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Supporting Information (SI)

Solar cells sensitized by doubly concerted companion dyes with optimized donors to achieve high efficiencies up to 12.5%: a record efficiency for iodine electrolyte-based DSSCs

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Contents

1 Experimental section

1.1 Materials and instrumentation

All reagents and solvents are commercially obtained without further purification unless otherwise stated. The FTO conducting glass (transparent Fluorine-doped SnO_2, transparency > 90% in the visible range, sheet resistance 15 Ω/square) was purchased from the Advanced Election Technology Co., Ltd. The TiO_2 paste (18 NR-T, 30 NR-D and 18 NR-AO) was purchased from the Greatcell Solar Industries Pty Ltd.

^{1}H NMR and ^{13}C NMR spectra were measured using Bruker AM 400 or Ascend 600 spectrometer with tetramethylsilane (TMS) used as the internal standard. HRMS data were collected using the Thermo Scientific Q Exactive combined quadrupole mass spectrometer. The Matrix-assisted laser desorption ionization-time-of-flight mass spectrometry (MALDI-TOF-MS) was performed by a Shimadzu-kratos model Axima CFR$^+$ mass spectrometer. UV-Vis absorption spectra and fluorescence spectra were recorded on a Shimadzu UV2600 spectrophotometer and Varian Cary Eclipse fluorescence spectrophotometer, respectively. IR spectra were measured using a Nicolet 6700 FTIR spectrometer with the ATR accessory. The cyclic voltammograms (CV) and differential pulse voltametric (DPV) of the dyes were measured in CH_2Cl_2 on a CorrTest electrochemical workstation using 0.1 M $TBAPF_6$ as the supporting electrolyte. A platinum ring, a platinum wire, and an Ag/AgCl electrode in saturated KCl solution were used as the working, counter and reference electrodes, respectively. The potentials were calibrated by using ferrocene/ferrocenium as the external reference. The scan rate was fixed at 100 mV s^{-1}.

The AM 1.5G sunlight simulator used in photovoltaic measurements was a 300 W xenon lamp (model No. 91160, Oriel) and was calibrated to 100 mW cm^{-2} by employing a Newport Oriel PV reference cell system (model 91150 V). The *J–V* curves were measured by a Keithley 2400 source meter (Inc. USA), and the action spectra of the incident monochromatic photon-to-electron conversion efficiency (IPCE) spectra were recorded by a Newport-74125 system (Newport Instruments). The intensity of monochromatic light was calibrated by a Si detector (Newport 71640). The electrochemical impedance spectroscopy (EIS) measurements were measured by a Zahner IM6e Impedance Analyzer (ZAHNER-Elektrik GmbH & CoKG, Kronach, Germany). The experimental EIS data were fitted by ZSimpWin software to give the chemical capacitances and the electron lifetimes.

1.2 Fabrication of the solar cells

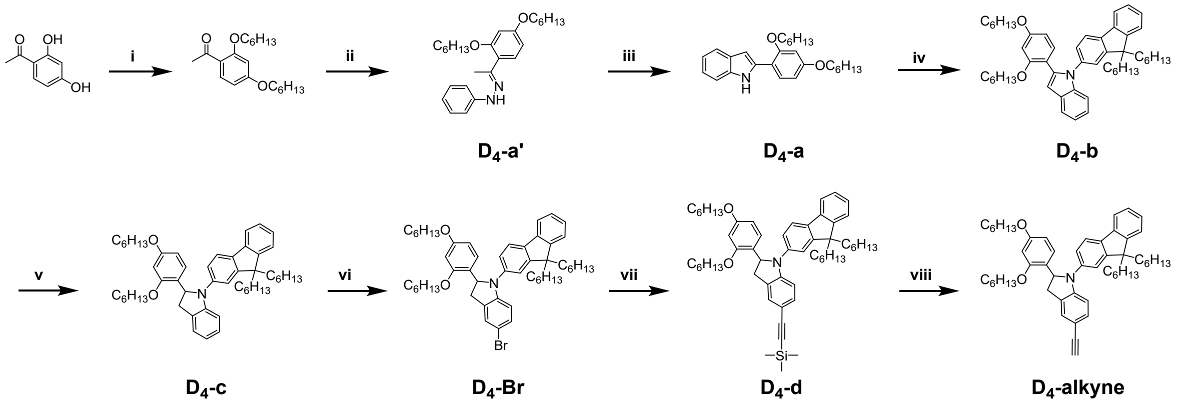
All the FTO glasses for photoanodes and counter electrodes were rinsed sequentially with detergent solution, deionized water, acetone and ethanol under ultrasonic conditions before use. For iodine-based electrolytes, TiO_2 photoanodes containing transmission and scattering layers were prepared by repetitive screen printing. After printing each layer, the TiO_2 photoanodes were left for 10 min and then dried at 130°C for 5 min. Later, the TiO_2 photoanodes were sintered with a programmed procedure at 275°C for 5 min, 325°C for 5 min, 375°C for 5 min, 450°C for 15 min, and 500°C for 15 min, respectively. After cooling to room temperature, the obtained photoanodes were chemically deposited with 40 mM $TiCl_4$ aqueous solution at 70°C for 30 min, rinsed with water and ethanol and then sintered again at 450°C for 30 min. The active area of the TiO_2 photoanode is 0.12 cm^2. Eventually, the photoanodes were immersed in a solution of the porphyrin dyes (0.2 mM), organic dyes (0.2 mM) and CC dyes (0.1 mM) in a mixture of chloroform and ethanol (v:v, 3:2) at 25°C for 12 h. For cobalt-based electrolyte, the FTO glass plates were immersed in 40 mM $TiCl_4$ aqueous solution at 70°C for 30 min, rinsed with water and ethanol and then sintered at 450°C for 30 min before screen printing. The remaining steps are the same as those for iodine-based electrolytes. The counter electrodes were made by spin-coating H_2PtCl_6 in 2-propanol onto FTO glass and then sintered at 400°C for 15 minutes. After injecting the electrolyte solution, fabrication of the DSSCs was accomplished by heat-sealing the two electrodes with Surlyn (25 μm). The iodine-based electrolyte contains 0.6 M 1-methyl-3-propylimidazolium iodide (PMII), 0.5 M 4-tert-butylpyridine (TBP), 0.1 M LiI and 0.05 M I_2 in acetonitrile. The cobalt-based electrolyte contains 0.22 M $[Co(bpy)_3](TFSI)_2$, 0.05 M $[Co(bpy)_3](TFSI)_3$, 0.1 M LiTFSI, and 0.5 M TBP in acetonitrile.

1.3 Theoretical calculation details

Density functional theory (DFT) calculations were carried out using Gaussian16 program package with a B3LYP/6-31G* and pm6 basis set.[1–4]

1.4 Synthetic section

The starting material 2,4-dihydroxyacetophenone was purchased from commercial source and used as received. 2-bromo-9,9-dihexyl-9H-fluorene was prepared according to reported methods.[5–6]



Scheme S1. Reaction conditions: i) 1-bromohexane, K_2CO_3, DMF, reflux; ii) phenylhydrazine, AcOH, EtOH, reflux; iii) $ZnCl_2$, o-DCB, 160°C; iv) 2-bromo-9,9-dihexyl-9H-fluorene, ^{t}BuONa, ^{t}Bu$_3$PHBF$_4$, Pd(OAC)$_2$, p-xylene, reflux; v) $NaBH_3CN$, AcOH/DCM, rt; vi) NBS, DCM, rt; vii) Trimethylsilylacetylene (TMSA), CuI, PPh_3, $Pd_2(PPh_3)_2Cl_2$, Piperdine, 80°C; viii) Tetrabutylammonium fluoride (TBAF), THF, rt.

Synthesis of 2,4-Dihexyloxyacetophenone. The mixture of 2,4-dihydroxyacetophenone (2.10 g, 13.8 mmol), K_2CO_3 (3.55 g, 25.7 mmol) and 1-bromohexane (4.6 mL, 32.7 mmol) in DMF (40 mL) was stirred at 110°C for 10 h. After cooling to room temperature, the solution was poured into water and extracted with ethyl acetate (EA) (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with petroleum ether (PE)/dichloromethane (DCM) (3/1, v/v) used as the eluent to give a yellow viscous liquid of 2,4-Dihexyloxyacetophenone (2.98 g, yield 68%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.82 (d, J = 8.7 Hz, 1H), 6.49 (dd, J = 8.8, 2.2 Hz, 1H), 6.42 (d, J = 2.1 Hz, 1H), 4.00 (dt, J = 12.9, 6.5 Hz, 4H), 2.59 (s, 3H), 1.80 (ddd, J = 27.8, 14.8, 6.8 Hz, 4H), 1.66 (s, 1H), 1.54 – 1.39 (m, 5H), 1.39 – 1.26 (m, 9H), 0.90 (t, J = 6.9 Hz, 7H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 197.70, 164.13, 160.70, 132.58, 120.90, 105.49, 99.20, 68.38, 33.89, 30.79, 29.12, 25.79, 22.57, 14.00. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{20}H_{32}O_3$, 320.2351; Found, 320.1934. FT-IR (ATR, cm^{-1}): 2928 (s), 2857 (s), 1662 (m), 1595 (s), 1571 (m), 1498 (m), 1466 (m), 1431 (m), 1388 (m), 1356 (m), 1254 (s), 1182 (s), 1136 (m), 1066 (m), 1019 (m), 963 (m), 827 (m), 726 (w), 643 (w), 583 (m).

Synthesis of compound D$_4$-a'. To the mixture of 2,4-Dihexyloxyacetophenone (3.65 g, 11.4 mmol) and phenylhydrazine (1.50 g, 13.8 mmol) in EtOH (10 mL) were added AcOH (0.65

mL, 11.3 mmol) under nitrogen. The reaction was stirred at 80°C for 3 h under nitrogen. After cooling to room temperature, the solution was concentrated under reduced pressure. The obtained phenylhydrazone derivative **D_4-a′** (3.55 g) was used for the next reaction without further purification.

Synthesis of compound D_4-a. The mixture of **D_4-a′** (2.26 g, 5.51 mmol) and $ZnCl_2$ (2.28 g, 16.8 mmol) in o-DCB (10 mL) was stirred at 160°C for 2 h under nitrogen. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (4/1, v/v) used as the eluent to give a white solid of **D_4-a** (1.53 g, yield 71%). ^1H NMR (600 MHz, acetone-d_6, ppm) δ 10.27 (s, 1H), 7.72 (d, J = 8.6 Hz, 1H), 7.51 (d, J = 7.8 Hz, 1H), 7.39 (dd, J = 8.0, 0.6 Hz, 1H), 7.11 – 7.02 (m, 1H), 7.01 – 6.95 (m, 1H), 6.85 (d, J = 1.3 Hz, 1H), 6.68 (d, J = 2.3 Hz, 1H), 6.61 (dd, J = 8.6, 2.3 Hz, 1H), 4.16 (t, J = 6.5 Hz, 2H), 4.02 (t, J = 6.5 Hz, 2H), 2.00 – 1.88 (m, 2H), 1.77 (dq, J = 13.2, 6.5 Hz, 2H), 1.61 – 1.45 (m, 4H), 1.45 – 1.28 (m, 9H), 1.07 – 0.83 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 159.76, 156.39, 136.46, 135.80, 128.91, 128.27, 121.18, 119.74, 113.52, 110.59, 106.37, 100.47, 98.18, 68.86, 68.16, 31.61, 29.26, 25.88, 22.62, 14.05. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{26}H_{35}NO_2$, 393.2668; Found, 393.2560. FT-IR (ATR, cm^{-1}): 3448 (s), 3046 (w), 2921 (s), 2852 (s), 1606 (m), 1573 (m), 1540 (w), 1435 (m), 1386 (w), 1348 (w), 1293 (s), 1249 (m), 1188 (m), 1140 (s), 1071 (m), 829 (m), 811 (m), 783 (m), 729 (s), 627 (m), 573 (m), 542 (s). mp 65–66°C.

Synthesis of compound D_4-b. The mixture of 2-bromo-9,9-dihexyl-9H-fluorene (1.39 g, 3.36 mmol), **D_4-a** (1.42 g, 3.61 mmol), ^{t}BuONa (324 mg, 3.38 mmol), $^tBu_3PHBF_4$ (52 mg, 0.18 mmol) and $Pd(OAc)_2$ (16.2 mg, 0.07 mmol) in p-xylene (20 mL) was stirred at 130°C for 3 h under nitrogen atmosphere. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (8/1, v/v) used as the eluent to give a yellow oil of **D_4-b** (949 mg, yield 37%). ^1H NMR (600 MHz, acetone-d_6, ppm) δ 7.86 (d, J = 8.0 Hz, 1H), 7.79 (dd, J = 12.0, 5.2 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.43 – 7.40 (m, 1H), 7.40 – 7.36 (m, 1H), 7.36 – 7.30 (m, 4H), 7.23 (d, J = 8.4 Hz, 1H), 7.14 (d, J = 1.7 Hz, 1H), 7.13 – 7.09 (m, 2H), 6.63 (s, 1H), 6.49 (dd, J = 8.4, 2.3 Hz, 1H), 6.44 (d, J = 2.2 Hz, 1H), 3.96 (t, J = 6.6 Hz, 2H), 3.78 (t, J = 6.6 Hz, 2H), 2.00 – 1.90 (m, 2H), 1.82 (td, J = 12.5, 5.0 Hz, 2H), 1.78 – 1.69 (m, 2H), 1.63 – 1.51 (m, 2H), 1.50 – 1.38 (m, 2H), 1.46 – 1.29 (m, 8H), 1.25 – 1.15 (m, 4H), 1.14 – 1.07 (m, 4H), 1.03 – 0.97 (m, 9H), 0.91 – 0.85 (m, 3H), 0.81 – 0.68 (m, 10H), 0.50 (s, 4H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 160.56, 157.82, 151.38, 150.92, 140.61, 139.29, 138.18, 137.95, 132.77, 128.54, 127.06, 126.87, 125.88, 122.87, 121.86, 121.57, 120.38, 120.16, 119.65, 114.95, 110.54, 104.42, 99.96, 68.13, 55.10, 40.43, 32.15, 30.88, 30.26, 28.04, 25.72, 23.76, 22.88, 21.82, 15.10, 12.26. HRMS (DART, m/z): $[M+H]^+$ calcd for $C_{51}H_{68}NO_2$, 726.5250; Found, 726.5245. FT-IR (ATR, cm^{-1}): 3045 (m), 2953 (m), 2922 (s), 2851 (s), 1609 (m), 1574 (m), 1495 (m), 1455 (s), 1423 (m), 1375 (m), 1295 (s), 1256 (m), 1185 (m), 1129 (m), 1070 (w), 1045 (m), 1022 (m), 919 (m), 830 (m), 785 (s), 736 (s), 620 (m), 469 (m). mp 59–60°C.

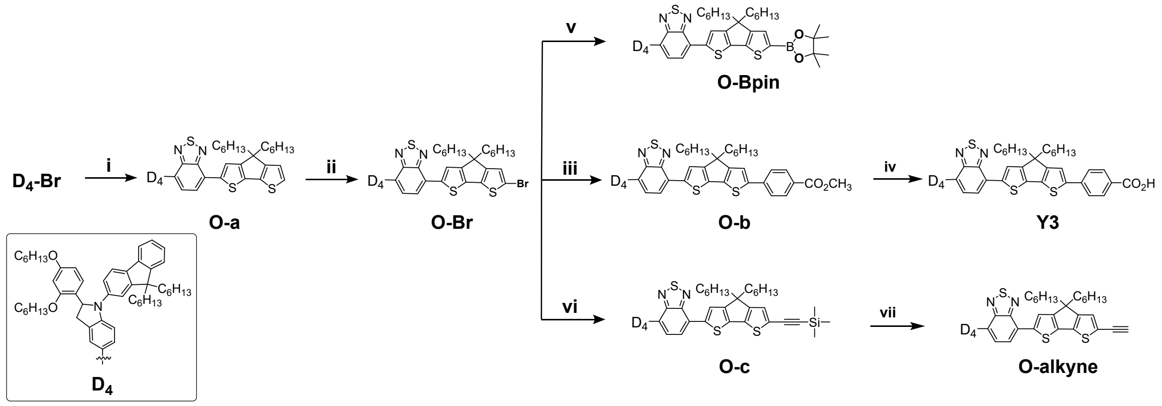
Synthesis of compound D_4-c. To the solution of **D_4-b** (695 mg, 0.96 mmol) in AcOH/DCM (7/7 mL) was added $NaBH_3CN$ (241 mg, 3.82 mmol) at 0°C under nitrogen. After the mixture was stirred for 4h at room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (4/1, v/v) used as the eluent to give a yellow oil of **D_4-c** (571 mg, yield 82%). ^{1}H NMR (600 MHz, Acetone, ppm) δ 7.62 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 7.3 Hz, 1H), 7.25 (dd, J = 7.4, 1.0 Hz, 1H), 7.22 – 7.17 (m, 3H), 7.15 (d, J = 8.4 Hz, 2H), 7.12 (d, J = 7.2 Hz, 1H), 7.09 (d, J = 7.6 Hz, 1H), 6.74 (td, J = 7.4, 0.5 Hz, 1H), 6.55 (d, J = 2.3 Hz, 1H), 6.32 (dd, J = 8.5, 2.3 Hz, 1H), 5.75 (dd, J = 9.4, 7.3 Hz, 1H), 4.09 (t, J = 6.3 Hz, 2H), 3.89 (td, J = 6.5, 2.0 Hz, 2H), 3.61 (dd, J = 15.6, 9.5 Hz, 1H), 2.94 (dd, J = 15.6, 7.2 Hz, 1H), 1.89 – 1.78 (m, 3H), 1.76 – 1.67 (m, 3H), 1.62 – 1.52 (m, 2H), 1.48 – 1.35 (m, 2H), 1.31 (tt, J = 7.7, 3.9 Hz, 6H), 1.17 – 1.02 (m, 5H), 0.98 (dd, J = 13.6, 6.7 Hz, 9H), 0.92 (t, J = 7.1 Hz, 10H), 0.77 (t, J = 7.3 Hz, 6H), 0.64 (dd, J = 6.9, 4.4 Hz, 2H), 0.48 – 0.35 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 159.32, 157.00, 151.47, 150.33, 148.20, 142.68, 141.23, 134.55, 130.05, 127.57, 127.08, 126.59, 125.77, 125.09, 123.02, 122.56, 119.90, 118.83, 118.18, 113.41, 108.28, 104.48, 99.52, 67.92, 61.55, 54.82, 40.47, 38.19, 31.56, 29.58, 25.86, 23.67, 22.62, 14.04. HRMS (DART, m/z): $[M+H]^+$ calcd for $C_{51}H_{70}NO_2$, 728.5407; Found, 728.5393. FT-IR (ATR, cm^{-1}): 2965 (m), 2924 (s), 2853 (s), 1603 (m), 1494 (m), 1477 (m), 1453 (s), 1381 (m), 1292 (m), 1259 (m), 1174 (s), 1114 (m), 1024 (m), 907 (m), 824 (m), 733 (s), 634 (w), 592 (w), 470 (w), 423 (w).

Synthesis of compound D_4-Br. To the solution of **D_4-c** (490 mg, 0.67 mmol) in DCM (10 mL) was added an DCM solution (10 mL) of NBS (119 mg, 0.67 mmol) dropwise at 0°C. After the mixture was stirred for 0.5 h at room temperature, the solution was poured into water and extracted with DCM (50 mL × 3). The combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (3/1, v/v) used as the eluent to give a yellow oil of **D_4-**

Br (482 mg, yield 89%). ^{1}H NMR (600 MHz, acetone-d$_6$, ppm) δ 7.61 (dd, *J* = 7.7, 2.5 Hz, 2H), 7.33 (d, *J* = 7.3 Hz, 1H), 7.23 (d, *J* = 7.4 Hz, 1H), 7.20 (d, *J* = 7.2 Hz, 2H), 7.18 (s, 1H), 7.17 (d, *J* = 3.7 Hz, 2H), 7.13 (d, *J* = 8.5 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.52 (d, *J* = 2.0 Hz, 1H), 6.32 (dd, *J* = 8.5, 2.1 Hz, 1H), 5.76 (dd, *J* = 9.2, 8.0 Hz, 1H), 4.05 (dd, *J* = 9.9, 5.8 Hz, 2H), 3.87 (td, *J* = 6.5, 1.8 Hz, 2H), 3.59 (dd, *J* = 16.0, 9.8 Hz, 1H), 3.00 (dd, *J* = 15.7, 7.0 Hz, 1H), 1.98 – 1.87 (m, 3H), 1.81 (dt, *J* = 12.4, 5.2 Hz, 3H), 1.72 – 1.65 (m, 2H), 1.53 (s, 2H), 1.44 – 1.34 (m, 7H), 1.34 – 1.26 (m, 9H), 1.10 (dt, *J* = 14.0, 7.0 Hz, 5H), 1.07 – 1.01 (m, 4H), 1.00 – 0.90 (m, 4H), 0.90 – 0.84 (m, 5H), 0.76 (td, *J* = 7.3, 3.4 Hz, 7H), 0.60 (d, *J* = 4.9 Hz, 2H), 0.42 (d, *J* = 4.2 Hz, 2H). ^{13}C NMR (151 MHz, CDCl$_3$, ppm) δ 159.52, 157.02, 151.59, 150.33, 147.42, 142.17, 141.05, 135.07, 132.52, 129.69, 127.81, 126.64, 125.97, 122.52, 119.99, 118.82, 118.34, 113.66, 110.07, 109.40, 104.46, 99.60, 67.94, 62.17, 54.85, 40.43, 37.73, 31.90, 30.92, 30.18, 28.75, 25.87, 23.67, 22.62, 14.60, 13.32. HRMS (DART, m/z): [M+H]$^+$ calcd for $C_{51}H_{69}BrNO_2$, 806.4512; Found, 806.4488. FT-IR (ATR, cm^{-1}): 2952 (m), 2924 (m), 2853 (m), 1610 (m), 1587 (m), 1494 (m), 1471 (s), 1454 (m), 1377 (w), 1292 (m), 1257 (m), 1173 (s), 1114 (m), 1024 (m), 831 (w), 801 (m), 736 (s), 634 (m), 594 (w).

Synthesis of compound D$_4$-d. The mixture of **D$_4$-Br** (285 mg, 0.35 mmol), Pd (PPh$_3$)$_2$Cl$_2$ (12.4 mg, 0.02 mmol), CuI (2.06 mg, 0.01 mmol) and PPh$_3$ (13.8 mg, 0.05 mmol) in piperidine (5 mL) was stirred at 80°C under nitrogen, and then TMSA (0.3 mL, 2.12 mmol) was added *via* a syringe over 10 min. After the mixture was stirred at 80°C for 8 h and cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na$_2$SO$_4$, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (6/1, v/v) used as the eluent to give a yellow oil of **D$_4$-d** (169 mg, yield 58%). ^{1}H NMR (600 MHz, Acetone, ppm) δ 7.63 (d, *J* = 8.1 Hz, 2H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.25 (td, *J* = 7.4, 1.1 Hz, 1H), 7.22 (dd, *J* = 3.2, 1.6 Hz, 1H), 7.21 – 7.19 (m, 2H), 7.19 – 7.16 (m, 2H), 7.13 (d, *J* = 8.5 Hz, 1H), 6.99 (d, *J* = 8.2 Hz, 1H), 6.51 (d, *J* = 2.0 Hz, 1H), 6.32 (dd, *J* = 8.5, 2.3 Hz, 1H), 5.82 – 5.74 (m, 1H), 4.04 (d, *J* = 5.9 Hz, 2H), 3.87 (td, *J* = 6.5, 2.4 Hz, 2H), 3.58 (dd, *J* = 15.8, 10.0 Hz, 1H), 3.01 (dd, *J* = 15.0, 6.4 Hz, 1H), 1.98 – 1.87 (m, 3H), 1.86 – 1.75 (m, 3H), 1.73 – 1.65 (m, 2H), 1.51 (s, 2H), 1.44 – 1.39 (m, 7H), 1.39 – 1.33 (m, 5H), 1.32 – 1.27 (m, 9H), 1.16 – 1.07 (m, 8H), 1.02 – 0.95 (m, 4H), 0.87 (m, 7H), 0.62 – 0.53 (m, 2H), 0.41 (m, 2H). ^{13}C NMR (151 MHz, CDCl$_3$, ppm) δ 159.28, 156.82, 151.32, 150.15, 148.36, 141.58, 140.82, 135.07, 131.70, 129.84, 128.31, 126.44, 125.81, 122.36, 119.74, 118.65, 113.93, 112.38, 107.32, 106.46, 104.27, 99.36, 90.99, 67.73, 61.80, 54.64, 40.24, 37.39, 31.35, 29.77, 27.53, 25.67, 23.45, 22.42, 13.86. MS (MALDI-TOF, m/z): [M]$^+$ calcd for $C_{56}H_{77}NO_2Si$, 823.5724; Found, 823.5968. FT-IR (ATR, cm^{-1}): 2920 (s), 2850 (s), 2192 (m) 1682 (m), 1600 (m), 1491 (s), 1463 (m), 1388 (w), 1294 (m), 1239 (m), 1175 (s), 1131 (m), 1001 (m), 888 (w), 810 (m), 721 (s), 635 (m), 538 (m).

***Synthesis of compound D_4*-alkyne**. To the solution of **D_4-d** (425 mg, 0.52 mmol) in THF (10 mL) was added TBAF (1 M, 1.3 mL) at room temperature. After the mixture was stirred for 0.5 h at room temperature, the solution was poured into water and extracted with DCM (50 mL × 3). The combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained crude product of **D_4-alkyne** (383 mg) was used for the next reaction without further purification.



Scheme S2. Reaction conditions: i) n-BuLi, trimethylborate, THF, -78 ^{o}C; then, 4-bromo-7-(4,4-dihexyl-4H-cyclopenta[2,1-b:3,4-b']dithiophen-2-yl)benzo[c][1,2,5]thiadiazole, Sphos, K_3PO_4, $Pd_2(dba)_3$, THF, reflux; ii) NBS, THF, rt; iii) Methyl 4-boronobenzoate acid, Sphos, K_3PO_4, $Pd_2(dba)_3$, THF, reflux; iv) LiOH·H$_2$O, THF, H_2O, reflux; v) bis(pinacolato)diboron, $Pd(PPh_3)_2Cl_2$, KOAc, 1,4-dioxane, 80 ^{o}C; vi) Trimethylsilylacetylene, CuI, PPh_3, $Pd_2(PPh_3)_2Cl_2$, Piperdine, refulx; vii) TBAF, THF, rt.

Synthesis of compound O-a. To the solution of **D$_4$-Br** (650 mg, 0.81 mmol) in dry THF (10 mL) was added n-BuLi (2.4 M in THF, 0.4 mL) dropwise at -78°C under nitrogen atmosphere. Stirring was continued at -78°C for 1 h and subsequently a solution of trimethylborate (0.15 mL, 1.27 mmol) was added dropwise. The reaction mixture was stirred at -78°C for 3 h followed by the addition of 4-bromo-7-(4,4-dihexyl-4H-cyclopenta[2,1-b:3,4-b']dithiophen-2-yl)benzo[c][1,2,5]thiadiazole[7] (375 mg, 0.67 mmol), Sphos (55.0 mg, 0.13 mmol), K_3PO_4 (426 mg, 2.01 mmol) and $Pd_2(dba)_3$ (36.8 mg, 0.04 mmol), and then stirred at 80°C for 10 h under nitrogen atmosphere. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (5/1, v/v) used as the eluent to give a purplish red solid of **O-a** (573 mg, yield 59%). ^{1}H NMR (600 MHz, CD_2Cl_2, ppm) δ 7.98 (s, 1H), 7.80 (d, J = 7.6 Hz, 1H), 7.74 (dd, J = 10.9, 2.6 Hz, 2H), 7.59 – 7.55 (m, 2H), 7.48 (dd, J = 7.8, 5.3 Hz, 2H), 7.23 – 7.18 (m, 2H), 7.18 – 7.16 (m, 1H), 7.15 (dd, J = 9.1, 2.9 Hz, 1H), 7.11 (td, J = 7.4, 1.0 Hz, 1H), 7.07 (dd, J = 8.4, 3.2 Hz, 2H), 6.91 (d, J = 4.8 Hz, 1H), 6.38 (d, J = 2.2 Hz, 1H), 6.21 (dd, J = 8.5, 2.3 Hz, 1H), 5.73 (dd, J = 9.2, 6.6 Hz, 1H), 3.95 (t, J = 6.3 Hz, 2H), 3.75 (t, J = 6.7 Hz, 2H), 3.66 (dd, J = 15.7, 9.6 Hz, 1H), 2.97 (dd, J = 15.5, 6.0 Hz, 1H), 1.88 – 1.79 (m, 8H), 1.80 – 1.67 (m, 6H), 1.66 – 1.54 (m, 3H), 1.33 – 1.24 (m, 7H), 1.23 – 1.14 (m, 6H), 1.13 – 0.96 (m, 24H), 0.93 – 0.86 (m, 7H), 0.84 – 0.76 (m, 7H), 0.69 (m, 14H), 0.62 – 0.47 (m, 2H), 0.38 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 158.41, 157.87, 157.59, 155.96, 153.15, 151.88, 151.65, 150.56, 149.33, 147.35, 141.18, 140.10, 138.59, 137.09, 135.65, 133.90, 131.24, 129.64, 129.64, 127.59, 127.11, 126.60, 125.55, 124.82, 124.47, 123.51, 121.66, 120.65, 118.98, 117.78, 117.28, 112.85, 112.51, 107.24, 103.49, 98.56, 66.93, 60.94, 53.86, 52.73, 39.45, 36.96, 31.08, 30.12, 29.08, 28.54, 28.51, 27.77, 24.84, 23.55, 22.68, 21.59, 13.03. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{78}H_{99}N_3O_2S_3$, 1205.6899; Found, 1205.6892. FT-IR (ATR, cm^{-1}): 2964 (m), 2922 (s), 2852 (m), 1607 (m), 1493 (m), 1458 (s), 1376 (m), 1259 (m), 1180 (m), 1081 (m), 1020 (m), 798 (s), 737 (m), 659 (w), 491 (w). mp 128–129°C.

Synthesis of compound O-Br. To the solution of **O-a** (530 mg, 0.44 mmol) in DCM (10 mL) was added an DCM solution (5 mL) of NBS (70.4 mg, 0.40 mmol) dropwise at 0°C. After the mixture was stirred for 1 h at room temperature, the solution was poured into water and extracted with DCM (50 mL × 3). The combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (9/1, v/v) used as the eluent to give a yellow oil of **O-Br** (474 mg, yield 84%). ^{1}H NMR (600 MHz, CD_2Cl_2, ppm) δ 7.95 (s, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.75 – 7.69 (m, 2H), 7.61 – 7.54 (m, 2H), 7.52 – 7.44 (m, 2H), 7.20 (t, J = 7.7 Hz, 1H), 7.18 – 7.14 (m, 2H), 7.12 (d, J = 7.3 Hz, 1H), 7.09 – 7.04 (m, 2H), 6.93 (d, J = 1.0 Hz, 1H), 6.38 (s, 1H), 6.20 (d, J = 8.5 Hz, 1H), 5.72 (d, J = 6.8 Hz, 1H), 3.94 (t, J = 6.1 Hz, 2H), 3.75 (t, J = 6.6 Hz, 2H), 3.66 (dd, J = 15.5, 9.7 Hz, 1H), 2.97 (dd, J = 15.0, 4.8 Hz, 1H), 1.86 – 1.73 (m, 11H), 1.63 – 1.54 (m, 2H), 1.45 (s, 3H), 1.29 (m, 7H), 1.19 (m, 6H), 1.13 – 0.96 (m, 22H), 0.91 (m, 9H), 0.79 (m, 7H), 0.74 – 0.61 (m, 13H), 0.62 – 0.45 (m, 2H), 0.37 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 159.44, 157.98, 157.05, 154.14, 152.90, 152.62, 151.58, 150.35, 148.44, 142.14, 141.11, 140.17, 137.50, 137.09, 134.96, 132.39, 130.68, 128.64, 128.04, 127.62, 126.54, 126.14, 125.40, 124.72, 122.67, 121.34, 120.00, 118.81, 118.33, 113.72, 111.49, 108.25, 104.51, 99.58, 67.95, 61.97, 54.76, 40.47, 37.93, 32.10, 31.24, 30.10, 29.66, 29.54, 29.14, 27.20, 25.87, 24.54, 23.61, 22.75, 22.17, 14.06. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{78}H_{98}BrN_3O_2S_3$, 1283.6005; Found, 1283.5254. FT-IR (ATR, cm^{-1}): 2924 (s), 2850 (s), 2190 (m), 1606 (m), 1467 (s), 1385 (m), 1291 (m), 1178 (s), 1130 (m), 1023 (m), 881 (w), 812 (m), 723 (m), 638 (m), 515 (w), 437 (m). mp 113–114°C.

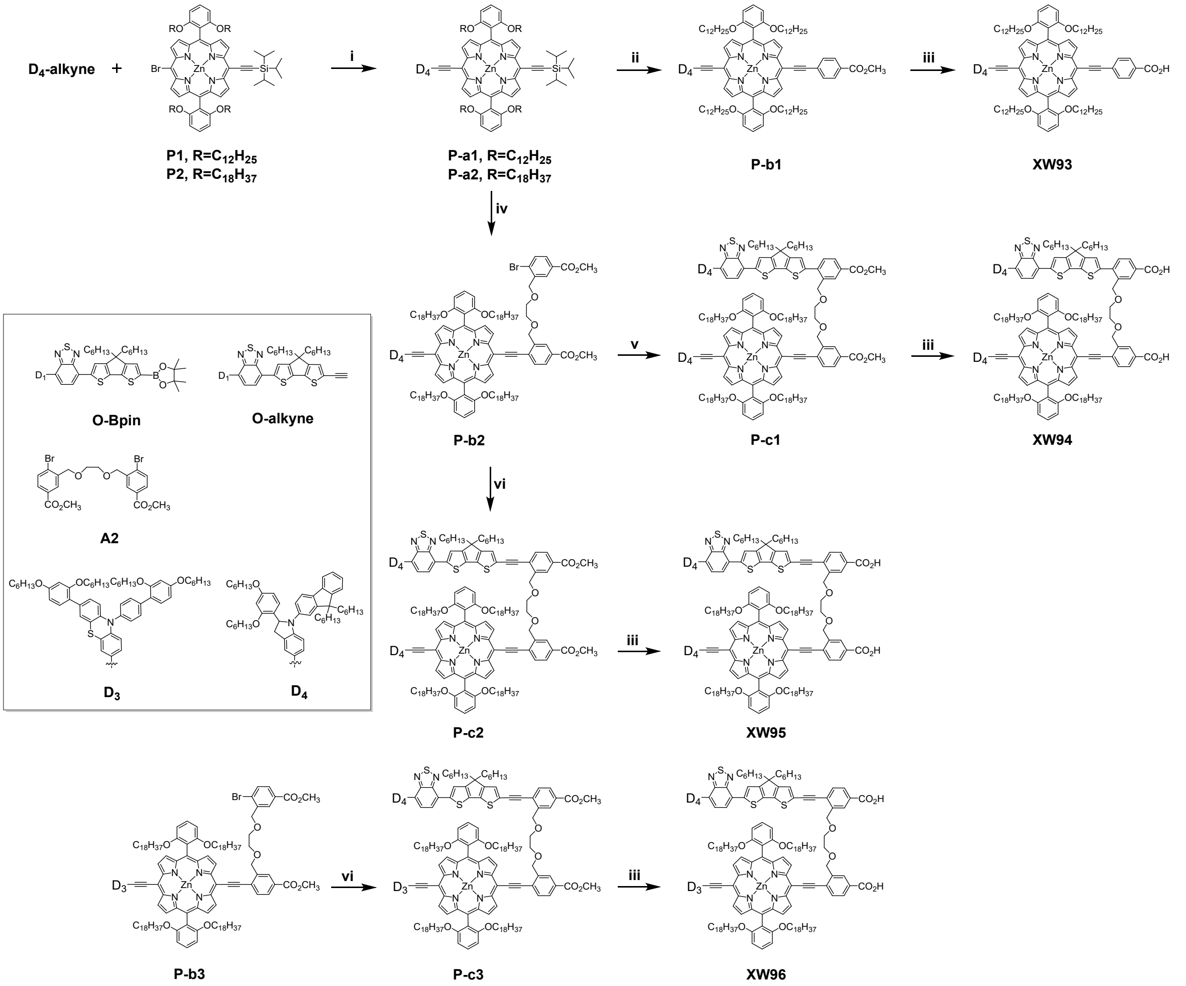
Synthesis of compound O-b. The mixture of **O-Br** (115 mg, 0.09 mmol) and 4-methoxyphenylboronic acid (64.1 mg, 0.36 mmol), K_3PO_4 (56.9 mg, 0.27 mmol), Sphos (3.7 mg, 0.01 mmol) and $Pd_2(dba)_3$ (4.5 mg, 0.01 mmol) in THF (10 mL) was stirred at 80°C for 6 h under nitrogen atmosphere. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (2/1, v/v) used as the eluent to give a dark purple solid of **O-b** (51.6 mg, yield 43%). ^{1}H NMR (600 MHz, CD_2Cl_2, ppm) δ 7.99 (s, 1H), 7.91 (d, *J* = 8.5 Hz, 2H), 7.82 (d, *J* = 7.5 Hz, 1H), 7.77 – 7.71 (m, 2H), 7.59 (t, *J* = 7.5 Hz, 3H), 7.52 – 7.47 (m, 2H), 7.30 (s, 1H), 7.24 – 7.18 (m, 2H), 7.17 (dd, *J* = 5.5, 1.6 Hz, 2H), 7.12 (td, *J* = 7.4, 0.9 Hz, 1H), 7.09 – 7.05 (m, 2H), 6.38 (d, *J* = 2.2 Hz, 1H), 6.21 (dd, *J* = 8.5, 2.2 Hz, 1H), 5.76 – 5.70 (m, 1H), 3.95 (t, *J* = 6.3 Hz, 2H), 3.79 (s, 3H), 3.75 (t, *J* = 6.7 Hz, 2H), 3.66 (dd, *J* = 15.8, 9.7 Hz, 1H), 2.98 (dd, *J* = 15.2, 5.4 Hz, 1H), 1.93 – 1.86 (m, 5H), 1.86 – 1.79 (m, 3H), 1.76 (m, 3H), 1.64 – 1.58 (m, 2H), 1.46 (s, 3H), 1.33 – 1.24 (m, 8H), 1.23 – 1.15 (m, 8H), 1.14 – 1.03 (m, 17H), 1.01 (m, 11H), 0.91 (m, 5H), 0.85 – 0.77 (m, 7H), 0.73 – 0.67 (m, 14H), 0.56 (m, 2H), 0.37 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 166.77, 160.00, 159.05, 157.02, 154.20, 152.69, 151.61, 150.39, 148.49, 143.43, 142.17, 141.06, 139.51, 137.97, 135.00, 132.59, 130.72, 130.34, 128.69, 128.10, 126.57, 126.15, 125.48, 124.69, 122.69, 121.45, 120.02, 118.96, 118.37, 113.60, 108.29, 104.54, 99.61, 67.98, 54.92, 54.28, 53.42, 52.07, 41.36, 40.50, 38.04, 36.08, 34.60, 31.55, 30.35, 29.65, 29.28, 27.68, 26.92, 26.45, 25.62, 25.29, 24.64, 23.72, 22.61, 20.58, 19.44, 18.77, 14.71, 13.67, 11.44. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{86}H_{105}N_3O_4S_3$, 1339.7267; Found, 1339.5566. FT-IR (ATR, cm^{-1}): 2925 (s), 2850 (s), 2197 (m) 1607 (m), 1579 (m), 1460 (s), 1385 (m), 1290 (m), 1247 (m), 1171 (m), 1133 (m), 1013 (m), 1002 (m), 882 (w), 831 (s), 793 (m), 725 (m), 635 (w), 576 (m), 442 (m). mp 117–118°C.

Synthesis of compound O-c. The mixture of **O-Br** (156 mg, 0.12 mmol), Pd $(PPh_3)_2Cl_2$ (5.3 mg, 0.01 mmol), CuI (1.0 mg, 0.01 mmol) and PPh_3 (4.8 mg, 0.02 mmol) in THF/Et_3N (10/10 mL) was stirred at 80°C under nitrogen atmosphere, and then TMSA (0.1 mL, 0.71 mmol) was added *via* a syringe over 10 min. After the mixture was stirred at 80°C for 8 h and cooled to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (5/1, v/v) used as the eluent to give a dark purple solid of **O-c** (118 mg, yield 75%). ^{1}H NMR (600 MHz, CD_2Cl_2, ppm) δ 7.97 (d, *J* = 12.9 Hz, 1H), 7.81 (dd, *J* = 7.5, 5.3 Hz, 1H), 7.77 – 7.72 (m, 2H), 7.58 (dd, *J* = 7.6, 2.1 Hz, 1H), 7.53 – 7.45 (m, 2H), 7.23 – 7.15 (m, 4H), 7.12 (ddd, *J* = 9.1, 8.1, 2.8 Hz, 1H), 7.09 – 7.03 (m, 2H), 6.38 (d, *J* = 1.6 Hz, 1H), 6.21 (dd, *J* = 8.6, 1.9 Hz, 1H), 5.72 (dd, *J* = 9.1, 6.7 Hz, 1H), 3.94 (t, *J* = 6.2 Hz, 2H), 3.75 (t, *J* = 6.6 Hz, 2H), 3.66 (dd, *J* = 15.6, 9.6 Hz, 1H), 2.97 (dd, *J* = 15.5, 5.9 Hz, 1H), 1.88 – 1.69 (m, 10H), 1.66 – 1.56 (m, 3H), 1.44 (m, 2H), 1.34 – 1.25 (m, 6H), 1.25 – 1.16 (m, 6H), 1.14 – 0.96 (m, 22H), 0.95 – 0.85 (m, 8H), 0.80 (m, 6H), 0.70 (m, 12H), 0.56 (m, 2H), 0.37 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 160.41, 159.51, 158.95, 158.67, 157.37, 157.05, 154.24, 152.73, 151.64, 150.42, 148.49, 142.22, 141.15, 139.67, 138.82, 138.18, 137.57, 136.74, 135.02, 132.72, 132.33, 130.74, 128.70, 128.15, 127.68, 127.30, 126.90, 126.40, 125.92, 125.59, 124.92, 124.61, 122.73, 121.72, 121.33, 120.05, 118.86, 118.41, 113.64, 108.32, 104.57, 99.93, 99.64, 99.11, 68.01, 62.03, 54.94, 54.17, 53.82, 40.53, 38.03, 31.97, 31.31, 30.08, 29.65, 29.63, 29.03, 26.07, 25.78, 24.60, 23.75, 23.14, 22.22, 14.11. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{83}H_{107}N_3O_2S_3Si$, 1301.7295; Found, 1301.5756. FT-IR (ATR, cm^{-1}): 2962 (m), 2922 (s), 2850 (s), 2128 (m), 2012 (m), 1603 (m), 1492 (m), 1470 (s), 1375 (m), 1246 (m), 1173 (m), 1115 (w), 1019 (m), 837 (m), 730 (m), 509 (m). mp 103–104°C.

