**Electronic Supplementary Information (ESI)**

# Efficient solar cells sensitized by a promising new type of porphyrins: dye-aggregation suppressed by double strapping

Kaiwen Zeng,[a] Yunyue Lu,[a] Weiqiang Tang,[b] Qingyun Liu[c], Weihong Zhu,[a] He Tian,[a] and Yongshu Xie*[a, d] Zhao, Shuangliang [b]

[a]*Key Laboratory for Advanced Materials and Feringa Nobel Prize Scientist Joint Research Center, School of Chemistry and Molecular Engineering, East China University of Science & Technology, 130 Meilong, Shanghai 200237, China.*

[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, P. R. China.*

[d]*Corresponding author: Yongshu Xie, E-mail: yshxie@ecust.edu.cn*

## Contents

## 1. Experimental Details

### 1.1 Materials and Reagents

All 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) was purchased from Geao Science and Educational Co. Ltd. $TiO_2$ paste (18NR-T and 18NR-AO) was purchased from Dyesol Ltd. The FTO conducting glass was washed with a detergent solution, deionized water, ethanol, and acetone successively under ultrasonication for 20 min before use.

### 1.2 Equipment and Apparatus

$^1H$ NMR and $^{13}C$ NMR spectra were obtained using a Bruker AM 400 spectrometer. 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.[1] A screen-printed double layer of $TiO_2$ particles was used as the photoelectrode, and the detailed procedure was reported in our previous work.[2] However, the dyes examined in this report were not fully soluble in the solvent used before (Toluene : EtOH = 1 : 4). Therefore, 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°C for the indicated time. For coadsorption, the films were then immersed into a 0.2 mM solution of the dyes with various concentrations of CDCA in a mixture of chloroform and ethanol (volume ratio of 3 : 2) at 25°C for 12 h. For cosensitization, the films were immersed into a 0.2 mM solution of porphyrin dyes in a mixture of chloroform and ethanol (volume ratio of 3 : 2) at 25°C for 12 h. Then, the porphyrin-sensitized films were washed with ethanol, dried in air, and immersed in a solution containing **Z1** (0.3 mM) in a mixture of chloroform and ethanol (volume ratio of 1 : 1) at 25°C for the indicated time. The counter electrode was also prepared according to the procedure reported in our previous work.[3, 4] The 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.

### 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[5, 6] and the 6-31G* basis set.[7] For zinc atoms, the Los Alamos effective core potential basis set (LANL2DZ) was used.[8] All calculations were carried out using the Gaussian09 program package.[9]

### 1.6 Measurement of the Dye Adsorption Amounts

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 dye.

### 1.7 Synthesis of Dyes

***Synthesis of compound 1.*** In a 250 mL three-necked flask, 2,6-dihydroxybenzaldehyde (4.00 g, 29.40 mmol), 6-bromo-1-hexene (14.38 g, 88.20 mmol), and $K_2CO_3$ (16.25 g, 117.60 mmol) were mixed in DMF (120 mL) under nitrogen. After the mixture was kept stirring at 80°C for 24 h, the resulting suspension was poured into water, extracted with $CH_2Cl_2$, and washed with water. The organic portions were combined and dried using anhydrous $Na_2SO_4$. After filtration, the solvent was removed by rotary evaporation. The residue was purified by column chromatography (silica gel, $CH_2Cl_2$ : PE = 1 : 2) to give **1** as a yellow oil (8.14 g, yield 92%). $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 10.53 (s, 1H), 7.35 – 7.39 (t, *J* = 8.4 Hz, 1H), 6.51 – 6.53 (d, *J* = 8.4 Hz, 2H), 5.78 – 5.85 (m, 2 H), 4.95 – 5.05 (m, 4H), 4.01 – 4.05 (t, *J* = 6.4 Hz, 4 H), 2.09 – 2.15 (m, 4H), 1.82 – 1.87 (m, 4H), 1.56 – 1.62 (m, 4H). $^{13}$C NMR ($CDCl_3$, 100 MHz): $\delta$ 25.24, 28.49, 33.35, 68.71, 104.57, 114.83, 135.58, 138.43, 161.62, 189.28. HRMS (ESI, *m/z*): $[M+H]^+$ calcd for $C_{19}H_{27}O_3$, 303.1960; Found, 303.1966.

***Synthesis of compound 2.*** To a solution of **1** (2.36 g, 7.80 mmol) and dipyrromethene (1.14 g, 7.80 mmol) in $CH_2Cl_2$ (1.5 L), was added trifluoroacetic acid (1.5 mL, 20 mmol) under nitrogen. The solution was stirred at room temperature for 4 h in dark. Then, DDQ (2,3-dichloro-5,6-dicyanobenzoquinone) (2.56 g, 11.61 mmol) was added and stirred at room temperature for

another 1 h. After the reaction was quenched by the addition of 3 mL triethylamine, the solvent was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, $CH_2Cl_2$ : PE = 1 : 3) to give compound **2** as purple powders (0.87 g, yield 26%). $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 10.15 (s, 2H), 9.27 – 9.28 (d, *J* = 4.8 Hz, 4 H), 8.97 – 8.98 (d, *J* = 4.4 Hz, 4H), 7.70 – 7.74 (t, *J* = 8.4 Hz, 2H), 7.02 – 7.04 (d, *J* = 8.4 Hz, 4H), 4.96 – 5.06 (m, 4 H), 4.31 – 4.40 (m, 4 H), 3.84 – 3.87 (t, *J* = 6.2 Hz, 8 H), 1.26 – 1.29 (m, 8 H), 0.92 – 0.96 (m,8 H), 0.50 – 0.51 (m, 8 H), -3.02 (s, 1 H). $^{13}$C NMR ($CDCl_3$, 100 MHz): $\delta$ 24.56, 28.14, 32.70, 68.58, 104.12, 105.55, 111.58, 113.90, 120.18, 130.20, 130.51, 131.03, 138.26, 145.09, 147.74, 160.22. HRMS (ESI, *m*/*z*): $[M+H]^+$ calcd for $C_{56}H_{63}N_4O_4$, 855.4849; Found, 855.4839.

***Synthesis of compound 3.*** To a solution of porphyrin **1** (2.06 g, 2.41 mmol) in $CH_2Cl_2$ (800 mL) was added NBS (0.94 g, 5.30 mmol) in $CH_2Cl_2$ (300 mL) dropwise at room temperature. After 1 h, 100 mL water was added to quench the reaction and the raw product was extracted using $CH_2Cl_2$ and water. The organic layers were combined and dried using anhydrous $Na_2SO_4$. Then the solvent was removed under reduced pressure and the residue was purified by column chromatography (silica gel, $CH_2Cl_2$ : PE = 2 : 3) to afford **3** as purple powders (2.09 g, yield 86%). $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 9.55 – 9.56 (d, *J* = 4.8 Hz, 4 H), 8.82 – 8.83 (d, *J* = 4.4 Hz, 4H), 7.71 – 7.75 (t, *J* = 8.4 Hz, 2H), 7.00 – 7.03 (d, *J* = 8.4 Hz, 4H), 4.50 – 5.07 (m, 4 H), 4.30 – 4.43 (m, 4 H), 3.87 – 3.90 (t, *J* = 6.2 Hz, 8 H), 1.29 – 1.33 (m, 8 H), 0.98 – 1.02 (m,8 H), 0.50 – 0.54 (m, 8 H), -2.55 (s, 2 H). $^{13}$C NMR ($CDCl_3$, 100 MHz): $\delta$ 24.49, 28.02, 32.57, 68.41, 102.36, 105.15, 113.85, 114.11, 119.96, 130.36, 138.01, 159.92. HRMS (ESI, *m*/*z*): $[M+H]^+$ calcd for $C_{56}H_{61}N_4O_4Br_2$, 1011.3060; Found, 1011.3071.

***Synthesis of compound 4.*** To a solution of porphyrin **3** (2.09 g, 2.06 mmol) in $CH_2Cl_2$ (350 mL) was added a $CH_3OH$ (50 mL) solution of $Zn(OAc)_2{\cdot}2H_2O$ (18.12 g, 82.50 mmol). After reflux overnight, the solution was poured into water, extracted with $CH_2Cl_2$, and the combined organic extracts were dried over anhydrous $Na_2SO_4$. Then the solvent was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, $CH_2Cl_2$ : PE = 1 : 1) to afford **4** as purple powders (2.20 g, yield 98%). $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 9.63 – 9.64 (d, *J* = 4.8 Hz 4H), 8.87 – 8.89 (d, *J* = 4.4 Hz, 4H), 7.69 – 7.73 (t, *J* = 8.4 Hz, 2H), 7.00 – 7.02 (d, *J* = 8.4 Hz, 4H), 4.58 – 4.68 (m, 4 H), 3.88 – 3.93 (m, 8H), 3.84 – 3.87 (t, *J* = 6.2 Hz, 8 H), 0.10 – 1.05 (m,8 H), 0.91 – 0.96 (m, 8 H), 0.25 – 0.32 (m, 8 H). $^{13}$C NMR ($CDCl_3$, 100 MHz): $\delta$ 24.37, 28.14, 32.45, 68.70, 103.93, 105.70, 113.65, 114.64, 121.31, 130.15, 132.70, 132.90, 138.11, 149.73, 151.36, 160.03. HRMS (FTICR-MS, *m*/*z*): $[M]^+$ calcd For $C_{56}H_{58}Br_2N_4O_4Zn$, 1072.2116; Found, 1072.2093.

***Synthesis of compound 5.*** A solution of **4** (600 mg, 0.56 mmol) and 2$^{nd}$ Generation Grubbs Catalyst (48 mg, 0.05 mmol) in $CH_2Cl_2$ (800 mL) were stirred at 40$^o$C for 24 h under nitrogen. Then the solvent was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, $CH_2Cl_2$ : PE = 2 : 3) to afford **5** as purple powders (249 mg, yield 45%). $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 9.65 – 9.67 (d, *J* = 4.8 Hz, 4H), 8.89 – 8.90 (d, *J* = 4.4 Hz, 4H), 7.70 – 7.74 (t, *J* = 8.4 Hz, 2H), 7.10 – 7.12 (d, *J* = 8.4 Hz, 4H), 3.84 – 3.87 (t, *J* = 5.4 Hz, 8H), 2.04 – 2.06 (m, 4H), 0.82 – 0.88 (m, 8H), -0.66 – -0.62 (m, 8H), -1.02 – -0.96 (m, 8H). HRMS (FTICR-MS, *m*/*z*): $[M+H]^+$ calcd for $C_{52}H_{51}Br_2N_4O_4Zn$, 1017.1563; Found, 1017.1575.

***Synthesis of compound 6.*** In a three-neck 250 mL flask, compound **5** (200 mg, 0.19 mmol), 3-ethynyl-10-hexyl-7-(4-(hexyloxy)-phenyl)-10*H*-phenothiazine[10] (114 mg, 0.24 mmol), $Pd_2(dba)_3$ (90 mg, 0.10 mmol), and $AsPh_3$ (121 mg, 0.39 mmol) were mixed in dry THF (100 mL) and $Et_3N$

(50 mL) under nitrogen. After the mixture was stirred at 55°C for 24 h, the solvent was removed under reduced pressure and the residue was purified by column chromatography (silica gel, $CH_2Cl_2$ : PE = 4 : 3), followed by recrystallization from $CH_2Cl_2$/$CH_3OH$ to afford the target compound as dark green powders (154 mg, yield 54%). $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 9.70 (d, $J$ = 4.4 Hz, 2H), 9.63 (d, $J$ = 4.4 Hz, 2H), 8.90 (d, $J$ = 4.4 Hz, 2H), 8.86 (d, $J$ = 4.4 Hz, 2H), 7.78 – 7.81 (m, 2H), 7.72 (t, $J$ =8.4 Hz, 2H), 7.48 (d, $J$ = 8.8 Hz, 2H), 7.36 – 7.39 (m, 2H), 7.12 (d, $J$ = 8.4 Hz, 4H), 7.01 (d, $J$ = 8.4 Hz, 1H), 6.96 (d, $J$ = 8.8 Hz, 3H), 3.97 – 4.01 (m, 4H), 3.85 (t, $J$ = 5.3 Hz, 8H), 1.94 – 1.96 (m, 4H), 1.89 – 1.92 (m, 2H), 1.79 – 1.82 (m, 2H), 1.46 – 1.53 (m, 4H), 1.34 – 1.40 (m, 8H), 0.90 – 0.94 (m, 6H), 0.82 – 0.88 (m, 8H), -0.77 – -0.73 (m, 8H), -0.98 – -0.92 (m, 8H). $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 160.46, 158.72, 152.37, 151.47, 150.66, 149.19, 145.34, 143.45, 135.79, 132.72, 132.61, 132.48, 132.41, 130.97, 130.34, 130.26, 127.84, 127.65, 125.70, 125.63, 125.22, 124.82, 124.59, 118.24, 115.80, 115.38, 115.17, 114.97, 109.74, 105.00, 100.16, 95.39, 93.00, 71.36, 68.26, 47.92, 31.75, 31.65, 30.89, 29.61, 29.42, 27.03, 26.83, 25.89, 25.36, 22.79, 22.77, 14.19. HRMS (FTICR-MS, $m/z$): $[M]^+$ calcd for $C_{84}H_{86}BrN_5O_5SZn$, 1419.4820; Found, 1419.4817.

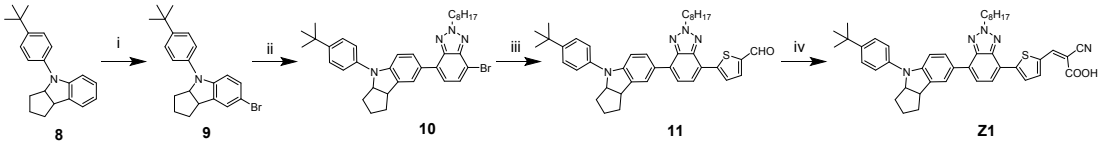
***Synthesis of compound 7a.*** In a three-neck 100 mL flask, **6** (66 mg, 0.046 mmol), methyl 4-ethynylbenzoate (15 mg, 0.092 mmol), $Pd_2(dba)_3$ (21 mg, 0.023 mmol), and $AsPh_3$ (28 mg, 0.092 mmol) were mixed in dry THF (15 mL) and $Et_3N$ (6 mL) under nitrogen. After the mixture was stirred at 55°C 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 the target compound as dark green powders (38 mg, yield 55%). $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 9.68 – 9.69 (m, 4H), 8.88 – 8.90 (d, $J$ = 4.4 Hz, 2H), 8.86 – 8.87 (d, $J$ = 4.4 Hz, 2H), 8.22 – 8.24 (d, $J$ = 8.4 Hz, 2H), 8.07 – 8.09 (d, $J$ = 8.4 Hz, 2H), 7.71 – 7.81 (m, 4H), 7.48 – 7.50 (d, $J$ = 8.4 Hz, 2H, phenyl), 7.36 – 7.39 (m, 2H), 7.13 – 7.15 (d, $J$ = 8.4 Hz, 2H), 7.01 – 7.03 (d, $J$ = 8.4 Hz, 1H), 6.95 – 6.97 (d, $J$ = 8.8 Hz, 3H, phenyl), 3.95 – 4.02 (m, 7H), 3.86 – 3.89 (t, $J$ = 6.4 Hz, 8H), 2.00 (m, 4H), 1.91 – 1.95 (m, 2H), 1.71 – 1.84 (m, 2H), 1.49 – 1.50 (m, 4H), 1.35 – 1.38 (m, 8H), 0.90 – 0.94 (m, 6H), 0.84 – 0.88 (m, 8H), -0.72 – -0.71 (m, 8H), -0.96 – -0.88 (m, 8H). $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 166.78, 160.33, 158.60, 151.77, 151.50, 150.74, 150.61, 145.33, 143.29, 135.69, 132.35, 132.27, 132.03, 131.37, 130.90, 130.84, 130.47, 130.25, 130.19, 129.89, 129.25, 127.64, 127.53, 125.59, 125.51, 125.13, 124.70, 124.44, 117.99, 115.70, 115.66, 115.27, 114.84, 109.80, 101.56, 99.10, 96.52, 95.77, 95.04, 92.88, 71.37, 68.13, 52.32, 47.80, 31.64, 31.54, 30.65, 29.73, 29.44, 29.30, 26.90, 26.71, 25.78, 25.30, 22.68, 22.65, 14.09. MS (MALDI-TOF): [M] calcd for $C_{94}H_{93}N_5O_7SZn$, 1499.6; Found, 1499.5.

***Synthesis of compound 7b.*** It was prepared according to the procedure same as that for **7a**, except that methyl 4-(7-ethynylbenzo[*c*][1,2,5]thiadiazol-4-yl)benzoate (27 mg, 0.092 mmol) was used instead of methyl 4-ethynylbenzoate. Brown powders, 49 mg, yield: 66%. $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 10.06 (d, $J$ = 4.4 Hz, 2H), 9.70 (d, $J$ = 4.4 Hz, 2H), 8.98 (d, $J$ = 4.4 Hz, 2H), 8.89 (d, $J$ = 4.4 Hz, 2H), 8.32 (d, $J$ = 7.4 Hz, 1H), 8.27 (d, $J$ = 8.4 Hz, 2H), 8.18 (d, $J$ = 8.4 Hz, 2H), 7.97 (d, $J$ = 7.4 Hz, 1H), 7.79 – 7.83 (m, 2H), 7.74 (t, $J$ = 8.4 Hz, 2H), 7.49 (d, $J$ = 8.6 Hz, 2H), 7.37 – 7.40 (m, 2H), 7.15 (d, $J$ = 8.4 Hz, 4H), 7.02 (d, $J$ = 8.4 Hz, 1H), 6.97 (d, $J$ = 8.6 Hz, 3H), 3.98 – 4.02 (m, 7H), 3.87 (t, $J$ = 5.3 Hz, 8H), 1.91 – 1.97 (m, 2H), 1.83 – 1.85 (m, 4H), 1.78 – 1.81 (m, 2H), 1.47 – 1.55 (m, 4H), 1.35 – 1.40 (m, 8H), 0.91 – 0.94 (m, 6H), 0.86 – 0.88 (m, 8H), -0.93 – -0.83 (m, 16H). MS (MALDI-TOF): [M] calcd for $C_{100}H_{95}N_7O_7S_2Zn$, 1633.6; Found, 1633.5.

***Synthesis of XW40.*** In a three-neck 100 mL flask, porphyrin carboxylate **7a** (37 mg, 0.025 mmol) and $LiOH{\cdot}H_2O$ (44 mg, 1.065 mmol) were mixed in THF (15 mL) and $H_2O$ (2 mL) under

nitrogen. After the mixture was refluxed for 12 h, the solution was poured into water, extracted with $CH_2Cl_2$, and the combined organic extracts were dried over anhydrous $Na_2SO_4$. Then the solvent was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, $CH_2Cl_2$ : MeOH = 15 : 1), followed by recrystallization from $CH_2Cl_2$/MeOH to afford the product as a dark green powder (31 mg, yield 84%). $^1$H NMR ($CDCl_3$ : DMSO-$d_6$ = 1 : 2, 400 MHz, ppm): $\delta$ 13.00 (s, 1H), 9.56 – 9.58 (m, 4H), 8.72 – 8.73 (d, *J* = 4.4 Hz, 2H), 8.69 – 8.70 (d, *J* = 4.4 Hz, 2H), 8.14 – 8.19 (m, 4H), 7.86 – 7.89 (m, 1H), 7.81 – 7.82 (m, 1H), 7.73 – 7.77 (t, *J* = 8.3 Hz, 2H), 7.54 – 7.56 (d, *J* = 8.8 Hz, 2H), 7.44 – 7.46 (m, 1H), 7.41 – 7.42 (m, 1H), 7.17 – 7.19 (d, *J* = 8.4 Hz, 5H), 7.09 – 7.11 (d, *J* = 8.4 Hz, 1H), 6.96 – 6.98 (d, *J* = 8.8 Hz, 2H), 3.98 – 4.01 (m, 4H), 3.90 – 3.93 (m, 8H), 1.82 – 1.85 (m, 2H), 1.73 – 1.77 (m, 2H), 1.44 – 1.51 (m, 4H), 1.34 – 1.35 (m, 8H), 1.24 – 1.25 (m, 4H), 0.85 – 0.92 (m, 14H), -0.03 – 0.01 (m, 8H), -1.02 – -0.94 (m, 8H). MS (MALDI-TOF): [M] calcd for $C_{93}H_{91}N_5O_7SZn$, 1485.6; Found, 1485.5.

