Electronic Supplementary Information

Molecular Engineering of New Phenothiazine-based D-A-π-A Dyes for Dye-Sensitized Solar Cells

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Experimental section

Synthesis and characterization of dyes.

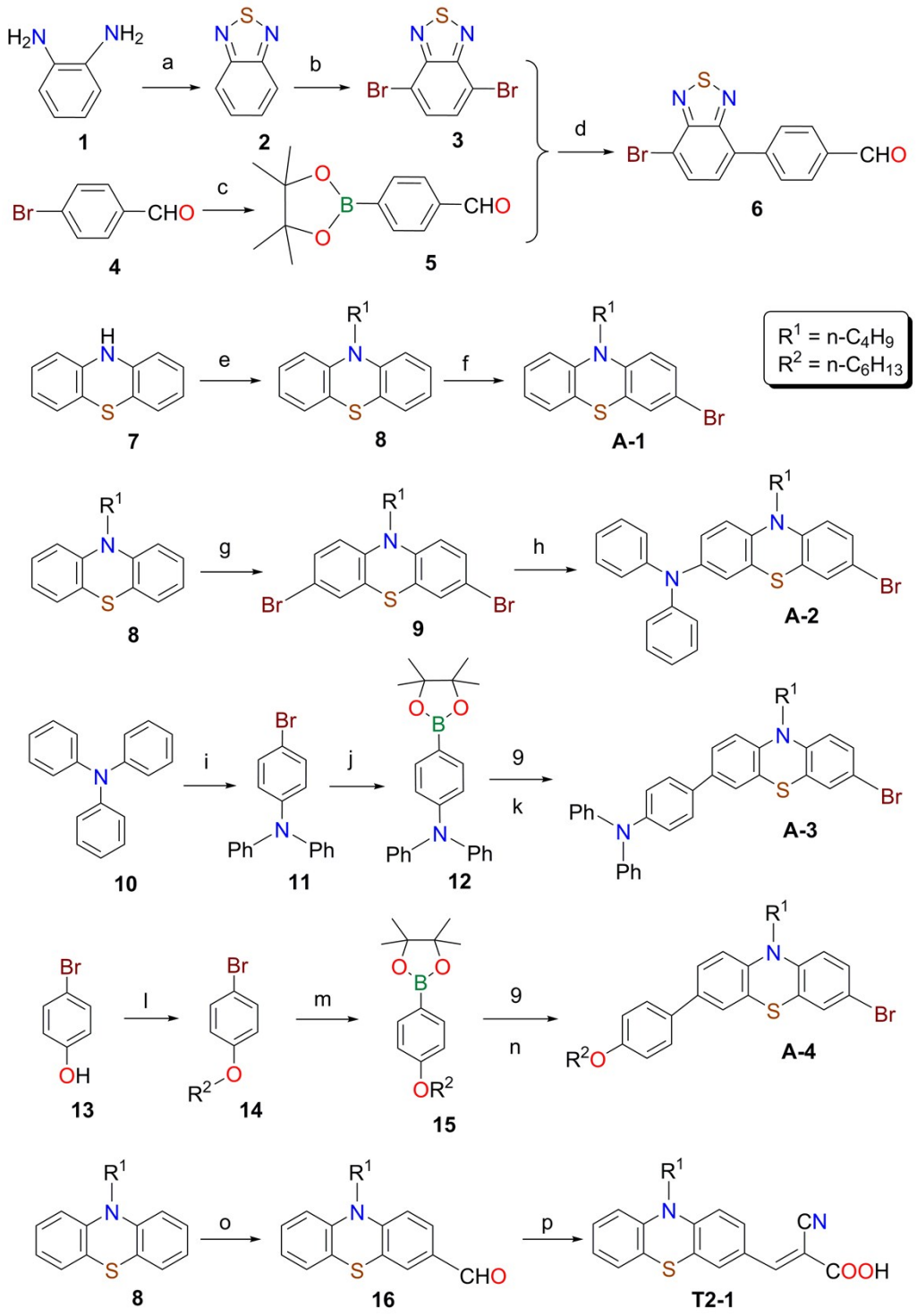

Figure S1 Synthetic routs of intermediates. (a) $SOCl_2$, NEt_3, CH_2Cl_2; (b) Br_2, HBr

(aq); (c) bis(pinacolato)diboron, $Pd(PPh_3)_2Cl_2$, KOAc, toluene; (d) $Pd(PPh_3)_4$, K_2CO_3, DME/H_2O; (e) NaH, n-BuBr, THF; (f) NBS, THF; (g) NBS, THF; (h) $Pd_2(dba)_3$, $^tBu_3P$, ^{t}BuOK, diphenylamine, 1,4-dioxane; (i) NBS, DMF; (j) bis(pinacolato)diboron, $Pd(PPh_3)_2Cl_2$, KOAc, toluene; (k) $Pd(PPh_3)_4$, K_2CO_3, DME/H_2O; (l) n-$C_6H_{13}Br$, K_2CO_3, acetone; (m) bis(pinacolato)diboron, $Pd(PPh_3)_2Cl_2$, KOAc, toluene; (n) $Pd(PPh_3)_4$, K_2CO_3, DME/H_2O; (o) DMF, $POCl_3$, CH_2Cl2; (p) cyanoacetic acid, piperidine, $CHCl_3$.

Dye of **T2-1**, compound **2**, **3**, **5**, **6**, **8**, **A-1**, **9**, **11**, **12**, **14**, **15** and **16** were synthesized according to literatures.[1-6] Their ^{1}H NMR spectra were consistent with that in references. The synthetic procedures and NMR data for other intermediates and new dyes are detailed as follows.

Preparation of A-2~4

A-2[4]**:** Under argon, 3,7-dibromo-10-butyl-10H-phenothiazine (compound **9**) (6.20 g, 15 mmol), $Pd_2(dba)_3$ (41.2 mg, 0.045mmol), $HP(t\text{-}Bu)_3BF_4$ (43.5 mg, 0.15mmol), and ^{t}BuOK (1.00 g, 9mmo) were dissolved in dry 1,4-dioxane (50 mL). The reaction mixture was stirred at 70 ˚C for 5 minutes and then diphenylamine (0.51 g, 3 mmol) was added and the mixture was heated to 105 ˚C for 14 h. After cooling to room temperature, solvents were removed by rotary evaporation. The residue was purified using column chromatography to give a pale green solid (1.00 g, 66.8 %). ^{1}H NMR (300 MHz, Acetone-d_6): δ 7.33 (dd, J = 6.9, 1.8 Hz, 1 H), 7.27 (m, 5 H), 7.00 (m, 7 H), 6.93 (2 H, m), 6.85 (1 H, d, J = 2.4 Hz), 3.91 (t, J = 7.2 Hz, 2 H), 1.77 (m, 2

H), 1.47 (m, 2 H), 0.93 (t, J = 7.2 Hz, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 147.82, 144.65, 143.09, 140.76, 130.03, 129.79, 129.36, 126.84, 125.22, 124.34, 124.21, 123.63, 122.55, 116.51, 116.09, 114.34, 47.39, 29.06, 20.35, 14.03.

A-3: Compound **12** (0.63 g, 1.7 mmol) was treated with **9** (2.81 g, 6.8 mmol) in the presence of $Pd(PPh_3)_4$ (0.10 g, 0.08 mmol), 1 N aqueous solution of K_2CO_3 (2.5 mL) and 1,2-dimethoxyethane (22.5 mL). The mixture was degassed for three times and refluxed for 48 h. After cooling and addition of AcOEt (50 mL), the mixture was washed with water and dried on magnesium sulfate. Solvents were removed by rotary evaporation and the residue was purified by silica gel column chromatography with petroleum ether:AcOEt (10:1, v:v) as eluent to give **A-3** as a pale yellow oil (0.64 g, 67.2%). ^{1}H NMR (300 MHz, Acetone-d_6): δ 7.48 (dd, J = 6.9, 2.4 Hz, 2H), 7.41 (dd, J = 8.1, 2.4 Hz, 1H), 7.35 (d, J = 2.4 Hz, 1H), 7.27 (m, 6H), 7.03 (m, 9H), 6.88 (d, J = 8.7 Hz, 1H), 3.88 (t, J = 6.9 Hz, 2H), 1.73 (m, 2H), 1.44 (m, 2H), 0.89 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, Acetone-d_6): δ 148.57, 147.91, 145.42, 144.61, 135.89, 134.47, 130.95, 130.29, 130.04, 127.95, 127.62, 126.52, 125.75, 125.20, 125.10, 124.67, 123.97, 117.99, 117.03, 114.78, 47.67, 29.55, 20.63, 14.14.

A-4: Compound **12** (0.61 g, 2 mmol) was treated with **9** (4.13 g, 10 mmol) in the presence of $Pd(PPh_3)_4$ (115.6 mg, 0.1 mmol), 1 N aqueous solution of K_2CO_3 (5 mL) and 1,2-dimethoxyethane (45 mL). The mixture was degassed for three times and refluxed for 48 h. After cooling and addition of AcOEt (80 mL), the mixture was washed with water and dried on magnesium sulfate. Solvents were removed by rotary evaporation and the residue was purified by silica gel column chromatography with

petroleum ether:AcOEt (10:1, v:v) as eluent to give **A-4** as a pale yellow oil (0.69 g, 67.5%). ^{1}H NMR (300 MHz, Acetone-d_6): δ 7.54 (dd, J = 6.9, 2.4 Hz, 2H), 7.44 (dd, J = 8.7, 2.4 Hz, 1H), 7.37 (d, J = 2.1 Hz, 1H), 7.31 (m, 2H), 7.08 (d, J = 8.1 Hz, 1H), 6.97 (m, 3H), 4.02 (t, J = 6.6 Hz, 2H), 3.95 (t, J = 6.9 Hz, 2H), 1.78 (m, 4H), 1.49 (m, 4H), 1.36 (m, 4H), 0.92 (m, 6H).

General synthetic procedure for compounds B-n[7-8]

A mixture of **A-n** (1.0 mmol), bis(pinacolato)diboron (0.31 g, 1.2 mmol), $Pd(PPh_3)_2Cl_2$ (17.8 mg, 25 μmol) and KOAc (0.30 g, 3 mmol) in dry toluene (25 mL) was heated to 120 °C under argon for 12 h. After cooling, the solvents were evaporated in vacuum. The residue was chromatographed with petroleum ether: AcOEt (10:1, v:v) to give **B-n** as a pale green oil.

B-1: 0.36 g, yield 94.5%. ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.49 (d, J = 8.1 Hz, 1H), 7.36 (s, 1H), 7.20 (t, J = 7.2 Hz, 1H), 7.13 (d, J = 7.8 Hz, 1H), 7.02 (m, 2H), 6.98 (t, J = 7.2 Hz, 1H), 3.84 (t, J = 6.9 Hz, 2H), 1.68 (m, 2H), 1.31 (s, 12 H), 0.92 (t, J = 7.8 Hz, 3H).

B-2: 0.47 g, yield 86.7 %. ^{1}H NMR (300 MHz, Acetone-d_6): δ 7.56 (dd, J = 1.2, 8.1 Hz, 1H), 7.41 (d, J = 1.2 Hz, 1H), 7.26 (m, 4H), 7.00 (m, 8H), 6.89 (dd, J = 8.7, 2.7 Hz, 1H), 6.84 (d, J = 2.7 Hz, 1H), 3.94 (t, J = 6.9 Hz, 2H), 1.73 (m, 2H), 1.48 (m, 2H), 1.30 (s, 12 H), 0.93 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 147.95, 147.83, 142.94, 140.64, 134.34, 133.97, 129.29, 125.90, 124.24, 124.09, 123.59, 123.52, 122.41, 115.99, 114.64, 83.75, 47.27, 29.85, 29.08, 24.98, 20.31, 14.01. HRMS (EIS): m/z $[M]^+$ calcd for $C_{34}H_{37}BN_2O_2S$: 548.2335; found: 548.2358.

B-3: 0.46 g, yield 73.7 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.56 (d, J = 8.7 Hz, 2H), 7.41 (m, 2H), 7.39 (d, J = 2.1 Hz, 1H), 7.32 (m, 5H), 7.03 (m, 10H), 3.90 (t, J = 6.9 Hz, 2H), 1.68 (m, 2H), 1.41 (m, 2H), 1.27 (s, 12 H), 0.88 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 147.85, 147.03, 143.68, 135.30, 134.17, 134.00, 129.63, 129.44, 129.23, 127.30, 125.28, 124.69, 124.50, 124.33, 124.20, 123.69, 123.02, 115.71, 114.75, 83.86, 47.37, 29.07, 25.35, 25.03, 20.33, 14.04. HRMS (EIS): m/z $[M]^+$ calcd for $C_{40}H_{41}BN_2O_2S$: 624.2976; found: 624.2964.

B-4: 0.43 g, yield 77.4 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.55 (m, 3H), 7.44 (m, 2H), 7.36 (d, J = 2.1 Hz, 1H), 7.06 (dd, J = 12.9, 8.1 Hz, 2H), 6.98 (d, J = 9.0 Hz, 2H), 4.01 (m, 4H), 1.74 (m, 4H), 1.48 (m, 4H), 1.35 (m, 16H), 0.92 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.67, 147.88, 143.49, 135.58, 134.34, 133.99, 132.50, 127.63, 125.53, 125.43, 125.29, 123.75, 115.70, 114.94, 114.73, 83.84, 68.25, 47.33, 31.80, 29.91, 29.46, 29.09, 25.94, 25.02, 22.82, 20.32, 14.26, 14.02. HRMS (EIS): m/z $[M+1]^+$ calcd for $C_{34}H_{44}BNO_3S$: 558.3208; found: 558.3192.

General synthetic procedure for compounds C-n

Compound **B-n** (0.5 mmol) was treated with **6** (0.6 mmol) in the presence of $Pd(PPh_3)_4$ (57.8 mg, 50 μmol), 1 N aqueous solution of K_2CO_3 (3 mL) and 1,2-dimethoxyethane (22 mL). The mixture was degassed for three times and refluxed for 48 h. After cooling and addition of AcOEt (50 mL), the mixture was washed with water and dried on magnesium sulfate. Solvents were removed by rotary evaporation and the residue was purified by silica gel column chromatography with petroleum ether:AcOEt (10:1, v:v) as eluent to give **C-n** as an orange solid.

C-1: 173.8 mg, yield 70.5 %. ^{1}H NMR (300 MHz, Acetone-d_6): δ 10.16 (s, 1H), 8.31 (d, J = 8.7 Hz, 2H), 8.09 (m, 3H), 7.96 (m, 3H), 7.22 (m, 3H), 7.10 (d, J = 6.9 Hz, 1H), 6.99 (t, J = 7.8 Hz, 1H), 4.06 (t, J = 6.9 Hz, 2H), 1.86 (m, 2H), 1.53 (m, 2H), 0.96 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 191.74, 153.62, 153.58, 145.46, 144.48, 143.10, 135.51, 132.93, 132.92, 130.80, 129.75, 129.59, 128.79, 128.22, 127.63, 127.35, 127.26, 126.53, 124.67, 124.00, 122.52, 115.33, 115.01, 47.16, 28.81, 20.12, 13.80. Anal. Calcd. for $C_{29}H_{23}N_3OS_2$ • 1/6 CH_2Cl_2: C, 68.99; H, 4.63; N, 8.28. Found: C, 69.15; H, 4.36; N, 8.07. HRMS (ESI): calcd for $C_{29}H_{23}N_3OS_2$ *m/z*: 493.1557, found: 493.1546.

C-2: 221.8 mg, yield 67.2 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 10.12 (s, 1H), 8.17 (d, J = 8.1 Hz, 2H), 8.06 (d, J = 8.1 Hz, 2H), 7.84 (d, J = 7.8 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H), 7.24 (m, 4H), 7.01 (m, 5H), 6.94 (m, 4H), 6.79 (d, J = 8.7 Hz, 1H), 3.90 (t, J = 6.9 Hz, 2H), 1.87 (m, 2H), 1.54 (m, 2H), 0.91 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 191.92, 153.90, 153.83, 147.79, 143.36, 143.00, 140.45, 136.86, 135.76, 133.24, 132.41, 131.02, 130.00, 129.83, 129.30, 129.03, 128.94, 128.50, 127.90, 126.77, 125.18, 124.43, 124.24, 123.55, 122.47, 115.99, 115.10, 47.43, 29.83, 20.40, 14.04. HRMS (EIS): m/z $[M]^+$ calcd for $C_{41}H_{32}N_4OS_2$: 660.1794; found: 660.1814.

C-3: 264.2mg, yield 71.8 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 10.07 (s, 1H), 8.12 (d, J = 8.1 Hz, 2H), 8.01 (d, J = 8.1 Hz, 2H), 7.81 (m, 3H), 7.70 (d, J = 7.5 Hz, 2H), 7.38 (m, 4H), 7.25 (t, J = 7.8 Hz, 4H), 7.11 (m, 4H), 7.01 (dd, J = 7.2, 12.9 Hz, 4H), 6.90 (d, J = 8.7 Hz, 1H), 3.90 (t, J = 6.9 Hz, 2H), 1.76 (m, 2H), 1.51 (m, 2H), 0.90 (t,

J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 192.05, 153.97, 153.91, 147.78, 147.07, 145.59, 143.52, 143.47, 135.82, 135.34, 133.95, 133.33, 131.17, 130.50, 130.09, 129.90, 129.43, 129.10, 128.57, 128.15, 127.96, 127.24, 126.88, 125.65, 125.50, 124.59, 124.51, 124.12, 123.05, 115.71, 115.25, 47.51, 29.08, 20.40, 14.06. HRMS (EIS): m/z $[M]^+$ calcd for $C_{47}H_{36}N_4OS_2$: 736.2325; found: 736.2313.