Synthesis of compound O-Bpin. The mixture of **O-Br** (210 mg, 0.16 mmol), bis(pinacolato)diboron (124 mg, 0.49 mmol), KOAc (48.1 mg, 0.49 mmol) and $Pd(PPh_3)_2Cl_2$ (11.5 mg, 0.02 mmol) in 1,4-dioxane (10 mL) was stirred at 80°C for 4 h under nitrogen atmosphere. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was rapidly passed through a short silica gel column chromatography with PE/DCM (1/1, v/v) used as the eluent to give the crude product **O-Bpin** (128 mg), which was used for the next reaction without further purification.

***Synthesis of compound O-*alkyne**. To the solution of **O-c** (109 mg, 0.08 mmol) in THF (10 mL) was added TBAF (1 M, 0.2 mL) at room temperature. After the mixture was stirred for 0.5 h at room temperature, the solution was poured into water and extracted with DCM (50 mL × 3). The combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained crude product of **O-alkyne** (95.1 mg) was used for the next reaction without further purification.

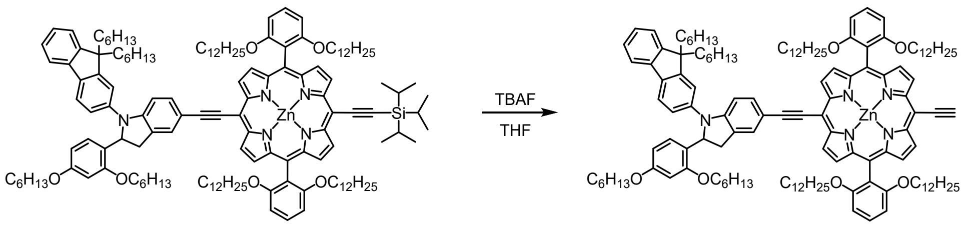
Synthesis of compound Y3. The intermediate **O-b** was hydrolyzed by $LiOH\cdot H_2O$ under nitrogen atmosphere to give **Y3** (refer to experimental section of the main text for more details).



Scheme S3. Reaction conditions: i) $Pd_2(dba)_3$, $AsPh_3$, $^tBu_3P$ HBF_4, THF/Et_3N, reflux; ii) TBAF, THF, rt; then, methyl 4-iodobenzoate, $Pd_2(dba)_3$, $AsPh_3$, $^tBu_3P$ HBF_4, THF/Et_3N, reflux; iii) $LiOH{\cdot}H_2O$, THF/H_2O, reflux. iv) TBAF, THF, rt; then, **A2**, $Pd_2(dba)_3$, $AsPh_3$, $^tBu_3P{\cdot}HBF_4$, THF/Et_3N, reflux; v) **O-Bpin**, $Pd_2(dba)_3$, Sphos, K_3PO_4, THF/Et_3N, reflux; vi) **O-alkyne**, $Pd_2(dba)_3$, $AsPh_3$, $^tBu_3P{\cdot}HBF_4$, THF/Et_3N.

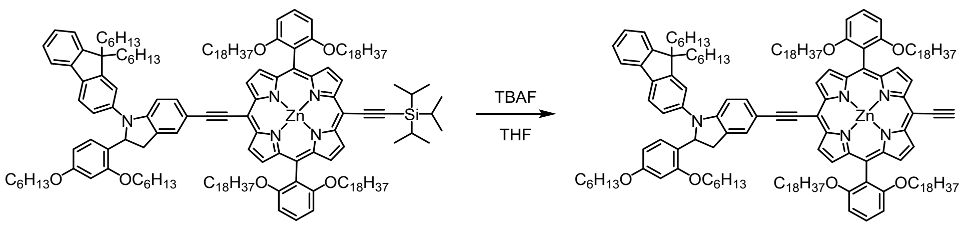
Synthesis of compound P-a1. The mixture of **D$_4$-alkyne** (346 mg, 0.46 mmol), porphyrin derivative **P1**[8] (558 mg, 0.37 mmol), $AsPh_3$ (226 mg, 0.74 mmol), $^tBu_3P{\cdot}HBF_4$ (13.5 mg, 0.05 mmol) and $Pd_2(dba)_3$ (25.8 mg, 0.03 mmol) in THF/Et_3N (10/10 mL) was stirred at 80°C for 12 h under nitrogen. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/DCM (3/1, v/v) used as the eluent to give a green tar of **P-a1** (425 mg, yield 53%). ^1H NMR (400 MHz, CD_2Cl_2, ppm) δ 9.61 (d, $J = 4.6$ Hz, 2H), 9.55 (d, $J = 4.6$ Hz, 2H), 8.73 (dd, $J = 8.7$, 4.6 Hz, 4H), 7.78 – 7.67 (m, 2H), 7.61 (t, $J = 8.4$ Hz, 2H), 7.52 (d, $J = 8.2$ Hz, 2H), 7.25 – 7.17 (m, 4H), 7.13 (ddd, $J = 8.6$, 4.5, 1.8 Hz, 3H), 6.93 (t, $J = 7.6$ Hz, 4H), 6.38 (d, $J = 2.2$ Hz, 1H), 6.24 (dd, $J = 8.5$, 2.2 Hz, 1H), 5.85 – 5.73 (m, 1H), 3.96 (t, *J* = 6.3 Hz, 2H), 3.76 (dd, *J* = 11.2, 6.0 Hz, 10H), 3.73 – 3.62 (m, 1H), 3.14 – 2.92 (m, 1H), 1.81 (m, 6H), 1.65 – 1.56 (m, 2H), 1.47 (m, 3H), 1.40 – 1.27 (m, 25H), 1.24 – 1.15 (m, 8H), 1.14 – 1.04 (m, 10H), 1.04 – 0.90 (m, 25H), 0.89 – 0.77 (m, 21H), 0.77 – 0.67 (m, 30H), 0.62 – 0.50 (m, 11H), 0.40 (m, 18H), 0.34 – 0.21 (m, 9H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 161.18, 160.02, 159.60, 157.16, 152.35, 151.59, 150.50, 148.52, 142.00, 141.18, 135.34, 132.02, 131.59, 130.67, 129.79, 128.27, 126.74, 126.08, 122.71, 121.18, 120.11, 118.85, 115.18, 114.21, 108.18, 105.40, 104.64, 102.34, 99.76, 97.57, 96.46, 91.26, 68.80, 68.06, 54.99, 53.43, 40.58, 37.96, 32.32, 31.21, 30.26, 28.27, 26.15, 25.81, 25.30, 23.80, 23.25, 22.32, 19.13, 14.15, 11.91. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{144}H_{203}N_5O_6SiZn$, 2190.4794; Found, 2190.5146. FT-IR (ATR, cm^{-1}): 2920 (s), 2850 (s), 2184 (m), 2135 (w), 1719 (m), 1585 (m), 1489 (m), 1453 (s), 1377 (m), 1339 (w), 1245 (m), 1206 (m), 1174 (w), 1097 (s), 997 (s), 880 (w), 791 (m), 736 (m), 710 (m), 653 (m), 571 (m). mp 132–134°C.

Synthesis of compound P-a2. The synthetic procedure resembles that for synthesizing compound **P-a1** except using the porphyrin derivative **P2**[8] (763 mg, 0.41 mmol) instead of the porphyrin derivative **P1**. A green tar of **P-a2** was obtained (632 mg, 61%). ^{1}H NMR (600 MHz, CD_2Cl_2, ppm) δ 9.53 (dd, *J* = 34.2, 4.3 Hz, 4H), 8.68 (dd, *J* = 12.3, 4.3 Hz, 4H), 7.78 – 7.67 (m, 1H), 7.60 (t, *J* = 8.6 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.17 (m, 2H), 7.16 – 7.07 (m, 4H), 6.91 (d, *J* = 8.7 Hz, 3H), 6.39 (d, *J* = 2.1 Hz, 4H), 6.24 (dd, *J* = 8.6, 2.2 Hz, 1H), 5.80 (t, *J* = 8.1 Hz, 1H), 3.97 (t, *J* = 6.2 Hz, 1H), 3.76 (dd, *J* = 15.2, 7.9 Hz, 2H), 3.69 (d, *J* = 9.7 Hz, 10H), 3.17 – 2.93 (m, 1H), 1.96 – 1.69 (m, 7H), 1.62 (m, 2H), 1.49 (s, 2H), 1.47 – 1.28 (m, 32H), 1.26 – 0.98 (m, 85H), 0.92 – 0.68 (m, 28H), 0.59 (m, 34H), 0.54 – 0.32 (m, 24H), 0.29 (s, 10H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 158.93, 158.51, 156.06, 151.23, 150.47, 149.39, 147.39, 140.91, 140.09, 134.23, 130.85, 130.45, 129.55, 128.66, 127.16, 125.64, 124.97, 121.63, 120.16, 119.01, 117.74, 113.97, 113.13, 109.16, 107.09, 104.30, 103.53, 101.07, 98.62, 96.36, 95.20, 90.27, 67.72, 66.97, 63.68, 53.89, 39.48, 36.87, 31.39, 29.86, 29.11, 27.18, 25.05, 24.72, 24.19, 22.71, 22.52 , 21.12, 18.05, 13.36, 12.57, 10.93. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{168}H_{251}N_5O_6SiZn$, 2526.8550; Found, 2526.7678. FT-IR (ATR, cm^{-1}): 2919 (s), 2849 (s), 2185 (w), 2136 (w), 1585 (m), 1489 (m), 1453 (s), 1377 (m), 1338 (w), 1294 (m), 1246 (m), 1208 (m), 1176 (m), 1097 (s), 1060 (m), 997 (s), 880 (m), 792 (m), 769 (m), 736 (s), 655 (m), 571 (m). mp 143–144°C.



P-a1 **P-a1'**

Synthesis of compound P-a1′. To the solution of **P-a1** (396 mg, 0.18 mmol) in THF (20 mL) was added TBAF (1 M, 0.5 mL) at room temperature. After the mixture was stirred for 0.5 h at room temperature, the solution was poured into water and extracted with DCM (50 mL × 3). The combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained crude product of **P-a1′**(351 mg) was used for the next reaction without further purification.



P-a2 **P-a2'**

Synthesis of compound P-a2′. The synthetic procedure resembles that for synthesizing compound **P-a1′**except using **P-a2** (576 mg, 0.23 mmol) instead of **P-a1**. The obtained crude product of **P-a2′**(513 mg) was used for the next reaction without further purification.

Synthesis of compound P-b1. The mixture of **P-a1′** (195 mg, 0.10 mmol), methyl 4-iodobenzoate (75.2 mg, 0.29 mmol), $AsPh_3$ (57.2 mg, 0.19 mmol) and $Pd_2(dba)_3$ (17.5 mg, 0.02 mmol) in THF/Et_3N (10/10 mL) was stirred at 80°C for 8 h under nitrogen. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/EA (5/1, v/v) used as the eluent to give a green solid of **P-b1** (139 mg, yield 67%). ^1H NMR (400 MHz, CD_2Cl_2, ppm) δ 9.70 (dd, J = 27.2, 4.5 Hz, 4H), 8.92 (dd, J = 11.5, 4.5 Hz, 4H), 8.08 (d, J = 8.2 Hz, 2H), 7.95 (d, J = 8.0 Hz, 2H), 7.81 (dd, J = 15.6, 7.2 Hz, 4H), 7.68 (d, J = 8.0 Hz, 2H), 7.46 – 7.24 (m, 7H), 7.11 (d, J = 8.5 Hz, 4H), 6.55 (d, J = 2.1 Hz, 1H), 6.40 (dd, J = 8.5, 2.2 Hz, 1H), 5.96 (s, 1H), 4.12 (t, J = 6.3 Hz, 2H), 4.04 – 3.89 (m, 13H), 3.84 (d, J = 6.0 Hz, 1H), 3.21 (dd, J = 15.4, 6.2 Hz, 1H), 2.08 – 1.85 (m, 6H), 1.87 – 1.70 (m, 2H), 1.64 (s, 2H), 1.46 (m, 8H), 1.36 (m, 13H), 1.31 – 0.78 (m, 48H), 0.81 – 0.66 (m, 34H), 0.66 – 0.52 (m, 31H), 0.50 – 0.32 (m, 9H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 167.75, 166.43, 159.95, 159.54, 157.10, 152.18, 151.18, 151.01, 149.75, 148.48, 141.88, 141.11, 135.30, 132.06, 131.54, 131.22, 130.15, 129.81, 129.41, 129.01, 128.55, 126.68, 126.02, 122.64, 120.93, 120.04, 118.81, 115.43, 114.07, 108.06, 105.22, 104.58, 102.71, 99.63, 98.62, 97.74, 96.68, 94.58, 91.19, 68.68, 68.50, 67.31, 54.93, 52.13, 40.52, 38.73, 37.85, 32.63, 31.29, 30.36, 30.07, 28.22, 26.08, 25.74, 25.25, 24.27, 23.45, 23.33, 22.15, 17.79, 14.99, 13.01, 10.97. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{143}H_{189}N_5O_8Zn$, 2168.3828; Found, 2168.4202. FT-IR (ATR, cm^{-1}): 2918 (s), 2852 (s), 2191 (w), 1720 (m), 1602 (m), 1578 (m), 1491 (m), 1464 (s), 1384 (m), 1269 (m), 1179 (s), 1130 (m), 1105 (w), 1017 (m), 882 (w), 767 (m), 698 (m), 577 (m), 516 (m). mp 159–160°C.

Synthesis of compound P-b2. The mixture of **P-a2′**(284 mg, 0.12 mmol), **A2**[9] (185 mg, 0.36 mmol), $AsPh_3$ (78.8 mg, 0.26 mmol), $^tBu_3P{\cdot}HBF_4$ (8.9 mg, 0.03 mmol) and $Pd_2(dba)_3$ (21.8 mg, 0.02 mmol) in THF/Et_3N (10/10 mL) was stirred at 80°C for 12 h under nitrogen atmosphere. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/EA (5/1, v/v) used as the eluent to give a green solid of **P-b2** (164 mg, yield 49%). ^1H NMR (600 MHz, CD_2Cl_2, ppm) δ 9.46 (dd, J = 14.3, 4.4 Hz, 4H), 8.62 (dd, J = 14.0, 4.4 Hz, 4H), 8.17 (s, 1H), 7.99 – 7.85 (m, 2H), 7.70 (s, 1H), 7.63 (d, J = 7.3 Hz, 1H), 7.60 (s, 1H), 7.54 (dd, J = 11.5, 5.7 Hz, 2H), 7.44 (d, J = 8.0 Hz, 2H), 7.29 (dt, J = 14.1, 5.0 Hz, 2H), 7.19 – 7.10 (m, 4H), 7.10 – 7.01 (m, 3H), 6.85 (t, J = 7.3 Hz, 4H), 6.31 (d, J = 2.2 Hz, 1H), 6.16 (dd, J = 8.6, 2.2 Hz, 1H), 5.72 (t, J = 7.9 Hz, 1H), 5.22 (s, 2H), 4.49 (s, 2H), 3.94 – 3.80 (m, 4H), 3.81 – 3.73 (m, 3H), 3.68 (dd, J = 17.0, 11.0 Hz, 12H), 3.65 – 3.54 (m, 1H), 3.34 (d, J = 11.0 Hz, 3H), 2.99 (d, J = 8.6 Hz, 1H), 1.84 – 1.74 (m, 7H), 1.73 – 1.64 (m, 2H), 1.62 – 1.48 (m, 3H), 1.41 (s, 10H), 1.32 – 1.20 (m, 7H), 1.18 – 0.93 (m, 76H), 0.95 – 0.82 (m, 19H), 0.77 (m, 15H), 0.72 – 0.59 (m, 23H), 0.61 – 0.46 (m, 37H), 0.38 (m, 25H), 0.23 (s, 10H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 166.80, 166.06, 159.77, 157.14, 152.93, 151.07, 151.18, 150.15, 148.55, 141.93, 141.15, 140.07, 138.06, 135.35, 132.51, 132.12, 131.58, 130.81, 130.59, 129.98, 129.58, 129.36, 128.87, 128.71, 128.10, 126.72, 126.07, 122.68, 120.97, 120.09, 118.84, 115.45, 114.14, 108.14, 105.24, 104.61, 102.80, 101.56, 99.69, 98.20, 97.80, 92.54, 91.33, 72.36, 71.78, 70.42, 68.69, 68.04, 54.97, 53.44, 52.22, 51.94, 40.55, 37.92, 36.11, 35.48, 34.71, 31.98, 31.65, 30.01, 28.95, 28.72, 27.26, 26.12, 25.79, 25.24, 23.78, 23.16, 22.15, 18.80, 14.68, 13.23, 11.48. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{179}H_{250}BrN_5O_{12}Zn$, 2804.7581; Found, 2804.4983. FT-IR (ATR, cm^{-1}): 2923 (s), 2852 (s), 2182 (w), 1714 (m), 1606 (m), 1573 (m), 1492 (m), 1468 (s), 1429 (m), 1381 (m), 1295 (m), 1248 (w), 1178 (m), 1099 (m), 999 (m), 883 (w), 797 (m), 715 (m), 583 (m), 440 (m). mp 182–184°C.

Synthesis of compound P-c1. The mixture of **P-b2** (82 mg, 0.03 mmol), **O-Bpin** (54 mg, 0.04 mmol), Sphos (3.2 mg, 0.01 mmol), K_3PO_4 (13.3 mg, 0.06 mmol) and $Pd_2(dba)_3$ (7.3 mg, 0.01 mmol) in THF (15 mL) was stirred at 80°C for 10 h under nitrogen atmosphere. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/EA (5/1, v/v) used as the eluent to give a black solid of **P-c1** (72 mg, yield 63%). ^{1}H NMR (400 MHz, CD_2Cl_2, ppm) δ 9.76 (dd, *J* = 4.4, 2.6 Hz, 4H), 8.91 (dd, *J* = 11.6, 4.5 Hz, 4H), 8.45 (s, 1H), 8.18 (d, *J* = 14.4 Hz, 3H), 7.98 (d, *J* = 7.5 Hz, 1H), 7.91 (d, *J* = 8.7 Hz, 3H), 7.86 (s, 1H), 7.78 (dd, *J* = 16.1, 7.7 Hz, 3H), 7.72 – 7.62 (m, 4H), 7.55 – 7.47 (m, 3H), 7.44 (s, 1H), 7.38 (dd, *J* = 14.2, 6.8 Hz, 3H), 7.36 – 7.33 (m, 5H), 7.30 (dd, *J* = 13.5, 6.0 Hz, 4H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.5 Hz, 4H), 6.56 (dd, *J* = 4.1, 2.2 Hz, 2H), 6.39 (ddd, *J* = 12.5, 8.6, 2.1 Hz, 2H), 5.97 (t, *J* = 8.2 Hz, 1H), 5.90 (dd, *J* = 9.1, 6.7 Hz, 1H), 5.52 (s, 2H), 4.68 (s, 2H), 4.13 (dd, *J* = 12.5, 6.1 Hz, 6H), 4.05 – 3.88 (m, 17H), 3.86 (d, *J* = 9.3 Hz, 2H), 3.29 – 3.20 (m, 1H), 3.14 (d, *J* = 15.9 Hz, 4H), 2.10 – 1.97 (m, 9H), 1.96 – 1.84 (m, 7H), 1.78 (m, 5H), 1.64 (m, 5H), 1.48 (m, 4.6 Hz, 13H), 1.43 – 1.22 (m, 12H), 1.15 (m, 96H), 1.10 – 0.97 (m, 26H), 0.97 – 0.85 (m, 67H), 0.77 (m, 42H), 0.59 (s, 6H), 0.50 – 0.38 (m, 9H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 165.70, 164.82, 158.91, 158.79, 158.12, 157.89, 156.02, 153.18, 151.66, 150.58, 149.41, 147.44, 141.01, 140.55, 139.78, 139.46, 138.92, 137.13, 134.72, 133.28, 131.40, 131.12, 130.50, 129.59, 128.59, 128.54, 127.69, 127.01, 125.56, 125.23, 124.24, 123.61, 122.11, 121.67, 120.51, 119.99, 119.01, 117.65, 114.41, 112.83, 107.16, 104.21, 103.50, 102.53, 101.76, 100.64, 98.59, 97.13, 96.65, 91.51, 90.34, 70.71, 68.98, 67.64, 67.49, 66.11, 53.88, 53.22, 52.36, 51.11, 50.55, 40.00, 38.80, 36.97, 31.28, 30.03, 29.42 27.25, 25.68, 24.67, 24.22, 23.65, 22.69, 22.21, 20.88, 15.10, 12.27. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{257}H_{348}N_8O_{14}S_3Zn$, 3930.5219; Found, 3930.5105. FT-IR (ATR, cm^{-1}): 2914 (s), 2862 (s), 2198 (w), 1727 (m), 1661 (m), 1635 (m), 1608 (m), 1499 (m), 1486 (s), 1381 (m), 1300 (m), 1269 (m), 1209 (w), 1103 (m), 1000 (m), 798 (w), 737 (m), 508 (m), 432 (m). mp > 300°C.

Synthesis of compound P-c2. The mixture of **P-b2** (95 mg, 0.03 mmol), **O-alkyne** (50.9 mg, 0.04 mmol), $AsPh_3$ (30 mg, 0.10 mmol)，$^tBu_3P\cdot HBF_4$ (3.8 mg, 0.01 mmol) and $Pd_2(dba)_3$ (8.2 mg, 0.01 mmol) in THF/Et_3N (10/10 mL) was stirred at 80°C for 10 h under nitrogen atmosphere. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/EA (5/1, v/v) used as the eluent to give a black solid of **P-c2** (54.9 mg, yield 41%). ^{1}H NMR (600 MHz, CD_2Cl_2, ppm) δ 9.66 (dd, *J* = 9.1, 4.4 Hz, 4H), 8.80 (dd, *J* = 18.2, 4.4 Hz, 4H), 8.33 (s, 1H), 8.07 (s, 2H), 8.01 (s, 1H), 7.83 (d, *J* = 7.5

Hz, 4H), 7.74 (s, 1H), 7.67 (t, *J* = 8.5 Hz, 2H), 7.61 (d, *J* = 7.5 Hz, 1H), 7.59 – 7.53 (m, 5H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.30 – 7.23 (m, 7H), 7.21 – 7.16 (m, 6H), 7.16 – 7.11 (m, 2H), 6.98 (d, *J* = 8.6 Hz, 4H), 6.47 – 6.40 (m, 2H), 6.32 – 6.23 (m, 2H), 5.85 (s, 1H), 5.82 – 5.73 (m, 1H), 5.41 (s, 2H), 4.79 (d, *J* = 10.0 Hz, 2H), 4.10 – 4.05 (m, 2H), 4.01 (dd, *J* = 13.5, 6.5 Hz, 4H), 3.99 – 3.95 (m, 2H), 3.88 (s, 3H), 3.87 – 3.79 (m, 12H), 3.78 – 3.69 (m, 2H), 3.20 (d, *J* = 13.4 Hz, 3H), 3.13 (s, 1H), 3.04 (dd, *J* = 15.5, 5.7 Hz, 1H), 1.95 – 1.76 (m, 17H), 1.72 – 1.62 (m, 5H), 1.59 – 1.47 (m, 4H), 1.43 – 1.31 (m, 14H), 1.30 – 1.20 (m, 98H), 1.17 – 1.02 (m, 30H), 1.01 – 0.85 (m, 74H), 0.84 – 0.71 (m, 13H), 0.67 – 0.57 (m, 22H), 0.56 – 0.41 (m, 9H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 166.75, 165.80, 159.85, 157.86, 157.05, 154.16, 152.65, 152.22, 151.15, 151.15, 149.77, 148.51, 142.14, 141.28, 140.54, 139.37, 137.39, 135.16, 132.74, 132.21, 132.00, 131.55, 131.17, 130.73, 130.53, 130.18, 129.79, 129.09, 128.67, 128.07, 126.92, 126.67, 126.40, 126.12, 125.72, 125.51, 124.91, 122.69, 122.17, 121.38, 121.00, 120.04, 118.86, 118.37, 115.49, 114.12, 113.61, 108.18, 105.27, 104.54, 102.76, 101.50, 99.62, 98.32, 97.74, 92.60, 91.86, 91.30, 71.80, 71.21, 70.50, 68.68, 68.44, 67.69, 62.03, 54.91, 54.16, 52.15, 51.66, 41.11, 40.18, 37.97, 32.37, 31.48, 30.01, 28.95, 28.66, 26.05, 25.66, 25.25, 24.57, 23.94, 23.33, 22.65, 14.71, 13.48. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{259}H_{348}N_8O_{14}S_3Zn$, 3954.5219; Found, 3954.5754. FT-IR (ATR, cm^{-1}): 3358 (m), 2922 (s), 2852 (m), 2187 (w), 1724 (m), 1606 (m), 1493 (m), 1466 (s), 1378 (m), 1295 (m), 1260 (m), 1205 (w), 1101 (s), 996 (m), 967 (m), 812 (m), 794 (m), 738 (m), 509 (m), 435 (m). mp > 300°C.

Synthesis of compound P-c3. The mixture of **P-b3**[10] (121 mg, 0.04 mmol), **O-alkyne** (66 mg, 0.05 mmol), $AsPh_3$ (25.5 mg, 0.08 mmol)，$^tBu_3P{\cdot}HBF_4$ (3.3 mg, 0.01 mmol) and $Pd_2(dba)_3$ (12.5 mg, 0.01 mmol) in THF/Et_3N (10/10 mL) was stirred at 80°C for 10 h under nitrogen atmosphere. After cooling to room temperature, the solution was poured into water and extracted with DCM (50 mL × 3) and the combined organic phase was dried over Na_2SO_4, filtered and then concentrated under reduced pressure. The obtained residue was purified by silica gel column chromatography with PE/EA (5/1, v/v) used as the eluent to give a black solid of **P-c3** (93 mg, yield 55%). ^{1}H NMR (400 MHz, CD_2Cl_2, ppm) δ 9.58 (dd, *J* = 30.4, 4.5 Hz, 4H), 8.74 (dd, *J* = 13.0, 4.5 Hz, 4H), 8.28 (s, 1H), 8.03 (s, 2H), 7.94 (s, 1H), 7.82 – 7.70 (m, 5H), 7.66 – 7.54 (m, 4H), 7.49 (dd, *J* = 7.8, 4.3 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 4H), 7.30 (t, *J* = 8.1 Hz, 3H), 7.25 – 7.14 (m, 6H) 7.12 – 7.04 (m, 5H), 7.00 – 6.89 (m, 5H), 6.58 – 6.48 (m, 2H), 6.46 – 6.32 (m, 4H), 6.31 – 6.14 (m, 2H), 5.73 (dd, *J* = 9.3, 6.6 Hz, 1H), 5.35 (s, 2H), 4.72 (s, 2H), 4.00 (d, *J* = 5.1 Hz, 2H), 3.99 – 3.89(m, 9H), 3.88 – 3.83(m, 9H), 3.82 – 3.74 (dd, *J* = 14.9, 11.1 Hz, 11H), 3.74 – 3.63 (m, 2H), 3.08 (d, *J* = 7.3 Hz, 3H), 2.99 (dd, *J* = 24.6, 8.4 Hz, 1H), 1.92 – 1.54 (m, 23H), 1.48 – 1.28 (m, 43H), 1.28 – 0.95 (m, 131H), 0.95 – 0.63 (m, 105H), 0.56

(m, 12H), 0.39 (m, 22H), 0.36 – 0.18 (m, 10H). ^{13}C NMR (151 MHz, $CDCl_3$, ppm) δ 165.76, 164.87, 159.46, 159.17, 158.89, 158.52, 156.84, 155.97, 153.14, 151.62, 150.96, 150.02, 149.84, 148.69, 147.48, 143.31, 141.06, 140.26, 139.17, 138.66, 137.83, 136.37, 133.97, 132.12, 131.73, 130.91, 130.16, 129.80, 129.35, 129.32, 128.77, 128.06, 127.09 (s), 126.90, 126.37, 125.62, 124.85, 124.49, 123.89, 121.66, 121.18, 120.34, 119.90, 119.04, 117.66, 116.94, 114.56, 112.57, 107.25, 104.80, 103.92, 103.50, 100.43, 99.35, 98.57, 97.52, 94.50, 92.00, 90.82, 70.77, 70.16, 69.48, 67.74, 66.65, 53.88, 53.14, 52.38, 51.73, 51.34, 50.68, 39.45, 36.94, 31.35 30.31, 28.41, 27.64, 26.19, 25.27, 24.43, 24.22, 23.54, 22.68, 21.61, 13.05. MS (MALDI-TOF, m/z): $[M]^+$ calcd for $C_{262}H_{348}N_8O_{16}S_4Zn$, 4054.4838; Found, 4054.5632. FT-IR (ATR, cm^{-1}): 3359 (m), 2923 (s), 2852 (s), 1660 (m), 1606 (m), 1467 (m), 1295 (m), 1263 (s), 1180 (w), 1100 (s), 1000 (m), 897 (w), 737 (s), 705 (m), 428 (m). mp > 300°C.

Synthesis of compound XW93–XW96. The intermediates **P-b1 and P-c1–P-c3** were hydrolyzed by $LiOH·H_2O$ under nitrogen to give **XW93–XW96**, respectively (refer to experimental section of the main text for more details).

2 Absorption and Emission spectra

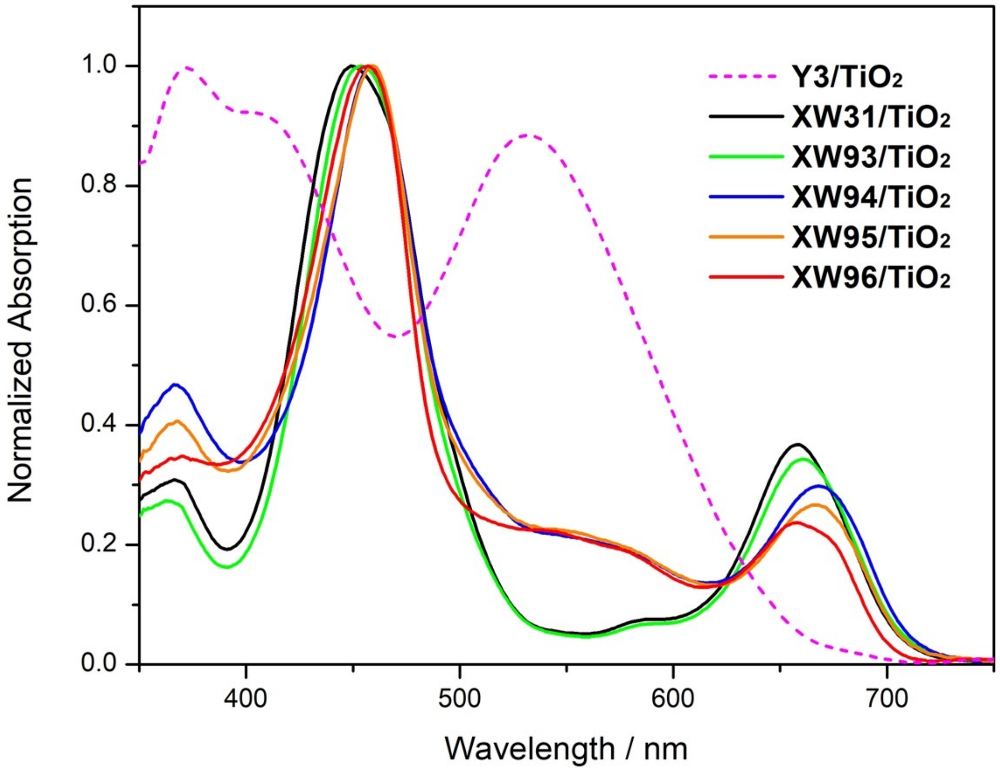


Figure S1 Normalized UV-visible spectra of sensitizers **Y3**, **XW31** and **XW93−XW96** adsorbed on TiO_2 films (2μm).

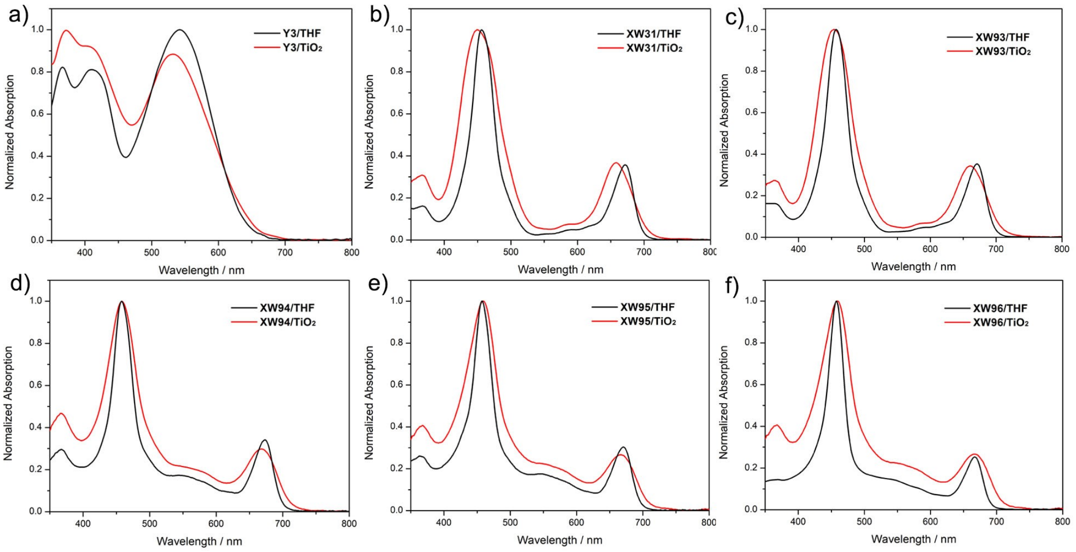


Figure S2 Normalized UV-visible spectra of sensitizers **Y3**, **XW31** and **XW93−XW96** in THF and on the TiO_2 films (2μm).

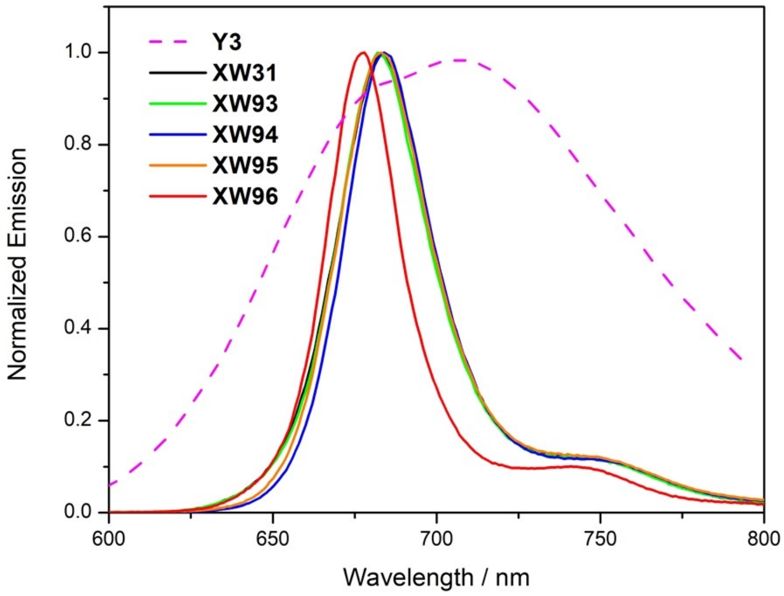


Figure S3 Fluorescence emission spectra of the dyes **Y3**, **XW31** and **XW93**–**XW96** in THF.

3 Electrochemical behavior

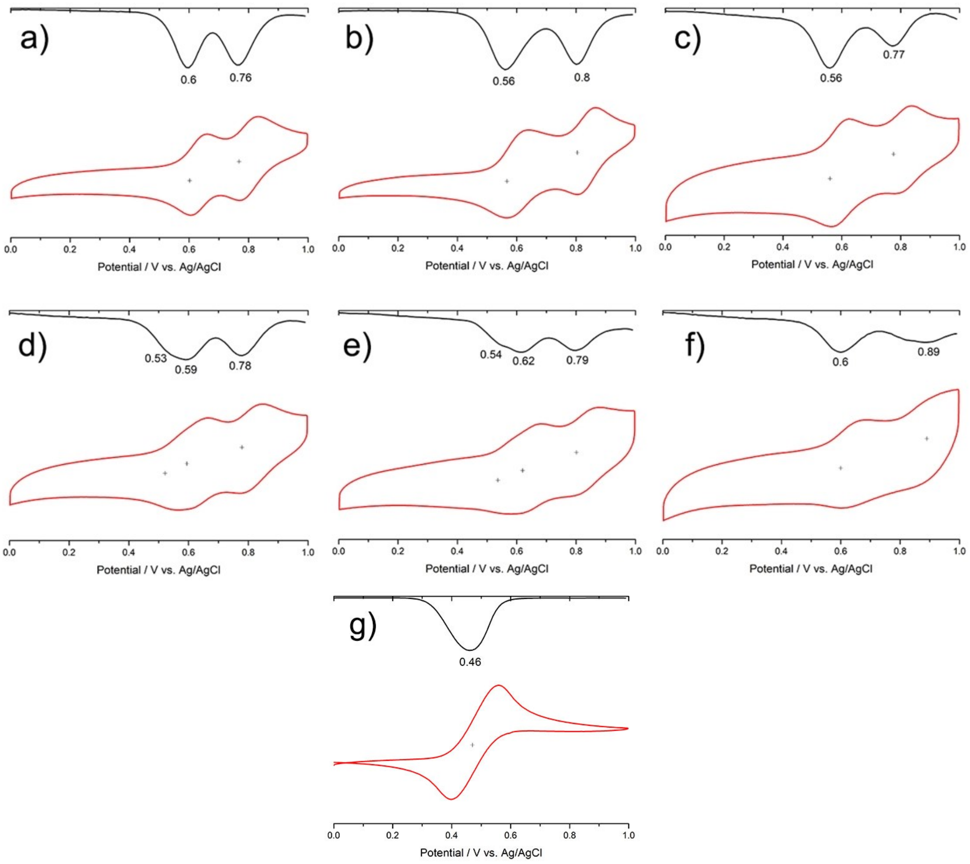


Figure S4 Cyclic voltammetry (CV) (red) and differential pulse voltammogram (DPV) (black) curves of (a) **Y3**, (b) **XW31**, (c) **XW93**, (d) **XW94**, (e) **XW95**, (f) **XW96** and g) ferrocene.

4 Theoretical calculation

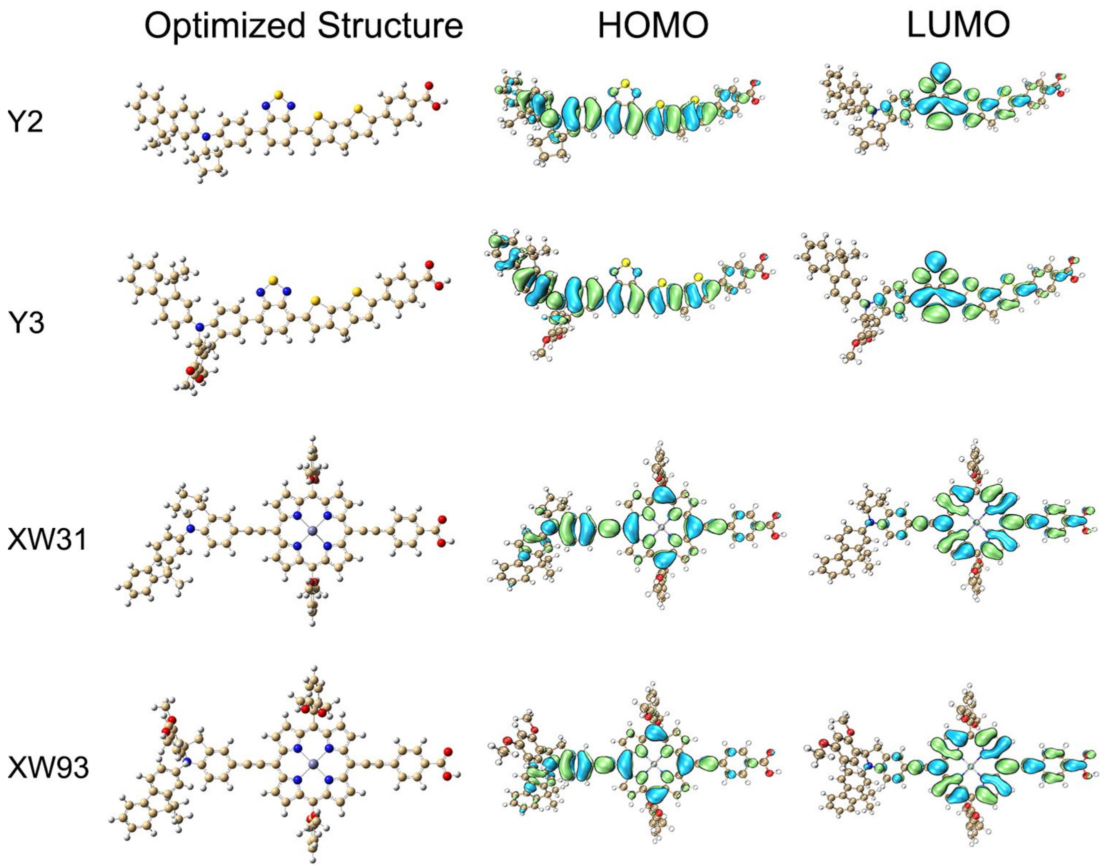


Figure S5 Optimized structures and frontier orbitals of the dyes **Y2**, **Y3**, **XW31** and **XW93**. For saving the computation time, the alkoxy chains in the molecules have been simplified to methoxy groups.

