Supporting Information

Cobalt-Catalyzed Carbon-Sulfur/Selenium Bond Formation: Synthesis of Benzo[*b*]thio/selenophene-fused Imidazo[1,2-*a*]pyridines

Tianyu Wang, Jichao Chen, Jia Wang, Shengtao Xu,* Aijun Lin, Hequan Yao, Sheng Jiang,* Jinyi Xu*

State Key Laboratory of Natural Medicines and Department of Medicinal Chemistry, China Pharmaceutical University, 24 Tong Jia Xiang, Nanjing 210009, P. R. China.
E-mail: jinyixu@china.com

Contents

Materials and Methods

General

All reactions were carried out in oven-dried glassware. Melting point (m.p.) was measured on a microscopic melting point apparatus. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-300 spectrometers, and were referenced to the residual peaks of $CDCl_3$ at 7.26 ppm (^{1}H NMR) and $CDCl_3$ at 77.23 ppm (^{13}C NMR). Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, brs = broad singlet, m = multiplet), coupling constant (Hz), and integration. High Resolution Mass measurement was performed on Agilent QTOF 6520 mass spectrometer with electron spray ionization (ESI) as the ion source. Flash column chromatography was carried out using commercially available 200-300 mesh under pressure.

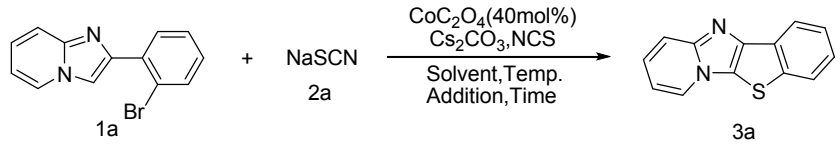
Materials

Unless otherwise indicated, all reagents were obtained from commercial suppliers used without further purification. PE refers to petroleum ether (b.p. 60-90 °C) and EA refers to ethyl acetate, and all reaction solvents were freshly distilled prior to use.

Preparation of Substrates

All substrates were synthesized according to the literature procedures and the ^{1}H NMR spectrum data for them showed good agreement with the literature data.[1]

Table S1 Optimization of Reaction Conditions[a]



Entry	Addition	Solvent	Temp.(°C)	Time(h)	Yield [b](%)
1	/	CH_3CN	120	5	70
2	/	H_2O	120	5	12
3	/	THF	120	5	trace
4	/	DMF	120	5	0
5	/	EtOH	120	5	22
6	/	DCE	120	5	0
7	/	CH_3CN	80	5	0
8	/	CH_3CN	100	5	trace
9	/	CH_3CN	130	5	76

10	/	CH_3CN	140	5	72
11	/	CH_3CN	130	1	42
12	/	CH_3CN	130	3	62
13	/	CH_3CN	130	10	72
14	1,10-phen	CH_3CN	130	5	82
15	EDTA	CH_3CN	130	5	trace
16	TBAI	CH_3CN	130	5	0
17	glycine	CH_3CN	130	5	34

[a]Reaction conditions: 1a (0.1 mmol), 2a (0.15 mmol), CoC_2O_4 (20 %mol), NCS (0.15 mmol), Cs_2CO_3 (0.15 mmol), CH_3CN (1.5 ml) at 130 °C for 5h. [b]Isolated yield.

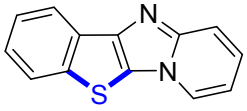
General Procedure for benzo[*b*]-thiophene/imidazo[1,2-*a*]pyridines

To a 15 mL sealed tube with a magnetic stirring bar were added 2-(2-iodophenyl)imidazo[1,2-*a*]pyridine derivatives (**1**, 0.3 mmol), NaSCN/KSeCN (**2**, 0.45 mmol), CoC_2O_4 (20 mol %), NCS (0.45 mmol), Cs_2CO_3(0.45 mmol), 1,10-phenanthroline (10 mol %) and CH_3CN (1.5 mL). The reaction mixture was placed in an oil bath at 130 °C and vigorously stirred for 5 h. Afterward it was cooled to ambient temperature, the solvents were removed under reduced pressure and the crude reaction mixture was purified by flash chromatography using *PE*/*EA* = 15:1 ~ 4:1 as an eluent to obtain the desired product.

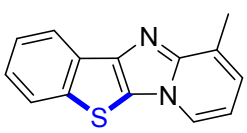
References

1. (a) C. Granchi, F. Rizzolio, S. Palazzolo, S. Carmignani, M. Macchia, G. Saccomanni, C. Manera, A. Martinelli, F. Minutolo and T. Tuccinardi, *J Med Chem*, 2016, **59**, 10299-10314; (b) K. Pericherla, P. Khedar, B. Khungar and A. Kumar, *Chem Commun (Camb)*, 2013, **49**, 2924-2926; (c) *WO Pat.*, 2016173557, 2016.

Analytical Data for the Products

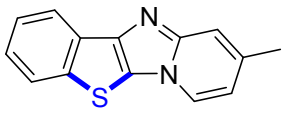


Compound **3a**: m.p.118-120; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 (d, *J* = 7.7 Hz, 1H), 8.07 (d, *J* = 6.7 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 9.3 Hz, 1H), 7.47 (d, *J* = 7.2 Hz, 1H), 7.36 (s, 1H), 7.28 – 7.17 (m, 1H), 6.86 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.96, 145.32, 139.67, 128.48, 124.97, 124.84, 123.88, 123.72, 123.66, 121.12, 117.79, 111.57. HRMS (ESI) calculated for $C_{13}H_8N_2S$ $[M + H]^+$ 225.0486, found 225.0483.