C-4: 205.0 mg, yield 61.3 %. ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.06 (s, 1H), 8.10 (d, *J* = 7.2 Hz, 2H), 8.00 (d, *J* = 7.2 Hz, 2H), 7.74 (m, 4H), 7.43 (d, *J* = 8.7 Hz, 2H), 7.31 (m, 2H), 6.93 (m, 4H), 3.96 (m, 4H), 1.79 (m, 4H), 1.45 (m, 8H), 0.97 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 192.12, 158.64, 153.91, 153.85, 147.08, 145.58, 143.44, 143.27, 135.73, 135.54, 133.26, 132.27, 131.07, 130.07, 129.86, 129.44, 129.09, 128.54, 127.91, 127.56, 126.84, 125.62, 125.49, 124.48, 115.67, 115.18, 114.88, 68.18, 47.43, 31.76, 29.40, 29.00, 25.90, 22.79, 20.37, 14.26, 14.05. HRMS (EIS): m/z $[M]^+$ calcd for $C_{41}H_{39}N_3O_2S_2$: 669.2478; found: 669.2467.

Synthesis of compounds PZ-n

A $CHCl_3$ (10 mL) solution of compound **C-n** (0.3 mmol), cyanoacetic acid (123.2 mg, 1.5 mmol) and piperidine (0.19 mL, 1.9 mmol) were charged sequentially into a three-necked flask under a nitrogen atmosphere and heated to reflux till no starting material **C-n** was detected by the TLC plate. After cooling to 0 °C, 2M HCl (5mL) were added dropwisely into the flask and stirred for 1h. The mixture was washed with water and dried on anhydrous magnesium sulfate. Solvents were removed by rotary evaporation, and the residue was purified by silica gel column chromatography with CH_2Cl_2:CH_3OH (10:1, v:v) as eluent to afford the dye **PZ-n** as a dark purple solid.

PZ-1: 116.3 mg, yield 69.2 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 14.07 (br, 1H), 8.42 (s, 1H), 8.23 (m, 4H), 8.06 (d, J = 7.2 Hz, 1H), 7.97 (d, J = 7.2 Hz, 1H), 7.91 (m, 2H), 7.31 (dd, J = 9.3, 40.5 Hz, 1H), 7.21 (m, 2H), 7.08 (d, J = 7.8 Hz, 1H), 6.99 (m, 1H), 3.95 (t, J = 6.9 Hz, 2H), 1.72 (m, 2H), 1.45 (m, 2H), 0.91 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$-CD_3OD): δ 164.06, 154.30, 153.80, 153.68, 145.64, 144.64, 143.86, 142.00, 133.16, 131.21, 130.97, 130.68, 129.77, 129.54, 128.86, 128.33, 127.72, 127.34, 126.80, 124.78, 124.11, 122.58, 116.55, 116.06, 115.45, 115.17, 47.20, 28.92, 20.14, 13.73. Anal. Calcd. for $C_{32}H_{24}N_4O_2S_2$ • 1/3 CH_2Cl_2 • 1/3 CH_3OH: C, 65.43; H, 4.37; N, 9.34. Found: C, 65.23; H, 4.05; N, 9.28. HRMS (ESI): m/z $[M+1]^+$ calcd for $C_{32}H_{24}N_4O_2S_2$ *m/z*: 561.1413, found: 560.1420.

PZ-2: 171.2 mg, yield 78.5 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 14.09 (br, 1H), 8.40 (s, 1H), 8.22 (m, 4H), 8.07 (d, J = 7.5 Hz, 1H), 7.98 (d, J = 7.5 Hz, 1H), 7.91 (m, 1H), 7.86 (d, J = 2.1 Hz, 1H), 7.28 (m, 4H), 7.20 (d, J = 8.7 Hz, 1H), 6.99 (m, 9H), 3.92 (t, J = 6.3 Hz, 2H), 1.74 (m, 2H), 1.44 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$-CD_3OD): δ 164.48, 158.89, 154.12, 153.81, 153.70, 153.68, 147.74, 142.89, 142.54, 141.94, 141.92, 141.81, 141.63, 140.48, 131.20, 130.70, 129.77, 129.40, 129.18, 128.86, 128.45, 127.02, 126.75, 125.14, 124.19, 123.47, 122.35, 116.24, 116.04, 115.97, 47.32, 28.92, 20.24, 13.82. Anal. Calcd. for $C_{44}H_{33}N_5O_2S_2$ • 1/4 CH_2Cl_2: C, 70.95; H, 4.51; N, 9.35. Found: C, 70.72; H, 4.24; N, 9.41. HRMS (ESI): m/z $[M]^+$ calcd for $C_{44}H_{33}N_5O_2S_2$ *m/z*: 727.2070, found:727.2078.

PZ-3: 174.4 mg, yield 72.4 %. ^{1}H NMR (400 MHz, DMSO-d_6): δ 14.05 (s, 1 H), 8.39 (s, 1H), 8.22 (dd, J = 18.3, 8.7 Hz, 4H), 8.06 (d, J = 7.5 Hz, 1H),

7.98 (d, *J* = 7.5 Hz, 1H), 7.91 (m, 2H), 7.58 (d, *J* = 8.7 Hz, 2H), 7.49 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.44 (d, *J* = 2.1 Hz, 1H), 7.32 (dd, *J* = 8.2, 7.5 Hz, 4 H), 7.20 (d, *J* = 8.6 Hz, 1H), 7.11 (d, *J* = 8.6 Hz, 1H), 7.04 (m, 8H), 3.97 (t, *J* = 6.9 Hz, 2H), 1.75 (m, 2H), 1.46 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$-CD_3OD): δ 164.39, 153.96, 153.81, 153.68, 147.63, 146.91, 145.39, 143.38, 141.87, 135.12, 133.80, 133.11, 131.13, 131.00, 130.73, 129.75, 129.22, 128.84, 128.39, 127.89, 127.76, 127.03, 126.81, 126.00, 125.71, 125.44, 125.23, 124.42, 124.29, 123.91, 122.85, 116.22, 115.56, 115.11, 47.26, 28.88, 20.13, 13.71. Anal. Calcd. for $C_{50}H_{37}N_5O_2S_2 \cdot CH_3OH$: C, 73.27; H, 4.9 4; N, 8.38. Found: C, 73.19; H, 4.69; N, 8.39. HRMS (ESI): m/z $[M+1]^+$ calc d for $C_{50}H_{37}N_5O_2S_2$ *m/z*: 804.2461, found: 804.2460.

PZ-4: 181.9 mg, yield 82.4 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 14.09 (br, 1H), 8.39 (s, 1H), 8.24 (d, *J* = 8.4 Hz, 2H), 8.20 (d, *J* = 8.4 Hz, 2H), 8.06 (d, *J* = 7.2 Hz, 1H), 7.98 (d, *J* = 7.2 Hz, 1H), 7.91 (m, 2H), 7.56 (m, *J* = 8.7 Hz, 2H), 7.44 (m, 2H), 7.20 (d, *J* = 8.1 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 1H), 6.97 (d, *J* = 8.7 Hz, 2H), 3.98 (m, 4H), 1.71 (m, 4H), 1.31 (m, 8H), 0.92 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$-CD_3OD): δ 164.88, 158.36, 153.93, 153.68, 153.57, 145.29, 143.07, 141.76, 135.24, 132.93, 132.14, 131.03, 130.80, 130.51, 129.63, 128.75, 128.28, 127.62, 127.27, 126.66, 125.34, 125.11, 124.26, 124.20, 118.85, 116.20, 115.46, 114.95, 114.71, 106.01, 68.06, 47.17, 31.48, 29.13, 28.78, 25.60, 22.48, 20.05, 13.79, 13.61. Anal. Calcd. for $C_{44}H_{40}N_4O_3S_{22} \cdot 1/3\ CH_2Cl_2$: C, 69.58; H, 5.36; N, 7.32. Found: C, 69.63; H, 5.22; N, 7.36. HRMS (ESI): m/z $[M+1]^+$ calcd for $C_{44}H_{40}N_4O_3S_2$ *m/z*: 737.2615, found:

737.2609.

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Results and discussion.

Photophysical and electrochemical properties.

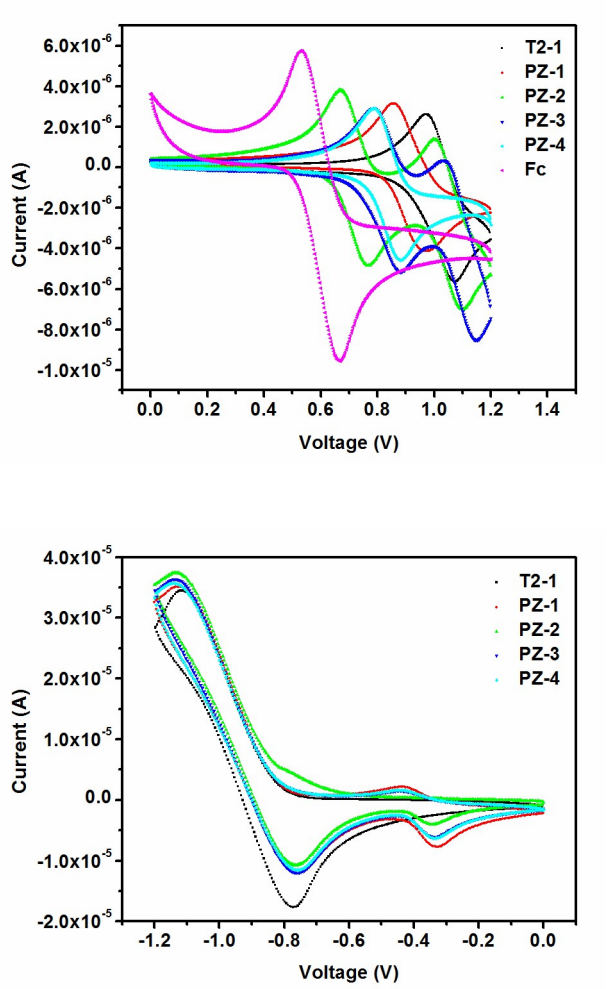
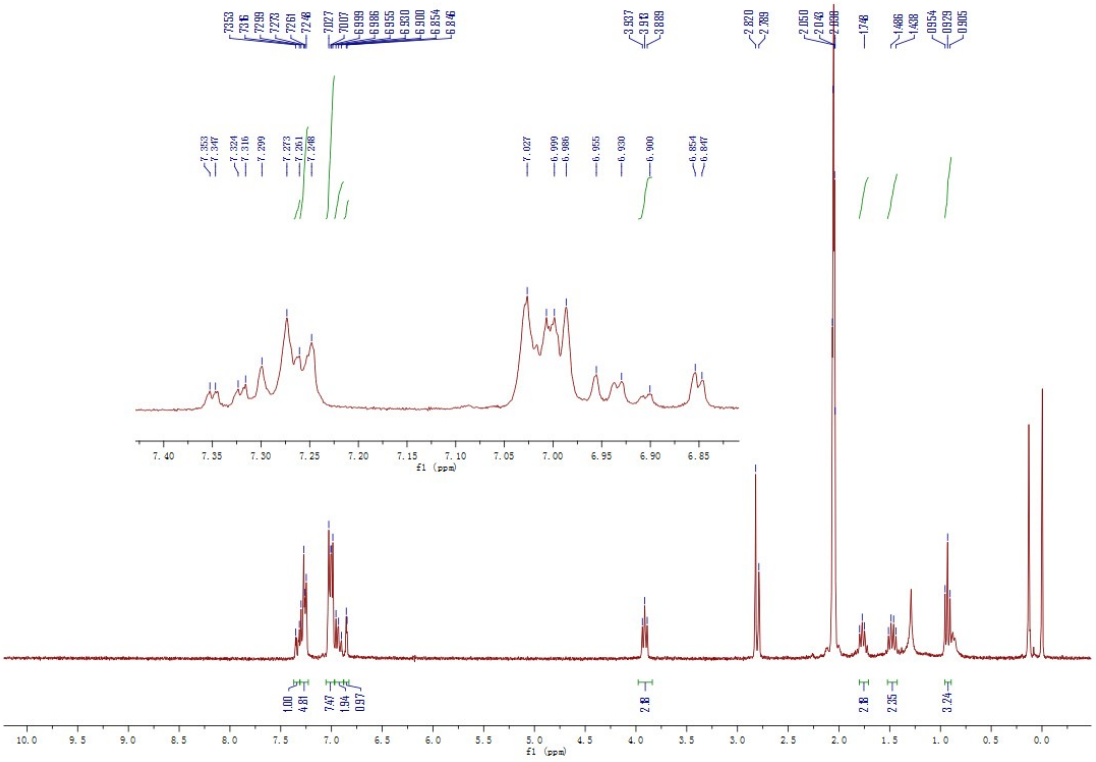


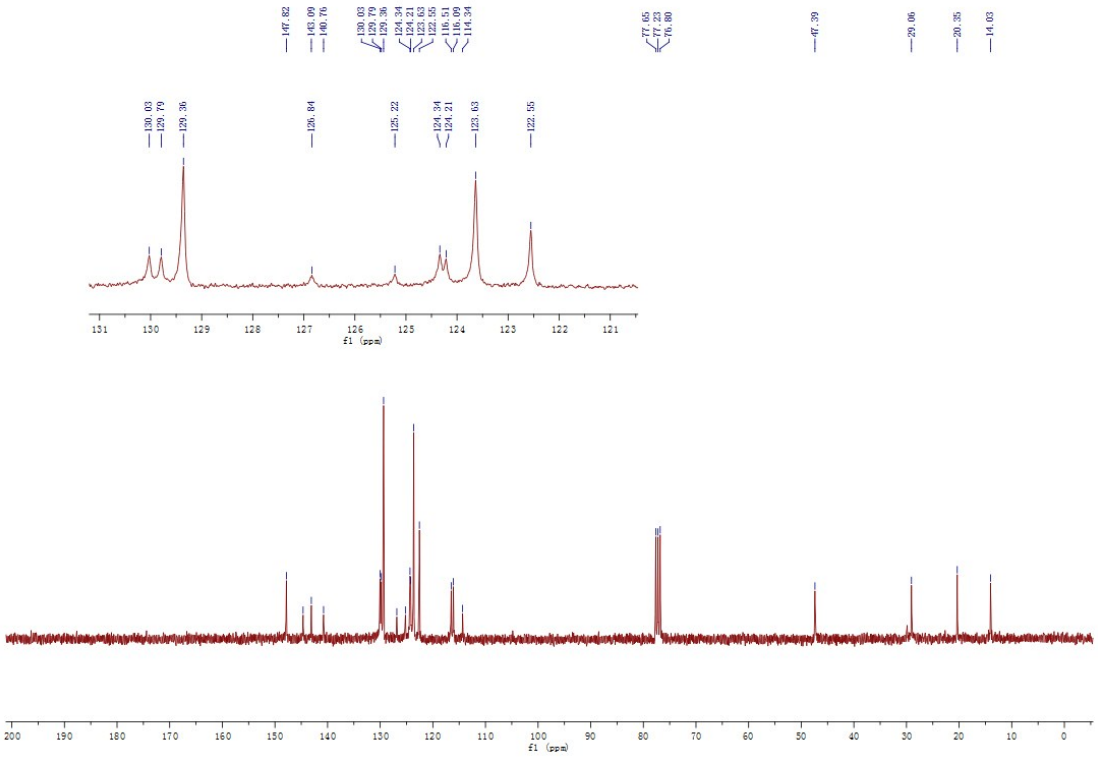
Figure S2. CV curves of organic dyes and Fc/Fc^{+} in THF.

NMR and HRMS spectra for our compounds.

