J = 6.6 Hz, 2H), 3.86 (t, J = 5.3 Hz, 8H), 2.06-2.08 (m, 4H), 1.78-1.82 (m, 2H), 1.67-1.74 (m, 4H), 1.46-1.49 (m, 2H), 1.32-1.37 (m, 8H), 1.22 (m, 8H), 0.79-0.93 (m, 17H), (-0.65)-(-0.62) (m, 8H), (-1.00)-(-0.92) (m, 8H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.32, 158.34, 157.91, 152.23, 151.26, 150.48, 149.07, 143.03, 141.00, 134.98, 132.56, 132.54, 132.36, 132.33, 130.90, 130.45, 130.19, 129.92, 128.86, 127.70, 127.23, 125.14, 125.03, 124.16, 120.11, 119.95, 117.95, 117.27, 115.76, 115.20, 114.95, 114.71, 109.65, 105.82, 104.69, 100.59, 95.86, 92.25, 71.26, 68.79, 68.10, 31.63, 31.44, 30.75, 29.48, 29.31, 29.16, 25.77, 25.58, 25.25, 22.65, 14.07. MS (MALDI-TOF): [M] calcd for $C_{96}H_{102}BrN_5O_7SZn$, 1611.60; Found, 1611.61. FT-IR (neat, cm^{-1}): 3754 (w), 3444 (br), 2921 (s), 2855 (m), 1653 (w), 1583 (m), 1465 (s), 1382 (w), 1312 (w), 1241 (m), 1094 (s), 999 (m), 966 (w), 878 (w), 791 (m), 722 (m), 631 (w), 482 (w). m.p.: 227–228^{o}C.

Synthesis of compound 4c. It was prepared in a similar way with that of **4a** using **3c** (168 mg, 0.217 mmol) as the starting material. Dark green powder, 153 mg, yield 45%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.67 (d, J = 4.4 Hz, 2H), 9.61 (d, J = 4.4 Hz, 2H), 8.85 (m, 4H), 7.71 (t, J = 8.4 Hz, 2H), 7.55 (s, 1H), 7.40 (t, J = 8.4 Hz, 2H), 7.17 (t, J = 8.4 Hz, 1H), 7.12 (d, J = 8.4 Hz, 4H), 7.04 (s, 1H), 6.88 (d, J = 8.4 Hz, 1H), 6.75 (d, J = 8.4 Hz, 2H), 6.60 (d, J = 8.4 Hz, 2H), 6.22 (d, J = 8.4 Hz, 1H), 6.16 (d, J = 8.4 Hz, 1H), 4.03 (t, J = 6.4 Hz, 4H), 3.90 (t, J = 6.4 Hz, 4H), 3.85 (t, J = 5.3 Hz, 8H), 1.98 (m, 4H), 1.65-1.74 (m, 8H), 1.32-1.39 (m, 16H), 1.23-1.28 (m, 8H), 0.82-0.91 (m, 20H), (-0.76)-(-0.70) (m, 8H), (-0.98)-(-0.94) (m, 8H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.33, 158.06, 157.27, 152.25, 151.24, 150.49, 149.08, 143.56, 140.56, 132.52, 132.33, 132.31, 130.96, 130.18, 129.83, 129.66, 128.99, 128.84, 128.04, 127.94, 127.62, 125.18, 121.02, 119.42, 118.44, 118.06, 116.89, 115.08, 114.95, 114.54, 109.69, 105.86, 105.59, 104.60, 100.86, 96.17, 91.97, 71.28, 68.84, 68.70, 31.59, 31.49, 30.70, 29.45, 29.20, 29.17, 25.84, 25.54, 25.26, 22.68, 22. MS (MALDI-TOF): [M] calcd for $C_{102}H_{114}BrN_5O_8SZn$, 1711.69; Found, 1711.70. FT-IR (neat, cm^{-1}): 3753 (w), 3448 (br), 2922 (s), 2856 (m), 1630 (w), 1585 (m), 1458 (s), 1383 (w), 1313 (w), 1244 (m), 1095 (s), 1000 (m), 969 (w), 883 (w), 786 (m), 725 (m), 630 (w), 484 (w). m.p.: 229–232^{o}C.

Synthesis of compound 4d. It was prepared in a similar way with that of **4a** using **3d** (185 mg, 0.217 mmol) as the starting material. Dark green powder, 169 mg, yield 48%. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 9.68 (d, J = 4.6 Hz, 2H), 9.62 (d, J = 4.6 Hz, 2H), 8.88 (d, J = 4.6 Hz, 2H), 8.85 (d, J = 4.6 Hz, 2H), 7.86 (d, J = 8.4 Hz, 2H), 7.72 (t, J = 8.4 Hz, 2H), 7.67 (d, J = 2.0 Hz, 1H), 7.50 (m, 4H), 7.41 (d, J = 9.2 Hz, 1H), 7.32 (d, J = 2.1 Hz, 1H), 7.21 (d, J = 8.0 Hz, 1H), 7.12 (d, J = 8.4 Hz, 4H), 7.07 (dd, J = 8.4, 2.1 Hz, 1H), 6.63 (m, 2H), 6.53 (m, 2H), 6.44 (d, J = 8.4 Hz, 1H), 6.36 (d, J = 8.4 Hz, 1H), 4.05 (m, 4H), 3.98 (m, 4H), 3.87 (t, J = 5.3 Hz, 8H), 2.06 (m, 4H), 1.75 – 1.88 (m, 8H), 1.45 – 1.54 (m, 8H), 1.34 – 1.42 (m, 16H), 0.91 – 0.97 (m, 12H), 0.83 – 0.90 (m, 8H), -0.67 – -0.62 (m, 8H), -0.99 – -0.91 (m, 8H). ^{13}C NMR ($CDCl_3$,100 MHz, ppm): δ 160.4, 160.3, 159.8, 157.2, 157.1, 152.3, 151.4, 150.6, 149.2, 144.6, 142.1, 139.0, 138.6, 133.3, 132.7, 132.6, 132.5, 132.0, 131.3, 131.0, 130.6, 130.4, 130.3, 129.4, 128.0, 127.8, 125.2, 122.4, 122.2, 120.3, 118.6, 117.9, 115.8, 115.2, 109.8, 105.6, 105.4, 104.9, 100.5, 100.4, 95.6, 92.8, 71.4, 68.6, 68.3, 68.3, 31.8, 31.7, 31.6, 30.9, 29.8, 29.6, 29.5, 29.4, 29.3, 29.2, 26.1, 26.0, 25.9, 25.9, 25.4, 22.8, 22.8, 14.3, 14.2, 14.2. MS (MALDI-TOF): [M] calcd for $C_{108}H_{118}BrN_5O_8SZn$, 1787.72; Found, 1787.62. FT-IR (neat, cm^{-1}): 3756 (w), 3449 (br), 2924 (s), 2858 (m), 16352 (w), 1601 (m), 1464 (s), 1384 (w), 1301 (m), 1245 (m), 1180 (m), 1091 (m), 1000 (m), 792 (w), 722 (w), 630 (w), 484 (w). m.p.: 221–223^{o}C.

Synthesis of compound 5a. In a three-neck 100 mL flask, **4a** (77 mg, 0.051 mmol), methyl 4-ethynylbenzoate (24 mg, 0.152 mmol), $Pd_2(dba)_3$ (23 mg, 0.025 mmol), and $AsPh_3$ (31 mg, 0.101 mmol) were mixed in dry THF (21 mL) and Et_3N (7 mL) under nitrogen. After the mixture was refluxed for 12 h, the solvent was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, CH_2Cl_2 : PE = 2 : 1). Recrystallization from CH_2Cl_2/MeOH to afford **5a** as a dark green powder (51 mg, yield 61%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.69 (d, J = 4.8 Hz, 4H), 8.90 (d, J = 4.4 Hz, 2H), 8.86 (d, J = 4.4 Hz, 2H), 8.23 (d, J = 8.4 Hz, 2H), 8.08 (d, J = 8.4 Hz, 2H), 7.79 (dd, J = 8.4, 2.0 Hz, 1H), 7.71-7.76 (m, 3H), 7.21-7.24 (m, 3H), 7.14 (d, J = 8.4 Hz, 4H), 7.00 (d, J = 8.4 Hz, 1H), 6.92 (d, J = 8.8 Hz, 1H), 6.62 (d, J = 8.4 Hz, 2H), 4.01 (s, 3H), 3.97 (t, J = 7.4 Hz, 2H), 3.92 (t, J = 6.3 Hz, 4H), 3.87 (t, J = 5.3 Hz, 8H), 1.95-1.98 (m, 2H), 1.91-1.93 (m, 4H), 1.64-1.71 (m, 4H), 1.52-1.56 (m, 2H), 1.37-1.41 (m, 8H), 1.27-1.32 (m, 8H), 0.85-0.95 (m, 17H), (-0.81)-(-0.77) (m, 8H), (-0.96)-(-0.88) (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.76, 160.34, 157.23, 151.77, 151.51, 150.72, 150.58, 145.62, 142.82, 132.34, 131.97, 131.36, 130.86, 130.67, 130.43, 130.35, 130.30, 130.23, 130.07, 129.88, 129.27, 129.24, 128.69, 128.40, 127.62, 127.28, 125.26, 125.16, 122.26, 119.04, 117.59, 115.64, 115.03, 114.31, 109.79, 105.49, 101.77, 99.01, 96.54, 96.03, 95.02, 92.64, 71.36, 68.74, 52.30, 47.78, 31.57, 30.64, 30.42, 29.44, 29.19, 26.91, 26.77, 25.87, 25.30, 25.16, 22.70, 14.16, 14.08. MS (MALDI-TOF): [M] calcd for $C_{100}H_{105}N_5O_8SZn$, 1599.70; Found, 1599.76. FT-IR (neat, cm^{-1}): 3452 (br), 2923 (s), 2858 (s), 2188 (w), 1719 (m), 1592 (m), 1458 (s), 1389 (w), 1338 (w), 1273 (s), 1243 (s), 1210 (w), 1095 (s), 1000 (m), 967 (w), 791 (w), 723 (w), 641 (w), 480 (w). m.p.: 172–173^{o}C.

Synthesis of compound 5b. It was prepared in a similar way with that of **5a** using **4b** (114 mg, 0.071 mmol) as the starting material. Dark green powder, 75 mg, yield 63%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.69 (d, J = 4.8 Hz, 2H), 9.66 (d, J = 4.8 Hz, 2H), 8.90 (d, J = 4.4 Hz, 2H), 8.85 (d, J = 4.4 Hz, 2H), 8.23 (d, J = 8.4 Hz, 2H), 8.08 (d, J = 8.4 Hz, 2H), 7.73 (t, J = 8.2 Hz, 2H), 7.58 (d, J = 2.0 Hz, 1H), 7.42 (d, J = 8.4 Hz, 4H), 7.18 (d, J = 2.4 Hz, 1H), 7.13 (d, J = 8.4 Hz, 4H), 7.01 (dd, J = 8.4, 2.0 Hz, 1H), 6.93 (d, J = 8.8 Hz, 2H), 6.76 (d, J = 8.8 Hz, 2H), 6.23 (d, J = 8.4 Hz, 1H), 6.18 (d, J = 8.4 Hz, 1H), 4.04 (t, J = 6.2 Hz, 4H), 3.97-4.01 (m, 5H), 3.86 (t, J = 5.3 Hz, 8H), 1.86-1.88 (m, 4H), 1.78-1.82 (m, 2H), 1.69-1.73 (m, 4H), 1.46-1.51 (m, 2H), 1.30-1.37 (m, 8H), 1.20-1.22 (m, 8H), 0.90-0.94 (m, 4H), 0.79-0.87 (m, 13H), (-0.86)-(-0.81) (m, 8H), (-0.95)-(-0.90) (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.76, 160.33, 158.35, 157.90, 151.78, 151.49, 150.69, 150.53, 143.14, 140.97, 135.01, 132.55, 132.32, 131.89, 131.35, 130.86, 130.53, 130.38, 130.21, 129.87, 129.28, 129.22, 128.92, 127.60, 127.23, 125.18, 125.03, 124.16, 120.13, 119.95, 117.93, 117.14, 115.77, 115.61, 115.20, 114.71, 110.16, 109.80, 105.82, 102.10, 98.90, 96.56, 96.39, 94.98, 92.28, 71.37, 68.80, 68.10, 52.30, 31.63, 31.44, 30.62, 29.43, 29.31, 29.15, 25.77, 25.58, 25.29, 22.66, 22.64, 14.07. MS (MALDI-TOF): [M] calcd for $C_{106}H_{109}N_5O_9SZn$, 1691.72; Found, 1691.78. FT-IR (neat, cm^{-1}): 3449 (br), 2921 (s), 2854 (m), 2186 (w), 1719 (m), 1597 (m), 1502 (w), 1468 (s), 1383 (w), 1312 (m), 1271 (m), 1242 (m), 1212 (w), 1178 (w), 1096 (s), 1000 (m), 973 (w), 794 (w), 720 (w), 631 (w), 482 (w). m.p.: 168–170^{o}C.

Synthesis of compound 5c. It was prepared in a similar way with that of **5a** using **4c** (72 mg, 0.042 mmol) as the starting material. Dark green powder, 45 mg, yield 60%. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.68 (d, J = 4.4 Hz, 2H), 9.66

(d, J = 4.8 Hz, 2H), 8.89 (d, J = 4.4 Hz, 2H), 8.84 (d, J = 4.4 Hz, 2H), 8.23 (d, J = 8.4 Hz, 2H), 8.08 (d, J = 8.4 Hz, 2H), 7.72 (t, J = 8.2 Hz, 2H), 7.56 (d, J = 2.0 Hz, 1H), 7.40-7.44 (m, 2H), 7.17 (t, J = 8.2 Hz, 1H), 7.13 (d, J = 8.4 Hz, 4H), 7.05 (d, J = 2.0 Hz, 1H), 6.88 (dd, J = 8.4, 2.0 Hz, 1H), 6.75 (d, J = 8.4 Hz, 2H), 6.60 (d, J = 8.4 Hz, 2H), 6.23 (d, J = 8.4 Hz, 1H), 6.16 (d, J = 8.4 Hz, 1H), 4.03 (t, J = 6.4 Hz, 4H), 4.01 (s, 3H), 3.90 (t, J = 6.4 Hz, 4H), 3.86 (t, J = 5.3 Hz, 8H), 1.93-1.94 (m, 4H), 1.66-1.73 (m, 8H), 1.35-1.43 (m, 10H), 1.28-1.32 (m, 6H), 1.24-1.27 (m, 8H), 0.84-0.91 (m, 20H), (-0.81)-(-0.76) (m, 8H), (-0.95)-(-0.89) (m, 8H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.9, 160.5, 158.2, 157.4, 151.9, 151.6, 150.8, 150.6, 132.4, 132.0, 131.5, 131.0, 130.5, 130.4, 130.3, 130.0, 129.8, 129.4, 129.3, 129.1, 128.2, 127.7, 127.3, 125.3, 119.5, 115.7, 115.2, 114.7, 110.3, 110.0, 106.0, 105.7, 102.5, 96.7, 95.1, 92.1, 71.5, 69.0, 68.8, 52.4, 31.7, 31.6, 30.7, 29.5, 29.3, 29.3, 26.0, 25.7, 25.4, 22.8, 22.7, 14.3, 14.2. MS (MALDI-TOF): [M] calcd for $C_{112}H_{121}N_5O_{10}SZn$, 1791.81; Found, 1791.84. FT-IR (neat, cm^{-1}): 3450 (br), 2957 (m), 2922 (s), 2857 (m),2188 (w), 1719 (w), 1592 (m), 1460 (s), 1385 (w), 1312 (w), 1263 (s), 1208 (w), 1096 (s), 1033 (m), 802 (s), 721 (w), 471 (w). m.p.: 167–169°C.

Synthesis of compound 5d. It was prepared in a similar way with that of **5a** using **4d** (200 mg, 0.110 mmol) as the starting material. Dark green powder, 128 mg, yield 61%. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 9.68 (d, J = 4.6 Hz, 2H), 9.65 (d, J = 4.6 Hz, 2H), 8.88 (d, J = 4.6 Hz, 2H), 8.84 (d, J = 4.6 Hz, 2H), 8.23 (d, J = 8.4 Hz, 2H), 8.08 (d, J = 8.4 Hz, 2H), 7.85 (d, J = 8.4 Hz, 2H), 7.72 (t, J = 8.4 Hz, 2H), 7.65 (d, J = 1.6 Hz, 1H), 7.48 – 7.50 (m, 3H), 7.40 (d, J = 8.8 Hz, 1H), 7.26 – 7.31 (m, 1H), 7.20 (d, J = 8.8 Hz, 1H), 7.13 (d, J = 8.4 Hz, 4H), 7.00 – 7.07 (m, 1H), 6.62 – 6.64 (m, 2H), 6.51 – 6.53 (m, 2H), 6.42 (d, J = 8.4 Hz, 1H), 6.34 (dd, J = 8.4, 3.0 Hz, 1H), 4.03 – 4.06 (m, 4H), 4.01 (s, 3H), 3.94 – 3.98 (m, 4H), 3.86 (t, J = 5.3 Hz, 8H), 1.99 (t, J = 3.3 Hz, 4H), 1.75 – 1.86 (m, 8H), 1.46 – 1.55 (m, 8H), 1.34 – 1.39 (m, 16H), 0.91 – 0.96 (m, 12H), 0.83 – 0.88 (m, 8H), -0.75 – -0.70 (m, 8H), -0.97 – -0.89 (m, 8H). ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 166.9, 160.4, 160.4, 160.3, 159.8, 157.2, 157.1, 156.3, 155.5, 151.9, 151.6, 150.8, 150.7, 144.6, 144.5, 142.5, 142.1, 139.1, 139.0, 138.6, 138.5, 133.7, 133.4, 132.4, 132.1, 131.5, 131.3, 130.9, 130.6, 130.5, 130.4, 130.3, 130.0, 129.4, 129.3, 127.9, 125.3, 123.6, 122.4, 122.4, 122.2, 120.3, 120.2, 118.8, 118.6, 118.0, 117.9, 115.8, 115.7, 109.8, 105.6, 105.4, 103.1, 101.7, 101.7, 100.6, 99.7, 99.0, 96.8, 96.0, 95.9, 95.1, 93.0, 92.9, 71.4, 69.7, 69.2, 68.6, 68.3, 68.3, 53.6, 52.4, 49.6, 31.8, 31.7, 31.7, 31.7, 31.6, 30.9, 29.6, 29.5, 29.4, 29.3, 29.3, 29.2, 26.1, 26.0, 26.0, 25.9, 25.9, 25.8, 25.4, 22.8, 22.8, 22.8, 22.7, 14.3, 14.2, 14.2, 14.2. MS (MALDI-TOF): [M] calcd for $C_{118}H_{125}N_5O_{10}SZn$, 1867.84; Found, 1867.88. FT-IR (neat, cm^{-1}): 3444 (br), 3054 (w), 2922 (s), 2853 (m), 2186 (w), 1729 (s), 1650 (s), 1597 (s), 1495 (w), 1464 (s), 1382 (w), 1339 (m), 1274 (s), 1247 (m), 1184 (s), 1099 (s), 990 (m), 882 (w), 854 (w), 793 (w), 764 (m), 738 (w), 694 (s), 596 (w), 555 (w), 527 (w), 475 (w). m.p.: 162–163°C.

Synthesis of compound XW48. In a 100 mL three-neck flask, **5a** (50 mg, 0.031 mmol) and $LiOH{\cdot}H_2O$ (52 mg, 1.248 mmol) were mixed in THF (15 mL) and H_2O (2 mL) under nitrogen. After refluxing for 6 h the mixture was poured into water, extracted with DCM, filtered, and dried over anhydrous Na_2SO_4. Then the solvent was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, DCM : MeOH = 15 : 1), followed by recrystallization from DCM/MeOH to afford the product as dark green powder (43 mg, yield 88%). ^{1}H NMR ($CDCl_3$: DMSO-d_6 = 1 : 2, 400 MHz, ppm): δ 13.04 (s, 1H), 9.56 (d, J = 4.4 Hz, 2H), 9.54 (d, J = 4.4 Hz, 2H), 8.72 (d, J = 4.4 Hz, 2H), 8.68 (d, J = 4.4 Hz, 2H), 8.20 – 8.10 (m, 4H), 7.89 – 7.82 (m, 1H), 7.78 – 7.67 (m, 4H), 7.16 (d, J = 8.4 Hz, 6H), 7.11 (m, 1H), 6.99 (d, J = 8.4 Hz, 1H), 6.65 (d, J = 8.4 Hz, 2H), 4.10 – 3.96 (m, 4H), 3.94 – 3.85 (m, 12H), 1.90 – 1.80 (m, 2H), 1.65 – 1.53 (m, 6H), 1.54 – 1.47 (m, 2H), 1.39 – 1.30 (m, 10H), 1.27 – 1.20 (m, 8H), 0.90 – 0.83 (m, 17H), -0.01 – 0.01 (m, 8H), -0.84 – -1.08 (m, 8H). MS (MALDI-TOF): [M] calcd for $C_{99}H_{103}N_5O_8SZn$, 1585.68; Found, 1585.61. FT-IR (neat, cm^{-1}): 3755 (w), 3448 (br), 2922 (s), 2854 (m), 2187 (w), 1695 (w), 1598 (m), 1504 (w), 1457 (s), 1383 (w), 1338 (w), 1242 (m), 1210 (m), 1168 (w), 1095 (s), 1000 (m), 971 (w), 793 (m), 729 (m), 615 (w), 477 (w). m.p.: 158–161°C.

Synthesis of compound XW49. It was prepared in a similar way with that of **XW48** using **5b** (100 mg, 0.059 mmol) as the starting material. Dark green powder, 88 mg, yield 89%.^{1}H NMR ($CDCl_3$: DMSO-d_6 = 1 : 2, 400 MHz, ppm): δ 13.01 (s, 1H), 9.57 (d, J = 4.8 Hz, 2H), 9.50 (d, J = 4.4 Hz, 2H), 8.72 (d, J = 4.4 Hz, 2H), 8.67 (d, J = 4.4 Hz, 2H), 8.12-8.19 (m, 4H), 7.74 (t, J = 8.4 Hz, 2H), 7.59 (d, J = 2.0 Hz, 1H), 7.45-7.50 (m, 4H), 7.20 (d, J = 2.1 Hz, 1H), 7.17 (d, J = 8.4 Hz, 4H), 7.08 (dd, J = 8.5, 2.1 Hz, 1H), 6.94 (d, J = 8.8 Hz, 2H), 6.89 (d, J = 8.8 Hz, 2H), 6.19 (d, J = 8.8 Hz, 1H), 6.12 (d, J = 8.4 Hz, 1H), 4.06 (t, J = 6.0 Hz, 4H), 3.98 (t, J = 6.4 Hz, 2H), 3.91 (t, J = 5.3 Hz, 8H), 1.71-1.78 (m, 2H), 1.60-1.67 (m, 4H), 1.43-1.47 (m, 2H), 1.25-1.35 (m, 12H), 1.15-1.17 (m, 8H), 0.86-0.91 (m, 11H), 0.75-0.79 (m, 6H), 0.00-0.01(m, 8H), (-1.02)-(-0.94) (m, 8H). [M] calcd for $C_{105}H_{107}N_5O_9SZn$, 1677.71; Found, 1677.60. FT-IR (neat, cm^{-1}): 3755 (w), 3448 (br), 2922 (s), 2854 (m), 2187 (w), 1695 (w), 1598 (m), 1504 (w), 1457 (s), 1383 (w), 1338 (w), 1242 (m), 1210 (m), 1168 (w), 1095 (s), 1000 (m), 971 (w), 793 (m), 729 (m), 615 (w), 477 (w). m.p.: 165–167°C.

Synthesis of compound XW50. It was prepared in a similar way with that of **XW48** using **5c** (76 mg, 0.042 mmol) as the starting material. Dark green powder, 66 mg, yield 88%. ^{1}H NMR (400 MHz, $CDCl_3$: DMSO-d_6 = 1 : 2, ppm): δ 9.57 (d, J = 4.5 Hz, 2H), 9.51 (d, J = 4.5 Hz, 2H), 8.74 (d, J = 4.5 Hz, 2H), 8.69 (d, J = 4.4 Hz, 2H), 8.18 (d, J = 1.5 Hz, 2H), 8.14 (d, J = 8.3 Hz, 2H), 7.74 (t, J = 8.3 Hz, 2H), 7.55 (d, J = 1.6 Hz, 1H), 7.48 (t, J = 8.6 Hz, 2H), 7.17 (m, 5H), 6.96 (d, J = 1.7 Hz, 1H), 6.88 (d, J = 8.5 Hz, 2H), 6.85 (dd, J = 8.6, 1.8 Hz, 1H), 6.64 (d, J = 8.4 Hz, 2H), 6.23 (d, J = 8.5 Hz, 1H), 6.12 (d, J = 8.5 Hz, 1H), 4.07 (t, J = 6.4 Hz, 4H), 3.95 – 3.89 (m, 12H), 2.60 – 2.56 (m, 4H), 1.70 – 1.60 (m, 8H), 1.44 – 1.18 (m, 24H), 0.92 – 0.87 (m, 14H), 0.82 (t, J = 6.7 Hz, 6H), 0.08 – -0.01 (m, 8H), -0.91 – -1.01 (m, 8H). [M] calcd for $C_{111}H_{119}N_5O_{10}SZn$, 1777.80; Found, 1777.71. FT-IR (neat, cm^{-1}): 3753 (w), 3448 (br), 2924 (s), 2859 (s), 2186 (m), 1725 (m), 1691 (m), 1634 (w), 1596 (s), 1507 (w), 1457 (s), 1382 (m), 1312 (m), 1242 (s), 1210 (m), 1170 (w), 1095 (s), 1000 (m), 969 (w), 947 (w), 855 (w), 792 (m), 728 (m), 635 (w), 553 (w), 486 (w). m.p.: 164–166°C.