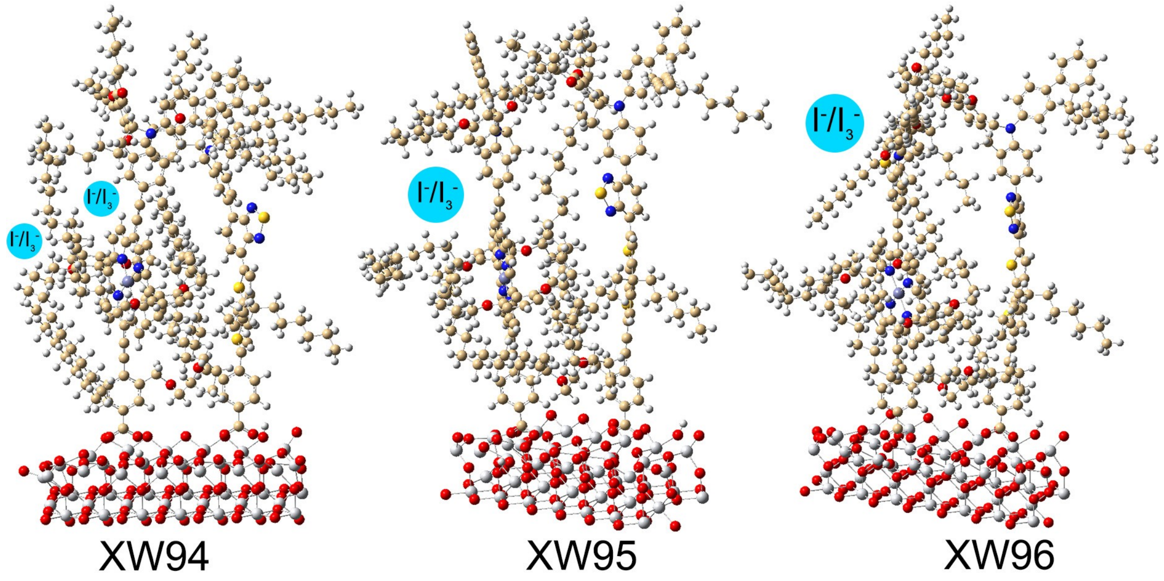


Figure S6 The optimized structures of the DCC dyes **XW94–XW96** adsorbed on TiO_2 films calculated using Gaussian 16 program package.

Table S1 Energy levels of frontier molecular orbitals for **Y2**, **Y3**, **XW31** and **XW93**.

	Y2	**Y3**	**XW31**	**XW93**
E_{LUMO+1} (eV)	-1.70	-1.70	-1.70	-1.70
E_{LUMO} (eV)	-2.48	-2.47	-2.18	-2.19
E_{HOMO} (eV)	-5.39	-5.30	-5.21	-5.21
E_{HOMO-1} (eV)	-5.89	-5.79	-5.75	-5.75
$E_{HOMO–LUMO}$ (eV)	2.91	2.83	3.03	3.02

Table S3 Photovoltaic Parameters of the DSSCs under AM1.5 Illumination [a]

Dye	Electrolyte	V_{OC} (mV)	J_{SC} (mA·cm^{-2})	$^bJ^{IPCE}$ (mA·cm^{-2})	$^cJ_{error}$ (%)	FF (%)	PCE (%)	Dye loading (10^{-7}mol cm^{-2})
Y3	I_3^-/I^-	747 ± 5	19.24 ± 0.25	16.66	13.4	70.63 ± 0.44	10.15 ± 0.21	1.77
XW31	I_3^-/I^-	718 ± 4	20.99 ± 0.29	17.68	15.8	69.58 ± 0.58	10.49 ± 0.26	1.28
XW93	I_3^-/I^-	734 ± 5	20.63 ± 0.34	17.23	16.5	70.88 ± 0.39	10.73 ± 0.19	1.19
XW94	I_3^-/I^-	750 ± 5	22.02 ± 0.04	18.86	14.3	71.72 ± 0.57	11.84 ± 0.04	1.04
XW95	I_3^-/I^-	759 ± 4	22.06 ± 0.11	19.13	13.3	72.04 ± 0.52	12.06 ± 0.14	0.99
XW96	I_3^-/I^-	782 ± 2	21.97 ± 0.18	18.60	15.3	72.52 ± 0.42	12.46 ± 0.13	0.93
XW93	$Co^{3+/2+}$	849 ± 1	14.83 ± 0.12	13.49	9.0	73.95 ± 0.29	9.31 ± 0.15	0.97

5 Photovoltaic properties

Table S2 Photovoltaic parameters of coadsorbed DSSCs based on **XW94**–**XW96** and CDCA.

Dye	Electrolyte	CDCA (mM)	V_{OC} (mV)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)	Dye loading (10^{-7} mol cm^{-2})
XW94	I_3^-/I^-	0.5	760 ± 3	21.86 ± 0.16	71.69 ± 0.42	11.91 ± 0.22	1.07
	I_3^-/I^-	1.0	762 ± 2	22.08 ± 0.19	72.72 ± 0.31	12.24 ± 0.09	0.90
	I_3^-/I^-	1.5	765 ± 2	21.62 ± 0.27	72.75 ± 0.30	12.03 ± 0.18	0.78
	$Co^{3+/2+}$	0.5	867 ± 4	16.46 ± 0.18	73.80 ± 0.13	10.53 ± 0.26	0.85
	$Co^{3+/2+}$	1.0	872 ± 2	16.50 ± 0.22	73.53 ± 0.21	10.58 ± 0.34	0.78
	$Co^{3+/2+}$	1.5	870 ± 5	16.29 ± 0.35	73.72 ± 0.17	10.45 ± 0.16	0.71
XW95	I_3^-/I^-	0.5	759 ± 2	21.81 ± 0.31	71.85 ± 0.45	11.89 ± 0.19	0.93
	I_3^-/I^-	1.0	768 ± 2	22.13 ± 0.14	71.58 ± 0.56	12.17 ± 0.17	0.87
	I_3^-/I^-	1.5	770 ± 1	21.76 ± 0.22	71.75 ± 0.38	12.02 ± 0.21	0.83
	$Co^{3+/2+}$	0.5	872 ± 3	16.72 ± 0.09	73.86 ± 0.29	10.77 ± 0.09	0.92
	$Co^{3+/2+}$	1.0	887 ± 1	16.98 ± 0.17	73.22 ± 0.23	11.03 ± 0.15	0.73
	$Co^{3+/2+}$	1.5	883 ± 4	16.33 ± 0.15	73.29 ± 0.35	10.57 ± 0.17	0.69
XW96	I_3^-/I^-	0.5	780 ± 2	21.94 ± 0.25	71.77 ± 0.28	12.28 ± 0.21	0.90
	I_3^-/I^-	1.0	784 ± 1	21.79 ± 0.27	71.92 ± 0.49	12.29 ± 0.16	0.78
	I_3^-/I^-	1.5	780 ± 1	21.63 ± 0.19	71.66 ± 0.35	12.09 ± 0.25	0.72
	$Co^{3+/2+}$	0.5	878 ± 2	16.04 ± 0.20	72.82 ± 0.35	10.26 ± 0.27	0.72
	$Co^{3+/2+}$	1.0	880 ± 5	16.48 ± 0.26	72.44 ± 0.46	10.51 ± 0.33	0.66
	$Co^{3+/2+}$	1.5	883 ± 3	15.89 ± 0.16	73.05 ± 0.30	10.25 ± 0.12	0.60

[a] The data were collected from three parallel cells (average values and errors). The TiO_2 electrode was dipped in a mixed dye solution with coadsorbent CDCA in a mixture of chloroform and ethanol (3/2, v/v).

XW94	$Co^{3+/2+}$	859 ± 3	16.14 ± 0.36	15.08	6.6	74.42 ± 0.14	10.32 ± 0.19	0.83
XW95	$Co^{3+/2+}$	867 ± 2	16.37 ± 0.32	15.36	6.2	73.69 ± 0.31	10.46 ± 0.17	0.87
XW96	$Co^{3+/2+}$	878 ± 3	15.98 ± 0.30	14.66	8.3	72.17 ± 0.47	10.13 ± 0.26	0.78

[a] The data were collected from three parallel cells (average values and errors). [b] The J^{IPCE} values were obtained by integrating the IPCE spectra. [c] The deviations between J_{SC} and J^{IPCE}.

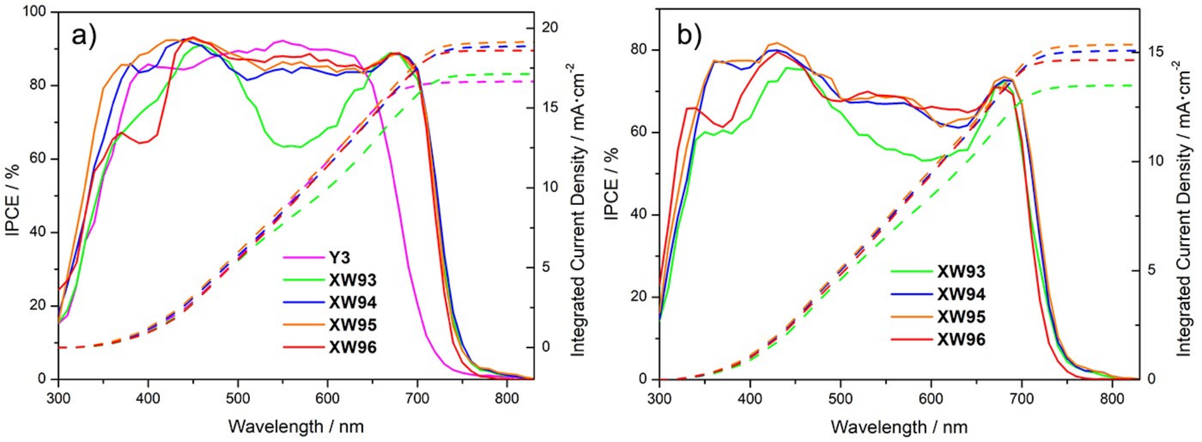


Figure S7 IPCE spectra and integral J_{SC} curves for the DSSCs based on I_3^-/I^- (a) and $Co^{3+/2+}$ (b) electrolytes, respectively.

6 Electrochemical impedance spectroscopy

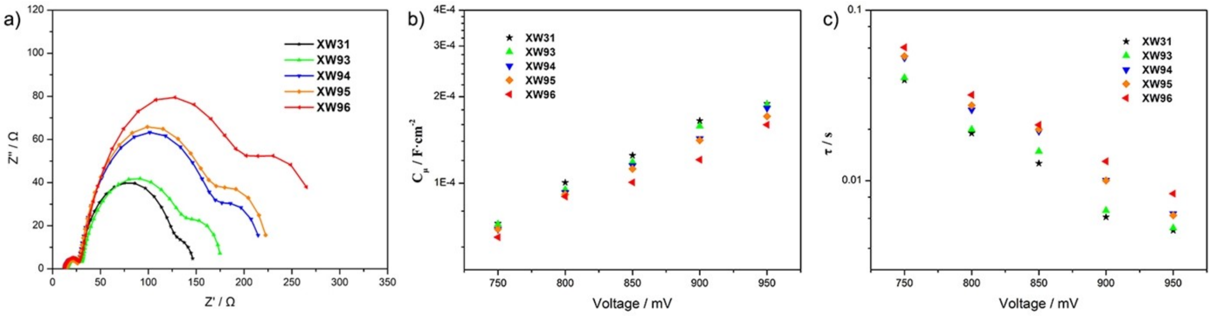


Figure S8 (a) Complex-plane plots at the bias voltage of −0.85 V, (b) plots of chemical capacitances versus bias voltages, and (c) electron lifetimes versus bias voltages for the DSSCs using the $Co^{3+/2+}$ electrolyte measured in the dark.

Table S4 Fitted EIS parameters for the DSSCs based on I_3^-/I^- and $Co^{3+/2+}$ electrolytes at the bias potentials of −0.75 V and −0.85 V, respectively. [a]

Dyes	Electrolytes	C_μ (mF cm^{-2})	R_{rec} (Ω cm^2)	R_{tr} (Ω cm^2)	τ (s)	η_{col}^{b} (%)
Y3	I_3^-/I^-	0.403	112.1	11.8	0.045	90.5
XW31	I_3^-/I^-	0.455	79.5	10.2	0.036	88.6
XW93	I_3^-/I^-	0.443	98.6	10.0	0.044	90.8
XW94	I_3^-/I^-	0.351	146.5	11.9	0.051	92.5
XW95	I_3^-/I^-	0.350	160.3	12.5	0.056	92.8
XW96	I_3^-/I^-	0.302	200.5	12.0	0.061	94.4
XW31	$Co^{3+/2+}$	0.125	105.2	10.9	0.013	90.6
XW93	$Co^{3+/2+}$	0.119	121.9	11.2	0.015	91.6
XW94	$Co^{3+/2+}$	0.115	152.9	12.7	0.018	92.3
XW95	$Co^{3+/2+}$	0.112	156.4	10.6	0.018	93.7
XW96	$Co^{3+/2+}$	0.101	193.5	10.2	0.020	95.0

a) R_{rec}: Charge recombination resistance, R_{tr}: transport resistance, η_{col}: charge collection efficiency; b) $\eta_{col} = (1 + R_{tr} / R_{rec})^{-1}$.

7 Characterization spectra for the compounds

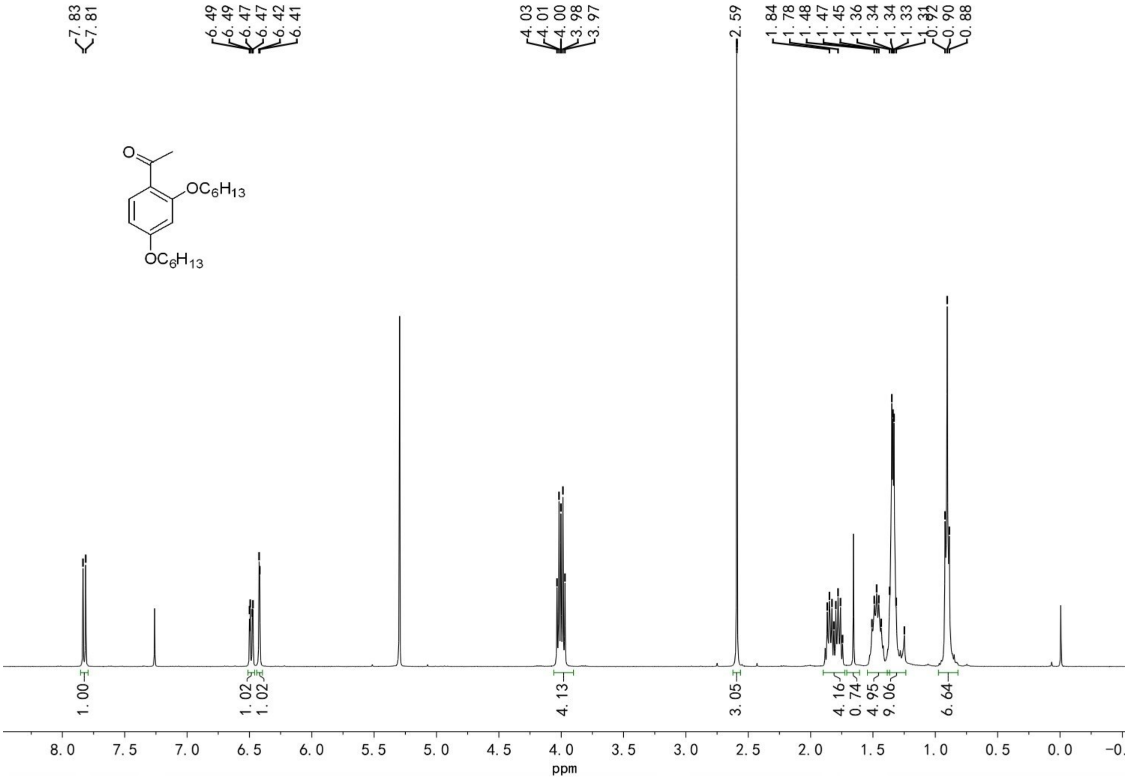


Figure S9 The ^{1}H NMR spectrum of compound 2,4-dihexyloxyacetophenone in $CDCl_3$.

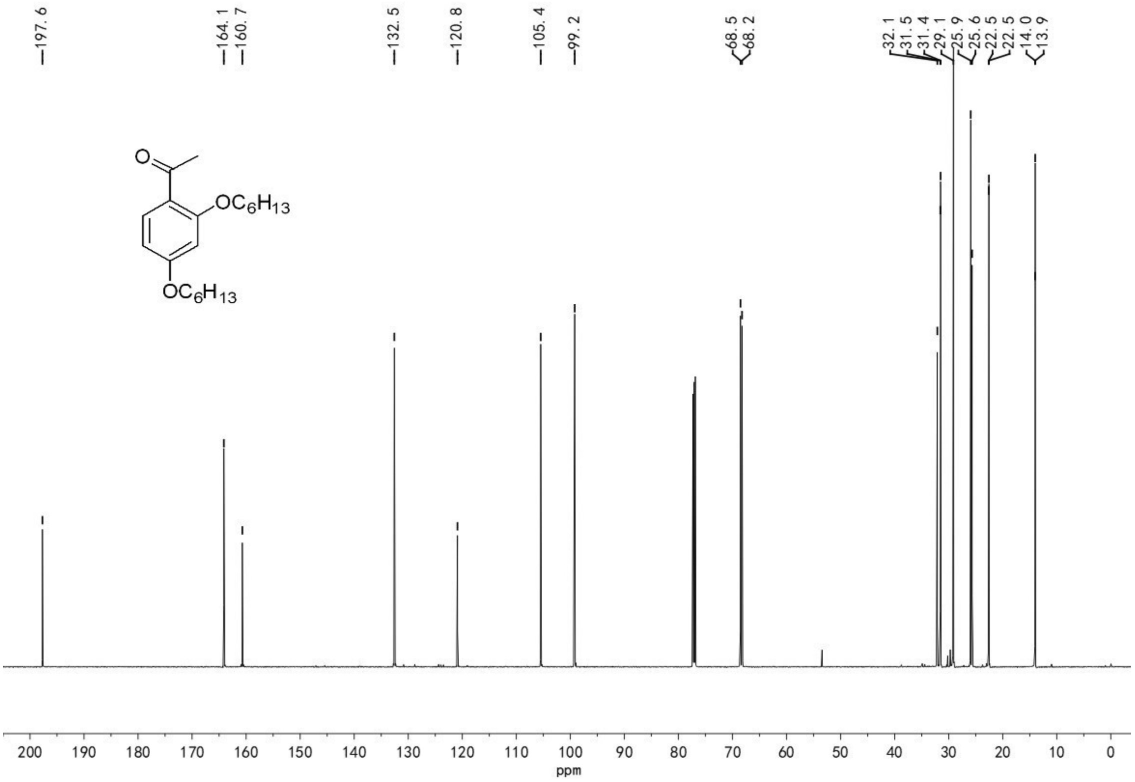


Figure S10 The ^{13}C NMR spectrum of compound 2,4-dihexyloxyacetophenone in $CDCl_3$.

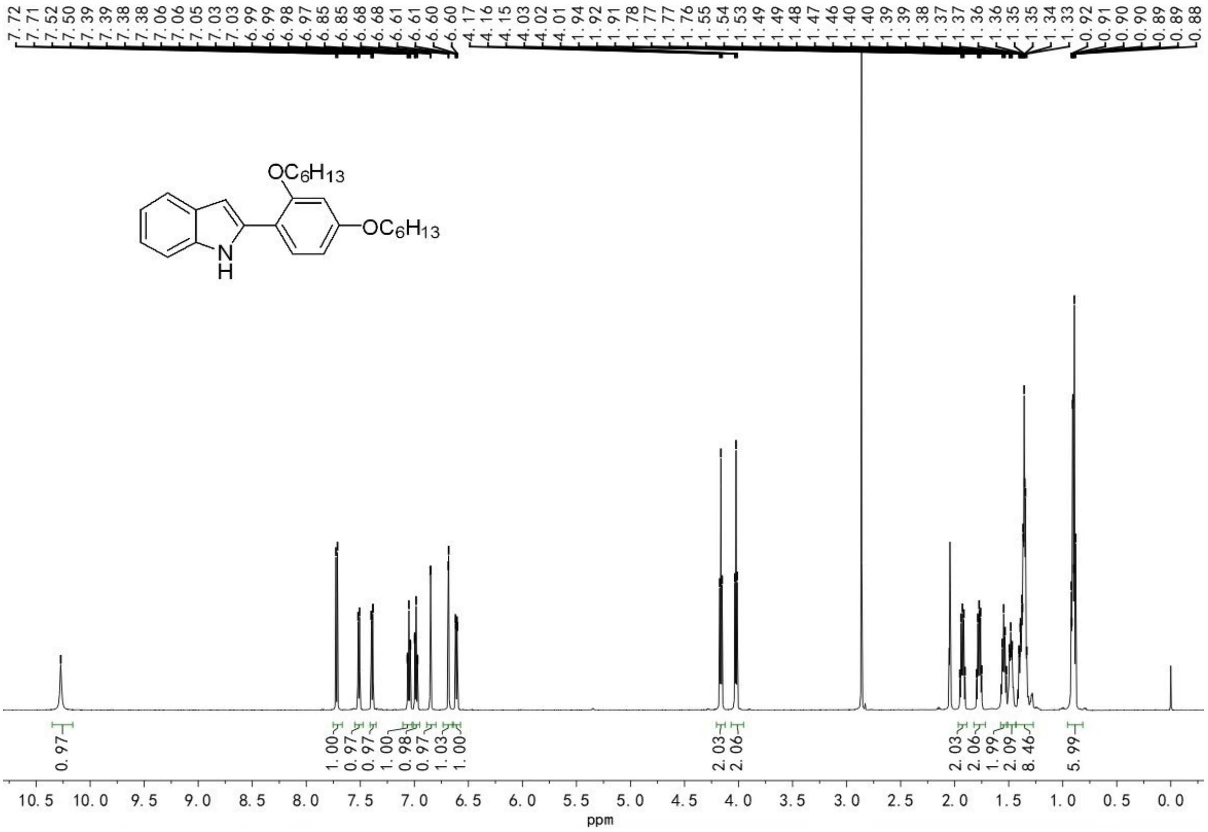


Figure S11 The ^{1}H NMR spectrum of compound **D$_4$-a** in acetone-d_6.

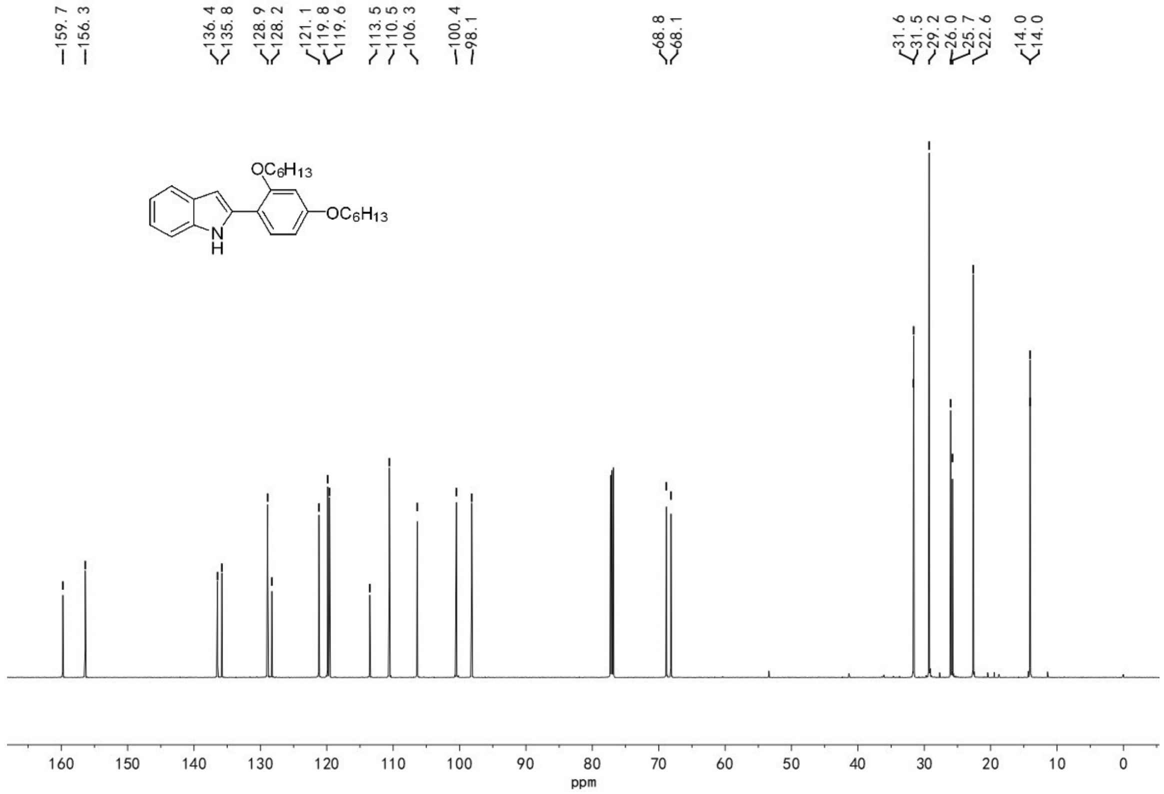


Figure S12 The ^{13}C NMR spectrum of compound **D$_4$-a** in CDCl$_3$.

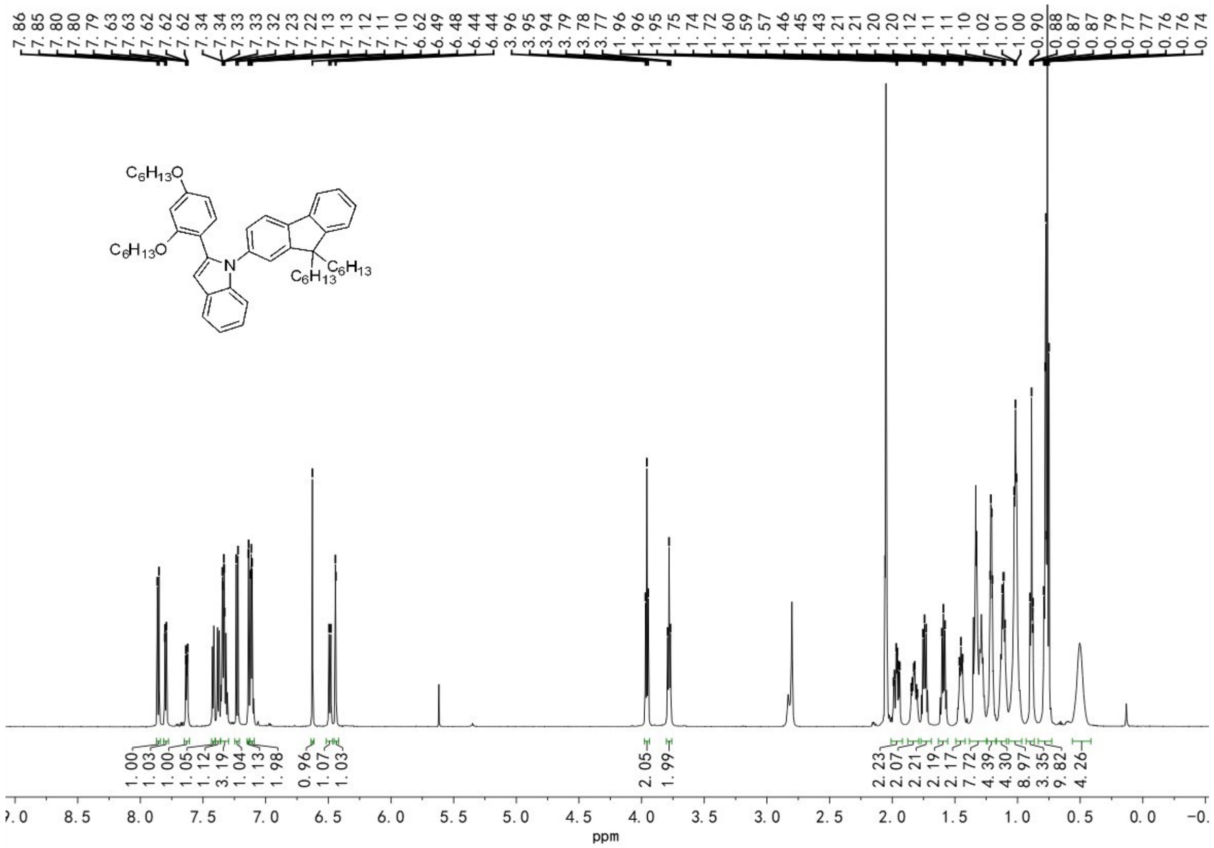


Figure S13 The ^{1}H NMR spectrum of compound **D_4-b** in acetone-d_6.

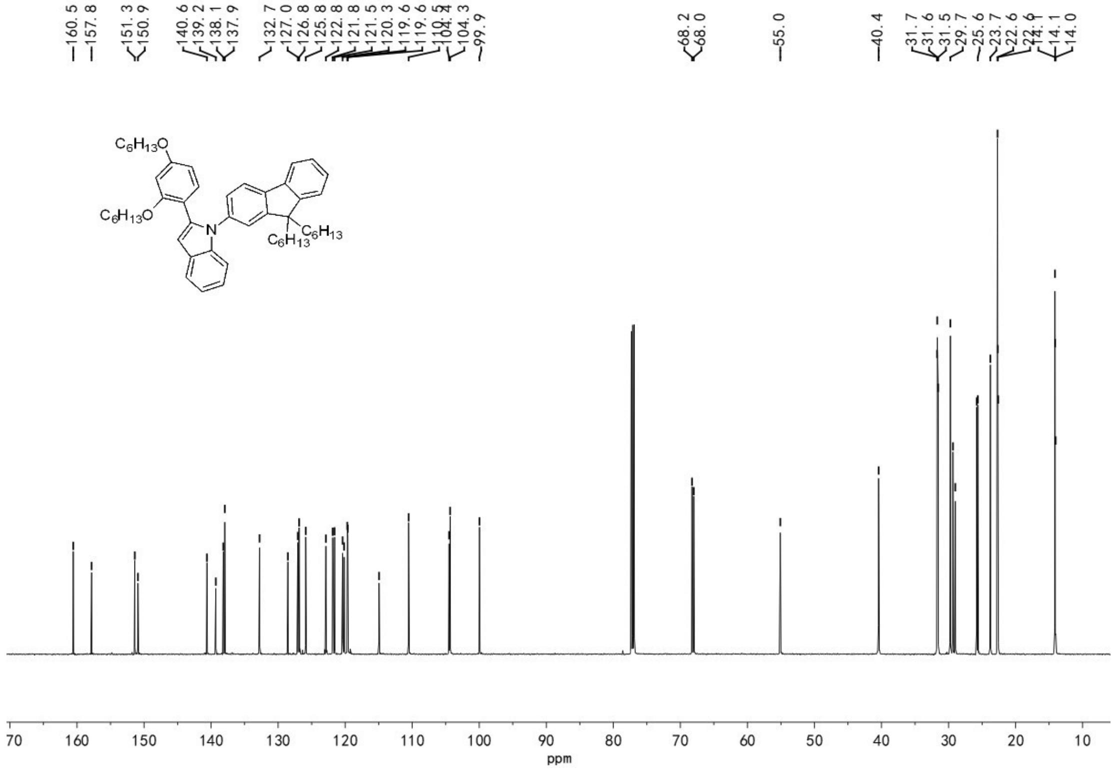


Figure S14 The ^{13}C NMR spectrum of compound **D_4-b** in $CDCl_3$.

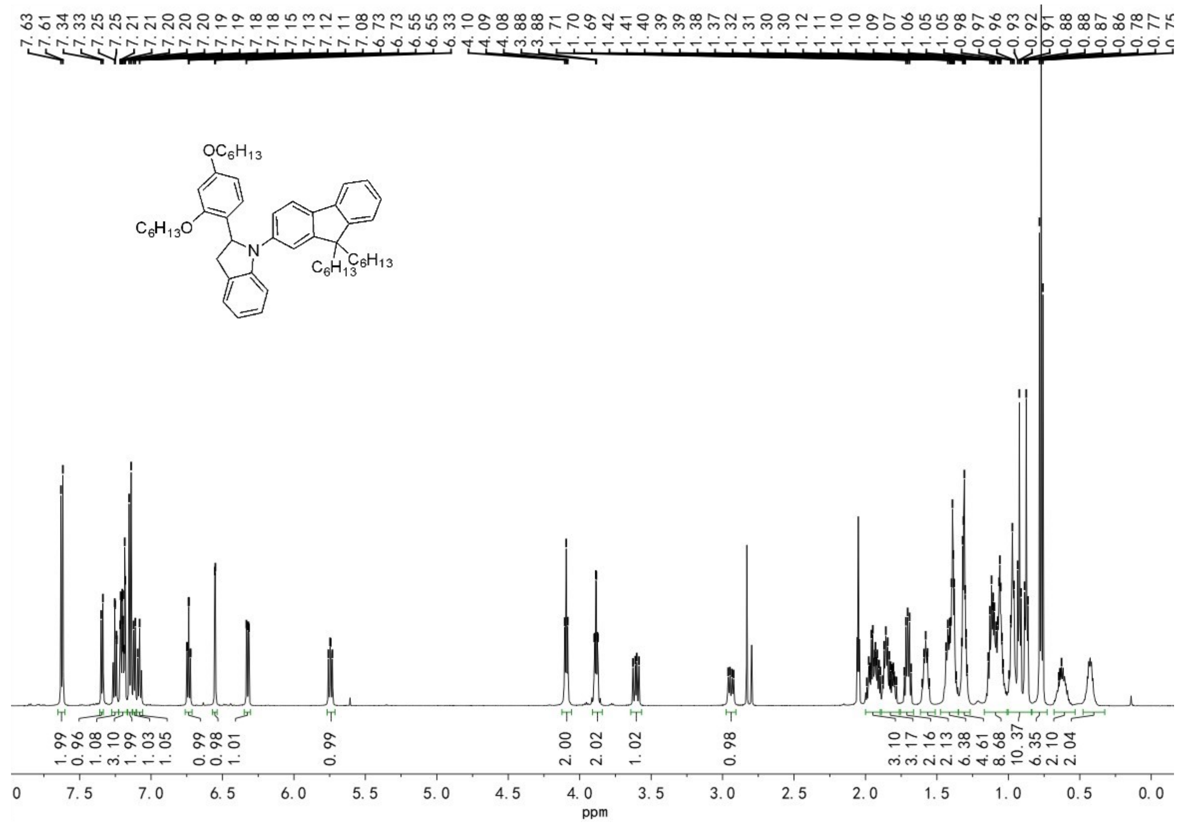


Figure S15 The ^{1}H NMR spectrum of compound **D_4-c** in acetone-d_6.

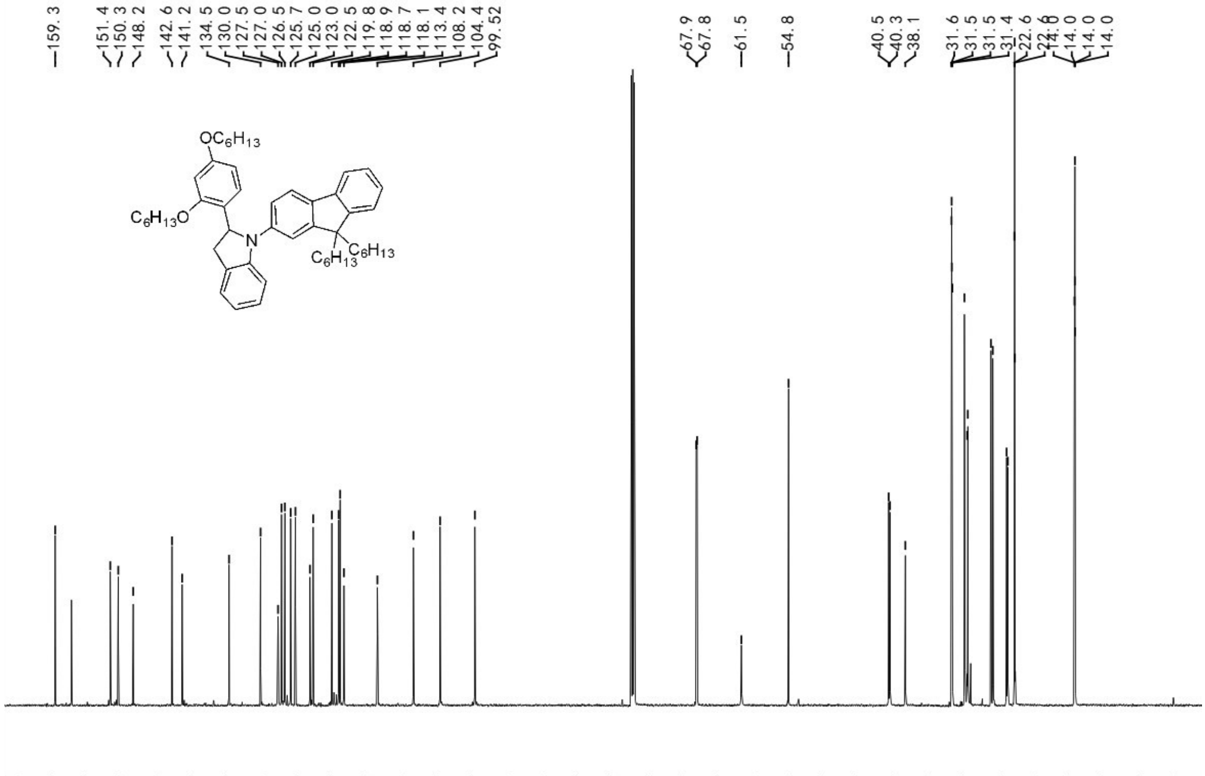


Figure S16 The ^{13}C NMR spectrum of compound **D_4-c** in $CDCl_3$.

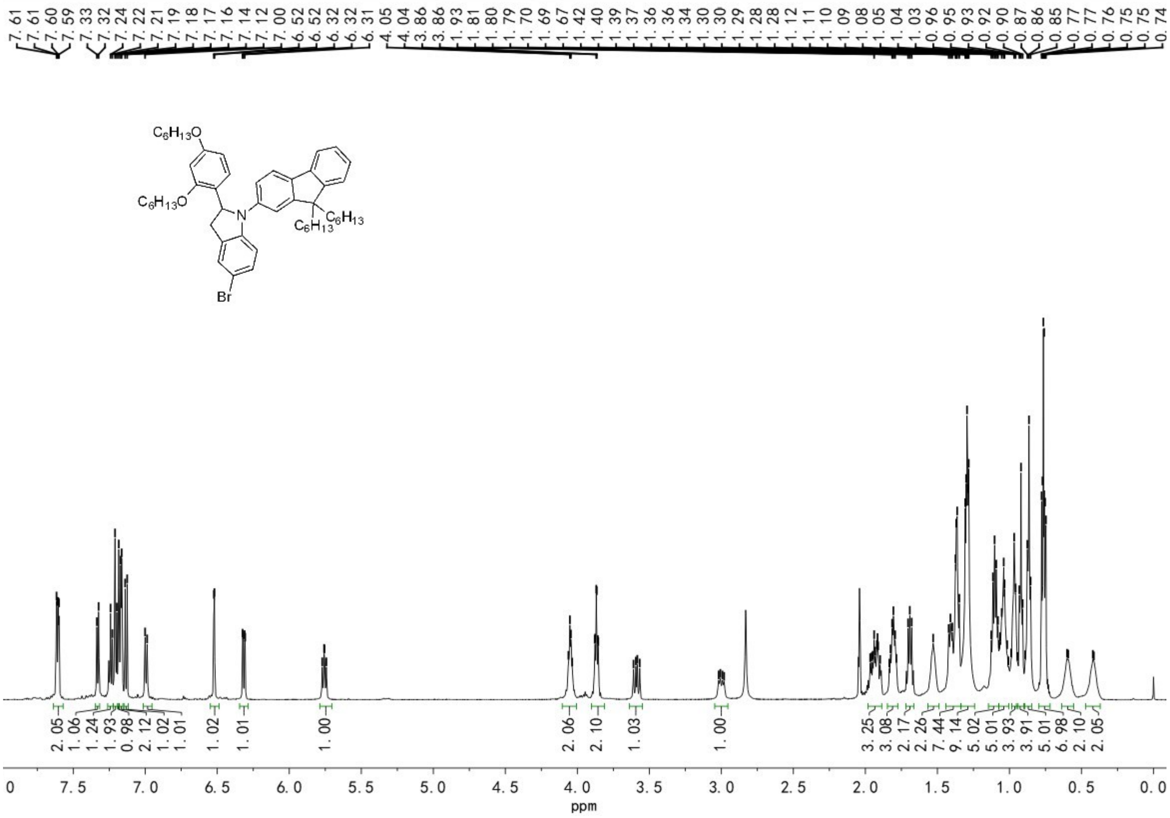


Figure S17 The ^{1}H NMR spectrum of compound $\mathbf{D_4}$**-Br** in acetone-d_6.