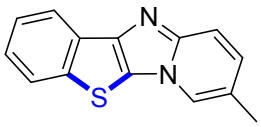


Compound **3b**: m.p.170-171; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.3 Hz, 1H), 7.99 (d, *J* = 6.7 Hz, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.50 (t, *J* = 7.0 Hz, 1H), 7.44 – 7.36 (m, 1H), 7.06 (d, *J* = 6.9 Hz, 1H), 6.83 (t, *J* = 6.8 Hz, 1H), 2.74 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.53, 144.85, 139.56, 128.75, 127.83, 124.73, 124.71, 123.69, 122.76,

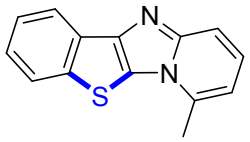
122.58, 121.53, 121.19, 111.53, 17.03. HRMS (ESI) calculated for $C_{14}H_{10}N_2S$ $[M + H]^+$ 239.0643, found 239.0641.



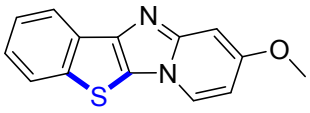
Compound **3c**: m.p.159-160; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (d, *J* = 7.8 Hz, 1H), 7.97 (d, *J* = 6.9 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 6.79 – 6.67 (m, 1H), 2.44 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.48, 145.14, 139.53, 135.02, 129.54, 124.75, 124.65, 123.69, 122.80, 121.46, 120.95, 116.13, 114.19, 21.08. HRMS (ESI) calculated for $C_{14}H_{10}N_2S$ $[M + H]^+$ 239.0643, found 239.0640.



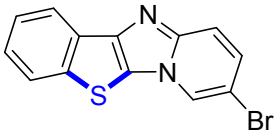
Compound **3d**: m.p.194-195; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.6 Hz, 1H), 7.89 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 9.3 Hz, 1H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 9.1 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.99, 144.92, 139.58, 128.52, 127.34, 124.87, 123.73, 123.44, 122.89, 121.57, 121.42, 121.09, 117.05, 17.76. HRMS (ESI) calculated for $C_{14}H_{10}N_2S$ $[M + H]^+$ 239.0643, found 239.0641.



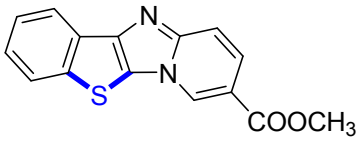
Compound **3e**: m.p.115-117; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.28 (d, *J* = 7.3 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 9.3 Hz, 1H), 7.53 (t, *J* = 7.0 Hz, 1H), 7.47 – 7.38 (m, 1H), 7.23 – 7.13 (m, 1H), 6.65 (d, *J* = 6.8 Hz, 1H), 2.93 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.62, 145.90, 140.95, 134.60, 130.69, 128.80, 125.45, 125.38, 125.16, 123.88, 121.70, 115.93, 111.09, 19.22. HRMS (ESI) calculated for $C_{14}H_{10}N_2S$ $[M + H]^+$ 239.0643, found 239.0641.



Compound **3f**: m.p.121-122; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.6 Hz, 1H), 7.95 (d, *J* = 7.4 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.1 Hz, 1H), 7.43 – 7.31 (m, 1H), 7.02 (d, *J* = 2.3 Hz, 1H), 6.76 – 6.55 (m, 1H), 3.90 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.48, 150.70, 139.16, 128.53, 124.87, 124.46, 124.08, 123.57, 121.20, 107.10, 95.14, 55.19. HRMS (ESI) calculated for $C_{14}H_{10}BrN_2S$ $[M + H]^+$ 255.0592, found 255.0590.

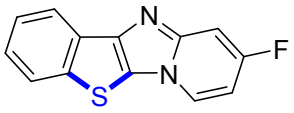


Compound **3g**: m.p.181-182; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 (d, *J* = 1.0 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 9.7 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.48 – 7.40 (m, 1H), 7.32 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.36, 146.11, 139.70, 128.16, 127.17, 125.41, 125.04, 123.76, 123.61, 122.31, 121.28, 118.32, 106.15. HRMS (ESI) calculated for $C_{13}H_7BrN_2S$ $[M + H]^+$ 302.9592, found 302.9590.

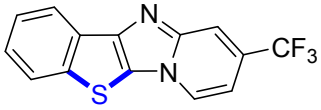


Compound **3h**: m.p.156-158; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.21 (d, *J* = 7.9 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H), 7.78 – 7.67 (m, 2H), 7.49 (t, *J* = 7.0 Hz, 1H), 7.44 – 7.37 (m, 1H), 3.96 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.09, 149.82, 147.36, 140.34, 128.65, 128.27, 125.99, 125.55, 124.26, 123.84,

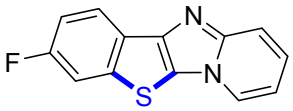
123.61, 121.82, 117.41, 116.03, 52.53. HRMS (ESI) calculated for $C_{15}H_{10}N_2O_2S$ [M + H]$^+$ 283.0541, found 283.0539.