Synthesis of compound XW51. It was prepared in a similar way with that of **XW48** using **5d** (80 mg, 0.043 mmol) as the starting material. Dark green powder, 67 mg, yield 85%. ^{1}H NMR ($CDCl_3$: DMSO-d_6 = 1 : 2, 400 MHz, ppm): δ 12.94 (s, 1H), 9.57 (d, J = 4.4 Hz, 2H), 9.52 (d, J = 4.4 Hz, 2H), 8.75 (d, J = 4.4 Hz, 2H), 8.71 (d, J = 4.4 Hz, 2H), 8.19 (d, J = 8.4 Hz, 2H), 8.13 (d, J = 8.4 Hz, 2H), 7.86 (d, J = 8.0 Hz, 2H), 7.74 (t, J = 8.2 Hz, 2H), 7.69 (d, J = 2.0 Hz, 1H), 7.61 – 7.65 (m, 1H), 7.56 (dd, J = 8.4, 2.0 Hz, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.38 – 7.40 (m, 1H), 7.27 – 7.29 (m, 1H), 7.16 (d, J = 8.4 Hz, 4H), 7.03 – 7.07 (m, 1H), 6.52 – 6.70 (m, 4H), 6.43 (d, J = 8.4 Hz, 1H), 6.31 (d, J = 8.4 Hz, 1H), 3.97 – 4.10 (m, 8H), 3.92 (t, J = 5.3 Hz, 8H), 1.74 – 1.82 (m, 8H), 1.46 – 1.52 (m, 8H), 1.35 – 1.39 (m, 16H), 0.90 – 0.96 (m, 20H), -0.02 – 0.04 (m, 8H), -1.00 – -0.92 (m, 8H). MS (MALDI-TOF): [M] calcd for $C_{117}H_{123}N_5O_{10}SZn$, 1853.83; Found, 1853.74. FT-IR (neat, cm^{-1}): 3753 (w), 3450 (br), 2922 (s), 2860 (s), 2187 (w), 1720 (w), 1690 (m), 1602 (s), 1499 (m), 1464 (s), 1384 (m), 1299 (m), 1242 (m), 1208 (m), 1176 (m), 1090 (s), 1001 (m), 971 (w), 827 (w), 792 (m), 720 (m), 628 (m), 481 (w). m.p.: 165–

166^{o}C.

2. Absorption and Emission Spectra

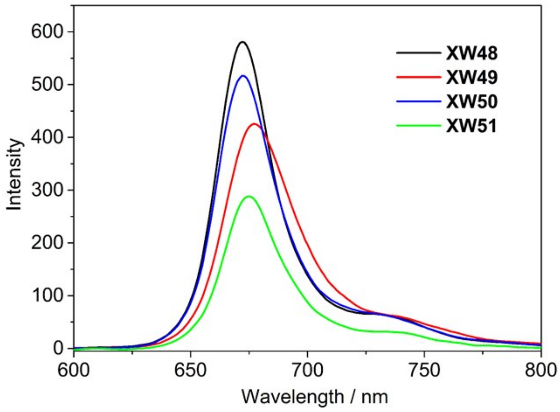

Figure S1. Emission spectra of **XW48~XW51** in THF. The spectra were used to calculate the wavelength at the intersection (λ_{inter}) of normalized absorption and emission spectra, and the corresponding $E_{0\text{-}0}$ values. Excitation wavelengths: 460 nm (**XW48**), 456 nm (**XW49**), and 455 nm (**XW50**) and 460 nm (**XW51**).

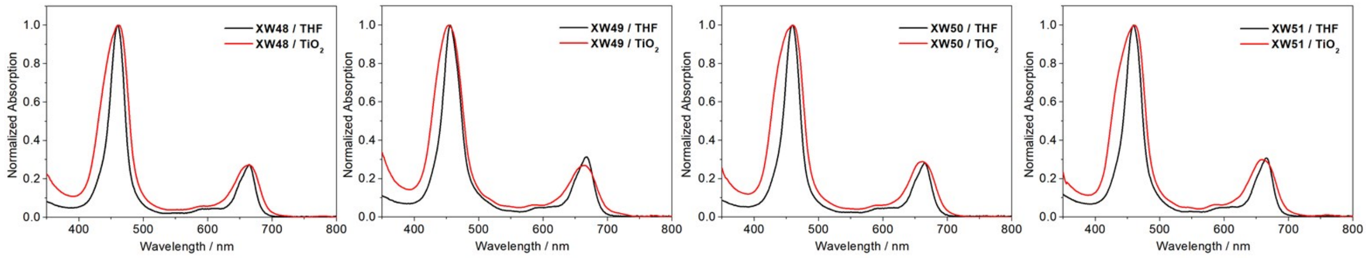

Figure S2. Normalized UV-visible spectra of porphyrins **XW48~XW51** in THF and on the TiO_2 films (3 µm).

3. Cyclic Voltammetry Curves

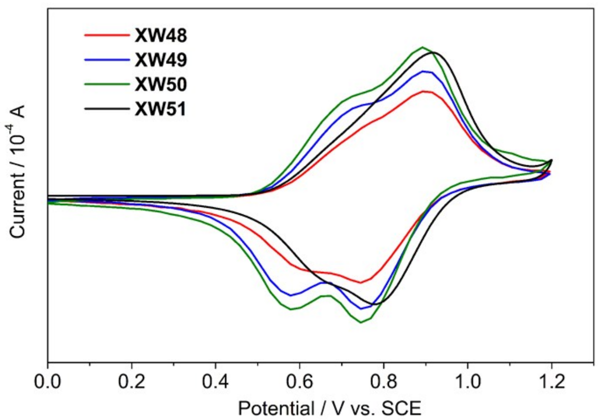

Figure S3. Cyclic voltammetry curves of the **XW48~XW51** adsorbed to a nanocrystalline TiO_2 film deposited on the conducting FTO glass.

4. The Photovoltaic Data for the DSSCs Coadsorbed with CDCA

Table S1. Photovoltaic parameters of the porphyrin sensitized solar cells coadsorbed with CDCA.

Dyes	CDCA	V_{oc}/mV	J_{sc}/mA cm^{-2}	Fill Factor (*FF*)	*PCE*/%	Dye loading amount (mol·cm^{-2})
XW51 (0.2 mM)	0 mM	781±2	20.07±0.13	0.702±0.003	11.1±0.1	1.96×10^{-7}
	1 mM	782±1	19.87±0.06	0.707±0.006	11.0±0.1	1.91×10^{-7}
	2 mM	765±2	18.92±0.16	0.718±0.004	10.4±0.1	1.68×10^{-7}
	3 mM	764±4	17.70±0.21	0.699±0.009	9.5±0.1	1.44×10^{-7}

5. Frontier Molecular Orbital Profiles

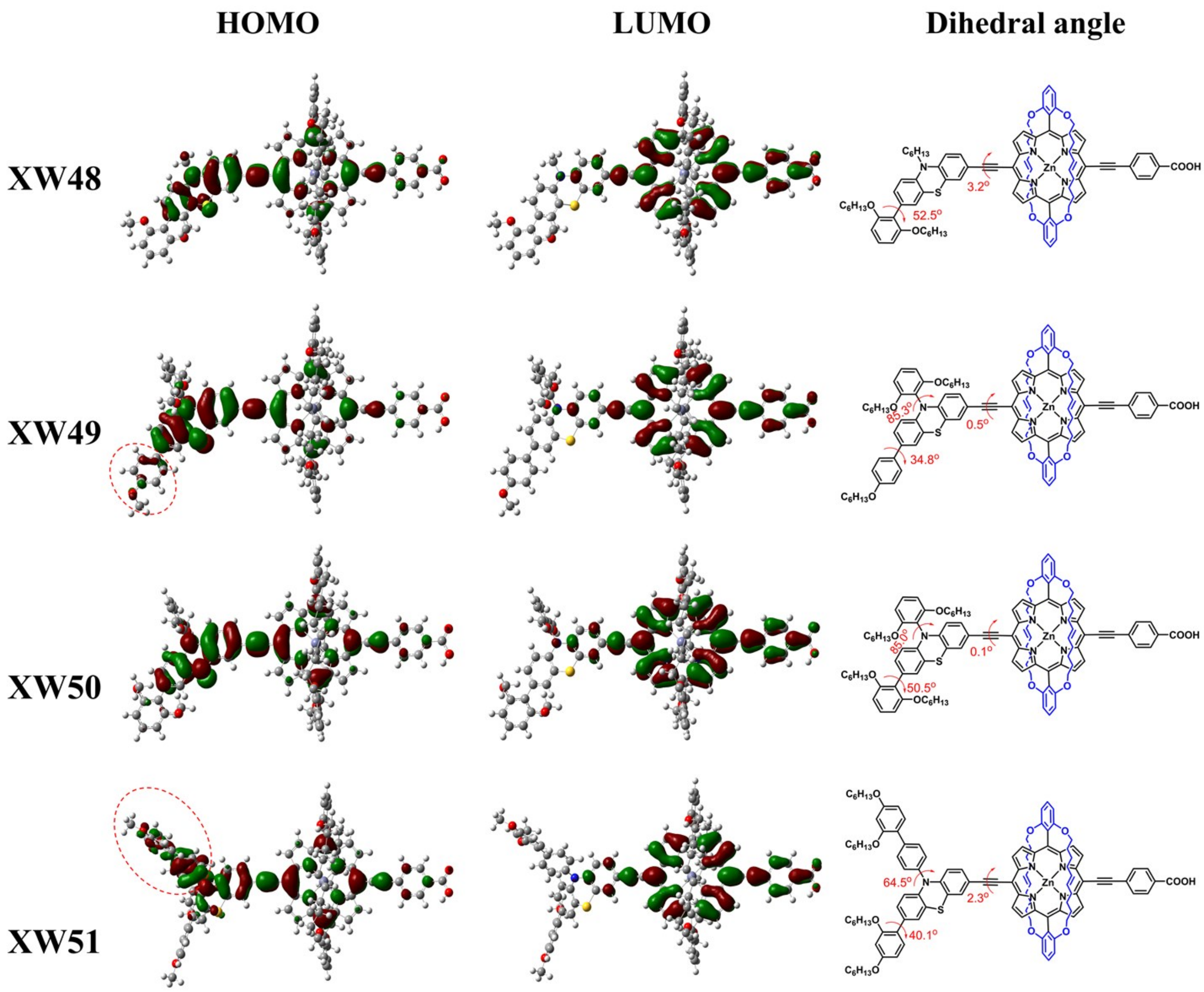

Figure S4. Frontier molecular orbital profiles and the selected dihedral angles for **XW48~XW51**.

6. *J*–V Curves and IPCE Action Spectra of DSSCs Using a Co^{3+}/Co^{2+} Electrolyte

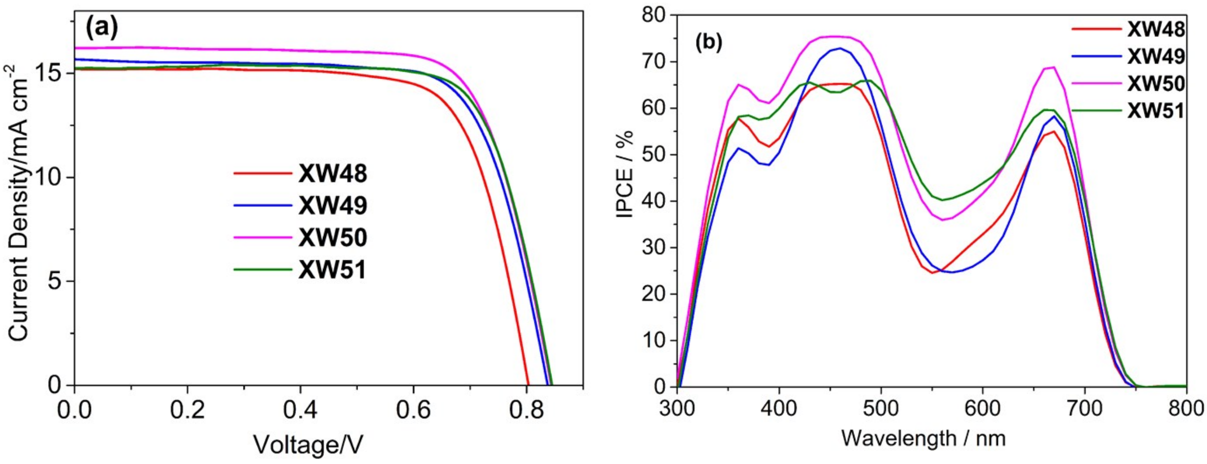

Figure S5. (a) J–V curves and (b) IPCE action spectra of DSSCs based on **XW48~XW51** using a Co^{3+}/Co^{2+} electrolyte.

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6. Characterization Spectra for the Compounds

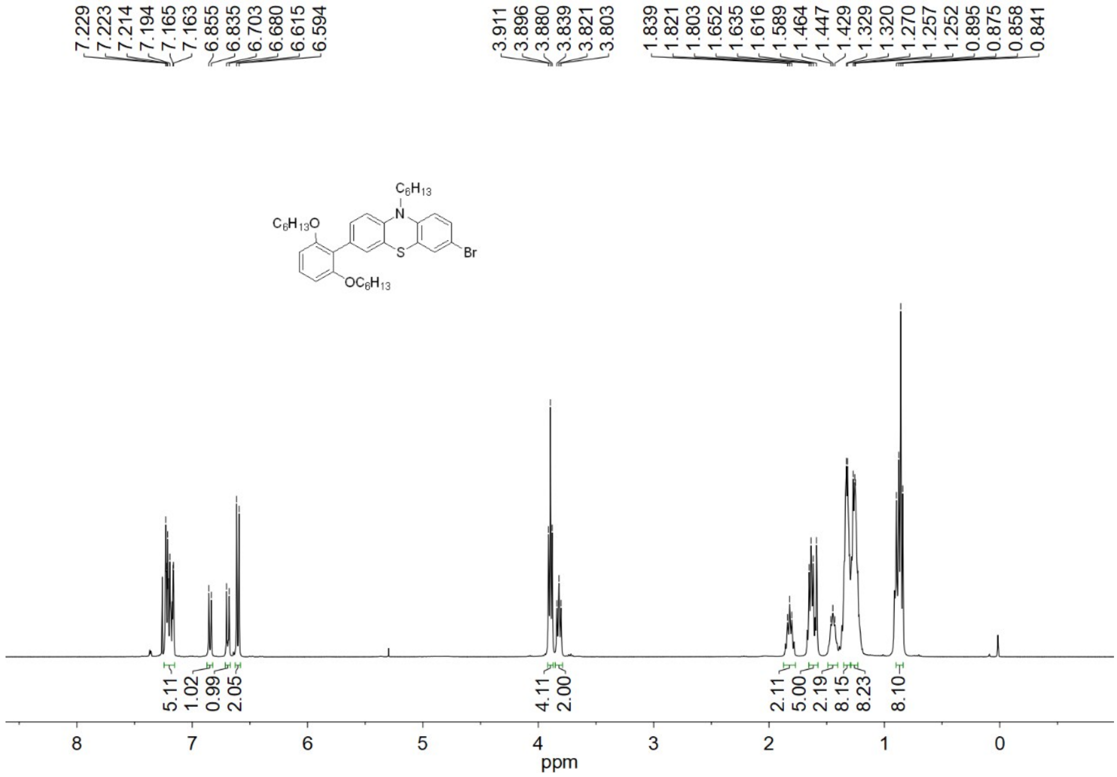


Figure S6. The ^{1}H NMR spectrum of **2a** in $CDCl_3$.

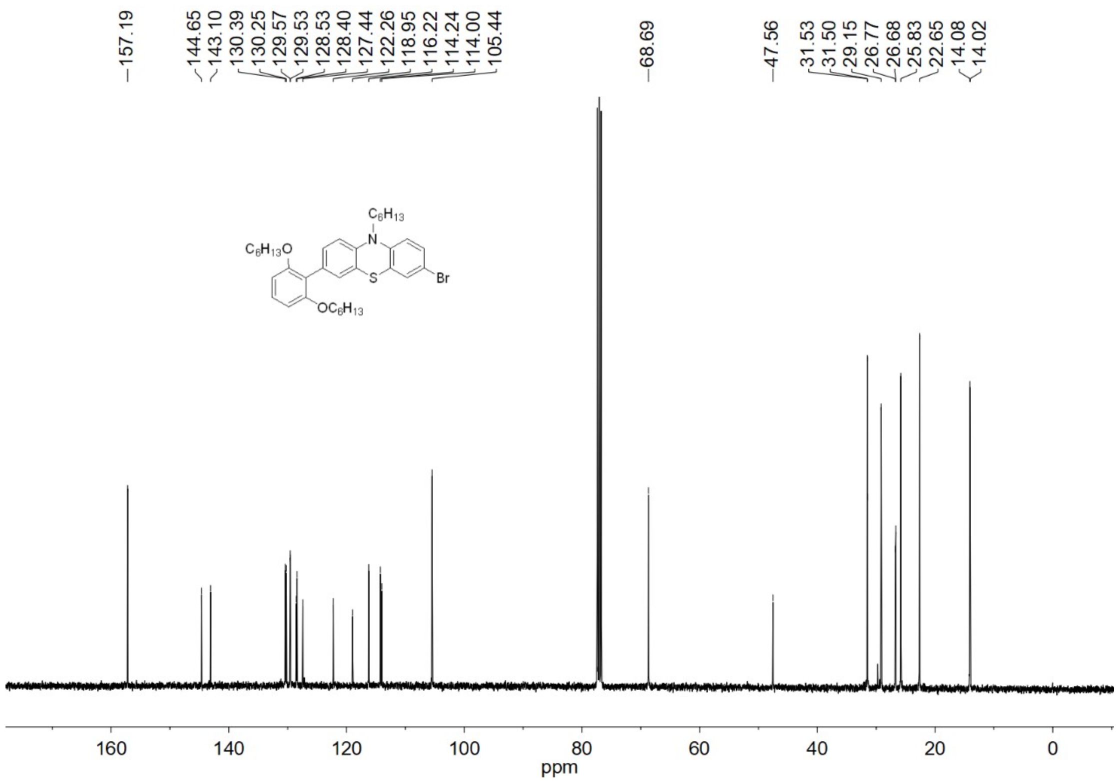


Figure S7. The ^{13}C NMR spectrum of **2a** in $CDCl_3$.

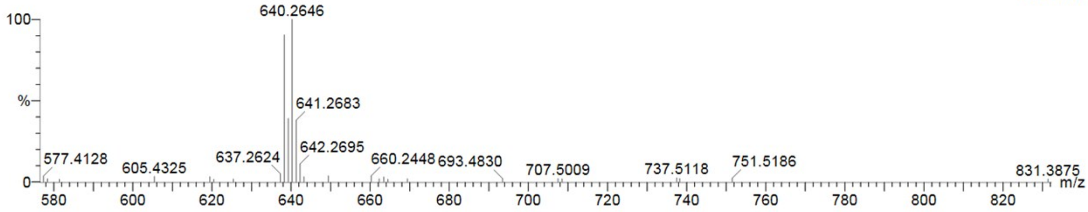
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-36 H: 0-100 N: 0-1 O: 0-2 S: 0-1 Br: 0-1

YS-XIE ECUST institute of Fine Chem 02-Jul-2017 12:42:38

XY-ZC-078 67 (0.916) Cm (66:67) 1: TOF MS ES+ 1.89e+003



Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
638.2668	638.2667	0.1	0.2	12.5	7.4	0.0	C36 H49 N O2 S Br

Figure S8. The HRMS of **2a**.

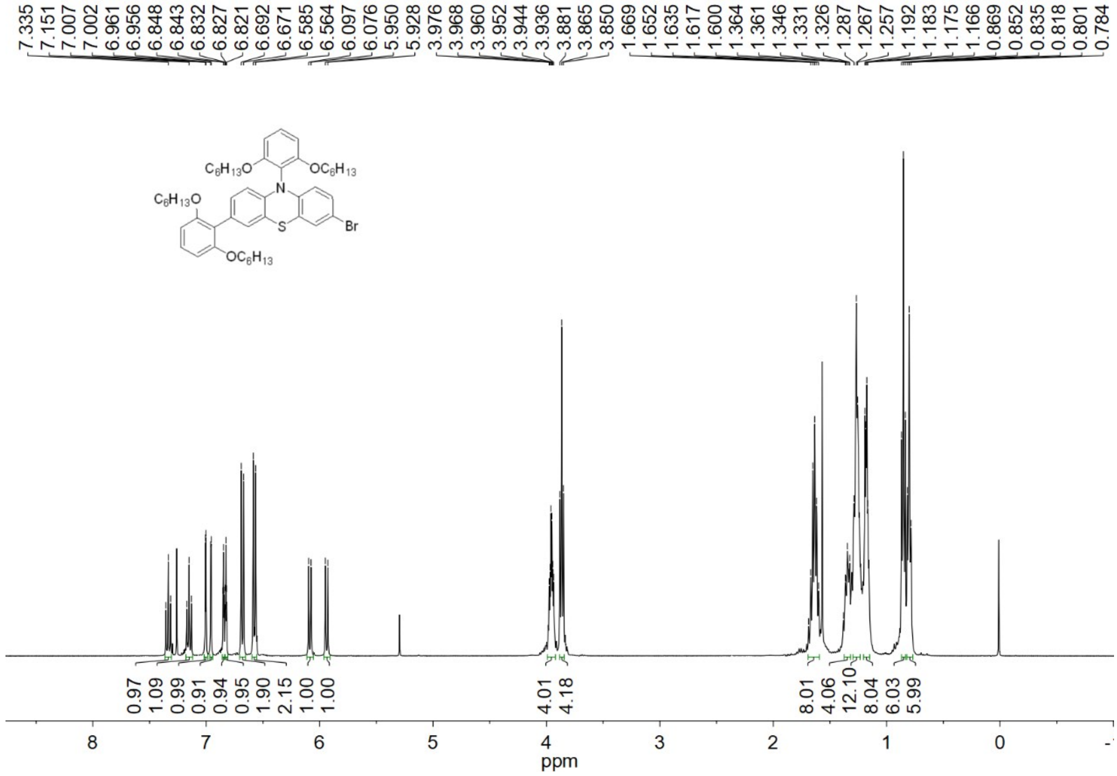


Figure S9. The ^1H NMR spectrum of **2c** in $CDCl_3$.

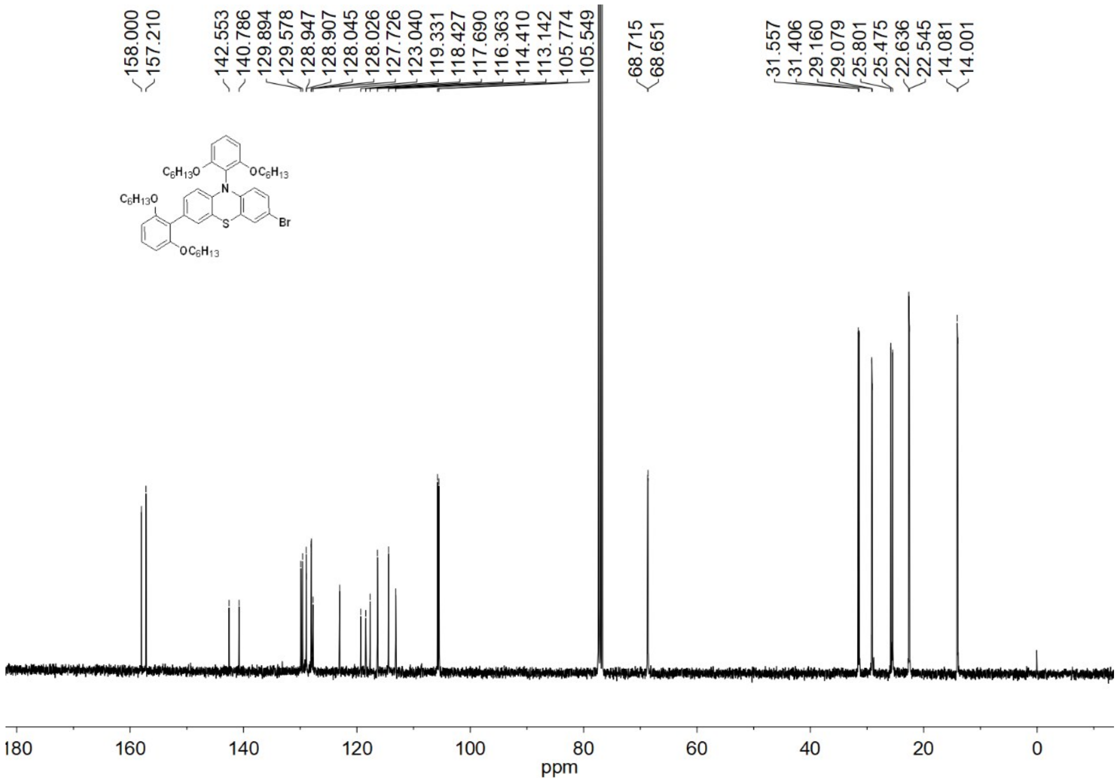


Figure S10. The ^{13}C NMR spectrum of **2c** in $CDCl_3$.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-48 H: 0-100 N: 0-1 O: 0-4 S: 0-1 Br: 0-1

YS-XIE ECUST institute of Fine Chem 02-Jul-2017 12:27:33
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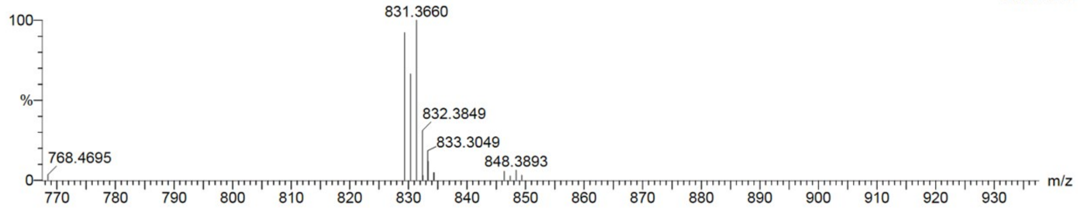


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
830.3816	830.3818	-0.2	-0.2	16.5	46.2	0.0	C48 H65 N O4 S Br

Figure S11. The HRMS of **2c**.