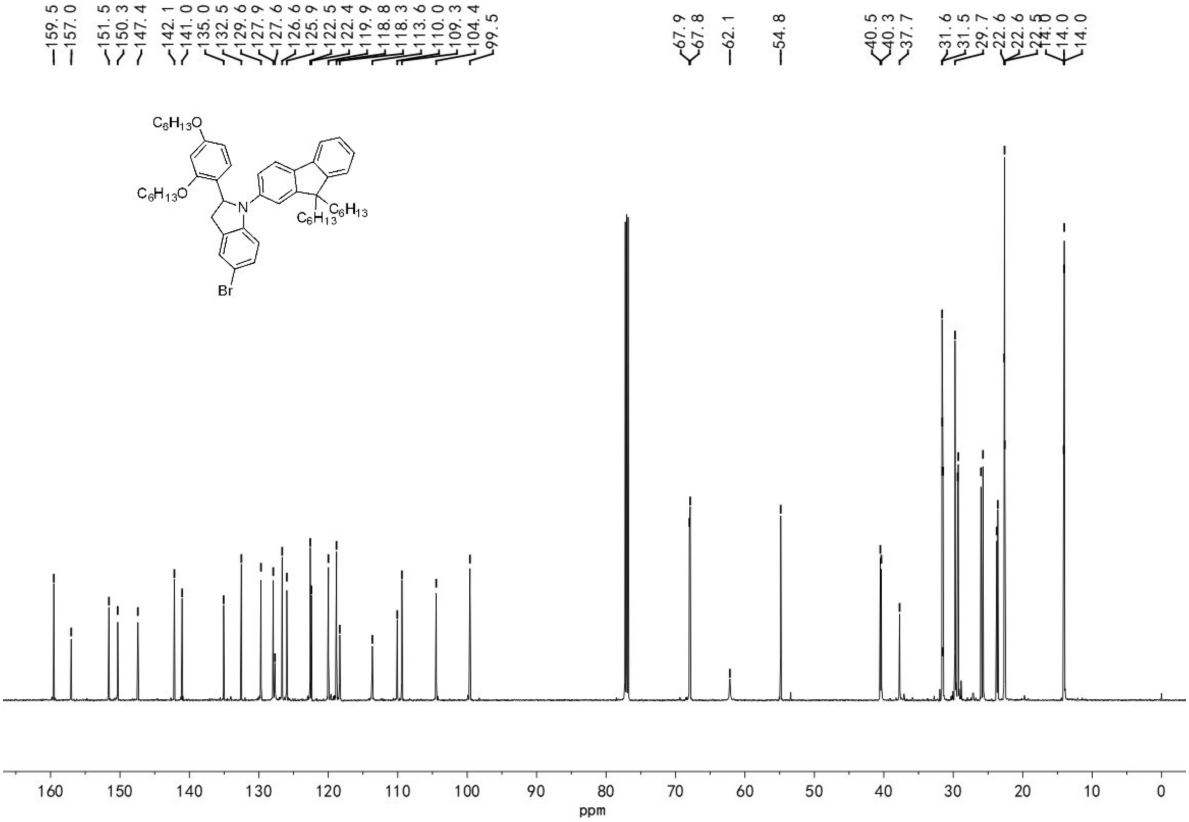


Figure S18 The ^{13}C NMR spectrum of compound $\mathbf{D_4}$**-Br** in $CDCl_3$.

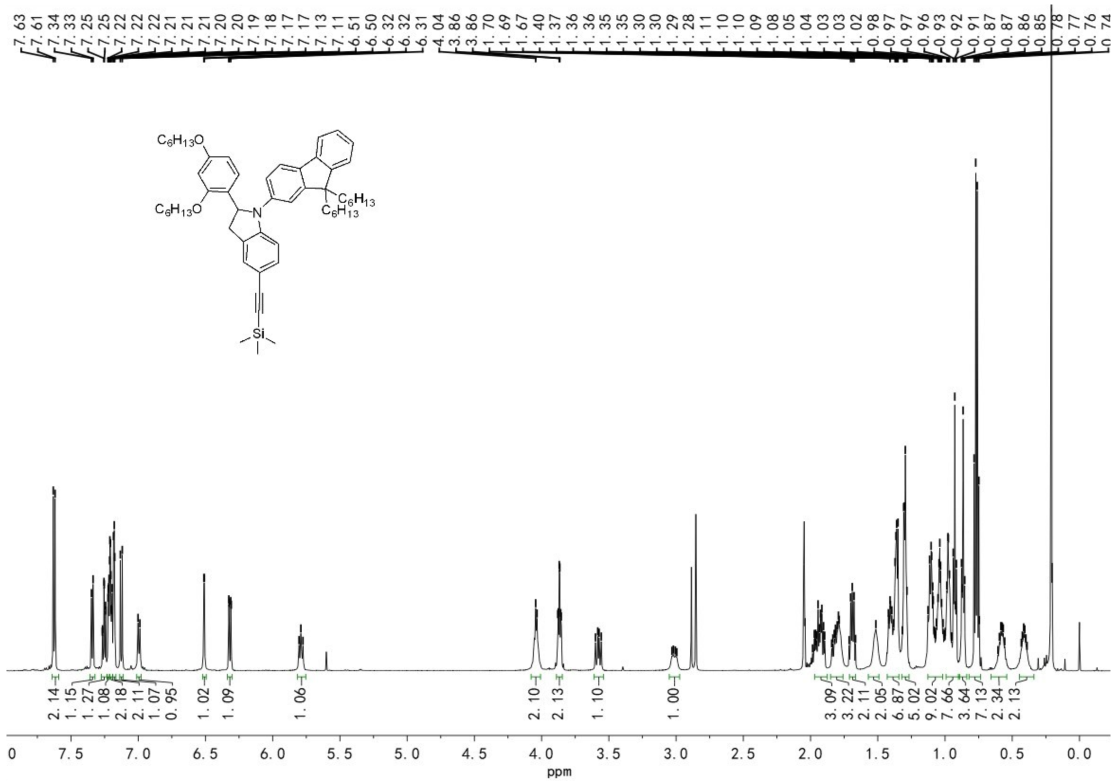


Figure S19 The ^{1}H NMR spectrum of compound **D_4-d** in acetone-d_6.

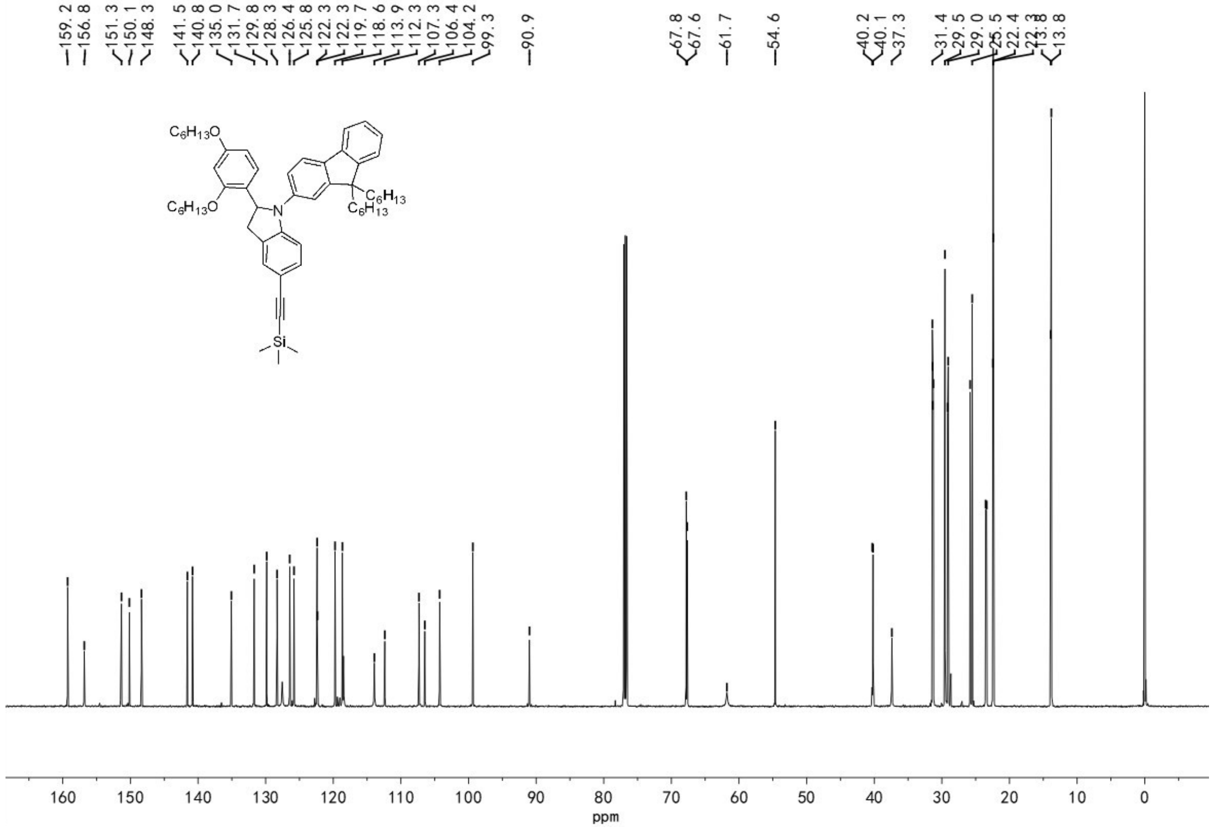


Figure S20 The ^{13}C NMR spectrum of compound **D_4-d** in $CDCl_3$.

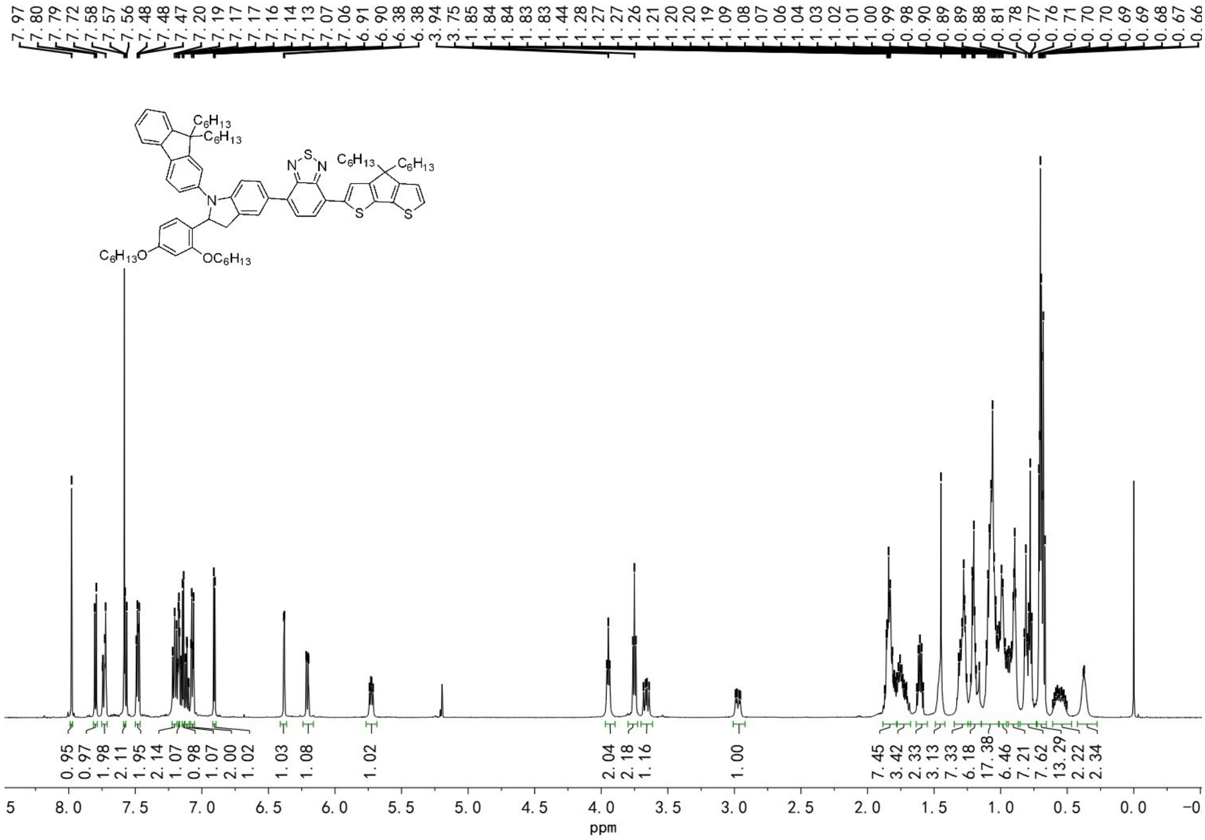


Figure S21 The ^{1}H NMR spectrum of compound **O-a** in CD_2Cl_2.

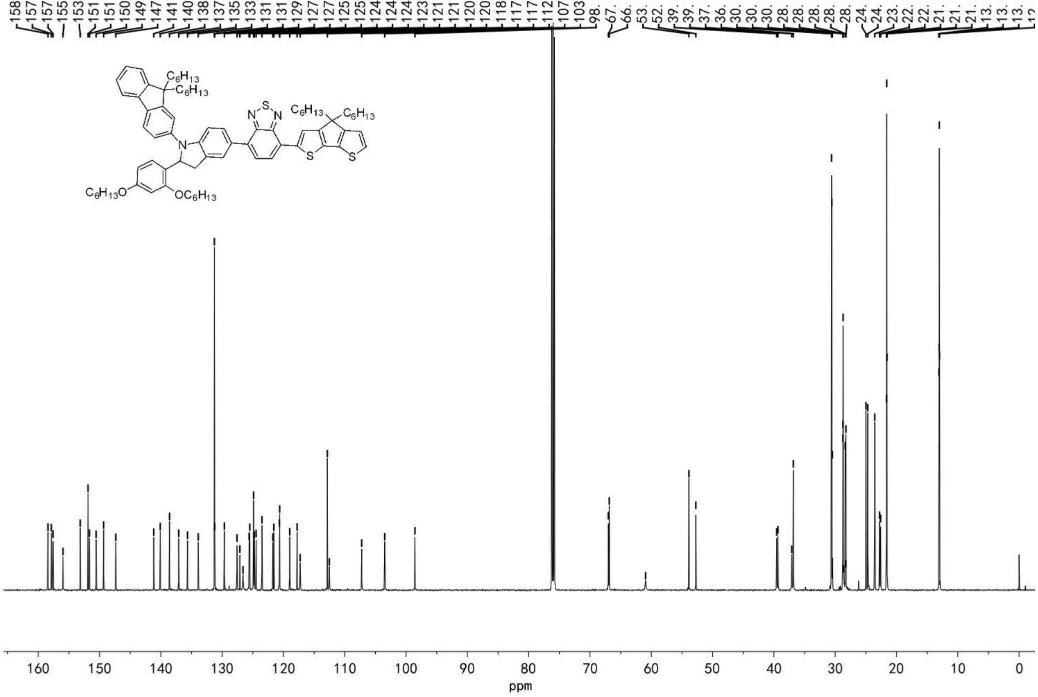


Figure S22 The ^{13}C NMR spectrum of compound **O-a** in $CDCl_3$.

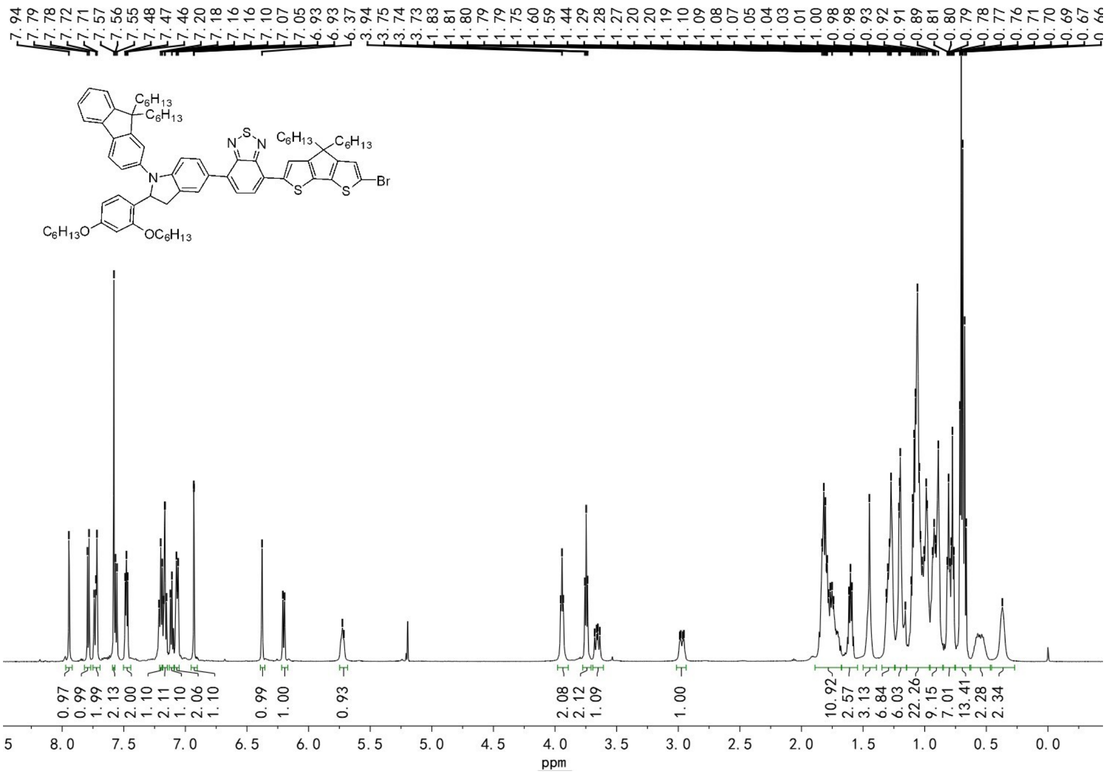


Figure S23 The ^{1}H NMR spectrum of compound **O-Br** in CD_2Cl_2.

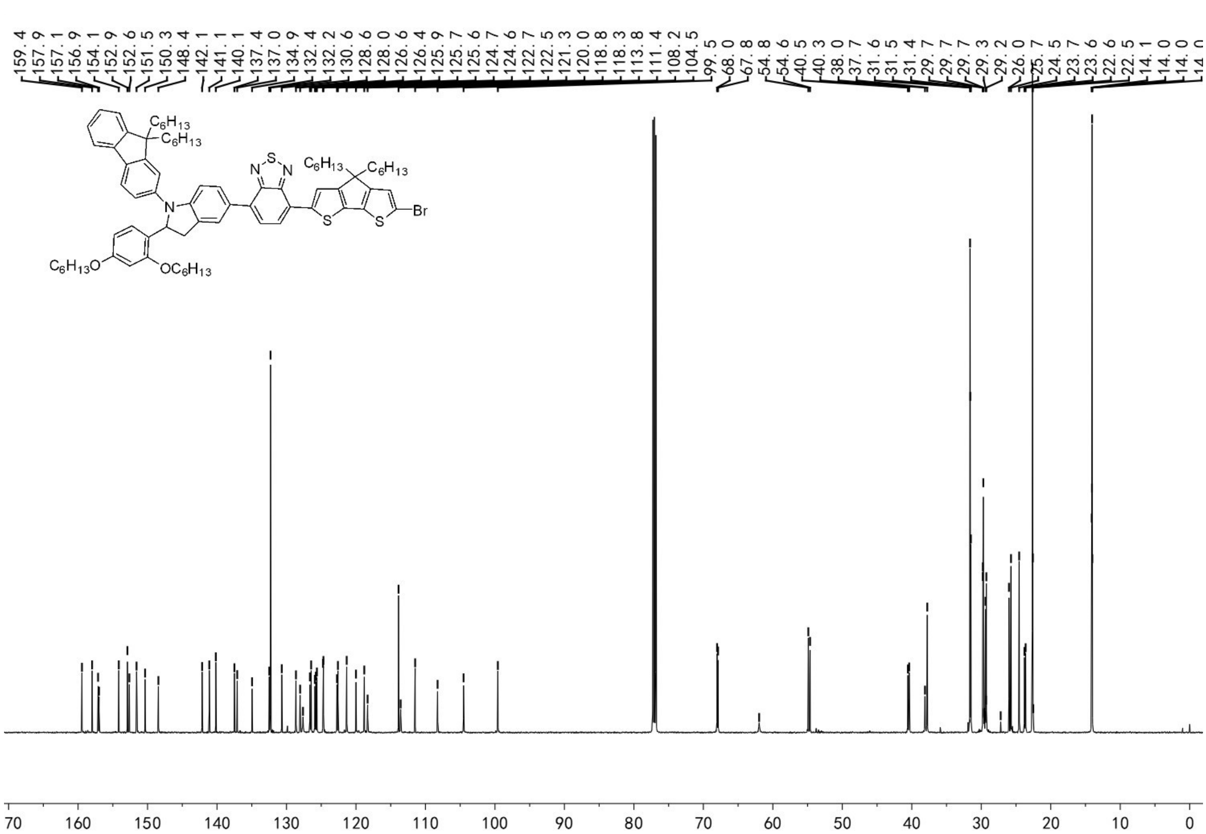


Figure S24 The ^{13}C NMR spectrum of compound **O-Br** in $CDCl_3$.

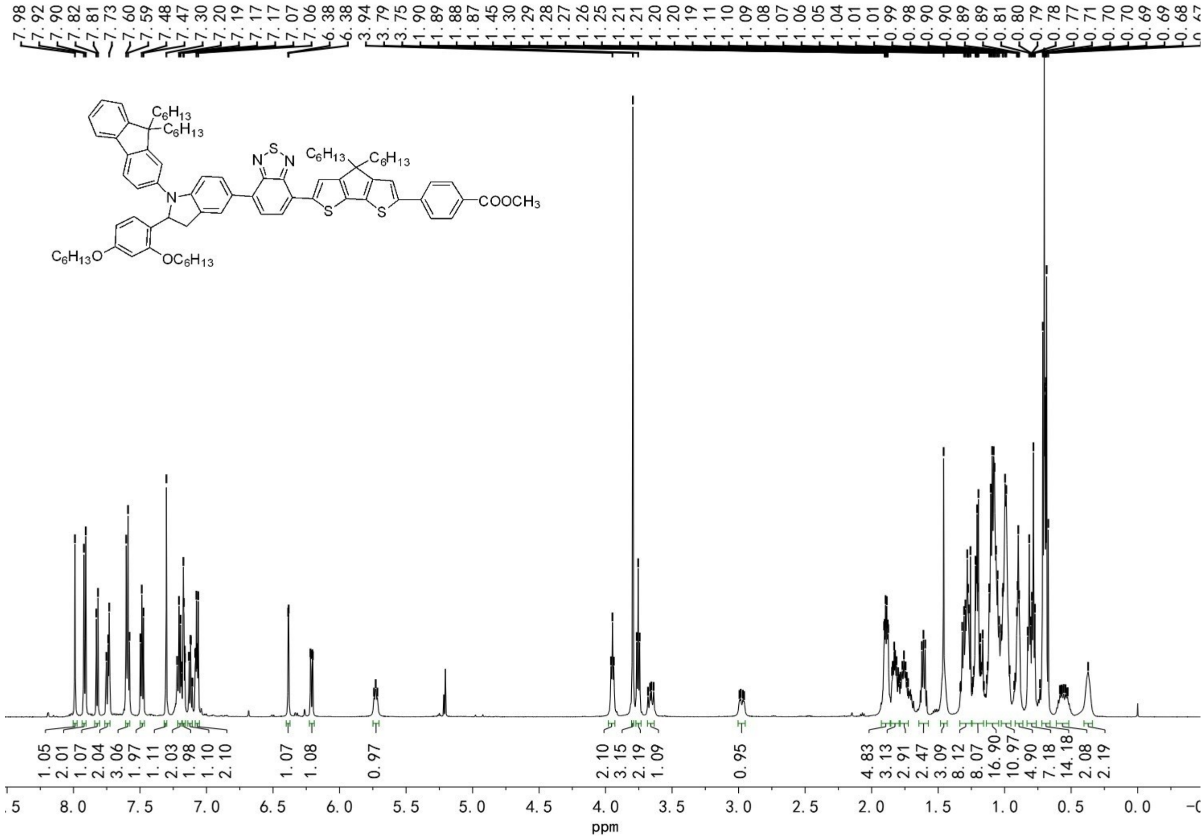


Figure S25 The ^{1}H NMR spectrum of compound **O-b** in CD_2Cl_2.

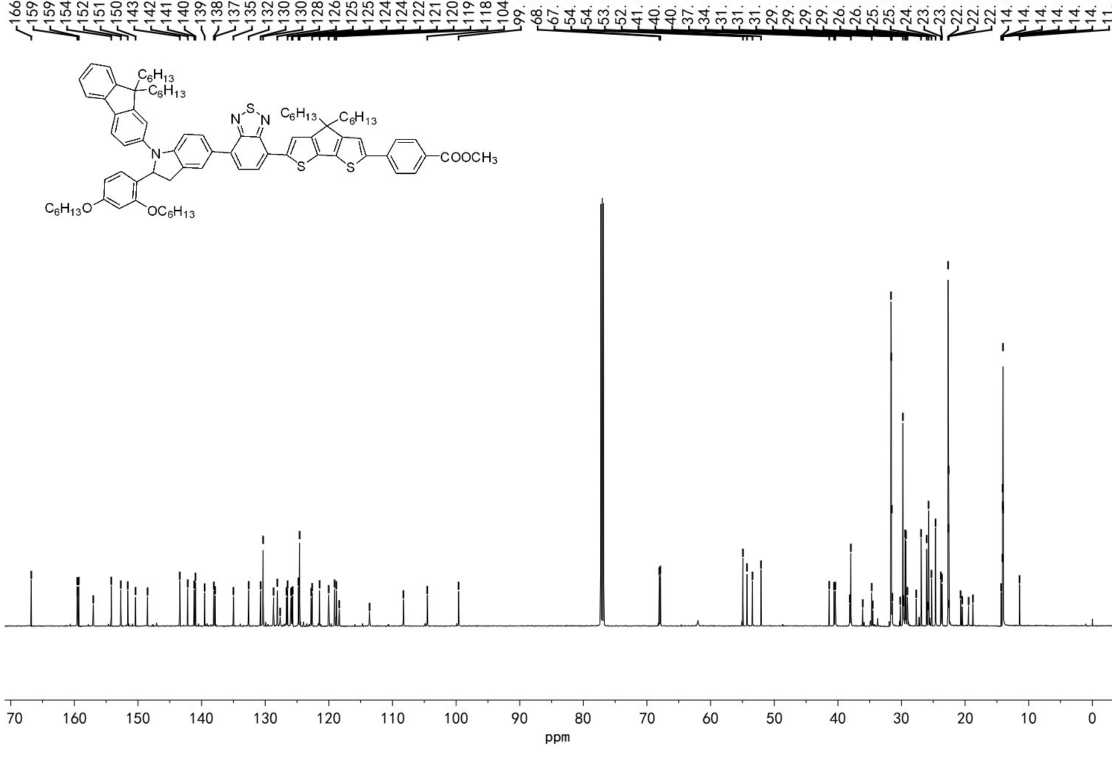


Figure S26 The ^{13}C NMR spectrum of compound **O-b** in $CDCl_3$.

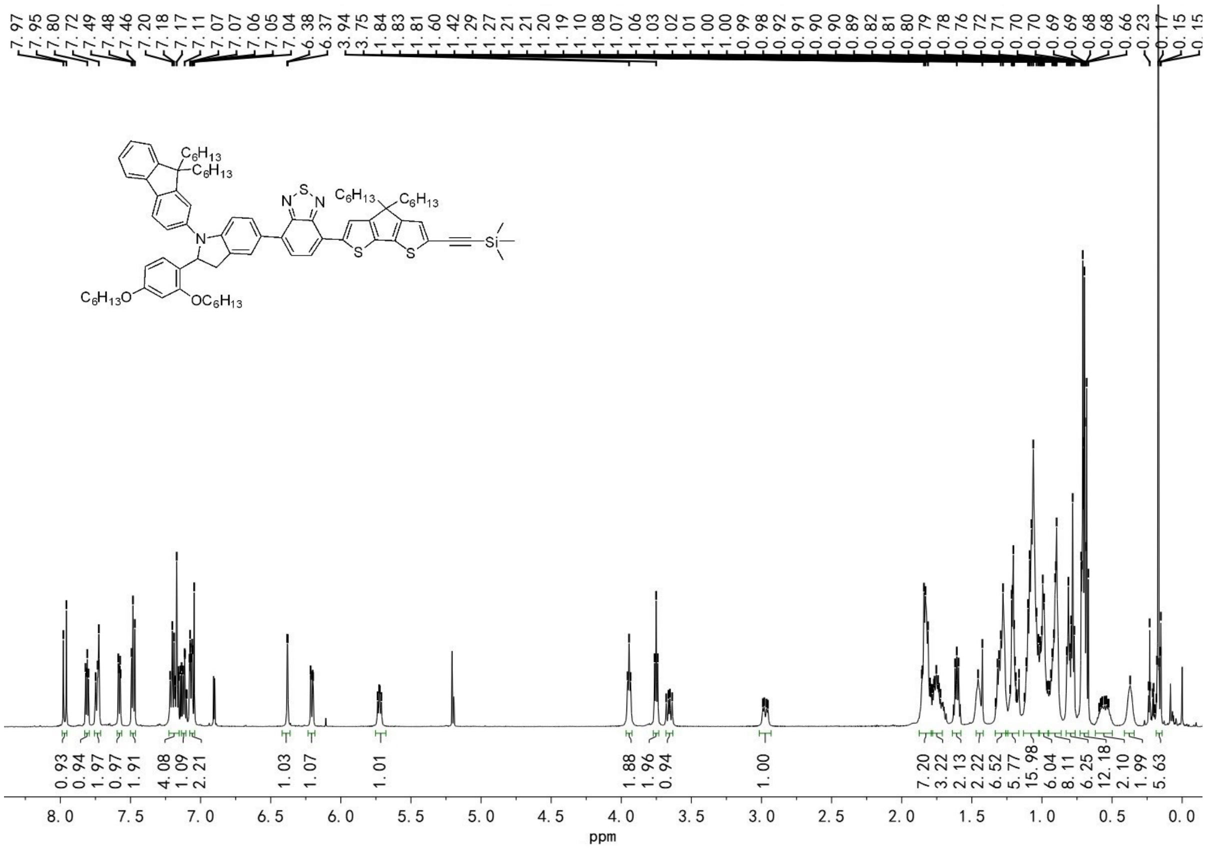


Figure S27 The ^{1}H NMR spectrum of compound **O-c** in CD_2Cl_2.

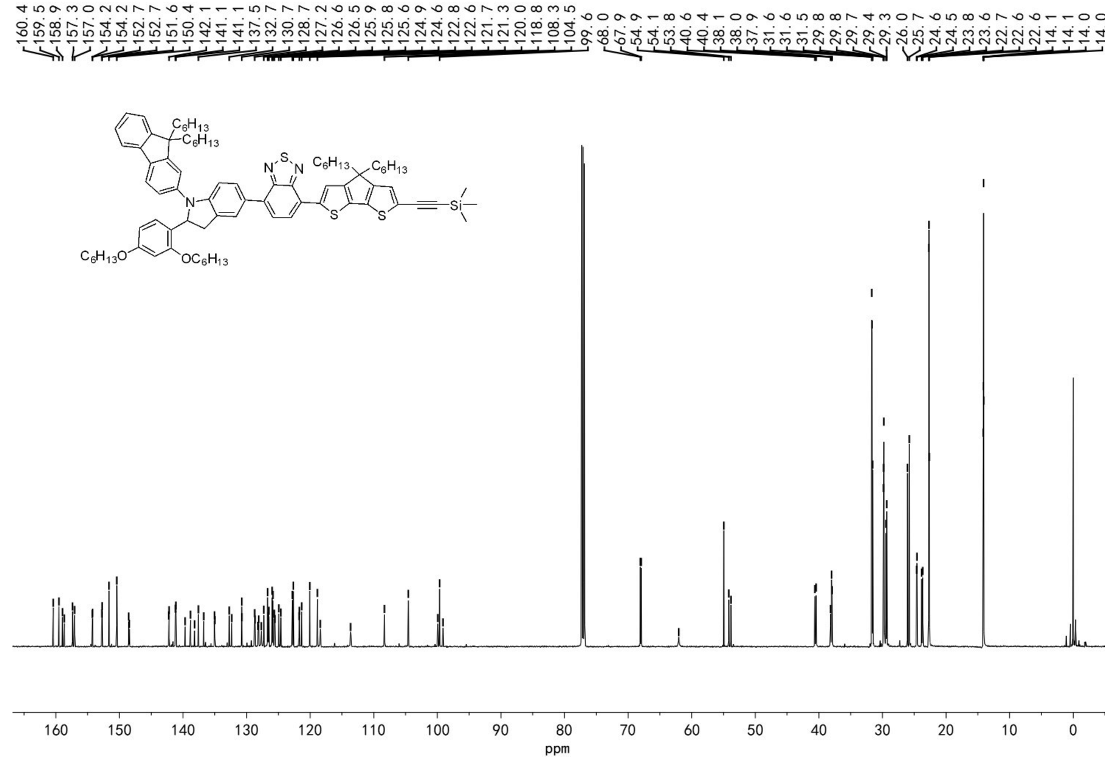


Figure S28 The ^{13}C NMR spectrum of compound **O-c** in $CDCl_3$.

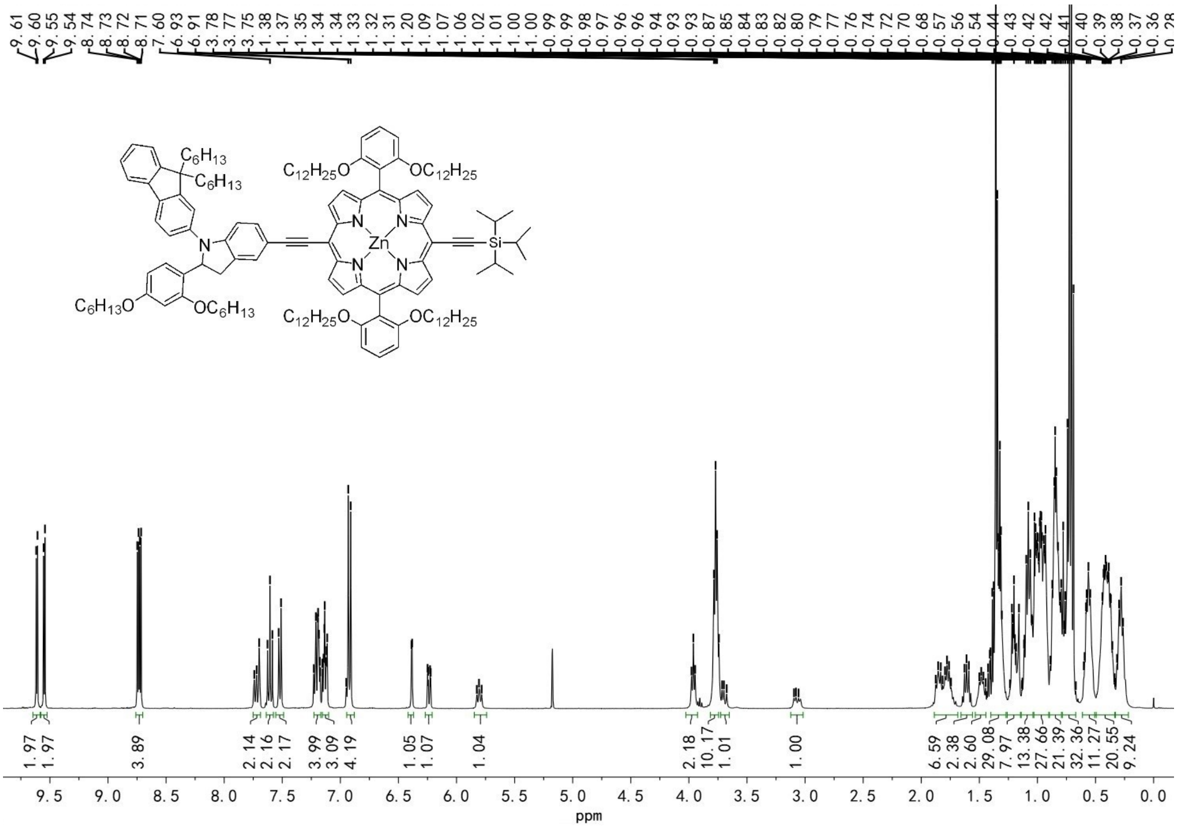


Figure S29 The ^1H NMR spectrum of compound **P-a1** in CD_2Cl_2.

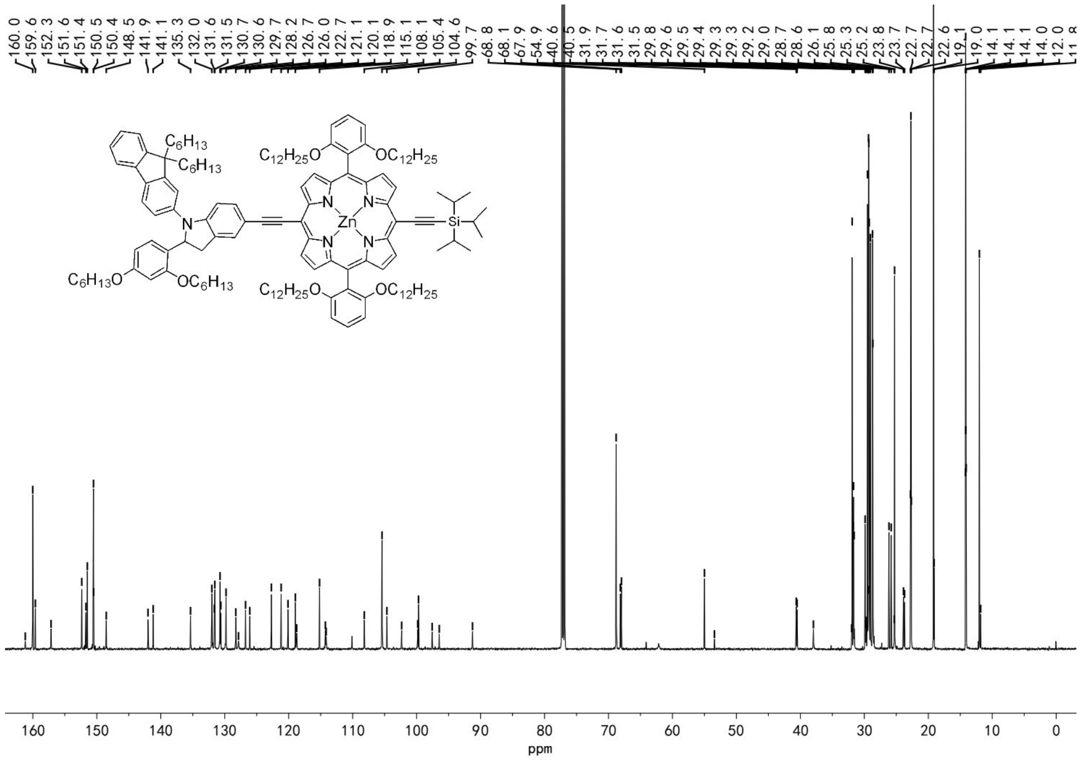


Figure S30 The ^{13}C NMR spectrum of compound **P-a1** in $CDCl_3$.

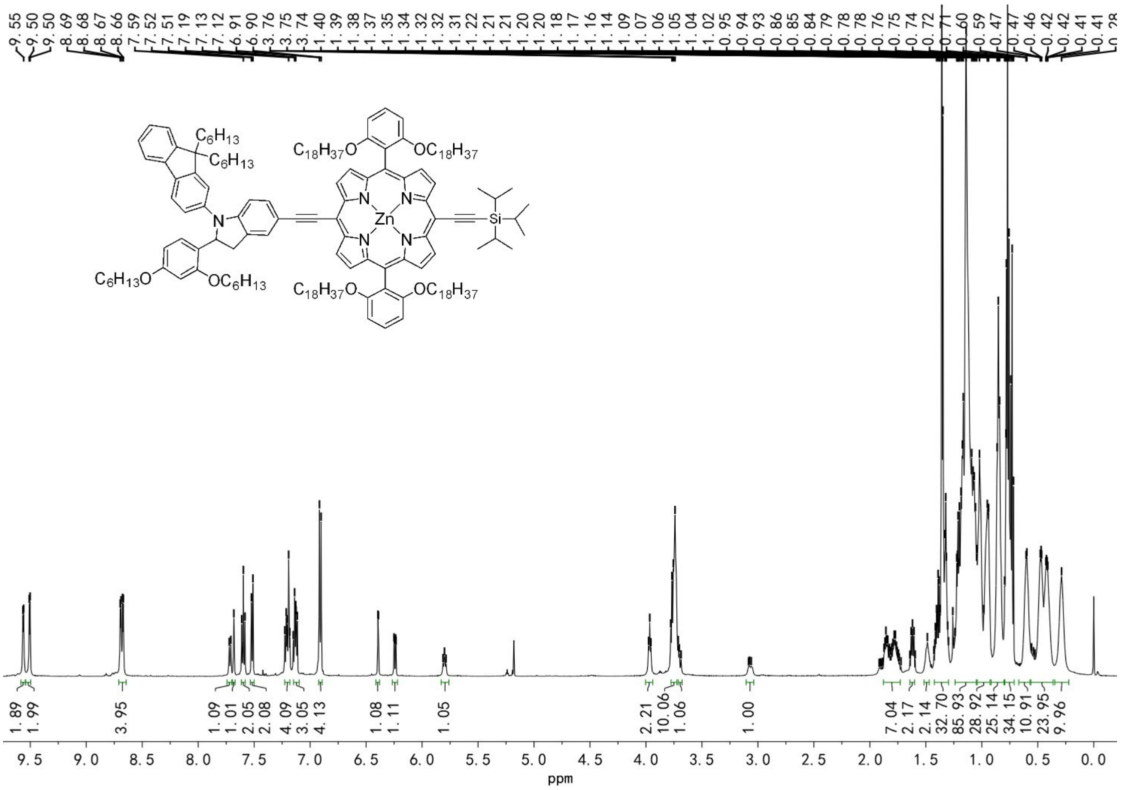


Figure S31 The ^1H NMR spectrum of compound **P-a2** in CD_2Cl_2.