***Synthesis of XW41.*** It was prepared according to the procedure same as that for XW40, except that 7b (49 mg, 0.030 mmol) was used instead of 7a. Brown powders, 42 mg, yield: 86%. $^1$H NMR (THF-$d_8$, 400 MHz, ppm): δ 12.96 (s, 1H), 9.93 (d, *J* = 4.4 Hz, 2H), 9.52 (d, *J* = 4.4 Hz, 2H), 8.77 (d, *J* = 4.4 Hz, 2H), 8.70 (d, *J* = 4.4 Hz, 2H), 8.32 (d, *J* = 7.2 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 2H), 8.12 (d, *J* = 8.0 Hz, 2H), 8.04 (d, *J* = 7.2 Hz, 1H), 7.74 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.70 (d, *J* = 2.0 Hz, 1H), 7.62 (t, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.8 Hz, 2H), 7.30 – 7.32 (m, 2H), 7.05 (d, *J* = 8.4 Hz, 5H), 6.96 (d, *J* = 8.6 Hz, 1H), 6.84 (d, *J* = 8.8 Hz, 2H), 3.95 (t, *J* = 7.2 Hz, 2H), 3.89 (t, *J* = 6.6 Hz, 2H), 3.83 (t, *J* = 5.3 Hz, 8H), 2.63 (t, *J* = 3.8 Hz, 4H), 1.92 – 1.97 (m, 2H), 1.79 – 1.83 (m, 2H), 1.40 – 1.47 (m, 4H), 1.26 – 1.29 (m, 8H), 0.77 – 0.84 (m, 14H), -0.09 – -0.04 (m, 8H), -0.90 – -0.80 (m, 8H). MS (MALDI-TOF): [M] calcd for $C_{99}H_{93}N_7O_7S_2Zn$, 1619.6; Found, 1619.6.




**Scheme S1. Synthesis Routes for Sensitizers Z1.** Reaction conditions: (i) NBS, acetone, 0°C; (ii) a: n-BuLi, THF, $B(OMe)_3$, -78°C; b: 4,7-dibromo-2-octyl-2H-benzo[d][1,2,3]triazole, $Pd(PPh_3)_4$, $K_2CO_3$, $H_2O$, THF, reflux; (iii) 5-formylthiophen-2-boronic acid, $Pd(PPh_3)_4$, 2 M $K_2CO_3$ aqueous solution, THF, 80°C; (iv) cyanoacetic acid, piperidine, acetonitrile, 80°C.

***Synthesis of 9.*** To a cold solution of **8**[11] (10.0 g, 34 mmol) in dry acetone at room temperature was added N-bromosuccinimide (6.11 g, 34 mmol). The reaction mixture was stirred at room temperature for 2 h under nitrogen atmosphere. then the mixture was poured into water, extracted with DCM and dried over anhydrous $Na_2SO_4$. The crude product was purified by recrystallization from $CHCl_3$ to obtain bromide **9** as white powder (11.58 g, yield 92%). $^1$H NMR (DMSO-$d_6$, 400 MHz, ppm): $\delta$ 7.35 (d, *J* = 9.2 Hz, 1H), 7.23 (s, 1H), 7.17 (d, *J* = 8.6 Hz, 2H), 7.09 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.78 (d, *J* = 8.5 Hz, 1H), 4.78 – 4.82 (m, 1H), 3.75 – 3.80 (m, 1H), 1.56 – 2.01 (m, 6H), 1.27 (s, 9H). $^{13}$C NMR (DMSO-$d_6$, 100 MHz, ppm): $\delta$ 146.4, 144.0, 139.4, 137.3, 129.5, 127.2, 125.9, 118.9, 108.5, 108.3, 68.2, 44.5, 34.6, 33.9, 33.2, 31.2, 23.9. HRMS (ESI, *m*/*z*): $[M + H]^+$ calcd for $C_{40}H_{47}N_4OS$, 631.3471 found, 631.3479.

***Synthesis of 10.*** To a solution of **9** (3.56 g, 9.60 mmol) in dry THF (40 mL) was added n-BuLi (4.41 mL, 10.56 mmol) dropwise at -78°C under argon in dark. After 30 min of stirring at -78°C,

$B(OMe)_3$ (1.52 g, 14.4 mmol) was added. The reaction mixture was stirred at the same temperature for 4 h, then gradually warmed up to room temperature and used for the next Suzuki coupling reaction without purification. The unpurified mixture was used to react with 4,7-dibromo-2-octyl-2H-benzo[d][1,2,3]triazole[12] (3.73 g, 9.60 mmol) through a Suzuki coupling reaction using $Pd(PPh_3)_4$ (221 mg, 0.19 mmol) and $K_2CO_3$ aqueous solution (5 mL, 2M) as catalysts in THF (40 mL) for 12 h. After cooling to room temperature, water was added and the reaction mixture was extracted with $CH_2Cl_2$. The combined organic layer was dried over anhydrous $Na_2SO_4$, evaporated under reduced pressure, and the residue was purified by column chromatography (silica gel, DCM : PE = 1 : 3) to obtain **10** as yellow oil (2.71 g, 47% for the two steps). $^1$H NMR ($CDCl_3$, 400 MHz, ppm): $\delta$ 7.74 – 7.78 (m, 2H), 7.58 (d, $J$ = 7.7 Hz, 1H), 7.36 – 7.40 (m, 3H), 7.27 (d, $J$ = 7.6 Hz, 2H), 7.08 (d, $J$ = 8.4 Hz, 1H), 4.82 – 4.86 (m, 1H), 4.77 (t, $J$ = 7.4 Hz, 2H), 3.90 – 3.95 (m, 1H), 2.09 – 2.19 (m, 3H), 1.94 – 1.99 (m, 2H), 1.80 – 1.89 (m, 1H), 1.66 – 1.71 (m, 1H), 1.52 – 1.57 (m, 1H), 1.34 (s, 9H), 1.25 – 1.30 (m, 10H), 0.85 – 0.87 (m, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm): $\delta$ 148.2, 144.7, 144.5, 144.4, 142.9, 140.3, 135.6, 131.6, 129.4, 128.2, 126.7, 126.2, 126.1, 124.8, 123.2, 119.4, 118.0, 107.9, 107.1, 69.2, 57.1, 56.8, 45.6, 35.2, 34.4, 34.0, 31.8, 31.6, 30.3, 30.2, 29.2, 29.1, 26.7, 24.6, 22.7, 14.2, 14.2. HRMS (ESI, $m/z$): $[M + H]^+$ calcd for $C_{35}H_{44}N_4Br$, 599.2749; found, 599.2751.

***Synthesis of 11.*** A mixture of **10** (0.91 g, 1.52 mmol), 4-formylphenylboronic acid (0.26 g, 1.67 mmol), $Pd(PPh_3)_4$ (87.8 mg, 0.08 mmol), $K_2CO_3$ (315 mg, 2.28 mmol), THF (30 ml) and $H_2O$ (3 ml) was refluxed for 12 h under argon. After cooling, water was added and the reaction mixture was extracted three times with $CH_2Cl_2$. The combined organic layer was washed with $H_2O$ and brine, dried over anhydrous $Na_2SO_4$, and evaporated under reduced pressure. The crude product was purified by column chromatography (silica gel, $CH_2Cl_2$ / PE = 2 / 3) to yield compound **11** as a red solid (307 mg, 0.48 mmol, 32%). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.94 (s, 1H), 8.15 (d, $J$ = 4.0 Hz, 1H), 7.88 (dd, $J$ = 8.4, 2.0 Hz, 1H), 7.84 (s, 1H), 7.78 – 7.82 (m, 2H), 7.54 (d, $J$ = 7.7 Hz, 1H), 7.38 (d, $J$ = 8.8 Hz, 2H), 7.27 (d, $J$ = 8.8 Hz, 2H), 7.09 (d, $J$ = 8.4 Hz, 1H), 4.83 – 4.88 (m, 1H), 4.80 (t, $J$ = 7.3 Hz, 2H), 3.92 – 3.96 (m, 1H), 2.15 – 2.23 (m, 2H), 2.07 – 2.13 (m, 1H), 1.95 – 1.99 (m, 2H), 1.81 – 1.89 (m, 1H), 1.66 – 1.72 (m, 1H), 1.53 – 1.59 (m, 1H), 1.40 – 1.43 (m, 4H), 1.35 (s, 9H), 1.26 – 1.29 (m, 6H), 0.86 – 0.88 (m, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm): $\delta$ 182.9, 150.4, 148.4, 144.8, 143.2, 142.5, 142.0, 140.1, 137.4, 135.6, 133.1, 128.6, 126.9, 126.8, 126.1, 124.9, 124.8, 122.3, 119.5, 107.9, 69.2, 56.9, 45.5, 34.3, 31.9, 31.5, 30.2, 29.2, 29.1, 26.7, 24.6, 22.7, 14.2. HRMS (ESI, $m/z$): $[M + H]^+$ calcd for $C_{40}H_{47}N_4OS$, 631.3471 found, 631.3479.

***Synthesis of Z1.*** A mixture of aldehyde **11** (75 mg, 0.12 mmol) and cyanoacetic acid (30 mg, 0.36 mmol) in acetonitrile (10 mL) was refluxed in the presence of piperidine (0.1 mL) for 7 h under argon. After cooling, water was added and the reaction mixture was extracted with $CH_2Cl_2$, dried over $Na_2SO_4$, and evaporated under reduced pressure. The crude product was purified by column chromatography (silica gel, $CH_2Cl_2$ / methanol = 15 / 1), to yield **Z1** as a deep red solid (61 mg, 73%). $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 13.75 (s, 1H), 8.41 (s, 1 H), 8.19 (d, $J$ = 3.7 Hz, 1 H), 7.92 – 8.01 (m, 4 H), 7.71 (d, J = 7.4 Hz, 1 H), 7.39 (d, $J$ = 7.7 Hz, 2 H), 7.28 (d, $J$ = 7.7 Hz, 2 H), 7.01 (d, $J$ = 8.3 Hz, 1 H), 4.91 (m, 1 H), 4.84 (t, $J$ = 7.2 Hz, 2 H), 3.91 (m, 1H), 2.10 (m, 3 H), 1.78 – 1.87 (m, 3 H), 1.64 (m, 1 H), 1.41 (m, 1 H), 1.29 (s, 9 H), 1.21 (m, 4 H),1.32 (m, 6 H), 0.79 (t, $J$ = 5.7 Hz, 3 H). HRMS (ESI, $m/z$): $[M + H]^+$ calcd for $C_{43}H_{48}N_5O_2S$, 698.3529; found, 698.3531.

## 2. Absorption and Emission Spectra

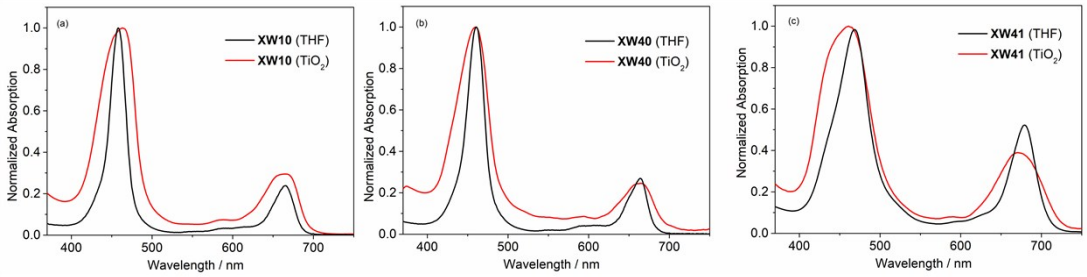



**Figure S1**. Normalized UV-visible spectra of the porphyrins in THF and on the $TiO_2$ films (3 µm).

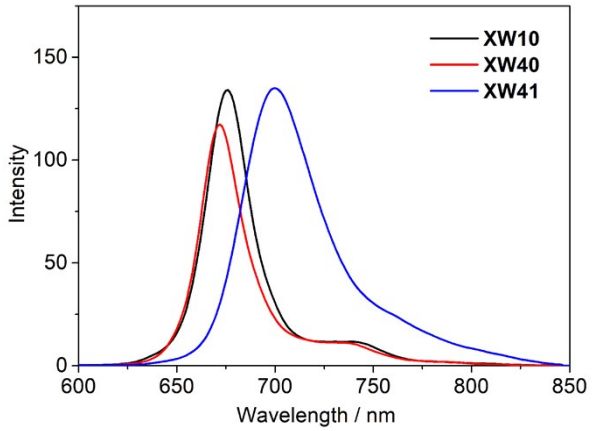



**Fig. S2** Emission spectra of **XW10**, **XW40**, **and XW41** in THF. The spectra were used to calculate the wavelength at the intersection ($\lambda_{inter}$) of normalized absorption and emission spectra, and the corresponding $E_{0\text{-}0}$ values. Excitation wavelengths: 459 nm (**XW10**), 461 nm (**XW40**), and 468 (**XW41**).

## 3. Cyclic Voltammetry Curves

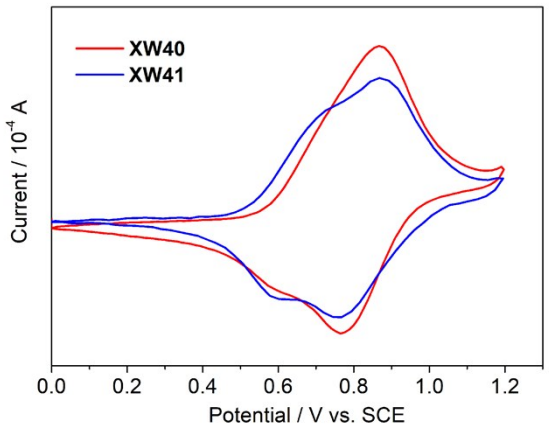



**Fig. S3** Cyclic voltammetry curves of the dyes adsorbed to a nanocrystalline $TiO_2$ film deposited on conducting FTO glass.

## 4. Crystal Structure of Compound 5

Single crystals **5** were obtained by slow diffusion of chloroform vapor to the corresponding $CHCl_3$/MeOH solutions. X-ray analyses of **5** were performed on a SMART APEX equipped with CCD detector (Bruker) using MoKα (graphite, monochromated, λ = 0.71073 Å) radiation and CuKα (graphite, monochromated, λ = 1.54178 Å) radiation. The structure was solved by the

direct method of SHELXS-97 and refined using the SHELXL-97 program.[13, 14] The positional parameters and thermal parameters of non-hydrogen atoms were refined anisotropically on $F^2$ by the full-matrix least-squares method. Hydrogen atoms were placed at calculated positions and refined riding on their corresponding carbon atoms. Crystal data: $C_{52}H_{54}Br_2N_4O_4Zn$, *Mr* = 1024.18, triclinic, space group: *P-1*, *a* = 8.8126(19), *b* = 15.058(3), *c* = 16.556(4), *α* = 84.489(10)°, *β* = 89.590(12)°, *γ* = 83.103(10)°, *V* = 2170.9(8) Å$^3$, *Z* = 2, $R_1$ = 0.0680, $wR_2$ = 0.1940 (all data), GOF = 1.000. CCDC 1867846 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

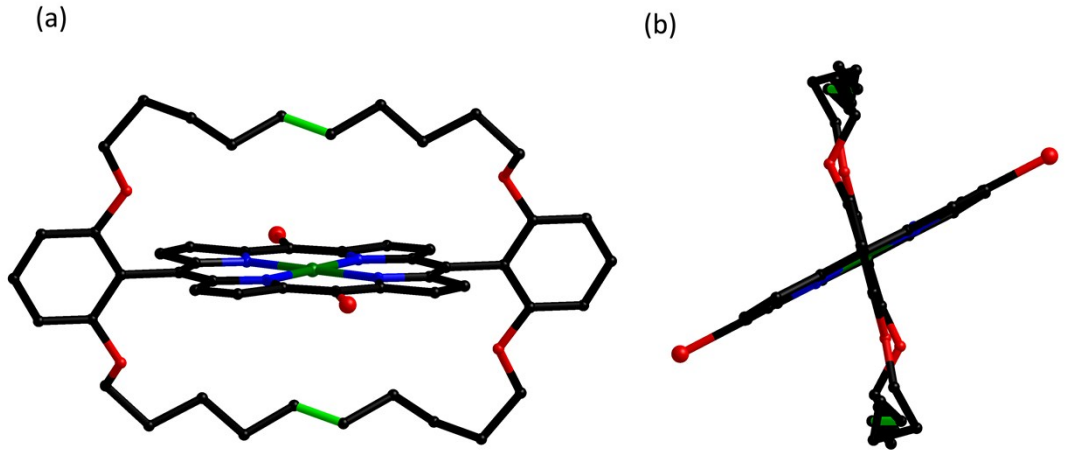



**Fig. S4** X-ray crystal structure for **5**. a) Top view, b) side view. (All hydrogen atoms are omitted for clarity)

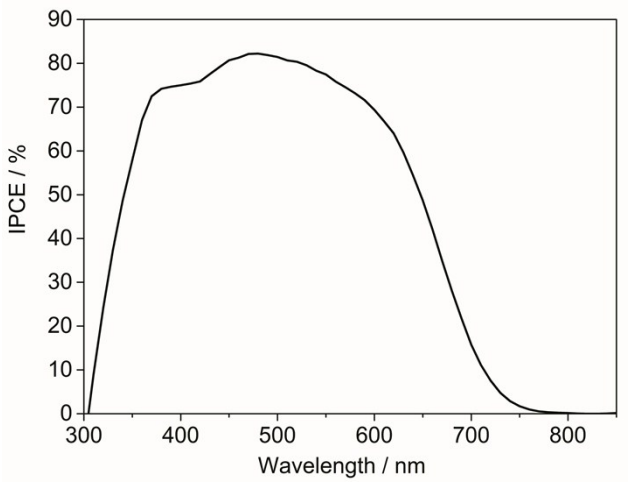



**Fig. S5** IPCE action spectra for the DSSCs based on **Z1**.

## 5. Performance of the DSSCs under the Optimized Conditions.

**Table S1.** The original photovoltaic data of the DSSCs based on **XW40** and **XW41** under the optimized conditions.[a]

| Dyes | | Time (h) | Voc (V) | Jsc (mA/cm$^2$) | Fill Factor | PCE | Dye loading amount (×10$^{-7}$ mol·cm$^{-2}$) | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Porphyrin | **Z1** |
| **XW40** | / | 12 h | 730±3 | 18.67±0.75 | 0.68±0.02 | 9.31±0.12 | 1.99 | \ |
| **XW40** [b] | **Z1** | 0.75 h | 741±2 | 19.13±0.33 | 0.68±0.02 | 9.65±0.04 | 1.89 | 1.71 |
| | | 1.5 h | 742±1 | 19.36±0.49 | 0.69±0.01 | 9.97±0.06 | 1.62 | 3.67 |
| | | 2.25 h | 718±2 | 17.25±0.26 | 0.73±0.01 | 8.98±0.02 | 1.43 | 4.69 |
| **XW40**/ CDCA [c] | **Z1** | 0.75 h | 739±1 | 19.74±0.35 | 0.68±0.01 | 9.91±0.04 | 1.87 | 1.10 |
| | | 1.5 h | 748±2 | 19.59±0.21 | 0.72±0.01 | 10.55±0.11 | 1.64 | 2.73 |
| | | 2.25 h | 725±3 | 19.31±0.14 | 0.69±0.01 | 9.58±0.22 | 1.40 | 4.64 |
| **XW41** | / | 12 h | 695±2 | 16.77±0.31 | 0.70±0.01 | 8.16±0.10 | 2.78 | \ |
| **XW41** [b] | **Z1** | 0.75 h | 728±3 | 18.32±0.13 | 0.73±0.01 | 9.71±0.01 | 2.65 | 1.96 |
| | | 1.5 h | 709±3 | 18.51±0.15 | 0.70±0.04 | 9.21±0.05 | 2.46 | 3.07 |
| | | 2.25 h | 704±1 | 16.76±0.10 | 0.74±0.04 | 8.78±0.03 | 2.11 | 4.61 |
| **XW41**/ CDCA [c] | **Z1** | 0.75 h | 704±1 | 17.34±0.16 | 0.71±0.01 | 8.60±0.13 | 2.60 | 1.31 |
| | | 1.5 h | 726±2 | 19.63±0.31 | 0.72±0.01 | 10.19±0.21 | 2.39 | 3.06 |
| | | 2.25 h | 707±2 | 18.31±0.19 | 0.71±0.01 | 9.23±0.15 | 2.09 | 5.37 |

[a] Under AM 1.5 illumination (power 100 mW cm$^{-2}$) with an active area of 0.16 cm$^2$. The parameters were obtained from the average values of three devices.