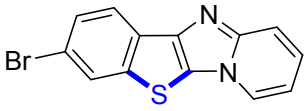
Compound **3i**: m.p.167-169; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.0 Hz, 1H), 8.09 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.1 Hz, 1H), 7.42 (t, *J* = 8.8 Hz, 2H), 6.82 (t, *J* = 6.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.82 (d, *J* =252 Hz, 1C), 140.06, 133.04, 132.24, 130.23, 128.95, 127.08, 125.56, 125.46, 125.34, 124.20, 121.63, 104.68 (d, *J* = 33.75 Hz, 1C), 102.15 (d, *J* = 24 Hz, 1C). HRMS (ESI) calculated for $C_{13}H_7FN_2S$ [M + H]$^+$ 243.0387, found 243.0384.



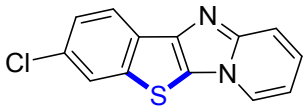
Compound **3j**: m.p.225-227; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.8 Hz, 1H), 8.19 (d, *J* = 7.1 Hz, 1H), 8.05 (s, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 7.1 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.96, 147.47, 140.47, 133.00, 128.54 (q, *J* = 315 Hz, 1C), 128.53, 126.39, 125.74, 124.76 (q, *J* = 180 Hz, 1C), 124.73, 124.35, 122.06, 116.31 (q, *J* = 10 Hz, 1C), 108.05 (q, *J* = 5.25 Hz, 1C). HRMS (ESI) calculated for $C_{14}H_7F_3N_2S$ [M + H]$^+$ 293.0355, found 293.0355.



Compound **3k**: m.p.181-183. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 – 8.15 (m, 1H), 8.12 (d, *J* = 8.2 Hz, 1H), 7.76 (d, *J* = 10.7 Hz, 1H), 7.57 (d, *J* = 8.3 Hz, 1H), 7.33 – 7.20 (m, 2H), 6.94 (t, *J* = 7.3 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.42, 159.16, 149.59, 141.07 (d, *J* = 4.5 Hz, 1C), 125.50, 125.47, 125.50, 124.45, 124.07, 122.38 (d, *J* = 9 Hz, 1C), 118.39, 113.79 (d, *J* = 23.25 Hz, 1C), 112.21, 110.84 (d, *J* = 25.5 Hz, 1C). HRMS (ESI) calculated for $C_{13}H_7FN_2S$ [M + H]$^+$ 243.0387, found 243.0384.

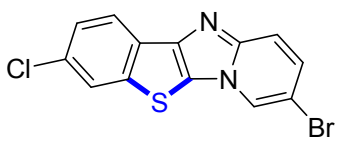


Compound **3l**: m.p.200-201; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.18 – 8.05 (m, 2H), 7.98 (s, 1H), 7.75 (d, *J* = 9.2 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 6.93 (t, *J* = 6.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.77, 145.25, 141.44, 128.76, 127.87, 127.56, 126.75, 124.78, 124.22, 122.59, 118.60, 118.53, 112.37. HRMS (ESI) calculated for $C_{13}H_7BrN_2S$ [M + H]$^+$ 302.9592, found 302.9588.

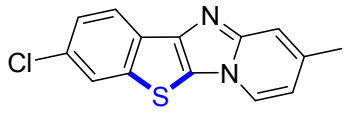


Compound **3m**: m.p.178-180; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 6.8 Hz, 1H), 7.82 (s, 1H), 7.74 (d, *J* = 9.3 Hz, 1H), 7.46 (d, *J* = 8.4Hz, 1H), 7.32 – 7.23 (m, 1H), 6.94 – 6.89 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.73, 145.28, 141.10, 131.04, 127.40, 126.27, 126.09, 124.74, 124.20, 123.90, 122.25, 118.50, 112.35. HRMS (ESI) calculated for $C_{13}H_7ClN_2S$ [M + H]$^+$ 259.0097, found 259.0095.

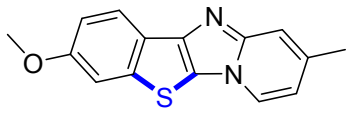
Compound **3n**: m.p.122-124; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.7 Hz, 1H), 8.10 (d, *J* = 6.8 Hz, 1H), 7.74 (d, *J* = 9.2 Hz, 1H), 7.36 (d, *J* = 2.3 Hz, 1H), 7.29 – 7.20 (m, 1H), 7.16 – 7.08 (m, 1H), 6.95 – 6.87 (m, 1H), 3.91 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.12, 149.40, 145.85, 141.78, 127.28, 123.89, 122.73, 122.14, 118.16, 114.12, 113.83, 111.98, 108.09, 55.70. HRMS (ESI) calculated for $C_{14}H_{10}BrN_2S$ [M + H]$^+$ 255.0592, found 255.0590.



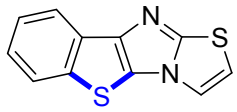
Compound **3o**: m.p.120-122; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.57 (d, *J* = 11.1 Hz, 2H), 7.43 (d, *J* = 9.5 Hz, 1H), 6.99 (d, *J* = 7.0 Hz, 1H), 6.66 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.12, 145.65, 144.60, 136.34, 135.26, 132.37, 131.51, 130.81, 127.35, 124.74, 123.51, 118.77, 108.74. HRMS (ESI) calculated for $C_{13}H_6BrClN_2S$ $[M + H]^+$ 336.9196, found 336.9199.