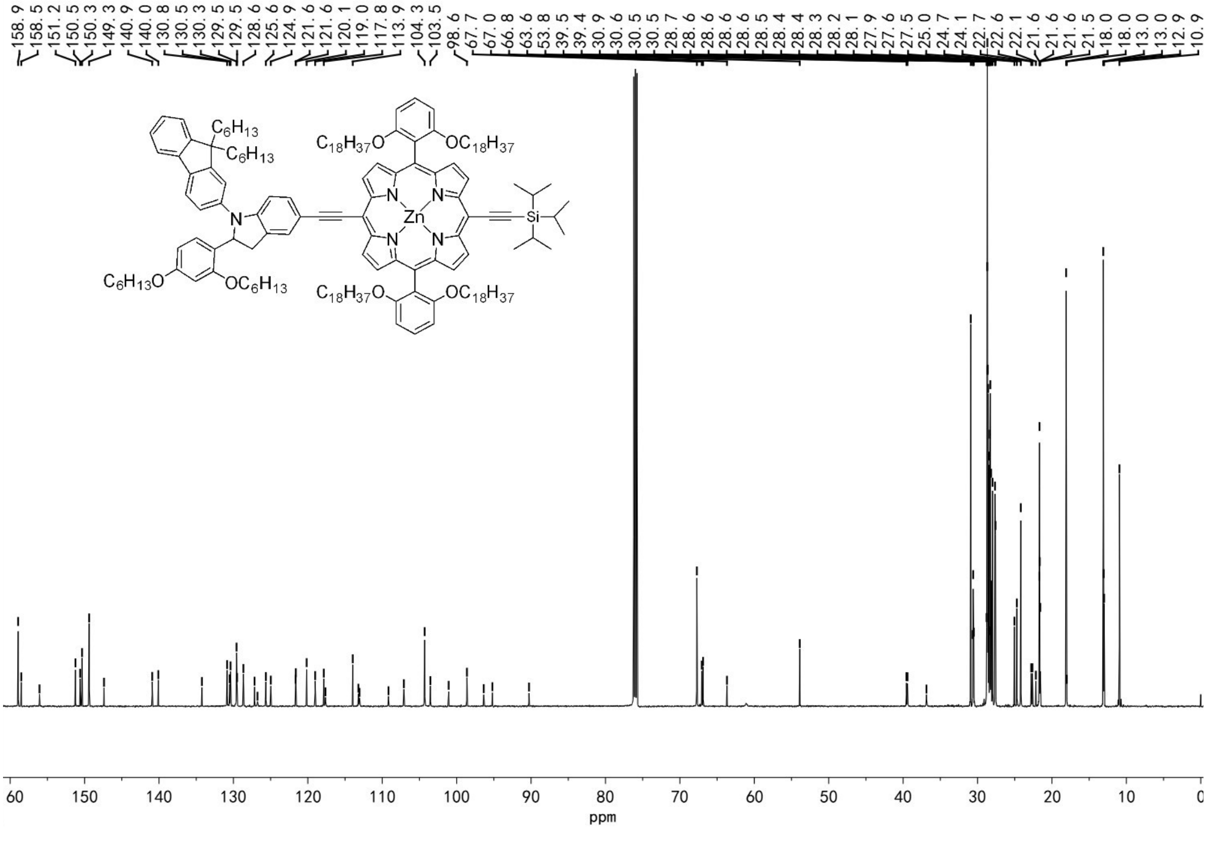


Figure S32 The ^{13}C NMR spectrum of compound **P-a2** in $CDCl_3$.

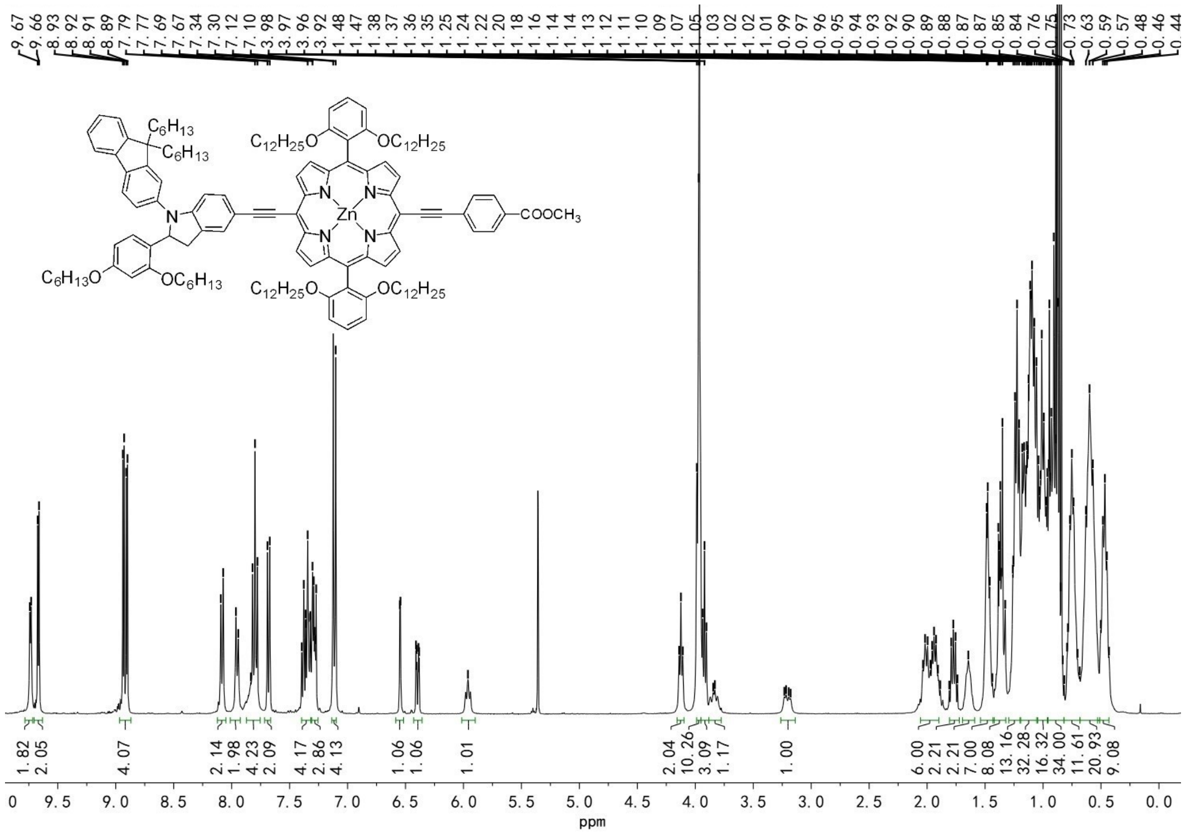


Figure S33 The ^1H NMR spectrum of compound **P-b1** in CD_2Cl_2.

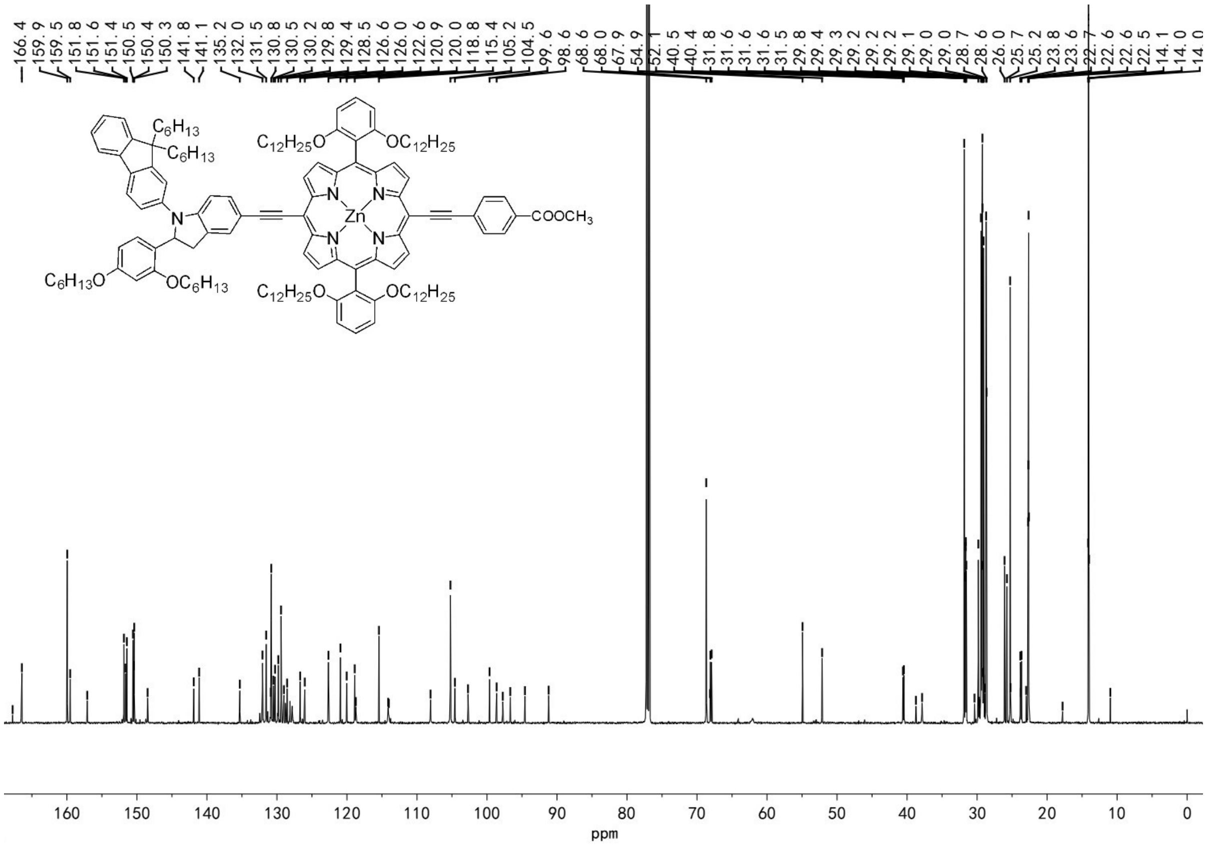


Figure S34 The ^{13}C NMR spectrum of compound **P-b1** in $CDCl_3$.

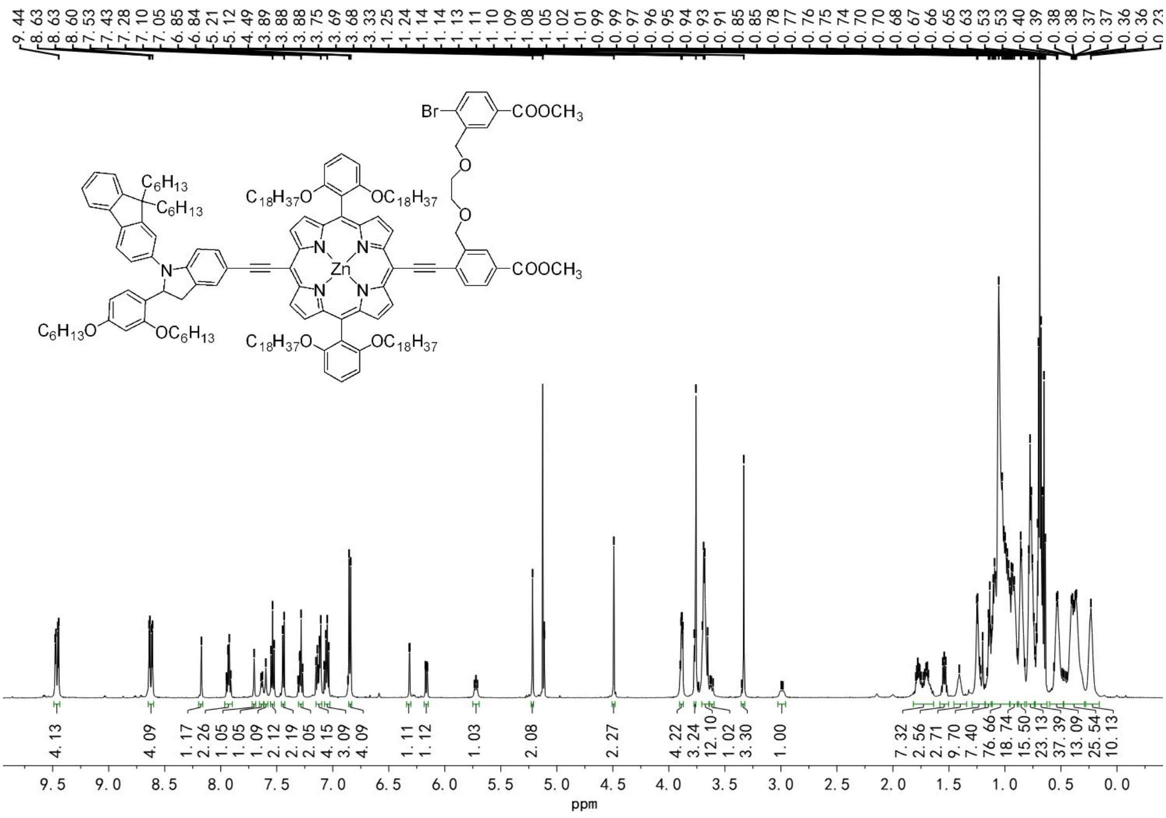


Figure S35 The ^{1}H NMR spectrum of compound **P-b2** in CD_2Cl_2.

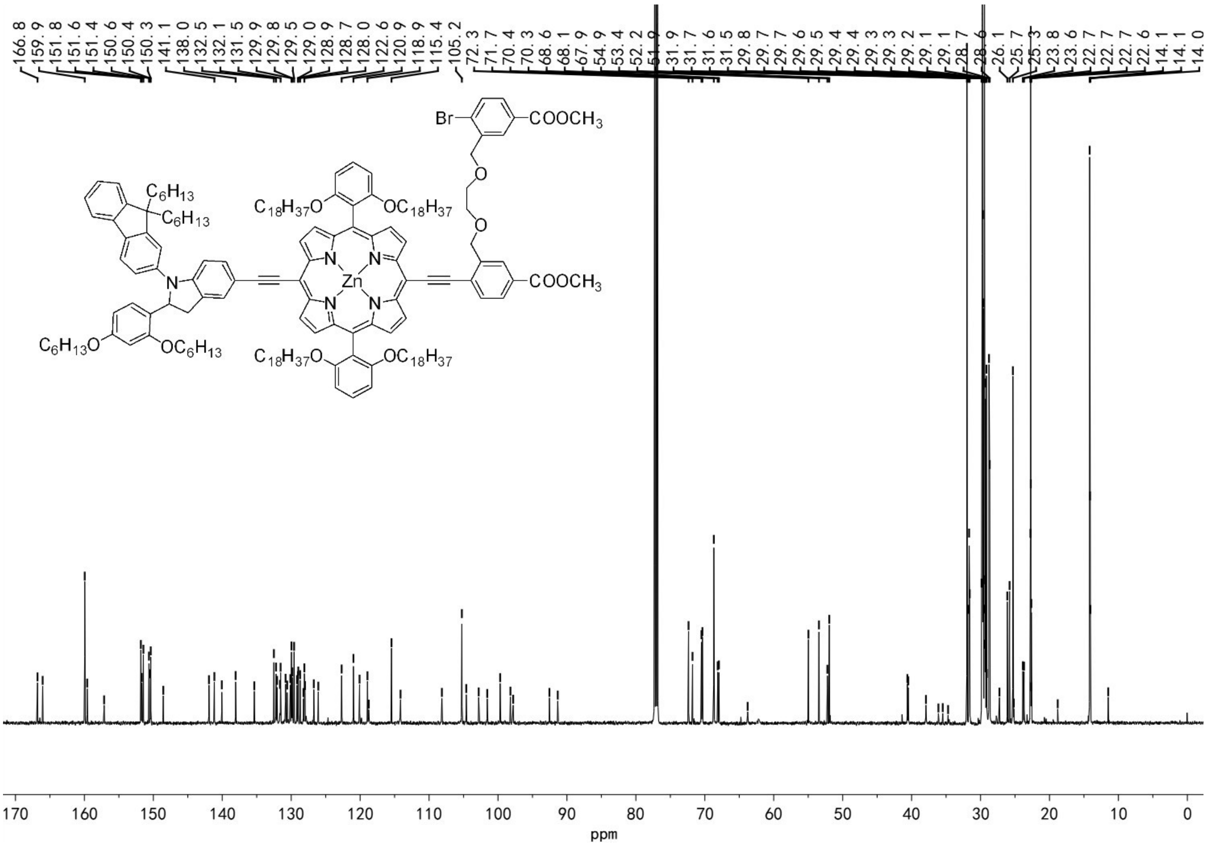


Figure S36 The ^{13}C NMR spectrum of compound **P-b2** in $CDCl_3$.

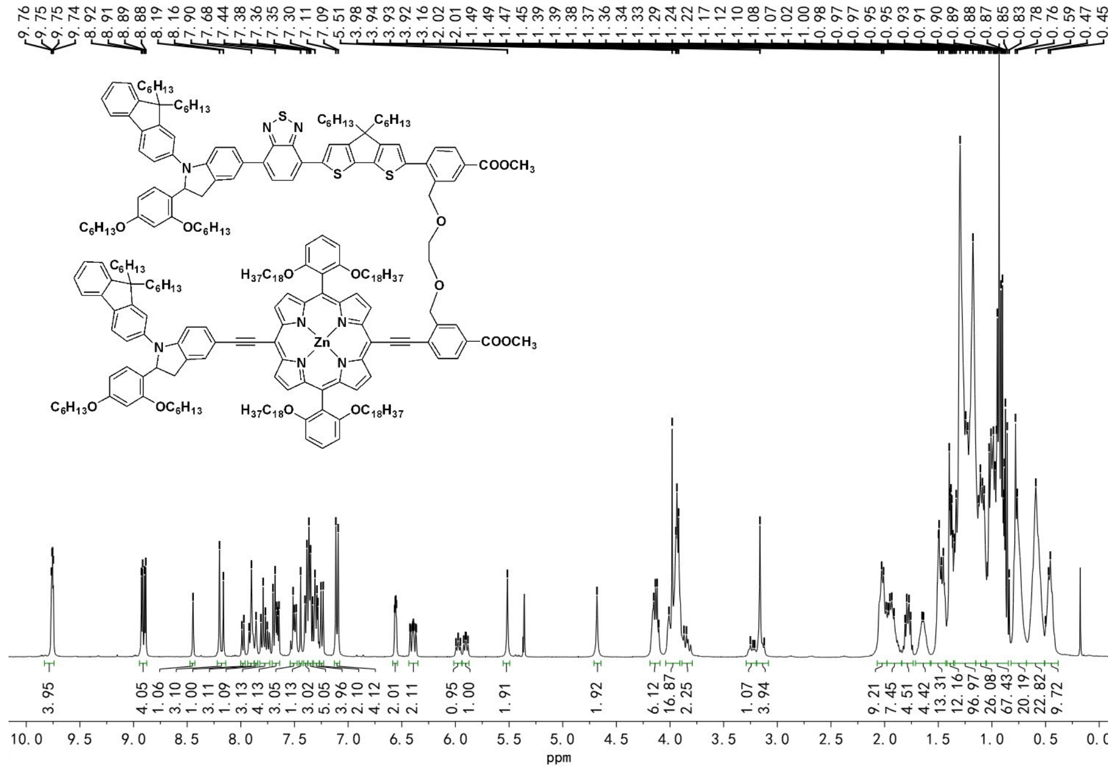


Figure S37 The ^{1}H NMR spectrum of compound **P-c1** in CD_2Cl_2.

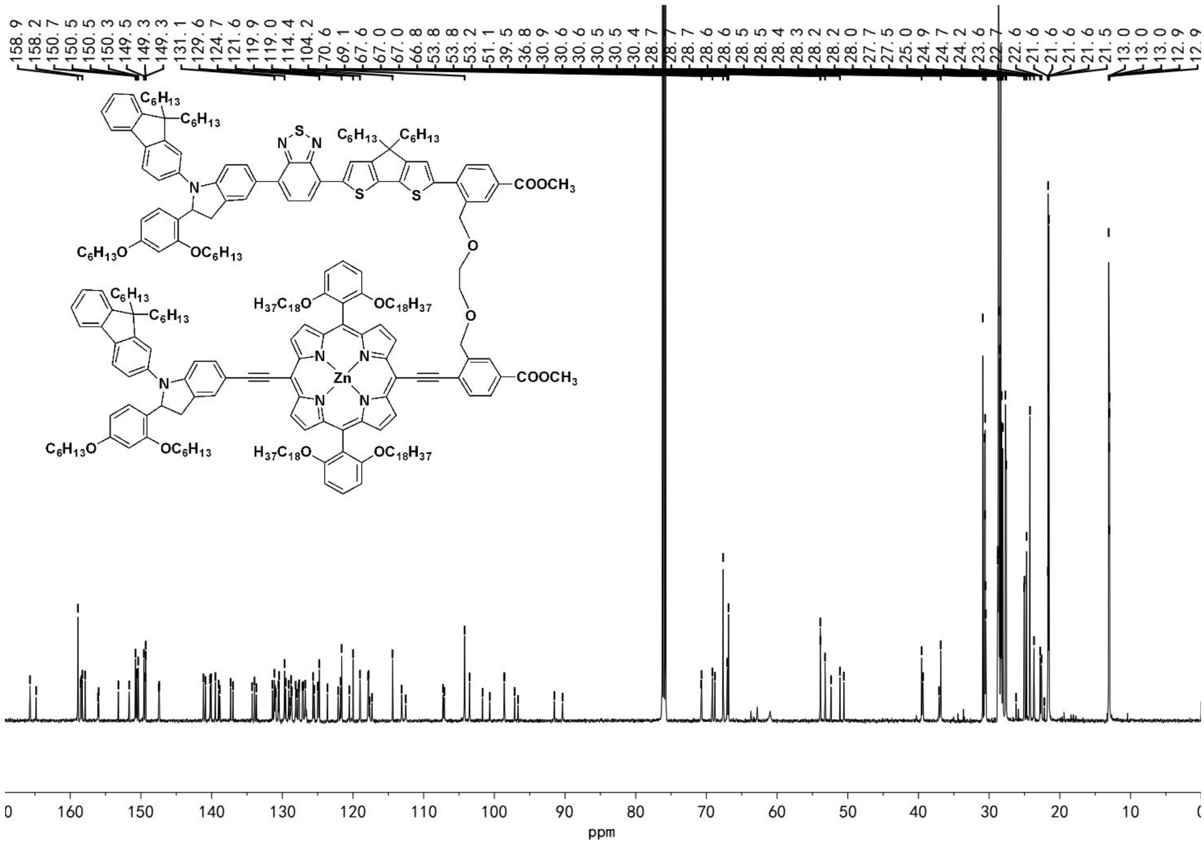


Figure S38 The ^{13}C NMR spectrum of compound **P-c1** in $CDCl_3$.

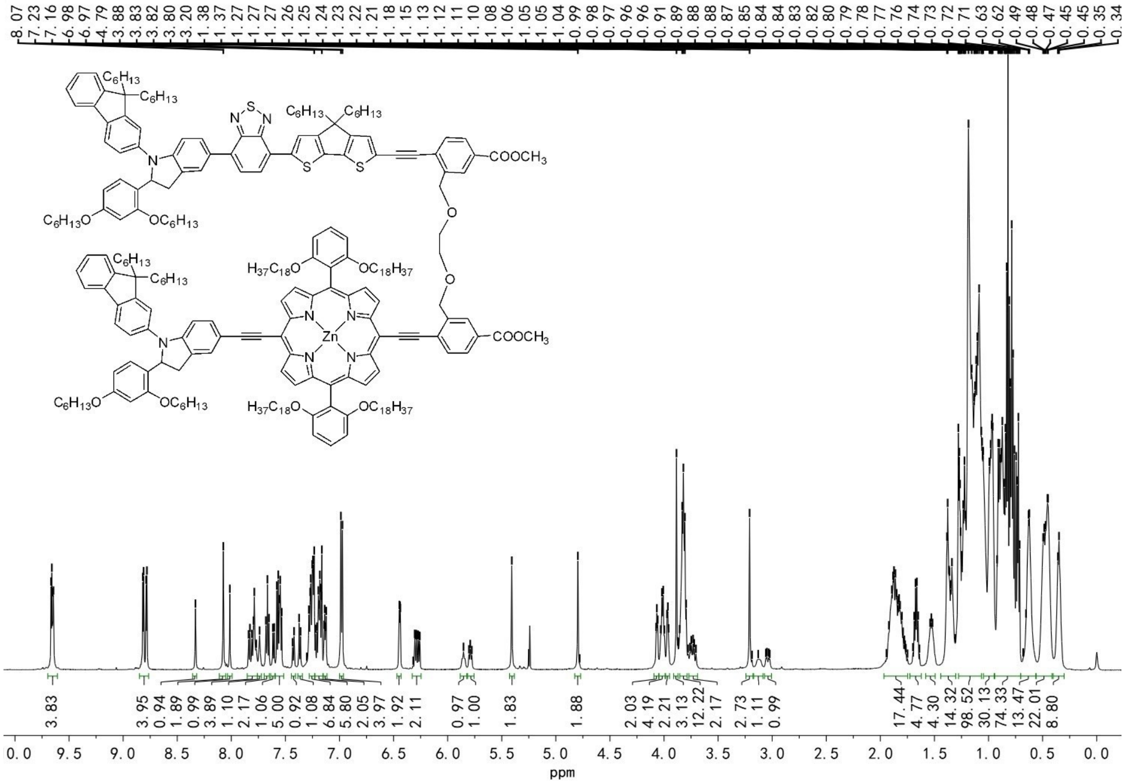


Figure S39 The ^1H NMR spectrum of compound **P-c2** in CD_2Cl_2.

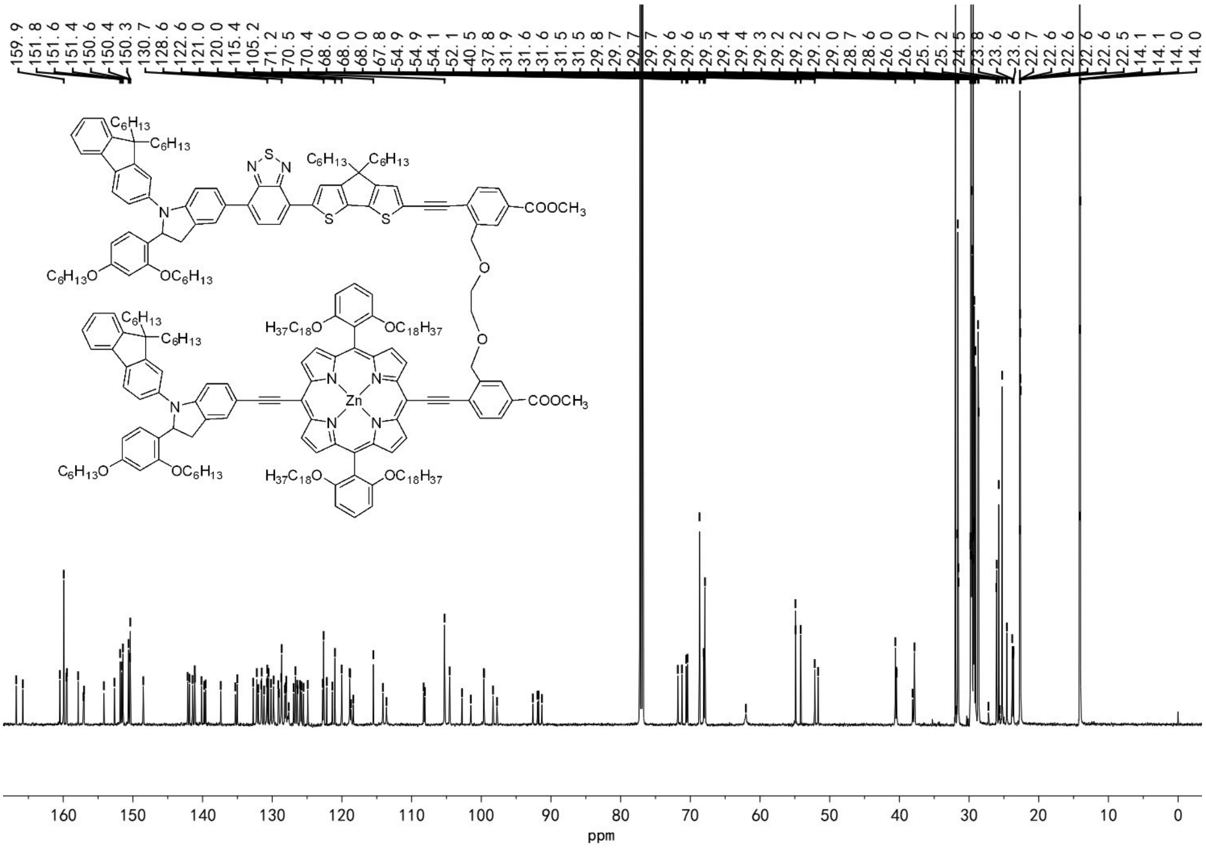


Figure S40 The ^{13}C NMR spectrum of compound **P-c2** in $CDCl_3$.

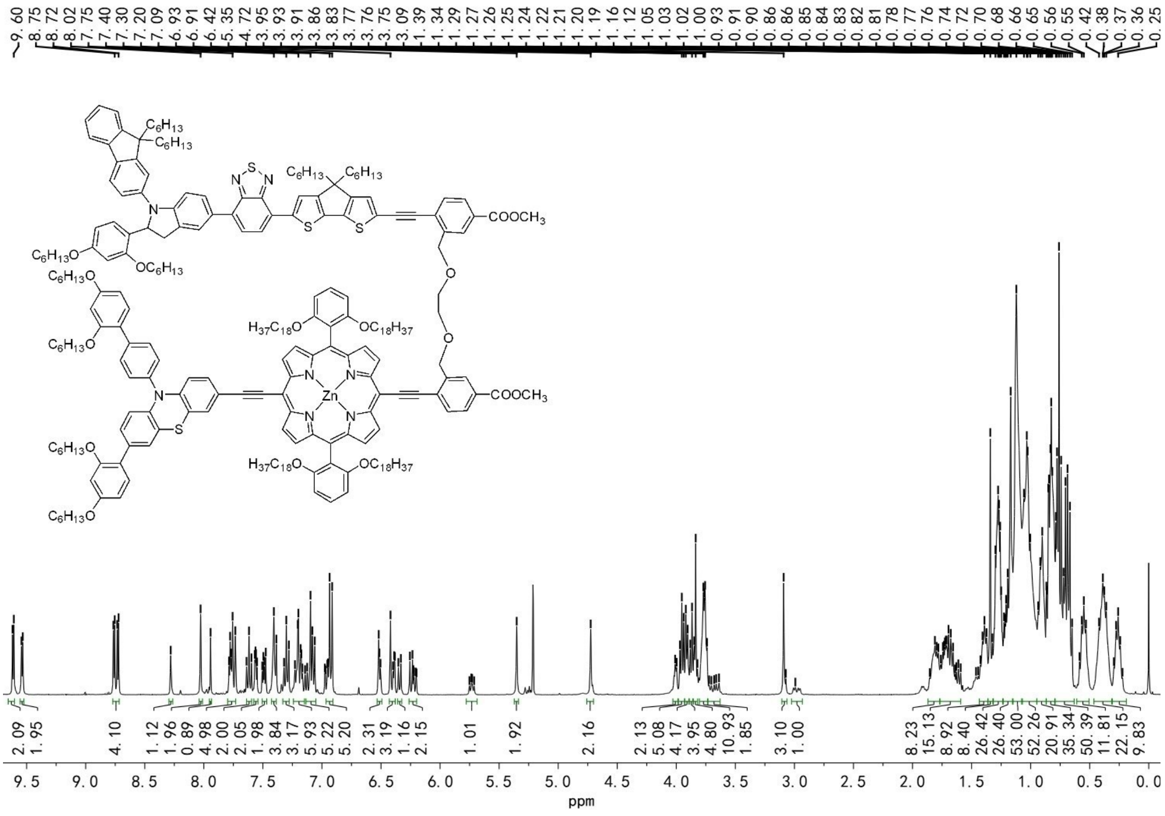


Figure S41 The ^{1}H NMR spectrum of compound **P-c3** in CD_2Cl_2.

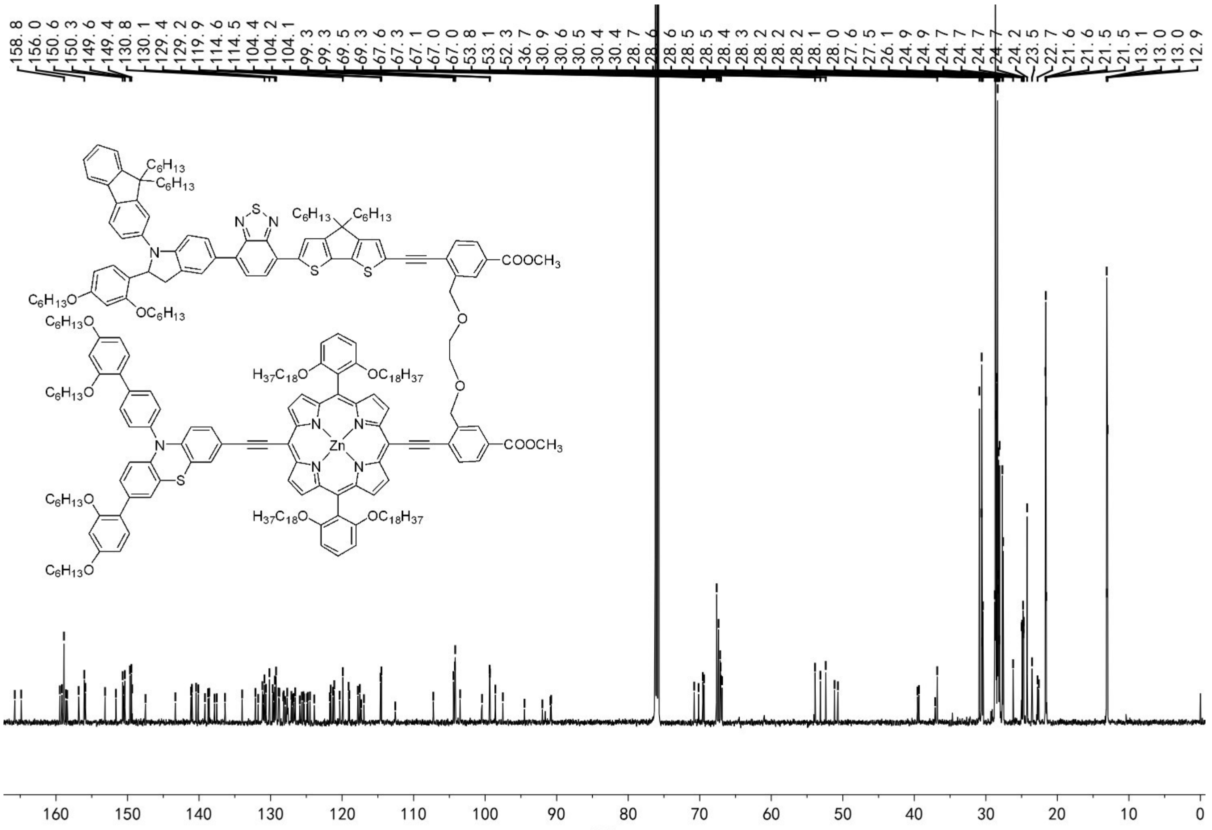


Figure S42 The ^{13}C NMR spectrum of compound **P-c3** in $CDCl_3$.

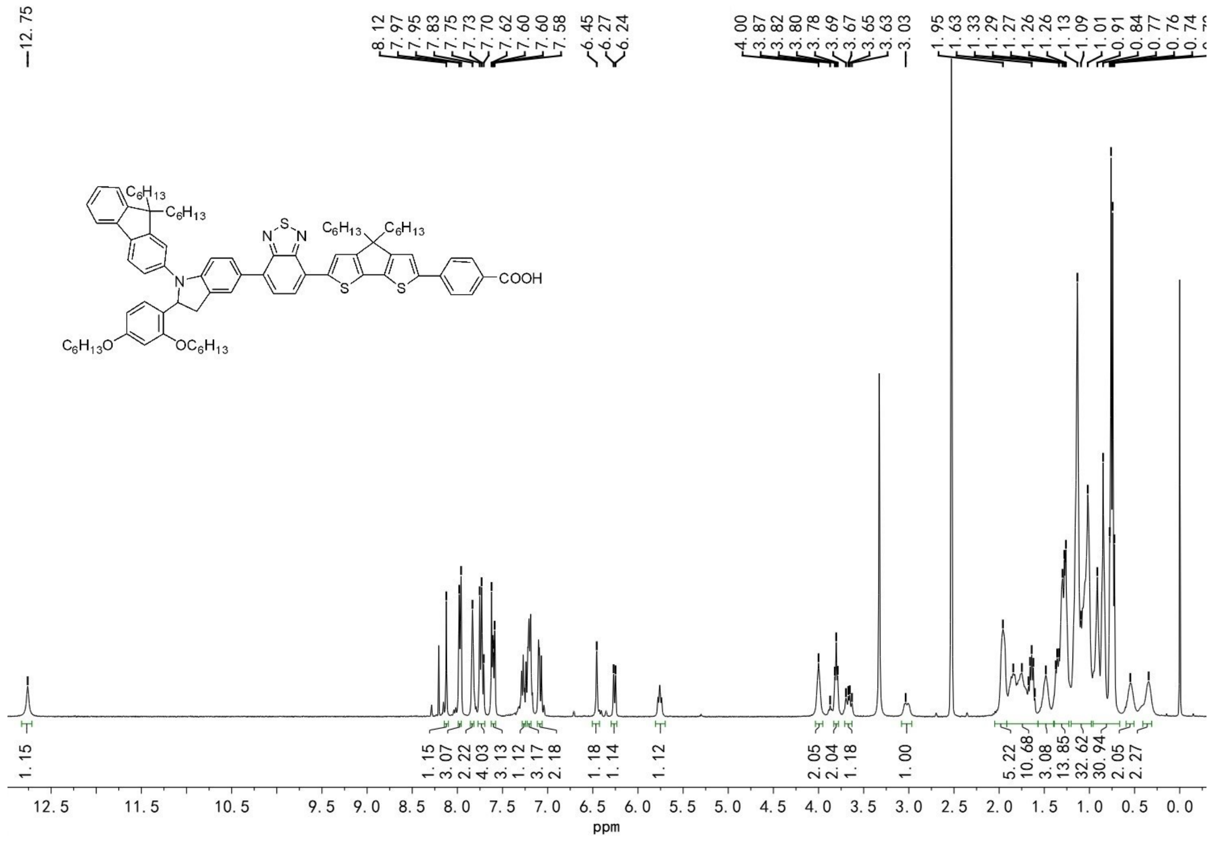


Figure S43 The ^1H NMR spectrum of **Y3** in $CDCl_3$/DMSO-d_6 (1/2, v/v).