[b] The cosensitization was performed through an optimized stepwise approach: the $TiO_2$ electrode was first dipped in 0.2 mM of the porphyrin dye in chloroform/ethanol (v/v, 3/2) for 12 h, rinsed with ethanol, and then immersed in a 0.3 mM solution of **Z1** in chloroform/ethanol (v/v, 1/1) for 1.5 h (**XW40** + **Z1**) or 0.75 h (**XW41** + **Z1**).

[c] The approach is similar to that of simple cosensitization approach, except that the $TiO_2$ electrode was first dipped in a cocktail solution of porphyrin (0.2 mM) and **Z1** (1.0 mM), then in **Z1** (0.3 mM) in chloroform/ethanol (v/v, 1/1) for 1.5 h for the optimized condition.

## 6. Photovoltaic Performance of the DSSCs Based on the Organic Dyes

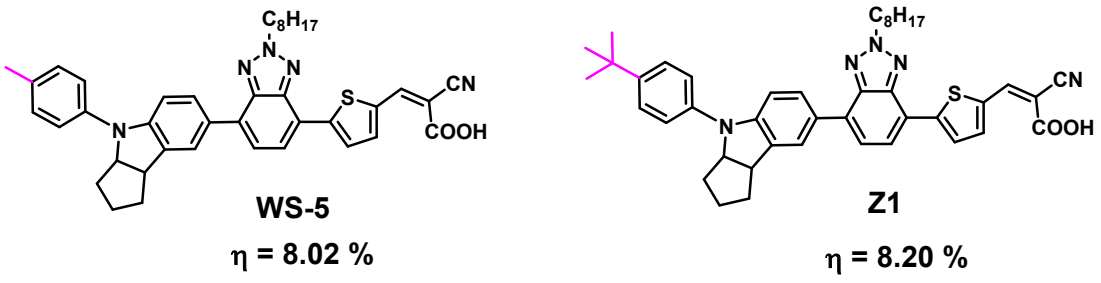



**Chart. S1** The conversion efficiencies improved by substitution of the metyl with the tert butyl group.

**Table S2.** The photovoltaic performance of the DSSCs based on **Z1**.

| Dyes | $V_{oc}$/V | $J_{sc}$/mA·cm$^{-2}$ | Fill Factor | PCE (%) |
|---|---|---|---|---|
| **WS5** [a] | 0.78 | 13.18 | 0.78 | 8.02 |
| **Z1** [b] | 0.79 | 13.30 | 0.78 | 8.20 |

[a] The data were reported in previous work. [15]

[b] The measurement procedure is identical to that of **WS5**[15].

## References


1. S. Ito, T. N. Murakami, P. Comte, P. Liska, C. Grätzel, M. K. Nazeeruddin and M. Grätzel, *Thin Solid Films*, 2008, **516**, 4613-4619.
2. Y. Wang, B. Chen, W. Wu, X. Li, W. Zhu, H. Tian and Y. Xie, *Angew. Chem., Int. Ed.*, 2014, **53**, 10779-10783.
3. H. Song, J. Zhang, J. Jin, H. Wang and Y. Xie, *J. Mater. Chem. C*, 2018, **6**, 3927-3936.
4. T. Wei, X. Sun, X. Li, H. Agren and Y. Xie, *ACS Appl. Mater. Interfaces*, 2015, **7**, 21956-21965.
5. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
6. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.
7. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.
8. P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270-283.
9. M. Frisch, G. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci and G. Petersson, *Inc., Wallingford, CT*, 2009, **200**.
10. Y. Xie, Y. Tang, W. Wu, Y. Wang, J. Liu, X. Li, H. Tian and W.-H. Zhu, *J. Am. Chem. Soc.*, 2015, **137**, 14055-14058.
11. G. Li, M. Liang, H. Wang, Z. Sun, L. Wang, Z. Wang and S. Xue, *Chem. Mater.*, 2013, **25**, 1713-1722.
12. Y. Liu, H. Cao, J. Li, Z. Chen, S. Cao, L. Xiao, S. Xu and Q. Gong, *J. Polym. Sci., Part A: Polym. Chem.*, 2007, **45**, 4867-4878.
13. G. M. Sheldrick, SHELXS97 and SHELXL97 Programs for Crystal Structure Solution and Refinement, University of Göttigen, Germany, 1997.
14. G. M. Sheldrick, *Acta Cryst. A*, 2008, **64**, 112-122.
15. Y. Cui, Y. Wu, X. Lu, X. Zhang, G. Zhou, F. B. Miapeh, W. Zhu and Z.-S. Wang, *Chem. Mater.*, 2011, **23**, 4394-4401.

## 7. Characterization Data for the Compounds

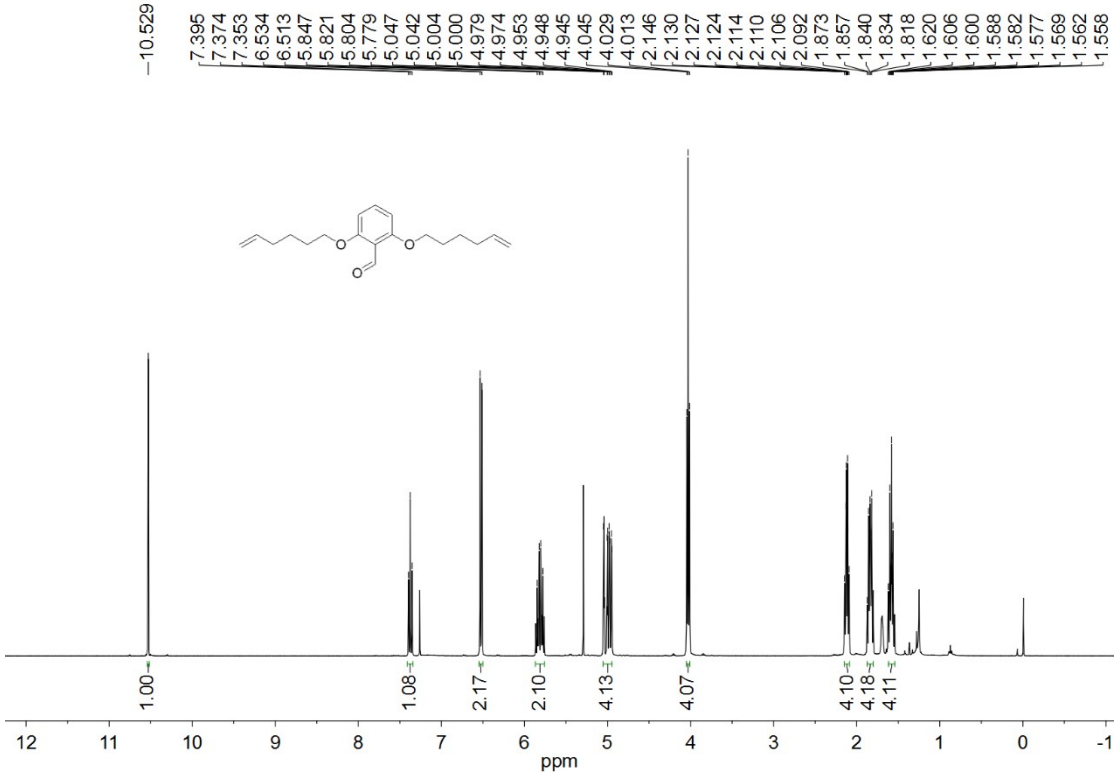



**Figure S6.** The $^{1}H$ NMR spectrum of **1** in $CDCl_3$

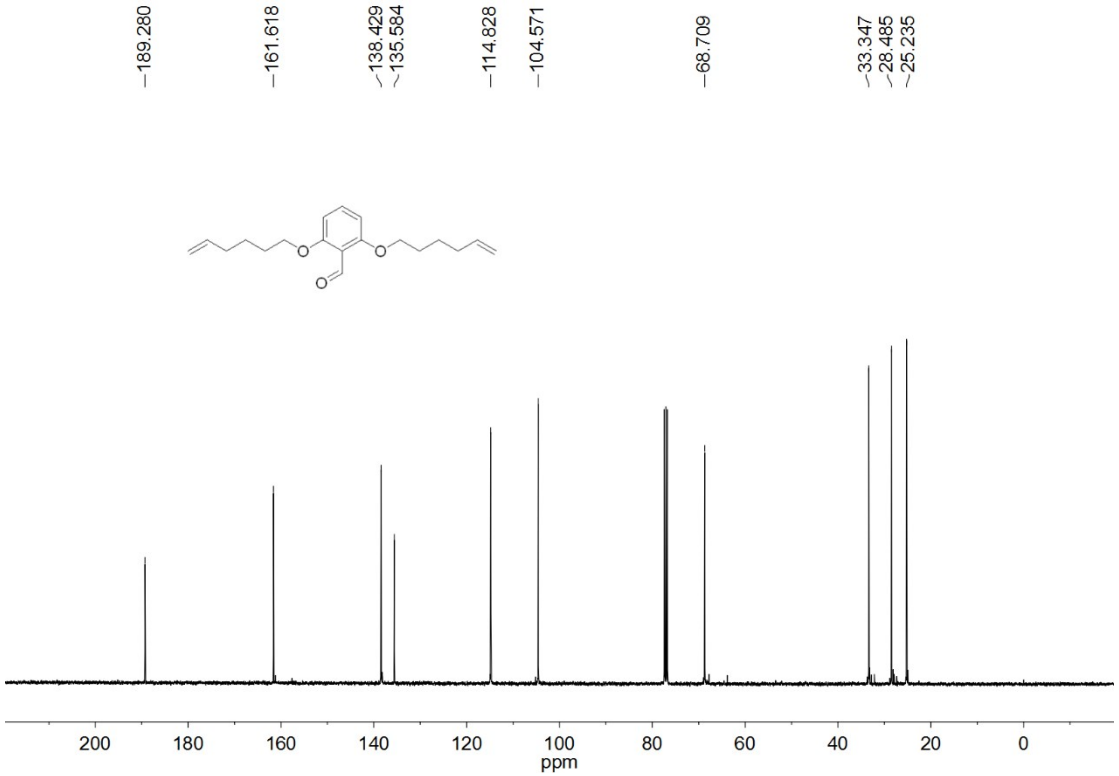



**Figure S7.** The $^{13}C$ NMR spectrum of **1** in $CDCl_3$

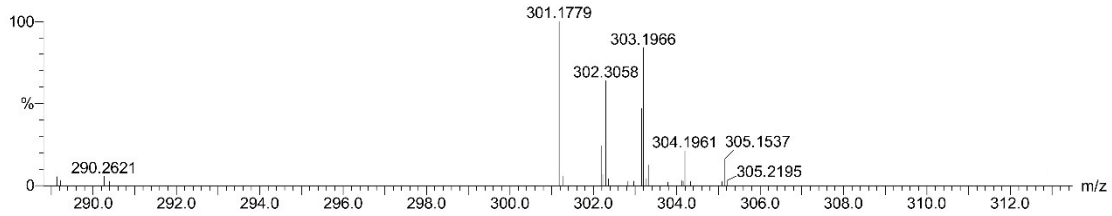



**Figure S8.** The HRMS of **1**

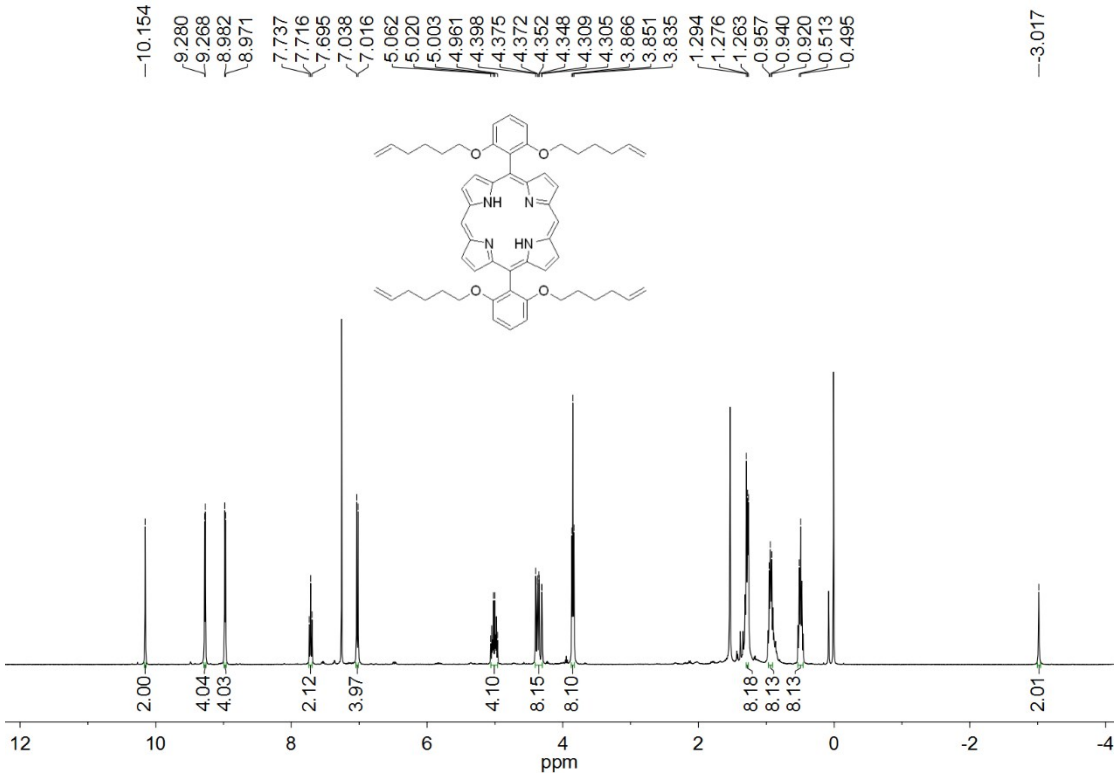



**Figure S9.** The $^{1}H$ NMR spectrum of **2** in $CDCl_3$

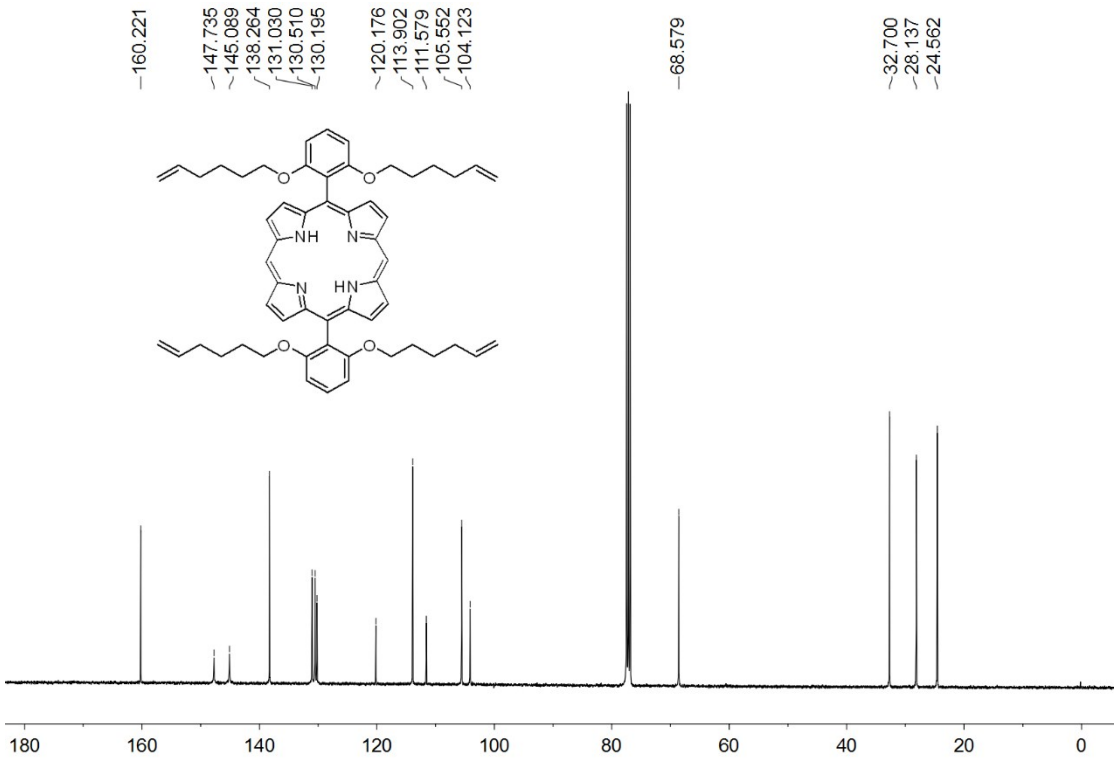
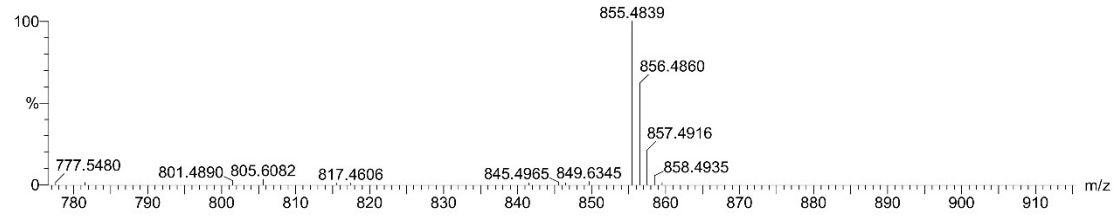



**Figure S10.** The $^{13}C$ NMR spectrum of **2** in $CDCl_3$




```
Minimum:                                    -1.5
Maximum:                    300.0   500.0   100.0

Mass        Calc. Mass      mDa     PPM     DBE     i-FIT   i-FIT (Norm)  Formula

855.4839    855.4849        -1.0    -1.2    27.5    9.1     0.0           C56  H63  N4  O4
```