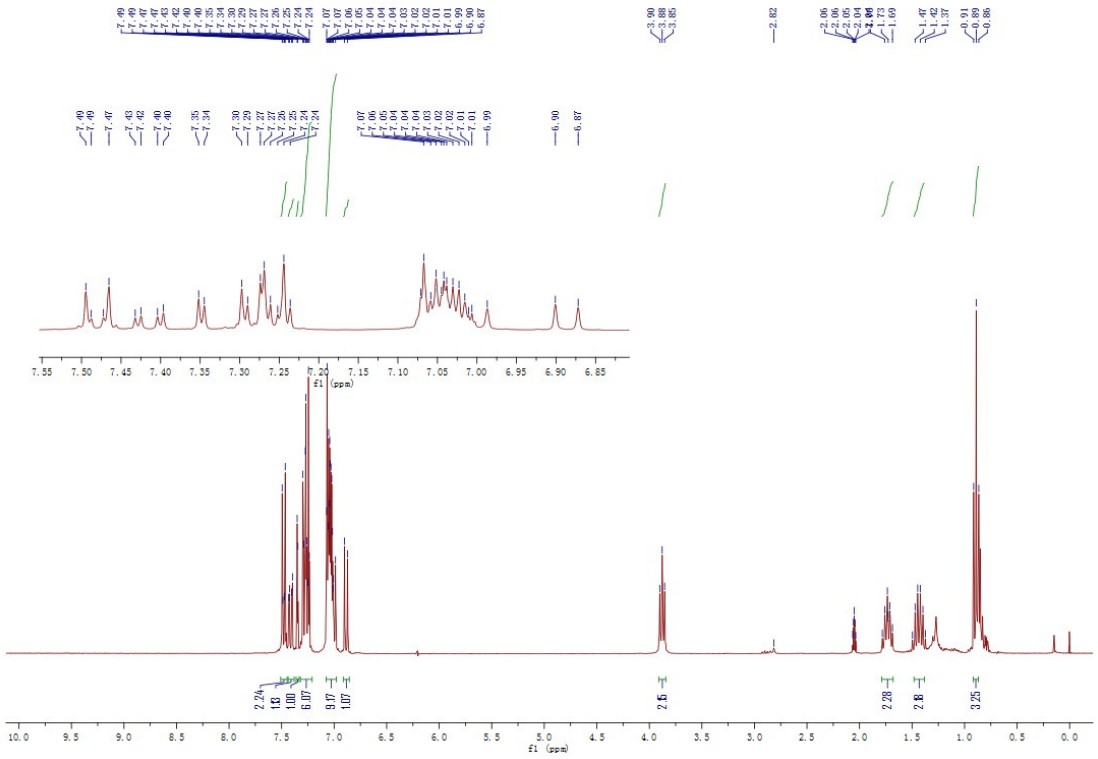
A2-^{1}H



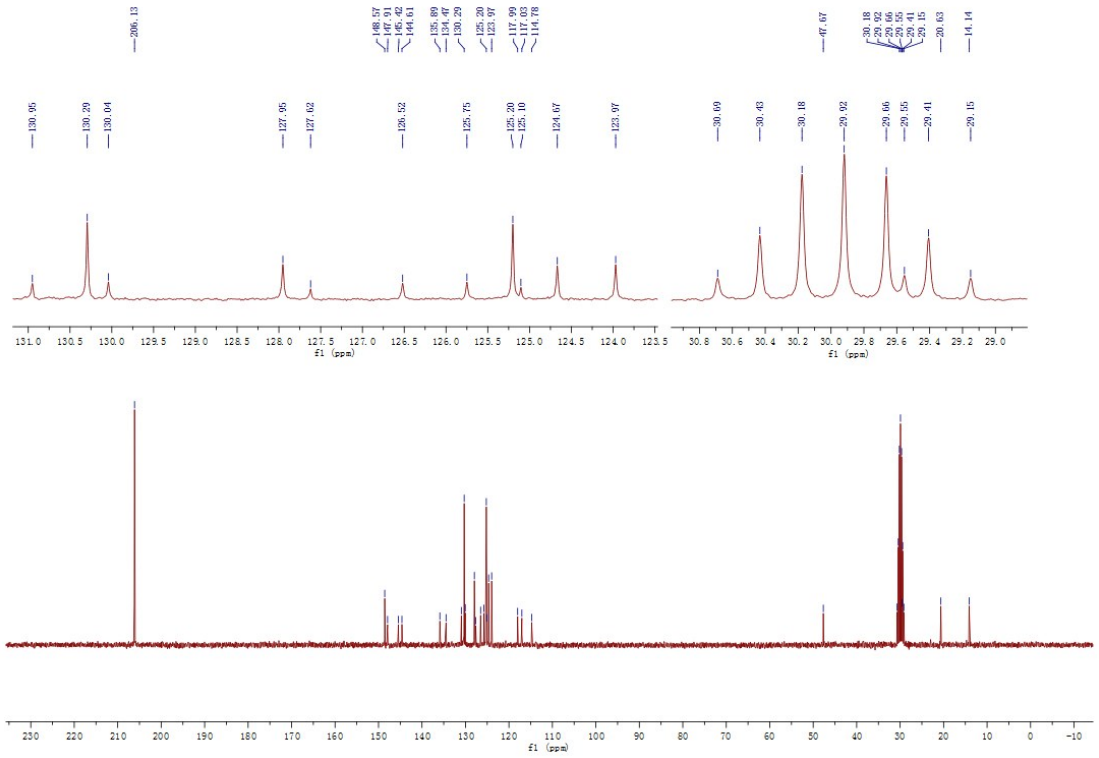
A2-^{13}C



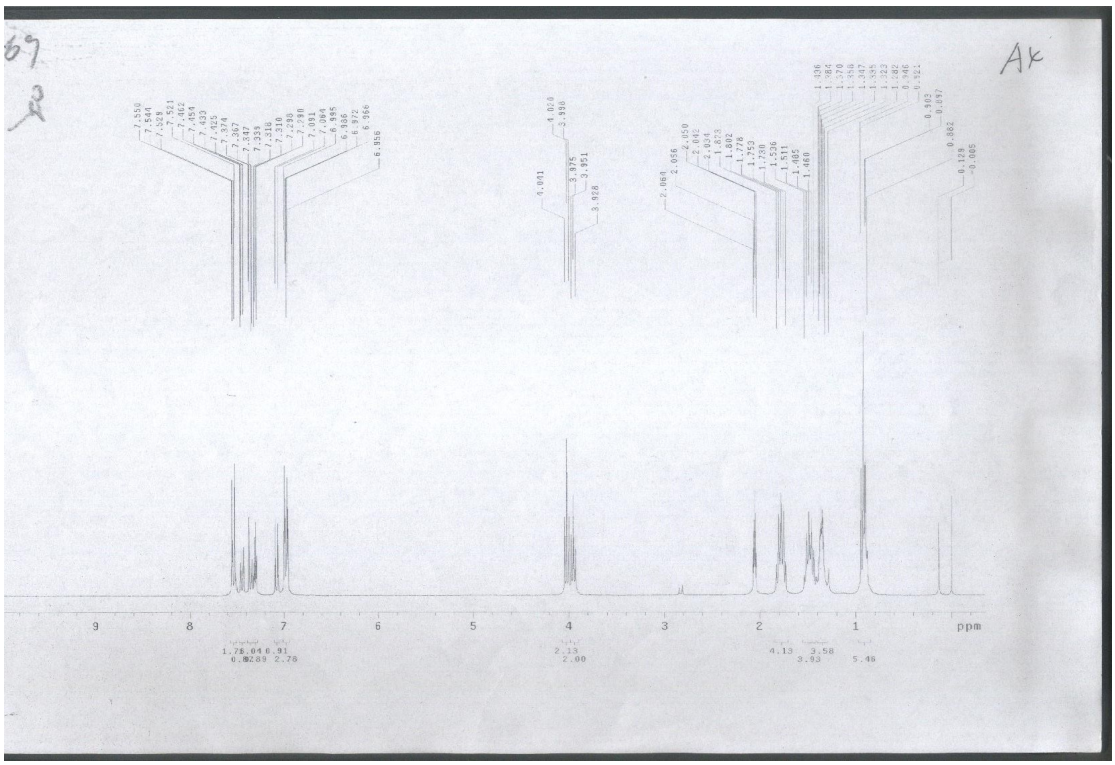
A3-^{1}H



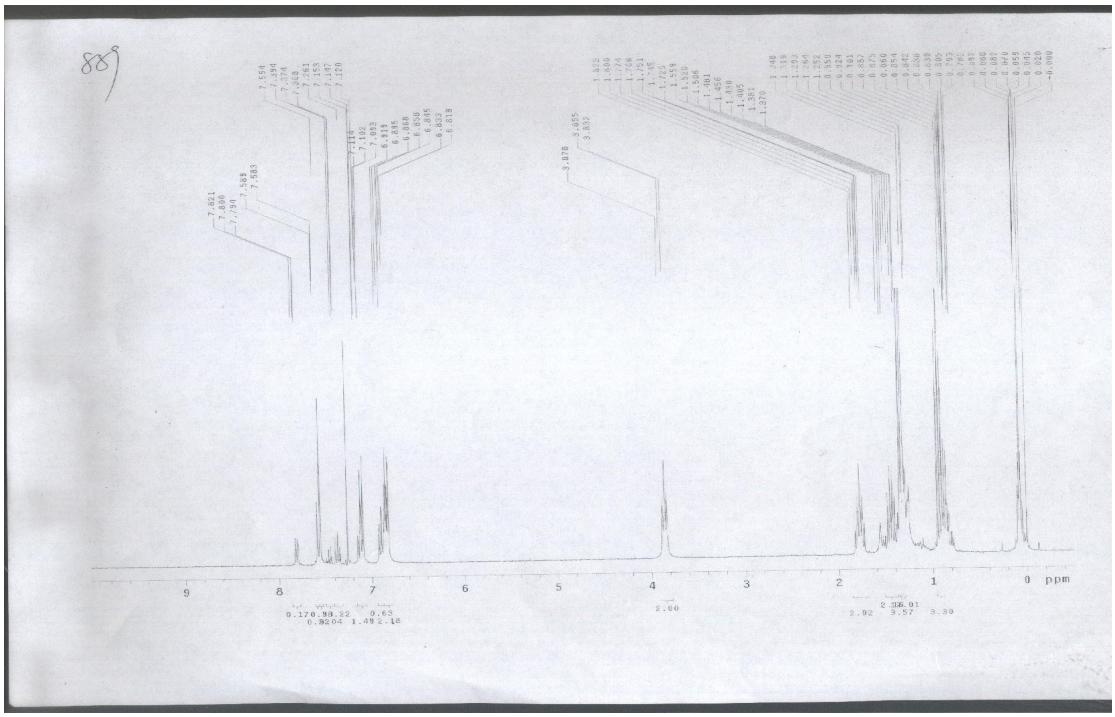
A3-^{13}C



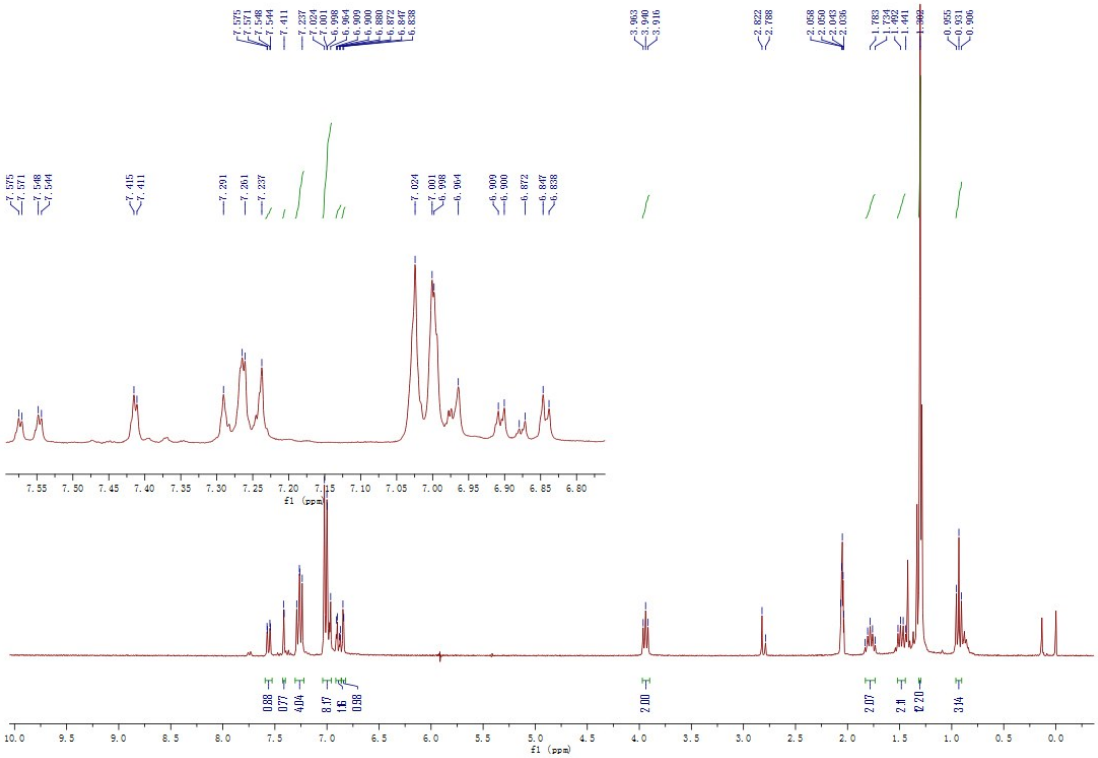
A4-^{1}H



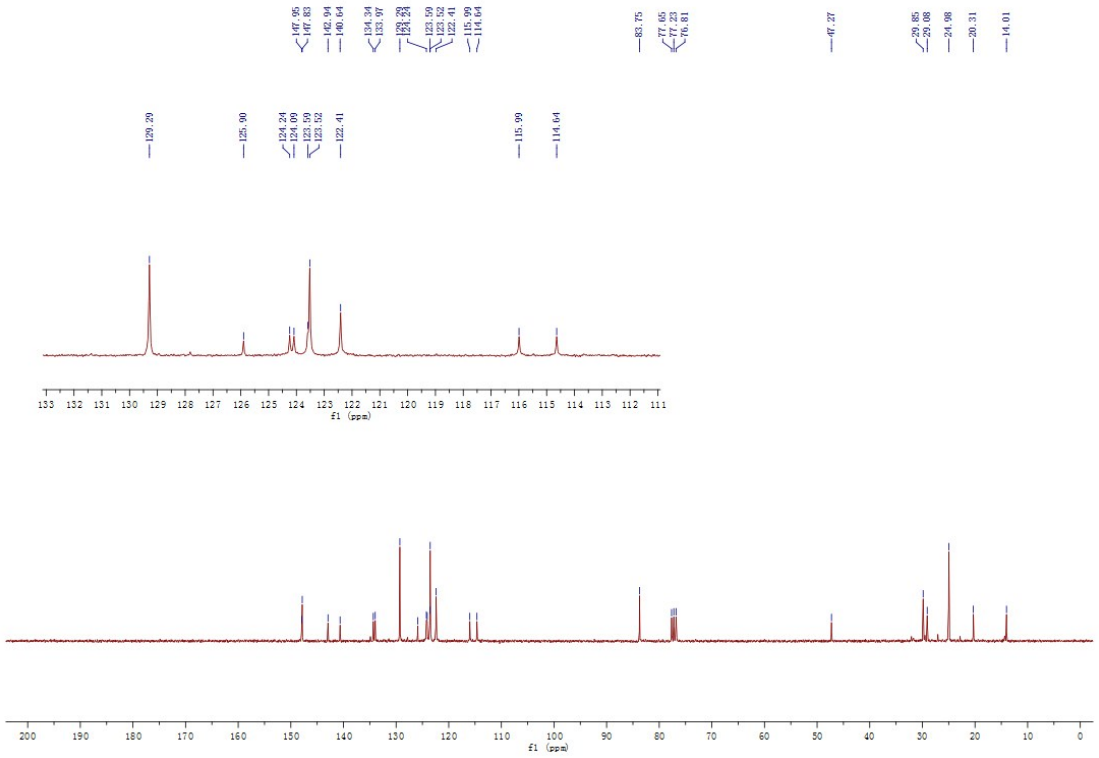
B1-^{1}H



B2-^{1}H



B2-^{13}C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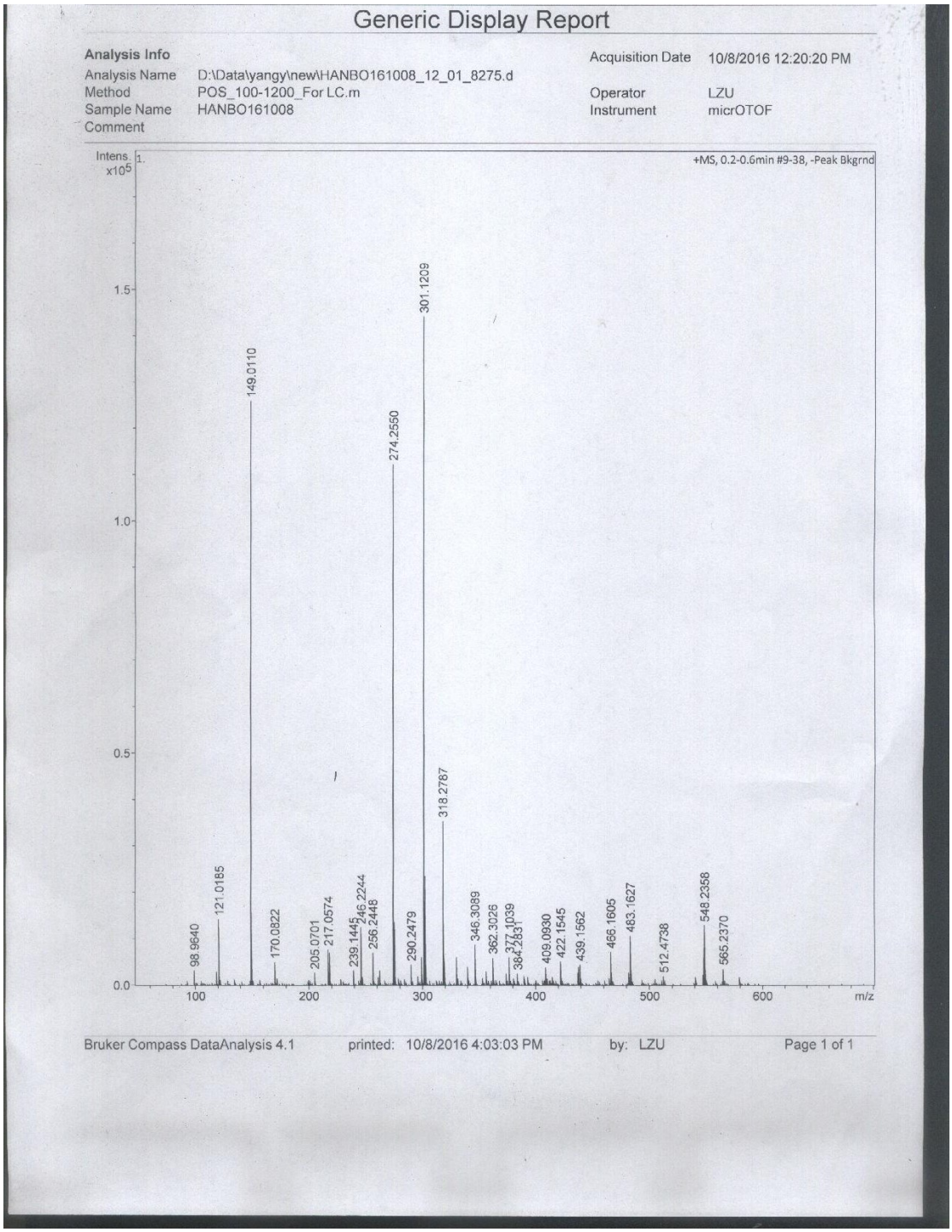
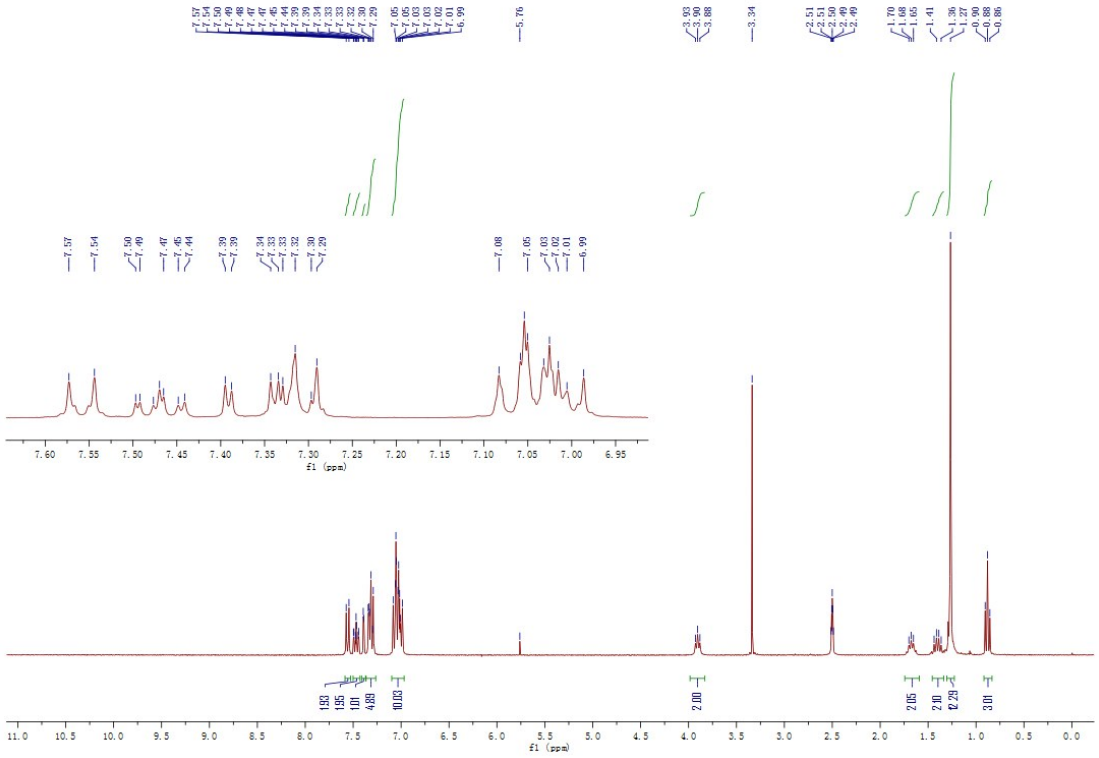
147.83
142.94
140.64
134.34
133.97
128.29
124.24
123.59
123.52
122.41
115.99
114.64
83.75
77.65
77.23
76.81
47.27
29.85
29.08
24.98
20.31
14.01
129.29
125.90
124.24
124.09
123.59
123.52
122.41
115.99
114.64
f1 (ppm)
f1 (ppm)