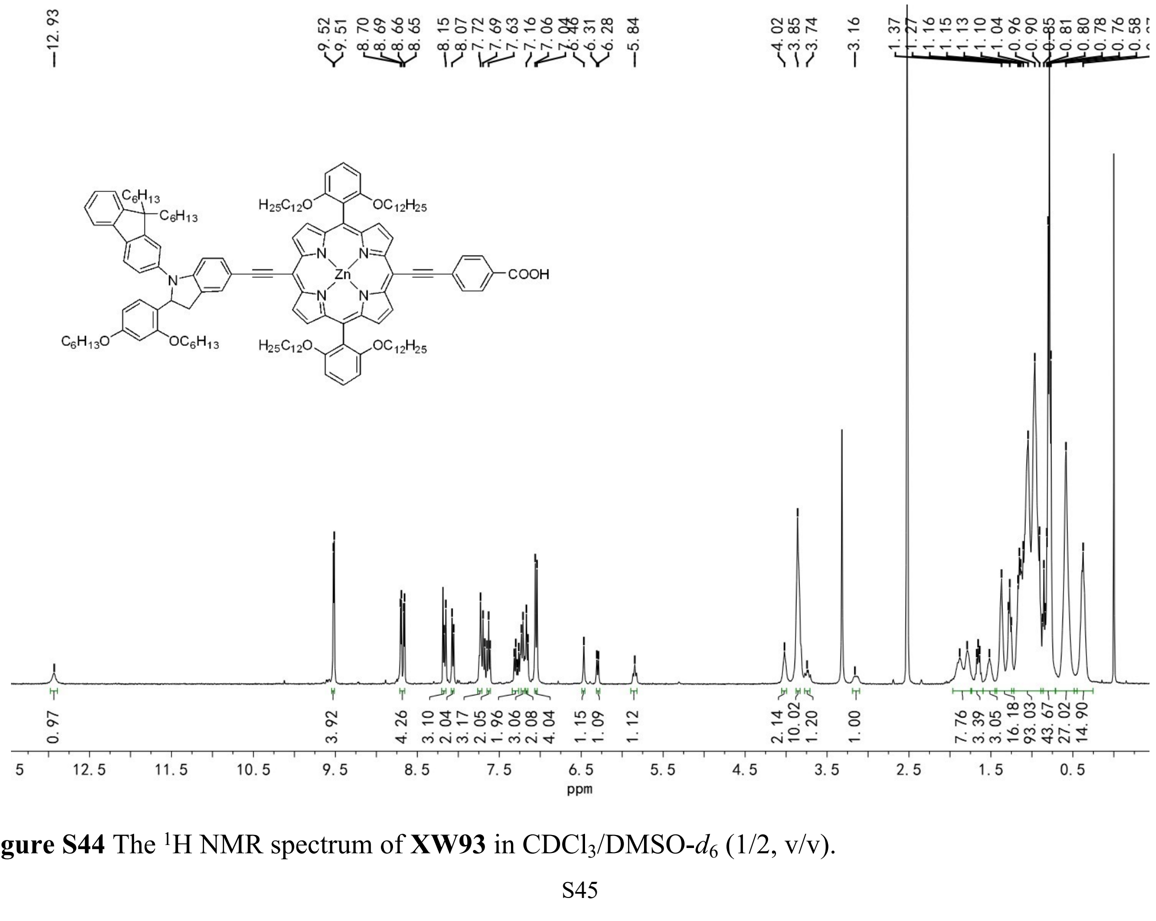


Figure S44 The ^1H NMR spectrum of **XW93** in $CDCl_3$/DMSO-d_6 (1/2, v/v).

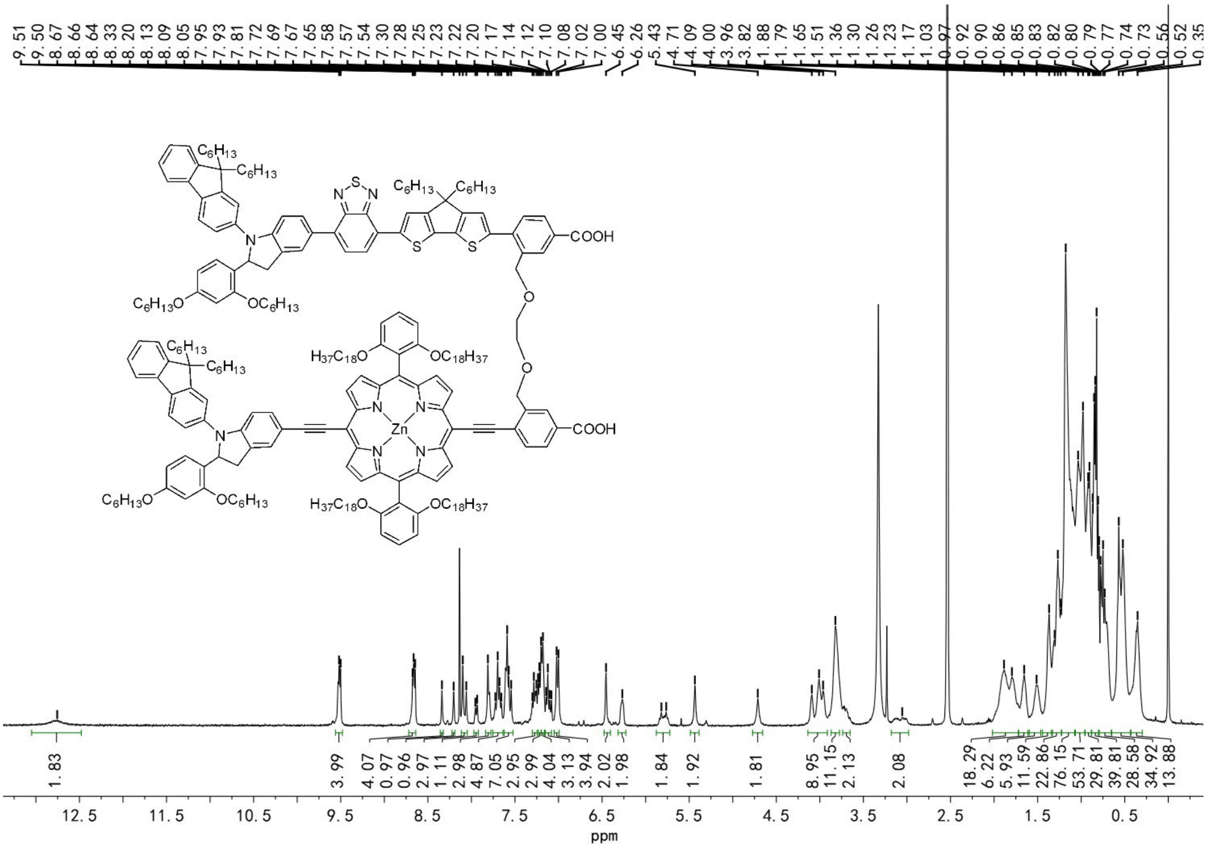


Figure S45 The ^{1}H NMR spectrum of **XW94** in $CDCl_3$/DMSO-d_6 (1/2, v/v).

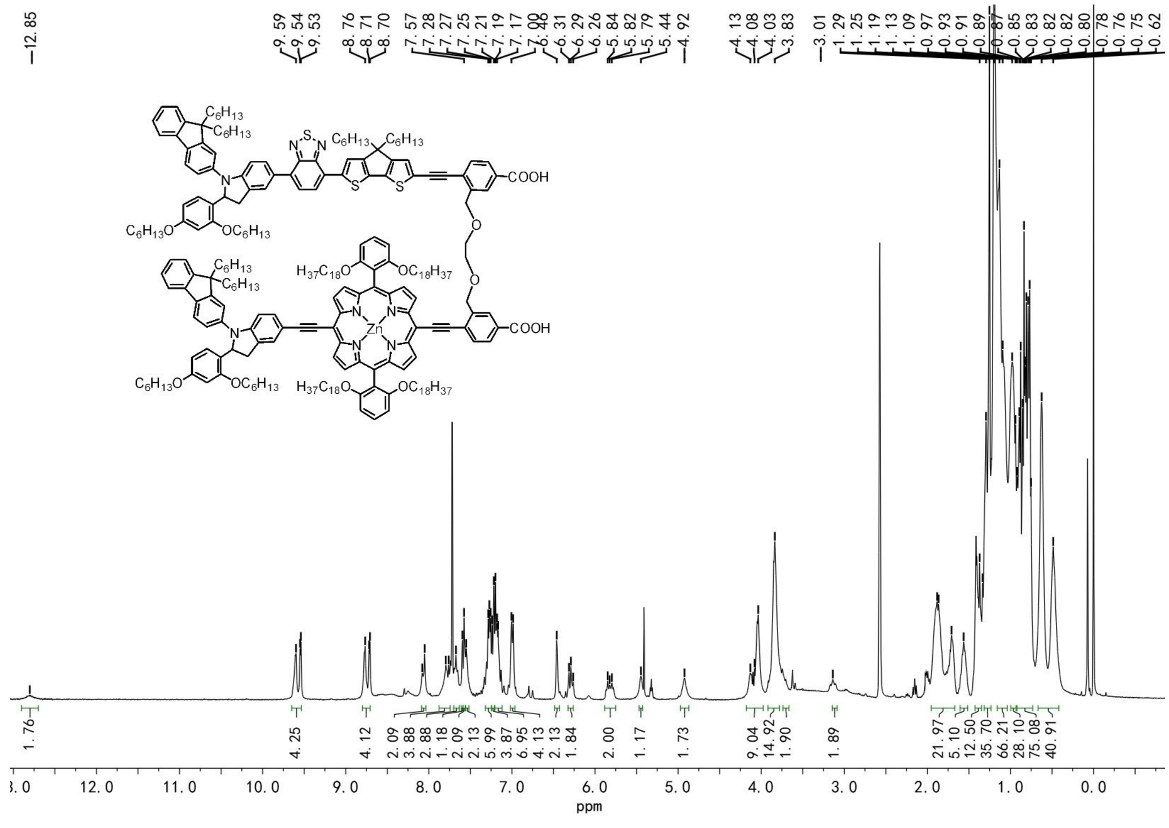


Figure S46 The ^{1}H NMR spectrum of **XW95** in $CDCl_3$/DMSO-d_6 (1/2, v/v).

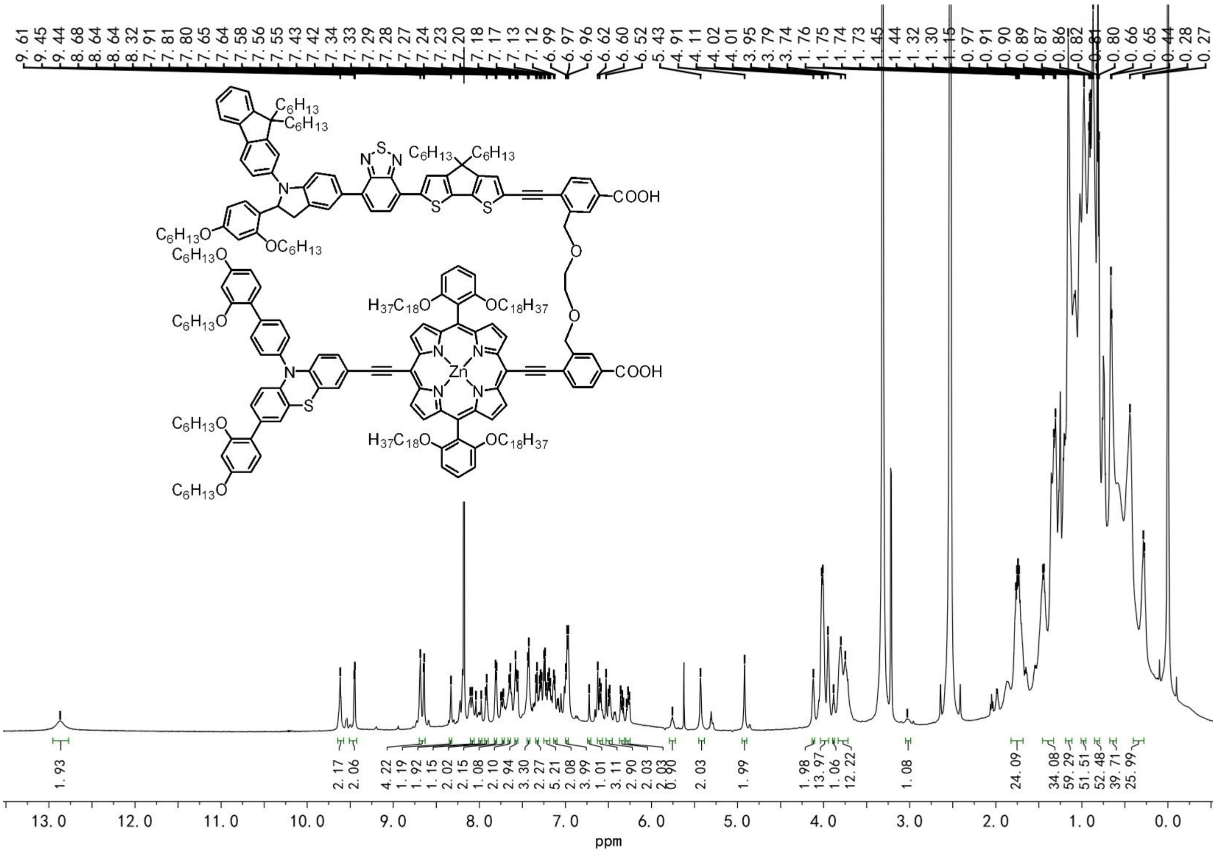


Figure S47 The ^{1}H NMR spectrum of **XW96** in $CDCl_3$/DMSO-d_6 (1/2, v/v).

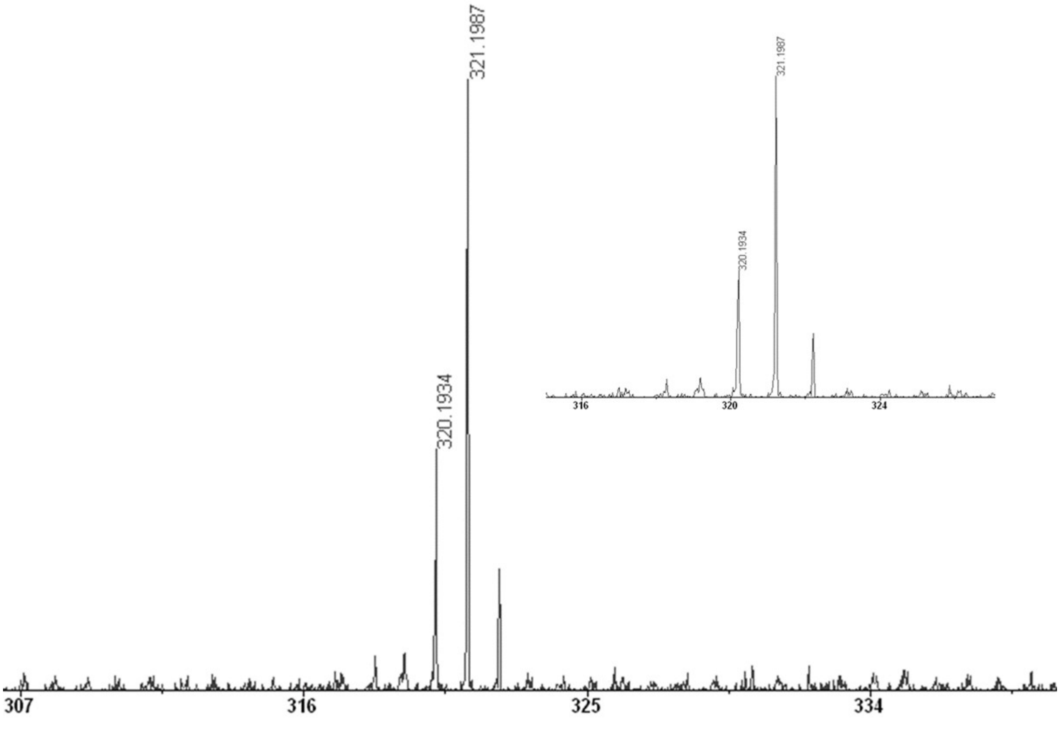


Figure S48 The MALDI-TOF MS of compound 2,4-dihexyloxyacetophenone.

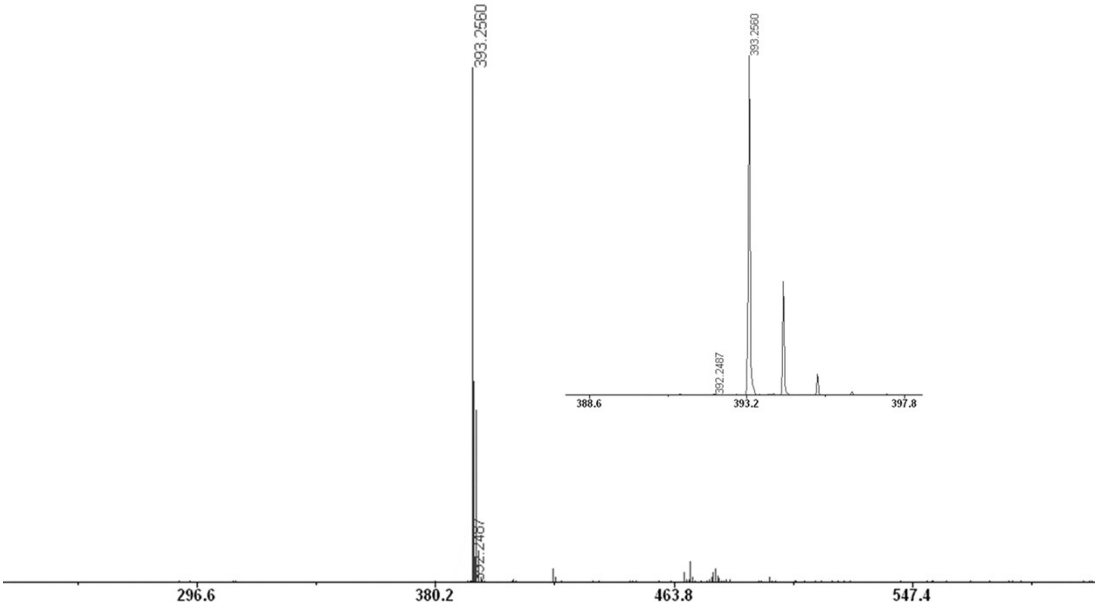


Figure S49 The MALDI-TOF MS of compound **D_4-a**.

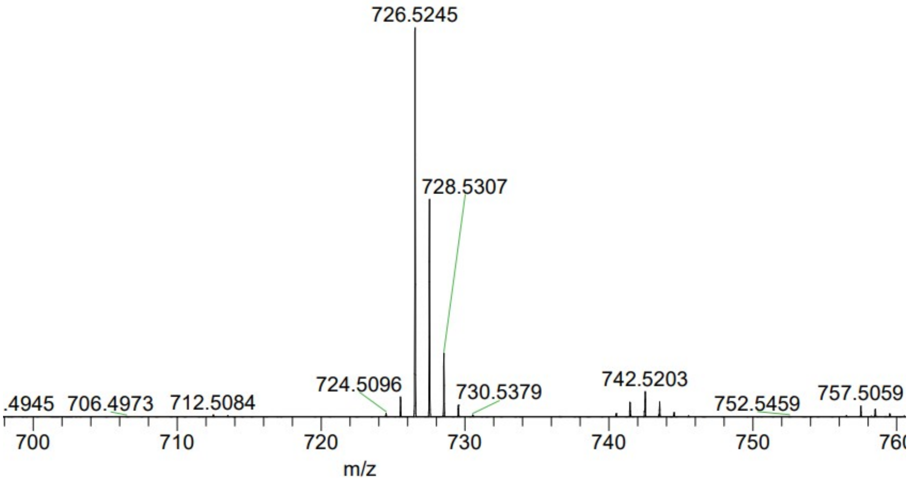


Figure S50 The HRMS of compound **D_4-b**.

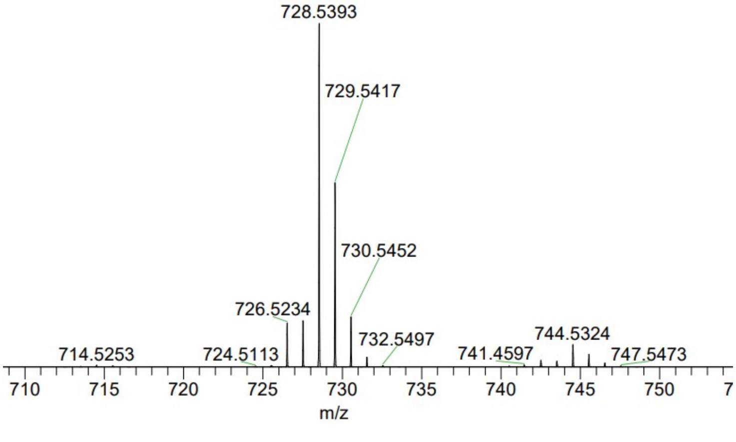


Figure S51 The HRMS of compound **D_4-c**.

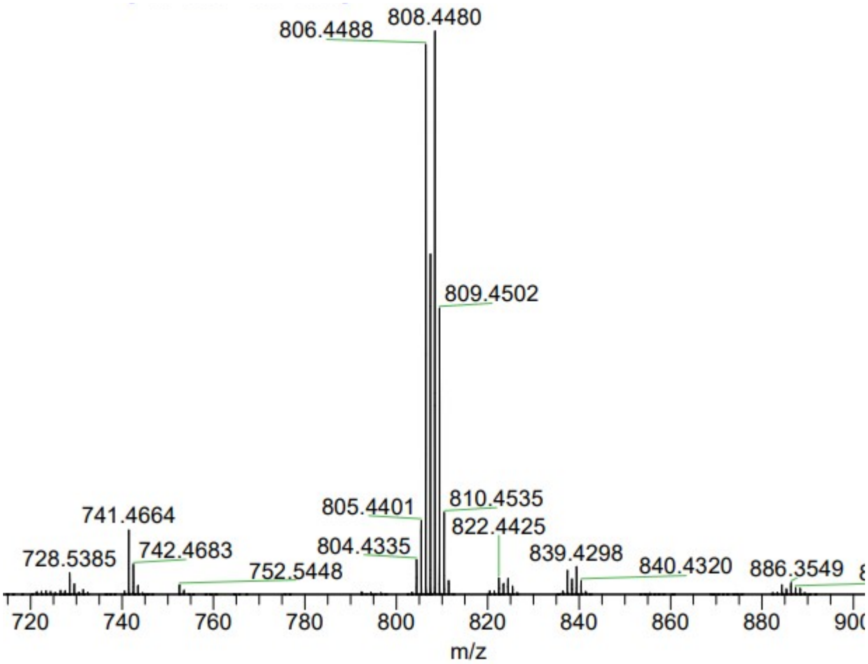


Figure S52 The HRMS of compound **D_4-Br**.

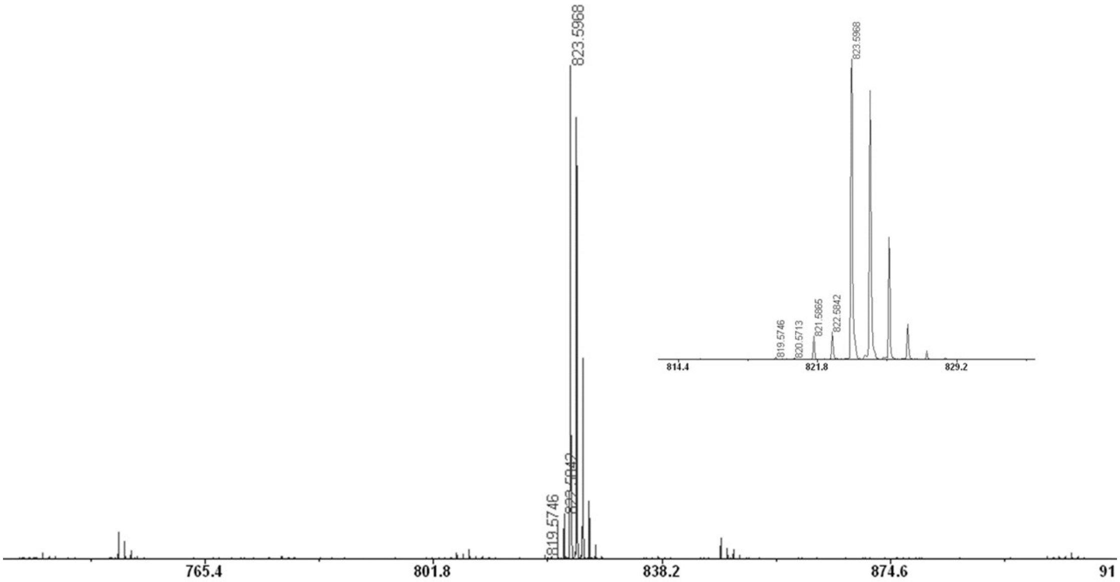


Figure S53 The MALDI-TOF MS of compound **D_4-d**.

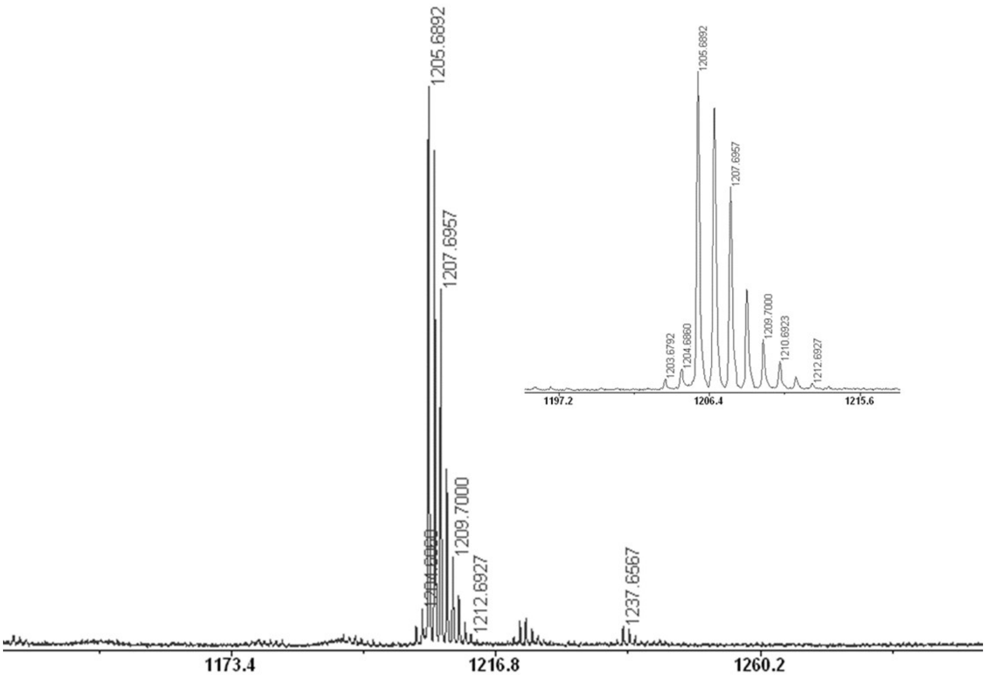


Figure S54 The MALDI-TOF MS of compound **O-a**.

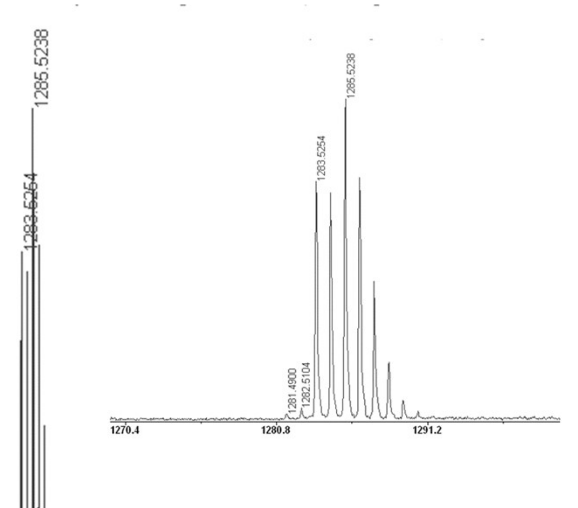


Figure S55 The MALDI-TOF MS of compound **O-Br**.

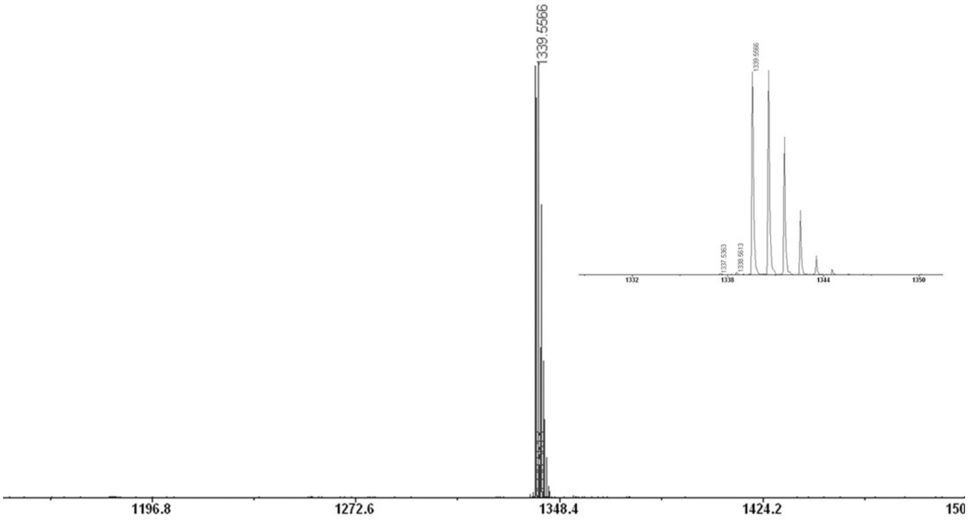


Figure S56 The MALDI-TOF MS of compound **O-b**.

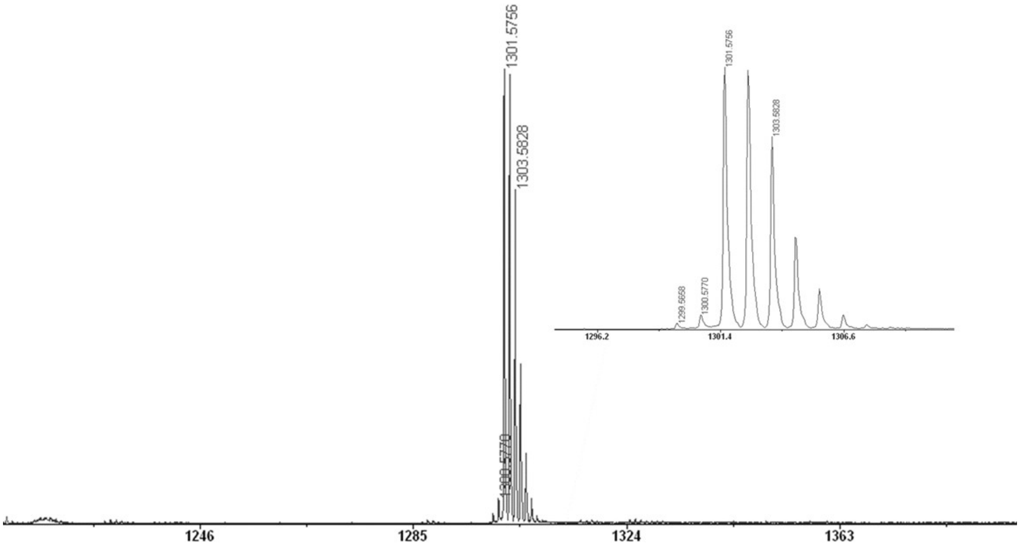


Figure S57 The MALDI-TOF MS of compound **O-c**.

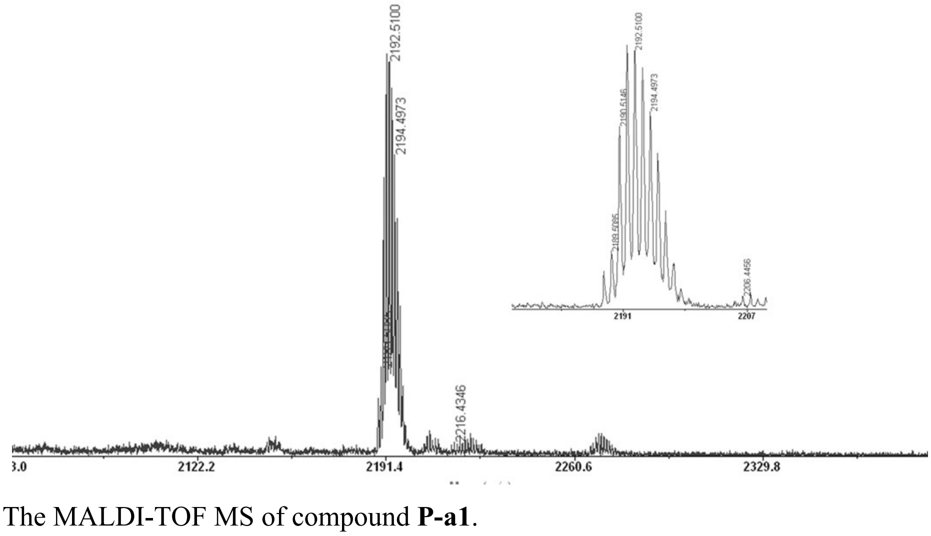


Figure S58 The MALDI-TOF MS of compound **P-a1**.

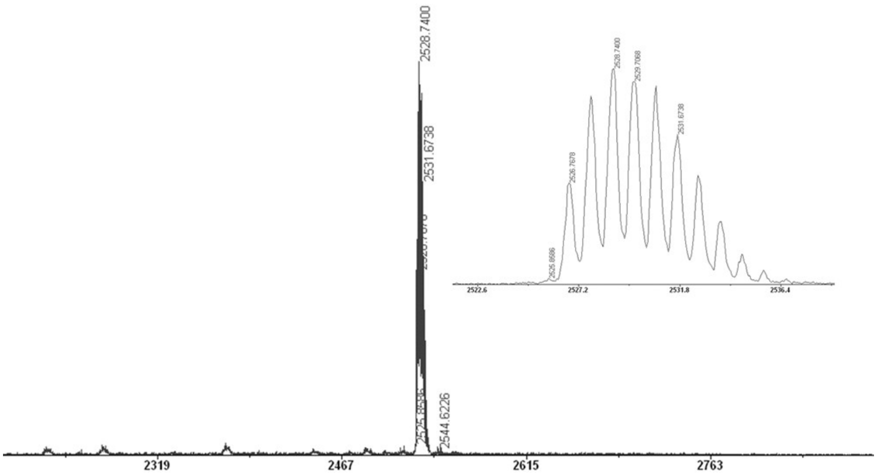


Figure S59 The MALDI-TOF MS of compound **P-a2**.

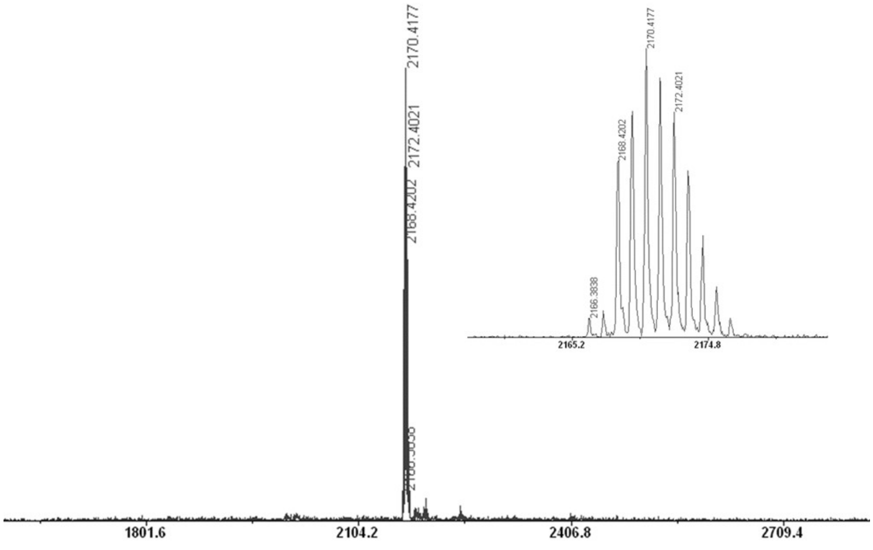


Figure S60 The MALDI-TOF MS of compound **P-b1**.

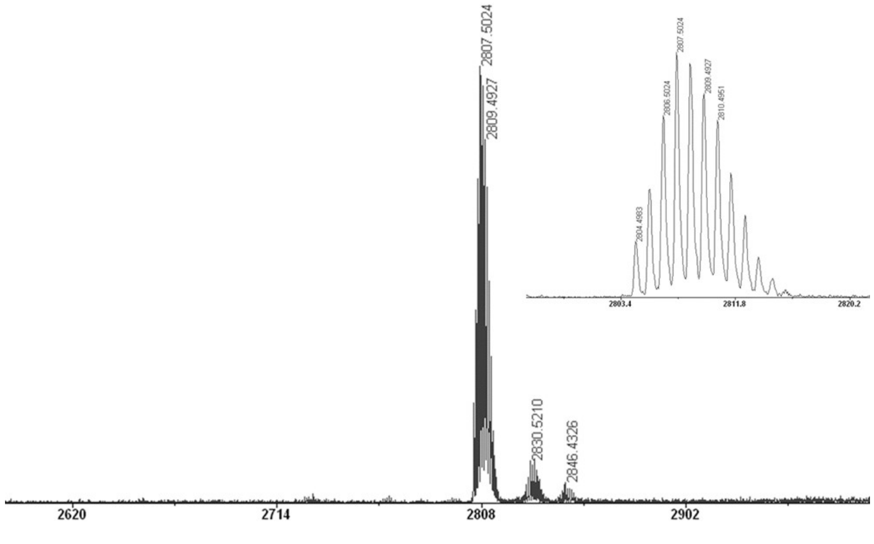


Figure S61 The MALDI-TOF MS of compound **P-b2**.

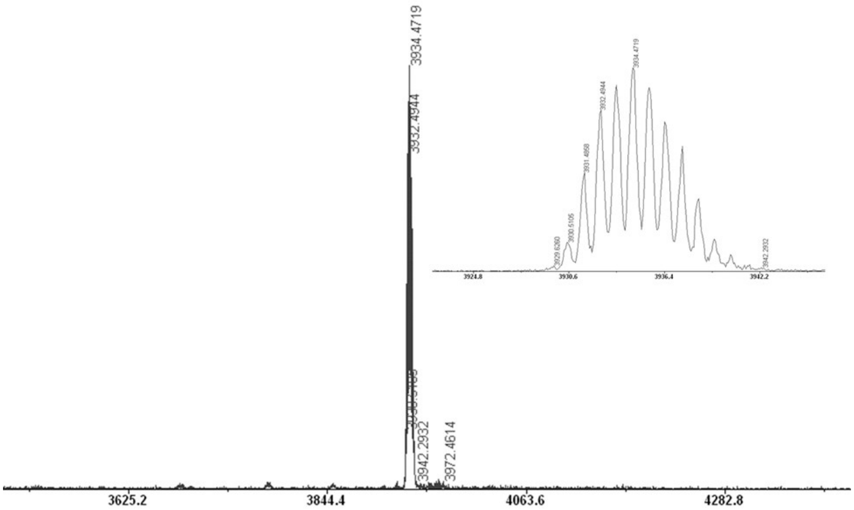


Figure S62 The MALDI-TOF MS of compound **P-c1**.

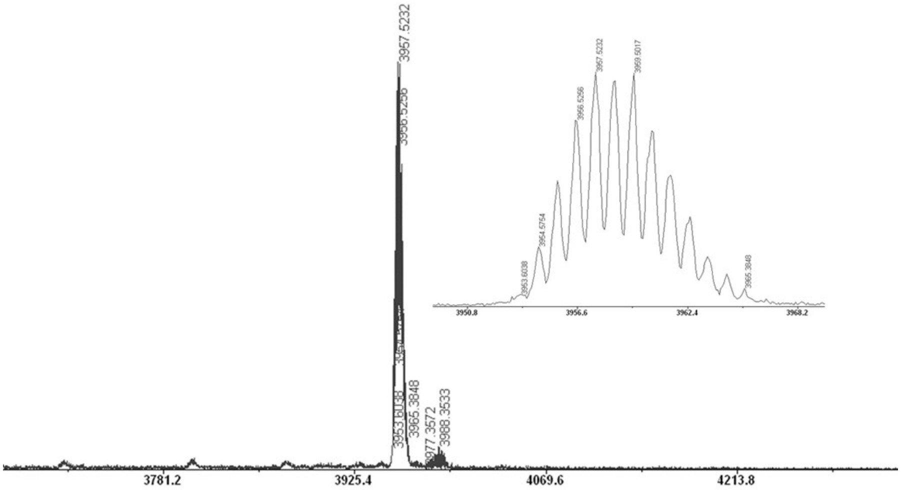


Figure S63 The MALDI-TOF MS of compound **P-c2**.

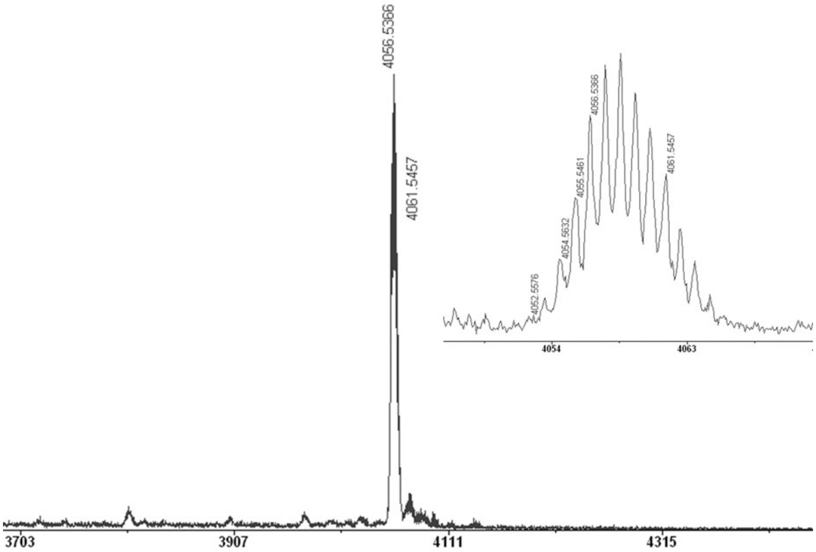


Figure S64 The MALDI-TOF MS of compound **P-c3**.