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

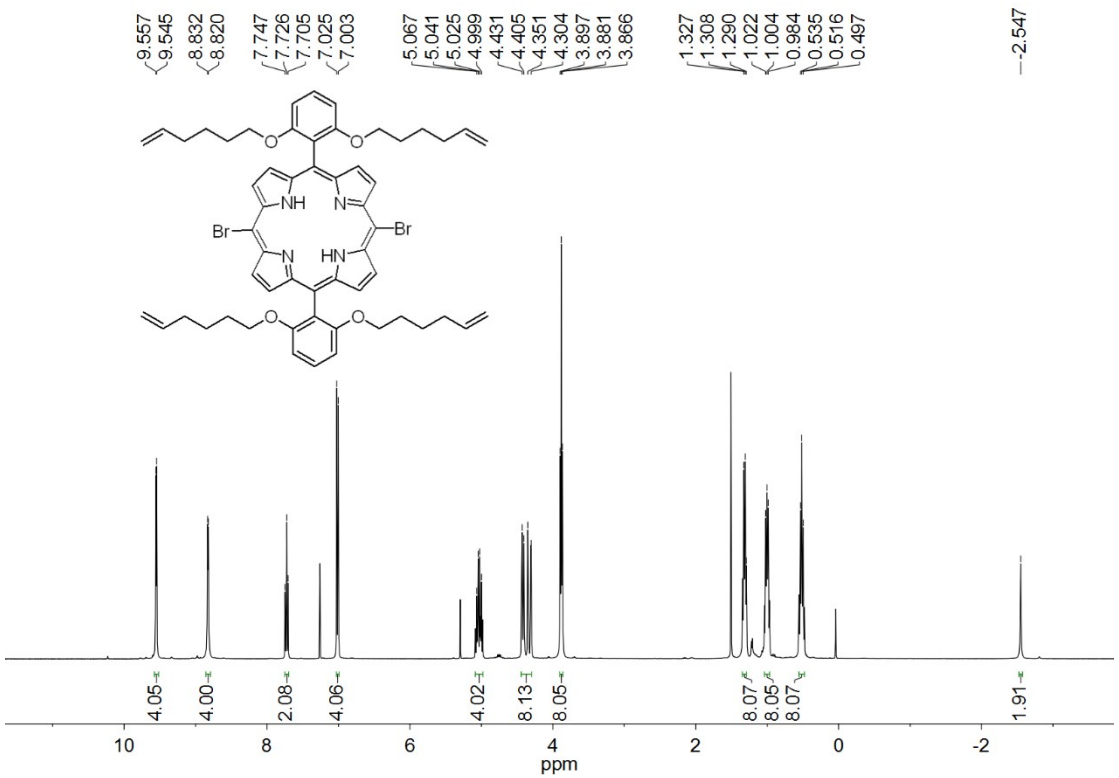



**Figure S12.** The $^{1}H$ NMR spectrum of **3** in $CDCl_3$

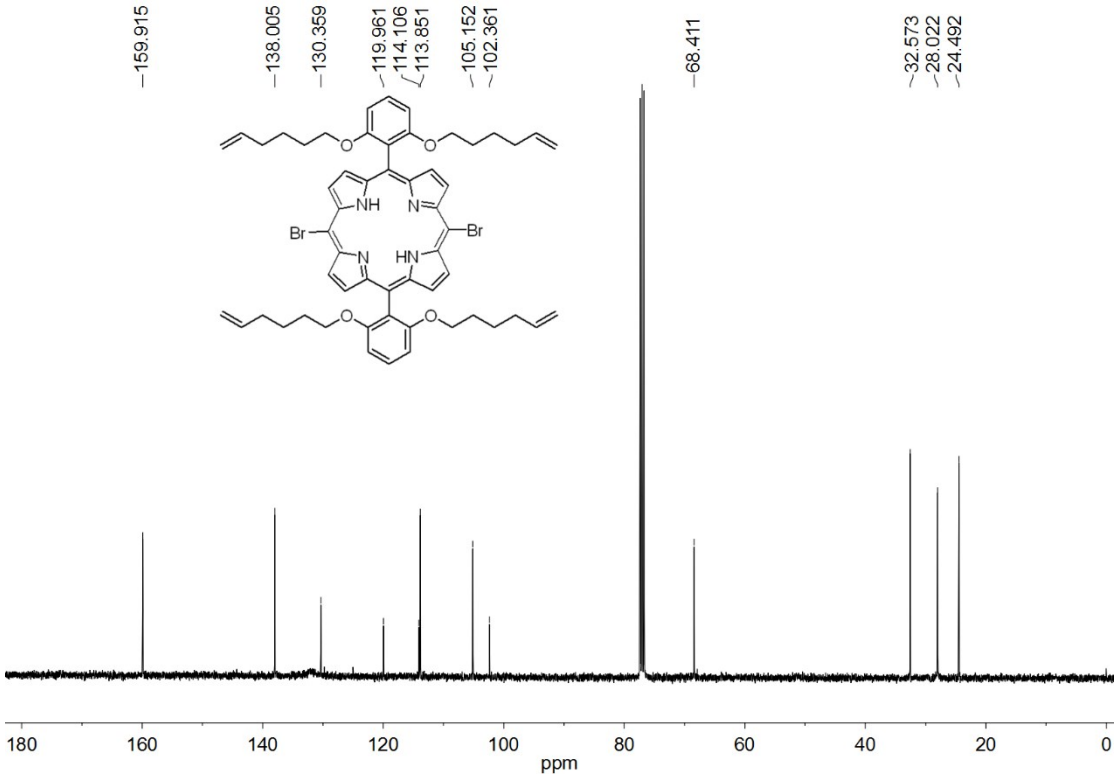
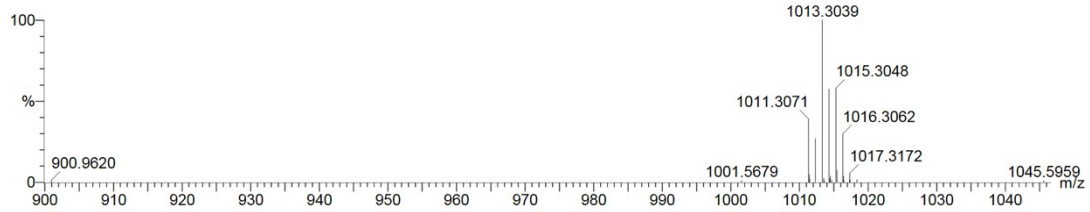



**Figure S13.** The $^{13}C$ NMR spectrum of **3** in $CDCl_3$




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 300.0 | 500.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1011.3071 | 1011.3060 | 1.1 | 1.1 | 27.5 | 74.9 | 0.0 | C56 H61 N4 O4 Br2 |