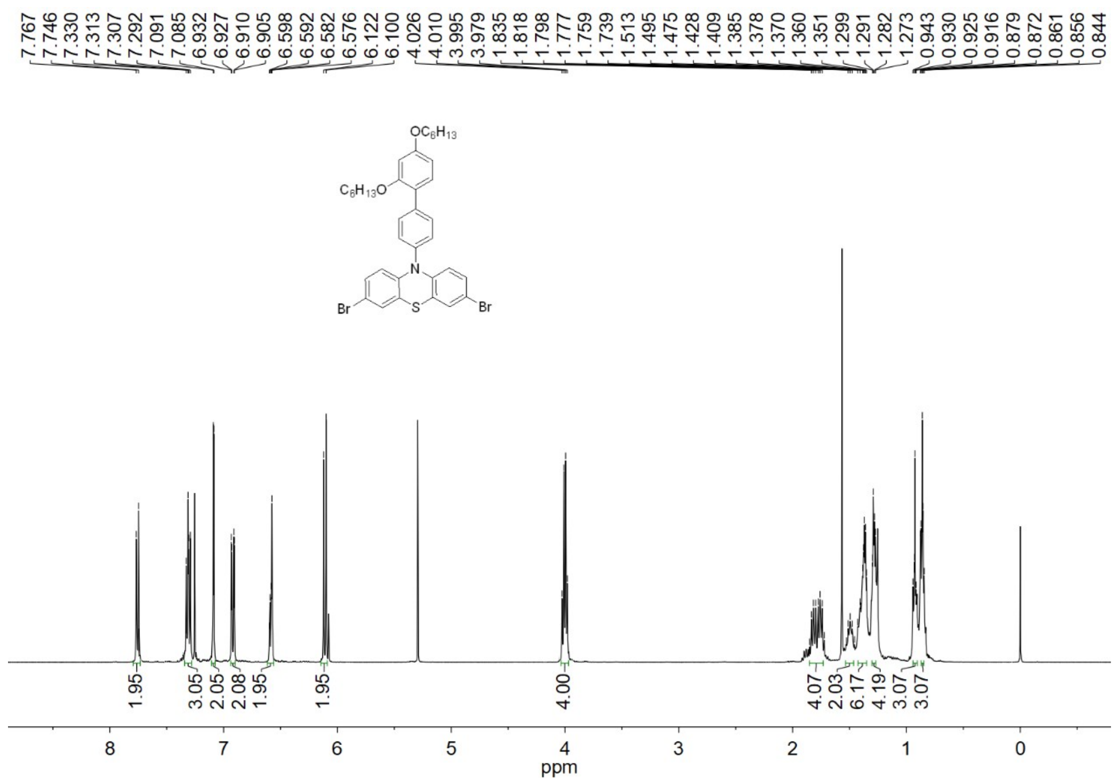


Figure S12. The ^{1}H NMR spectrum of **1c** in $CDCl_3$.

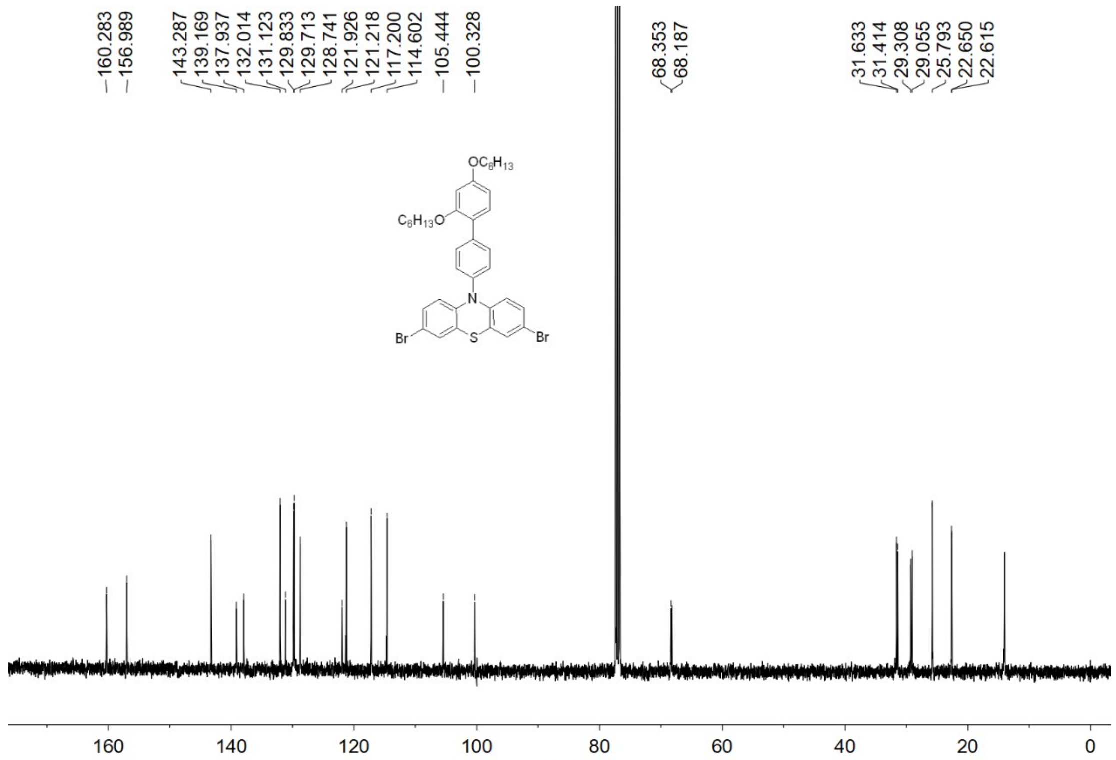


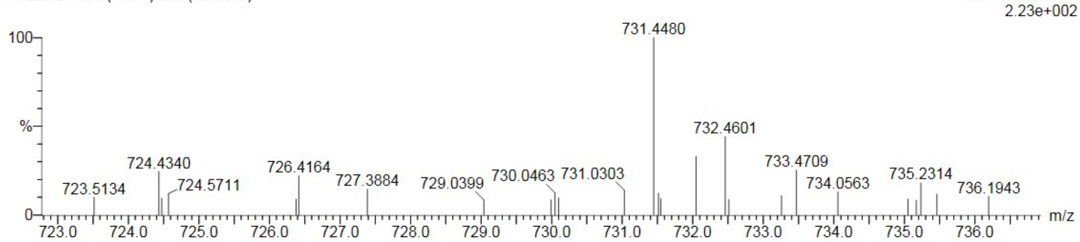
Figure S13. The ^{13}C NMR spectrum of **1c** in $CDCl_3$.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
64 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-36 H: 0-39 N: 0-1 O: 0-2 Na: 0-1 S: 0-1 Br: 0-2

YS-XIE
XY-ZD-21 126 (1.441) Cm (126:133) 1: TOF MS ES+ 2.23e+002



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
730.0992	730.0966	2.6	3.6	16.5	42.0	0.0	C36 H39 N O2 Na S Br2

Figure S14. The HRMS of **1c**.

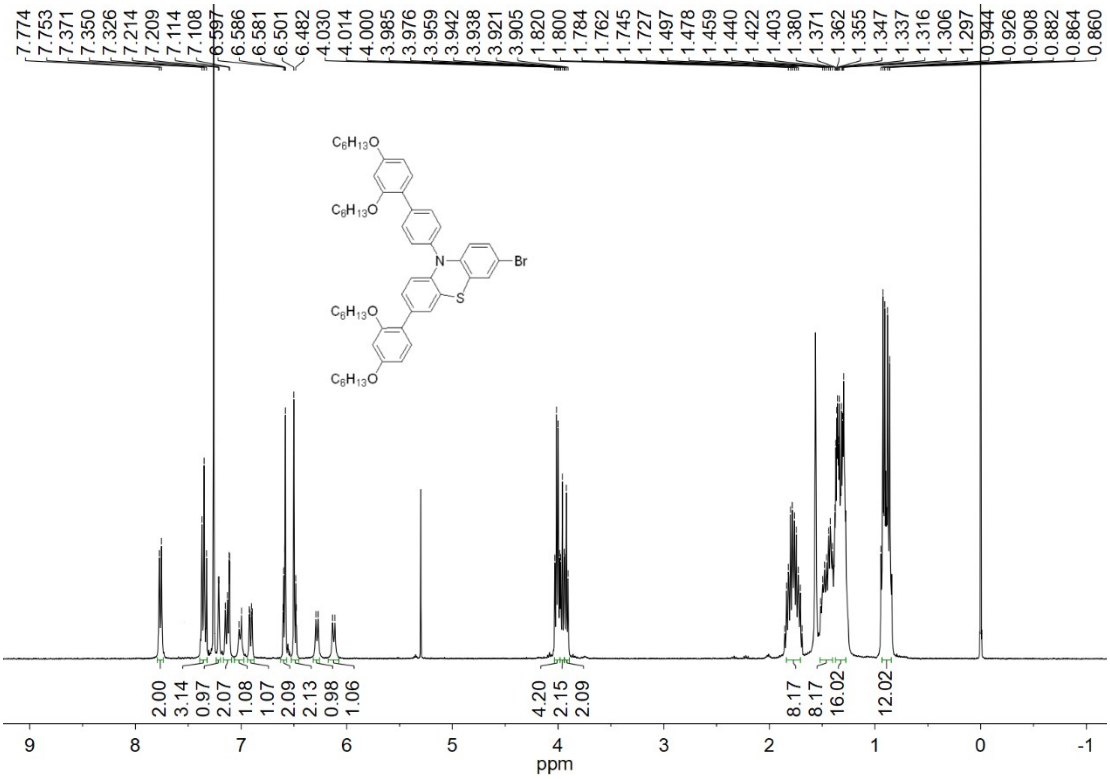


Figure S15. The ^{1}H NMR spectrum of **2d** in $CDCl_3$.

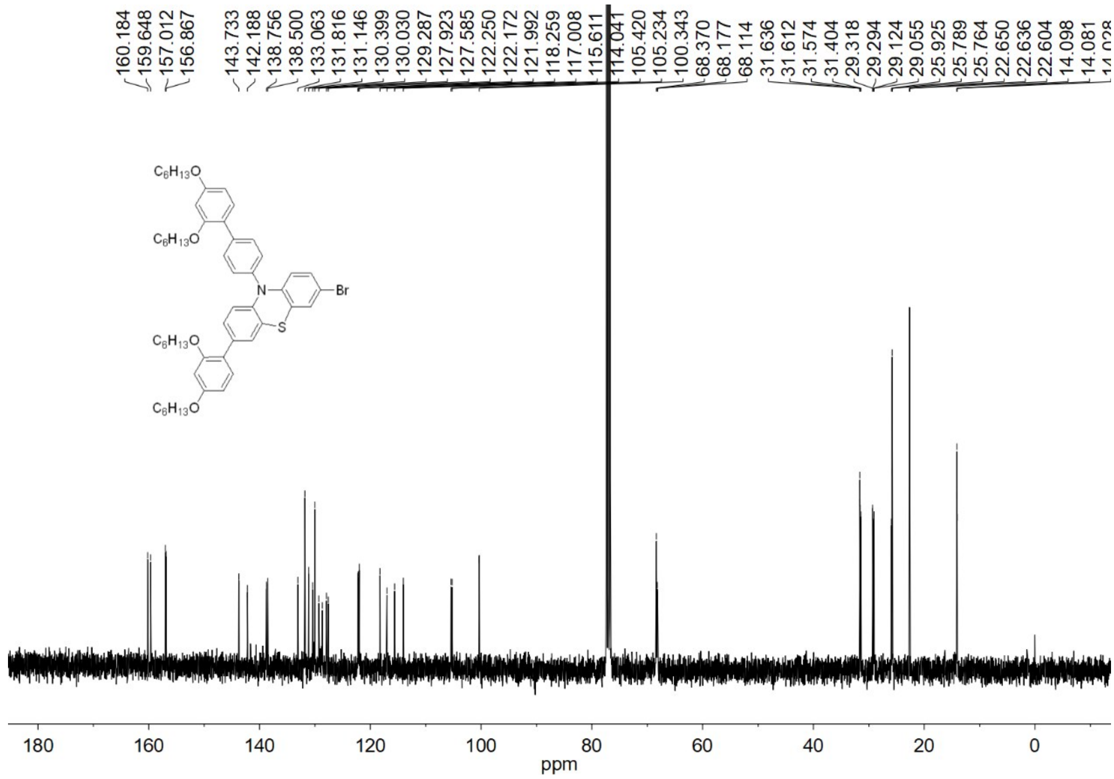


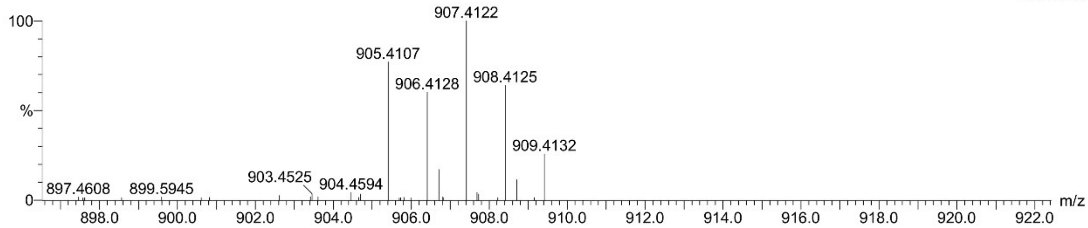
Figure S16. The ^{13}C NMR spectrum of **2d** in $CDCl_3$.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-54 H: 0-99 N: 0-1 O: 0-4 S: 0-1 Br: 0-1

YS-XIE
XY-ZD-22 112 (1.273) Cm (110:113) 1: TOF MS ES+ 1.11e+003



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
906.4128	906.4131	-0.3	-0.3	20.5	54.4	0.0	C54 H69 N O4 S Br

Figure S17. The HRMS of **2d**.

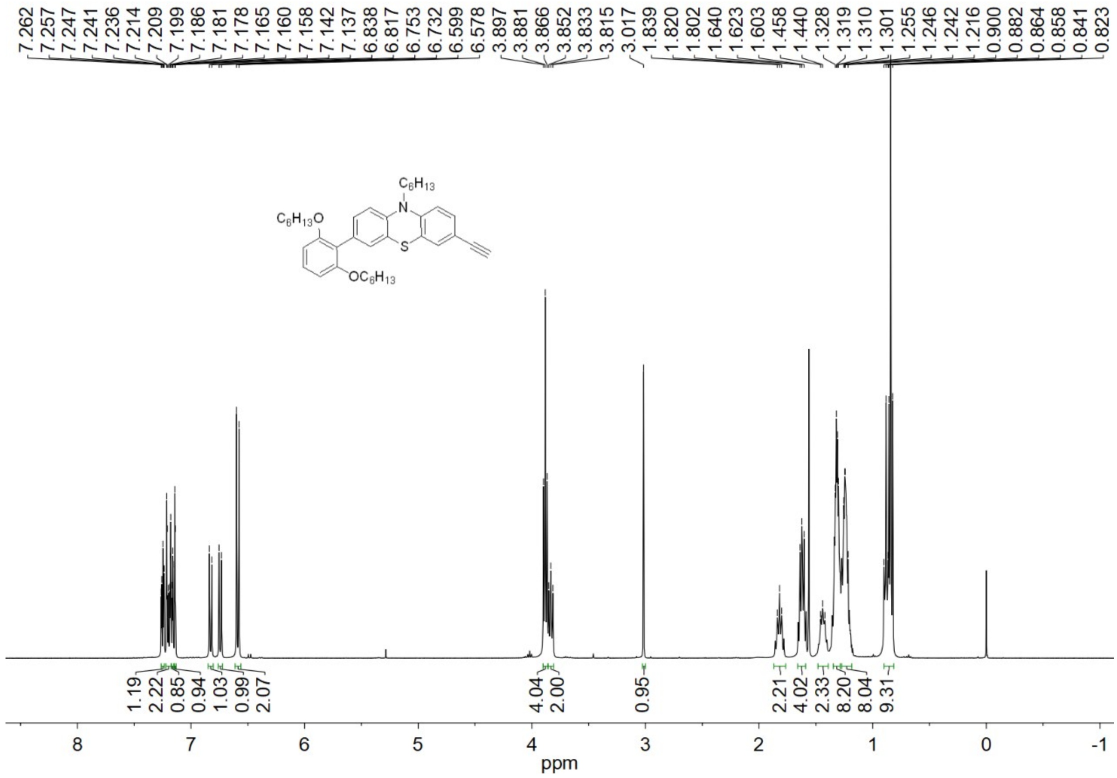


Figure S18. The ^{1}H NMR spectrum of **3a** in $CDCl_3$.

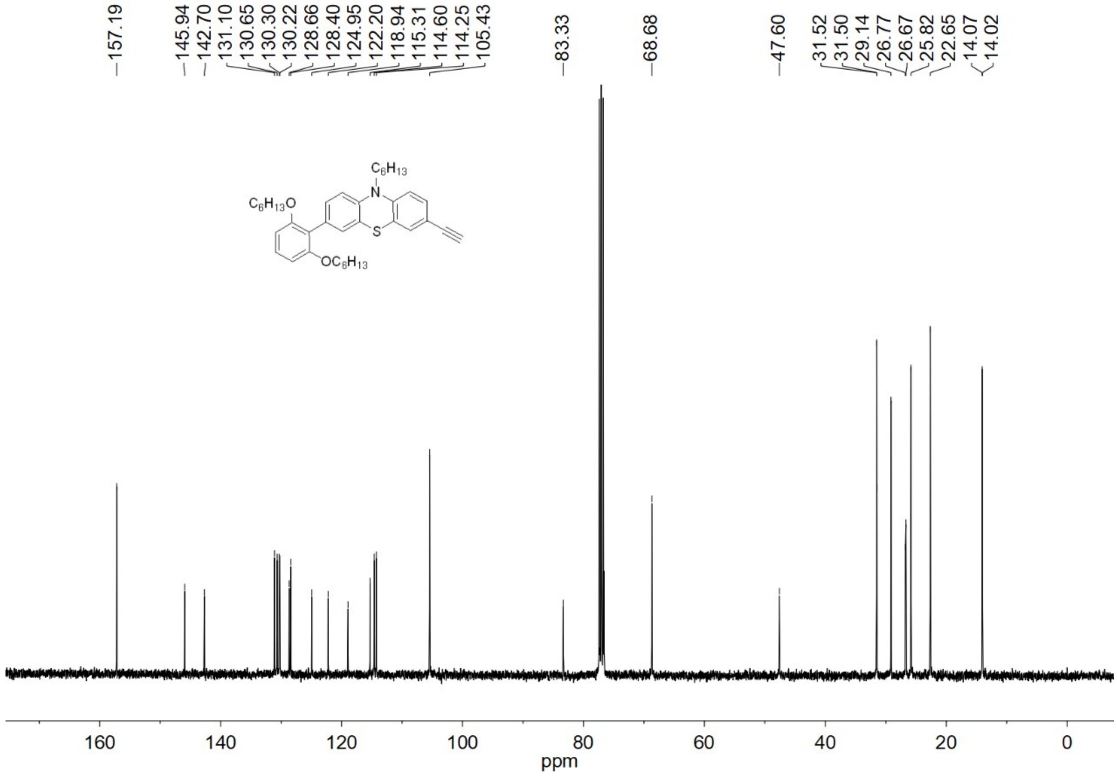
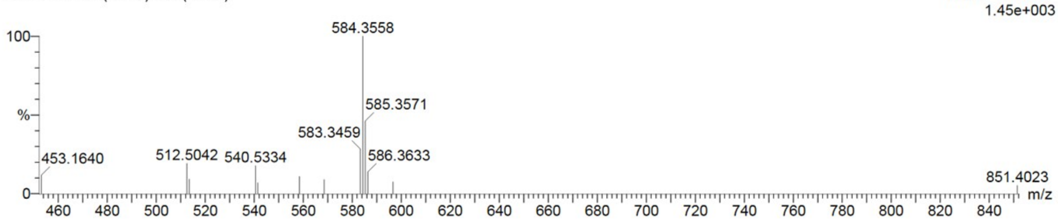


Figure S19. The ^{13}C NMR spectrum of **3a** in $CDCl_3$.

Elemental Composition Report — **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-38 H: 0-100 N: 0-1 O: 0-2 S: 0-1
YS-XIE ECUST institute of Fine Chem 02-Jul-2017
12:21:29
XY-ZC-099 55 (0.775) Cm (55:56) 1: TOF MS ES+
1.45e+003



Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
584.3558	584.3562	-0.4	-0.7	14.5	9.3	0.0	C38 H50 N O2 S

Figure S20. The HRMS of **3a**.

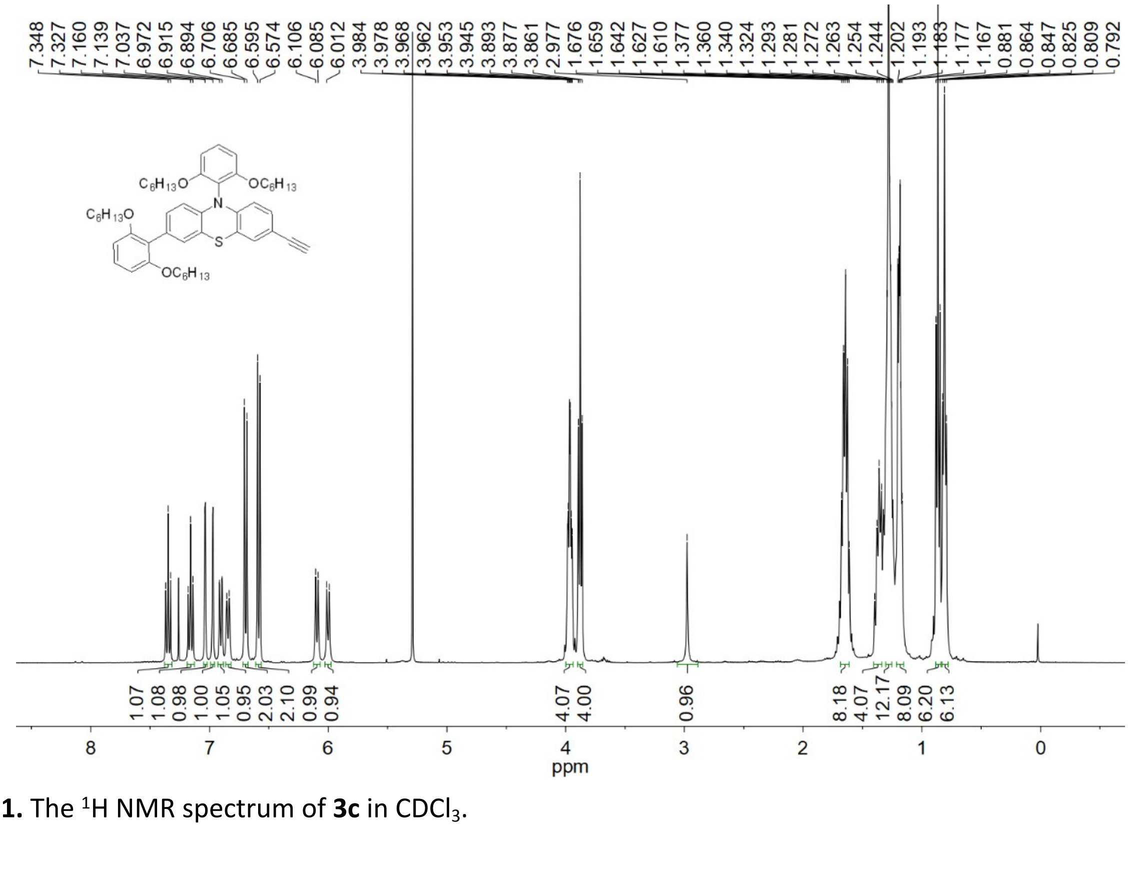


Figure S21. The ^1H NMR spectrum of **3c** in $CDCl_3$.