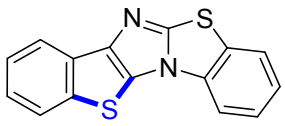
Compound **3p**: m.p.187-188; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 6.6 Hz, 1H), 7.82 (s, 1H), 7.49 (d, *J* = 5.1 Hz, 1H), 7.47 (d, *J* = 8.7 Hz, 1H), 6.77 (d, *J* = 6.7 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.19, 144.95, 140.92, 135.85, 130.62, 127.63, 125.90, 123.78, 123.26, 122.04, 121.87, 116.74, 114.91, 21.60. HRMS (ESI) calculated for $C_{14}H_9ClN_2S$ $[M + H]^+$ 273.0248, found 273.0252.



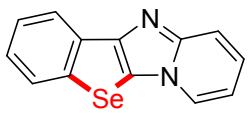
Compound **3q**: m.p.144-146; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.7 Hz, 1H), 7.93 (d, *J* = 6.9 Hz, 1H), 7.46 (s, 1H), 7.32 (d, *J* = 2.3 Hz, 1H), 7.16 – 7.03 (m, 1H), 6.74 – 6.62 (m, 1H), 3.88 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.16, 150.07, 145.73, 141.81, 135.29, 133.17, 123.30, 123.11, 122.24, 116.75, 114.83, 113.97, 108.31, 55.91, 21.74. HRMS (ESI) calculated for $C_{15}H_{12}N_2OS$ $[M + H]^+$ 269.0738, found 269.0749.



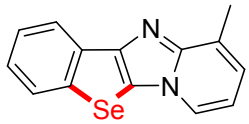
Compound **3r**: m.p.185-186; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 (d, *J* = 7.3 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.54 (d, *J* = 4.6 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.0 Hz, 1H), 6.93 (d, *J* = 4.6 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.91, 147.19, 138.09, 131.83, 128.73, 124.80, 123.94, 123.52, 120.17, 116.73, 111.63. HRMS (ESI) calculated for $C_{11}H_6N_2S_2$ $[M + H]^+$ 231.0045, found 231.0048.



Compound **3s**: m.p.186-188; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.9 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.69 (d, *J* = 7.9 Hz, 1H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.46 (t, *J* = 7.3 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.48, 146.41, 138.32, 130.59, 128.68, 128.23, 125.91, 124.88, 124.33, 123.78, 123.76, 123.53, 121.90, 120.03, 112.09. HRMS (ESI) calculated for $C_{15}H_8N_2S_2$ $[M + H]^+$ 281.0202, found 281.0207.

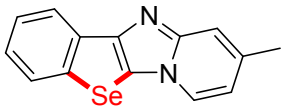


Compound **4a**: m.p.176-177; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.28 (d, *J* = 7.5 Hz, 1H), 8.08 (d, *J* = 6.8 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 9.2 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.29 – 7.22 (m, 1H), 6.91 (t, *J* = 6.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.01, 147.56, 139.78, 130.52, 126.53, 125.40, 125.37, 124.18, 123.90, 122.57, 117.82, 111.74. HRMS (ESI) calculated for $C_{13}H_8BrN_2Se$ $[M + H]^+$ 272.9931, found 272.9934.

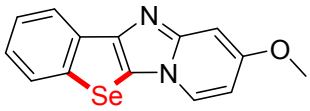


Compound **4b**: m.p.188-190; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 – 8.27 (m, 1H), 7.90 – 7.78 (m, 2H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 6.98 (d, *J* = 6.9 Hz, 1H), 6.73 (t, *J* = 6.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.02, 147.51, 140.18, 131.26, 128.26,

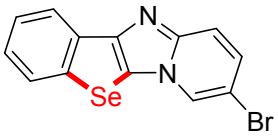
126.98, 125.71, 125.60, 123.22, 123.16, 122.52, 118.92, 112.14, 17.44. HRMS (ESI) calculated for $C_{14}H_{10}N_2Se$ $[M + H]^+$ 287.0082, found 287.0090.



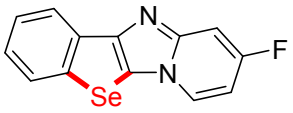
Compound **4c**: m.p.184-186; ^1H NMR (300 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.6 Hz, 1H), 7.90 – 7.79 (m, 2H), 7.52 – 7.42 (m, 2H), 7.30 (t, *J* = 7.6 Hz, 1H), 6.65 (d, *J* = 6.9 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.31, 147.11, 139.71, 134.86, 130.64, 126.43, 125.19, 124.93, 123.14, 122.34, 121.35, 115.92, 114.17, 20.96. HRMS (ESI) calculated for $C_{14}H_{10}N_2Se$ $[M + H]^+$ 287.0082, found 287.0085.