**Figure S14.** The HRMS of **3**

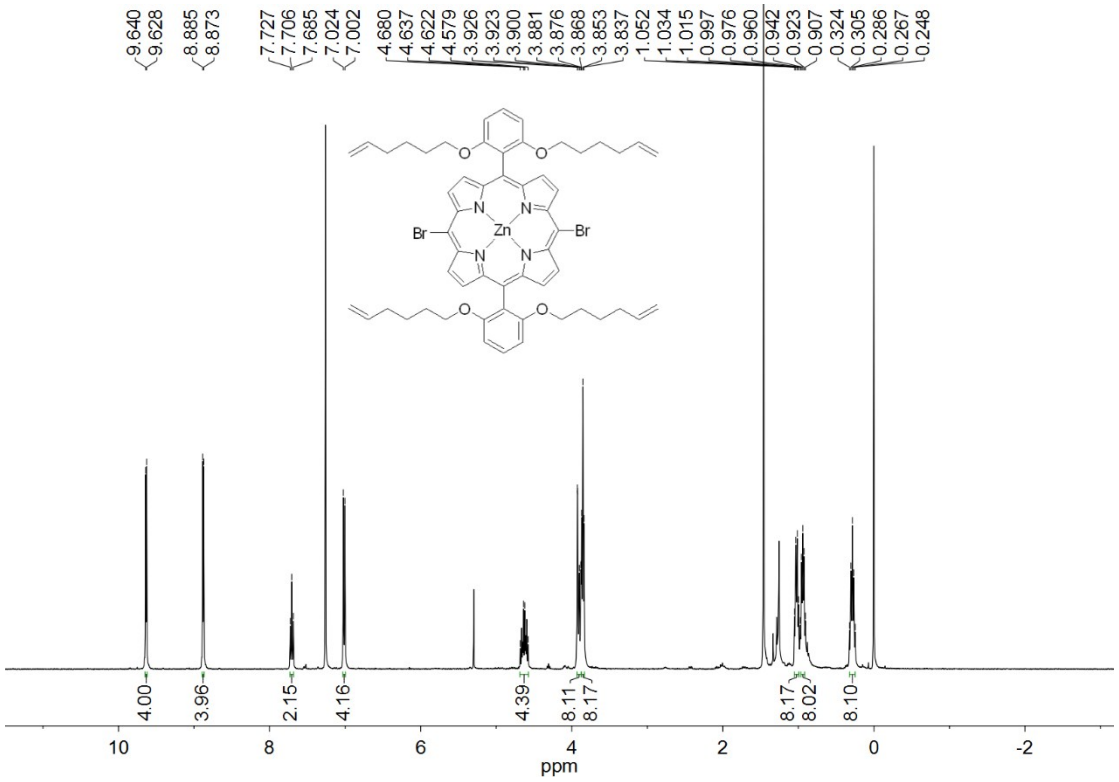



**Figure S15.** The $^{1}H$ NMR spectrum of **4** in $CDCl_3$

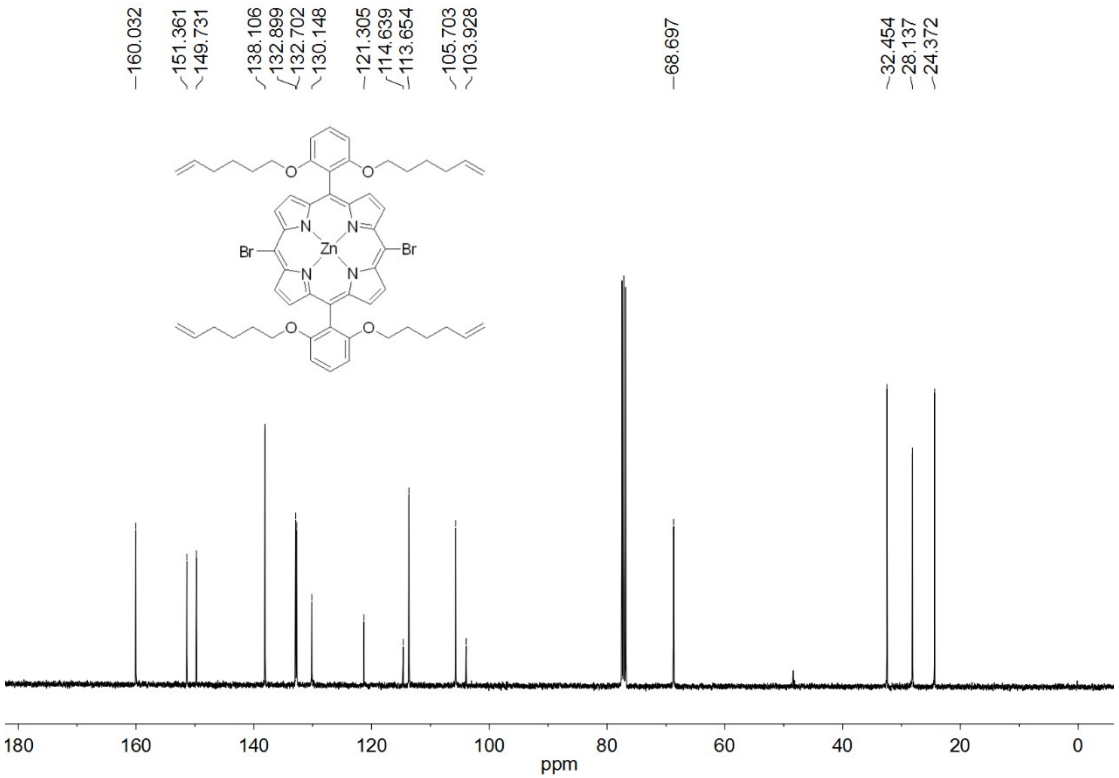



**Figure S16.** The $^{13}C$ NMR spectrum of **4** in $CDCl_3$

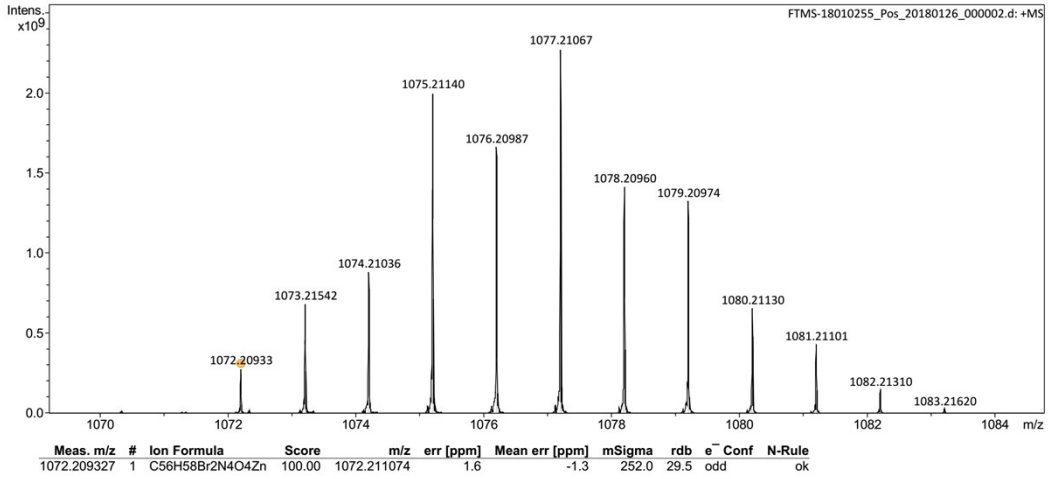



**Figure S17.** The FTICR-MS of **4**

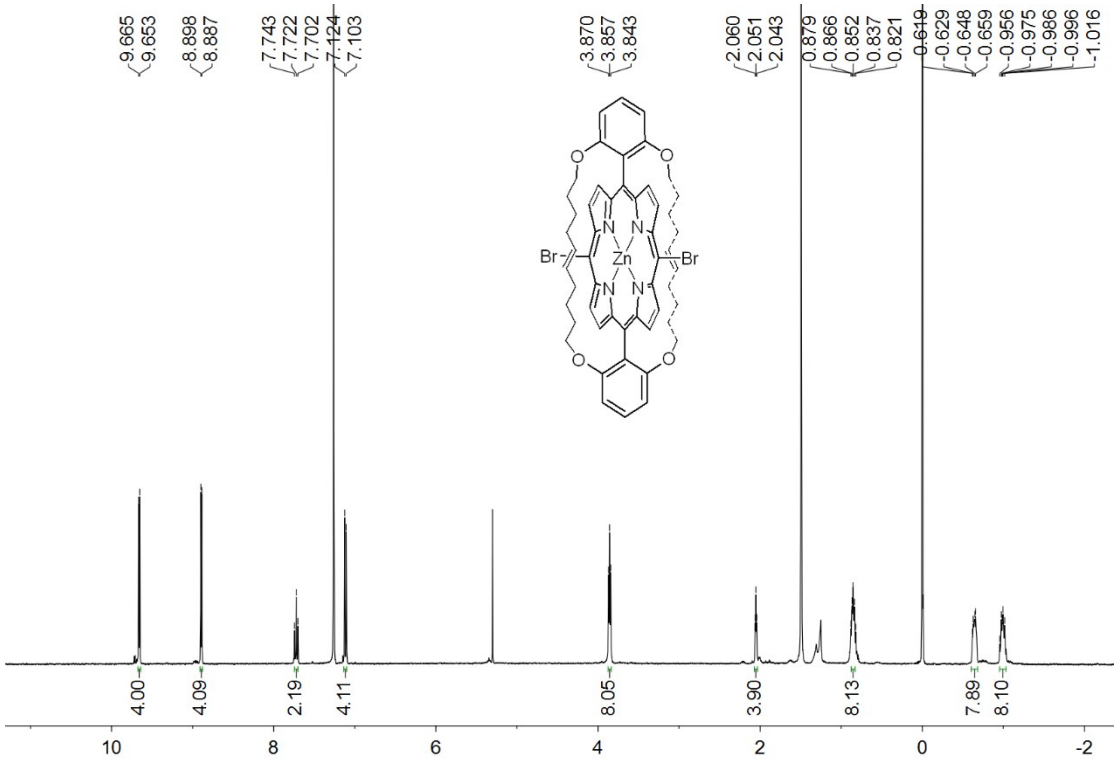



**Figure S18.** The $^{1}H$ NMR spectrum of **5** in $CDCl_3$

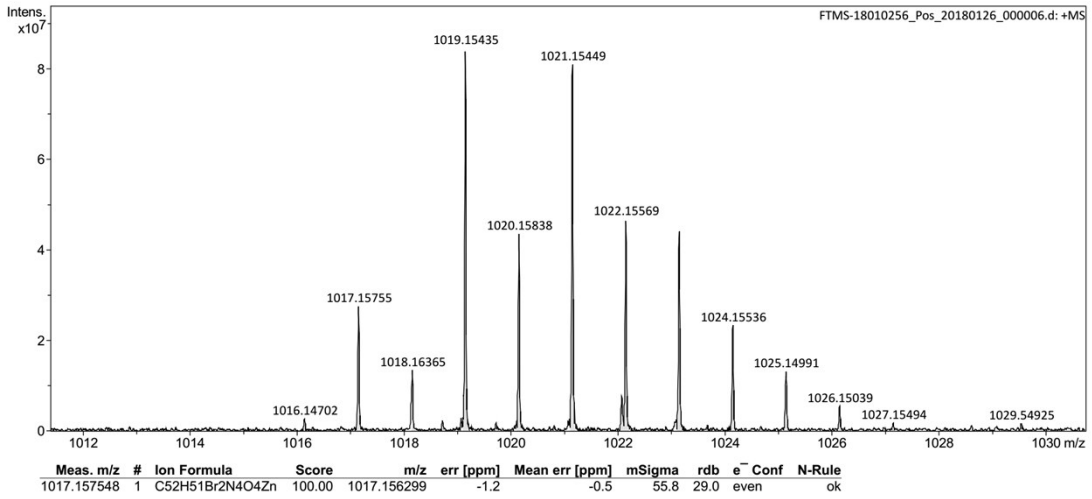



**Figure S19.** The FTICR-MS of **5**

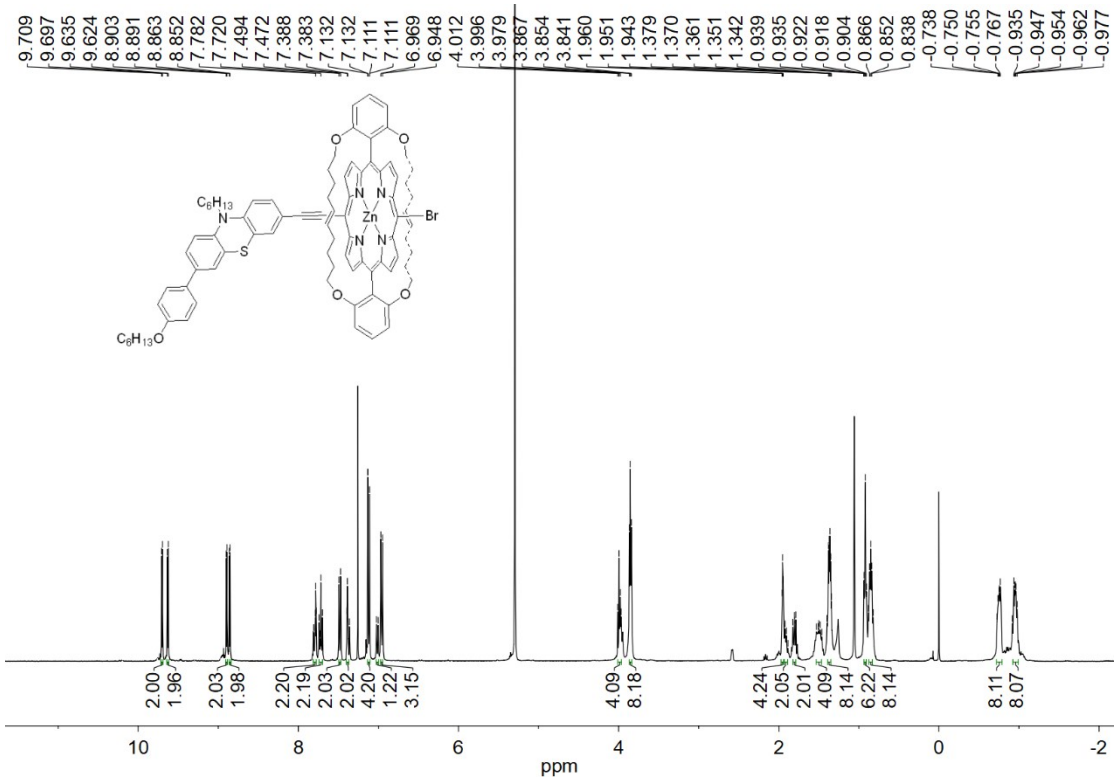



**Figure S20.** The $^{1}H$ NMR spectrum of **6** in $CDCl_3$

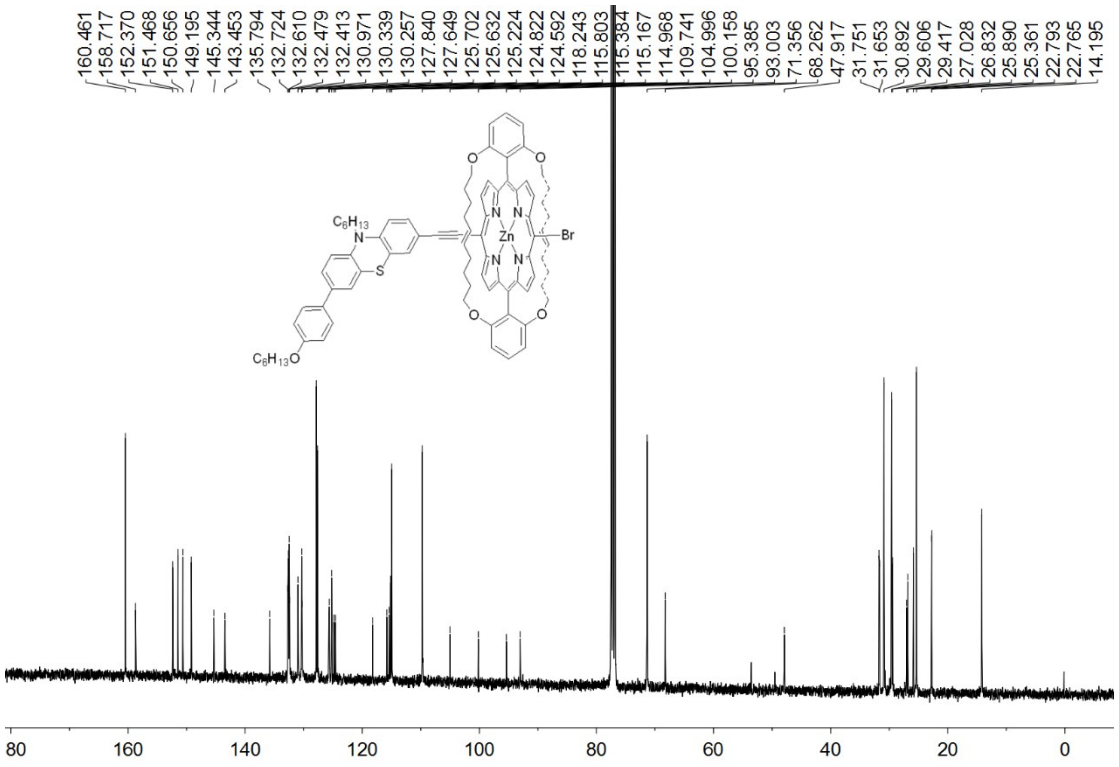



**Figure S21.** The $^{13}C$ NMR spectrum of **6** in $CDCl_3$

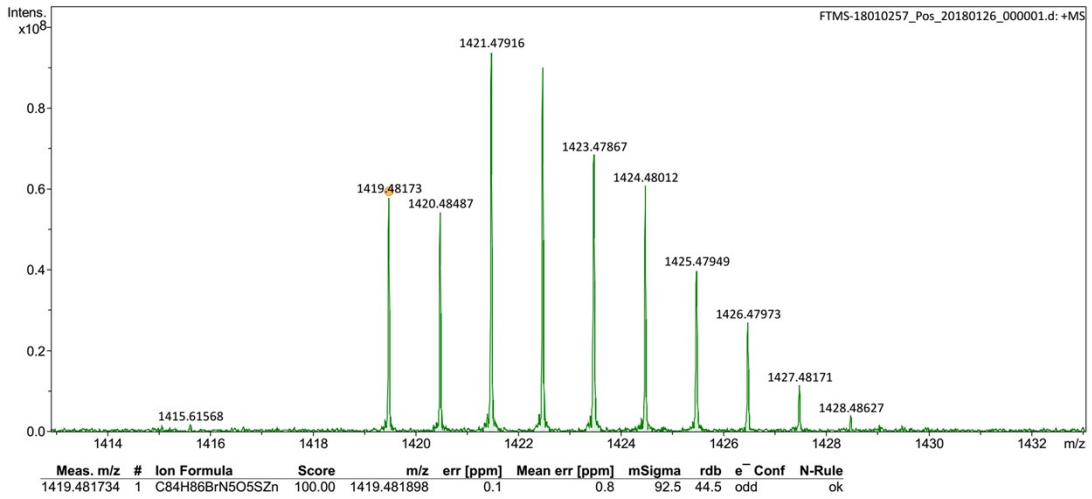



**Figure S22.** The FTICR-MS of **6**

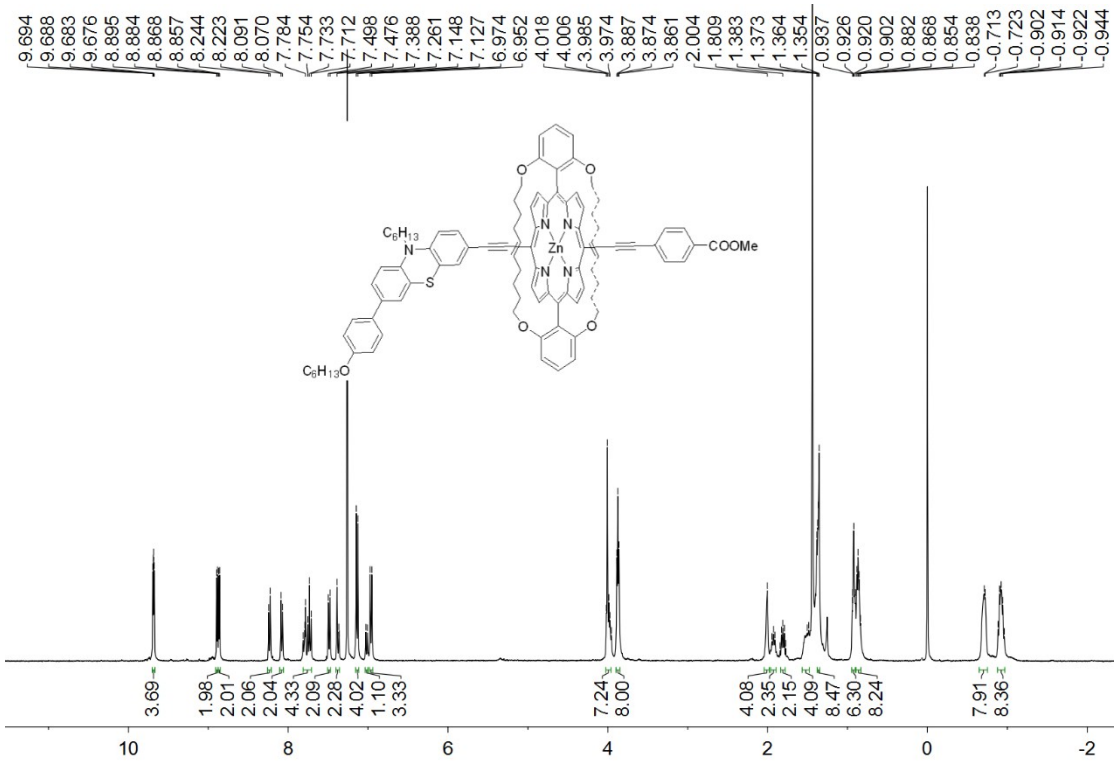



**Figure S23.** The $^{1}H$ NMR spectrum of **7a** in $CDCl_3$

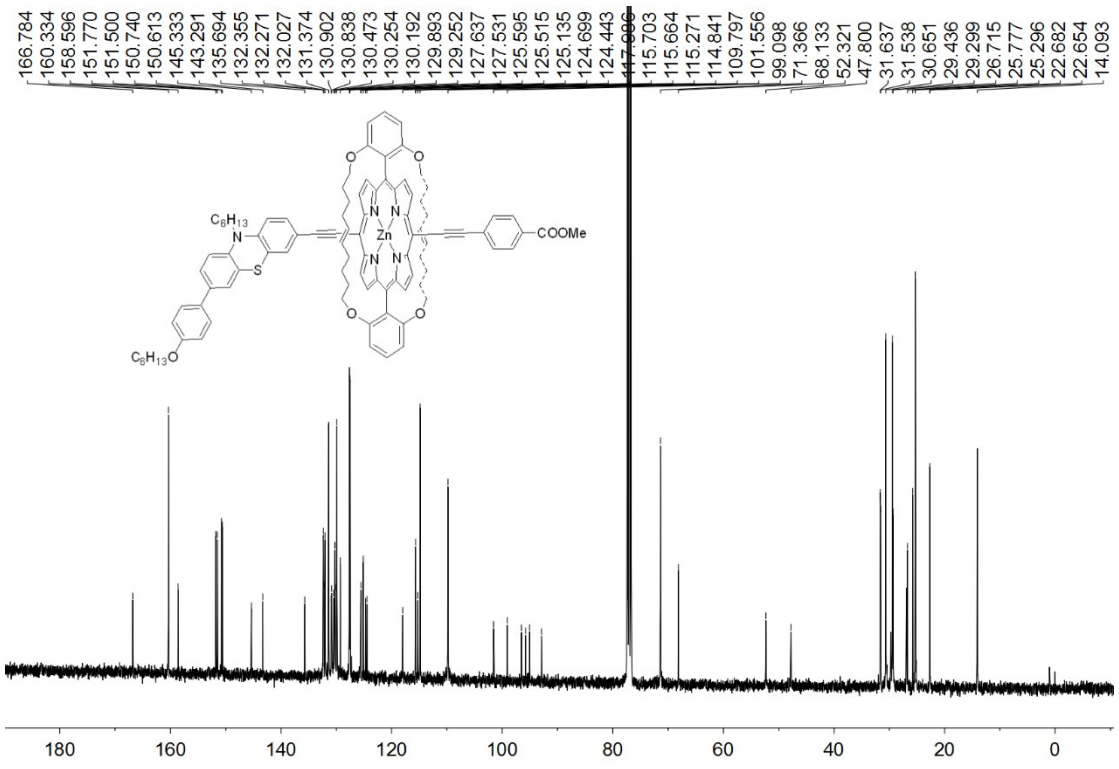



**Figure S24.** The $^{13}C$ NMR spectrum of **7a** in $CDCl_3$

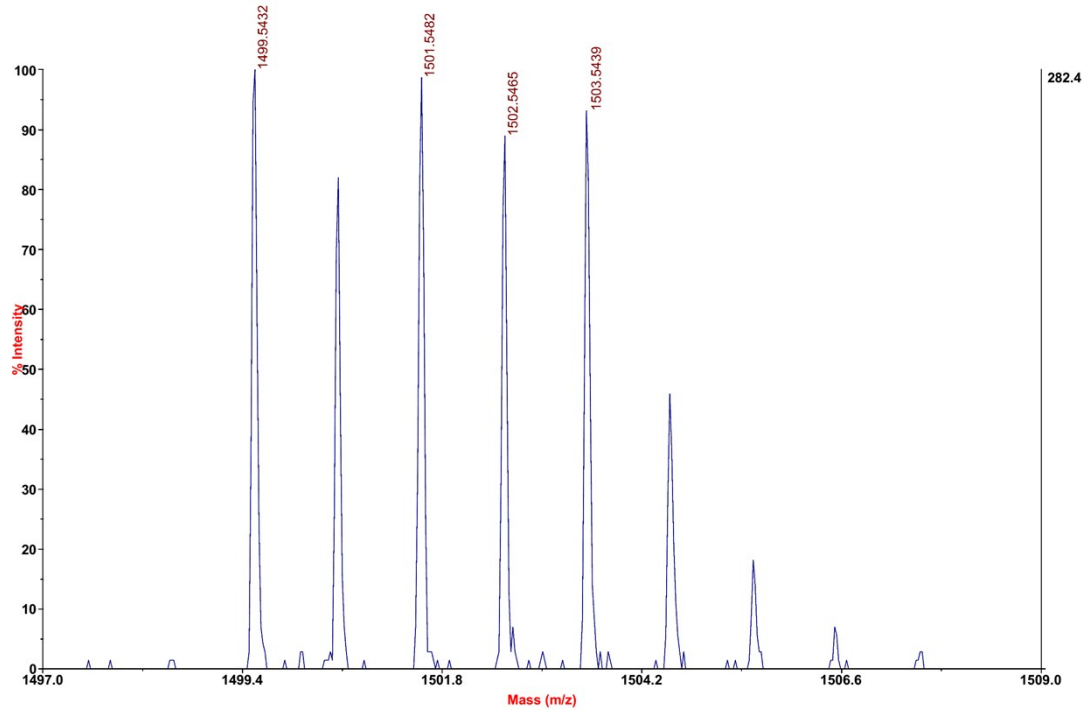



**Figure S25.** The MALDI-TOF MS of compound **7a**

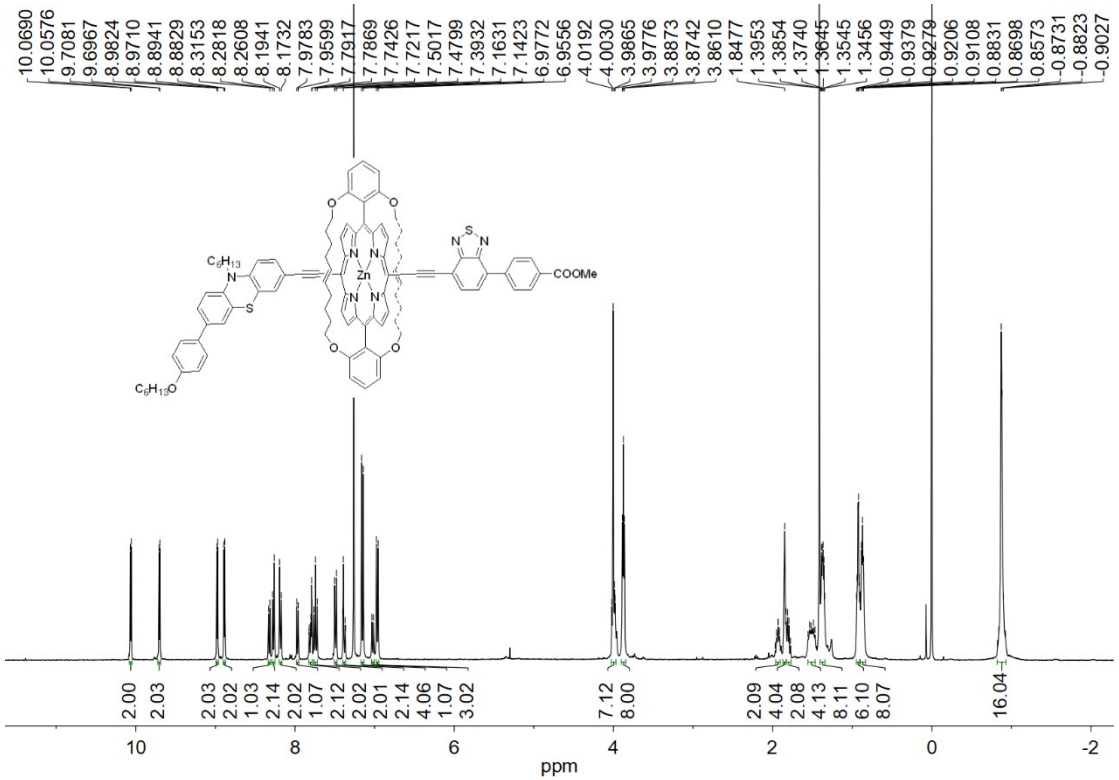



**Figure S26.** The $^{1}$H NMR spectrum of **7b** in $CDCl_3$

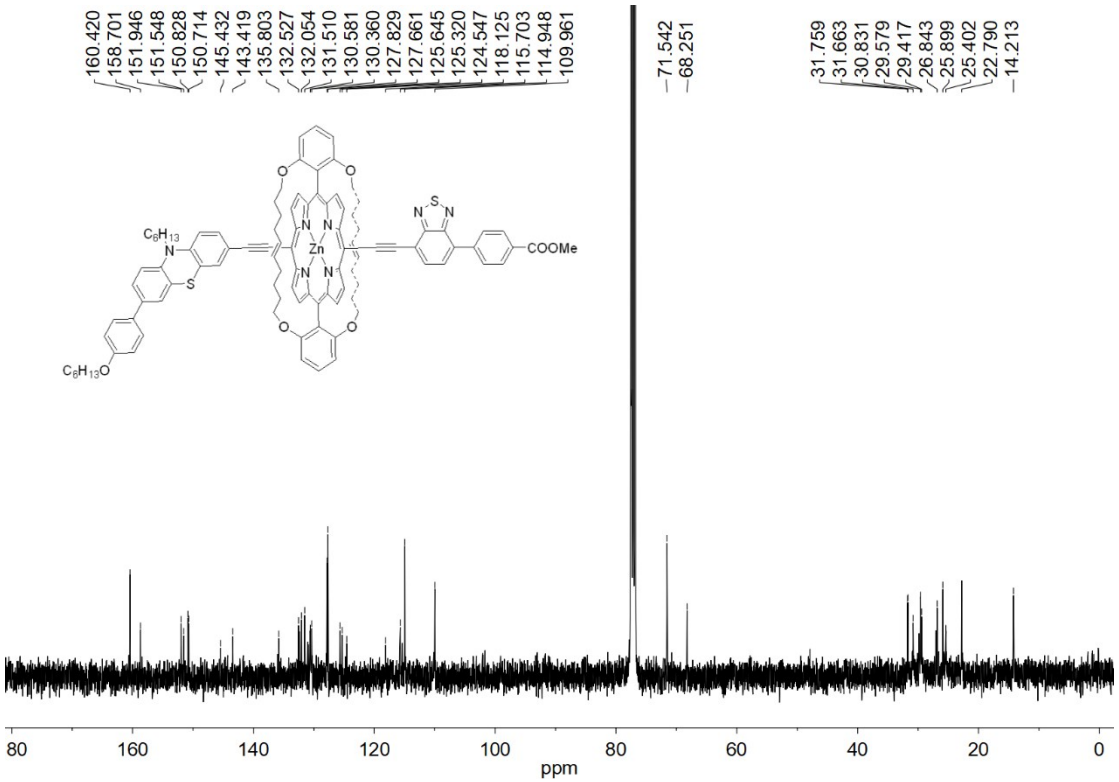



**Figure S27.** The $^{13}$C NMR spectrum of **7b** in $CDCl_3$

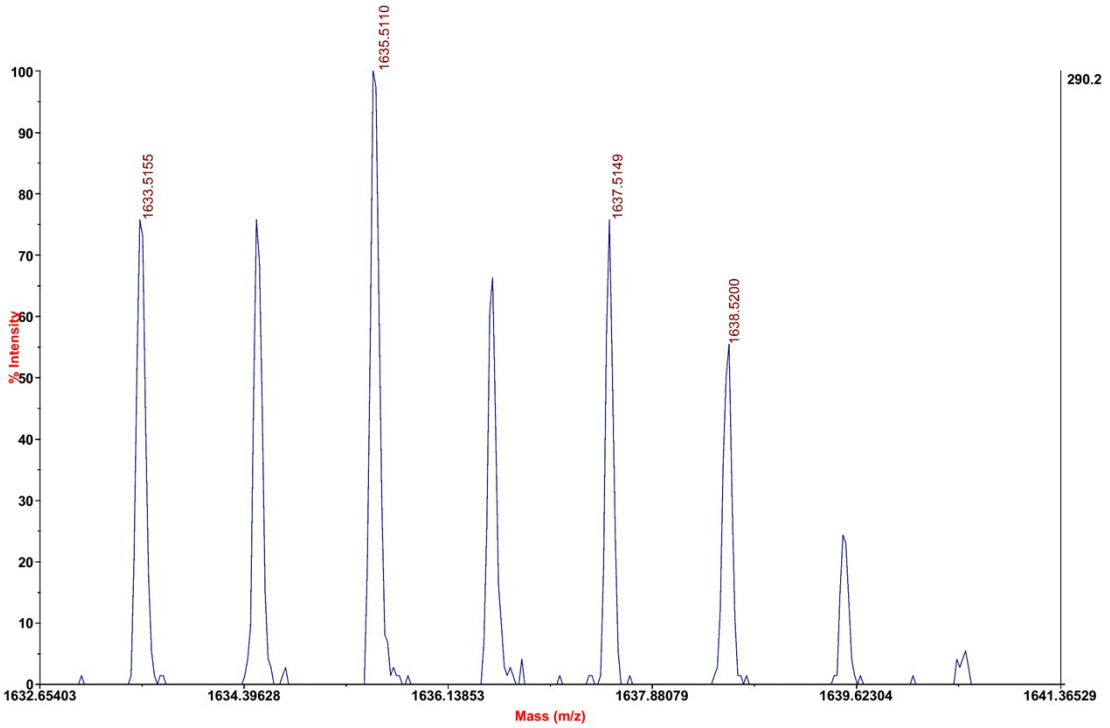



**Figure S28.** The MALDI-TOF MS of compound **7b**

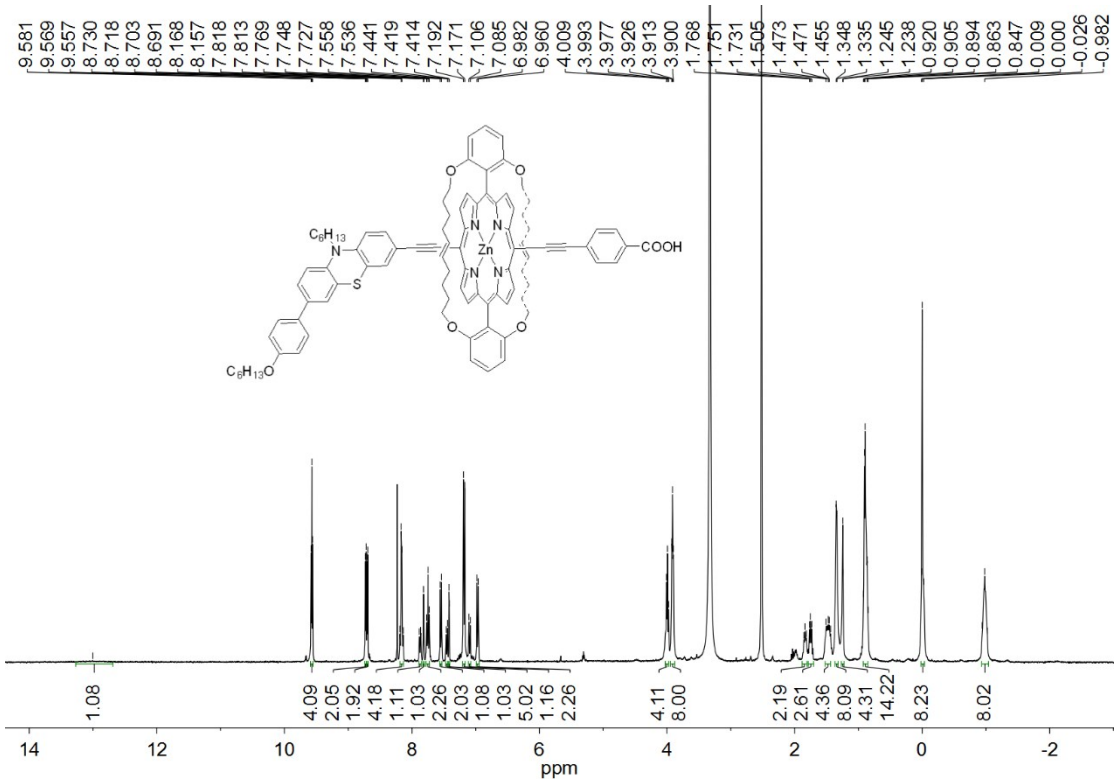



**Figure S29.** The $^{1}$H NMR spectrum of **XW40** in $CDCl_3$ : DMSO-$d_6$ (1 : 2)

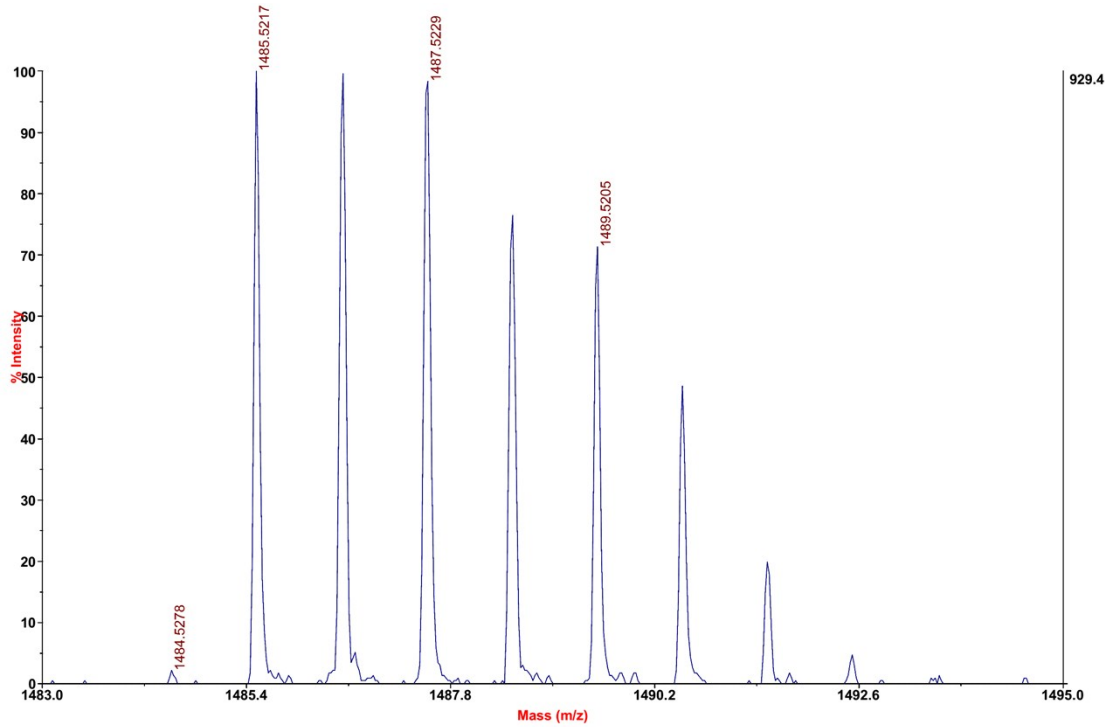



**Figure S30.** The MALDI-TOF MS of compound **XW40**

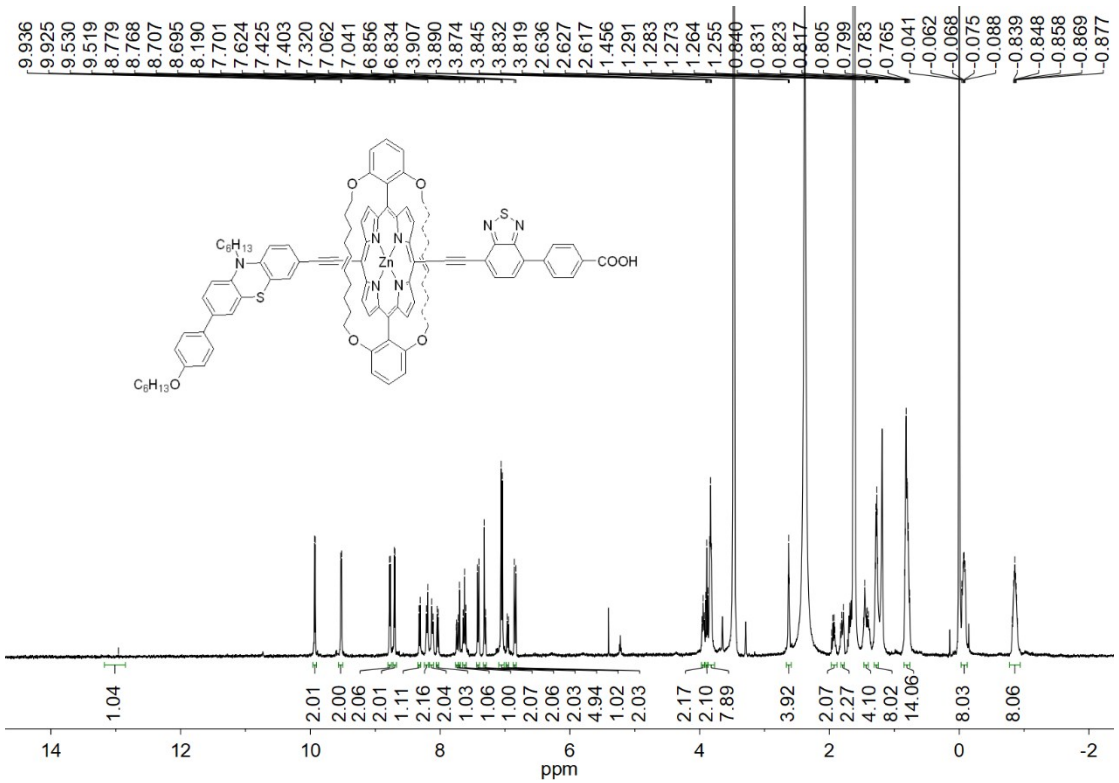



**Figure S31.** The $^{1}$H NMR spectrum of **XW41** in THF-$d_8$

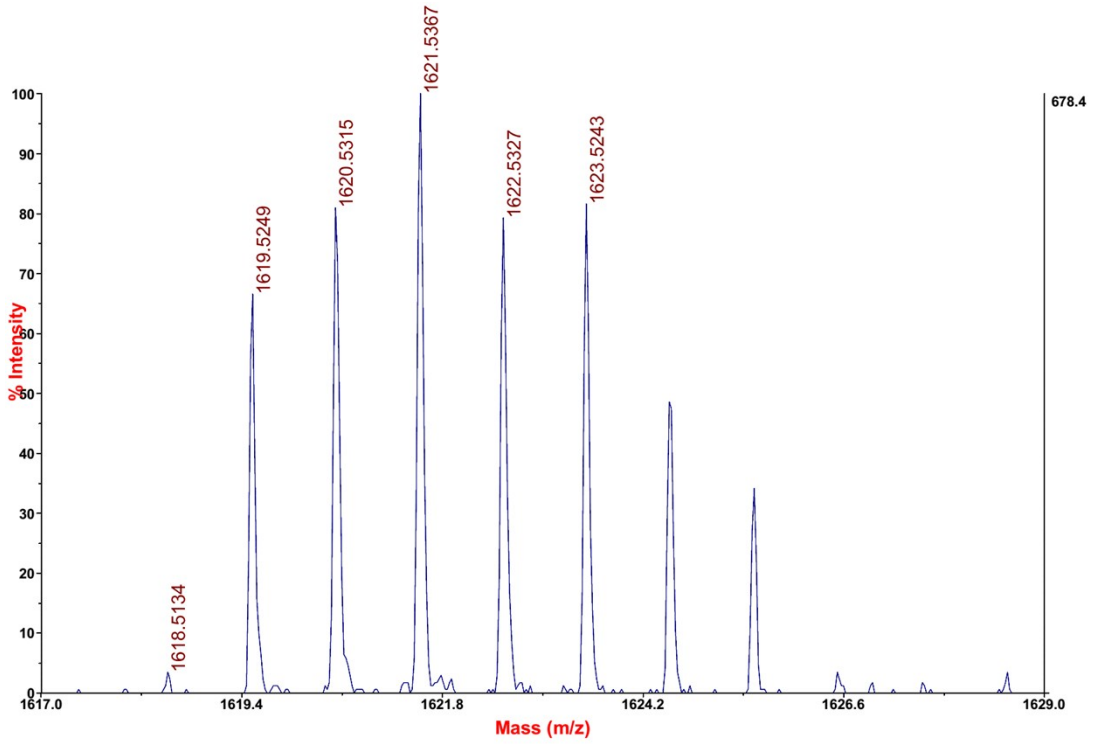



**Figure S32.** The MALDI-TOF MS of compound **XW41**

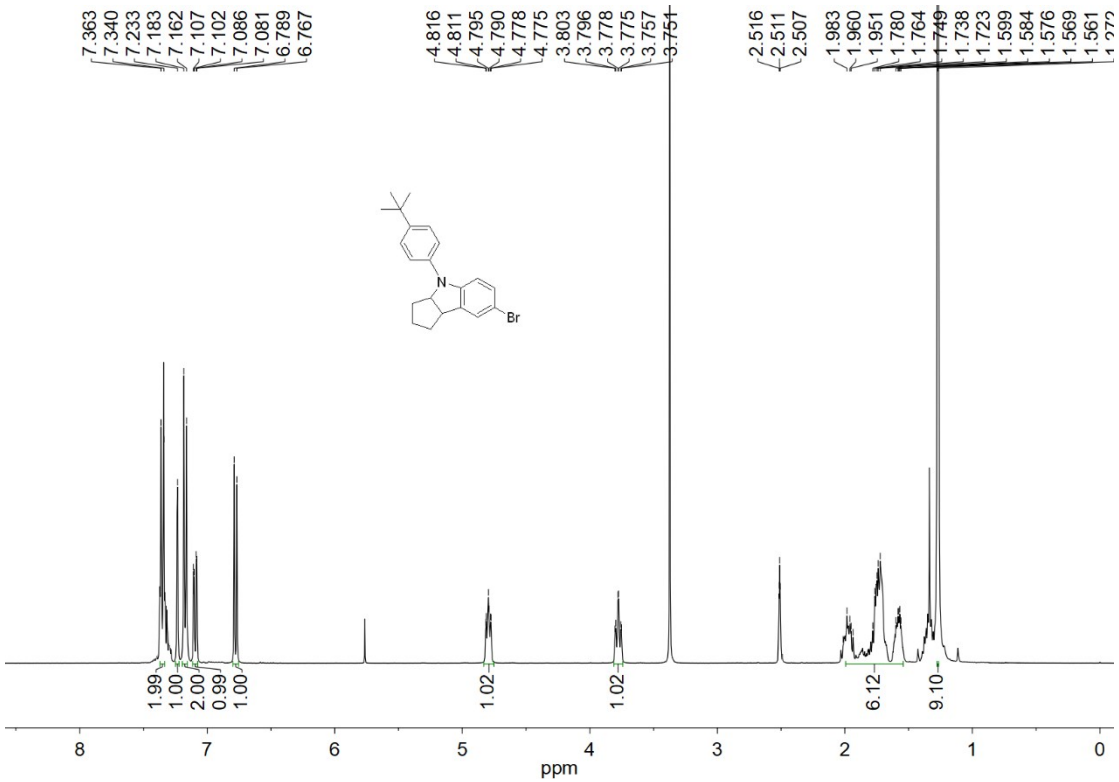



**Figure S33.** The $^{1}H$ NMR spectrum of **9** in $CDCl_3$

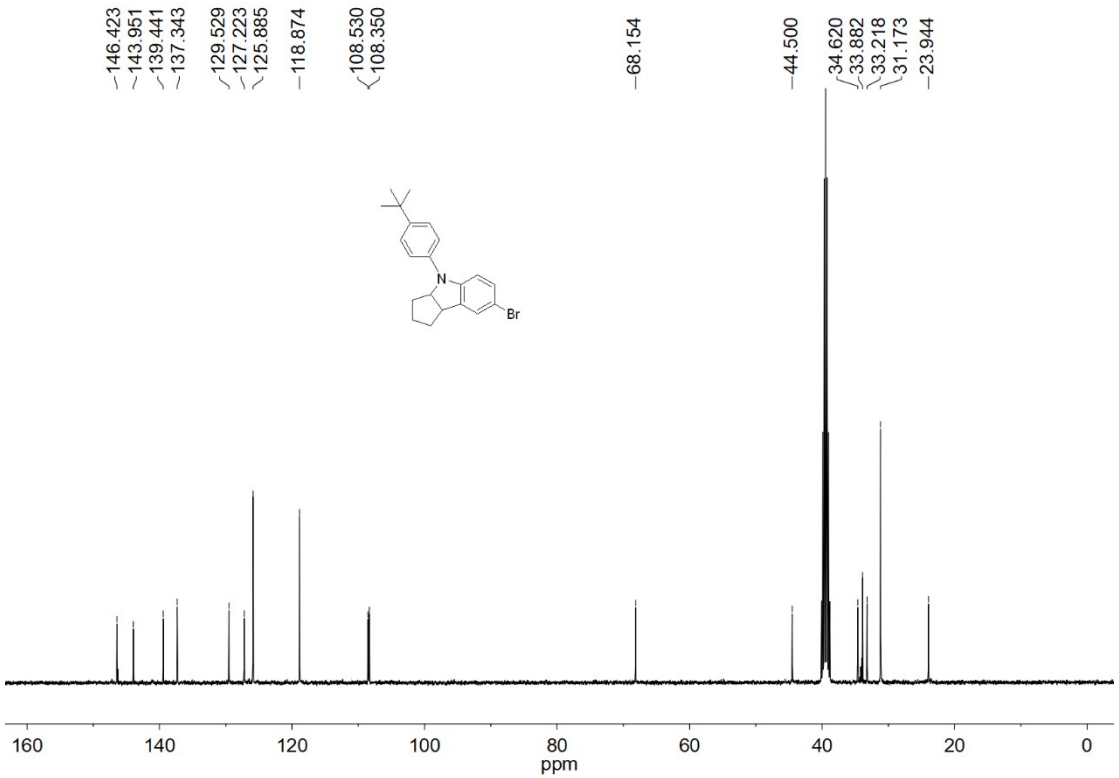



**Figure S34.** The $^{13}C$ NMR spectrum of **9** in $CDCl_3$

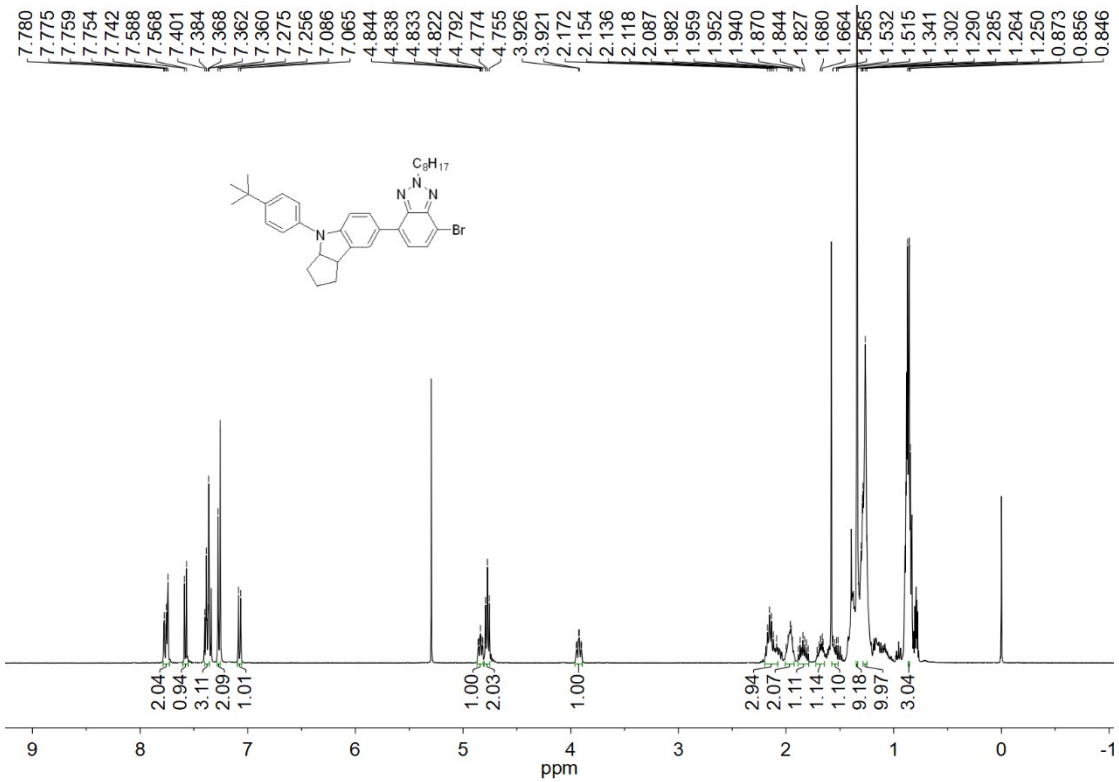



**Figure S35.** The $^{1}H$ NMR spectrum of **10** in $CDCl_3$

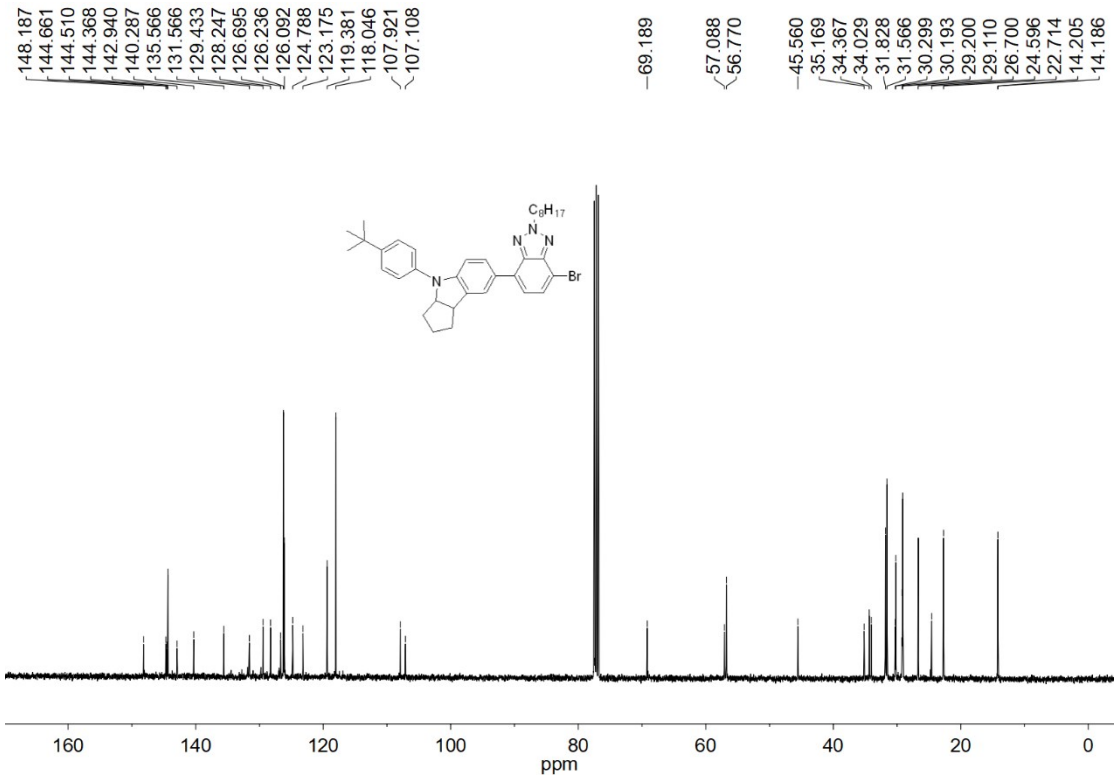



**Figure S36.** The $^{13}C$ NMR spectrum of **10** in $CDCl_3$

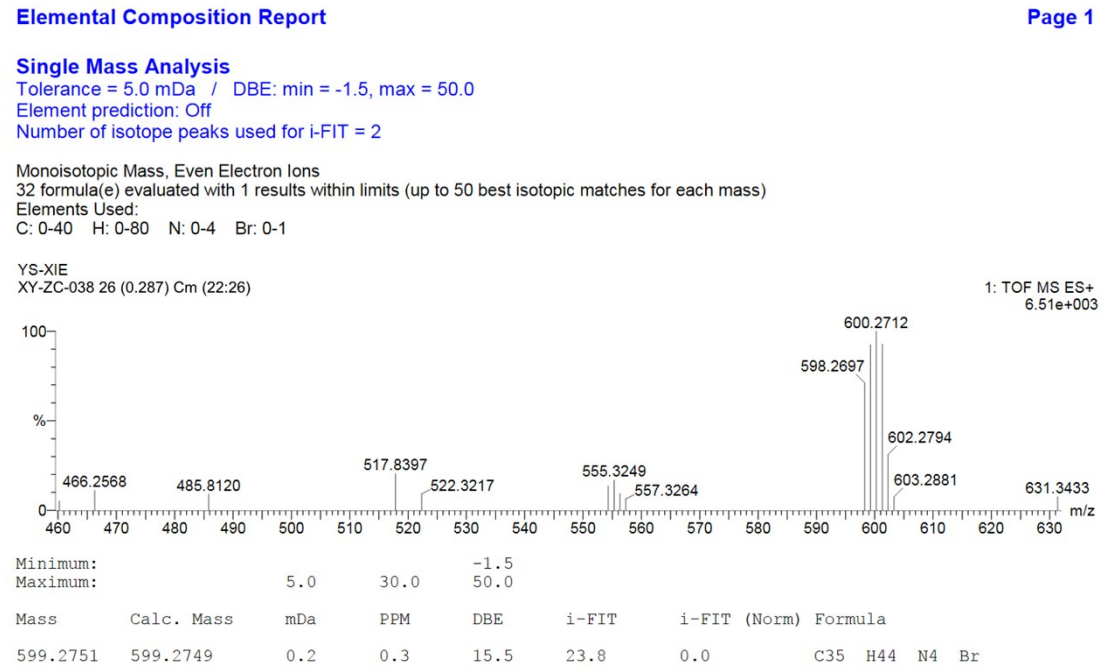



**Figure S37.** The HRMS of **10**

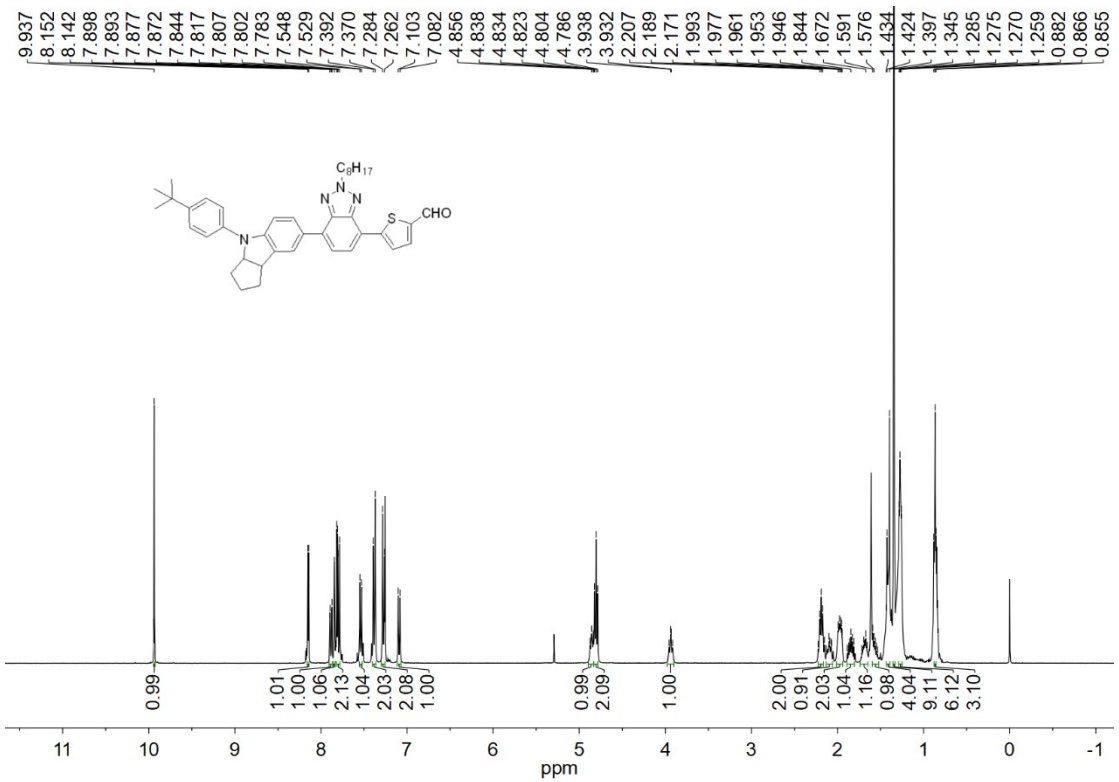



**Figure S38.** The $^{1}H$ NMR spectrum of **11** in $CDCl_3$

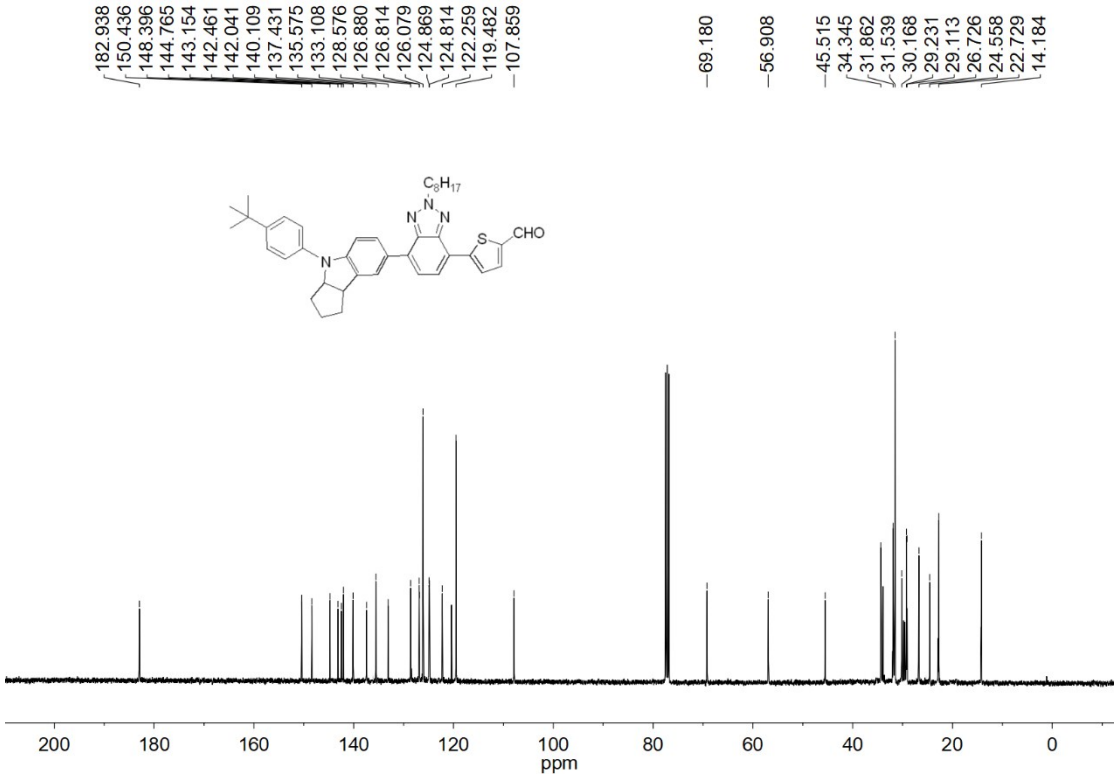
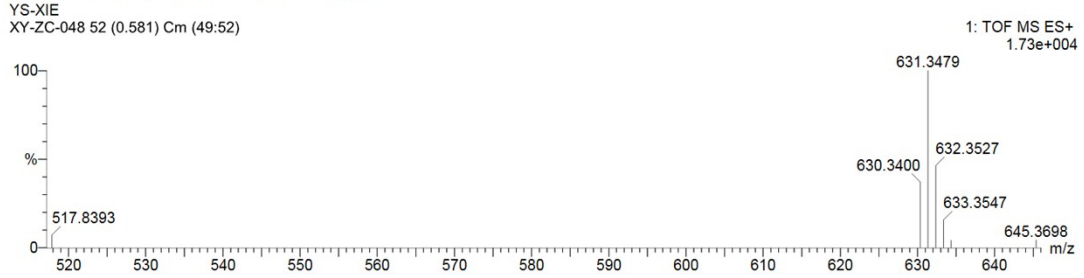



**Figure S39.** The $^{13}C$ NMR spectrum of **11** in $CDCl_3$

**Elemental Composition Report** **Page 1**

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