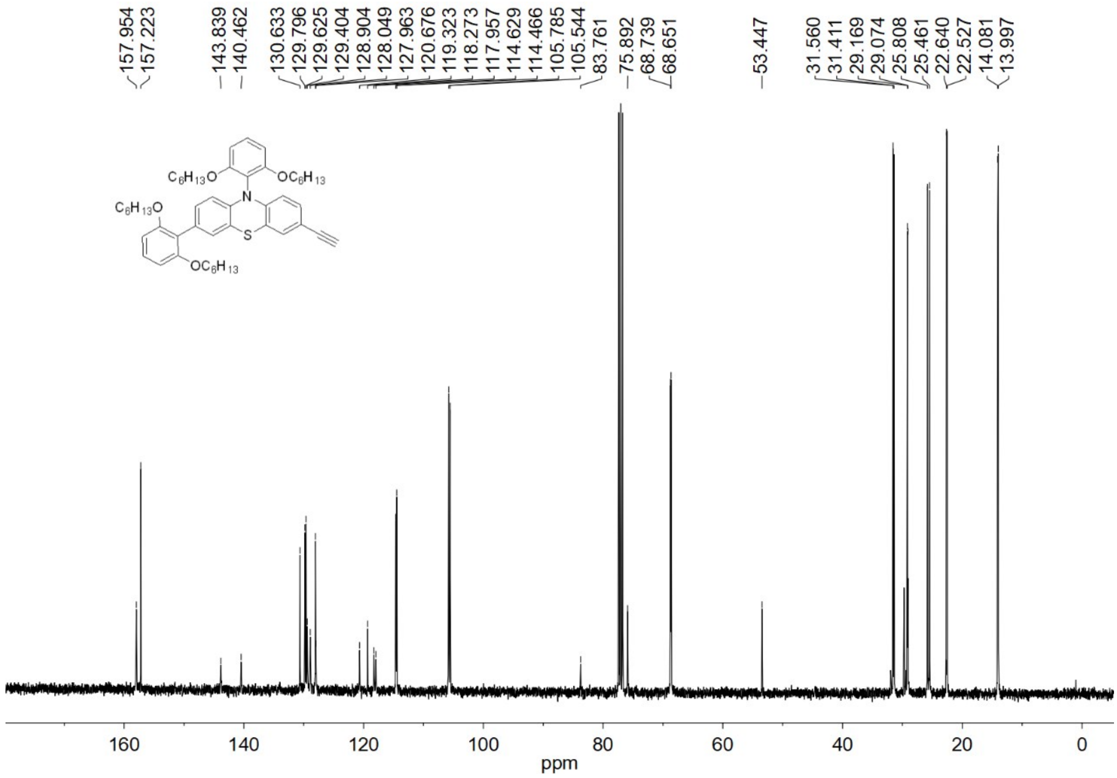
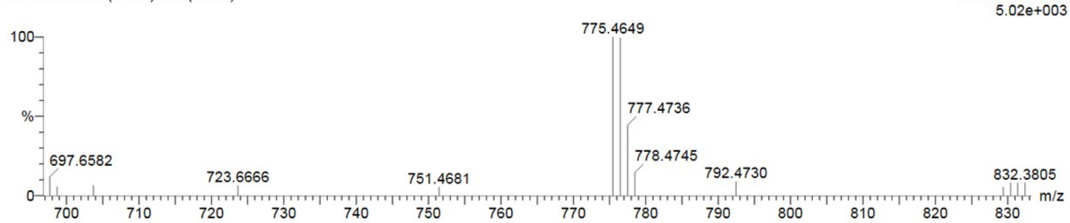


Figure S22. The ^{13}C NMR spectrum of **3c** in $CDCl_3$.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-1 O: 0-4 S: 0-1
YS-XIE ECUST institute of Fine Chem 02-Jul-2017 12:34:36
XY-ZC-102 96 (1.265) Cm (95:97) 1: TOF MS ES+ 5.02e+003



Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
776.4707	776.4713	-0.6	-0.8	18.5	15.4	0.0	C50 H66 N O4 S

Figure S23. The HRMS of **3c**.

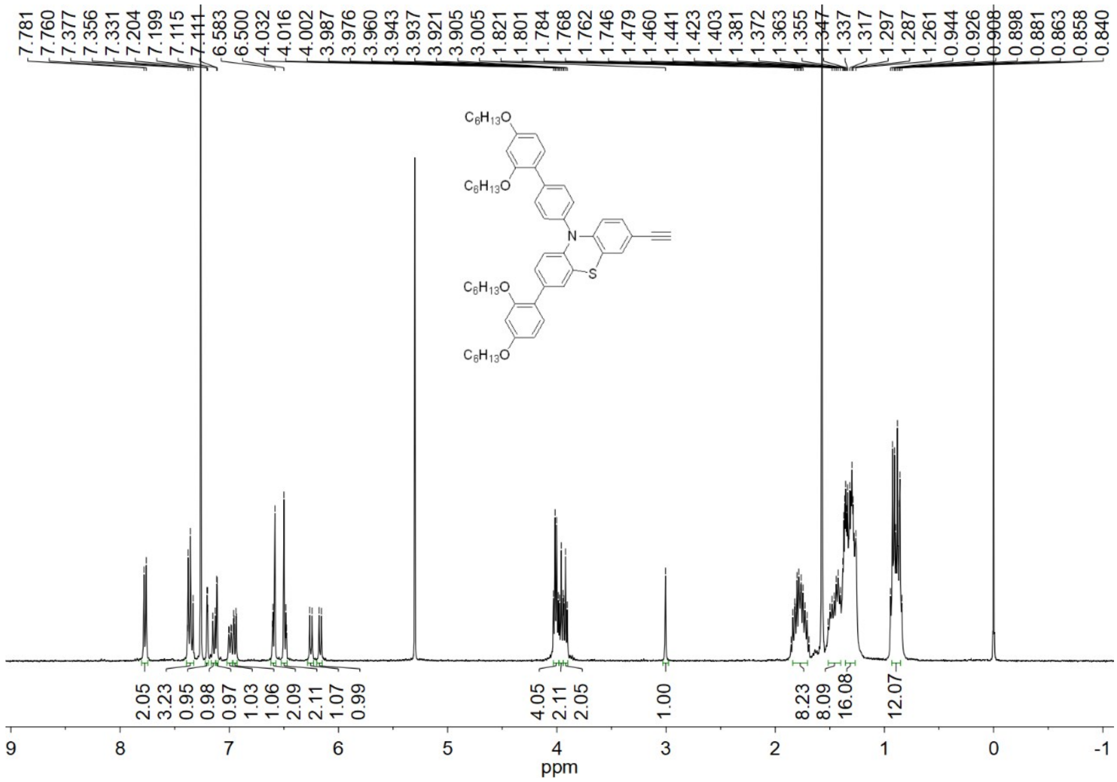


Figure S24. The ^{1}H NMR spectrum of **3d** in $CDCl_3$.

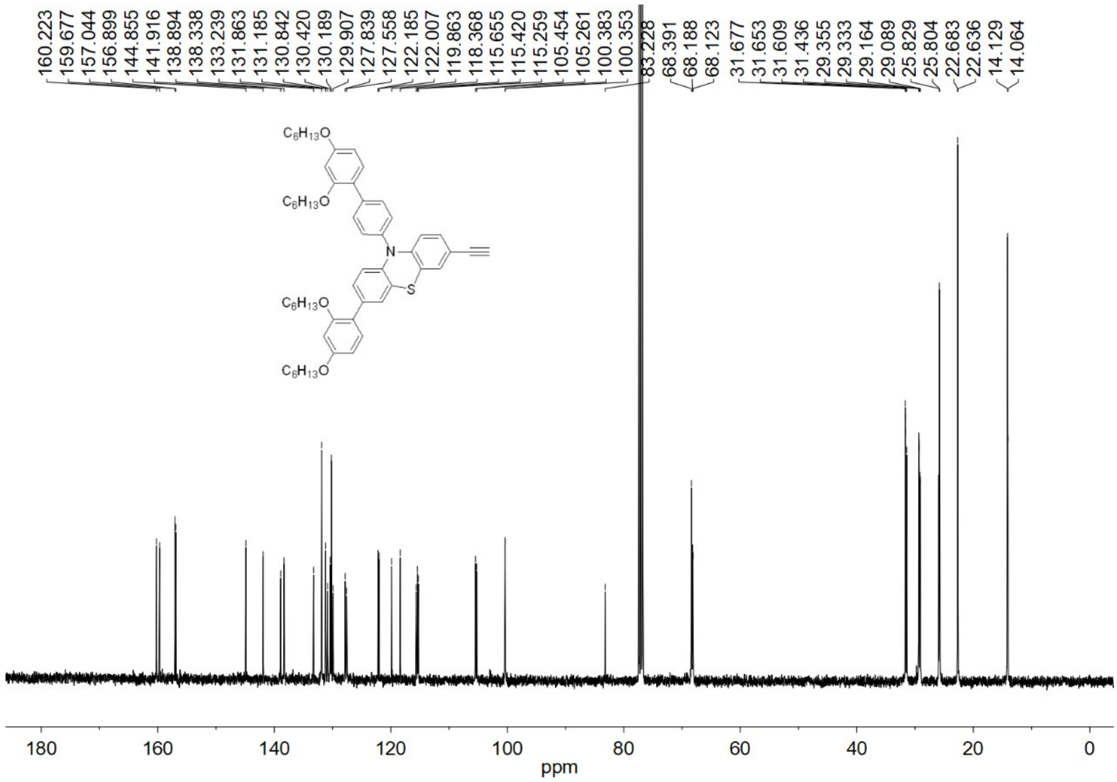


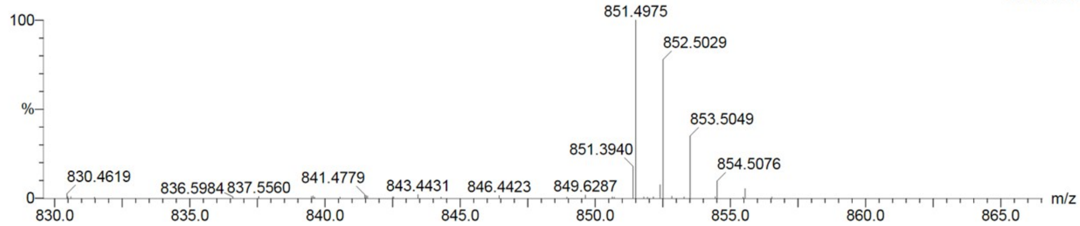
Figure S25. The ^{13}C NMR spectrum of **3d** in $CDCl_3$.

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
116 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-56 H: 0-99 N: 0-1 O: 0-4 S: 0-1 Br: 0-1

YS-XIE
XY-ZD-25 52 (0.581) Cm (50:54) 1: TOF MS ES+ 3.36e+003



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
852.5029	852.5026	0.3	0.4	22.5	27.8	0.0	C56 H70 N O4 S

Figure S26. The HRMS of **3d**.

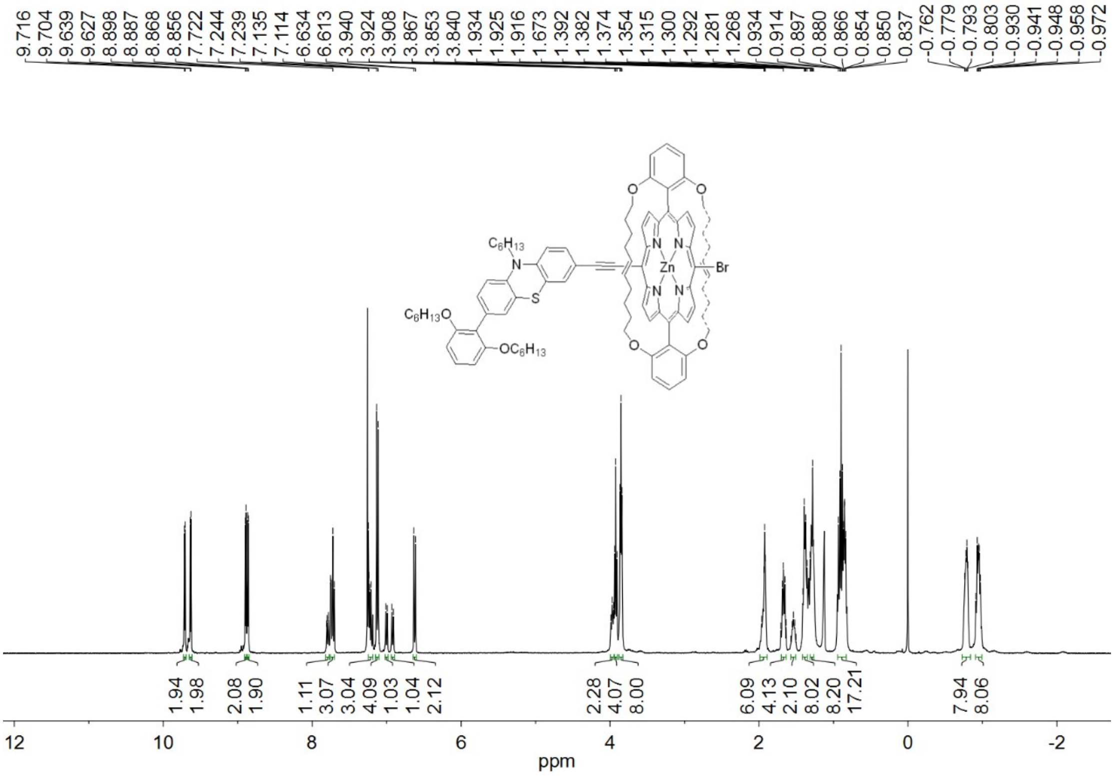


Figure S27. The ^1H NMR spectrum of **4a** in $CDCl_3$.

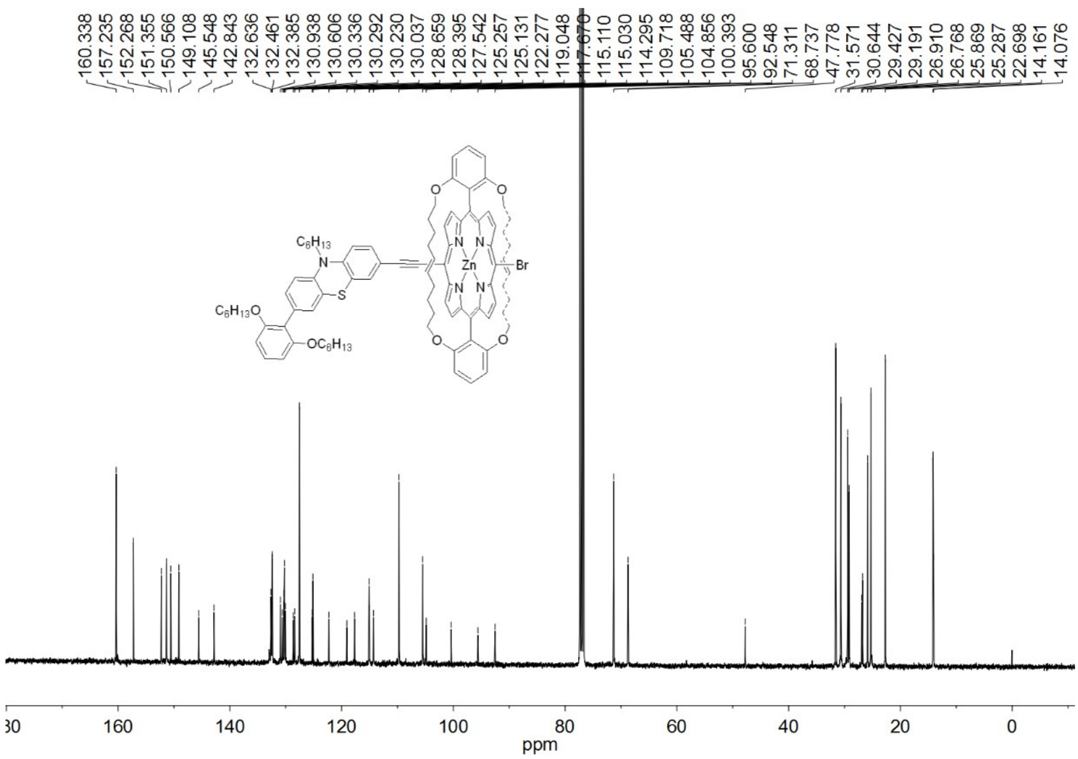


Figure S28. The ^{13}C NMR spectrum of **4a** in $CDCl_3$.

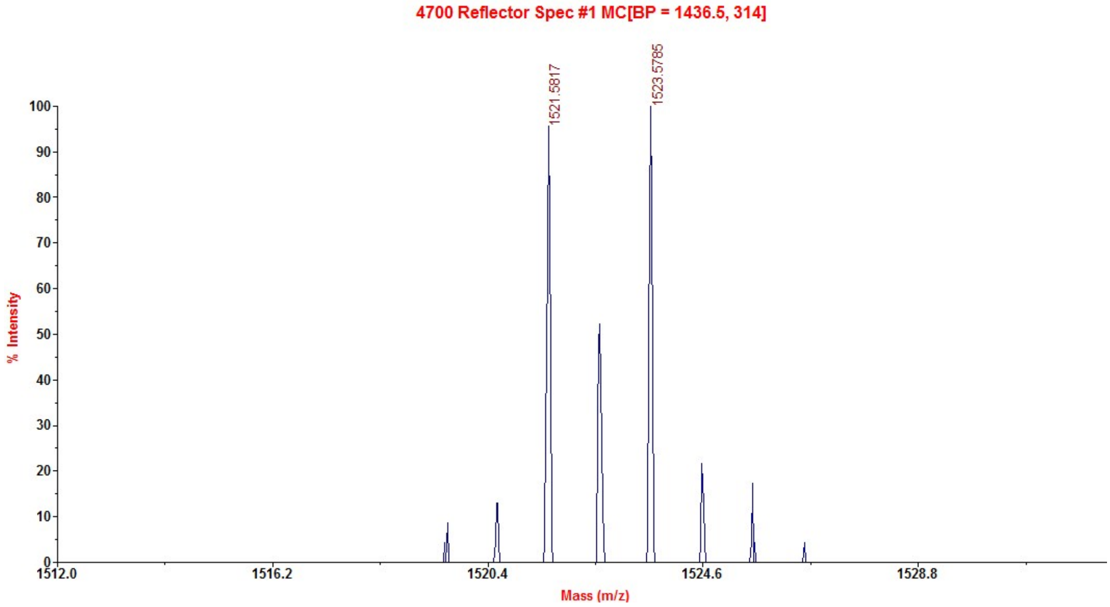


Figure S29. The HRMS of **4a**.

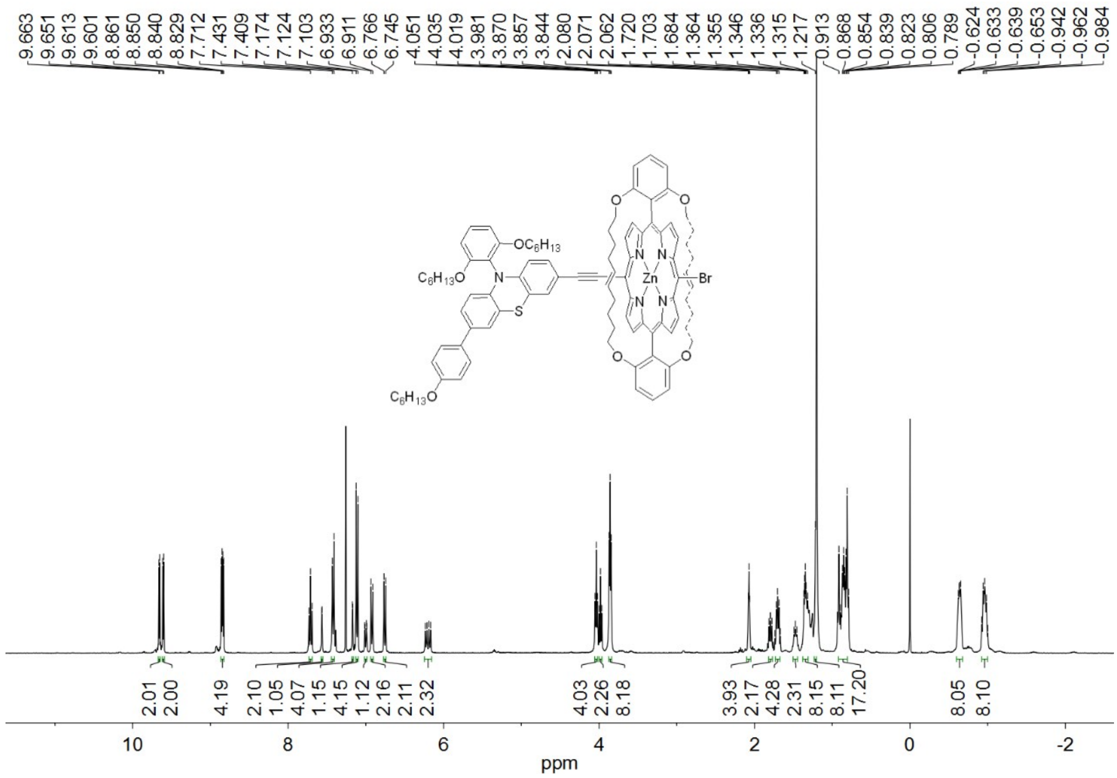


Figure S30. The ^{1}H NMR spectrum of **4b** in $CDCl_3$.

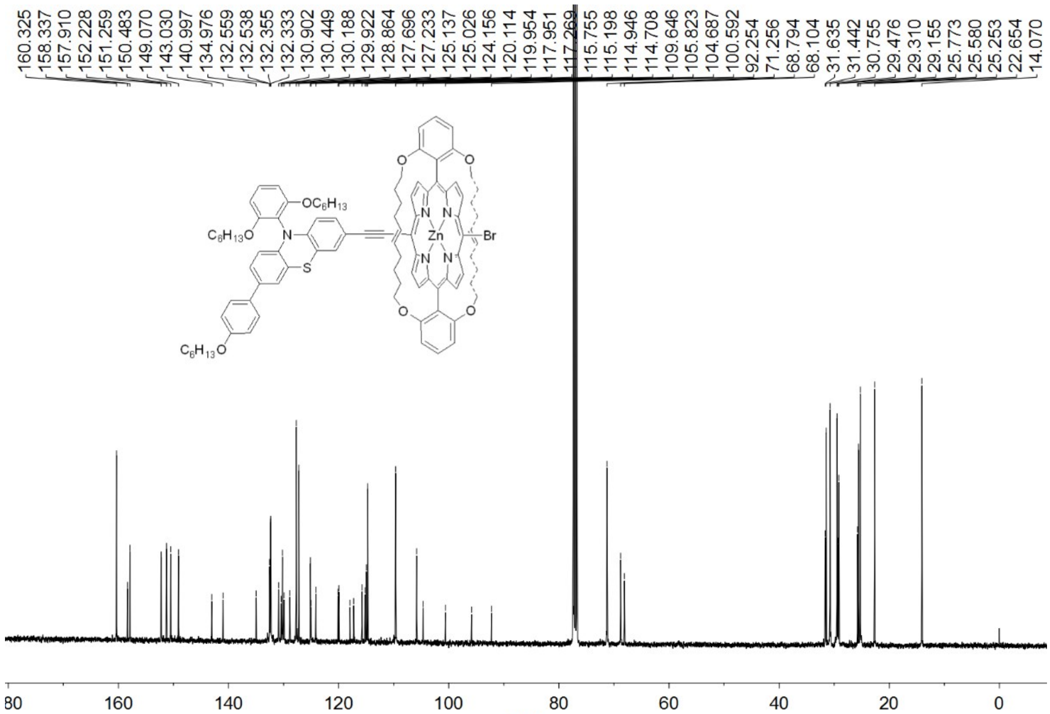


Figure S31. The ^{13}C NMR spectrum of **4b** in $CDCl_3$.

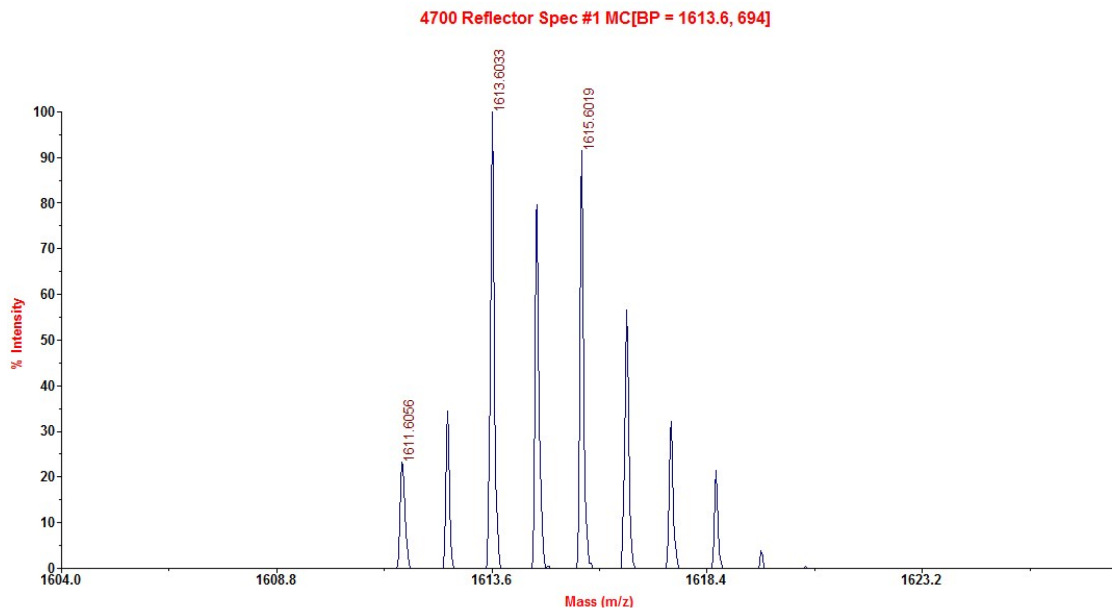


Figure S32. The HRMS of **4b**.