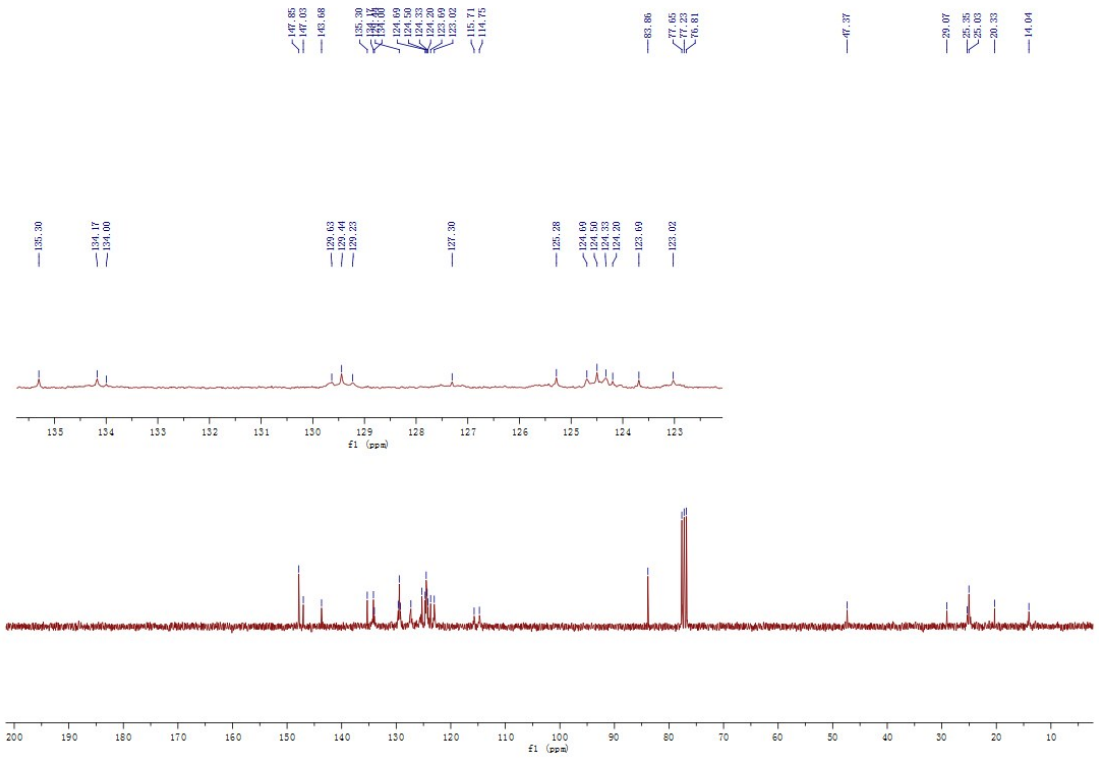
B2-HRMS


Generic Display Report
Analysis Info
Analysis Name D:\Data\yangy\new\HANBO161008_12_01_8275.d
Method POS_100-1200_For LC.m
Sample Name HANBO161008
Comment
Acquisition Date 10/8/2016 12:20:20 PM
Operator LZU
Instrument micrOTOF
Intens. x10^5
+MS, 0.2-0.6min #9-38, -Peak Bkgrnd
301.1209
149.0110
274.2550
318.2787
121.0185
98.9640
170.0822
205.0701
217.0574
239.1445
246.2244
256.2448
290.2479
346.3089
362.3026
377.1039
384.2831
409.0930
422.1545
439.1562
466.1605
483.1627
512.4738
548.2358
565.2370
m/z
Bruker Compass DataAnalysis 4.1 printed: 10/8/2016 4:03:03 PM by: LZU Page 1 of 1

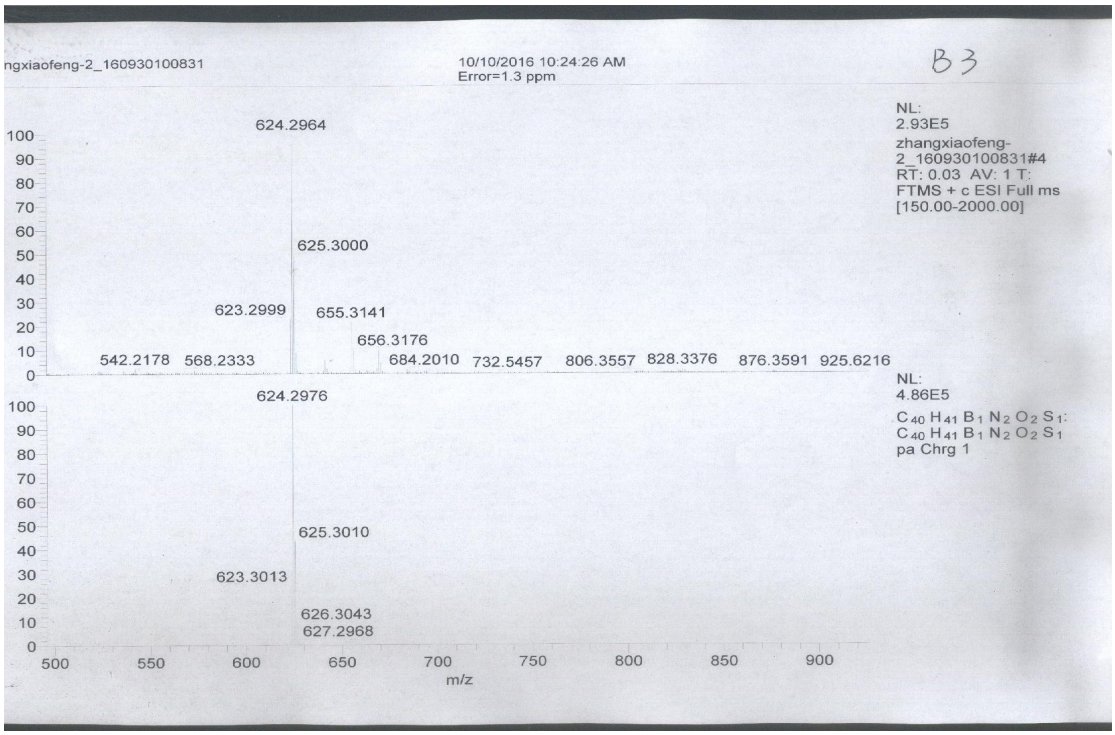
B3-^{1}H



B3-^{13}C



B3-HRMS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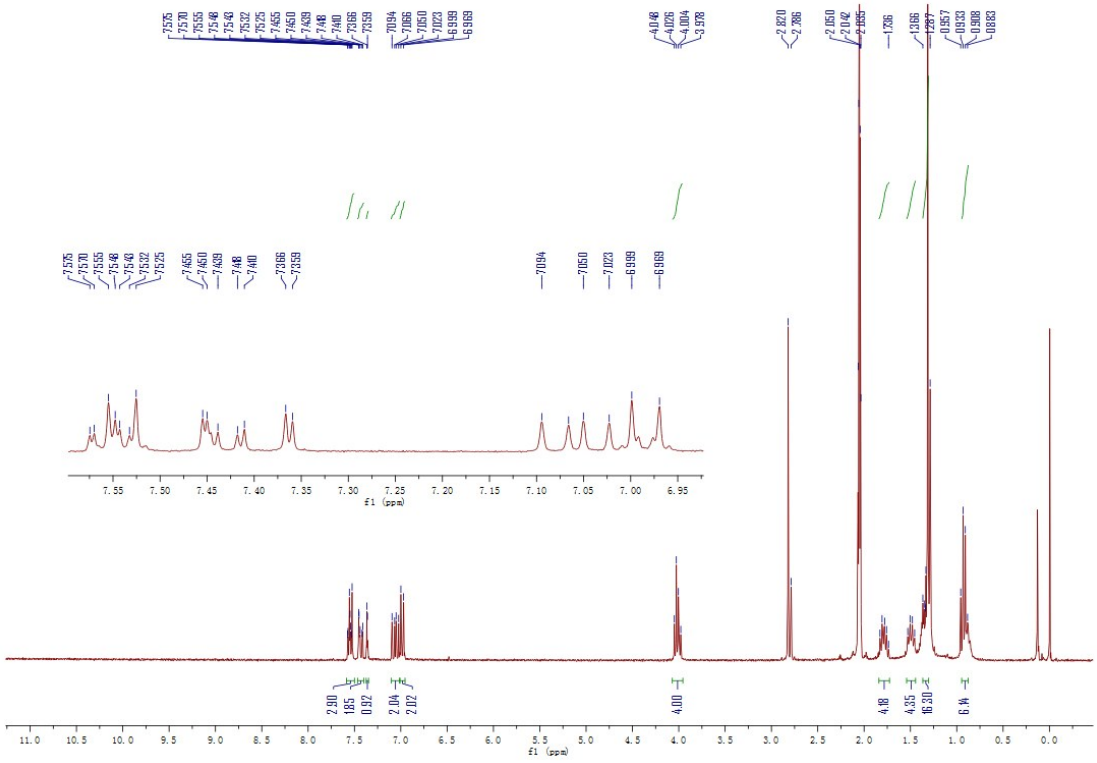
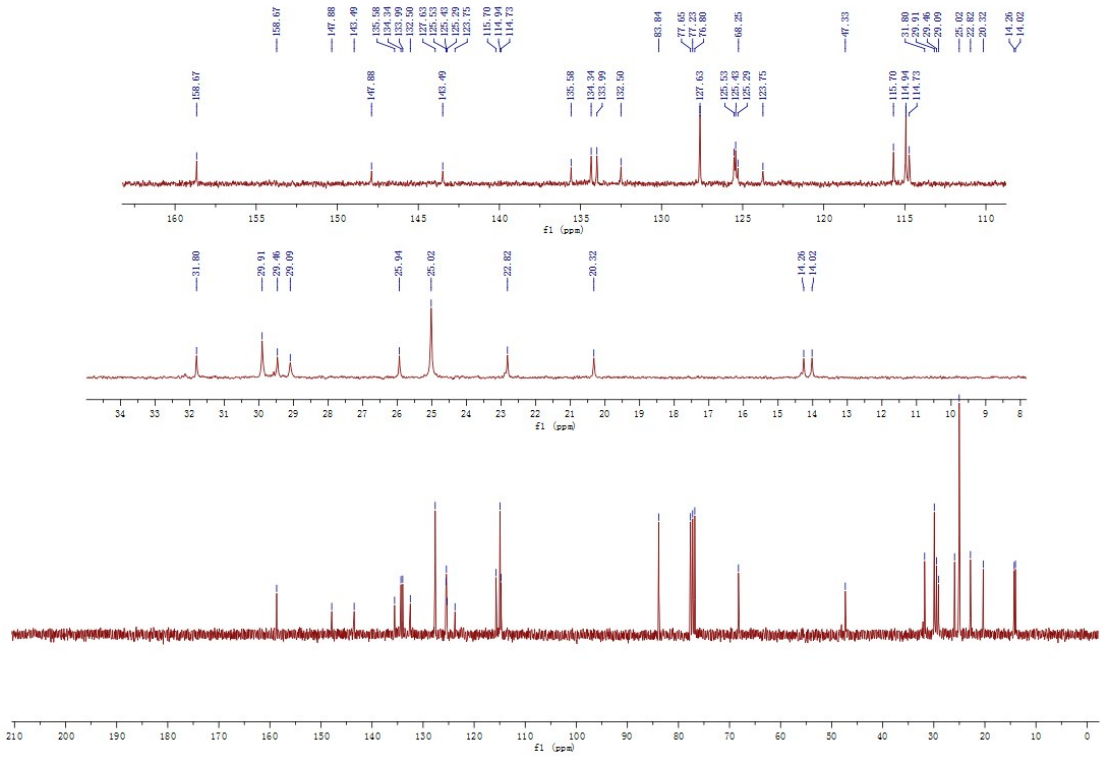
10/10/2016 10:24:26 AM
Error=1.3 ppm
B3
NL:
2.93E5
zhangxiaofeng-2_160930100831#4
RT: 0.03 AV: 1 T:
FTMS + c ESI Full ms
[150.00-2000.00]
624.2964
625.3000
623.2999
655.3141
656.3176
542.2178
568.2333
684.2010
732.5457
806.3557
828.3376
876.3591
925.6216
NL:
4.86E5
C40 H41 B1 N2 O2 S1:
C40 H41 B1 N2 O2 S1
pa Chrg 1
624.2976
625.3010
623.3013
626.3043
627.2968
m/z

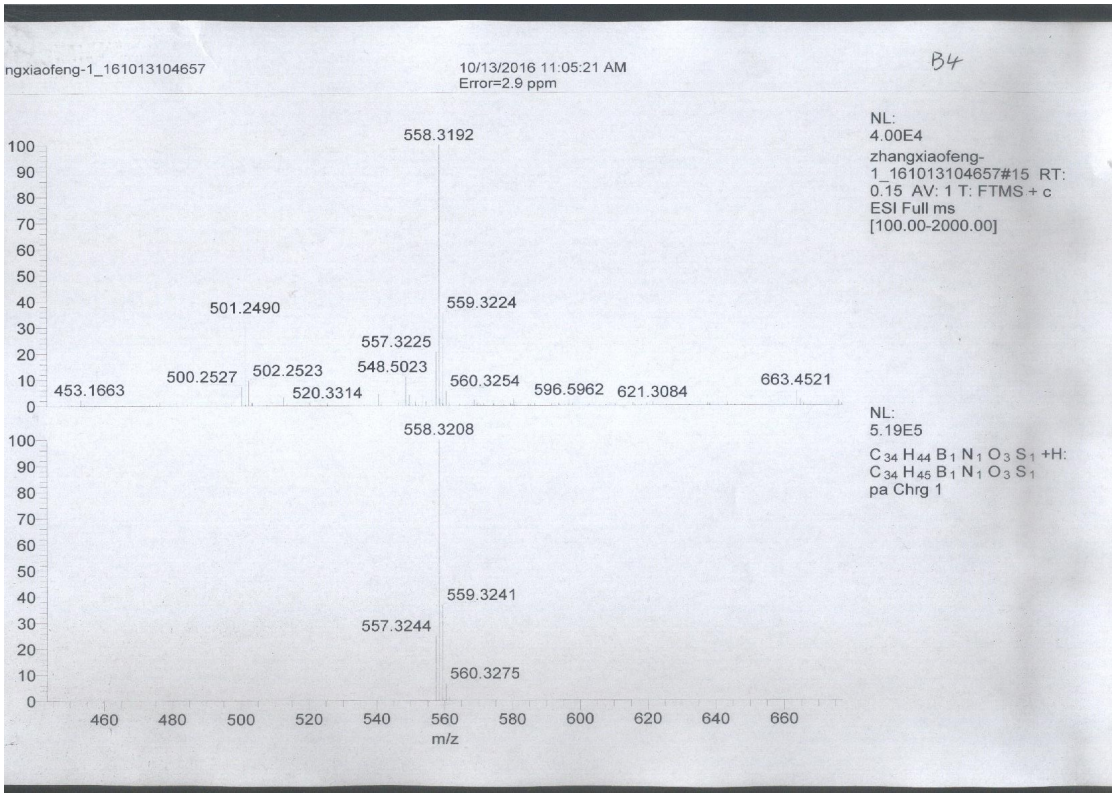
B4-^{1}H


f1 (ppm)