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-80 N: 0-4 O: 0-1 S: 0-1
YS-XIE
XY-ZC-048 52 (0.581) Cm (49:52)




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 30.0 | 50.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 631.3479 | 631.3471 | 0.8 | 1.3 | 19.5 | 11.0 | 0.0 | C40 H47 N4 O S |

**Figure S40.** The HRMS of **11**

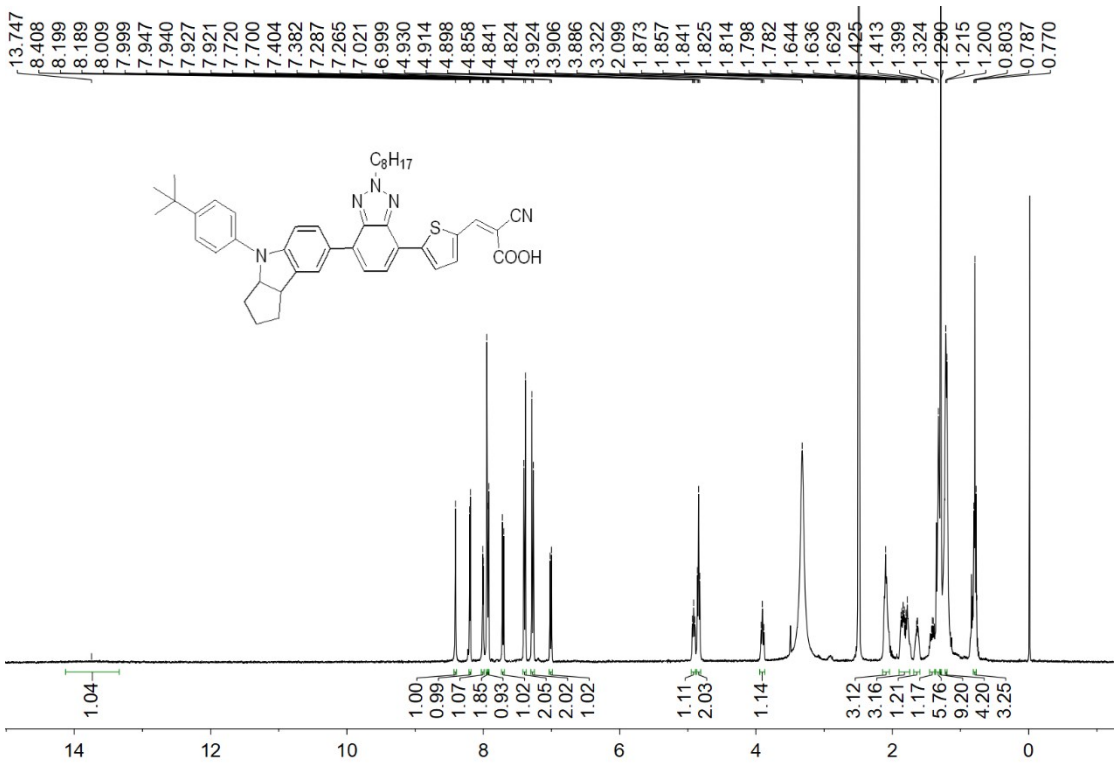
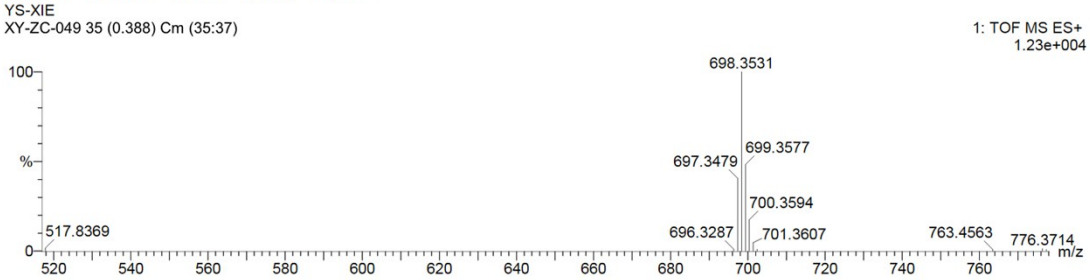



**Figure S41.** The $^{1}H$ NMR spectrum of **Z1** in $CDCl_3$

**Elemental Composition Report** **Page 1**

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

Monoisotopic Mass, Even Electron Ions
35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-43 H: 0-80 N: 0-5 O: 0-2 S: 0-1
YS-XIE
XY-ZC-049 35 (0.388) Cm (35:37)




| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | | | | | |
| Maximum: | | 5.0 | 30.0 | 50.0 | | | | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula | | | | |
| 698.3531 | 698.3529 | 0.2 | 0.3 | 22.5 | 12.1 | 0.0 | C43 | H48 | N5 | O2 | S |

**Figure S42.** The HRMS of **Z1**

## 8. Cartesian coordinates of the optimized structures for XW40 and XW41

**XW40** (the hexyloxy and hexyl chains in the phenothiazine moiety were replaced by methoxy and methyl groups, respectively)

| Row | Symbol | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -0.55535037 | 3.48597534 | 0.26817254 |
| 2 | C | 0.58760101 | 4.18328599 | 0.53096696 |
| 3 | C | 1.6920827 | 3.25873336 | 0.39163359 |
| 4 | N | 1.19941462 | 2.01525111 | 0.06688 |
| 5 | C | -0.16263322 | 2.12554331 | -0.01288768 |
| 6 | C | -0.93612976 | -2.53075117 | -0.76731375 |
| 7 | C | -1.65963562 | -1.37575338 | -0.69235744 |
| 8 | C | -0.71639007 | -0.3042345 | -0.47951802 |
| 9 | N | 0.55422083 | -0.81127087 | -0.44631323 |
| 10 | C | 0.45679024 | -2.17172432 | -0.61546242 |
| 11 | C | -1.06511496 | 1.06328355 | -0.29800175 |
| 12 | C | 5.15299969 | -2.96295774 | -0.51517521 |
| 13 | C | 4.00183769 | -3.68564897 | -0.6198299 |
| 14 | C | 2.90155894 | -2.7452776 | -0.57210666 |
| 15 | N | 3.40731151 | -1.46930655 | -0.43218609 |
| 16 | C | 4.76768861 | -1.57537041 | -0.3834721 |
| 17 | C | 1.537139 | -3.0857428 | -0.64534667 |
| 18 | C | 5.5395337 | 3.05766907 | 0.5237676 |
| 19 | C | 6.26791285 | 1.92919808 | 0.29151931 |
| 20 | C | 5.32336114 | 0.86250883 | 0.04621144 |
| 21 | N | 4.04946923 | 1.35340323 | 0.11258885 |
| 22 | C | 4.14136502 | 2.69539389 | 0.4127023 |
| 23 | C | 3.05768056 | 3.58498124 | 0.57160663 |
| 24 | C | 5.67496487 | -0.49535958 | -0.19089663 |
| 25 | Zn | 2.30251494 | 0.27045202 | -0.17307674 |
| 26 | C | 1.18987223 | -4.54723533 | -0.67787557 |
| 27 | C | 3.38173411 | 4.98319443 | 1.01780596 |
| 28 | C | 0.7210141 | -5.14959318 | 0.51644338 |
| 29 | C | 0.42825447 | -6.51736457 | 0.56848539 |