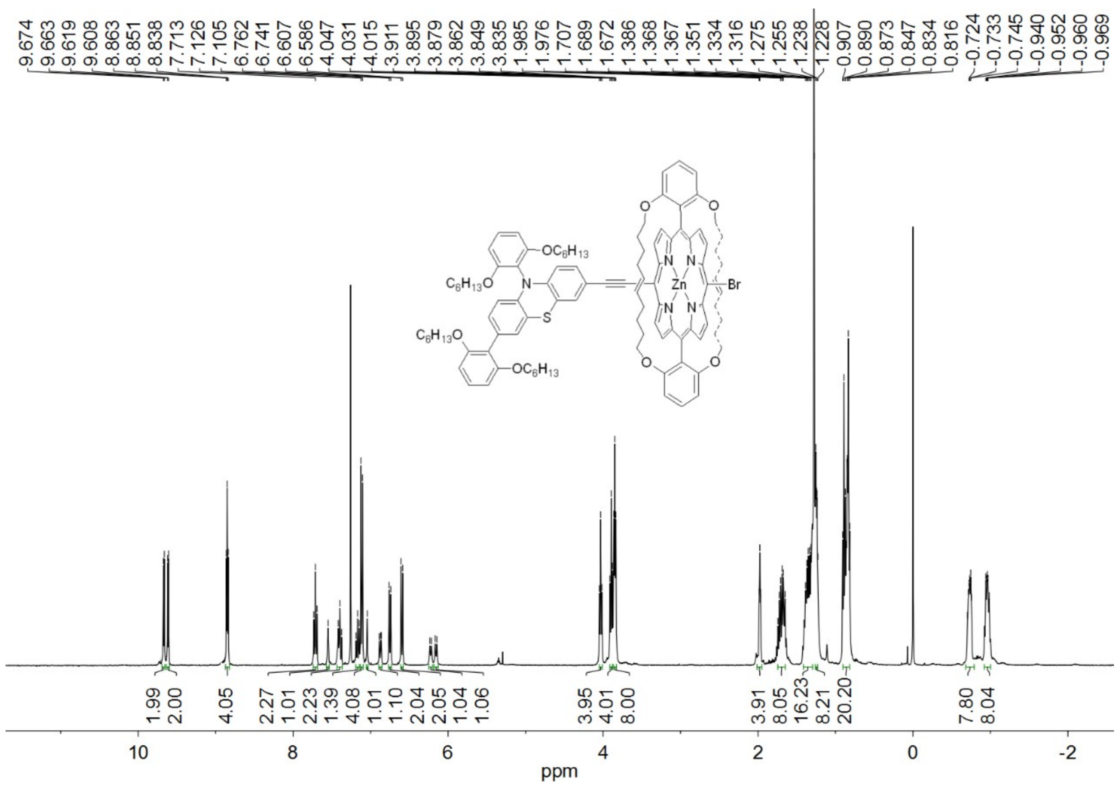


Figure S33. The ^{1}H NMR spectrum of **4c** in $CDCl_3$.

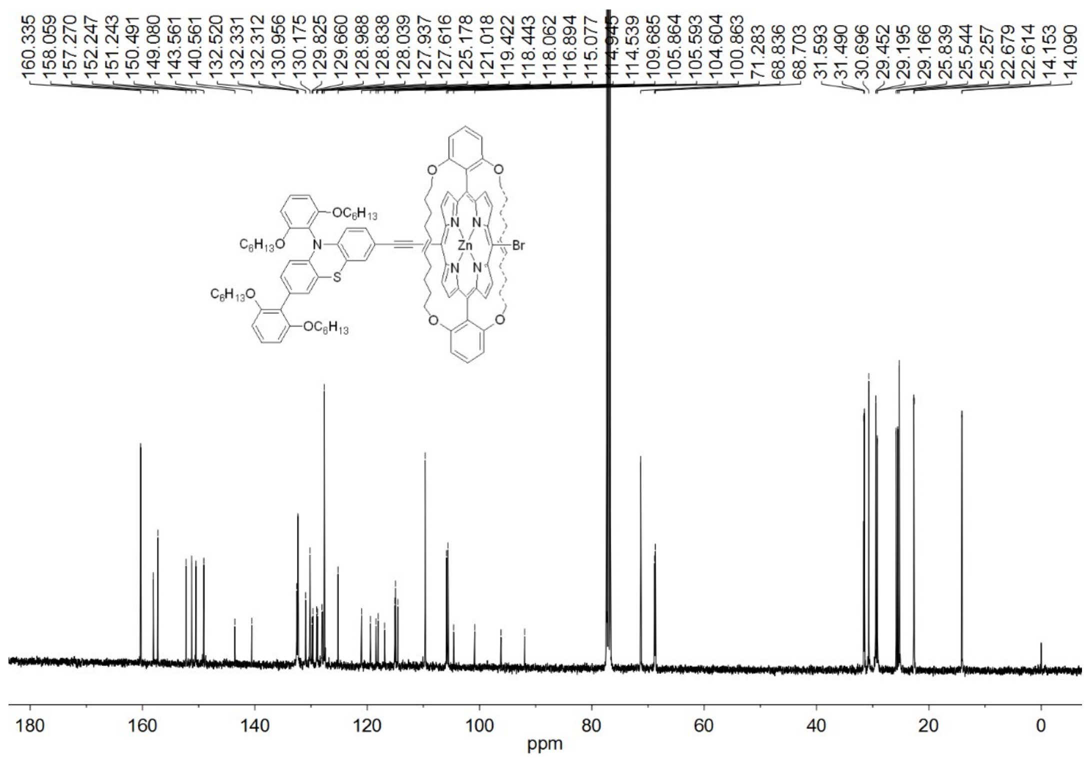


Figure S34. The ^{13}C NMR spectrum of **4c** in $CDCl_3$.

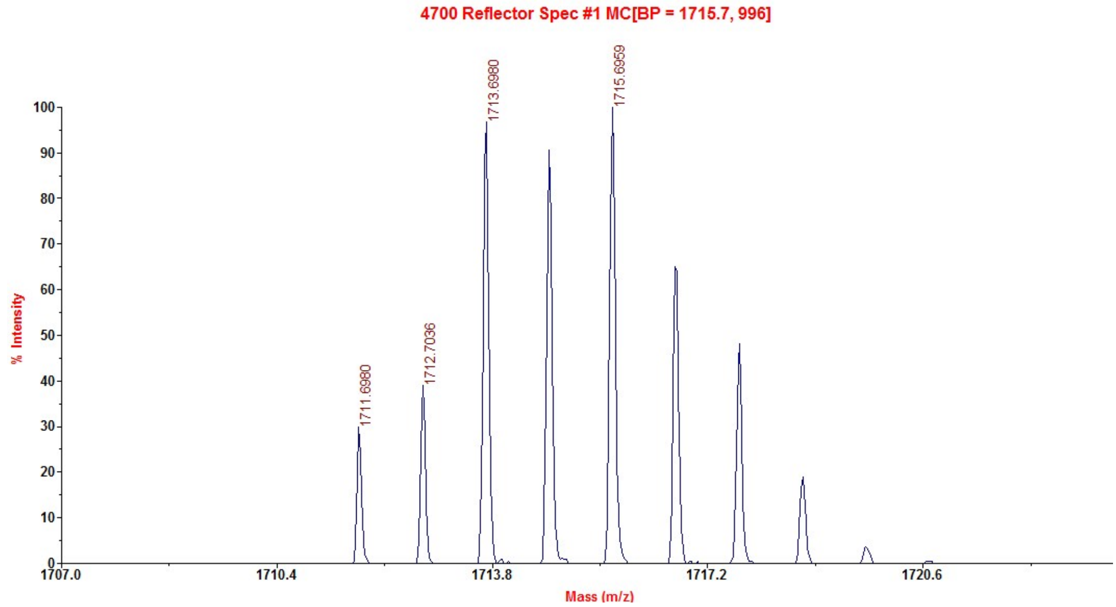


Figure S35. The HRMS of **4c**.

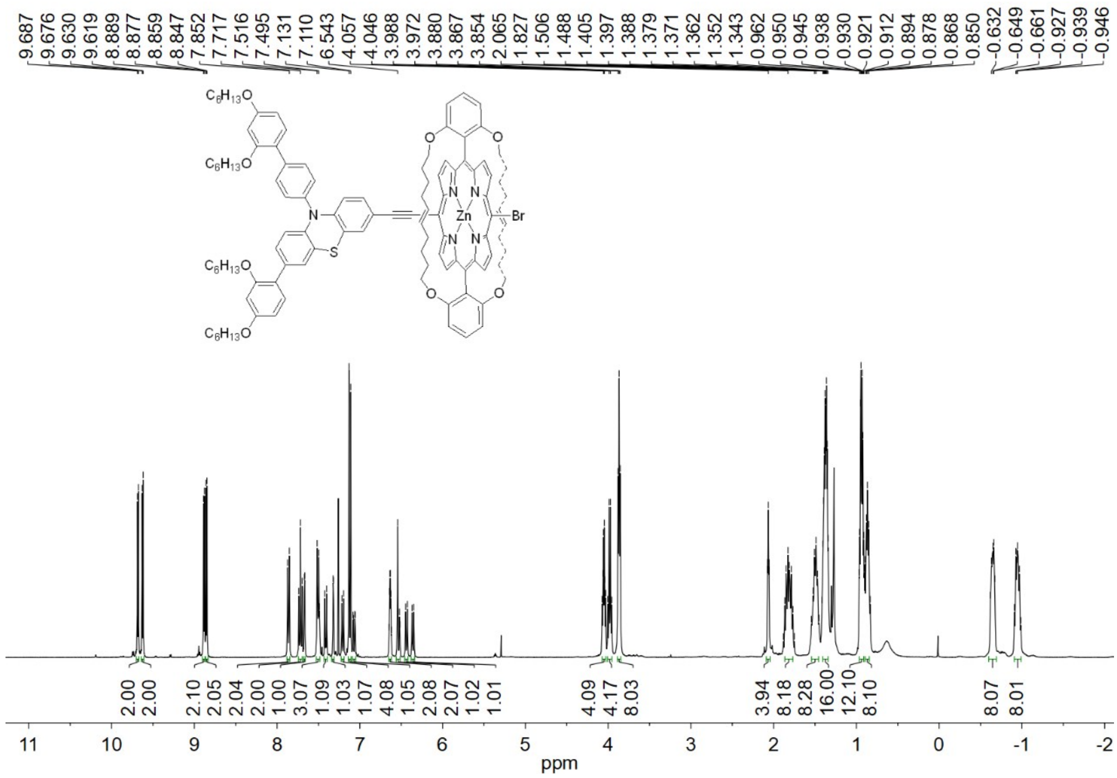


Figure S36. The ^{1}H NMR spectrum of **4d** in $CDCl_3$.

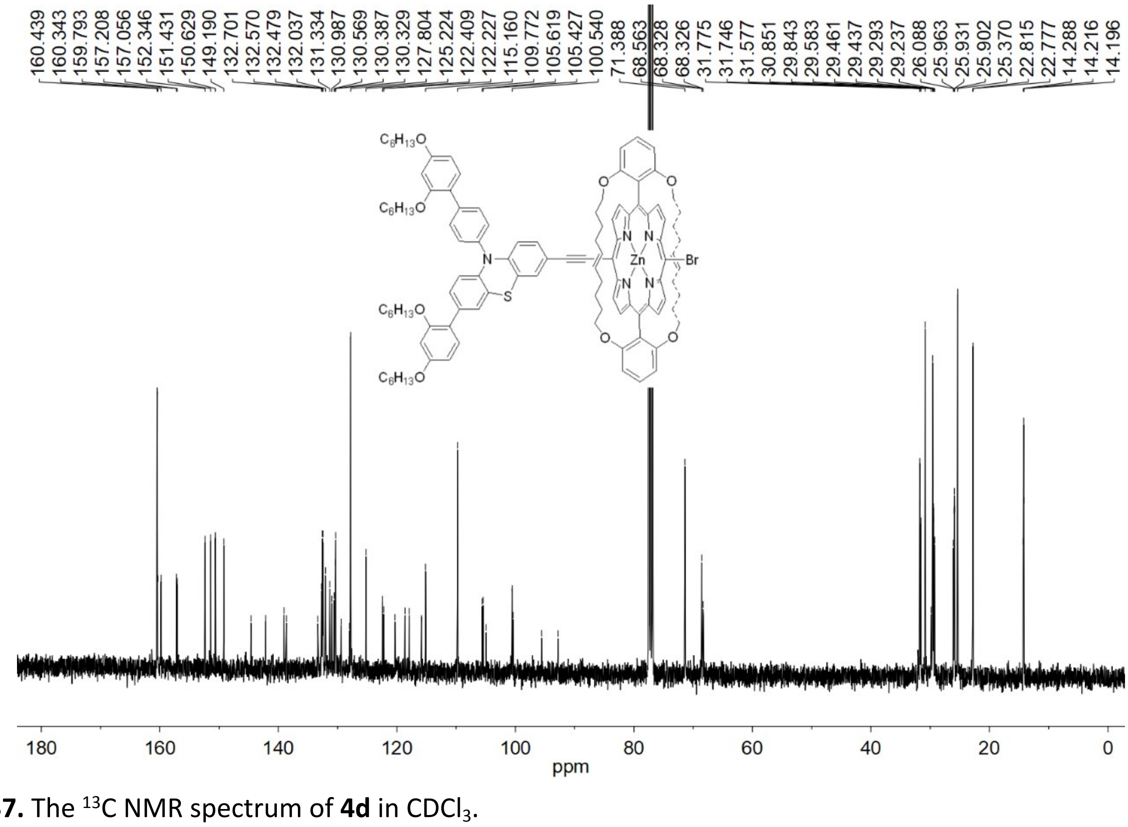


Figure S37. The ^{13}C NMR spectrum of **4d** in $CDCl_3$.

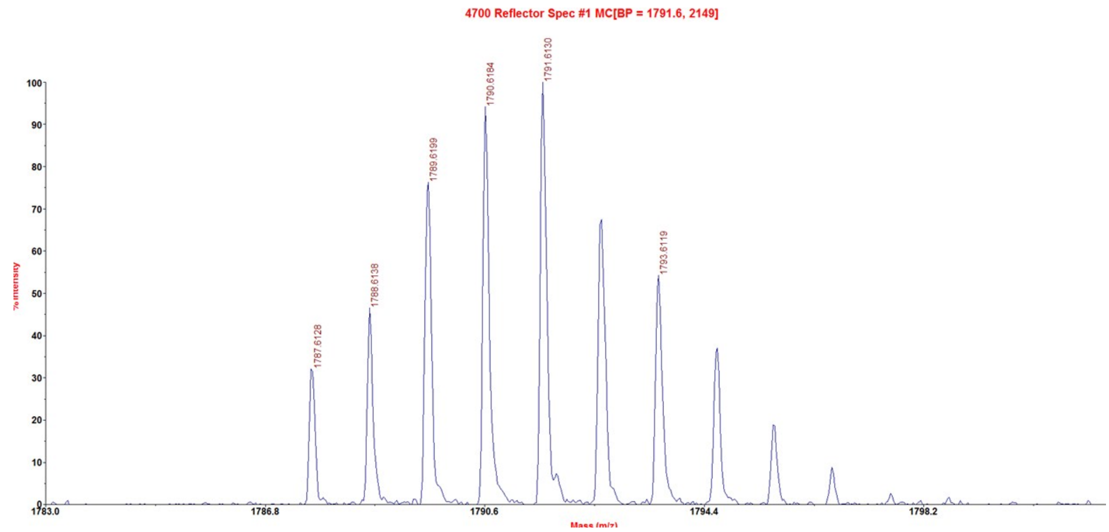


Figure S38. The HRMS of **4d**.

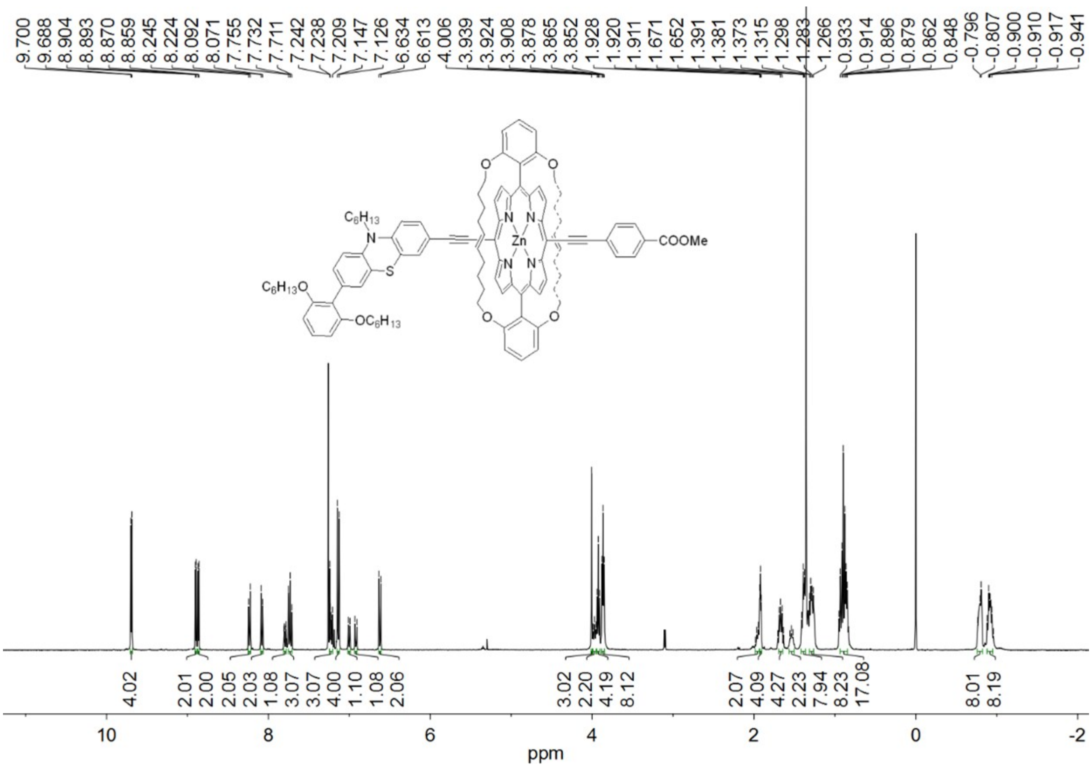


Figure S39. The ^{1}H NMR spectrum of **5a** in $CDCl_3$.

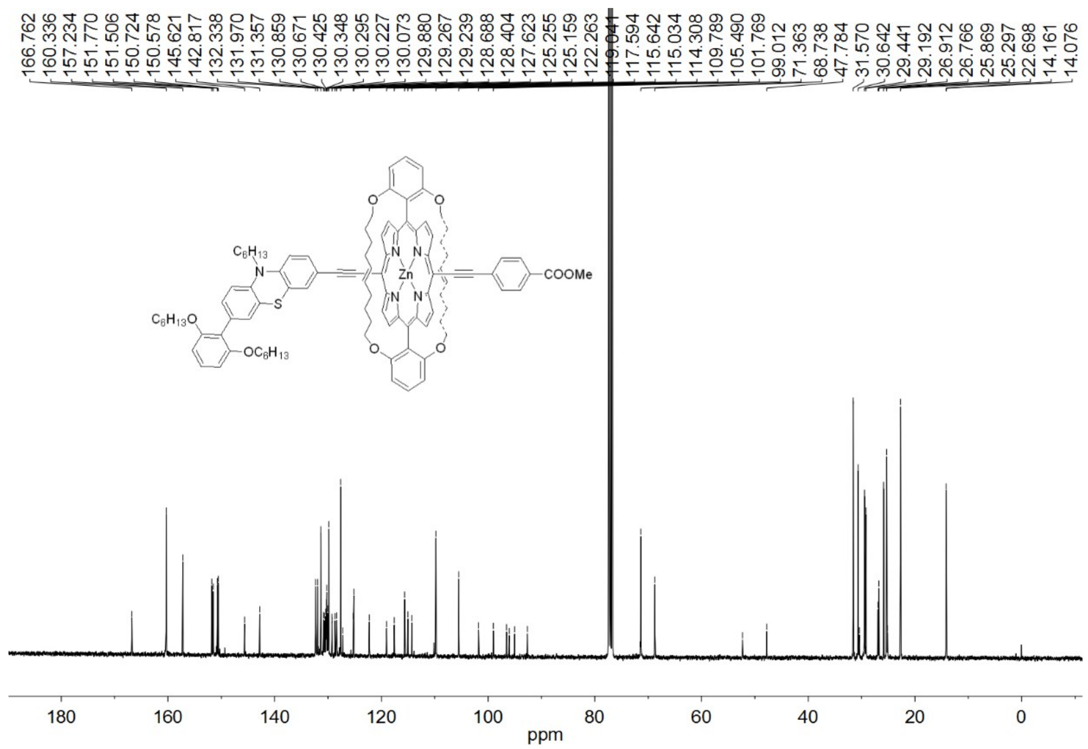


Figure S40. The ^{13}C NMR spectrum of **5a** in $CDCl_3$.

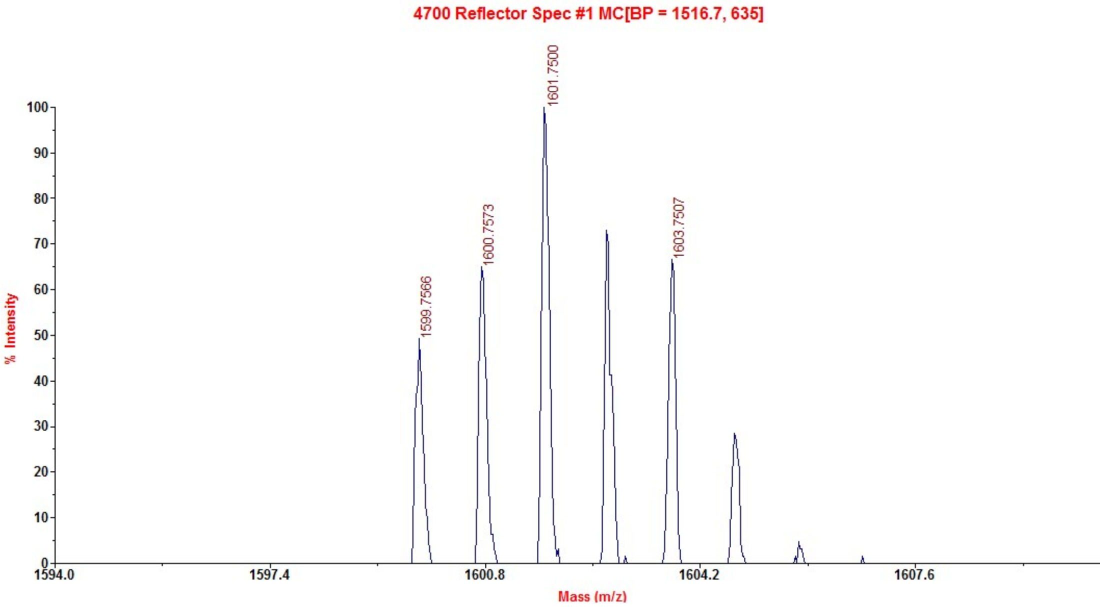


Figure S41. The HRMS of **5a**.

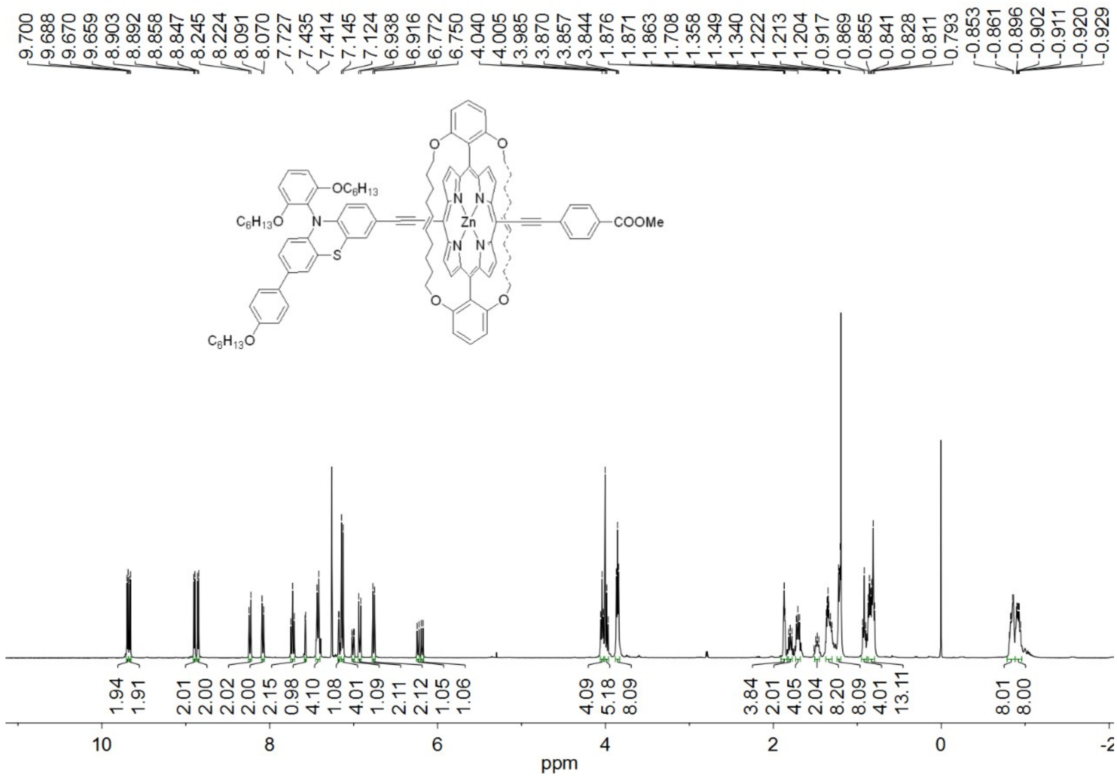


Figure S42. The ^{1}H NMR spectrum of **5b** in $CDCl_3$.