B4-^{13}C

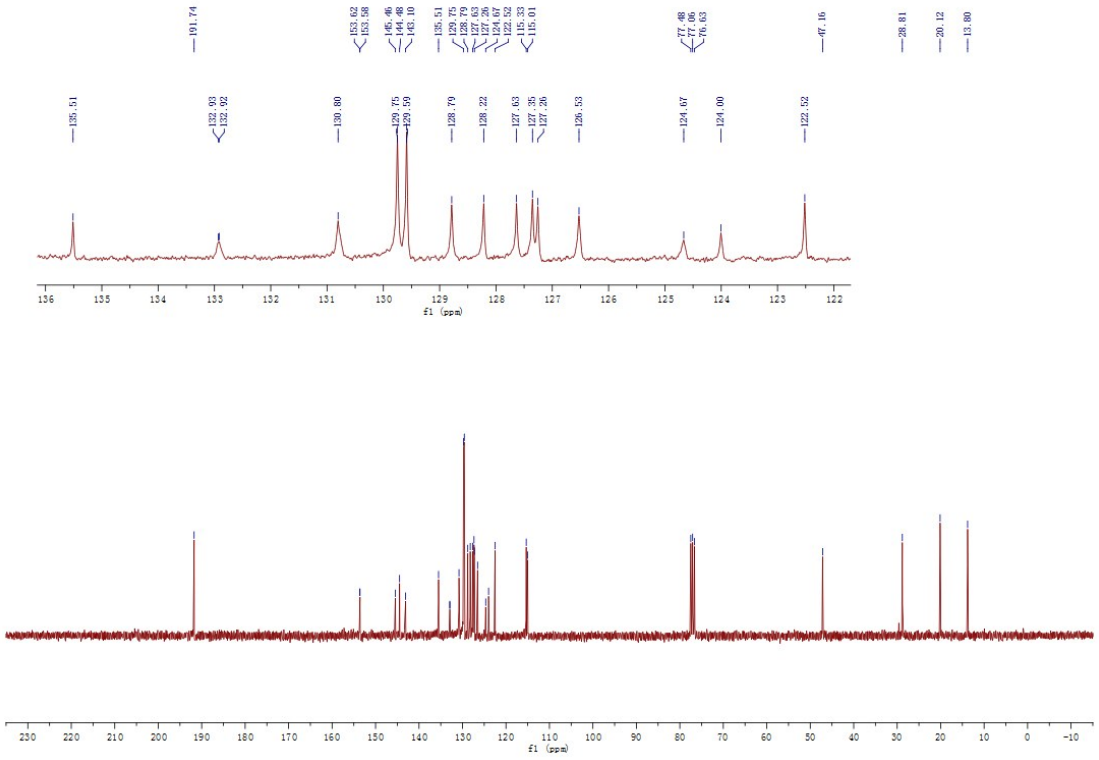


B4-HRMS

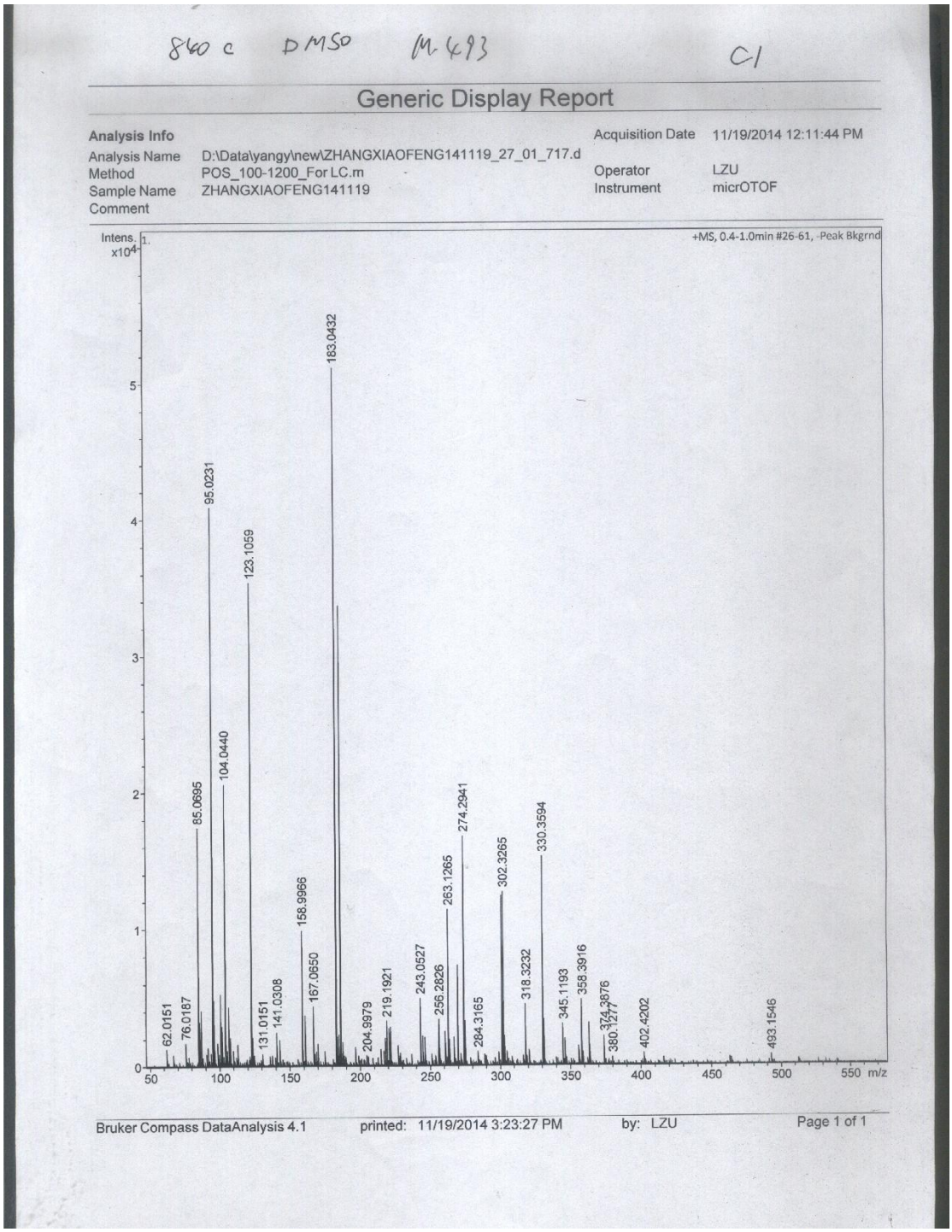


C1-^{1}H

C1-^{13}C



C1-HRMS


860 c DMSO M.493 C1
Generic Display Report
Analysis Info
Analysis Name D:\Data\yangy\new\ZHANGXIAOFENG141119_27_01_717.d
Method POS_100-1200_For LC.m
Sample Name ZHANGXIAOFENG141119
Comment
Acquisition Date 11/19/2014 12:11:44 PM
Operator LZU
Instrument micrOTOF
Intens. x10^4
+MS, 0.4-1.0min #26-61, -Peak Bkgrnd
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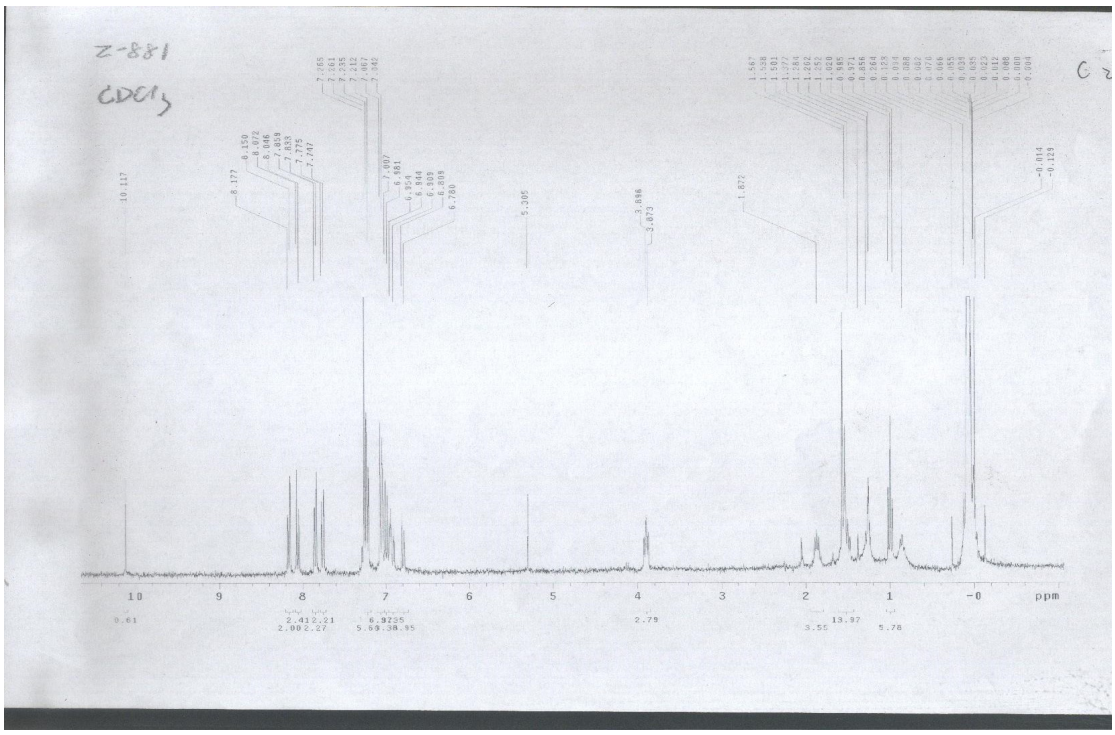
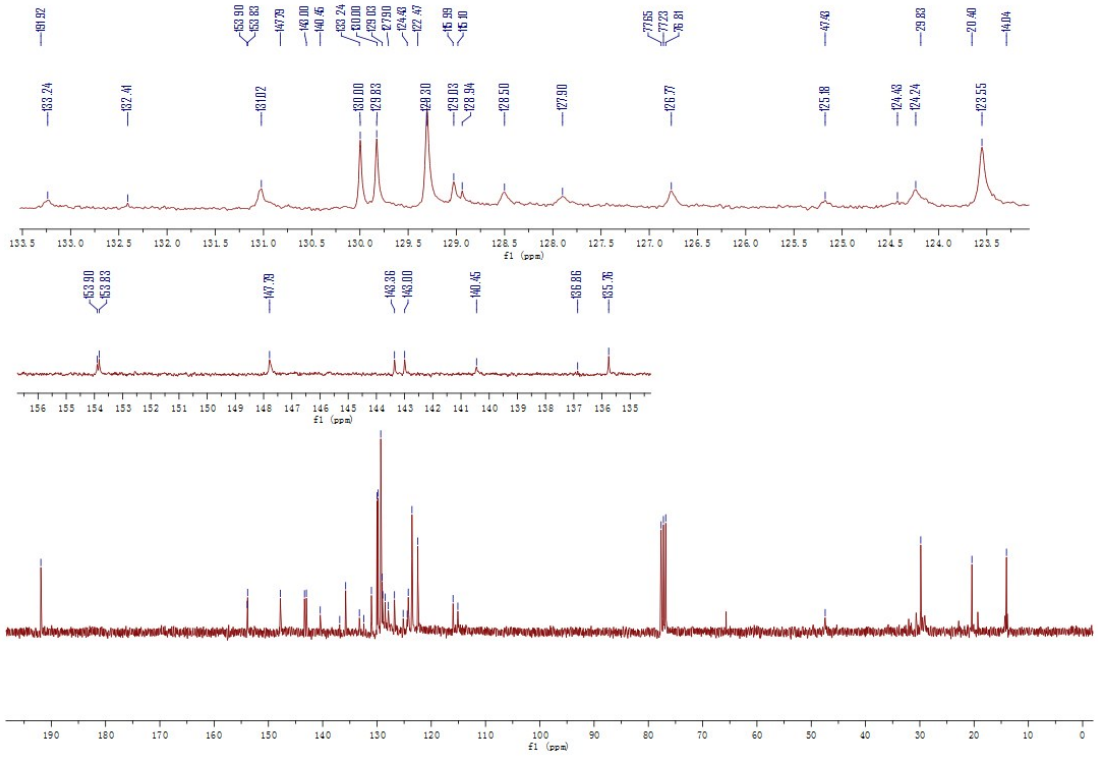
95.0231
123.1059
104.0440
85.0695
274.2941
330.3594
302.3265
263.1265
158.9966
167.0650
62.0151
76.0187
131.0151
141.0308
204.9979
219.1921
243.0527
256.2826
284.3165
318.3232
345.1193
358.3916
374.3876
380.1277
402.4202
493.1546
m/z
Bruker Compass DataAnalysis 4.1
printed: 11/19/2014 3:23:27 PM
by: LZU
Page 1 of 1