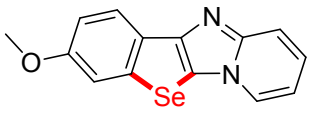
Compound **4d**: m.p.118-119; ^1H NMR (300 MHz, $CDCl_3$) δ 8.20 (d, *J* = 7.1 Hz, 1H), 7.84 (d, *J* = 7.3 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.29 (t, *J* = 7.7 Hz, 1H), 7.00 (s, 1H), 6.58 (d, *J* = 4.9 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.74, 150.99, 147.63, 140.08, 131.21, 126.93, 125.73, 125.21, 125.01, 122.70, 117.01, 107.35, 95.50, 55.50. HRMS (ESI) calculated for $C_{14}H_{10}N_2OSe$ $[M + H]^+$ 303.0031, found 303.0038.



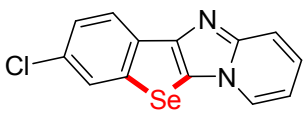
Compound **4e**: m.p.180-182; ^1H NMR (300 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.8 Hz, 1H), 8.22 (s, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 10.4 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 6.9 Hz, 1H), 7.33 – 7.27 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.29, 147.33, 139.78, 130.06, 127.08, 126.46, 125.73, 125.49, 124.02, 122.72, 118.16, 118.09, 106.21. HRMS (ESI) calculated for $C_{13}H_7BrN_2Se$ $[M + H]^+$ 350.9031, found 350.9032.



Compound **4f**: m.p.181-182. ^1H NMR (300 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.0 Hz, 1H), 8.07 – 7.99 (m, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.42 – 7.32 (m, 2H), 6.85 – 6.76 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.92 (d, *J* =250.5 Hz, 1C), 140.29, 133.10, 132.29, 130.88, 130.32, 127.85 (d, *J* = 12.75 Hz, 1C), 125.98, 125.94, 125.79, 123.08, 104.81 (d, *J* = 29.25 Hz, 1C), 102.07 (d, *J* = 24 Hz, 1C). HRMS (ESI) calculated for $C_{13}H_7FN_2Se$ $[M + H]^+$ 290.9831, found 290.9832.

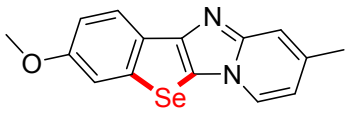


Compound **4g**: m.p.158-160; ^1H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.6 Hz, 1H), 8.01 (d, *J* = 6.8 Hz, 1H), 7.71 (d, *J* = 9.2 Hz, 1H), 7.38 (d, *J* = 2.3 Hz, 1H), 7.23 – 7.16 (m, 1H), 7.13 – 7.03 (m, 1H), 6.91 – 6.82 (m, 1H), 3.88 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.17, 149.32, 147.79, 141.62, 124.42, 124.31, 123.92, 123.41, 117.96, 116.36, 113.67, 112.08, 111.30, 55.65. HRMS (ESI) calculated for $C_{14}H_{10}N_2OSe$ $[M + H]^+$ 303.0031, found 303.0038.

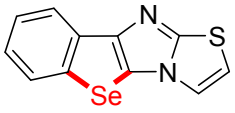


Compound **4h**: m.p.172-174; ^1H NMR (300 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.3 Hz, 1H), 7.93 (d, *J* = 6.7 Hz, 1H), 7.73 (s, 1H), 7.64 (d, *J* = 9.3 Hz, 1H), 7.37 (d, *J* = 7.3 Hz, 1H), 7.16 (t, *J* = 8.0 Hz, 1H), 6.80 (t, *J* = 6.6 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.17, 146.68, 140.51, 130.87, 128.98, 126.13, 126.03, 124.22, 124.15, 123.47, 123.08, 117.92, 111.98. $C_{13}H_7ClN_2Se$ $[M + H]^+$ 306.9541, found 306.9542.

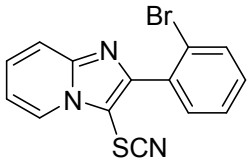
Compound **4i**: m.p.185-187; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.18 (q, *J* = 8.6, 5.3 Hz, 1H), 8.02 (d, *J* = 6.8 Hz, 1H), 7.73 (d, *J* = 9.2 Hz, 1H), 7.57 (q, *J* = 9.5, 3.4 Hz, 1H), 7.28 – 7.19 (m, 2H), 6.88 (t, *J* = 6.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.81 (d, *J* = 245.25 Hz, 1C), 149.53, 147.13, 141.00, 140.88, 127.38 (d, *J* = 2.25 Hz, 1C), 124.48 (d, *J* = 5.25 Hz, 1C), 123.64 (d, *J* = 9 Hz, 1C), 118.27, 114.21, 113.91 (d, *J* = 1.5 Hz, 1C), 113.58, 112.32. HRMS (ESI) calculated for $C_{13}H_7FN_2Se$ $[M + H]^+$ 290.9831, found 290.9833.



Compound **4j**: m.p.169-171; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 6.8 Hz, 1H), 7.48 (s, 1H), 7.39 (d, *J* = 2.3 Hz, 1H), 7.12 – 7.07 (m, 1H), 6.72 (d, *J* = 8.5 Hz, 1H), 3.90 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 178.52, 157.97, 149.76, 147.24, 141.45, 135.23, 124.55, 123.59, 123.49, 116.34, 114.79, 113.58, 111.29, 55.64, 21.45. HRMS (ESI) calculated for $C_{15}H_{12}N_2OSe$ $[M + H]^+$ 317.0188, found 317.0196.