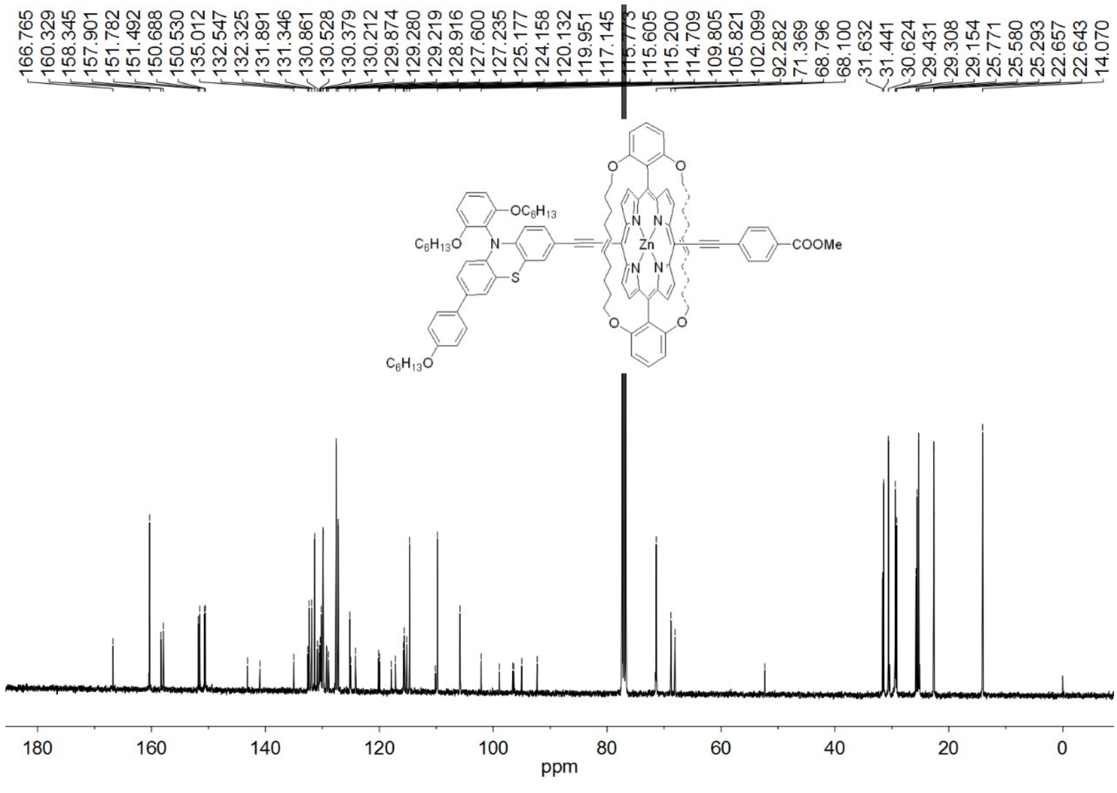


Figure S43. The ^{13}C NMR spectrum of **5b** in $CDCl_3$.

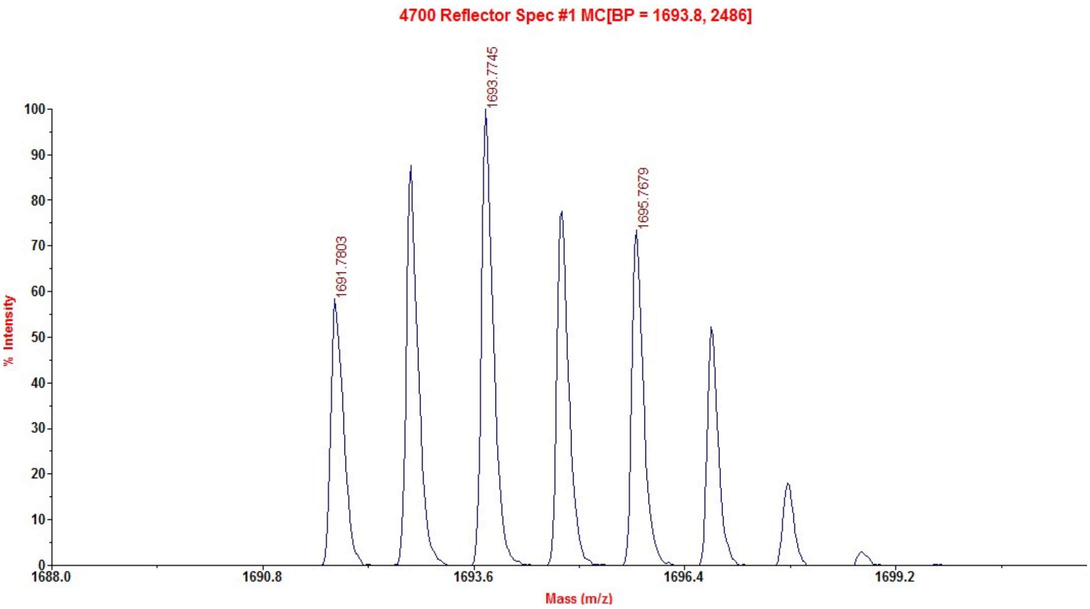


Figure S44. The HRMS of **5b**.

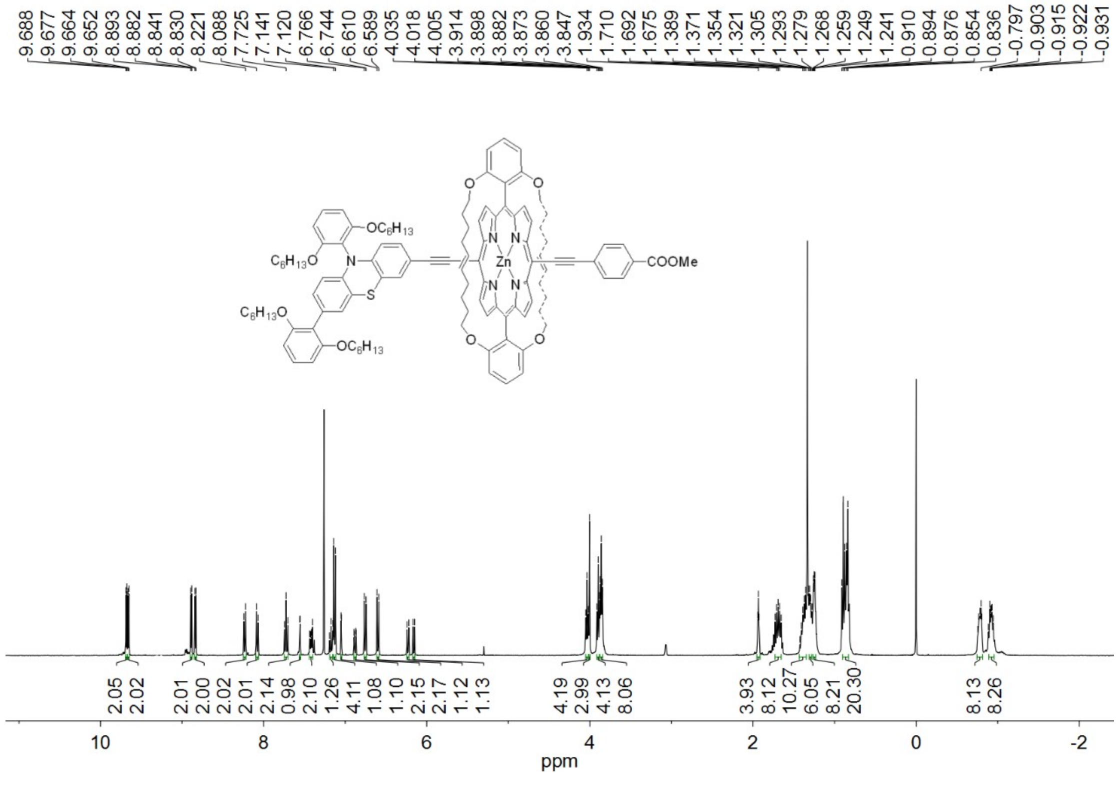


Figure S45. The ^{1}H NMR spectrum of **5c** in $CDCl_3$.

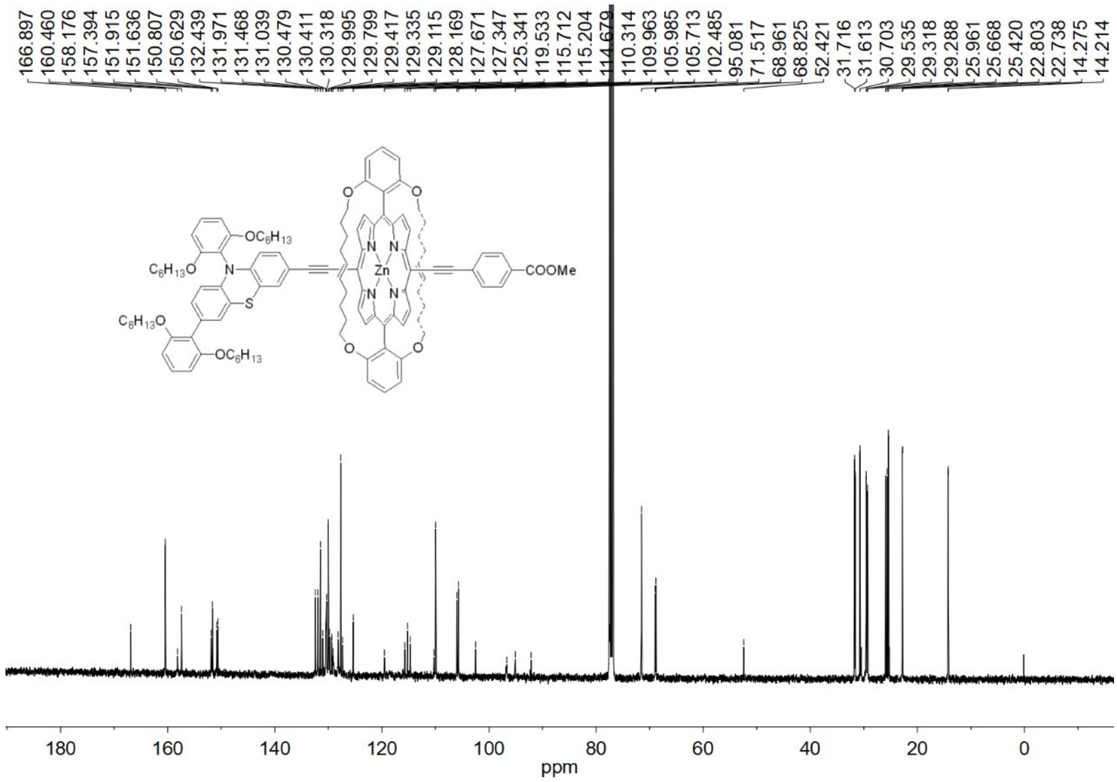


Figure S46. The ^{13}C NMR spectrum of **5c** in $CDCl_3$.

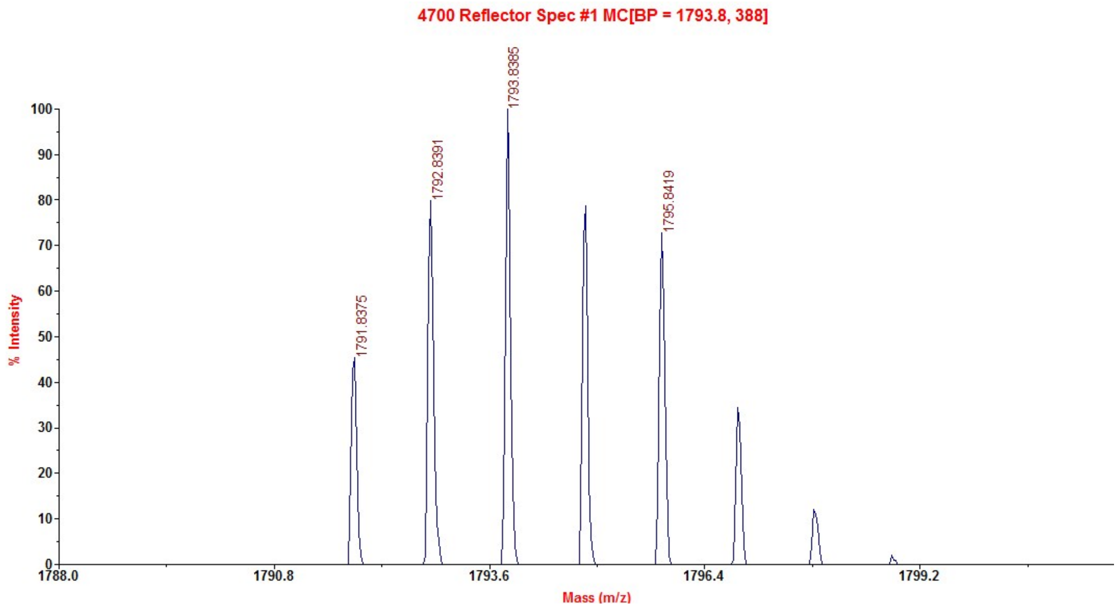


Figure S47. The HRMS of **5c**.

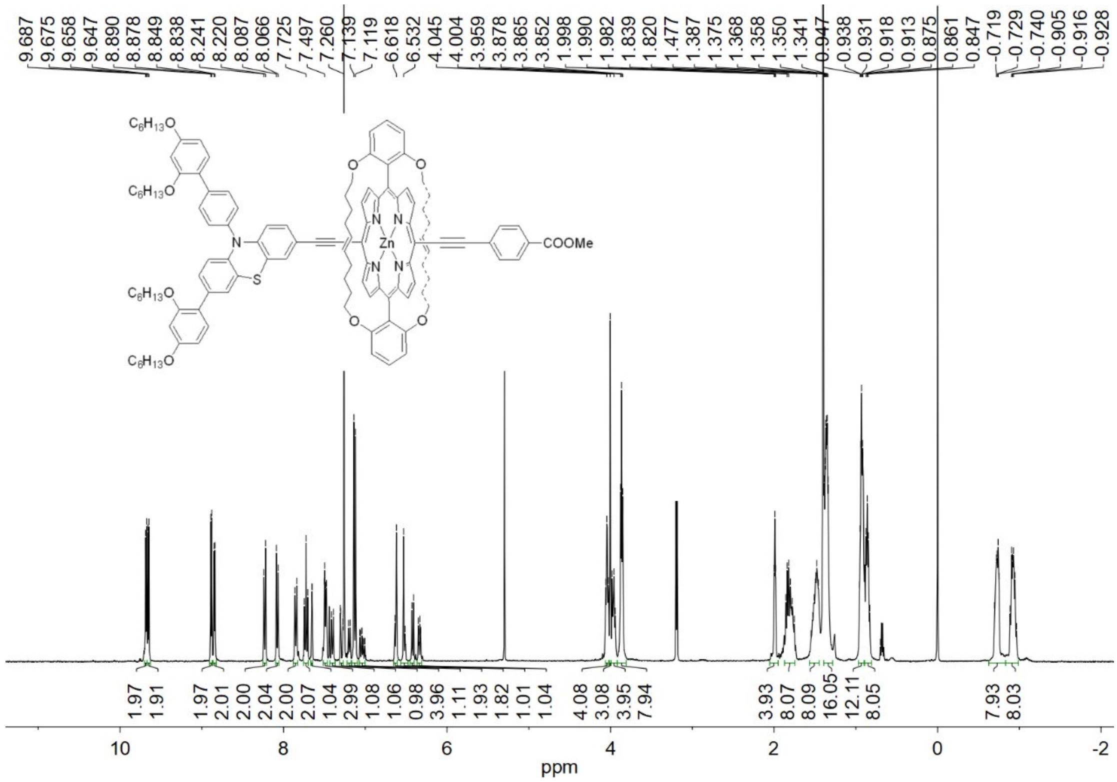


Figure S48. The ^{1}H NMR spectrum of **5d** in $CDCl_3$.

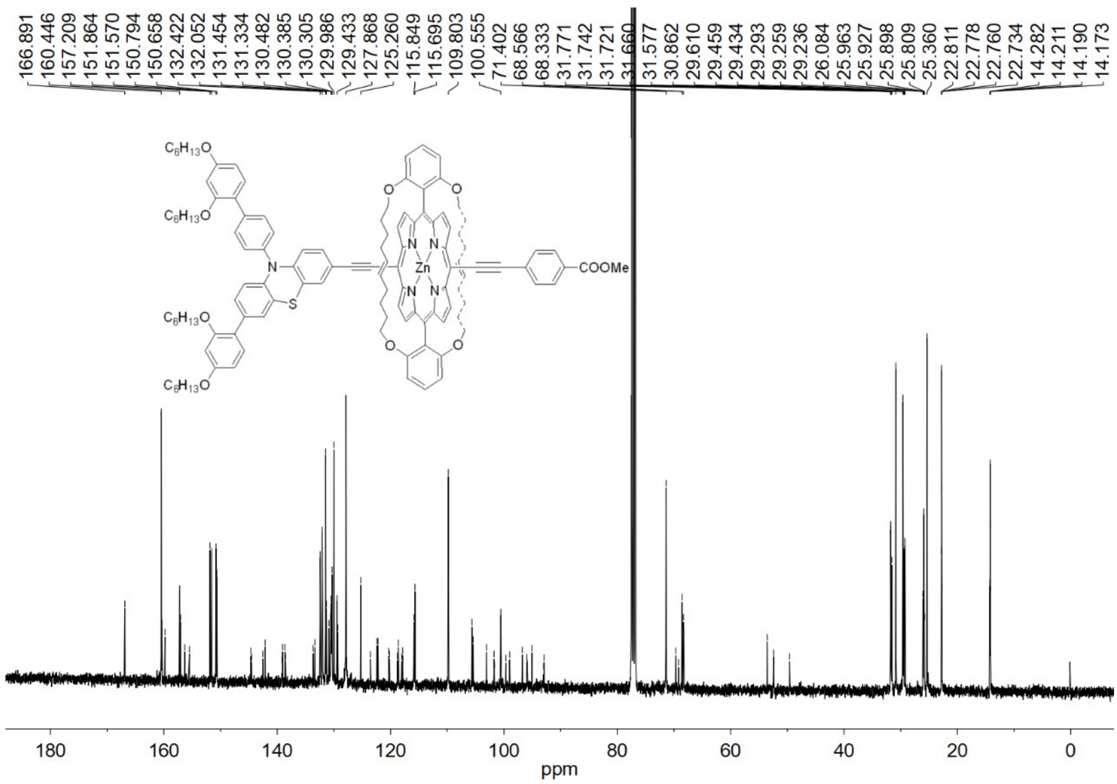


Figure S49. The ^{13}C NMR spectrum of **5d** in $CDCl_3$.

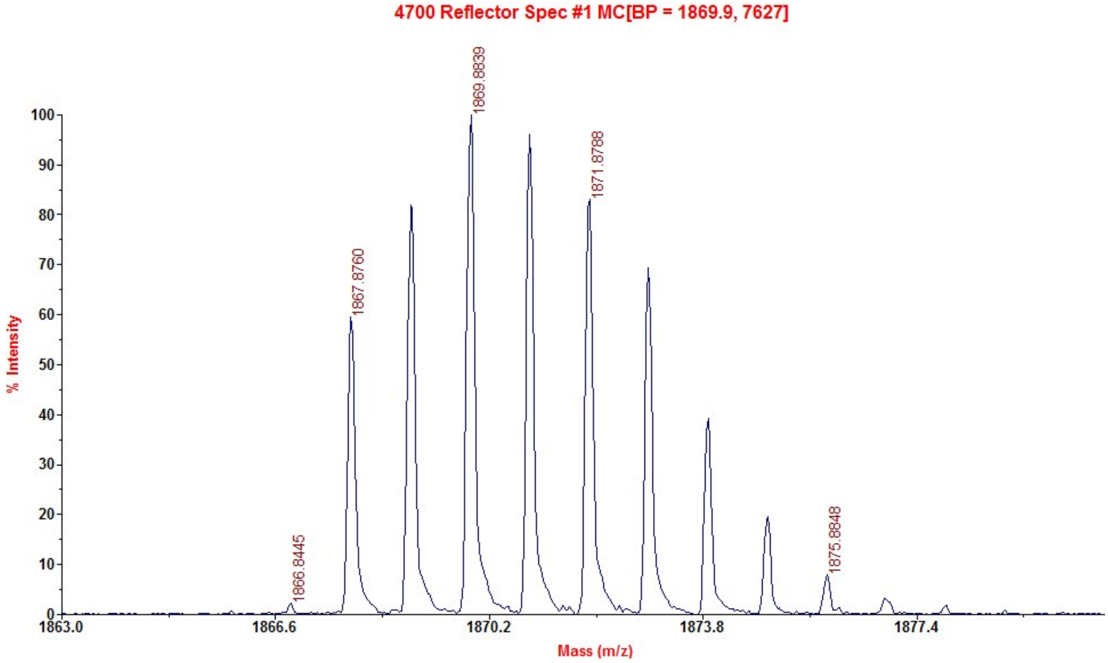


Figure S50. The HRMS of **5d**.

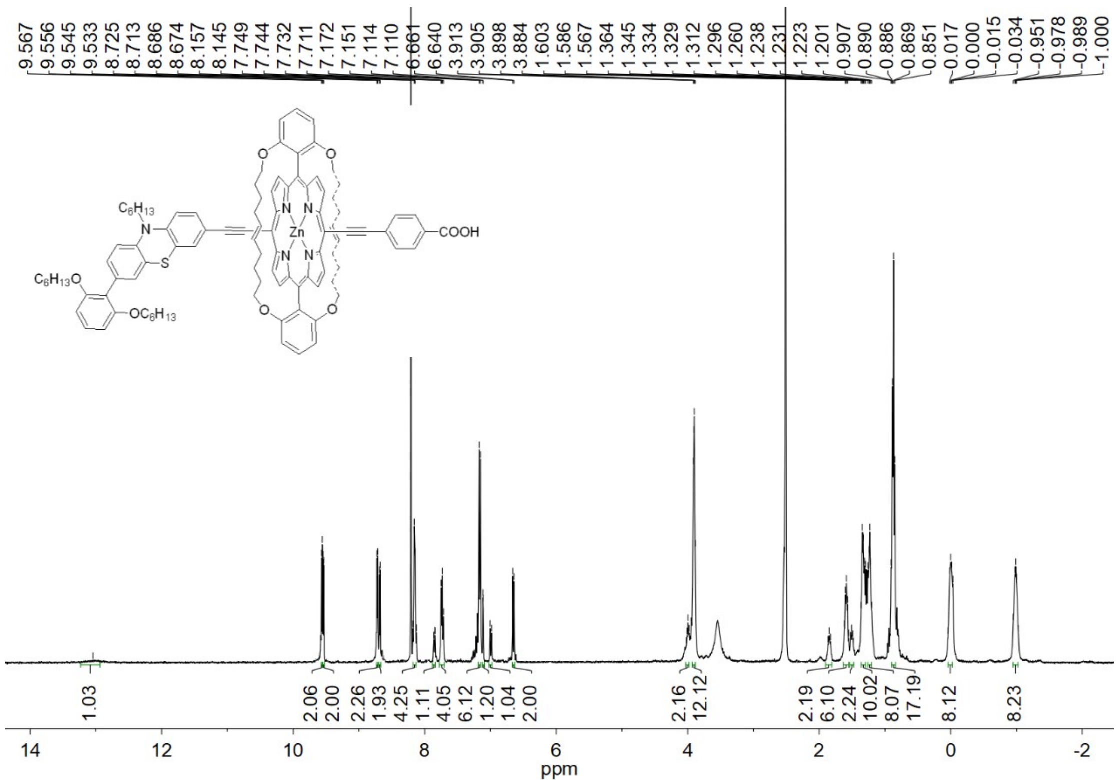


Figure S51. The ^{1}H NMR spectrum of **XW48** in $CDCl_3$.

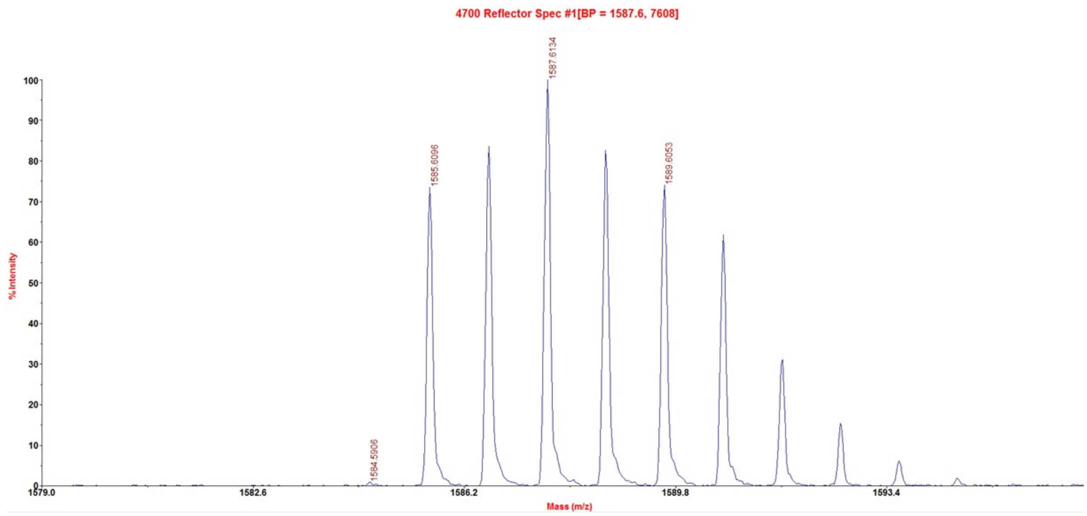


Figure S52. The HRMS of **XW48**.

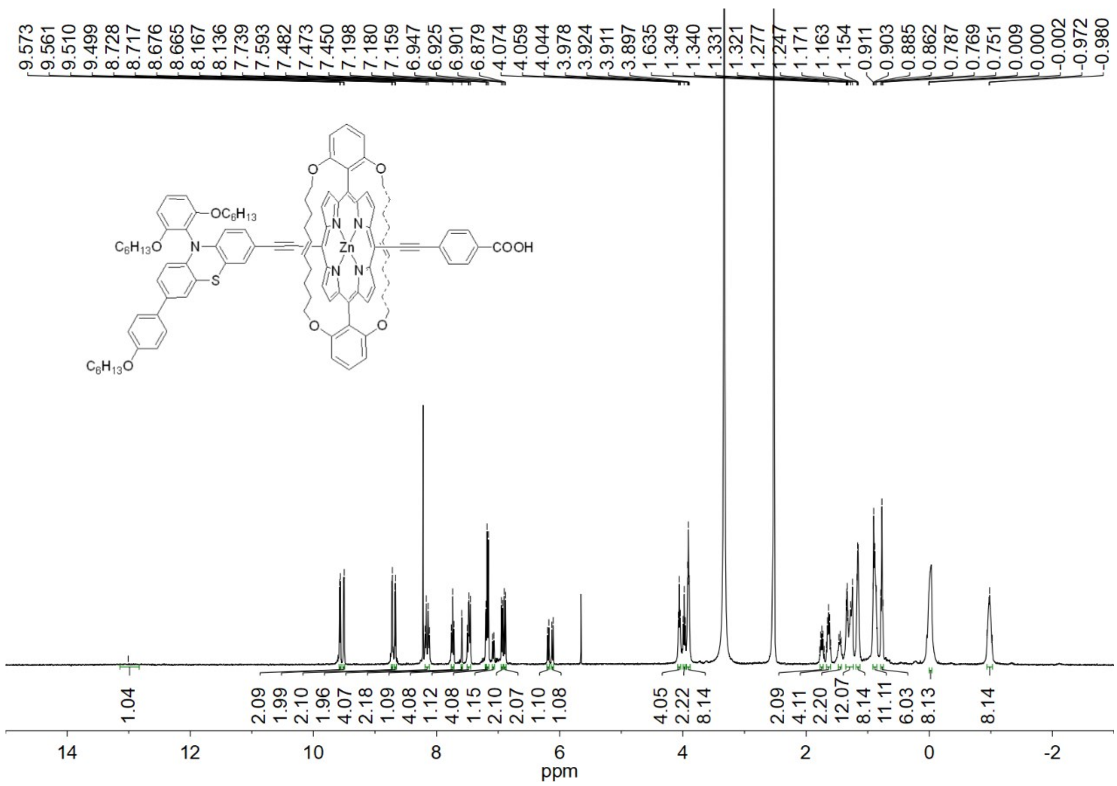


Figure S53. The ^{1}H NMR spectrum of **XW49** in $CDCl_3$.