| 30 | C | 0.60293203 | -7.29906991 | -0.57560919 |
| 31 | C | 1.06438119 | -6.734429 | -1.76029373 |
| 32 | C | 1.36420397 | -5.36695741 | -1.80891882 |
| 33 | C | 3.23191342 | 6.10983564 | 0.17580984 |
| 34 | C | 3.52827197 | 7.39706147 | 0.63613345 |
| 35 | C | 3.97883384 | 7.59059381 | 1.94029048 |
| 36 | C | 4.13728629 | 6.49816771 | 2.79129954 |
| 37 | C | 3.84238286 | 5.21068288 | 2.335495 |
| 38 | O | 4.06891099 | 4.1604025 | 3.2006212 |

| | | | | |
|---|---|---|---|---|
| 39 | O | 2.71370686 | 6.00681219 | -1.0943682 |
| 40 | O | 1.9321096 | -4.89103932 | -2.9688292 |
| 41 | O | 0.60183672 | -4.30973758 | 1.58378739 |
| 42 | C | 1.17804882 | -3.95314062 | -3.76159144 |
| 43 | C | 2.15932162 | -3.20260316 | -4.65765874 |
| 44 | C | 1.57388989 | -1.89105917 | -5.19858762 |
| 45 | C | 2.62661102 | -1.00465584 | -5.91118653 |
| 46 | C | 2.23245132 | 0.45327807 | -5.9025848 |
| 47 | C | 2.63053968 | 1.28853507 | -4.93736093 |
| 48 | C | 2.15065346 | 2.69520927 | -4.67516167 |
| 49 | C | 3.18016353 | 3.55131065 | -3.90961113 |
| 50 | C | 2.53017578 | 4.67294546 | -3.08768792 |
| 51 | C | 3.4935949 | 5.31966727 | -2.09586443 |
| 52 | C | 2.90510174 | 3.56410058 | 3.80600548 |
| 53 | C | 3.35838633 | 2.38377001 | 4.65814125 |
| 54 | C | 2.18662912 | 1.46241668 | 5.02465704 |
| 55 | C | 2.57331481 | 0.34672076 | 6.01480811 |
| 56 | C | 1.47300046 | -0.66651342 | 6.20051011 |
| 57 | C | 1.6265876 | -1.99481603 | 6.17602138 |
| 58 | C | 0.52116119 | -3.0029861 | 6.36502312 |
| 59 | C | 0.54602753 | -4.15548658 | 5.3390449 |
| 60 | C | 0.47455233 | -3.68715596 | 3.88004815 |
| 61 | C | 0.42024942 | -4.85171594 | 2.89748131 |
| 62 | C | -12.28344265 | 1.53135973 | 0.14776433 |
| 63 | C | -12.08437019 | 0.15695536 | -0.05325291 |
| 64 | C | -10.85528078 | -0.24046257 | -0.60914038 |
| 65 | C | -9.88903889 | 0.69263542 | -0.97551455 |
| 66 | C | -10.09367724 | 2.07089566 | -0.76925511 |
| 67 | C | -11.3072834 | 2.46851787 | -0.18717179 |
| 68 | S | -8.41477584 | 0.15030093 | -1.82031452 |
| 69 | C | -7.28194012 | 1.3722768 | -1.18654946 |
| 70 | C | -7.74163809 | 2.689893 | -0.96211174 |
| 71 | N | -9.0998486 | 3.00571754 | -1.14364741 |
| 72 | C | -5.94515346 | 1.03963096 | -1.00965688 |
| 73 | C | -4.99684911 | 2.01955387 | -0.64345262 |
| 74 | C | -5.45328257 | 3.33400248 | -0.42723997 |
| 75 | C | -6.79848728 | 3.65659527 | -0.56753761 |
| 76 | C | -13.11973696 | -0.84071301 | 0.30988713 |
| 77 | C | -3.62386183 | 1.68380982 | -0.50398908 |
| 78 | C | -14.4864441 | -0.55810547 | 0.16685613 |
| 79 | C | -15.47239461 | -1.48672775 | 0.50780149 |
| 80 | C | -15.10059351 | -2.74222874 | 1.00487471 |
| 81 | C | -13.7377491 | -3.0452384 | 1.15418408 |
| 82 | C | -12.77013585 | -2.10997342 | 0.81296336 |