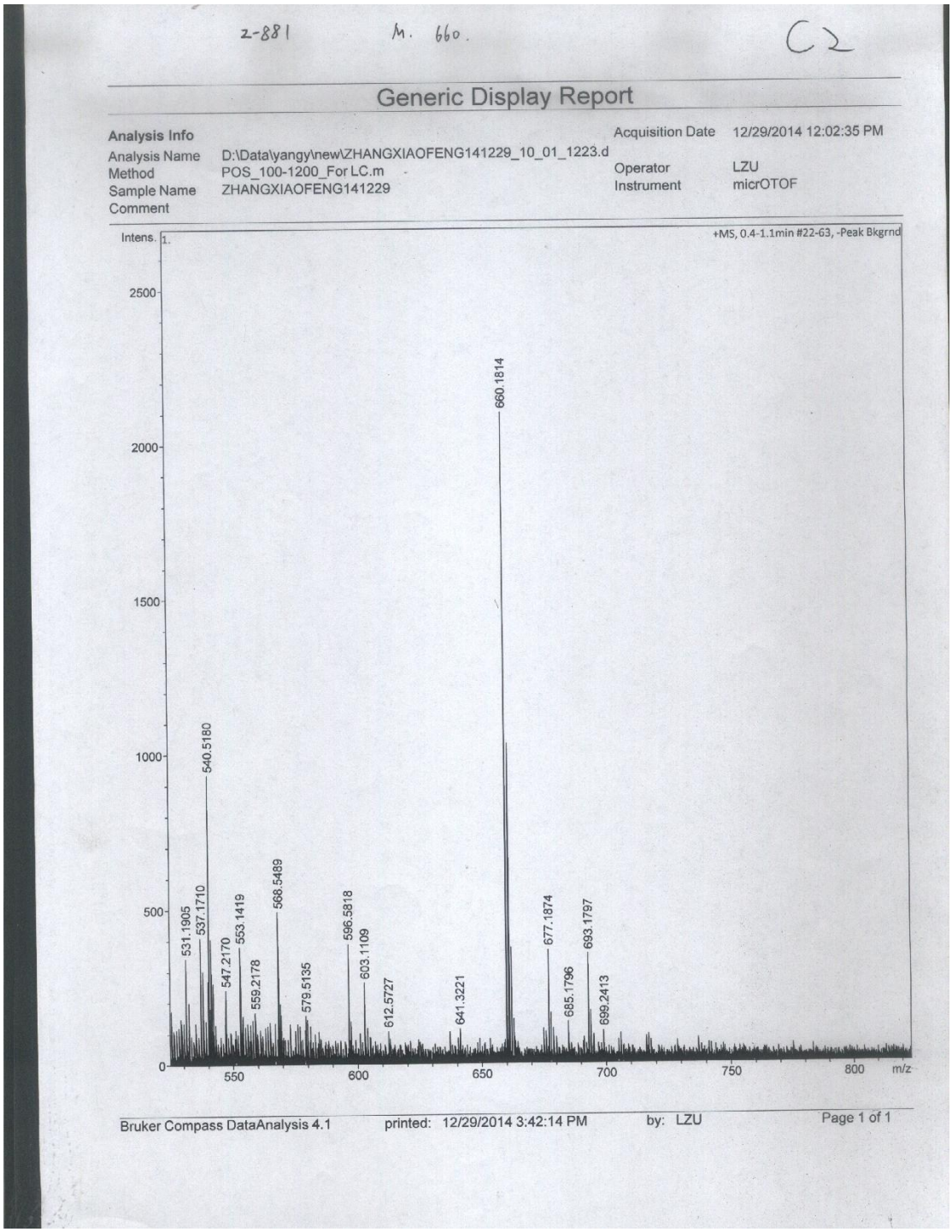
C2-^{1}H



C2-^{13}C



C2-HRMS


z-881
M. 660.
C2
Generic Display Report
Analysis Info
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Comment
Acquisition Date 12/29/2014 12:02:35 PM
Operator LZU
Instrument micrOTOF
Intens.
+MS, 0.4-1.1min #22-63, -Peak Bkgrnd
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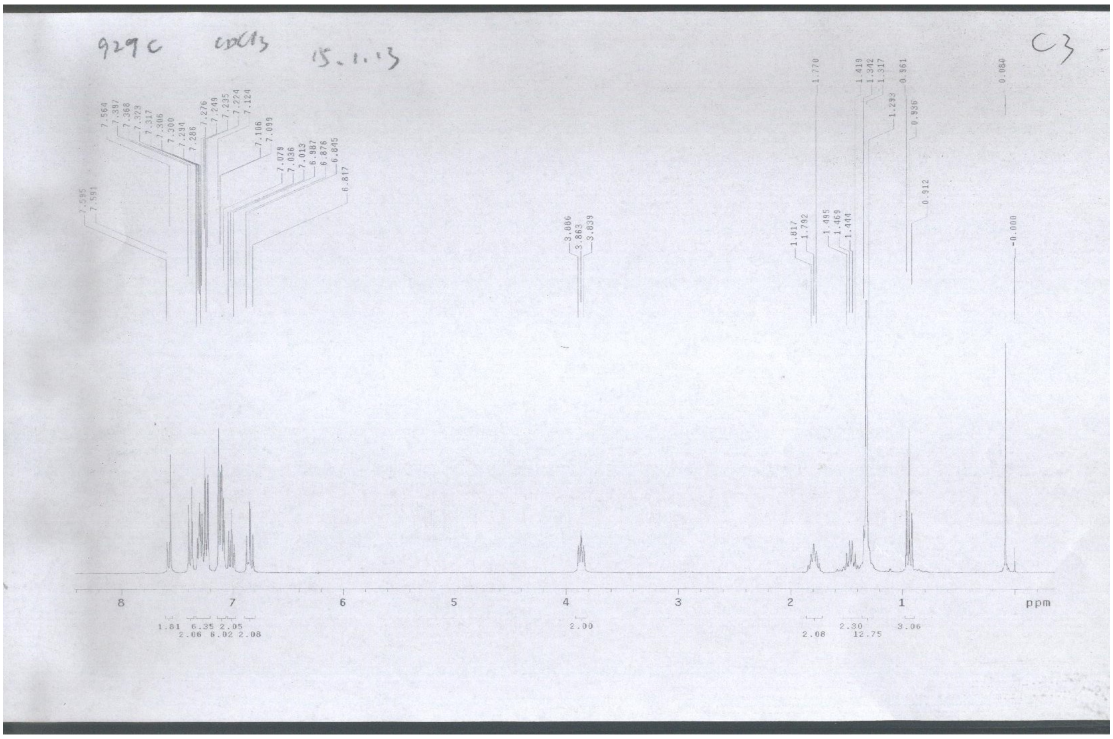
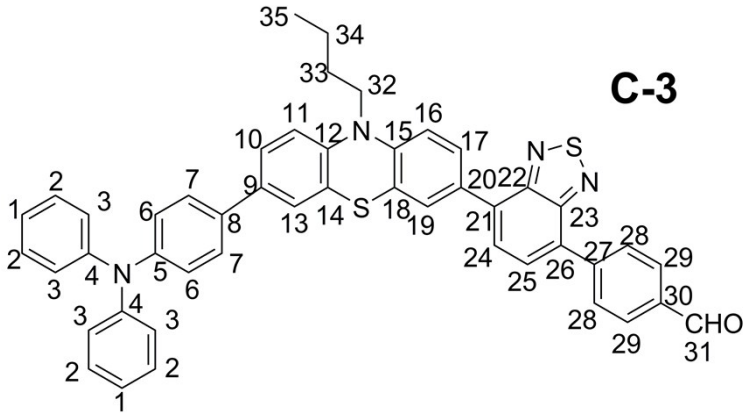
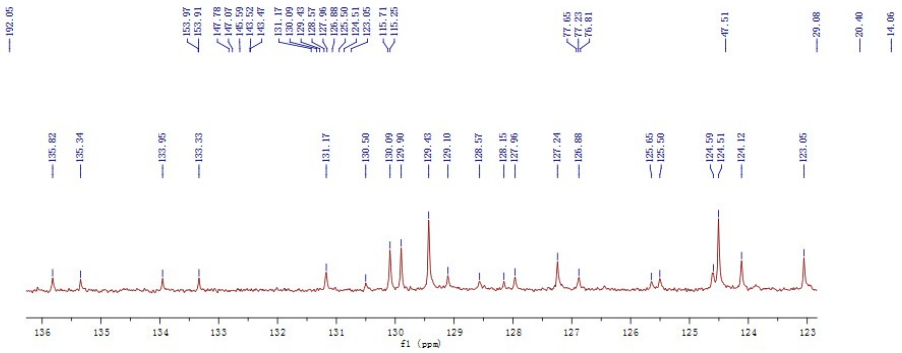
2000
1500
1000
500
0
660.1814
540.5180
531.1905
537.1710
547.2170
553.1419
559.2178
568.5489
579.5135
596.5818
603.1109
612.5727
641.3221
677.1874
685.1796
693.1797
699.2413
550
600
650
700
750
800
m/z
Bruker Compass DataAnalysis 4.1
printed: 12/29/2014 3:42:14 PM
by: LZU
Page 1 of 1

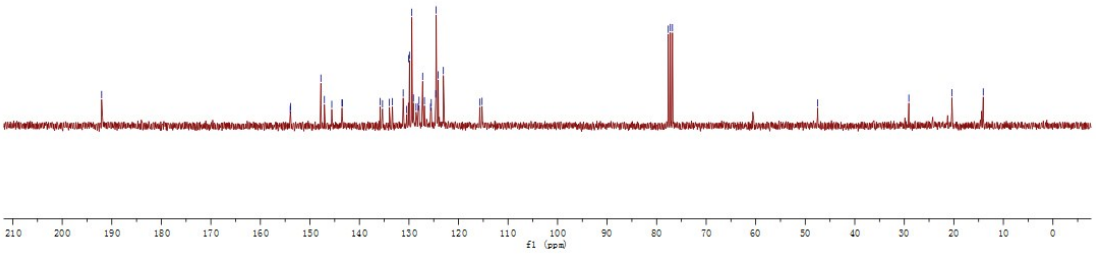
C3-^{1}H



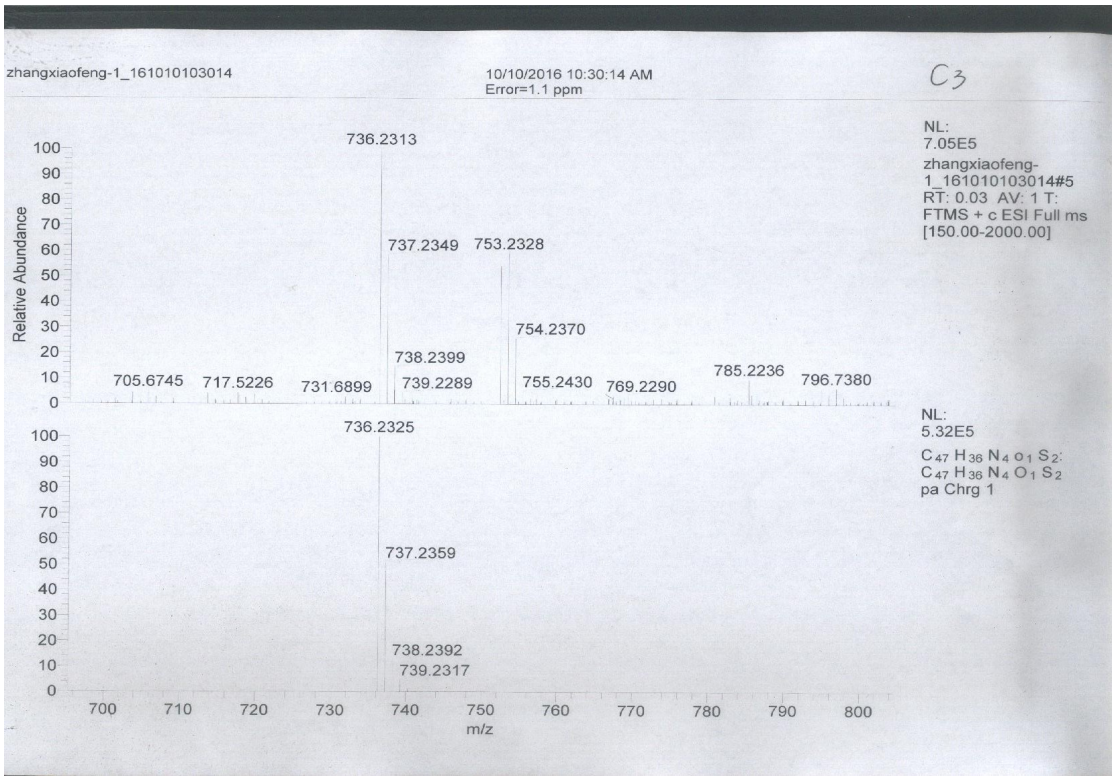
C3-^{13}C







C3-HRMS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10/10/2016 10:30:14 AM
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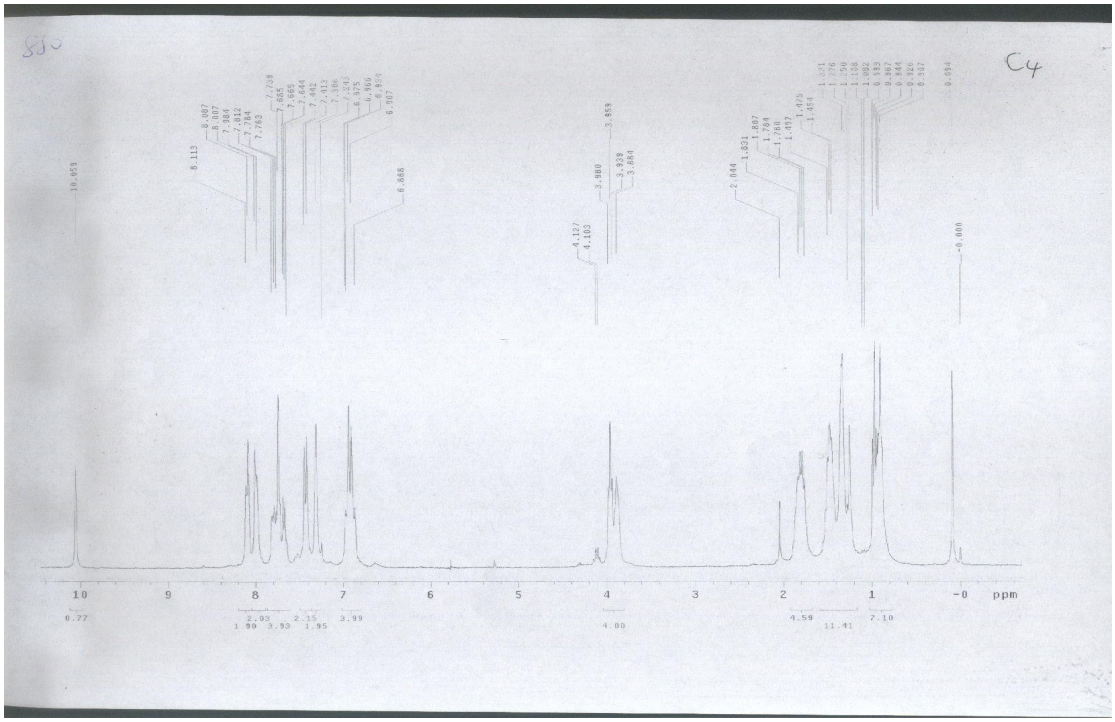
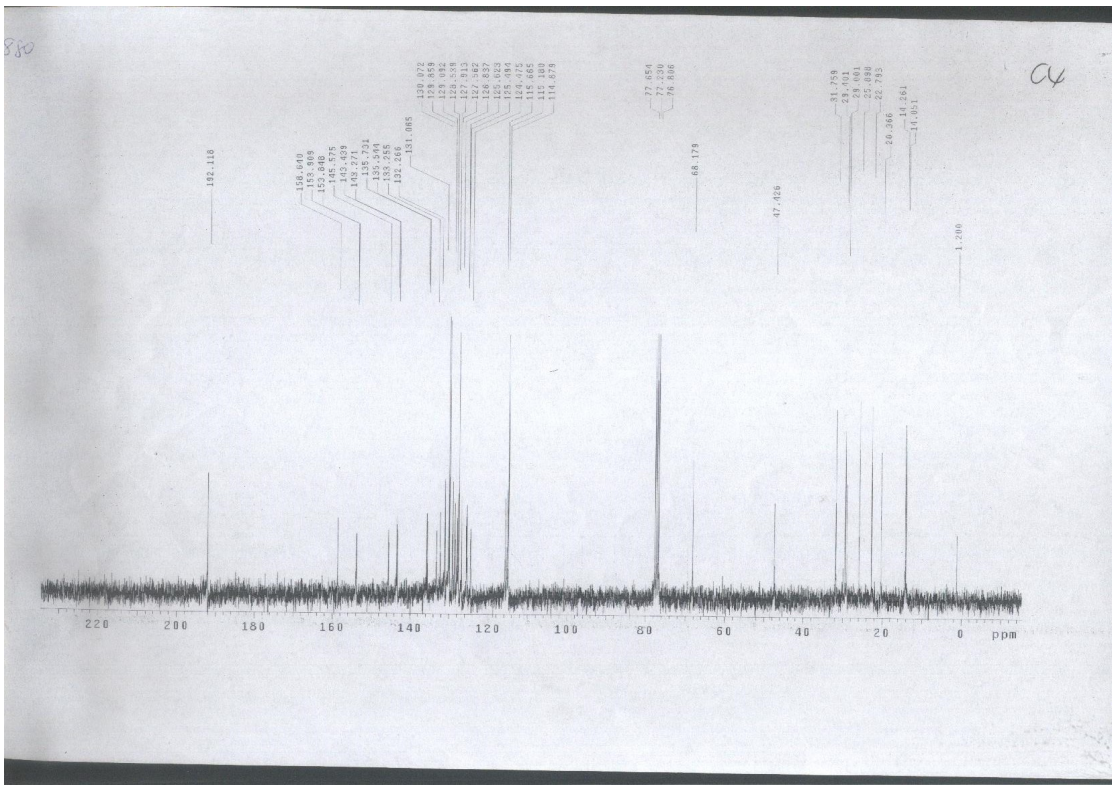
C3
NL:
7.05E5
zhangxiaofeng-1_161010103014#5
RT: 0.03 AV: 1 T:
FTMS + c ESI Full ms
[150.00-2000.00]
736.2313
737.2349
753.2328
754.2370
738.2399
705.6745
717.5226
731.6899
739.2289
755.2430
769.2290
785.2236
796.7380
NL:
5.32E5
C47 H36 N4 o1 S2:
C47 H36 N4 O1 S2
pa Chrg 1
736.2325
737.2359
738.2392
739.2317
Relative Abundance
m/z