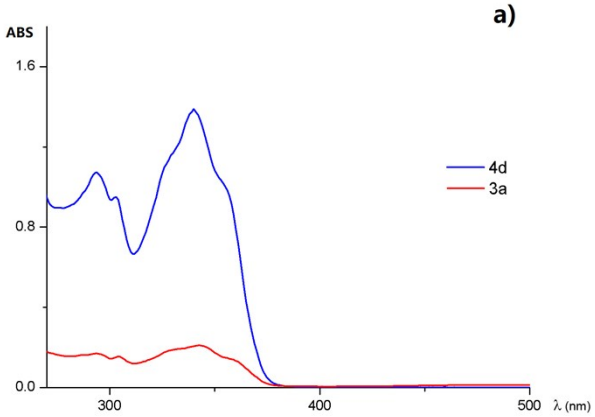


Compound **4k**: m.p.213-215; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 7.7 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.38 (m, 2H), 7.33 – 7.22 (m, 1H), 6.91 (d, *J* = 4.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.61, 149.26, 138.53, 130.72, 126.30, 125.29, 124.30, 121.68, 117.11, 116.57, 111.74. HRMS (ESI) calculated for $C_{11}H_6N_2SSe$ $[M + H]^+$ 278.9490, found 278.9494.



Compound **5a**: m.p.132-135; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.45 (d, *J* = 6.8 Hz, 1H), 7.81 (d, *J* = 9.1 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.43 (m, 3H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.20 (t, *J* = 6.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.66, 147.26, 132.89, 132.53, 131.75, 130.39, 127.37, 127.02, 123.95, 122.93, 118.11, 114.23, 107.25; HRMS (ESI) calculated for $C_{14}H_8BrN_3S$ [M + H]+ 329.9701, found 329.9700.

Ultraviolet absorption and fluorescence emission spectra of compounds **3a** and **4d**.