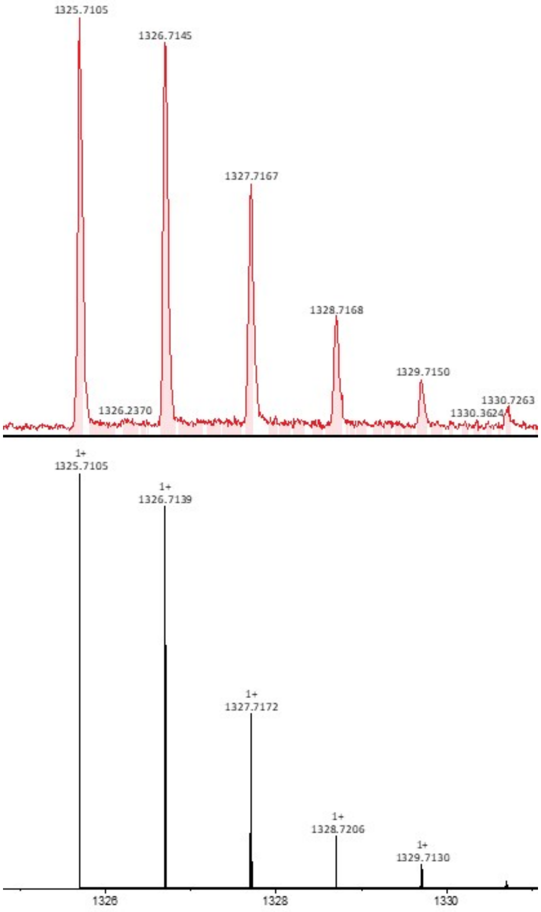


Figure S65 The MALDI-TOF MS of **Y3**.

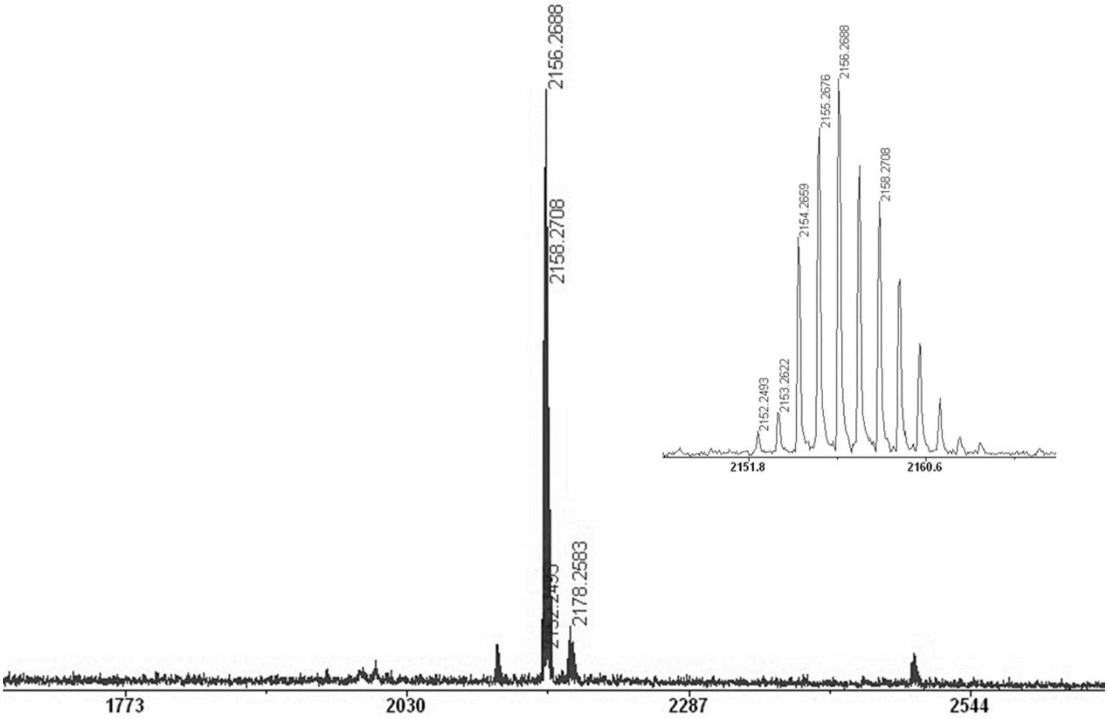


Figure S66 The MALDI-TOF MS of **XW93**.

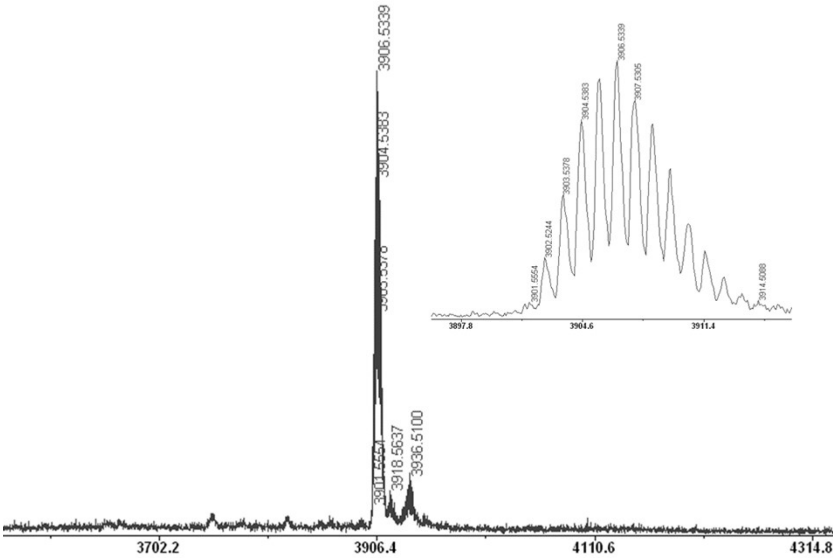


Figure S67 The MALDI-TOF MS of **XW94**.

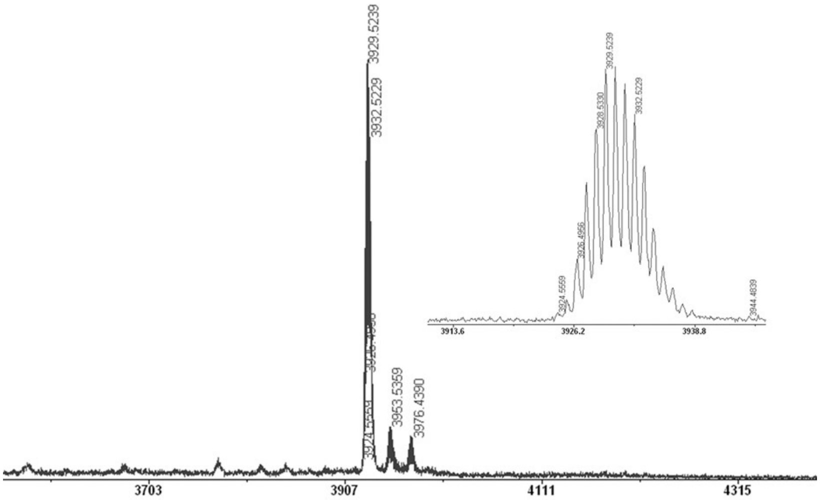


Figure S68 The MALDI-TOF MS of **XW95**.

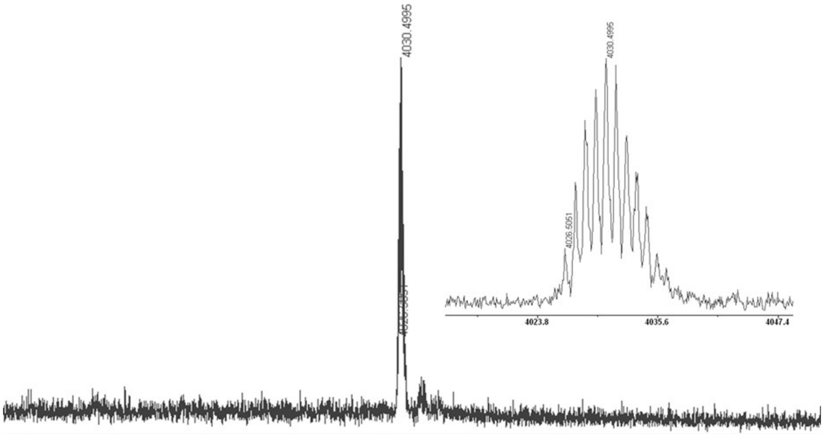


Figure S69 The MALDI-TOF MS of **XW96**.

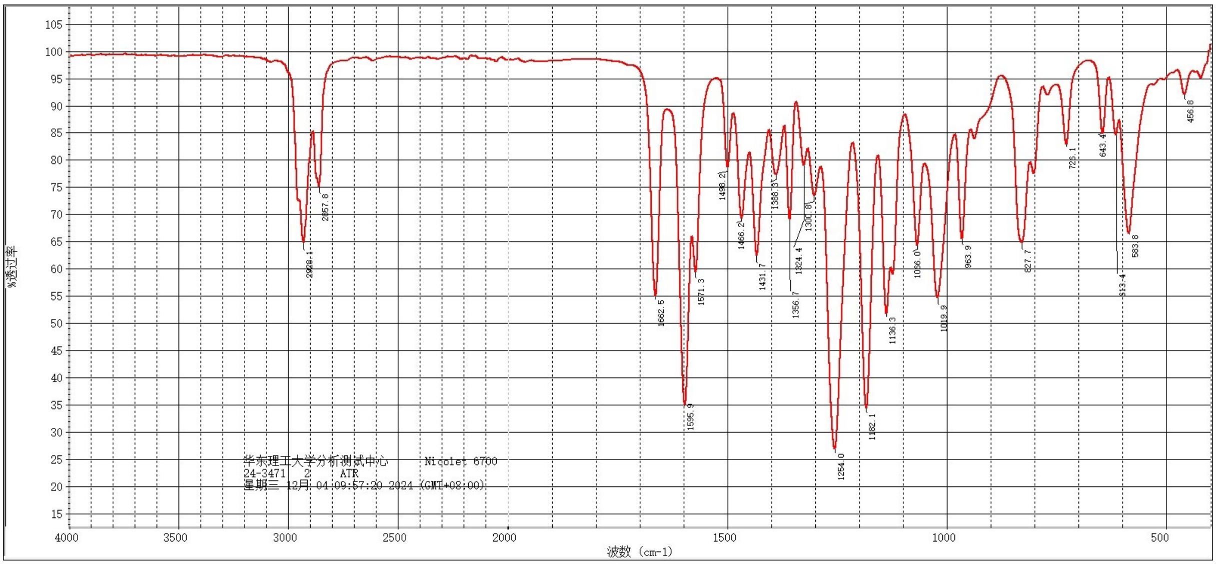


Figure S70 The IR spectrum of 2,4-dihexyloxyacetophenone.

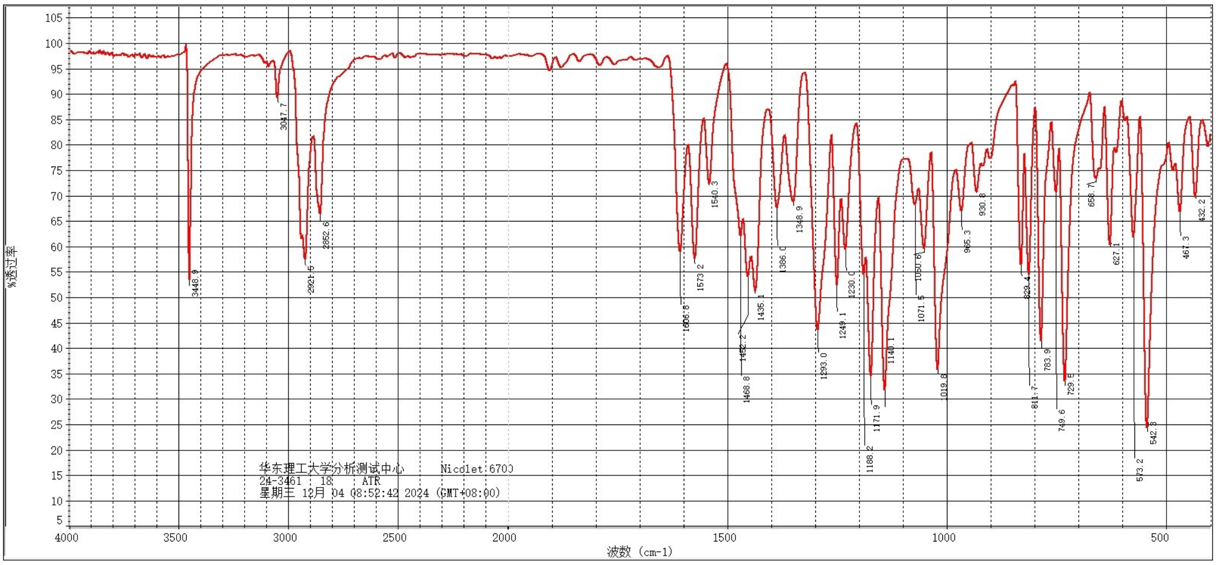


Figure S71 The IR spectrum of compound **D_4-a**.

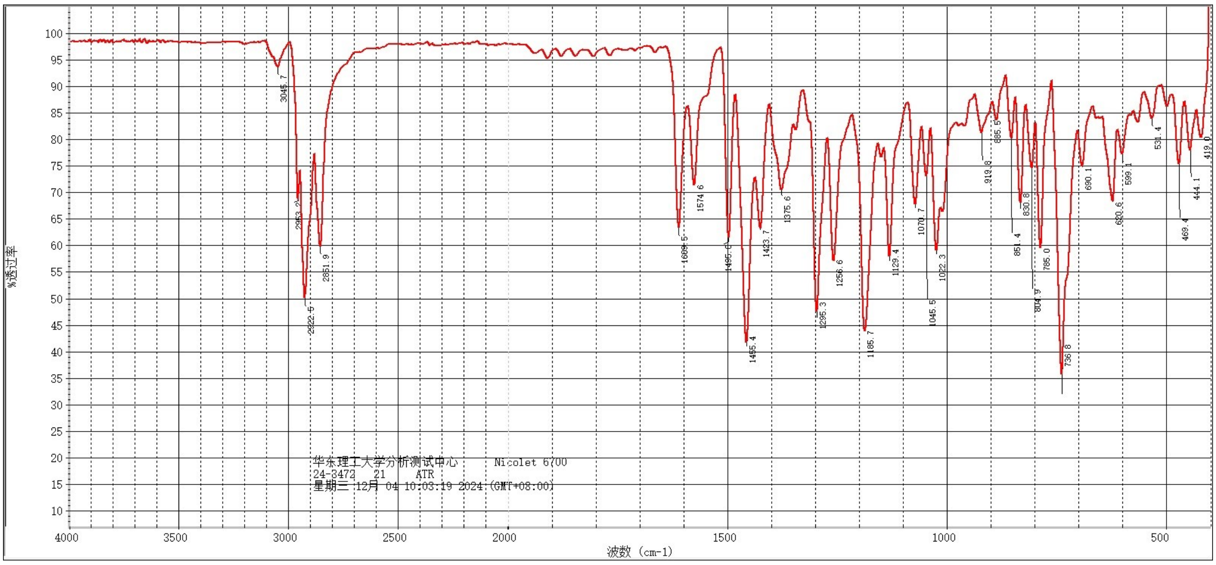


Figure S72 The IR spectrum of compound **D$_4$-b**.

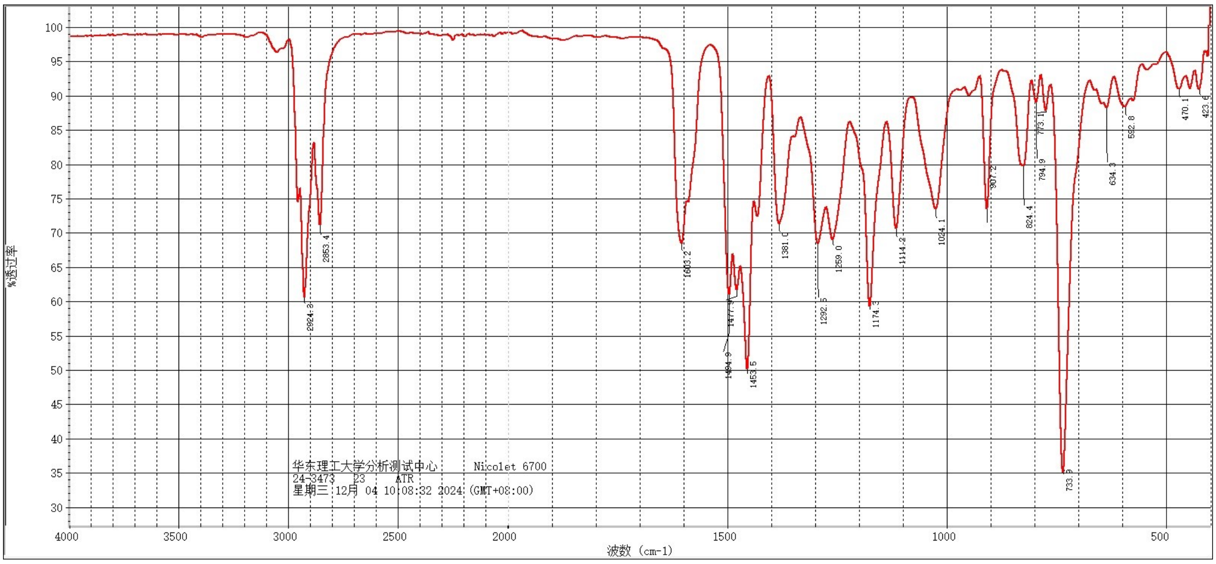


Figure S73 The IR spectrum of compound **D$_4$-c**.

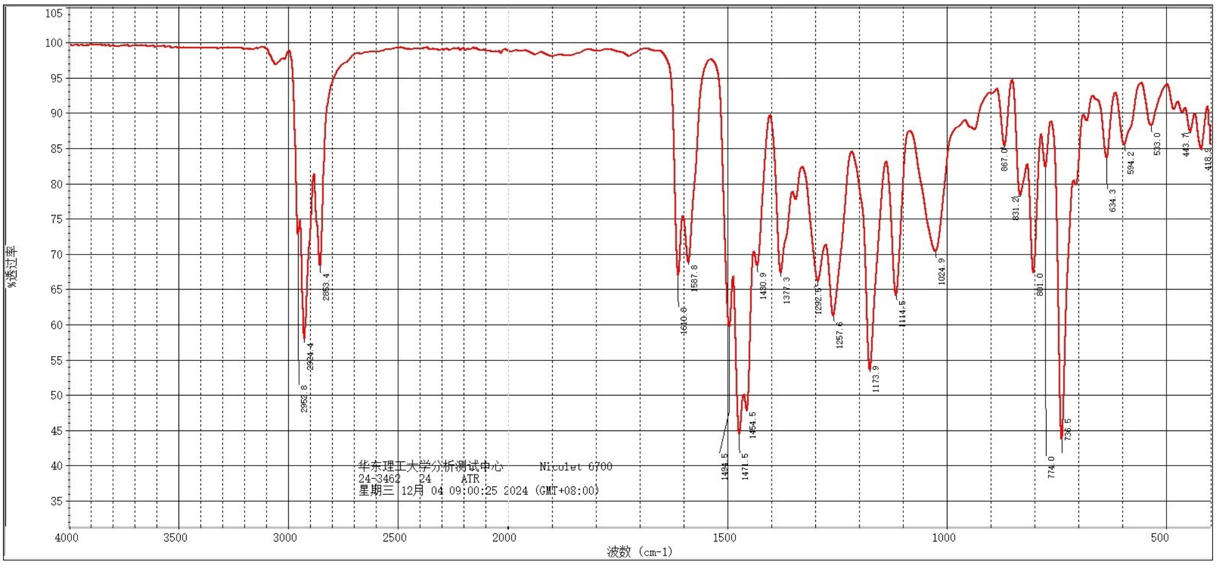


Figure S74 The IR spectrum of compound **D_4-Br**.

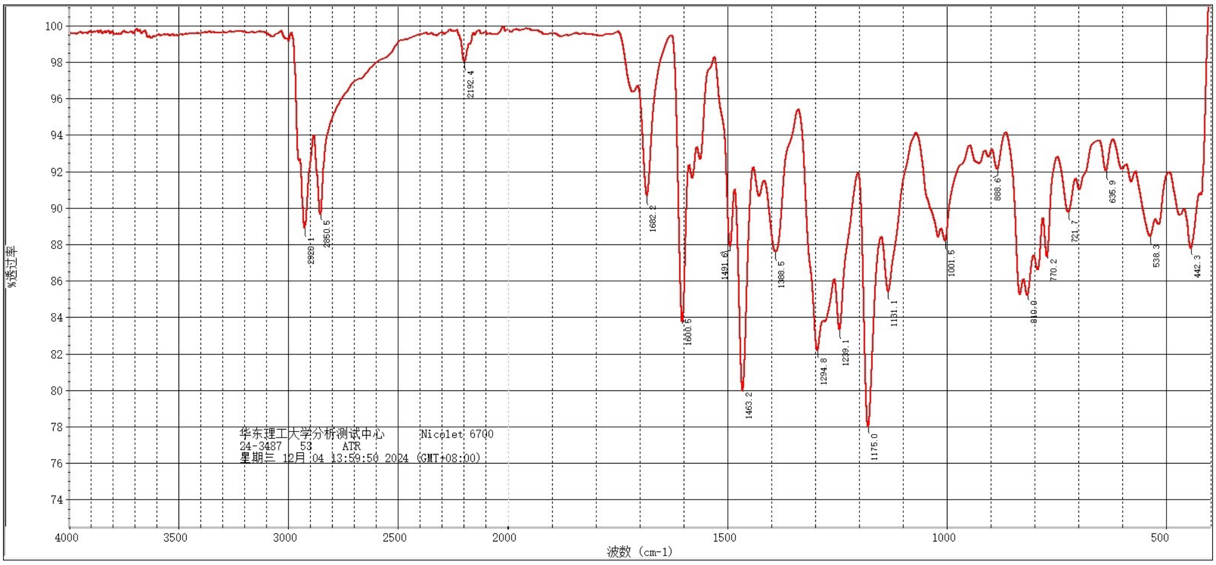


Figure S75 The IR spectrum of compound **D_4-d**.

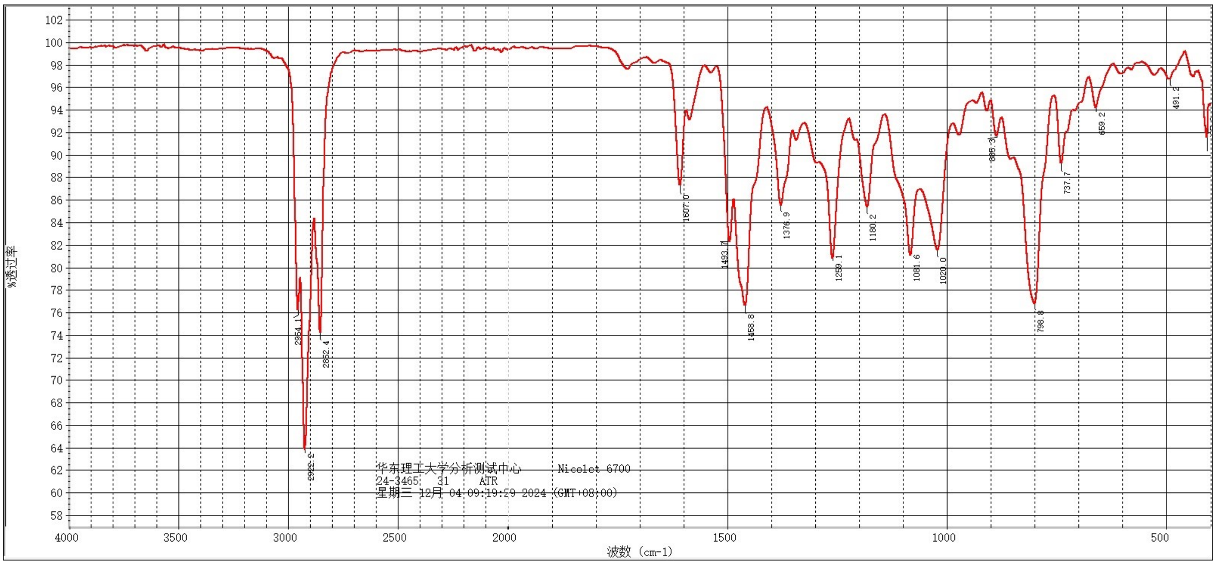


Figure S76 The IR spectrum of compound **O-a**.

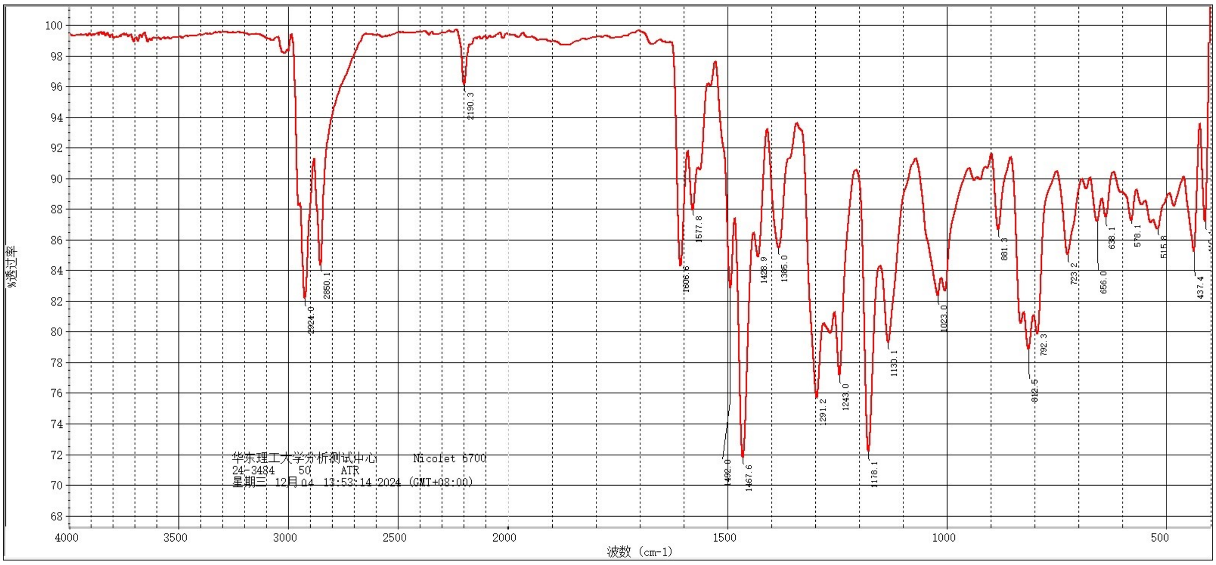


Figure S77 The IR spectrum of compound **O-Br**.

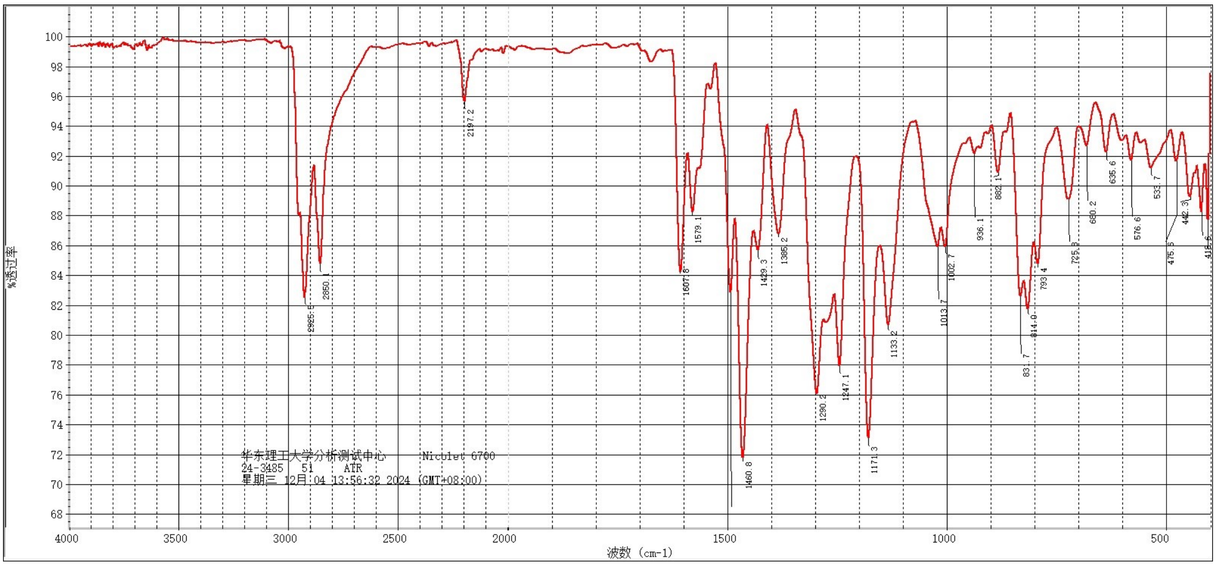


Figure S78 The IR spectrum of compound **O-b**.

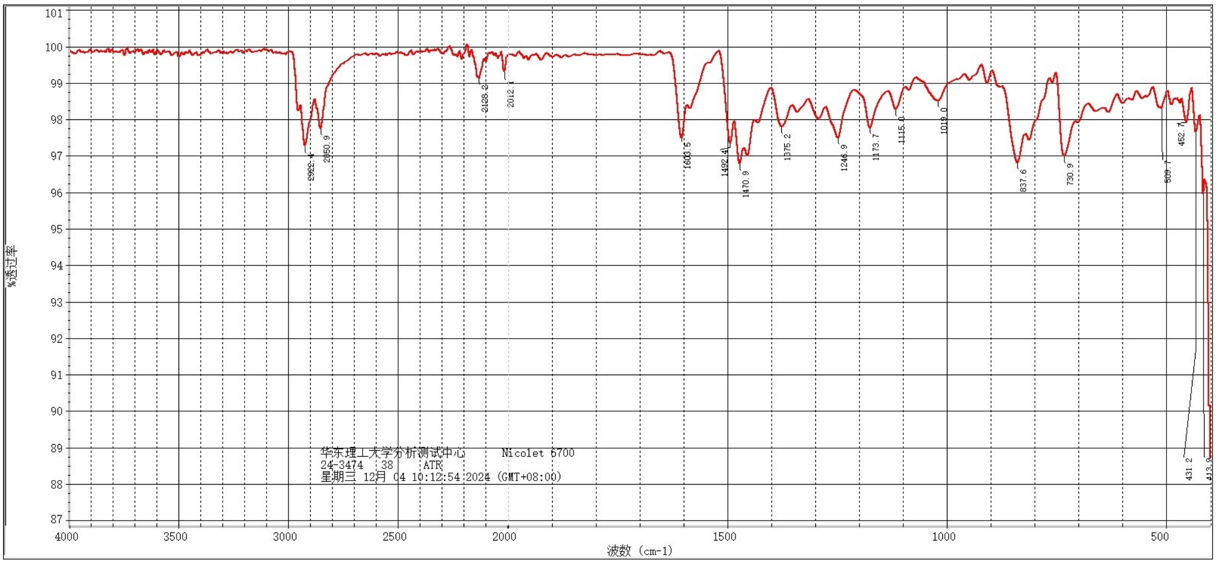


Figure S79 The IR spectrum of compound **O-c**.

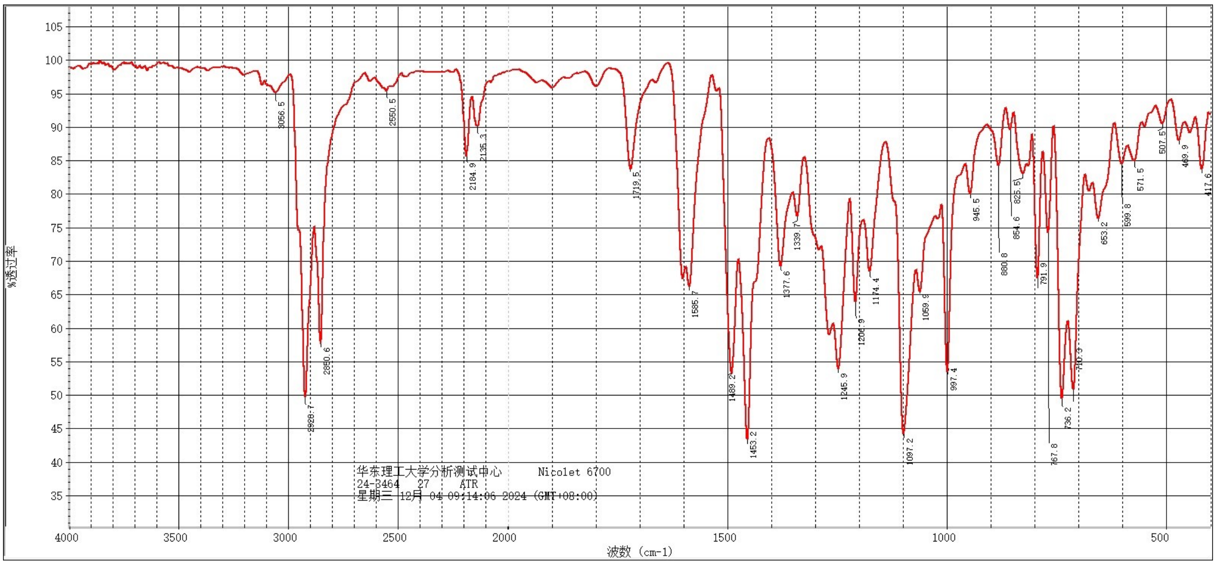


Figure S80 The IR spectrum of compound **P-a1**.

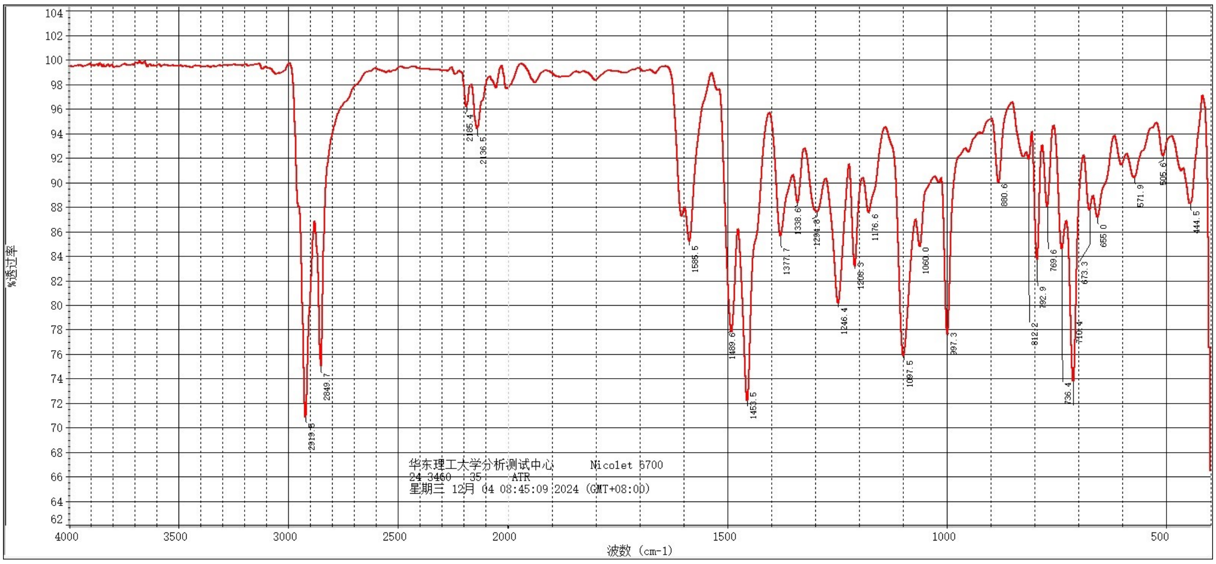


Figure S81 The IR spectrum of compound **P-a2**.

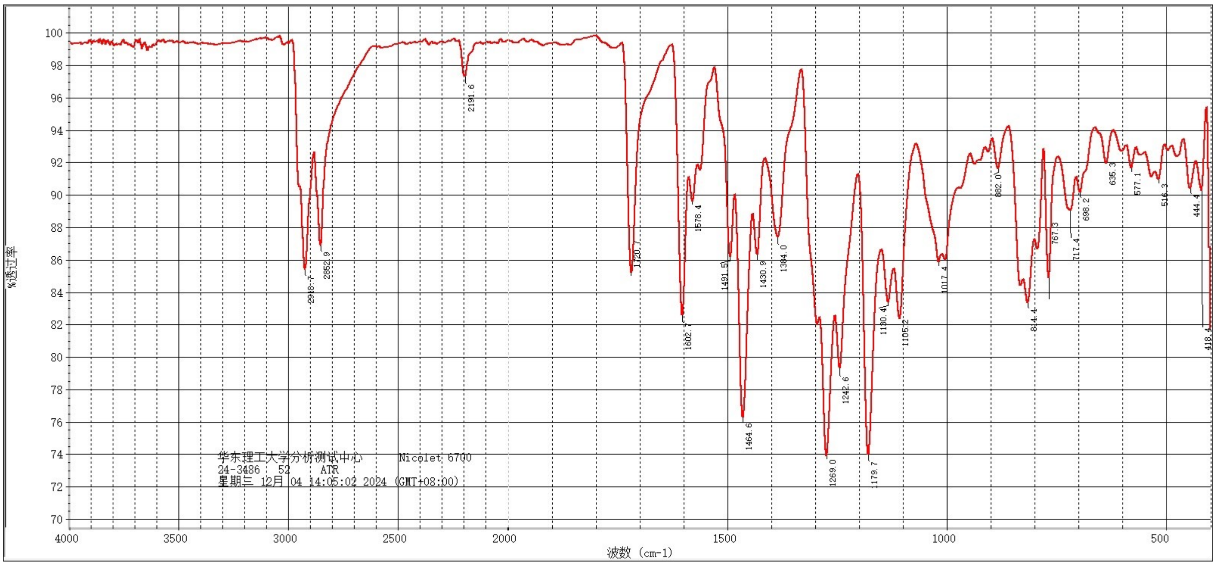


Figure S82 The IR spectrum of compound **P-b1**.

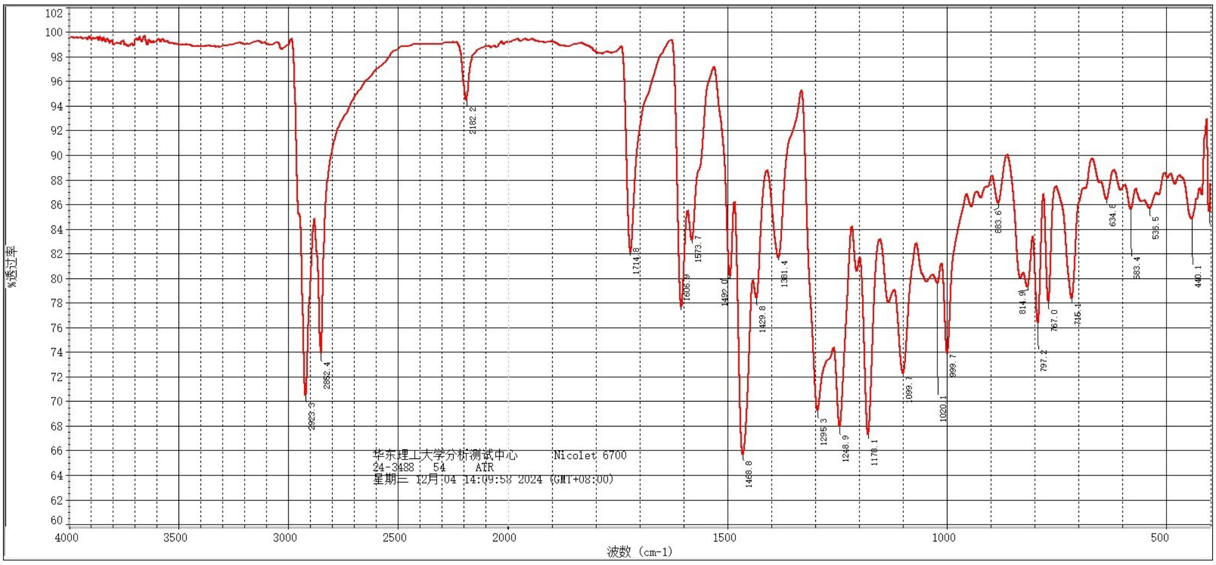


Figure S83 The IR spectrum of compound **P-b2**.

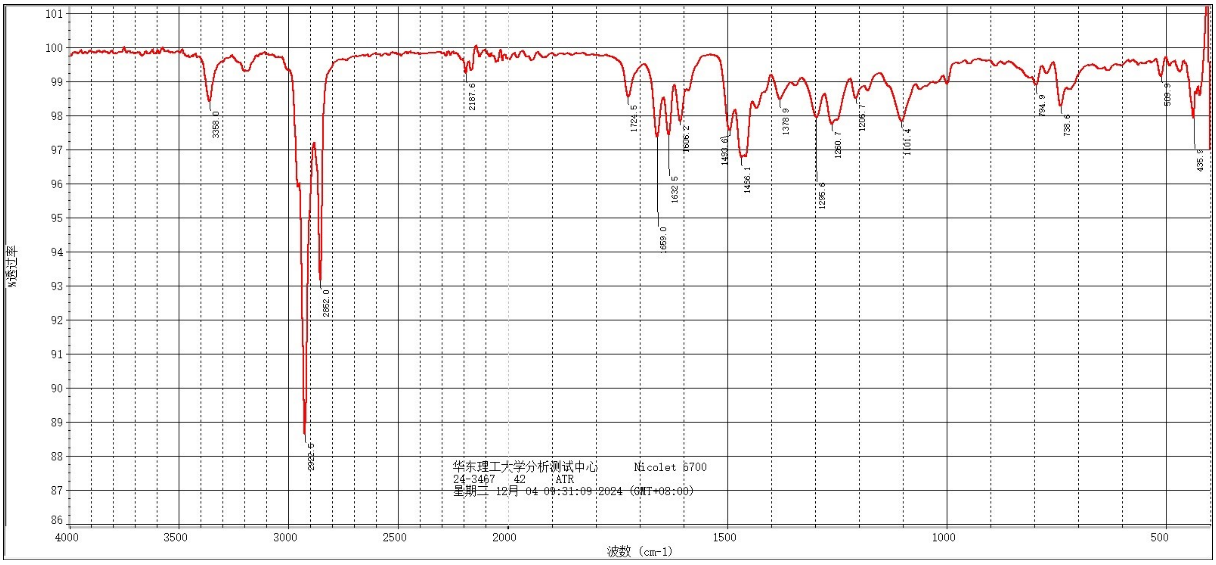


Figure S84 The IR spectrum of compound **P-c1**.