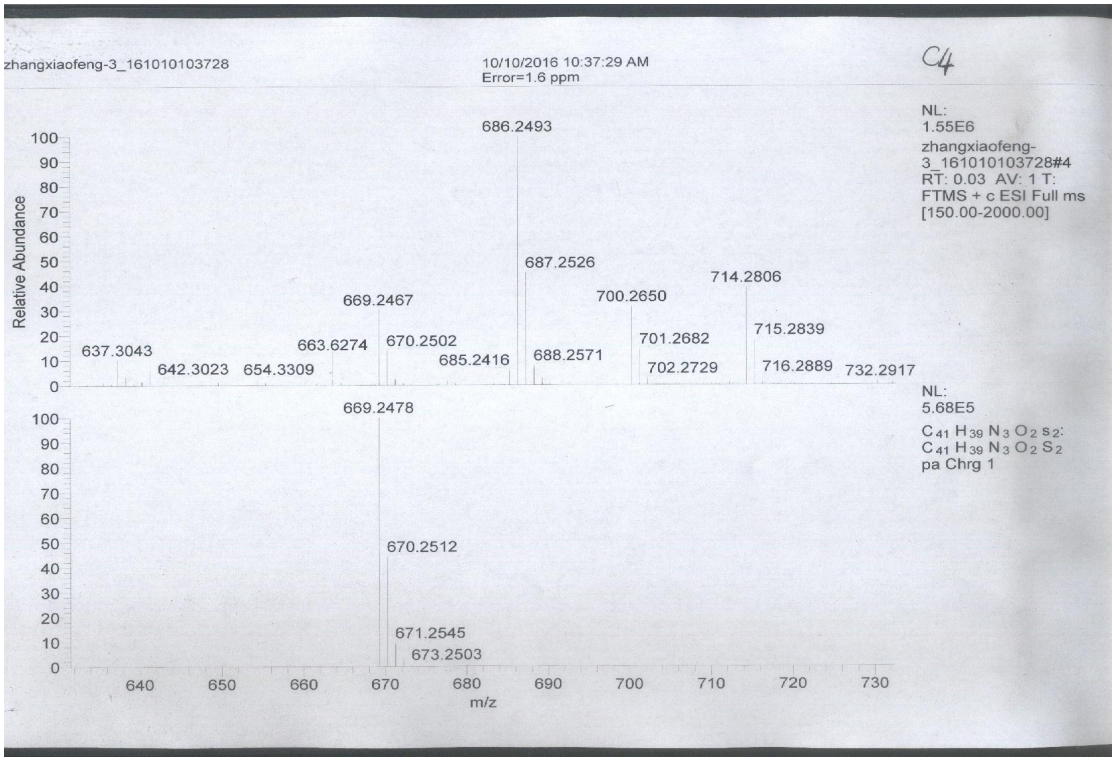
C4-^{1}H


C4
ppm

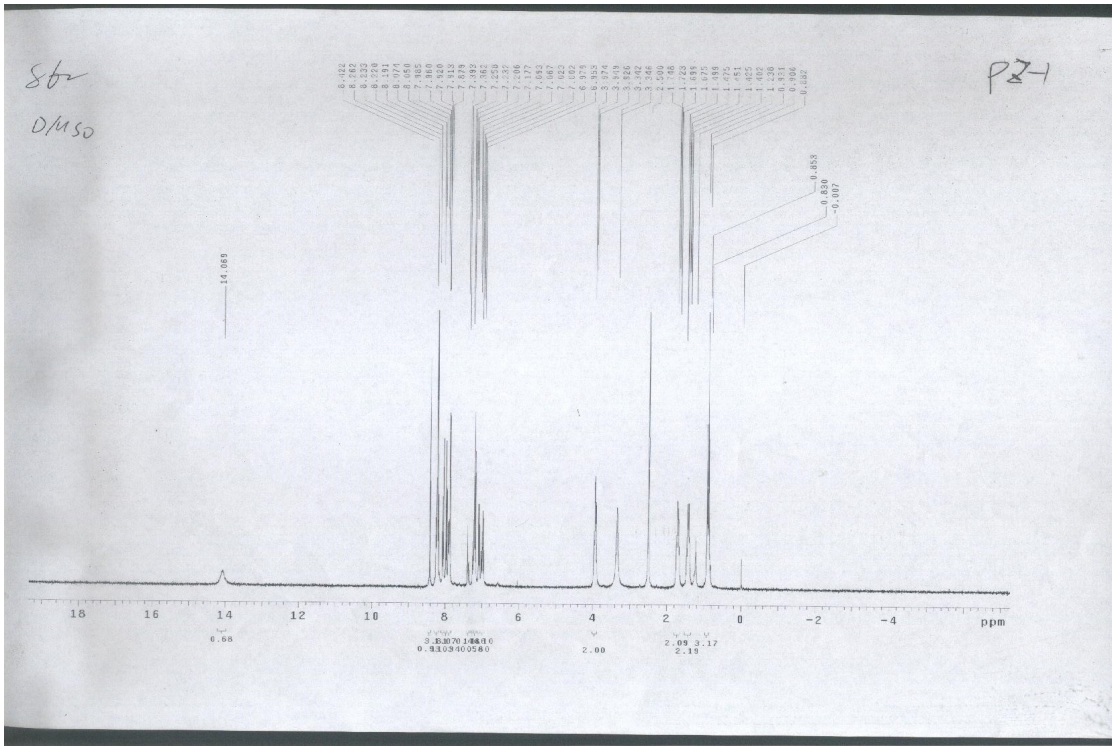
C4-^{13}C



C4-HRMS



PZ-1-^{1}H


Sbr
DMSO
PZ-1
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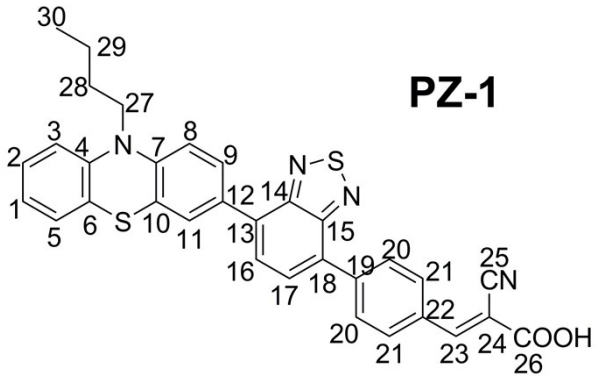
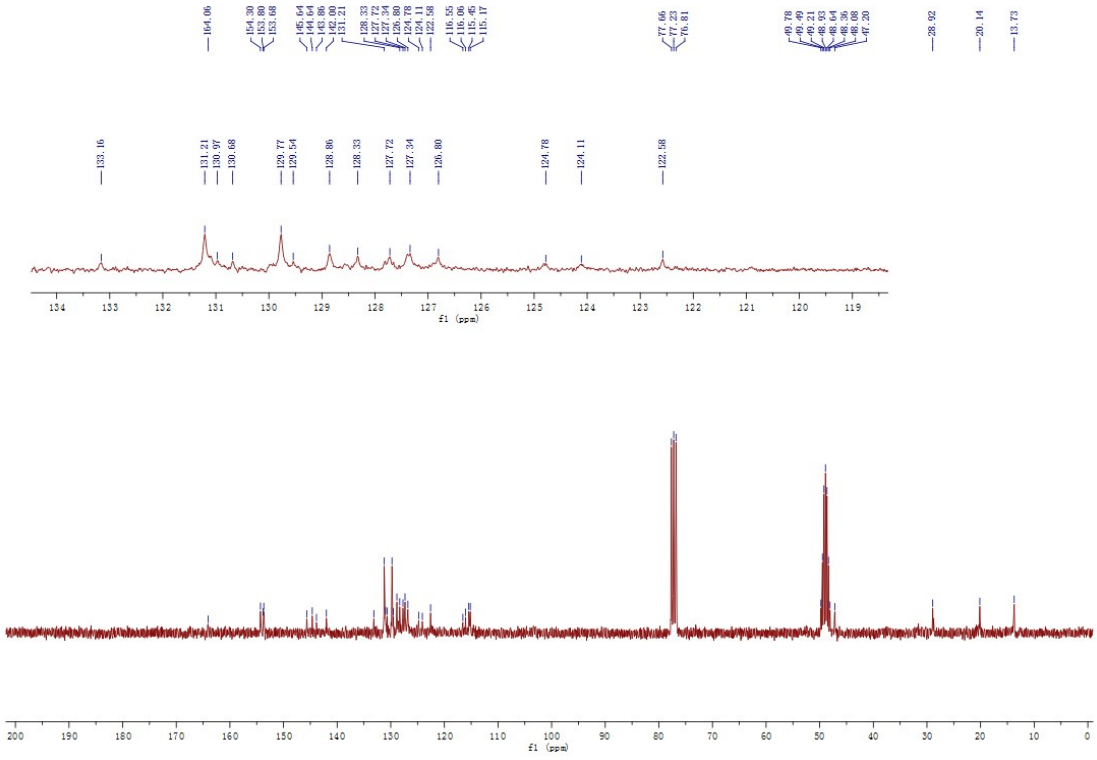
0.858
0.830
0.807
18
16
14
12
10
8
6
4
2
0
-2
-4
ppm
6.68
2.00
2.09
3.17
2.19

PZ-1-^{13}C


PZ-1
30
29
28
27
N
S
N
S
CN
COOH
26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144.64
143.86
142.00
131.21
128.33
127.72
127.34
126.80
124.78
124.11
122.58
116.55
116.06
115.45
115.17
77.66
77.23
76.81
49.78
49.49
49.21
48.93
48.64
48.36
48.08
47.20
28.92
20.14
13.73
133.16
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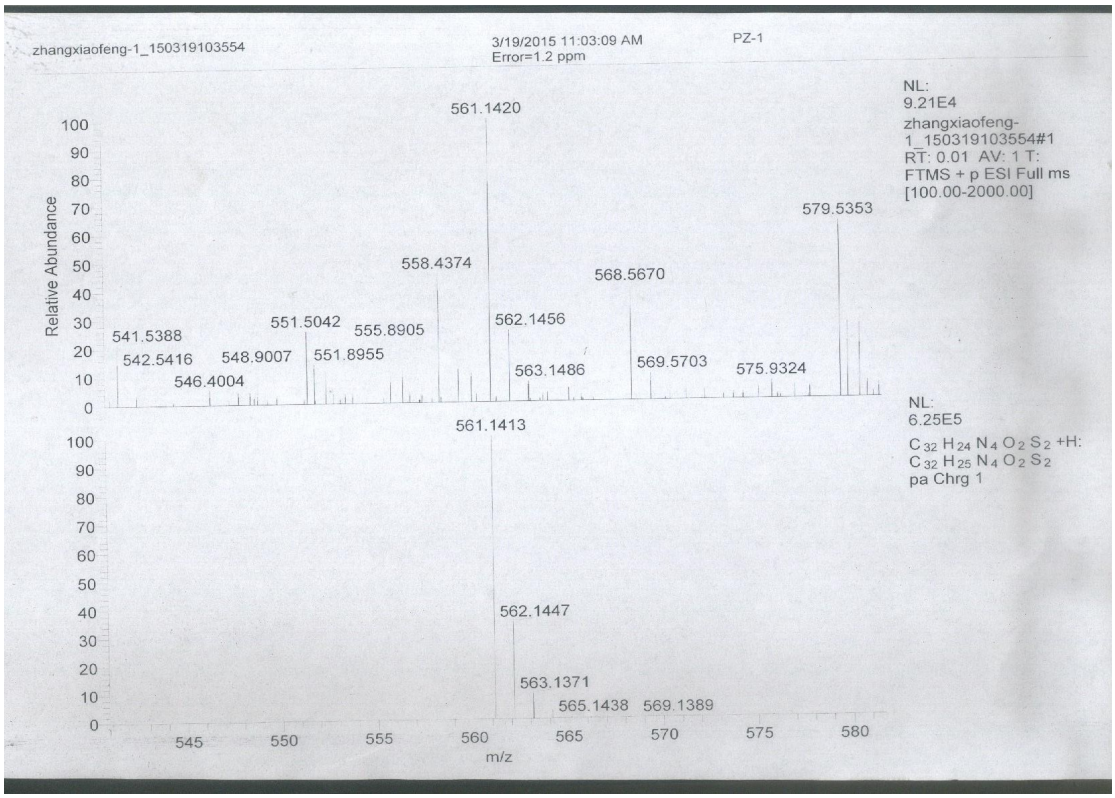
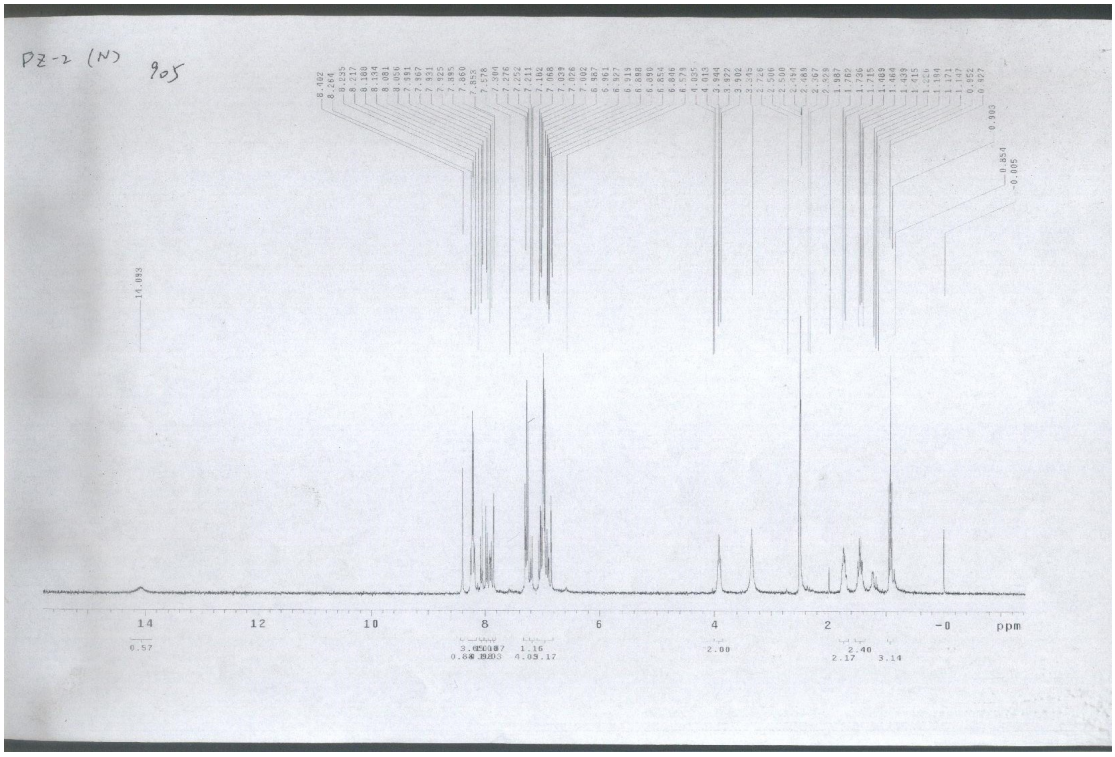
130.68
129.77
129.54
128.86
128.33
127.72
127.34
126.80
124.78
124.11
122.58
f1 (ppm)
f1 (ppm)

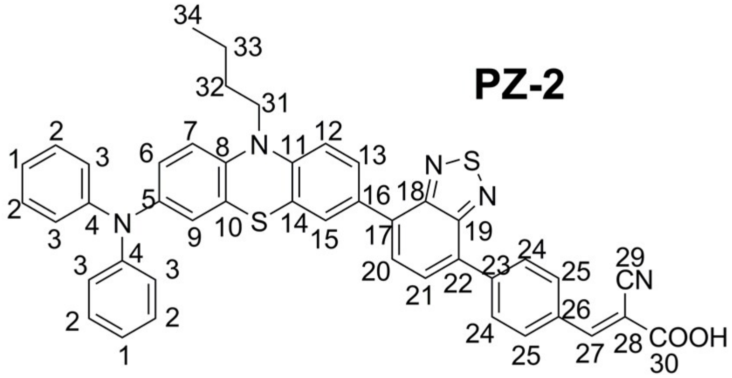
PZ-1-HRMS

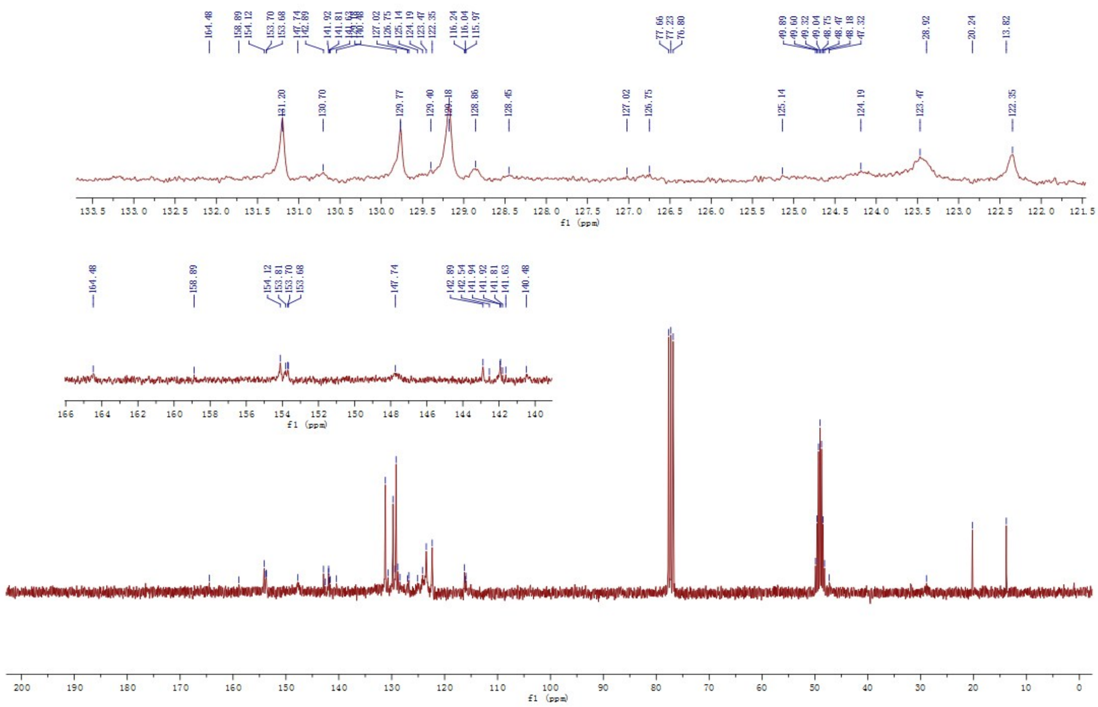


PZ-2-^{1}H



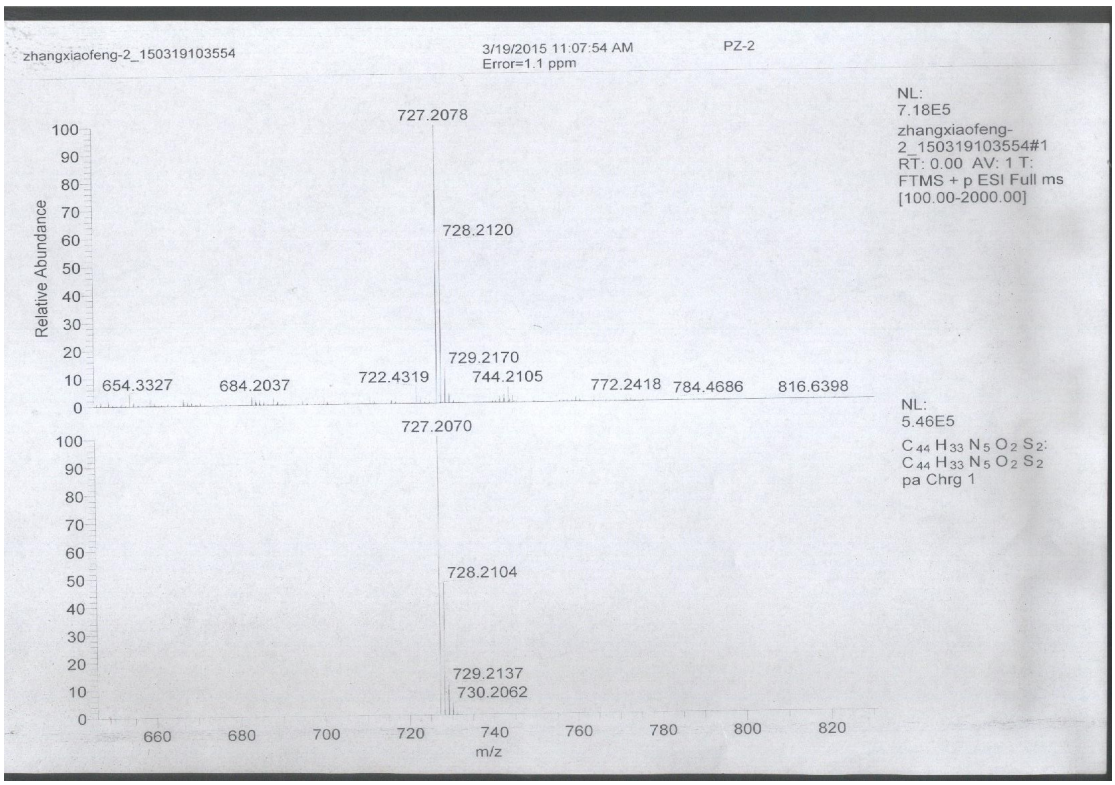
PZ-2-^{13}C



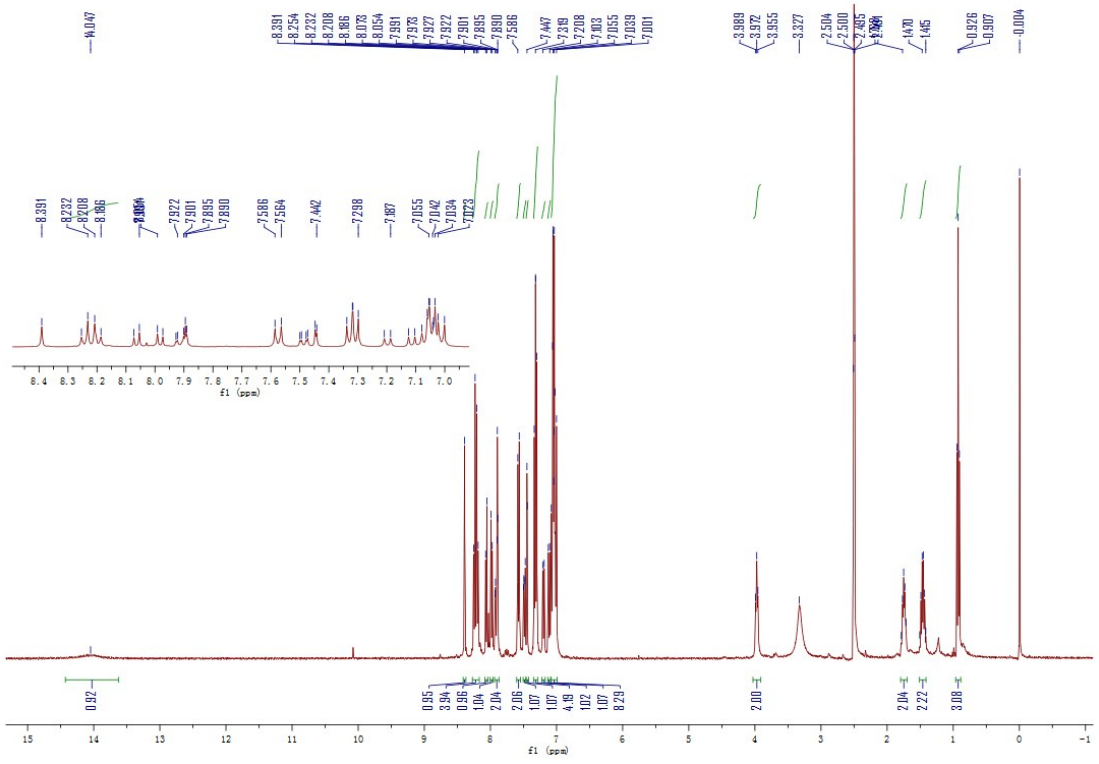


164.48
158.89
154.12
153.70
153.68
147.74
142.89
141.92
141.81
127.02
126.75
125.14
124.19
123.47
122.35
116.24
116.04
115.97
77.66
77.23
76.80
49.89
49.60
49.32
49.04
48.75
48.47
48.18
47.32
28.92
20.24
13.82
131.20
130.70
129.77
129.40
129.18
128.86
128.45
127.02
126.75
125.14
124.19
123.47
122.35
f1 (ppm)
164.48
158.89
154.12
153.81
153.70
153.68
147.74
142.89
142.54
141.92
141.81
141.63
140.48
f1 (ppm)
f1 (ppm)