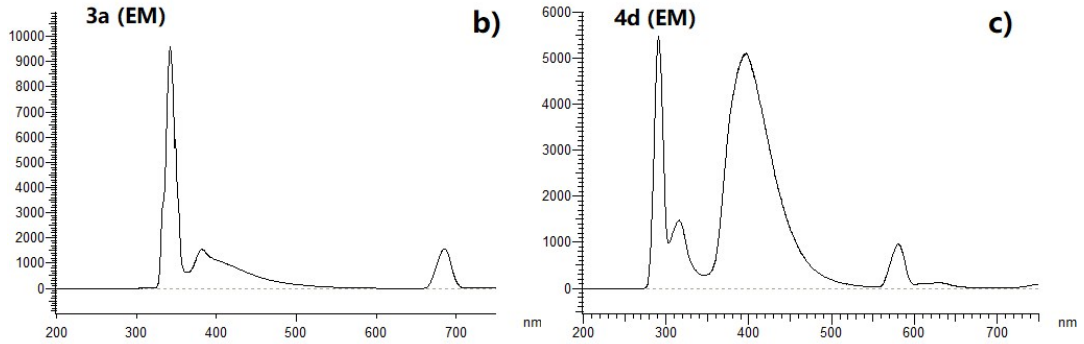
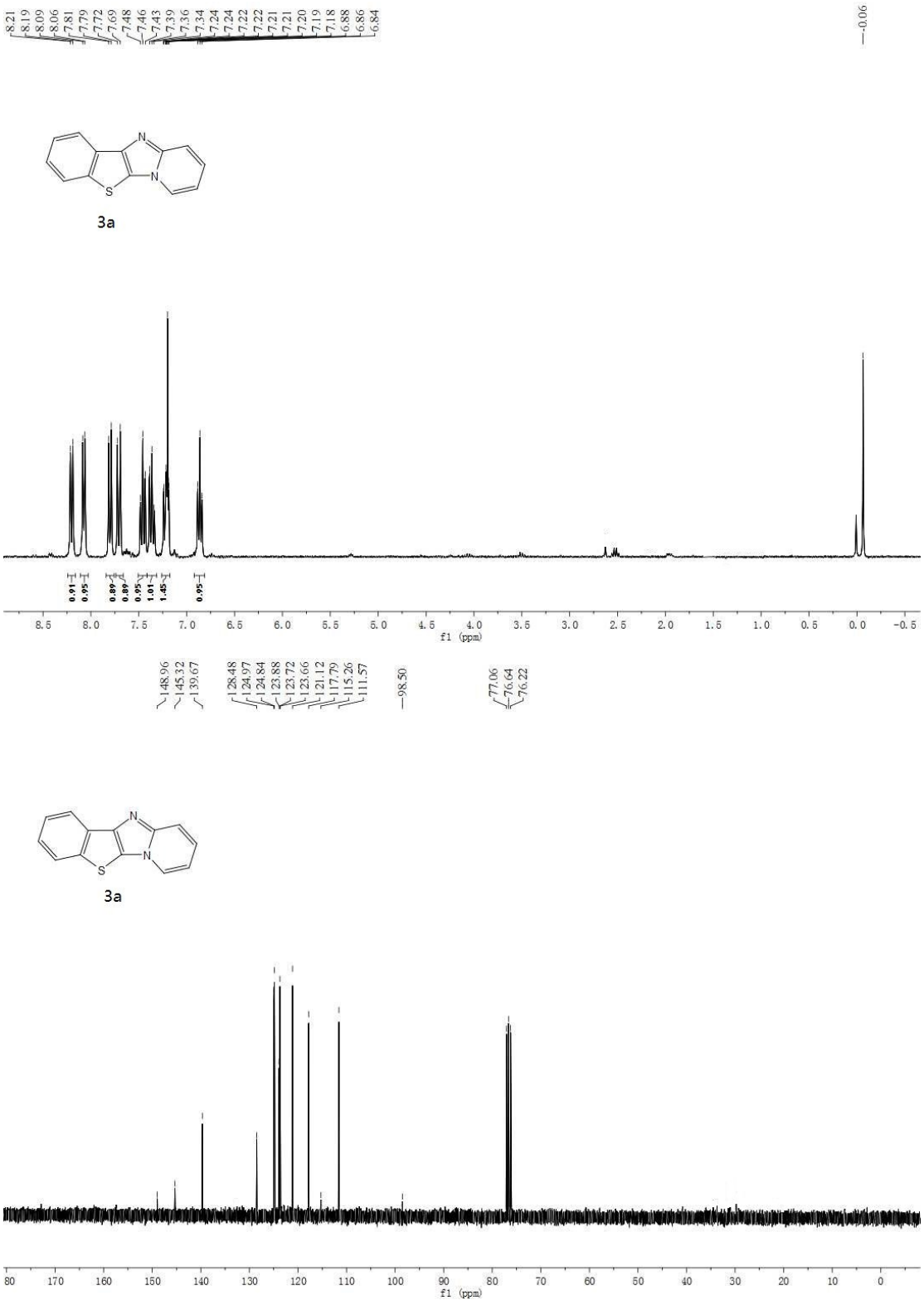
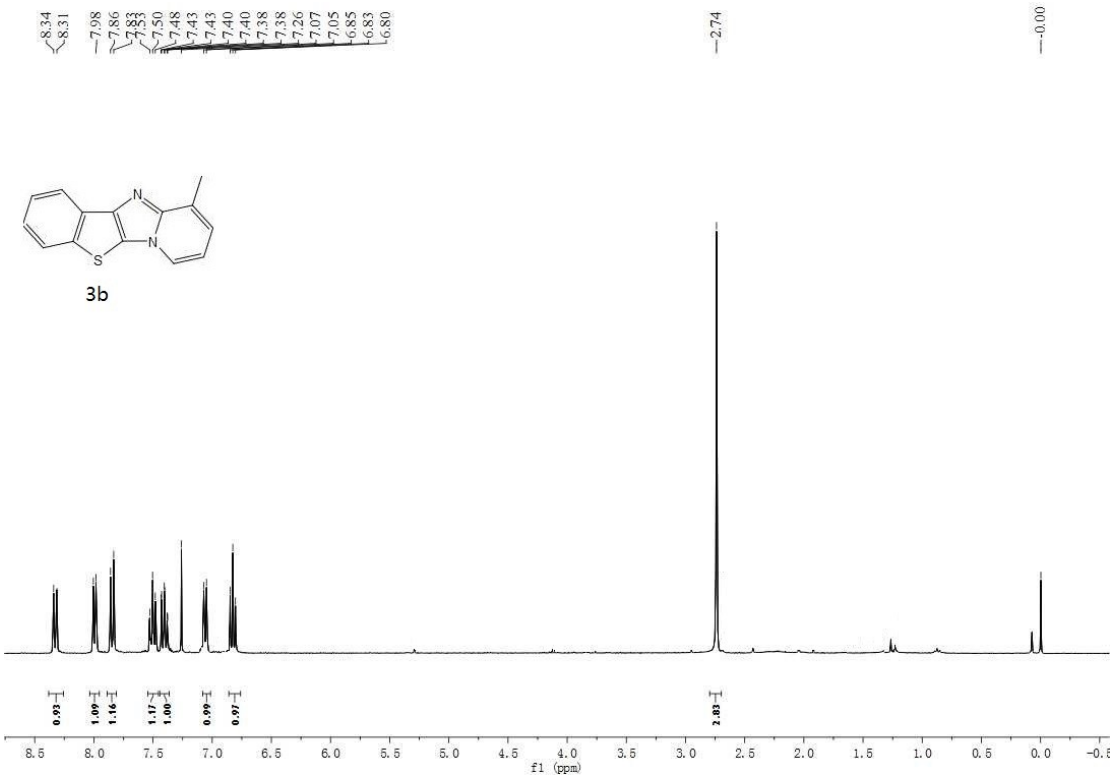