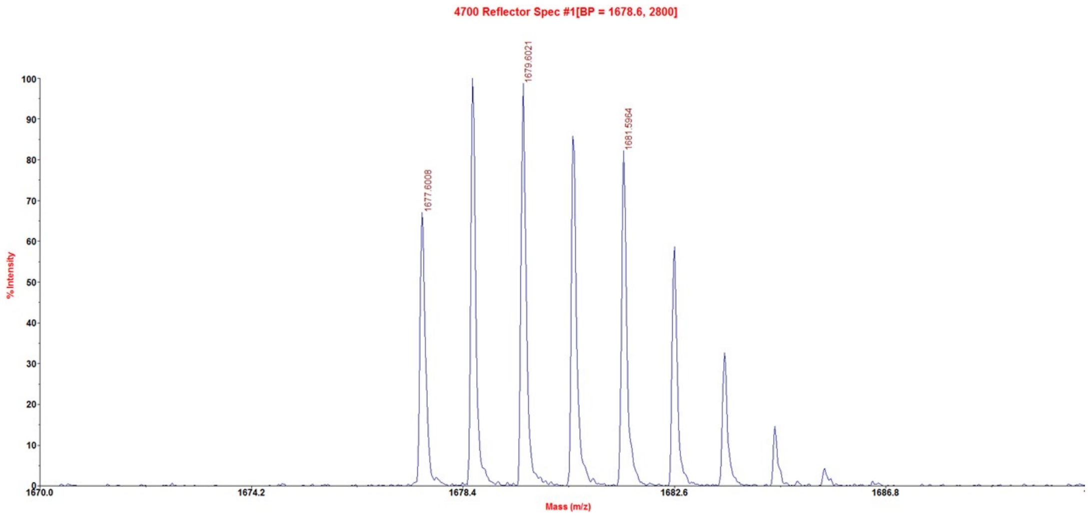


Figure S54. The HRMS of **XW49**.

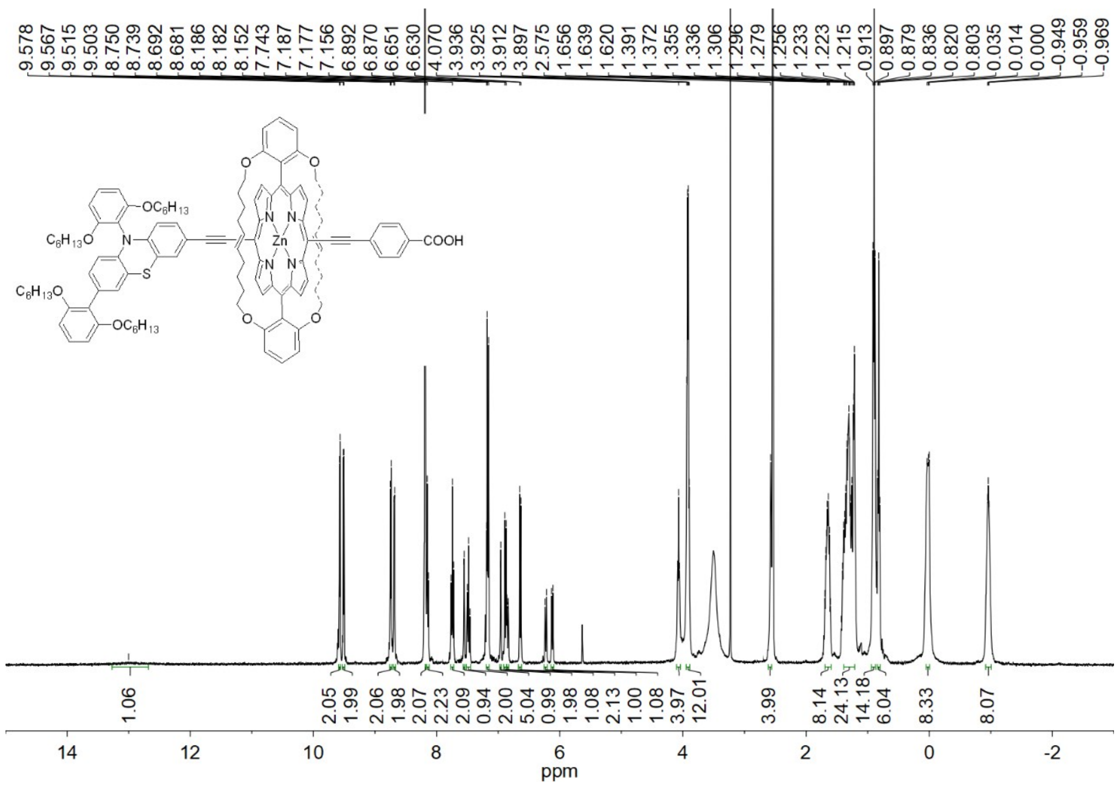


Figure S55. The [1]H NMR spectrum of **XW50** in $CDCl_3$.

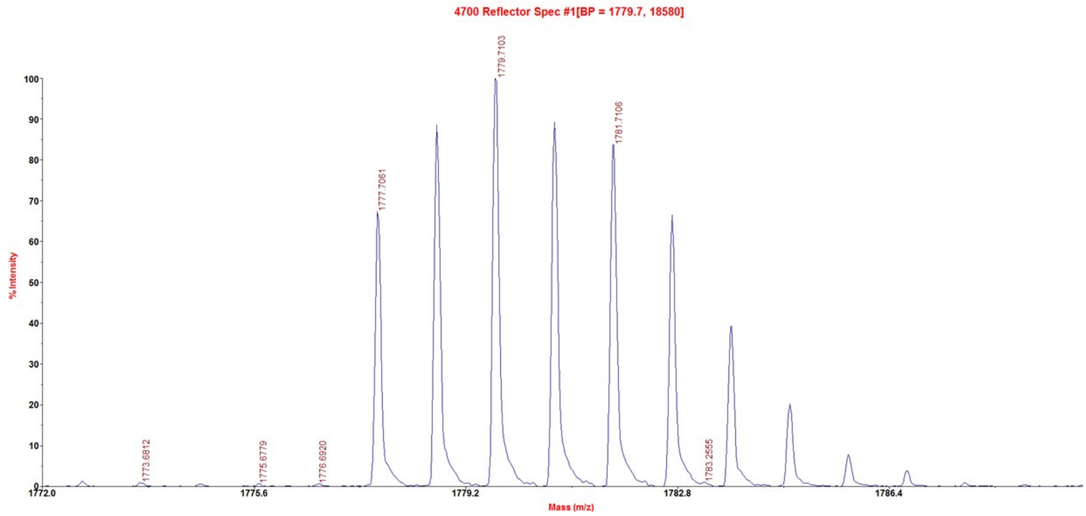


Figure S56. The HRMS of **XW50**.

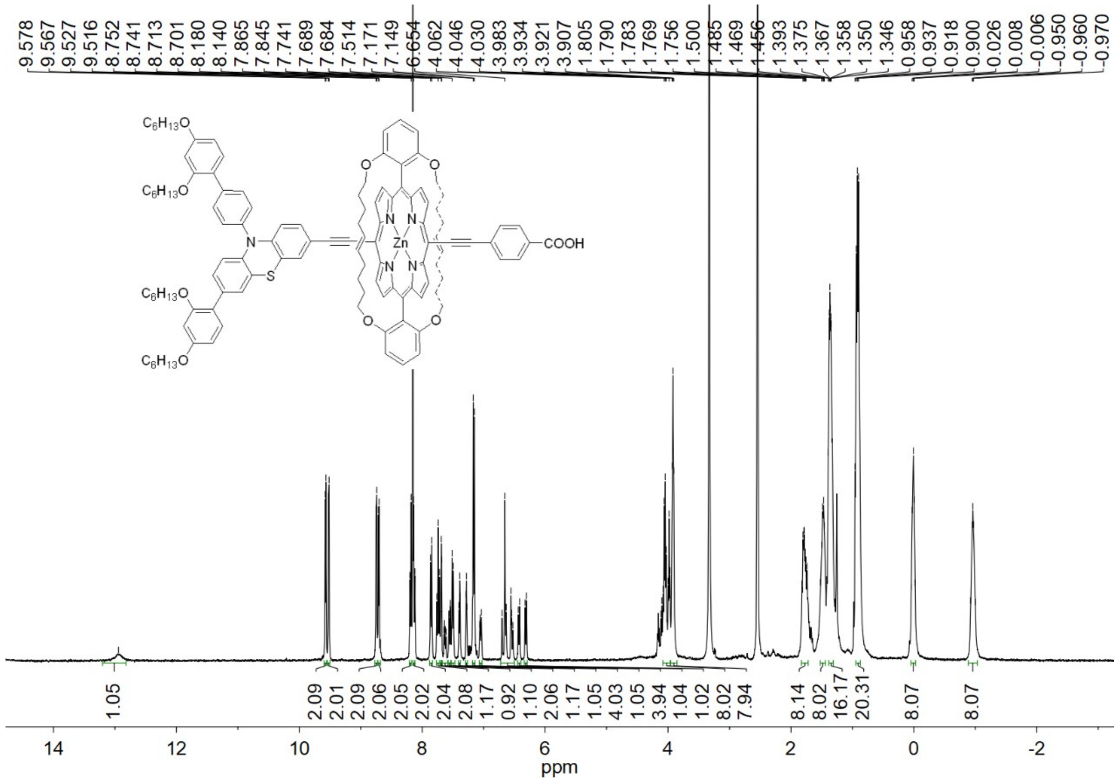


Figure S57. The ^{1}H NMR spectrum of **XW51** in $CDCl_3$.

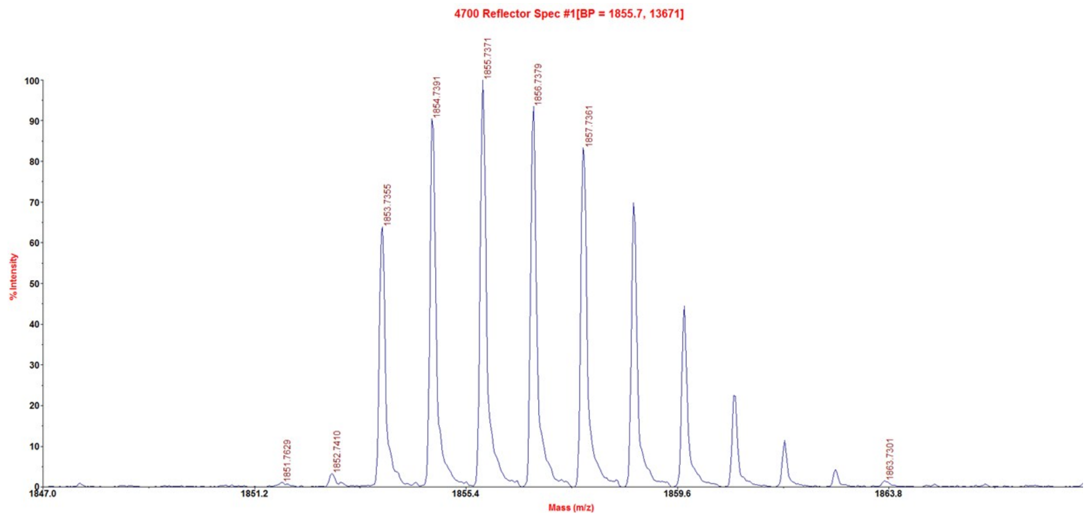


Figure S58. The HRMS of **XW51**.

7. Cartesian Coordinates of the Optimized Structures for XW48~XW51

XW48 (the hexyloxy and hexyl chains in the phenothiazine moiety were replaced by methoxy and methyl groups, respectively)

XW48			
C	12.19016309	1.28909153	-0.4325777
C	11.97579461	-0.09245202	-0.33221268
C	10.77262372	-0.52288997	0.25098425
C	9.84344694	0.38972301	0.7446907
C	10.0600721	1.77696944	0.63895734
C	11.24654533	2.20776645	0.02566933
S	8.39926968	-0.19990025	1.61098581
C	7.25924302	1.08268209	1.12811172
C	7.73094406	2.40815349	0.99260896
N	9.10126373	2.68945771	1.14036146
C	5.91100629	0.78295706	0.97946418
C	4.96512417	1.80165501	0.73213572
C	5.43414747	3.12367967	0.60731892
C	6.7888598	3.41640503	0.7186289
C	9.50731953	4.07787805	1.33253686
C	12.97327816	-1.07815612	-0.83545565
C	14.32586542	-1.03895361	-0.41039221
C	15.25434797	-1.97781184	-0.87628828
C	14.84829688	-2.97282938	-1.76814099
C	13.5284768	-3.03735608	-2.20214257
C	12.60548177	-2.09769661	-1.73267503
C	3.58291293	1.49802954	0.60975937
C	2.39454157	1.24341737	0.50495483
C	0.54768022	3.44282119	0.13692478
C	-0.58145096	4.18995397	-0.0366621
C	-1.69668498	3.27066918	-0.07652866
N	-1.22800051	1.98541726	0.07258038
C	0.13109699	2.0615155	0.20470161
C	0.77638809	-2.65759084	0.65303588
C	1.53283308	-1.52166502	0.63715262
C	0.62267381	-0.41380011	0.45664875
N	-0.65888922	-0.88330051	0.3659316
C	-0.60111105	-2.25259723	0.48255969
C	1.00819237	0.95410318	0.38453985
C	-5.29920754	-2.93070785	0.06228341
C	-4.17083102	-3.67651315	0.2352103
C	-3.05238531	-2.75657245	0.27503585
N	-3.52456821	-1.47117186	0.12507288

C	-4.88197192	-1.54845727	-0.00567714
C	-1.70336537	-3.13098451	0.44104103
C	-5.53012488	3.16851984	-0.45290287
C	-6.28506253	2.03137669	-0.43751521
C	-5.37317403	0.92592557	-0.25588602
N	-4.09366902	1.39530335	-0.16422334
C	-4.14909314	2.76625384	-0.28049831
C	-3.04732286	3.64289028	-0.23996649
C	-5.75845306	-0.44251721	-0.18358201
Zn	-2.37652129	0.25574072	0.09997634
C	-1.44634879	-4.60277264	0.58156398
C	-3.35392008	5.10527037	-0.38139254
C	-1.23071898	-5.40160143	-0.55951159
C	-1.13678868	-6.79724758	-0.44687927
C	-1.23208552	-7.38127797	0.81517477
C	-1.40104469	-6.61467746	1.96700569
C	-1.49468313	-5.21952879	1.84804218
C	-3.65236317	5.88806614	0.74921589
C	-4.01298563	7.23303441	0.61515474
C	-4.06431214	7.80869046	-0.65491073
C	-3.74900523	7.05916709	-1.78882717
C	-3.38902385	5.71465544	-1.64903918
O	-3.02081635	4.95921449	-2.73825819
O	-3.53824914	5.29912747	1.98712566
O	-1.63432227	-4.37100834	2.90754361
O	-1.12490504	-4.72222726	-1.73828781
C	-1.62360337	-4.90194532	4.23897069
C	-1.36522685	-3.78145488	5.24096351
C	-2.44450931	-2.69687746	5.39892591
C	-2.55157609	-1.70202654	4.2231012
C	-3.3843355	-0.49108214	4.55658941
C	-2.93007153	0.76787132	4.54941652
C	-3.72275349	2.00745306	4.87068737
C	-3.89994066	2.92044421	3.64080412
C	-4.45021276	4.31207029	3.9812077
C	-4.75104812	5.16196231	2.75246695
C	-4.05197398	4.66916648	-3.70166361
C	-3.50777841	3.64908602	-4.69456533
C	-3.04857889	2.34148005	-4.03526254
C	-2.62175066	1.25675519	-5.04431886
C	-1.93587355	0.09536287	-4.37438892
C	-2.39780705	-1.15786802	-4.28899408
C	-1.67807794	-2.29060792	-3.60364958
C	-1.33358884	-3.44758549	-4.56612959

C	-0.3365399	-4.48135895	-4.01549739
C	-0.83110766	-5.44442086	-2.94123198
C	-7.14483675	-0.72909491	-0.30007314
C	-8.3356031	-0.97467646	-0.40001306
C	-9.72174311	-1.2573129	-0.51673156
C	-10.19784896	-2.58295738	-0.41613707
C	-11.55600247	-2.85517317	-0.52283626
C	-12.47930194	-1.81819565	-0.73714015
C	-12.00687091	-0.50106	-0.8590167
C	-10.6541784	-0.21876877	-0.74247008
O	14.6426858	-0.05238825	0.47825361
C	15.97632164	0.02239036	0.96963964
O	11.29367756	-2.20958407	-2.15465557
C	10.97050082	-1.41107404	-3.29686653
C	-13.94752496	-2.04457133	-0.87870326
O	-14.70141781	-1.24458027	-1.39613871
O	-14.45310308	-3.20926097	-0.39959433
H	13.10306185	1.65814528	-0.88765189
H	10.56622855	-1.584187	0.33619978
H	11.43998481	3.26610709	-0.10555227
H	5.57745724	-0.24535954	1.07718147
H	4.72950297	3.92375645	0.4041546
H	7.11319365	4.44138334	0.58371301
H	10.50733689	4.0955525	1.77024069
H	9.52068422	4.66121507	0.40056516
H	8.8206095	4.55511567	2.03467861
H	16.28463803	-1.94695373	-0.5436229
H	15.57384879	-3.70008067	-2.12165848
H	13.19176015	-3.80481175	-2.89168135
H	1.56895963	3.78859742	0.21326168
H	-0.65431709	5.26452644	-0.12918193
H	1.11492596	-3.67774096	0.76918816
H	2.60572159	-1.43457413	0.73690885
H	-6.32046427	-3.27683276	-0.01370933
H	-4.09908711	-4.75077002	0.32737046
H	-5.87683572	4.18526404	-0.57101853
H	-7.35763591	1.94388048	-0.53928601
H	-1.00807547	-7.42319769	-1.32076005
H	-1.17122071	-8.46265718	0.9036314
H	-1.47293004	-7.10164033	2.93126528
H	-4.23041374	7.8213015	1.50112918
H	-4.33609487	8.85529579	-0.7603369
H	-3.76119259	7.51103191	-2.77572397
H	-0.8225678	-5.64554833	4.32977003

H	-2.58074242	-5.40487878	4.43898339
H	-0.40377977	-3.31203252	4.99313997
H	-1.22553496	-4.27620011	6.21178492
H	-2.21015828	-2.12937983	6.30939796
H	-3.42151001	-3.1691572	5.57719562
H	-2.96805425	-2.22134745	3.35155394
H	-1.54323522	-1.37640439	3.93432945
H	-4.42362837	-0.67735306	4.83946818
H	-1.88810125	0.94163909	4.26768338
H	-3.20102736	2.5744659	5.65745895
H	-4.70571481	1.73592856	5.27850958
H	-4.56579898	2.42384995	2.92210943
H	-2.93590972	3.03800677	3.13279455
H	-3.73666763	4.84623999	4.62314443
H	-5.38395331	4.22372247	4.55409682
H	-5.12480023	6.15187004	3.04675312
H	-5.51418717	4.67927784	2.12741065
H	-4.92823507	4.26610286	-3.17653994
H	-4.35502392	5.59066032	-4.2168896
H	-2.6736376	4.09737073	-5.25119486
H	-4.30278845	3.4485428	-5.42641476
H	-3.85402111	1.94214416	-3.40423462
H	-2.21283716	2.56090302	-3.36078557
H	-1.93417897	1.70814126	-5.7765759
H	-3.49685437	0.90757296	-5.60871659
H	-0.97743403	0.32854376	-3.9029862
H	-3.35374562	-1.4025902	-4.75927665
H	-2.28458484	-2.68054549	-2.77729947
H	-0.75214065	-1.90938959	-3.15243352
H	-0.89391613	-3.01824498	-5.47624172
H	-2.25624479	-3.95484817	-4.8835266
H	0.55532878	-3.96675846	-3.63343202
H	0.00425593	-5.11246968	-4.84757011
H	-0.04439084	-6.18213427	-2.74214014
H	-1.73021207	-5.98457494	-3.27117546
H	-9.49235599	-3.3923707	-0.25984471
H	-11.87735748	-3.89245908	-0.47245581
H	-12.72168925	0.29439426	-1.0400824
H	-10.30084241	0.80386687	-0.8267955
H	16.69384222	0.20435447	0.16007941
H	15.98972818	0.86623821	1.66123024
H	16.25826384	-0.89201616	1.50583423
H	9.92097199	-1.60824544	-3.52580696
H	11.59166934	-1.68938208	-4.15804183

H	11.10308612	-0.34317649	-3.08531549
H	-13.78533198	-3.69636004	0.11152707

XW49 (the hexyloxy chains in the phenothiazine moiety were replaced by methoxy and methyl groups, respectively)

XW49			
C	-11.79053436	-0.10879651	0.55117577
C	-11.46723929	1.25224484	0.43730404
C	-10.17871163	1.5645242	-0.02734202
C	-9.26625543	0.5706624	-0.37707954
C	-9.58707681	-0.79298175	-0.23457438
C	-10.8718998	-1.10640708	0.23627599
S	-7.73494797	1.05725705	-1.14729167
C	-6.70722548	-0.30725314	-0.6428116
C	-7.26190219	-1.5966406	-0.48048728
N	-8.65167844	-1.80954781	-0.54899497
C	-5.33775741	-0.09587908	-0.52926024
C	-4.45017986	-1.16908665	-0.30522823
C	-5.00053072	-2.45979435	-0.17809874
C	-6.37184299	-2.66282565	-0.25100852
C	-9.1337269	-3.14648864	-0.73263384
C	-12.437508	2.31672292	0.7887861
C	-13.81825416	2.15209605	0.55821321
C	-14.73159922	3.14437029	0.88816941
C	-14.29374093	4.34851467	1.46223641
C	-12.92634395	4.53584691	1.69988035
C	-12.02105614	3.5262902	1.36518121
C	-9.43244402	-3.59137056	-2.03629734
C	-9.90734859	-4.89570919	-2.23868655
C	-10.07626524	-5.73495045	-1.13875347
C	-9.78753053	-5.31643183	0.15992222
C	-9.31354736	-4.01309839	0.36385843
C	-3.04942639	-0.95338587	-0.22278856
C	-1.84420418	-0.7744592	-0.15799826
C	-0.13092339	-3.06626029	0.28978549
C	0.9536291	-3.87633919	0.46596152
C	2.1266842	-3.03339589	0.40810549
N	1.73666446	-1.72972571	0.20196744
C	0.37108737	-1.72253114	0.12353271
C	0.0205623	2.99190596	-0.6029695
C	-0.80860085	1.91410232	-0.48468212
C	0.03239715	0.75979909	-0.26575565
N	1.34500028	1.14430444	-0.25300307
C	1.37364013	2.50390979	-0.45852136
C	-0.43929309	-0.57193918	-0.09475059

C	6.12071844	2.88214893	-0.28569696
C	5.0367424	3.6913434	-0.45753284
C	3.8601173	2.84880439	-0.3939009
N	4.2537831	1.5445841	-0.18637277
C	5.61774271	1.53779276	-0.11504931
C	2.53256517	3.30449072	-0.5230666
C	5.97227131	-3.17428614	0.61527233
C	6.79989077	-2.09577201	0.49243425
C	5.95627629	-0.94332811	0.27581339
N	4.64554956	-1.32712473	0.26962
C	4.61457448	-2.68861935	0.47495051
C	3.45626687	-3.48730414	0.53802838
C	6.42748207	0.3880678	0.09835006
Zn	2.99569412	-0.09124435	0.00853332
C	2.36522475	4.77914082	-0.74496471
C	3.67186833	-4.95629591	0.75913745
C	2.40202323	5.31516503	-2.04794387
C	2.39420075	6.70396289	-2.24937356
C	2.31972756	7.5469377	-1.14173811
C	2.23530746	7.04623722	0.15639648
C	2.24401485	5.65652934	0.3513529
C	3.7258801	-5.48801539	2.06071349
C	4.00263606	-6.8429315	2.27153621
C	4.21475254	-7.68063872	1.1760599
C	4.14274803	-7.18171342	-0.12499495
C	3.86581571	-5.82587527	-0.3301085
O	3.73447467	-5.30858069	-1.59796976
O	3.45999573	-4.64353516	3.11359091
O	2.13846408	5.05645012	1.57231078
O	2.44166803	4.39755004	-3.05707583
C	1.94500235	5.8674804	2.73831572
C	1.44241101	5.00439125	3.89080185
C	2.4003293	3.946948	4.46535365
C	2.63837463	2.71717359	3.56266161
C	3.31602899	1.58416498	4.28915979
C	2.77965164	0.37195864	4.47391869
C	3.41846288	-0.78890694	5.18959275
C	3.72620812	-1.96129873	4.23683511
C	4.12299637	-3.25511077	4.960625
C	4.55045467	-4.37091898	4.01470776
C	4.91808388	-5.3007666	-2.41901604
C	4.6177124	-4.51130844	-3.687486
C	4.16896434	-3.06888054	-3.41653234
C	4.00189085	-2.22288302	-4.69476007