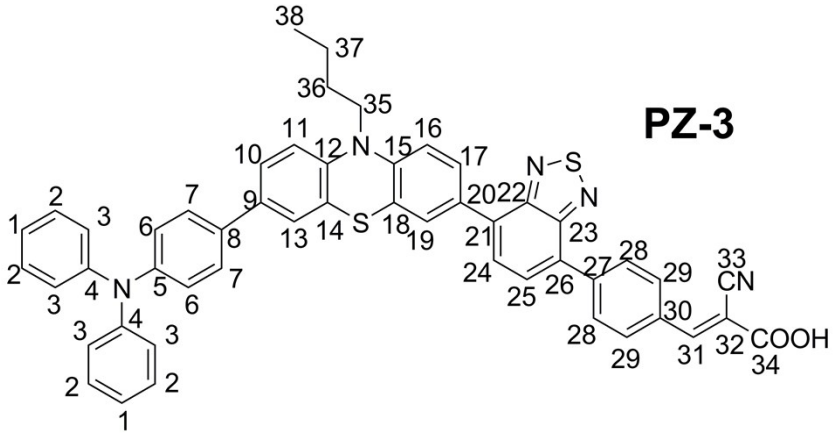
PZ-2-HRMS

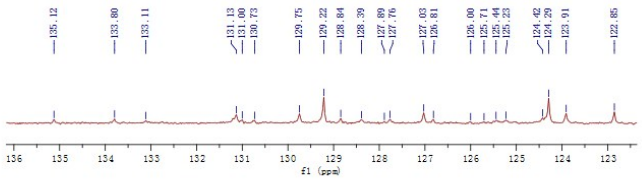


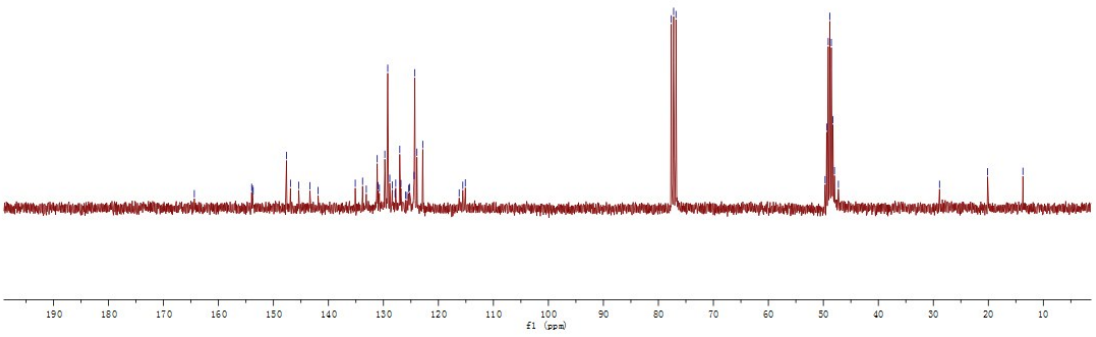
PZ-3-^{1}H



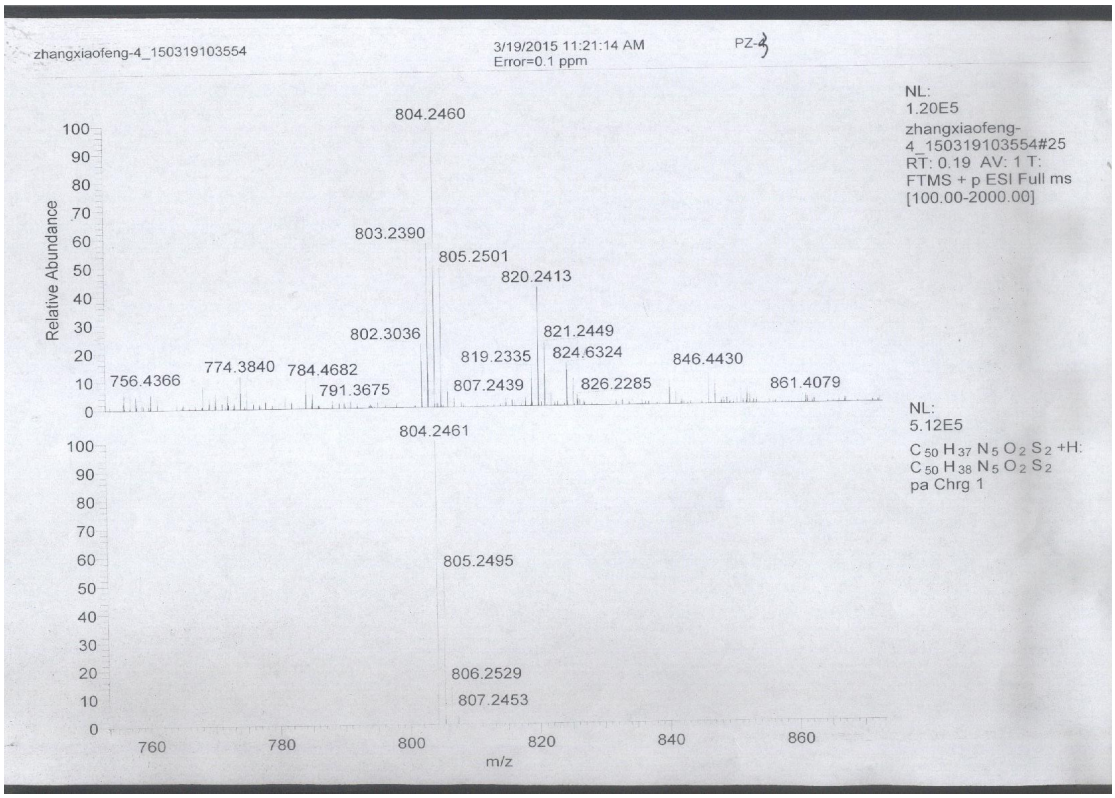
PZ-3-^{13}C



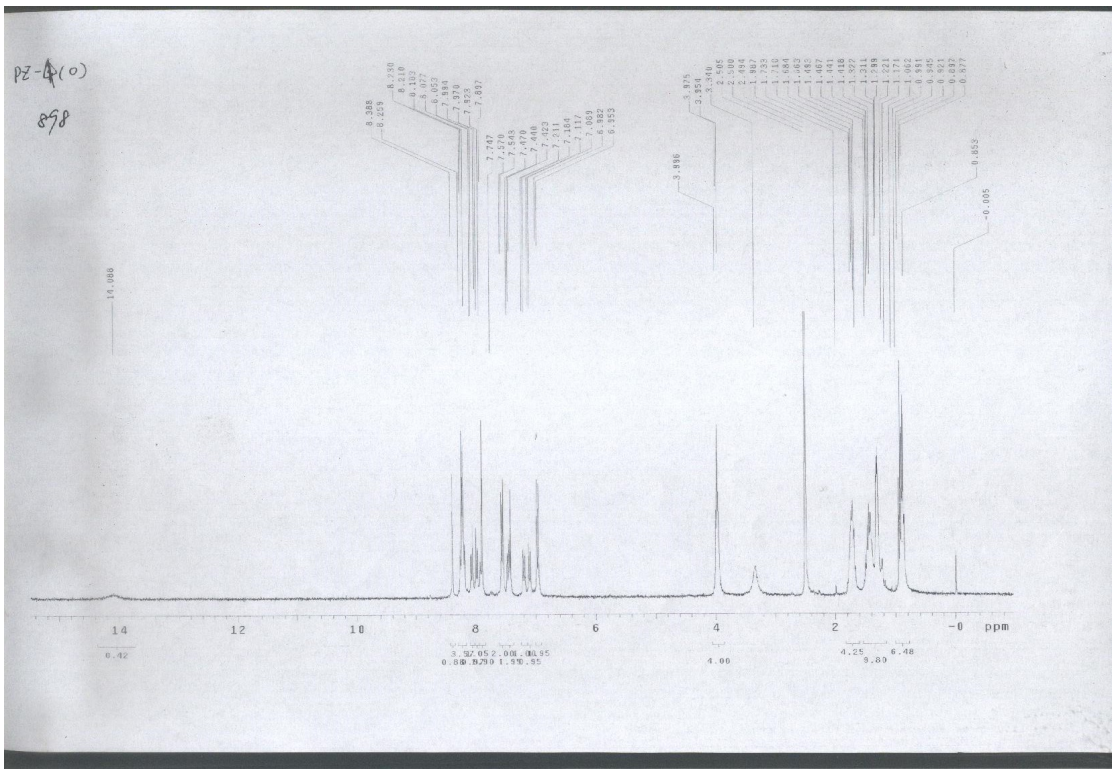




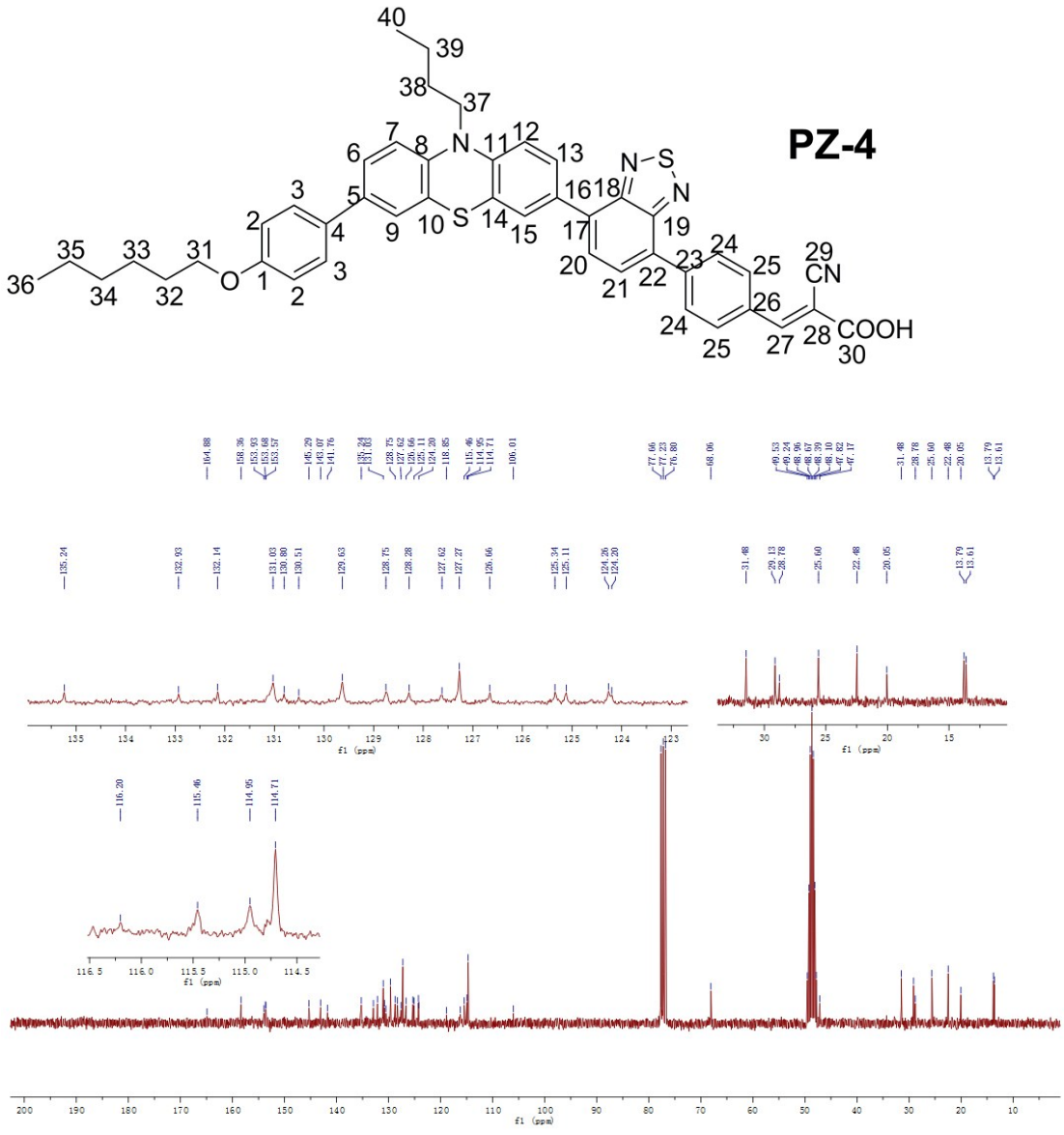
PZ-3-HRMS



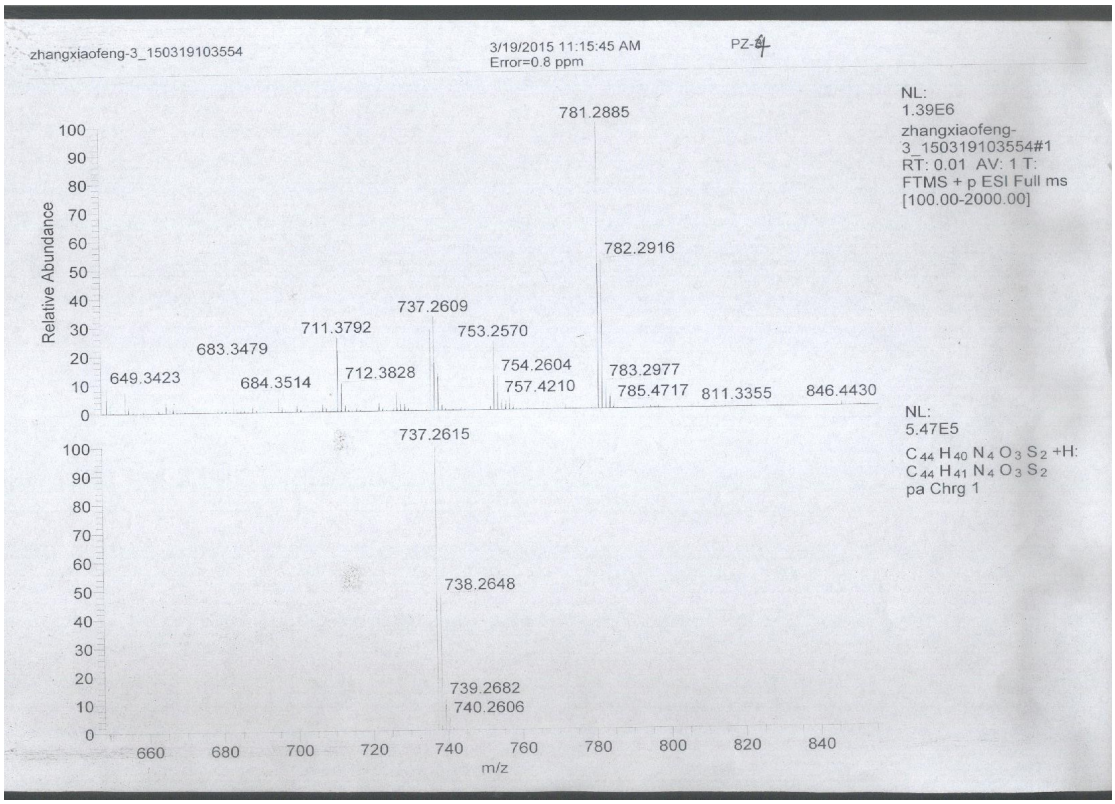
PZ-4-^{1}H



PZ-4-^{13}C



PZ-4-HRMS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pa Chrg 1
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Relative Abundance
m/z