| | | | | |
|---|---|---|---|---|
| 83 | C | -2.44344464 | 1.39585005 | -0.3967894 |
| 84 | C | 7.06069651 | -0.80983924 | -0.19836427 |
| 85 | C | 8.24984405 | -1.08079357 | -0.20215989 |
| 86 | C | 9.63434827 | -1.39528651 | -0.19556739 |
| 87 | C | 10.07309907 | -2.71766104 | -0.42423413 |
| 88 | C | 11.42769033 | -3.02513439 | -0.40093267 |
| 89 | C | 12.38444195 | -2.02662046 | -0.15393811 |
| 90 | C | 11.95246477 | -0.70577912 | 0.0498582 |
| 91 | C | 10.60171068 | -0.39152648 | 0.03888117 |
| 92 | C | -9.47882424 | 4.41187435 | -1.24064621 |
| 93 | O | -15.97317002 | -3.72561577 | 1.36730399 |
| 94 | C | -17.36801134 | -3.46891158 | 1.24145431 |
| 95 | C | 13.85386546 | -2.28794834 | -0.12796184 |
| 96 | O | 14.69079426 | -1.41601037 | -0.25104996 |
| 97 | O | 14.26164368 | -3.57072333 | 0.04377454 |
| 98 | H | -1.57266273 | 3.85126333 | 0.27359347 |
| 99 | H | 0.67542571 | 5.22877062 | 0.78777971 |
| 100 | H | -1.30967021 | -3.53396283 | -0.91661663 |
| 101 | H | -2.73162319 | -1.2566956 | -0.76350259 |
| 102 | H | 6.17002797 | -3.32906478 | -0.51288274 |
| 103 | H | 3.90325009 | -4.75650355 | -0.72334885 |
| 104 | H | 5.91215974 | 4.04645377 | 0.74983811 |
| 105 | H | 7.343295 | 1.82044674 | 0.29238818 |
| 106 | H | 0.07438871 | -6.9721776 | 1.48597171 |
| 107 | H | 0.37488387 | -8.36061931 | -0.53520287 |
| 108 | H | 1.21655839 | -7.33131654 | -2.65354635 |
| 109 | H | 3.39516623 | 8.23043563 | -0.04629417 |
| 110 | H | 4.208744 | 8.59224993 | 2.29229458 |
| 111 | H | 4.49079924 | 6.61897083 | 3.81034946 |
| 112 | H | 0.6548093 | -3.25079709 | -3.10567984 |
| 113 | H | 0.42304443 | -4.50041412 | -4.3434818 |
| 114 | H | 2.50540307 | -3.85129001 | -5.47279498 |
| 115 | H | 3.03842693 | -2.9677134 | -4.04419568 |
| 116 | H | 1.1735675 | -1.32169686 | -4.34988119 |
| 117 | H | 0.72498184 | -2.08616919 | -5.86790147 |
| 118 | H | 2.79215072 | -1.36852705 | -6.93379917 |
| 119 | H | 3.5817138 | -1.11074856 | -5.37949902 |
| 120 | H | 1.52615863 | 0.79250573 | -6.66276274 |
| 121 | H | 3.32470568 | 0.8956988 | -4.18880861 |
| 122 | H | 1.24428087 | 2.62946164 | -4.05194871 |
| 123 | H | 1.83788307 | 3.18580375 | -5.60601297 |
| 124 | H | 3.93450802 | 3.95258108 | -4.59951462 |
| 125 | H | 3.72192929 | 2.89402068 | -3.21457512 |
| 126 | H | 1.70899167 | 4.24480983 | -2.5000287 |

| | | | | |
|---|---|---|---|---|
| 127 | H | 2.08631074 | 5.43604002 | -3.74016382 |
| 128 | H | 4.16206458 | 6.04540434 | -2.57914203 |
| 129 | H | 4.11464278 | 4.55583568 | -1.61897634 |
| 130 | H | 2.38505669 | 4.31848765 | 4.41332927 |
| 131 | H | 2.21418976 | 3.22650881 | 3.02545878 |
| 132 | H | 3.86063714 | 2.75047286 | 5.56296969 |
| 133 | H | 4.10467158 | 1.8156258 | 4.0880883 |
| 134 | H | 1.78984826 | 1.00952137 | 4.10542789 |
| 135 | H | 1.3643519 | 2.05182381 | 5.45548744 |
| 136 | H | 2.82220922 | 0.81440679 | 6.98057664 |
| 137 | H | 3.48628619 | -0.1587165 | 5.67232608 |
| 138 | H | 0.47278119 | -0.25714303 | 6.36383257 |
| 139 | H | 2.62715818 | -2.40663878 | 6.01966961 |
| 140 | H | -0.45066582 | -2.4927372 | 6.32907854 |
| 141 | H | 0.5992731 | -3.45025471 | 7.36796196 |
| 142 | H | -0.28941291 | -4.83482944 | 5.55663666 |
| 143 | H | 1.46499526 | -4.74189472 | 5.48208685 |
| 144 | H | 1.35480736 | -3.07751395 | 3.64401168 |
| 145 | H | -0.40332042 | -3.04558027 | 3.72809315 |
| 146 | H | -0.54349625 | -5.37466879 | 2.96266645 |
| 147 | H | 1.21725016 | -5.57987431 | 3.10373639 |
| 148 | H | -13.20179642 | 1.87999456 | 0.6106521 |
| 149 | H | -10.66242763 | -1.29236329 | -0.79830206 |
| 150 | H | -11.49323967 | 3.51505769 | 0.0246488 |
| 151 | H | -5.6205999 | 0.01785605 | -1.17958249 |
| 152 | H | -4.74709064 | 4.10343252 | -0.13205961 |
| 153 | H | -7.11494004 | 4.67217082 | -0.36162091 |
| 154 | H | -14.7956837 | 0.39964023 | -0.24237728 |
| 155 | H | -16.51549081 | -1.22571082 | 0.37134902 |
| 156 | H | -13.46036053 | -4.01754858 | 1.5500859 |
| 157 | H | -11.72339621 | -2.35958917 | 0.96227841 |
| 158 | H | 9.34294745 | -3.49489153 | -0.62435216 |
| 159 | H | 11.72528495 | -4.04899682 | -0.61301269 |
| 160 | H | 12.69560568 | 0.06495177 | 0.22377417 |
| 161 | H | 10.27740747 | 0.6297556 | 0.21067391 |
| 162 | H | -9.52896463 | 4.91723448 | -0.26550601 |
| 163 | H | -8.75361851 | 4.93304607 | -1.86885952 |
| 164 | H | -17.67722628 | -2.62056162 | 1.86449687 |
| 165 | H | -17.64702391 | -3.2734747 | 0.19864171 |
| 166 | H | 13.51332545 | -4.14949231 | 0.26631445 |
| 167 | H | -17.87072989 | -4.37366414 | 1.58665328 |
| 168 | H | -10.45652789 | 4.48129693 | -1.72152096 |

**XW41** (the hexyloxy and hexyl chains in the phenothiazine moiety were replaced by methoxy and

methyl groups, respectively)

| Row | Symbol | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.05059359 | 3.46229521 | 0.15686885 |
| 2 | C | -0.92748241 | 4.22949063 | 0.04938305 |
| 3 | C | 0.20197157 | 3.3264158 | -0.00125906 |
| 4 | N | -0.25378495 | 2.03088539 | 0.08772708 |
| 5 | C | -1.61761645 | 2.08574891 | 0.19187074 |
| 6 | C | -2.20212491 | -2.61412841 | 0.84803012 |
| 7 | C | -2.9768594 | -1.49776254 | 0.71685642 |
| 8 | C | -2.08000253 | -0.39026043 | 0.49018968 |
| 9 | N | -0.78842317 | -0.84277759 | 0.46759806 |
| 10 | C | -0.82591484 | -2.19926519 | 0.68878653 |
| 11 | C | -2.48295753 | 0.96748889 | 0.34983771 |
| 12 | C | 3.88022414 | -2.83002659 | 0.31398409 |
| 13 | C | 2.77150996 | -3.57968628 | 0.57503686 |
| 14 | C | 1.63282535 | -2.68563259 | 0.53619644 |
| 15 | N | 2.0753096 | -1.40743308 | 0.26300315 |
| 16 | C | 3.43242472 | -1.4674355 | 0.13213932 |
| 17 | C | 0.29305663 | -3.06437857 | 0.74680491 |
| 18 | C | 4.04078529 | 3.25263741 | -0.35985778 |
| 19 | C | 4.79850748 | 2.11985688 | -0.38602262 |
| 20 | C | 3.89276775 | 1.00858465 | -0.19335 |
| 21 | N | 2.61302674 | 1.47136186 | -0.07285259 |
| 22 | C | 2.66394277 | 2.8456476 | -0.16441026 |
| 23 | C | 1.55856684 | 3.72005944 | -0.10092338 |
| 24 | C | 4.28898414 | -0.35615166 | -0.11097777 |
| 25 | Zn | 0.91245573 | 0.31373125 | 0.19475242 |
| 26 | C | 0.0353899 | -4.49048365 | 1.14583149 |
| 27 | C | 1.85629082 | 5.19309028 | -0.08479489 |
| 28 | C | -0.22144369 | -4.76085856 | 2.51355805 |
| 29 | C | -0.40553911 | -6.07063731 | 2.9708941 |
| 30 | C | -0.33440053 | -7.12813756 | 2.06148545 |
| 31 | C | -0.08596725 | -6.89258013 | 0.71372067 |
| 32 | C | 0.10485565 | -5.58119186 | 0.25717239 |
| 33 | C | 1.52646069 | 6.04798636 | -1.16120595 |
| 34 | C | 1.81637044 | 7.41500053 | -1.11347317 |
| 35 | C | 2.43705403 | 7.96076743 | 0.00850842 |
| 36 | C | 2.7685221 | 7.14268052 | 1.0871327 |
| 37 | C | 2.48134139 | 5.77574281 | 1.04221489 |
| 38 | O | 2.8809196 | 5.00679127 | 2.11482958 |
| 39 | O | 0.83809187 | 5.58650411 | -2.26062558 |
| 40 | O | 0.46542623 | -5.43604245 | -1.0613662 |
| 41 | O | -0.25154674 | -3.66635309 | 3.32591898 |
| 42 | C | -0.38775443 | -4.67933487 | -1.94468629 |

| | | | | |
|---|---|---|---|---|
| 43 | C | 0.4940508 | -3.92961887 | -2.94017133 |
| 44 | C | -0.24153442 | -2.78201689 | -3.64535201 |
| 45 | C | 0.71114272 | -1.84343554 | -4.41313296 |
| 46 | C | 0.17049503 | -0.44287083 | -4.56167198 |
| 47 | C | 0.46615509 | 0.45174435 | -5.5104407 |
| 48 | C | 0.03149822 | 1.89470356 | -5.4129835 |
| 49 | C | 1.11273159 | 2.78072698 | -4.74160062 |
| 50 | C | 0.5255806 | 4.01508977 | -4.04356138 |
| 51 | C | 1.55492949 | 4.75189926 | -3.19227707 |
| 52 | C | 1.84280858 | 4.55935838 | 3.00845768 |
| 53 | C | 2.47713935 | 3.67691563 | 4.07767095 |
| 54 | C | 1.42577976 | 2.8551012 | 4.83634637 |
| 55 | C | 2.00718885 | 2.06563011 | 6.02492852 |
| 56 | C | 1.00778902 | 1.11296639 | 6.62925693 |
| 57 | C | 1.24206277 | -0.16714936 | 6.93752575 |
| 58 | C | 0.23753698 | -1.11292747 | 7.54629935 |
| 59 | C | 0.19545064 | -2.49975685 | 6.87161143 |
| 60 | C | -0.10190433 | -2.44829497 | 5.36740578 |
| 61 | C | -0.21113988 | -3.83670128 | 4.74775481 |
| 62 | C | -13.61533633 | 1.06187111 | -1.04312363 |
| 63 | C | -13.38243685 | -0.31537487 | -0.90846802 |
| 64 | C | -12.19792903 | -0.70691471 | -0.25924994 |
| 65 | C | -11.30944721 | 0.23205906 | 0.25812452 |
| 66 | C | -11.54882344 | 1.61306712 | 0.11971813 |
| 67 | C | -12.7147846 | 2.00718473 | -0.55469847 |
| 68 | S | -9.9007825 | -0.31429888 | 1.20621622 |
| 69 | C | -8.76381433 | 0.98588027 | 0.76389087 |
| 70 | C | -9.2539854 | 2.29900168 | 0.58120707 |
| 71 | N | -10.63501832 | 2.55424591 | 0.64983623 |
| 72 | C | -7.40397051 | 0.71195801 | 0.69346271 |
| 73 | C | -6.46673405 | 1.74634056 | 0.48081308 |
| 74 | C | -6.95441793 | 3.05620122 | 0.30857068 |
| 75 | C | -8.3185837 | 3.32240248 | 0.34213285 |
| 76 | C | -14.3388382 | -1.32050576 | -1.43224947 |
| 77 | C | -5.07445325 | 1.46906419 | 0.43812304 |
| 78 | C | -15.72251828 | -1.08962958 | -1.41133273 |
| 79 | C | -16.63517933 | -2.02546832 | -1.90315459 |
| 80 | C | -16.17042576 | -3.23604408 | -2.43234247 |
| 81 | C | -14.7892952 | -3.48706774 | -2.46104937 |
| 82 | C | -13.89510112 | -2.54498479 | -1.97078499 |
| 83 | C | -3.87783874 | 1.23543298 | 0.40095553 |
| 84 | C | 5.67322102 | -0.62475806 | -0.26260163 |
| 85 | C | 6.86754253 | -0.8292967 | -0.40605537 |
| 86 | C | 8.25375462 | -1.02939082 | -0.58094979 |

| | | | | |
|---|---|---|---|---|
| 87 | C | 8.85323872 | -2.28161303 | -0.54417214 |
| 88 | C | 10.24734566 | -2.46223605 | -0.72073422 |
| 89 | C | 11.13830874 | -1.42370046 | -0.94349201 |
| 90 | C | 10.56156174 | -0.10547255 | -0.99020464 |
| 91 | C | 9.13283381 | 0.08907829 | -0.81426839 |
| 92 | N | 11.2183731 | 1.04095748 | -1.21377312 |
| 93 | S | 10.1040742 | 2.24561055 | -1.18898687 |
| 94 | N | 8.74783392 | 1.36468035 | -0.90139448 |
| 95 | C | 12.58441168 | -1.67518747 | -1.12534896 |
| 96 | C | 13.01910205 | -2.84190918 | -1.78318667 |
| 97 | C | 14.37340782 | -3.12367504 | -1.92815776 |
| 98 | C | 15.34037944 | -2.24113506 | -1.42336904 |
| 99 | C | 14.91569078 | -1.06362562 | -0.79071507 |
| 100 | C | 13.5629771 | -0.785955 | -0.63794481 |
| 101 | C | -11.07948387 | 3.93657321 | 0.79769969 |
| 102 | O | -16.9661951 | -4.22200183 | -2.9367952 |
| 103 | C | -18.3749124 | -4.0149853 | -2.9422191 |
| 104 | C | 16.81001674 | -2.47138301 | -1.55715878 |
| 105 | O | 17.6382683 | -1.58918427 | -1.45434166 |
| 106 | O | 17.22569378 | -3.73914446 | -1.80418732 |
| 107 | H | -3.07759808 | 3.79331784 | 0.21984561 |
| 108 | H | -0.86995513 | 5.30705338 | 0.00472741 |
| 109 | H | -2.53154234 | -3.62664583 | 1.03426632 |
| 110 | H | -4.05368029 | -1.42490498 | 0.77633722 |
| 111 | H | 4.90846245 | -3.15941157 | 0.26043434 |
| 112 | H | 2.72475022 | -4.64115088 | 0.77096573 |
| 113 | H | 4.38023558 | 4.27287566 | -0.46750316 |
| 114 | H | 5.86919642 | 2.03685575 | -0.51569443 |
| 115 | H | -0.59581557 | -6.26934025 | 4.01878513 |
| 116 | H | -0.47818164 | -8.14546643 | 2.41497173 |
| 117 | H | -0.02066271 | -7.70447175 | -0.00309589 |
| 118 | H | 1.54169859 | 8.03026502 | -1.96437332 |
| 119 | H | 2.66128613 | 9.02312743 | 0.0426602 |
| 120 | H | 3.2524364 | 7.54083734 | 1.97330836 |
| 121 | H | -0.99089908 | -3.97442513 | -1.36626679 |
| 122 | H | -1.07274469 | -5.37686578 | -2.44598842 |
| 123 | H | 0.92472695 | -4.63020235 | -3.66746698 |
| 124 | H | 1.3330718 | -3.51067268 | -2.371453 |
| 125 | H | -0.76016526 | -2.19076495 | -2.8773049 |
| 126 | H | -1.02350396 | -3.16583357 | -4.31411034 |
| 127 | H | 0.98600704 | -2.26584012 | -5.3883476 |
| 128 | H | 1.64948372 | -1.78069168 | -3.83861119 |
| 129 | H | -0.4728545 | -0.11174471 | -3.74131493 |
| 130 | H | 1.11882266 | 0.173317 | -6.34010638 |

| | | | | |
|---|---|---|---|---|
| 131 | H | -0.88026085 | 1.94296247 | -4.80285489 |
| 132 | H | -0.22722692 | 2.30216245 | -6.3990761 |
| 133 | H | 1.87758102 | 3.07027307 | -5.47479717 |
| 134 | H | 1.62507805 | 2.17369623 | -3.98412192 |
| 135 | H | -0.27350151 | 3.68712681 | -3.36677972 |
| 136 | H | 0.06713416 | 4.70205751 | -4.76664408 |
| 137 | H | 2.22192803 | 5.37972381 | -3.79980588 |
| 138 | H | 2.17366713 | 4.03502962 | -2.64233674 |
| 139 | H | 1.34658423 | 5.4332095 | 3.45411353 |
| 140 | H | 1.08962617 | 3.9953021 | 2.44702373 |
| 141 | H | 3.05949522 | 4.29625121 | 4.77244381 |
| 142 | H | 3.18596314 | 2.99806048 | 3.5863182 |
| 143 | H | 0.94830873 | 2.1553049 | 4.13648178 |
| 144 | H | 0.6258193 | 3.5141653 | 5.20392211 |
| 145 | H | 2.34673784 | 2.7872963 | 6.7846983 |
| 146 | H | 2.89953276 | 1.51014068 | 5.70615013 |
| 147 | H | 0.01333936 | 1.52427363 | 6.82014587 |
| 148 | H | 2.23780186 | -0.57930443 | 6.75398342 |
| 149 | H | -0.76015021 | -0.65456206 | 7.51898878 |
| 150 | H | 0.47743481 | -1.2687845 | 8.60944396 |
| 151 | H | -0.55892439 | -3.11366056 | 7.38245417 |
| 152 | H | 1.15999267 | -3.00360242 | 7.02885952 |
| 153 | H | 0.69677879 | -1.90264573 | 4.85111194 |
| 154 | H | -1.03241969 | -1.89603297 | 5.18139936 |
| 155 | H | -1.11797431 | -4.35070525 | 5.09407627 |
| 156 | H | 0.65533959 | -4.45791415 | 5.01495959 |
| 157 | H | -14.49714073 | 1.40922186 | -1.57313359 |
| 158 | H | -11.98221443 | -1.76184097 | -0.11738942 |
| 159 | H | -12.92062614 | 3.05867556 | -0.71822948 |
| 160 | H | -7.0556424 | -0.30757489 | 0.82559072 |
| 161 | H | -6.25606547 | 3.86744336 | 0.12937788 |
| 162 | H | -8.65543507 | 4.33813653 | 0.17264207 |
| 163 | H | -16.10582295 | -0.16924765 | -0.97975336 |
| 164 | H | -17.69553221 | -1.80565455 | -1.85713026 |
| 165 | H | -14.43850535 | -4.42406275 | -2.88298029 |
| 166 | H | -12.83035072 | -2.75265075 | -2.02861922 |
| 167 | H | 8.23465703 | -3.15503045 | -0.36568305 |
| 168 | H | 10.63167138 | -3.4749084 | -0.65034744 |
| 169 | H | 12.28992719 | -3.52038138 | -2.21409145 |
| 170 | H | 14.65795865 | -4.01598228 | -2.48010522 |
| 171 | H | 15.66378188 | -0.37574298 | -0.4113757 |
| 172 | H | 13.25838431 | 0.12253873 | -0.13330885 |
| 173 | H | -10.43968344 | 4.43982977 | 1.52542161 |
| 174 | H | -11.05763498 | 4.50376139 | -0.14386392 |

| | | | | |
|---|---|---|---|---|
| 175 | H | -18.76525524 | -3.88708271 | -1.92499549 |
| 176 | H | -18.64932007 | -3.1424048 | -3.54791629 |
| 177 | H | 16.48895564 | -4.36879756 | -1.73013678 |
| 178 | H | -12.10055455 | 3.9390189 | 1.18405345 |
| 179 | H | -18.80726492 | -4.91346726 | -3.38520519 |