C	3.30417128	-0.91583033	-4.4246396
C	3.84131802	0.30629307	-4.5202372
C	3.10454649	1.58944506	-4.23451099
C	3.03105276	2.52170707	-5.46290264
C	2.03917549	3.69084248	-5.33828373
C	2.41468992	4.84748144	-4.41771026
C	7.83314014	0.58652497	0.1436895
C	9.04045253	0.75686045	0.18570188
C	10.44516947	0.9529871	0.2387406
C	10.99821589	2.24473112	0.09845009
C	12.37380607	2.43256065	0.14632703
C	13.23947041	1.3428244	0.33810204
C	12.69141751	0.0593413	0.49781632
C	11.32012584	-0.13898263	0.44140585
O	-15.26612852	5.26150941	1.74842331
C	-14.87450592	6.50580792	2.31869656
O	-9.22900796	-2.68785576	-3.02772375
C	-9.51235222	-3.07728506	-4.36993234
O	-8.99808062	-3.48962274	1.57756432
C	-9.15336245	-4.31045873	2.73375449
C	14.72353821	1.47777005	0.41796844
O	15.44719551	0.63036181	0.90225123
O	15.28112831	2.61047317	-0.07971941
H	-12.76563171	-0.4020281	0.92871103
H	-9.89220094	2.60319436	-0.16505712
H	-11.15754254	-2.14339004	0.36049476
H	-4.94311585	0.90893713	-0.64421064
H	-4.3438085	-3.30698503	-0.00773013
H	-6.76137926	-3.66631633	-0.13671135
H	-14.17956442	1.24060468	0.09049032
H	-15.79267581	3.01294859	0.6983878
H	-12.55717302	5.44947789	2.1513537
H	-10.96823536	3.681815	1.58385301
H	-10.14167346	-5.25451329	-3.23305094
H	-10.44372328	-6.74494121	-1.29751302
H	-9.93029604	-5.9944504	0.99201354
H	-1.17476403	-3.34642958	0.27182363
H	0.96044277	-4.94637474	0.61946264
H	-0.25392505	4.02356238	-0.77364114
H	-1.88806976	1.89517257	-0.53943986
H	7.16472271	3.16221938	-0.27298112
H	5.03101813	4.76081224	-0.61217261
H	7.87951713	-2.0771712	0.54312905
H	2.45923947	7.1270719	-3.24374814

H	2.32509914	8.62284178	-1.29443846
H	2.17968018	7.72994793	0.99395938
H	4.03100589	-7.23315956	3.28407009
H	4.42154098	-8.73499936	1.33709142
H	4.27981453	-7.83656	-0.97975657
H	1.19649722	6.64049459	2.52591017
H	2.88952173	6.36823268	2.9956248
H	0.50593974	4.52320695	3.57842246
H	1.17630639	5.70474496	4.6942228
H	1.97436676	3.59861005	5.41568543
H	3.36274301	4.41599682	4.71654042
H	3.23342808	3.02103328	2.69296594
H	1.67481907	2.36752163	3.16857025
H	4.30521796	1.79416489	4.70417796
H	1.78848263	0.17407211	4.05722037
H	2.73699626	-1.14549448	5.97775041
H	4.33940365	-0.46552102	5.69313777
H	4.52878944	-1.65980767	3.55017798
H	2.8487362	-2.16209587	3.61141822
H	3.28526322	-3.60718416	5.57773263
H	4.96155545	-3.06744803	5.64578011
H	4.81054464	-5.27863075	4.57582117
H	5.73755167	-4.83165202	-1.85824886
H	5.21436317	-6.32986622	-2.66283845
H	3.84612716	-5.0374204	-4.26579448
H	5.52997676	-4.51849252	-4.30036017
H	4.892082	-2.57356701	-2.75463077
H	3.2200907	-3.09234913	-2.86842369
H	3.41429576	-2.8006952	-5.42517633
H	4.9835245	-2.04271758	-5.15323966
H	2.26320555	-1.00133455	-4.10173709
H	4.88056912	0.4036755	-4.84487031
H	3.58301817	2.12547584	-3.40601687
H	2.08552821	1.35267398	-3.89997708
H	2.72644167	1.92257514	-6.33135517
H	4.0334089	2.90912114	-5.69653318
H	1.05630887	3.30948413	-5.03050955
H	1.89953003	4.13543063	-6.33308923
H	1.66456888	5.64018131	-4.52647312
H	3.39590629	5.26723811	-4.68246981
H	10.33843775	3.09482008	-0.0404112
H	12.75553569	3.44733935	0.0683299
H	13.36247284	-0.77702835	0.66094959
H	10.90757545	-1.13623658	0.55527137

H	-15.79506494	7.07573393	2.45392216
H	-14.38764025	6.36554028	3.2917605
H	-14.19963257	7.05715738	1.65228047
H	-9.27793437	-2.20698955	-4.98402889
H	-10.56986125	-3.33841628	-4.494498
H	-8.88715359	-3.92275482	-4.68035384
H	-8.84610658	-3.69150084	3.57744681
H	-10.19728099	-4.61781088	2.8664397
H	-8.51377406	-5.19916607	2.67986729
H	14.62471261	3.14402868	-0.55806793
H	5.428931	-4.06557039	3.43063294
H	6.25569367	-4.2031219	0.78589616

XW50 (the hexyloxy chains in the phenothiazine moiety were replaced by methoxy and methyl groups, respectively)

XW50			
C	-11.58564476	-0.12648183	-0.68530573
C	-11.23768982	-1.48085143	-0.57552584
C	-9.95375912	-1.78052567	-0.09305849
C	-9.06638957	-0.77402112	0.28483888
C	-9.40645835	0.58509585	0.14379213
C	-10.68688181	0.88265875	-0.34930549
S	-7.54085359	-1.24269479	1.07804221
C	-6.52598439	0.14110755	0.6022286
C	-7.09809135	1.42252098	0.43754908
N	-8.49271503	1.61386785	0.48034714
C	-5.15132316	-0.04762059	0.51268689
C	-4.2770564	1.0409111	0.31202017
C	-4.84551611	2.32356169	0.18361385
C	-6.22106336	2.50421469	0.23198576
C	-8.99673	2.9447903	0.64956491
C	-12.18843575	-2.56255814	-0.95244985
C	-13.51340668	-2.5849316	-0.46386267
C	-14.40842734	-3.59653804	-0.81901615
C	-14.00262703	-4.61810854	-1.67662223
C	-12.70097239	-4.62565404	-2.17589179
C	-11.80883421	-3.61277914	-1.81716776
C	-9.32729872	3.39042212	1.94518049
C	-9.82244898	4.68943443	2.13300089
C	-9.97956805	5.52265946	1.0268045
C	-9.65922034	5.10330866	-0.26416026
C	-9.16479358	3.80542615	-0.45353334
C	-2.8717389	0.84896344	0.25033202
C	-1.66258153	0.69382915	0.19922436
C	0.0023415	3.03046583	-0.19166345

C	1.06972629	3.86662171	-0.34970198
C	2.26036208	3.04790643	-0.30457329
N	1.89785197	1.73274622	-0.12240087
C	0.53265744	1.69491024	-0.04857812
C	0.28320422	-3.03876638	0.58731198
C	-0.56878459	-1.97690483	0.48869194
C	0.24741454	-0.80081015	0.29343941
N	1.56817008	-1.15651105	0.27589673
C	1.62564946	-2.51924022	0.45359504
C	-0.25309089	0.52297532	0.14463389
C	6.37969762	-2.79475009	0.26748948
C	5.31300716	-3.62945056	0.42448829
C	4.1189673	-2.81057995	0.37735544
N	4.48519141	-1.49481717	0.19368127
C	5.84856856	-1.4582341	0.1223452
C	2.80141414	-3.29643538	0.49960796
C	6.10195842	3.27390832	-0.5106409
C	6.95236795	2.21085008	-0.4110923
C	6.13362359	1.03650586	-0.21868089
N	4.81489523	1.39201659	-0.20392928
C	4.75495635	2.75668554	-0.3800201
C	3.58007491	3.53204875	-0.42604912
C	6.63354332	-0.28771159	-0.06893921
Zn	3.19181335	0.11773694	0.03635465
C	2.66605841	-4.77879833	0.6906664
C	3.76497377	5.0093624	-0.61828693
C	2.71264538	-5.34061005	1.98244722
C	2.73502156	-6.73308791	2.15541745
C	2.6809646	-7.55462897	1.0306631
C	2.58812478	-7.02936065	-0.25712375
C	2.56682137	-5.63609728	-0.42368907
C	3.81013224	5.56731249	-1.90921523
C	4.05838352	6.93162267	-2.09320416
C	4.25061116	7.752395	-0.98134363
C	4.18684964	7.22683494	0.30960997
C	3.9384836	5.86172073	0.48788932
O	3.81587424	5.31836539	1.74574608
O	3.56373738	4.73830648	-2.97904343
O	2.4515371	-5.01401586	-1.63279593
O	2.73101317	-4.44329563	3.01021505
C	2.27035188	-5.8051176	-2.81436484
C	1.74558262	-4.92960314	-3.9474038
C	2.67864066	-3.83994093	-4.50221943
C	2.89129189	-2.62342821	-3.5755155

C	3.54463431	-1.46274035	-4.28012137
C	2.98315738	-0.25878835	-4.44252765
C	3.59888876	0.92850166	-5.1347344
C	3.88383374	2.08652566	-4.15773904
C	4.2576951	3.40243597	-4.85326948
C	4.66147317	4.50564211	-3.88245201
C	5.0011321	5.30952676	2.56442894
C	4.71273674	4.49356431	3.81881771
C	4.27978558	3.05130277	3.52220088
C	4.13362241	2.17763384	4.78422172
C	3.45953916	0.86316934	4.4908636
C	4.02146654	-0.34966811	4.55839016
C	3.31002709	-1.64135847	4.2481994
C	3.26296802	-2.60248209	5.45531303
C	2.30187205	-3.79404957	5.30441184
C	2.70901872	-4.92155125	4.36136163
C	8.04294723	-0.45612339	-0.11923421
C	9.25311834	-0.60365668	-0.16509786
C	10.66051582	-0.77808073	-0.22299492
C	11.23269354	-2.06141809	-0.08192235
C	12.60963952	-2.23160823	-0.1503499
C	13.45810258	-1.13123652	-0.35736469
C	12.89371451	0.14968033	-0.47551736
C	11.5195464	0.32765249	-0.41886563
O	-9.13248725	2.49328958	2.94425829
C	-9.4446252	2.88549758	4.27919596
O	-8.81725097	3.28209509	-1.65849073
C	-8.95880715	4.09697374	-2.82058845
O	-13.9682722	-1.58005741	0.36919854
C	-13.68859811	-1.7916149	1.75694283
O	-10.52088156	-3.67670759	-2.31425421
C	-10.3098262	-2.919664	-3.51055529
C	14.94447818	-1.24393296	-0.42688815
O	15.69512182	-0.30153786	-0.27014161
O	15.47211864	-2.46840247	-0.67989998
H	-12.56912576	0.14716559	-1.0506804
H	-9.64699513	-2.81557129	0.01086551
H	-10.98786905	1.91596298	-0.46736692
H	-4.74306104	-1.04694884	0.62781057
H	-4.19946249	3.18230798	0.03128889
H	-6.62407438	3.50228936	0.11724792
H	-15.41519727	-3.56486178	-0.41399669
H	-14.69766081	-5.40537864	-1.95409263
H	-12.35617399	-5.4085944	-2.8442931

H	-10.08136895	5.04885006	3.1210186
H	-10.36281552	6.5284703	1.17432762
H	-9.79320362	5.77670846	-1.10144554
H	-1.04726592	3.28797869	-0.17185517
H	1.05404549	4.93918096	-0.48368967
H	0.030742	-4.07924186	0.73720437
H	-1.64849451	-1.9821819	0.54200068
H	7.42931609	-3.05266912	0.24999003
H	5.32977953	-4.70143905	0.55959729
H	6.36342606	4.31193022	-0.6591489
H	8.03213762	2.21618093	-0.46196703
H	2.80807524	-7.17499181	3.14102912
H	2.70969819	-8.63305569	1.16135369
H	2.54934315	-7.69681286	-1.10863893
H	4.08018507	7.34176282	-3.09802641
H	4.43519964	8.81382444	-1.12155278
H	4.30832458	7.867452	1.17743087
H	1.53885266	-6.59762033	-2.61513442
H	3.22408216	-6.2807682	-3.08499681
H	0.79984973	-4.47544309	-3.62274277
H	1.4923401	-5.6188652	-4.76445642
H	2.24319931	-3.48209237	-5.44469101
H	3.65068511	-4.28246372	-4.76429385
H	3.49361428	-2.93155102	-2.71235627
H	1.92085733	-2.30245221	-3.17373361
H	4.53816354	-1.64405402	-4.69833545
H	1.98798235	-0.0893205	-4.02291173
H	2.91052436	1.28783092	-5.91558949
H	4.52589746	0.63335632	-5.64447447
H	4.69081688	1.78559772	-3.47602999
H	3.00191701	2.25799114	-3.52995037
H	3.41494593	3.75159587	-5.46517731
H	5.1013931	3.24520936	-5.53979263
H	4.9059504	5.42995427	-4.42310372
H	5.54394905	4.20429	-3.30234263
H	5.82497117	4.8602758	1.99391138
H	5.28571798	6.33758332	2.82609396
H	3.93695067	5.00012087	4.40883719
H	5.62660019	4.4995941	4.42931591
H	5.00412787	2.57861237	2.84525479
H	3.32639927	3.07349709	2.98181186
H	3.53878716	2.73008536	5.52826281
H	5.12050692	2.00671344	5.23491509
H	2.41551873	0.93473041	4.17452758

H	5.06410864	-0.43270392	4.87605411
H	3.79518356	-2.14861552	3.40559186
H	2.28426689	-1.41896121	3.92438607
H	2.94415503	-2.03128321	6.33739498
H	4.27545203	-2.96878452	5.67911976
H	1.30990312	-3.43202321	5.00255083
H	2.17213961	-4.26274677	6.28945761
H	1.97778736	-5.73406794	4.45022342
H	3.69896896	-5.32296759	4.62193088
H	10.58723731	-2.91714675	0.0864638
H	13.0107464	-3.23136778	-0.00448839
H	13.55332591	0.99874854	-0.61899253
H	11.09284199	1.31994789	-0.52353845
H	-9.2110016	2.02094019	4.90167511
H	-10.50721317	3.13465813	4.38353943
H	-8.83516737	3.73975489	4.59673854
H	-8.62534172	3.47948689	-3.65538007
H	-10.00366916	4.38984073	-2.97662589
H	-8.33240776	4.9943366	-2.7564196
H	-14.16214285	-2.71480593	2.1150175
H	-12.60900805	-1.84327689	1.94151687
H	-14.1077738	-0.93614189	2.29103589
H	-9.26453756	-3.06767954	-3.78992996
H	-10.49473385	-1.85195903	-3.34285788
H	-10.95980863	-3.27757656	-4.31939388
H	14.77957184	-3.10597934	-0.92148009

XW51 (the hexyloxy chains in the phenothiazine moiety were replaced by methoxy and methyl groups, respectively)

XW51			
C	1.0093233	-0.30226112	-0.14746396
C	-0.46330516	-2.37755267	-1.5359105
C	-1.46061026	-3.15080788	-2.05520666
C	-2.71487855	-2.55806117	-1.64545609
N	-2.45829687	-1.43986596	-0.88505157
C	-1.10015962	-1.30696333	-0.80339883
C	-1.2260279	2.63916549	1.89883566
C	-0.29247778	1.82028818	1.33354056
C	-1.01431198	0.78508814	0.62785999
N	-2.35906827	0.98461348	0.77127146
C	-2.52489958	2.1122331	1.54215235
C	-0.41164983	-0.27518578	-0.10498048
C	-7.28869899	2.014438	1.45847972
C	-6.29155966	2.78082768	1.98563589

C	-5.03501493	2.18243667	1.5834388
N	-5.29440647	1.06558546	0.8211375
C	-6.65172204	0.94086605	0.73000351
C	-3.75829471	2.67626353	1.92459621
C	-6.52869134	-3.01375418	-1.95544809
C	-7.46152859	-2.1880229	-1.39725345
C	-6.7380419	-1.15480895	-0.69353245
N	-5.39435202	-1.36038822	-0.82887553
C	-5.22631754	-2.4903175	-1.59675885
C	-3.99192817	-3.0532978	-1.97956375
C	-7.34078405	-0.08635583	0.02816506
Zn	-3.87691973	-0.18714596	-0.0298497
C	-3.74202898	3.91653246	2.7691307
C	-4.0581039	-4.29306325	-2.82320025
C	-3.78097092	3.82369372	4.17498021
C	-3.91492236	4.9769674	4.96320356
C	-3.98137211	6.22004532	4.33604529
C	-3.90114351	6.34760826	2.95029591
C	-3.76712864	5.19083331	2.16721795
C	-4.10404638	-4.20602444	-4.22690446
C	-4.23781177	-5.35555512	-5.01268146
C	-4.3140026	-6.6053714	-4.39702839
C	-4.24787578	-6.71892268	-3.00791025
C	-4.11414639	-5.56626202	-2.22664703
O	-3.99345232	-5.64277645	-0.8582829
O	-3.97400055	-2.96244091	-4.80099225
O	-3.65251431	5.19845762	0.80750375
O	-3.6795489	2.56054256	4.68125847
C	-3.60669205	6.45190106	0.11345952
C	-3.06475215	6.24311512	-1.29679016
C	-3.92151367	5.42981864	-2.28203448
C	-3.96593504	3.9100669	-2.01368943
C	-4.54892082	3.13141074	-3.1646034
C	-3.89182902	2.19381417	-3.85774642
C	-4.43433909	1.38839018	-5.00883963
C	-4.56838962	-0.10735389	-4.65978674
C	-4.85716232	-1.0001178	-5.87417867
C	-5.1235893	-2.45454007	-5.50552602
C	-5.14565069	-6.11631743	-0.13449639
C	-4.88956777	-5.92462519	1.35546615
C	-4.60597172	-4.46695199	1.74281334
C	-4.48656083	-4.24302887	3.26363852
C	-3.9429387	-2.87849076	3.59600372
C	-4.60199419	-1.88744265	4.20822069

C	-4.01597306	-0.53357508	4.51564067
C	-3.98067265	-0.2267201	6.02832679
C	-3.118022	0.9818199	6.43010848
C	-3.64680051	2.37433474	6.10226756
C	-8.76053274	-0.04082749	0.04657242
C	9.98018999	2.39874618	-1.83911843
C	9.56705629	3.52199219	-1.09772772
C	8.5599353	3.33658786	-0.13580968
C	8.02954285	2.07009803	0.11609865
C	8.47605753	0.9505688	-0.60107679
C	9.42840174	1.1414184	-1.61041446
S	6.73319464	1.84791371	1.32771017
C	5.78473809	0.626589	0.43216288
C	6.47311508	-0.35015899	-0.31093735
N	7.89708539	-0.32931732	-0.33477668
C	4.39234464	0.64595276	0.46671691
C	3.64876748	-0.32529974	-0.23387876
C	4.34279545	-1.2840475	-1.00369023
C	5.73132262	-1.27939859	-1.05485233
C	8.67247215	-1.41998589	0.13503642
C	10.16820937	4.86842642	-1.28275523
C	10.43378787	5.42937673	-2.56169073
C	10.98839203	6.70282585	-2.67714499
C	11.29337757	7.45503935	-1.53141369
C	11.0386761	6.92979531	-0.2622063
C	10.48244815	5.65162334	-0.16692742
C	8.07061679	-2.62085767	0.55756382
C	8.84217437	-3.68245174	1.02196125
C	10.24270668	-3.61174481	1.10215909
C	10.83337755	-2.40197617	0.69862341
C	10.07564595	-1.33287777	0.23075402
C	11.03238683	-4.74834643	1.64060959
C	10.56689648	-5.47020577	2.75875399
C	11.26852736	-6.53640214	3.30476928
C	12.49437783	-6.9256871	2.74438587
C	12.98563387	-6.23510174	1.63215692
C	12.26197599	-5.16484844	1.09464156
C	2.22787399	-0.31610707	-0.18670105
C	-9.97956324	0.00018679	0.05923954
C	-11.39827977	0.04861861	0.06860799
C	-12.07874159	1.09339186	0.73125215
C	-13.4672973	1.13689641	0.74036003
C	-14.2192469	0.14484064	0.08918835
C	-13.54481986	-0.88593029	-0.58592099

C	-12.15924581	-0.9425779	-0.5924026
O	10.09872019	4.66821711	-3.64233581
C	10.30546805	5.20007013	-4.94697129
O	11.83551877	8.6821662	-1.77219848
C	12.16534076	9.50234024	-0.65529081
O	13.12678539	-7.97315907	3.34665911
C	14.37928243	-8.39702809	2.81888292
O	12.82012633	-4.51594498	0.00719496
C	12.32718857	-4.96066495	-1.26042906
C	-15.71122172	0.14292844	0.04204328
O	-16.35366693	-0.50131542	-0.76320488
O	-16.37196794	0.90425913	0.95000328
H	0.60440466	-2.51421701	-1.63517262
H	-1.35867922	-4.04039209	-2.6608237
H	-1.05651318	3.52064816	2.50132558
H	0.7840769	1.9031998	1.38498831
H	-8.35637997	2.15638994	1.55026368
H	-6.39423767	3.66988679	2.59117774
H	-6.70660274	-3.89511151	-2.5549976
H	-8.53812611	-2.26678853	-1.45399104
H	-3.98217331	4.91469635	6.04191728
H	-4.09682798	7.11353968	4.94368981
H	-3.95818233	7.32888508	2.4965647
H	-4.2617582	-5.26579393	-6.09418972
H	-4.40924393	-7.50007413	-5.0059336
H	-4.2792849	-7.69180309	-2.52750091
H	-2.94084135	7.14117347	0.64675821
H	-4.61272951	6.8951469	0.09437248
H	-2.06539233	5.79441092	-1.21919483
H	-2.91936072	7.24964703	-1.71216743
H	-3.50865273	5.58955921	-3.28698808
H	-4.94413112	5.83363264	-2.30498255
H	-4.54298933	3.72480238	-1.09963513
H	-2.94786222	3.54945533	-1.81372461
H	-5.57512066	3.37807102	-3.44904416
H	-2.86497818	1.95729013	-3.56643413
H	-3.75650434	1.48945945	-5.87079157
H	-5.40775132	1.78588481	-5.32615504
H	-5.36529479	-0.2279817	-3.91356806
H	-3.645851	-0.4535293	-4.17974823
H	-4.01458205	-0.95469235	-6.57743328
H	-5.73993122	-0.63323471	-6.41637612
H	-5.30940282	-3.05651545	-6.40519582
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H	-5.32600597	-7.17488339	-0.36507236
H	-4.04791767	-6.56051828	1.6616892
H	-5.77531291	-6.29608429	1.88965062
H	-5.3995233	-3.81758277	1.34905658
H	-3.6788564	-4.14660864	1.25375029
H	-3.8151559	-5.00980373	3.68067241
H	-5.46519456	-4.38944665	3.74016884
H	-2.9124552	-2.69775918	3.27869007
H	-5.63175099	-2.05772093	4.5329307
H	-4.58559563	0.251674	4.00409041
H	-2.99474381	-0.4840782	4.11428694
H	-3.57777286	-1.10613729	6.54813839
H	-5.00510419	-0.09282015	6.40505141
H	-2.11577522	0.88138524	5.99242153
H	-2.98158869	0.96393124	7.51998321
H	-2.97914071	3.11846226	6.55325427
H	-4.65517019	2.52664214	6.51334737
H	10.73331733	2.51389679	-2.60915989
H	8.1706867	4.19161477	0.40833645
H	9.7498457	0.29117922	-2.20376133
H	3.87514577	1.41246359	1.03459477
H	3.78226147	-2.0178555	-1.57343623
H	6.25471649	-2.00614355	-1.66755703
H	11.1918356	7.14860772	-3.64257899
H	11.27018056	7.48313622	0.63955171
H	10.30435979	5.23719419	0.82136819
H	6.99431615	-2.73445205	0.53521372
H	8.33382591	-4.59526509	1.32110015
H	11.90984293	-2.28736766	0.75912623
H	10.58600856	-0.41749269	-0.04013054
H	9.63438854	-5.16427221	3.22452032
H	10.89447059	-7.0679953	4.17413643
H	13.92481813	-6.49793053	1.16040908
H	-11.50769399	1.87007305	1.22916816
H	-13.94958542	1.97695362	1.23378677
H	-14.12920744	-1.64160938	-1.09957979
H	-11.64825209	-1.74867893	-1.10891108
H	11.36680288	5.40449238	-5.13294113
H	9.95735197	4.43127422	-5.63835157
H	9.72594435	6.11843144	-5.10004202
H	12.57427365	10.42386813	-1.07235379
H	11.2776263	9.73626304	-0.0551448
H	12.91925509	9.02511766	-0.01742377

H	14.70209727	-9.22919381	3.4464087
H	14.28144036	-8.74028902	1.78148884
H	15.1257252	-7.59448739	2.8658353
H	12.53955025	-6.02726171	-1.40971937
H	11.24784034	-4.79044573	-1.35007498
H	12.85139155	-4.37570454	-2.0194621
H	-15.76296748	1.26401428	1.61627369