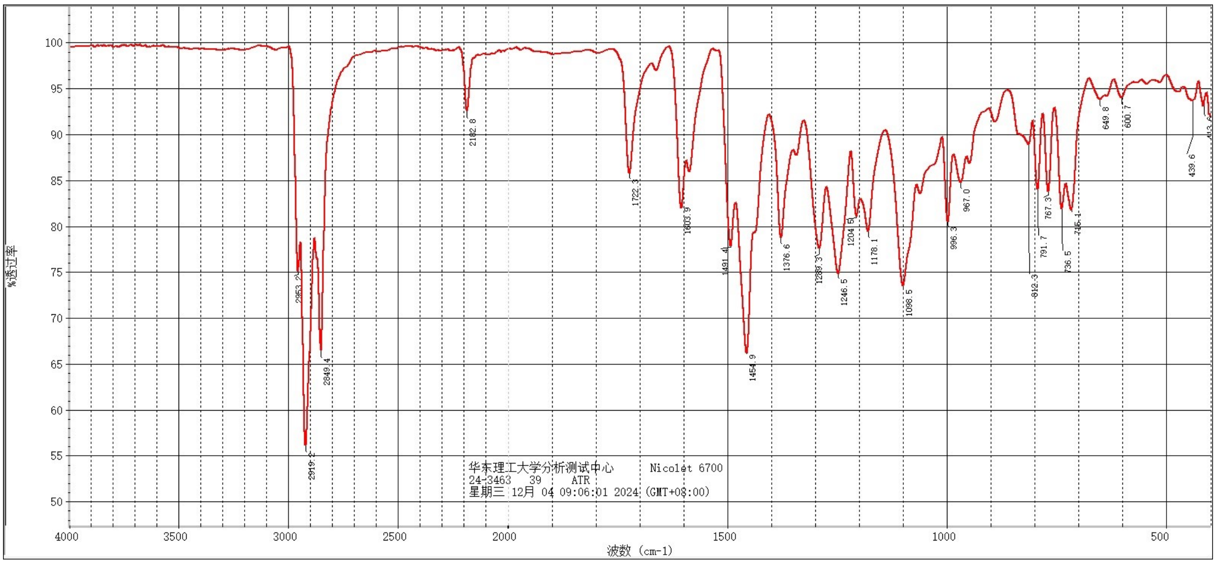


Figure S85 The IR spectrum of compound **P-c2**.

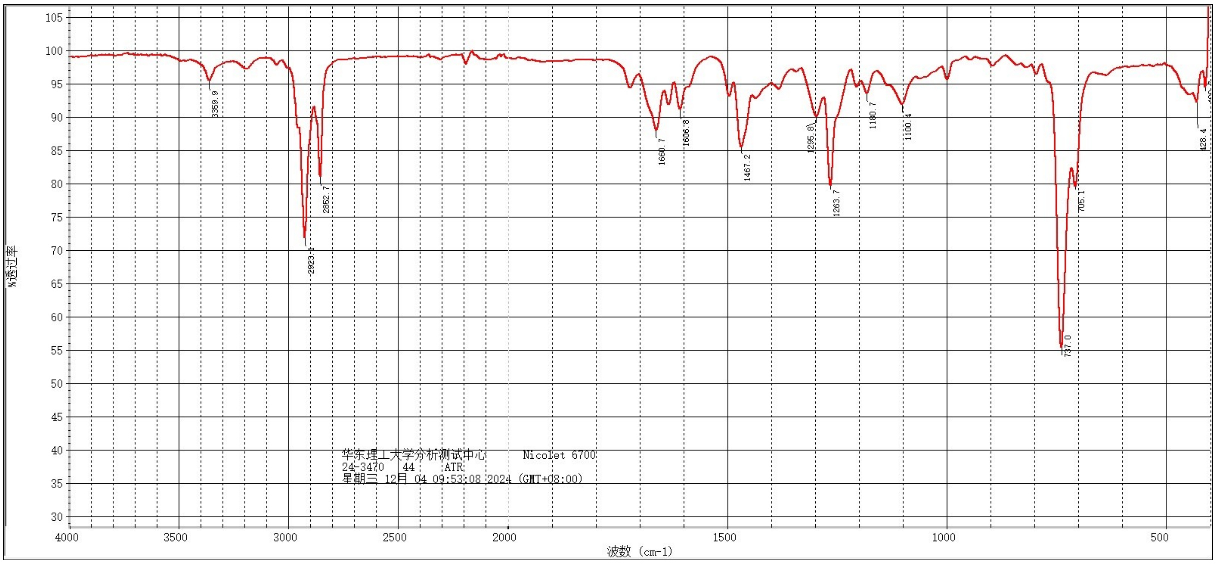


Figure S86 The IR spectrum of compound **P-c3**.

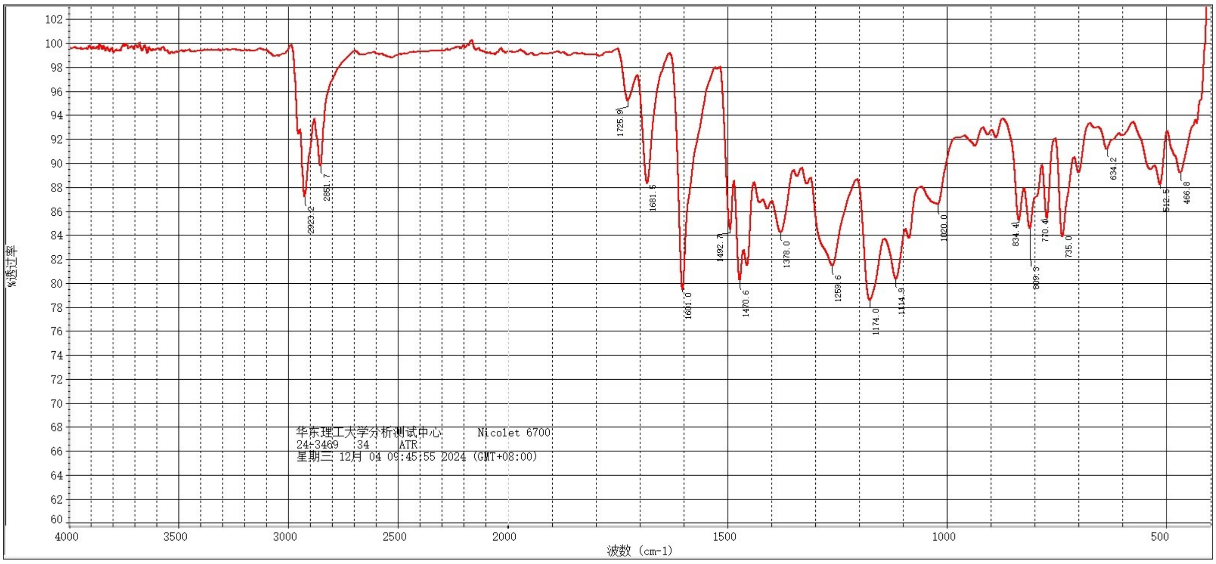


Figure S87 The IR spectrum of **Y3**.

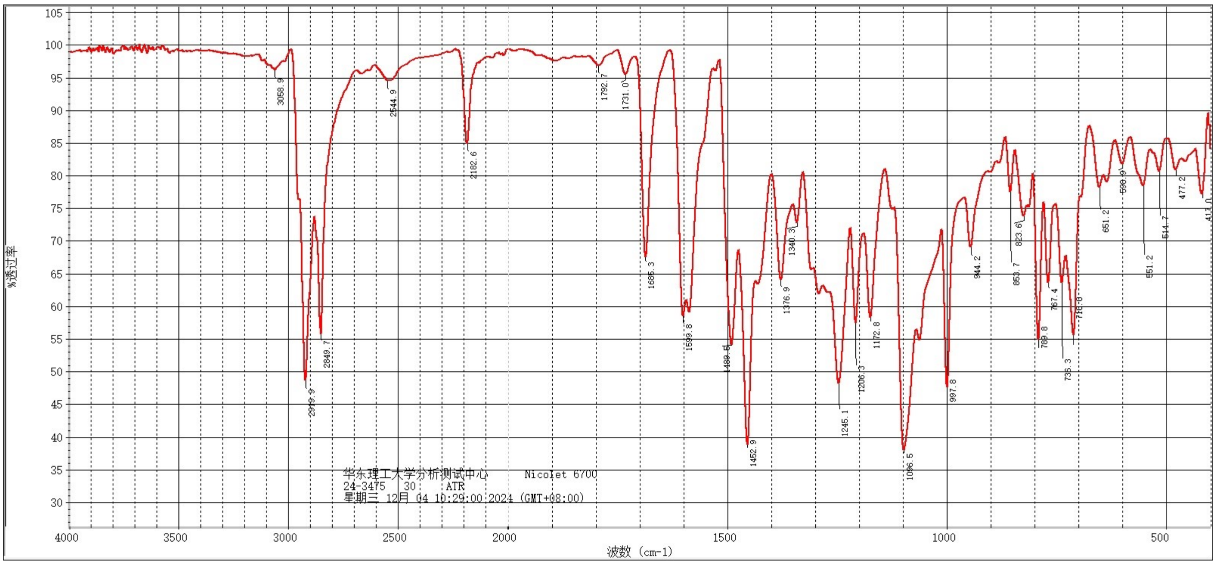


Figure S88 The IR spectrum of **XW93**.

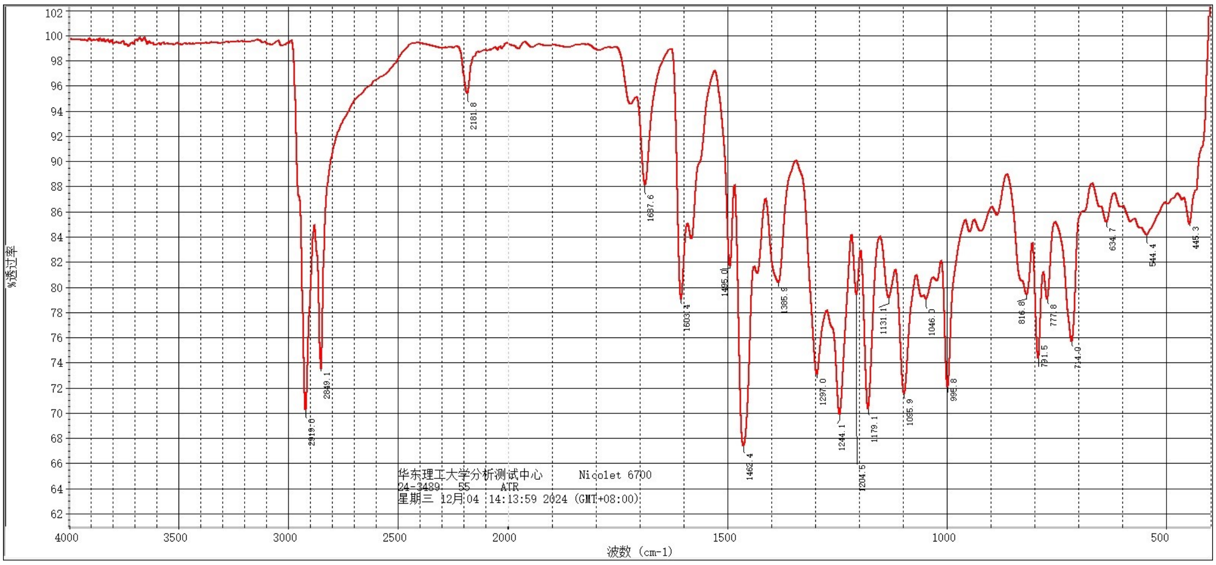


Figure S89 The IR spectrum of **XW94**.

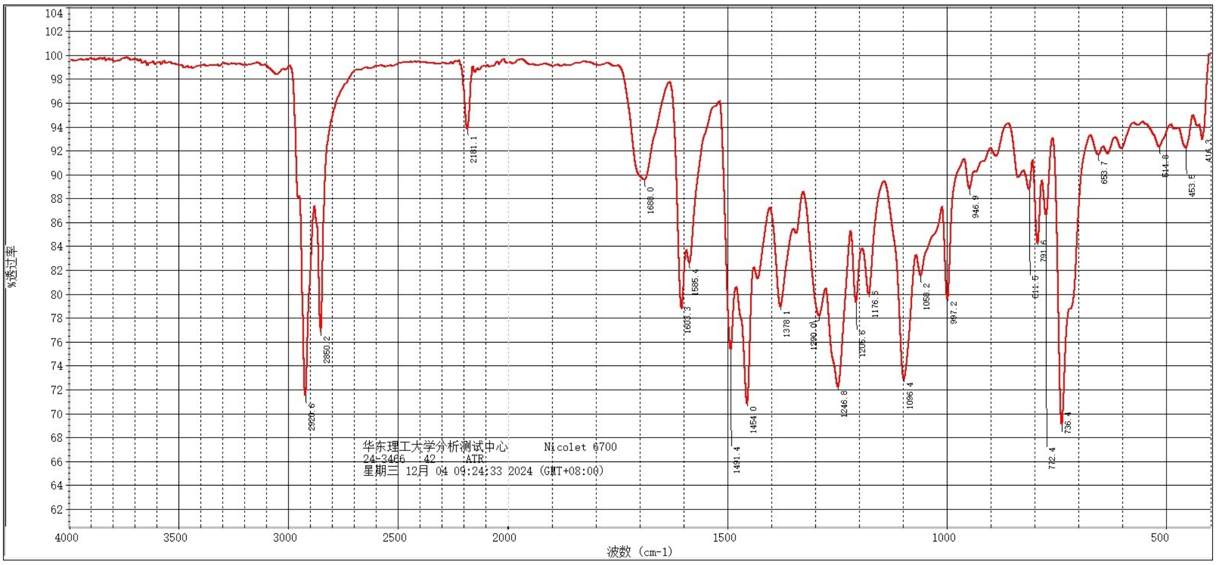


Figure S90 The IR spectrum of **XW95**.

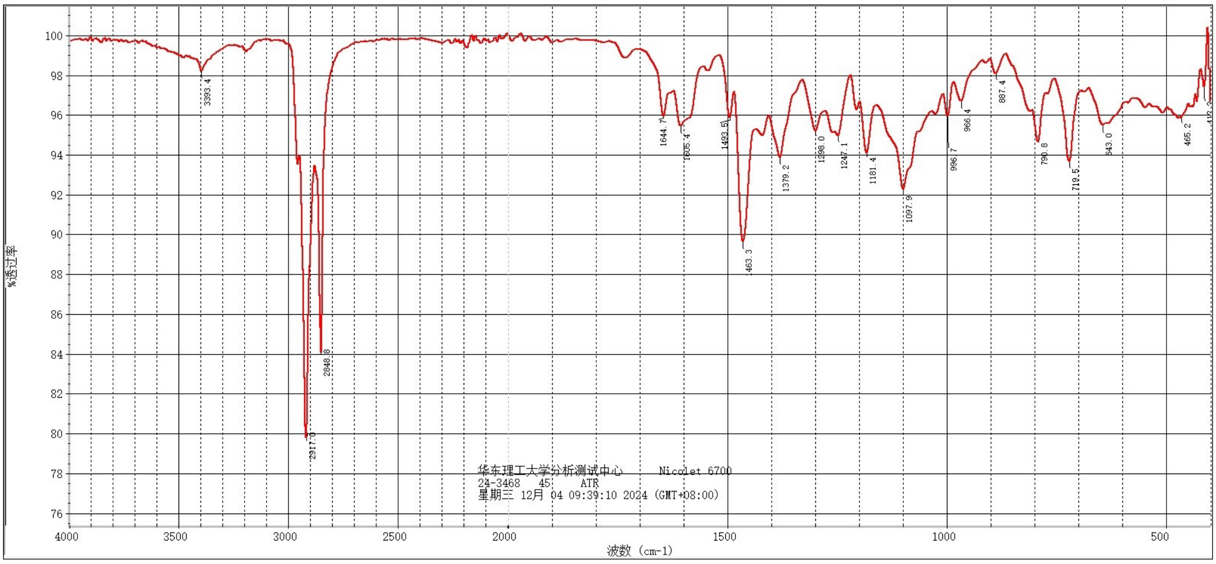


Figure S91 The IR spectrum of **XW96**.

8 Cartesian coordinates of the optimized structures

Y2

0 1

C	-4.37888400	2.00002100	-0.72745300
C	-5.12555400	0.79877100	-0.61768800
C	-3.00402600	1.98531700	-0.64046200
C	-2.31554900	0.76997200	-0.42284400
C	-3.07355700	-0.40835100	-0.32250200
H	-2.44641000	2.91594800	-0.76735000
H	-2.55887400	-1.35374300	-0.15531100
H	-5.01560600	-1.34422200	-0.28999200
N	-6.49791600	1.06973500	-0.69441000
C	-4.46540400	-0.41078900	-0.41015300
C	-5.37941400	3.06682200	-1.04607500
H	-5.54674900	3.00930200	-2.14251900
C	-6.63278400	2.48951700	-0.41136800
C	-0.85377200	0.76895600	-0.28118000
C	-0.02557700	-0.34349100	-0.65437600
C	-0.16126800	1.86109100	0.21744900
C	1.41973900	-0.28587700	-0.51350800
C	1.24301100	1.91609800	0.35419700
H	-0.73064500	2.73035700	0.55227600
C	2.08689600	0.87231000	0.00581900
H	1.67015600	2.83126200	0.76717800
N	-0.43812000	-1.50297700	-1.16697200
N	2.02703800	-1.39685700	-0.91861200
S	0.87403100	-2.41895100	-1.43311400
C	3.52789800	0.94454000	0.15879200
C	4.25756400	2.02027400	0.65859700
S	4.58513500	-0.38241300	-0.28922800
C	5.63868600	1.77835200	0.68002300
H	3.78929800	2.94560100	0.99400800
C	5.96010100	0.51341000	0.19409600
C	7.38351400	0.34731400	0.24962800
C	7.96076700	1.50194600	0.77097000
S	8.54968300	-0.84359800	-0.13407400
C	9.36187500	1.41414700	0.85621800
C	9.85084300	0.19836700	0.39954500
H	10.01189500	2.21129100	1.21777300
C	6.88967900	2.51368800	1.08685900
H	7.02412400	3.44949800	0.51816900

H	6.88111700	2.78721200	2.15562900
C	11.23357400	-0.25378600	0.33150600
C	12.24817300	0.43540700	1.02332800
C	11.60030400	-1.38503000	-0.42282900
C	13.56867100	0.01850600	0.95766600
H	11.99303300	1.30169000	1.63588600
C	12.91849600	-1.80690700	-0.48282000
H	10.83774300	-1.93270500	-0.98239600
C	13.91773000	-1.10886800	0.20400000
H	14.34389100	0.56092000	1.50080100
H	13.20467500	-2.68249600	-1.06890900
C	15.31142500	-1.59854900	0.10411800
O	15.65632600	-2.56396400	-0.53201500
O	16.18289300	-0.85361100	0.80261300
H	17.05118800	-1.26112800	0.66698700
C	-5.47386300	4.52723100	-0.65310000
H	-5.16448700	4.66777300	0.39460000
H	-4.85792100	5.19392500	-1.27261800
C	-7.71276900	3.41170500	-0.93841600
H	-7.94171600	3.15973500	-1.98535400
H	-8.65616400	3.37944700	-0.37611500
C	-7.00180000	4.79616100	-0.82837100
H	-7.39482600	5.37388000	0.02096300
H	-7.19712400	5.39922900	-1.72698700
H	-6.55128400	2.64304600	0.68879800
C	-7.52395500	0.14400000	-0.50595800
C	-7.50246200	-1.08618700	-1.18960300
C	-8.60803600	0.44536300	0.33677600
C	-8.52607500	-2.01252400	-1.02659900
H	-6.68223100	-1.29484500	-1.87806400
C	-9.63386200	-0.47508000	0.48331900
H	-8.63081500	1.39287800	0.87811200
C	-9.59941100	-1.70884600	-0.18799500
H	-8.49095200	-2.95954500	-1.57057500
C	-10.89020100	-0.35252000	1.33061800
C	-10.80227800	-2.46295300	0.16377300
C	-11.56834100	-1.68489800	1.05217500
C	-11.75723600	0.82076100	0.85891300
C	-10.54546900	-0.20513900	2.81712900
C	-11.24074300	-3.72764800	-0.22903300
C	-12.77122900	-2.16741900	1.54993100
H	-11.22898300	1.77691200	1.00023200
H	-12.69664000	0.86556800	1.43144100
H	-12.00789600	0.71968700	-0.20705500

H	-9.91996100	-1.04216600	3.15966600
H	-9.99731900	0.73238100	2.99981000
H	-11.46099400	-0.18606400	3.42843000
C	-12.45066600	-4.20636200	0.27347400
H	-10.64893600	-4.33557700	-0.91775200
C	-13.21096300	-3.43463200	1.15544400
H	-13.37179900	-1.56957400	2.24111800
H	-12.80762000	-5.19501900	-0.02495400
H	-14.15632200	-3.82491200	1.53974900

Y3

0 1

C	-3.79107200	1.28548400	-1.29024000
C	-4.50441100	0.30901700	-0.56904400
C	-2.41394300	1.32276500	-1.25241900
C	-1.69156800	0.38252200	-0.48338000
C	-2.42279300	-0.58135300	0.23097900
H	-1.87997000	2.06898200	-1.84532700
H	-1.88580100	-1.31058300	0.83627200
H	-4.34298300	-1.36475100	0.80959800
N	-5.86725300	0.50884100	-0.72864400
C	-3.81496500	-0.62610000	0.20689000
C	-6.90233000	-0.37231500	-0.43648800
C	-8.20075100	0.12246600	-0.19895300
C	-6.68743700	-1.76501500	-0.42105100
C	-9.25915500	-0.74050200	0.06493300
H	-8.37222500	1.19932500	-0.19971600
C	-7.74401500	-2.61503700	-0.14450400
H	-5.70182600	-2.16609000	-0.65982800
C	-9.03472500	-2.11567100	0.10427900
H	-10.25485800	-0.32954300	0.24885600
C	-7.72750600	-4.13409800	-0.07527500
C	-9.92924900	-3.24416400	0.35676500
C	-9.18163700	-4.43303300	0.25558100
C	-11.29192300	-3.28834500	0.65296900
C	-9.79197200	-5.66484200	0.44912200
C	-11.89902000	-4.52908700	0.84735100
H	-11.87640000	-2.36836500	0.73225600
C	-11.15750000	-5.70867200	0.74691900
H	-9.21801200	-6.59244400	0.37144300
H	-12.96540700	-4.57947700	1.08050900
H	-11.64855400	-6.67226200	0.90226200
C	-6.79209700	-4.62306000	1.03664100
H	-5.74942600	-4.34295400	0.81885300
H	-6.83535300	-5.71947000	1.12820300
C	-7.32839000	-4.74667200	-1.42282000
H	-7.99450200	-4.39711700	-2.22495400
H	-6.29562600	-4.47016400	-1.68650800
C	-4.77470700	2.13693900	-2.04127200
H	-4.54053100	3.20919500	-2.02556100
H	-4.83286700	1.82000600	-3.09678500
C	-6.10065400	1.83359600	-1.30770000
H	-6.93768900	1.77892600	-2.01887500

H	-7.07237000	-4.18531000	2.00582200
H	-7.38462300	-5.84555200	-1.38219600
C	-0.22668600	0.45219300	-0.42036200
C	0.60914300	-0.69617400	-0.20560900
C	0.46258200	1.64463600	-0.57800300
C	2.05734700	-0.57715700	-0.17226900
C	1.86927900	1.75903800	-0.54540000
H	-0.11053100	2.56420800	-0.71111000
C	2.72023600	0.68243300	-0.34513100
H	2.29329000	2.75592300	-0.67574600
N	0.20105500	-1.95404900	-0.03674900
N	2.67103700	-1.74008900	0.02321400
S	1.52028800	-2.87970200	0.15000100
C	4.16405200	0.82048300	-0.30886700
C	4.89007900	1.99957300	-0.45743200
S	5.23024700	-0.55096600	-0.06037100
C	6.27554600	1.80031500	-0.37189400
H	4.41616700	2.96722300	-0.62190200
C	6.60406400	0.46401600	-0.15780200
C	8.03153600	0.34750000	-0.08357500
C	8.60438800	1.60575200	-0.24766500
S	9.20643500	-0.87418300	0.14588000
C	10.00906800	1.57175400	-0.18701300
C	10.50524100	0.29240800	0.02011400
H	10.65581500	2.44092200	-0.30927900
C	7.52563400	2.63856200	-0.44822400
H	7.62118400	3.15317600	-1.41943700
H	7.54997800	3.41902200	0.33117700
C	11.89327000	-0.13302700	0.13517600
C	12.91823600	0.81136100	0.33687700
C	12.25512900	-1.49125500	0.04805300
C	14.24356700	0.41772400	0.43837400
H	12.66807600	1.86920600	0.43251100
C	13.57848100	-1.88627500	0.15704000
H	11.48396200	-2.24675700	-0.12245800
C	14.58771900	-0.93680200	0.35052400
H	15.02684600	1.16037900	0.59686900
H	13.86081400	-2.93866200	0.08756300
C	15.98634900	-1.41068900	0.45659800
O	16.32732500	-2.56596400	0.38753900
O	16.86751700	-0.41480800	0.64132300
H	17.73826300	-0.83571200	0.69641900
C	-6.41540600	2.87868400	-0.25904300
C	-6.94619100	4.11797200	-0.67415000

C	-6.18586900	2.68872700	1.09571600
C	-7.23724700	5.11431100	0.25090000
O	-7.14130500	4.24825700	-2.00591300
C	-6.46417600	3.67715700	2.04372900
H	-5.78484800	1.72920600	1.42913600
C	-6.99332400	4.89487500	1.61545100
H	-7.65287600	6.07810000	-0.03954600
C	-7.68980800	5.43936400	-2.49786100
H	-6.26937000	3.48024400	3.09711700
O	-7.30684800	5.92182600	2.43133700
H	-7.04608500	6.30791500	-2.27454000
H	-8.69538100	5.62740400	-2.08316900
H	-7.76844900	5.32414300	-3.58624600
C	-7.09045800	5.77577000	3.80669700
H	-7.68433400	4.94653800	4.23004700
H	-6.02488300	5.60177400	4.03859300
H	-7.40726200	6.71528700	4.27708900

XW31

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C	0.85464300	-1.97722500	-0.28445000
C	0.02009200	-3.05546800	-0.27433000
C	-1.32394300	-2.53893200	-0.22854300
N	-1.29405900	-1.17272900	-0.20730100
C	0.01699200	-0.80732900	-0.24074600
C	-0.87551500	3.85145100	-0.07586100
C	0.20619000	3.02372000	-0.14047500
C	-0.30526300	1.67848500	-0.16870500
N	-1.66581800	1.69531500	-0.12414900
C	-2.04310800	3.00772300	-0.06883600
C	0.50469600	0.52034200	-0.22777300
C	-6.68938000	2.12585400	0.07158200
C	-5.85609300	3.20336500	0.05887500
C	-4.51002200	2.68799200	0.01154100
N	-4.54093000	1.31895100	-0.00828100
C	-5.84965700	0.95461400	0.02749000
C	-3.36160500	3.48668000	-0.01118500
C	-4.96016200	-3.70665500	-0.14047500
C	-6.04040400	-2.87952200	-0.07304700
C	-5.52722200	-1.53243900	-0.04434200
N	-4.16915700	-1.54870600	-0.09084800
C	-3.79023100	-2.86349300	-0.14833900
C	-2.47634700	-3.34059000	-0.20744600
C	-6.33579900	-0.37355800	0.01629200
C	-3.55156100	4.96235200	0.02909000
C	-2.28352100	-4.81578800	-0.25085300
C	-1.99333700	-5.45899800	-1.46478300
C	-1.80869800	-6.84752900	-1.51003300
C	-1.91953800	-7.58128000	-0.33312900
C	-2.20704100	-6.97111800	0.88375300
C	-2.38781300	-5.58180000	0.92123900
C	-3.83654700	5.61036900	1.24164400

C	-4.01672400	6.99968200	1.28260300
C	-3.90663400	7.72919100	0.10301600
C	-3.62404000	7.11415500	-1.11259100
C	-3.44762700	5.72421600	-1.14572700
O	-3.91875500	4.81070600	2.32100400
O	-3.17438100	5.02855800	-2.26493300
O	-2.66615800	-4.89115100	2.04235400
O	-1.91141500	-4.65527600	-2.54107600
C	-7.74119400	-0.55704600	0.06490000
Zn	-2.91778300	0.07315600	-0.10792900
C	-8.95124600	-0.71482700	0.10831400
C	-10.35687800	-0.89726800	0.15906700
C	-10.91344200	-2.19233400	0.14798600
C	-12.28769900	-2.36945900	0.19796500
C	-13.13989800	-1.25975800	0.26023100
C	-12.59572800	0.03035800	0.27152100
C	-11.22380700	0.21349100	0.22173100
C	1.91039400	0.70351200	-0.27233100
C	3.12125700	0.85921000	-0.31102400
C	6.45851200	2.49504400	-0.36295200
C	7.31626100	1.37766700	-0.41917400
C	5.08954200	2.33878800	-0.32444900
C	4.52680600	1.04146100	-0.35271900
C	5.39547900	-0.06347800	-0.43496100
C	-2.81607200	-5.58017900	3.25053100
C	-1.59522300	-5.20939200	-3.78607400
C	-4.23036100	5.37041400	3.56465600
C	-3.02763400	5.71233100	-3.47646100
H	1.94149800	-1.96114900	-0.31427800
H	0.28248900	-4.11085000	-0.29189300
H	-0.89108100	4.93813200	-0.03223500
H	1.26106200	3.28665700	-0.16341400
H	-7.77618800	2.11023500	0.10300900
H	-6.11916400	4.25862300	0.07556200
H	-4.94542700	-4.79330100	-0.18571400

H	-7.09509600	-3.14301400	-0.04905500
H	-1.58531300	-7.35407400	-2.44810400
H	-1.77726900	-8.66420700	-0.36536700
H	-2.28496800	-7.57217700	1.78881600
H	-4.23687900	7.51000600	2.21938900
H	-4.04613800	8.81257100	0.13196300
H	-3.54719500	7.71184800	-2.01997700
H	-12.71493600	-3.37319000	0.18910100
H	-13.27877000	0.88078800	0.32024000
H	-10.79956200	1.21906700	0.23041900
H	4.43109800	3.20905900	-0.27850000
H	4.96556100	-1.06603900	-0.48160300
H	-3.05018300	-4.82614700	4.01239600
H	-3.64236600	-6.31133200	3.20630200
H	-1.88999500	-6.10649900	3.54172700
H	-0.60741300	-5.70278300	-3.77674000
H	-2.35502400	-5.93944000	-4.11641700
H	-1.56907300	-4.37682300	-4.50016900
H	-5.21654000	5.86704400	3.55575500
H	-4.25769900	4.54055500	4.28186400
H	-3.46745500	6.09918800	3.89069700
H	-2.79859300	4.95464900	-4.23623700
H	-3.95355700	6.23981700	-3.76595200
H	-2.19929800	6.44156000	-3.43849600
H	7.41631000	-0.79182900	-0.56432800
N	8.63614500	1.78560000	-0.47472500
C	6.77765700	0.08589200	-0.47077500
C	9.77000300	0.97749400	-0.44112400
C	10.92047000	1.35347700	-1.16044300
C	9.80433100	-0.19381700	0.33994200
C	12.07457500	0.57775100	-1.12770400
H	10.90389300	2.26372700	-1.76129500
C	10.95065700	-0.96971100	0.35695700
H	8.94018200	-0.46392900	0.94865400
C	12.09169000	-0.59557500	-0.37495700

H	12.95290700	0.89066800	-1.69749400
C	11.19452500	-2.26266000	1.11886900
C	13.13478500	-1.59603600	-0.15301600
C	12.62735300	-2.57828000	0.71852200
C	14.43716400	-1.68937300	-0.64437500
C	13.41817600	-3.65359400	1.10054500
C	15.22616000	-2.77256500	-0.25769500
H	14.83531000	-0.92906800	-1.32085100
C	14.72297400	-3.74748100	0.60717300
H	13.03178900	-4.42048300	1.77756300
H	16.24802500	-2.86008000	-0.63460500
H	15.35443500	-4.58967700	0.89987400
C	10.23220900	-3.36220400	0.65429400
H	9.19065600	-3.09278600	0.89015000
H	10.45705300	-4.31486800	1.15836800
C	11.07584200	-2.04655300	2.63201300
H	11.76188300	-1.25654700	2.97052000
H	10.04998600	-1.75413600	2.90532800
H	-10.24780600	-3.05594900	0.09931600
H	10.31116000	-3.52005500	-0.43119700
H	11.31993300	-2.97163600	3.17681800
C	8.72674000	3.24110700	-0.62509500
H	9.02684100	3.48874400	-1.65880600
C	7.28684400	3.74494800	-0.33211300
H	6.96633300	4.46531400	-1.10070300
C	9.64349700	3.92482200	0.40741600
H	10.59015600	4.27861800	-0.02486500
H	9.90137200	3.19200400	1.18795800
C	7.38992800	4.45522900	1.02736800
H	6.59220700	5.19693500	1.18064900
H	7.30738600	3.71023100	1.83635400
C	8.79354100	5.04875600	1.00260200
H	9.14965000	5.37687500	1.99063800
H	8.81307800	5.93196700	0.34117500
C	-14.61415300	-1.39585800	0.31536900

O	-15.38735300	-0.47132200	0.37031500
O	-15.02667500	-2.67294800	0.29848500
H	-15.99407300	-2.64168800	0.33756900

XW93

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C	0.03841500	-2.32613800	0.34125200
C	0.94773200	-3.31710800	0.56547500
C	2.25225600	-2.71963500	0.43637200
N	2.12549100	-1.39034200	0.14506500
C	0.79136200	-1.12730600	0.08001300
C	1.35365300	3.47855000	-0.91905400
C	0.33258400	2.59108300	-0.74877700
C	0.93732600	1.31973900	-0.44824800
N	2.29341000	1.43879100	-0.43696100
C	2.57758400	2.74584400	-0.71767400
C	0.21087100	0.13119300	-0.20264000
C	7.27542500	2.23608000	-0.48189400
C	6.36715200	3.22742300	-0.70069800
C	5.06145000	2.62007300	-0.62343600
N	5.18993400	1.28316500	-0.35589000
C	6.52144700	1.02595800	-0.26760600
C	3.85904700	3.31312600	-0.80103500
C	5.96367500	-3.60269900	0.63330600
C	6.98341700	-2.71419200	0.47084600
C	6.37616800	-1.43113500	0.21840100
N	5.02199900	-1.54481700	0.22948700
C	4.73669300	-2.85983300	0.48392200
C	3.45907300	-3.42030600	0.58974600
C	7.10091800	-0.23741000	-0.00568100
C	3.94441900	4.76792800	-1.10347200
C	3.37112100	-4.87566600	0.88876600
C	3.56087500	-5.34598100	2.19806400
C	3.47899400	-6.71585900	2.48267700
C	3.20383100	-7.60446900	1.44806400
C	3.00979500	-7.16701900	0.14162700
C	3.09585500	-5.79590000	-0.13541800
C	4.25879000	5.20775000	-2.39934800

C	4.34118700	6.57687500	-2.68742700
C	4.10414900	7.49569000	-1.66992700
C	3.78939900	7.08897400	-0.37712000
C	3.71134000	5.71813800	-0.09636800
O	4.46656000	4.23597000	-3.30686900
O	3.41796500	5.21586600	1.11728700
O	2.92850800	-5.26564300	-1.36096900
O	3.81857500	-4.40157000	3.12163800
C	8.51649300	-0.31268000	0.03512800
Zn	3.65791300	-0.05331400	-0.10466600
C	9.73538000	-0.37652300	0.07024000
C	11.15129000	-0.44871500	0.11092900
C	11.80089400	-1.67435700	0.36168700
C	13.18514900	-1.74330000	0.40136200
C	13.95480800	-0.59204900	0.19209300
C	13.31791600	0.62967500	-0.05770500
C	11.93557900	0.70465800	-0.09862600
C	-1.20484100	0.20686900	-0.24329300
C	-2.42401800	0.27118800	-0.27835100
C	2.61933300	-6.10786500	-2.43429900
C	4.04923900	-4.78575900	4.44683600
C	4.81625500	4.58558900	-4.61554400
C	3.14269800	6.09259100	2.17199600
H	-1.04722500	-2.38677200	0.35208300
H	0.76091000	-4.36228200	0.80149700
H	1.29310600	4.53682000	-1.16277800
H	-0.73804400	2.76711400	-0.82076300
H	8.36047900	2.30392700	-0.46120900
H	6.55384100	4.28118900	-0.89506300
H	6.02550000	-4.66995600	0.83379000
H	8.05451000	-2.89712400	0.51196200
H	3.62348100	-7.08849500	3.49595400
H	3.13851000	-8.67300300	1.66710000
H	2.79848100	-7.88724800	-0.64773800
H	4.58333200	6.92606500	-3.69037200

H	4.16715600	8.56380500	-1.89167300
H	3.61215600	7.83221300	0.39918600
H	13.68451100	-2.69356100	0.59560200
H	13.93762100	1.51422600	-0.21796100
H	11.43905400	1.65692500	-0.29328600
H	2.51469000	-5.46339100	-3.31605700
H	3.42008000	-6.84439300	-2.62333600
H	1.66983400	-6.64769500	-2.27203300
H	3.17126300	-5.28977400	4.88791100
H	4.92441200	-5.45338500	4.53432500
H	4.24864000	-3.86440600	5.00822100
H	5.76191600	5.15464200	-4.64953100
H	4.94849900	3.64495700	-5.16463900
H	4.02568000	5.17859200	-5.10823500
H	2.91984400	5.46819700	3.04622500
H	4.00683400	6.73910600	2.40586100
H	2.26786200	6.73122500	1.95717500
H	11.19950800	-2.57050700	0.52453400
C	15.43586100	-0.61317000	0.22434200
O	16.14013000	0.35077700	0.04989200
O	15.94048100	-1.83207000	0.47142300
H	16.90355400	-1.72789700	0.46932200
C	-3.83939800	0.34882500	-0.32040200
C	-4.48693100	1.57795900	-0.59021300
C	-4.62996400	-0.79144000	-0.08467000
C	-5.86312300	1.63364100	-0.62759800
H	-3.88738700	2.47387600	-0.76488900
H	-4.13323100	-1.73658000	0.14333300
C	-6.02023300	-0.74221800	-0.11896600
C	-6.63963300	0.47915700	-0.40387300
C	-6.78862100	2.78464100	-0.90147700
H	-6.60267200	-1.63667000	0.10102800
N	-7.98664600	0.80498500	-0.44012900
H	-6.49313500	3.71988000	-0.40893500
H	-6.84946900	2.97917100	-1.98597700

C	-8.13895500	2.25979100	-0.36430700
C	-9.07284500	-0.05582600	-0.55287100
H	-8.96776700	2.57427800	-1.01505100
C	-8.40991400	2.74273200	1.04422700
C	-10.34313500	0.35148200	-0.09749800
C	-8.93759700	-1.31849500	-1.16401000
C	-8.86903900	4.06334800	1.23135600
C	-8.20428300	1.95827100	2.16964400
C	-11.45108800	-0.47916600	-0.22775700
H	-10.45314100	1.32343100	0.38437700
C	-10.04308600	-2.14340900	-1.27725400
H	-7.97448400	-1.62399400	-1.57459900
C	-9.11583400	4.55782600	2.50712000
O	-9.04217200	4.78270500	0.09950300
C	-8.43876200	2.43491800	3.46221300
H	-7.85760100	0.93128200	2.03628900
C	-11.30543200	-1.73756600	-0.80936300
H	-12.42348400	-0.13941900	0.13711300
C	-10.11381500	-3.53185400	-1.89368100
C	-8.89759000	3.74195400	3.62798200
H	-9.47543400	5.57082500	2.68174300
C	-9.51513400	6.09744100	0.19703100
H	-8.26412900	1.78052800	4.31518300
C	-12.26491500	-2.80917300	-1.07106500
C	-11.58539000	-3.86690700	-1.70506700
C	-9.21726400	-4.51648600	-1.13404300
C	-9.73909500	-3.49858800	-3.37992000
O	-9.16334900	4.31373100	4.81988700
H	-8.82545200	6.73718000	0.77462500
H	-10.51355300	6.13819100	0.66609700
H	-9.58617500	6.48354100	-0.82761800
C	-13.63045700	-2.90600100	-0.80189300
C	-12.26654700	-5.01997000	-2.07074900
H	-8.15845000	-4.22644700	-1.22297800
H	-9.32395600	-5.53422600	-1.54048900

H	-9.47991800	-4.54284100	-0.06642300
H	-10.37765200	-2.79172100	-3.92934100
H	-8.69018300	-3.19003700	-3.51114500
H	-9.85805400	-4.49490000	-3.83330100
C	-8.96313600	3.56205600	5.98387800
C	-14.30892300	-4.06762300	-1.17082700
H	-14.16226800	-2.08756700	-0.31038400
C	-13.63493700	-5.11707300	-1.79992200
H	-11.74575500	-5.84525500	-2.56427600
H	-9.60287500	2.66218500	6.00673900
H	-7.90970100	3.25003100	6.09490700
H	-9.23225700	4.21013000	6.82761100
H	-15.37847100	-4.15811100	-0.96602700
H	-14.18144000	-6.02006200	-2.08224300

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