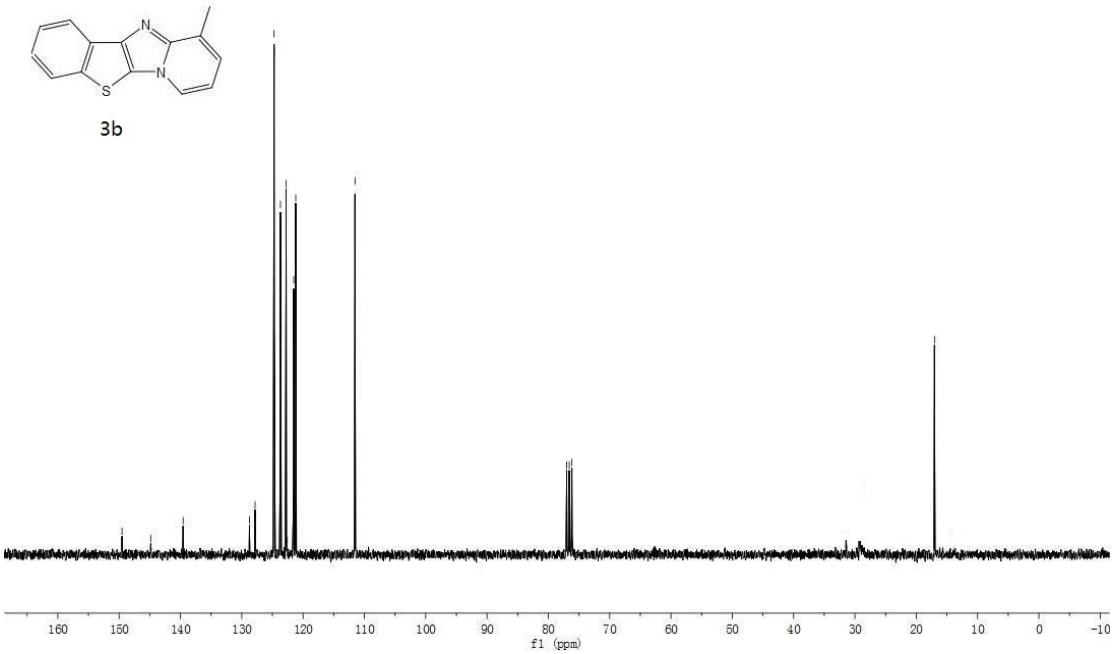
Figure S1. a) The Ultraviolet absorption spectra of compound **3a (**1µM, λ_{abs} = 344nm) and **4d** (1µM, λ_{abs} = 288nm, 340nm) in methanol. b) The fluorescence spectra of compound **3a** (1nM) in methanol. c) The fluorescence spectra of compound **4d** (1µM) in methanol.

Copies of ^{1}H and ^{13}C NMR spectra for the title compounds

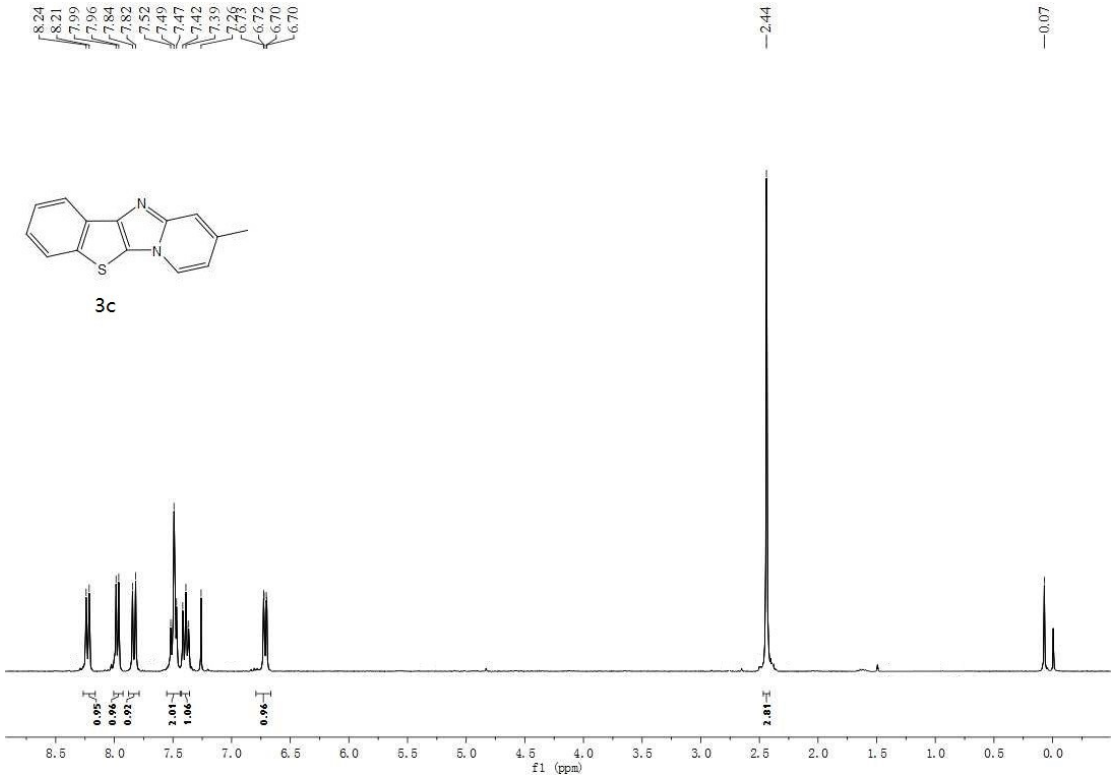



8.34
8.31
7.98
7.86
7.83
7.55
7.50
7.48
7.43
7.43
7.40
7.40
7.38
7.38
7.26
7.07
7.05
6.85
6.83
6.80
2.74
0.00
0.93
1.09
1.16
1.17
1.00
0.99
0.97
2.83
f1 (ppm)

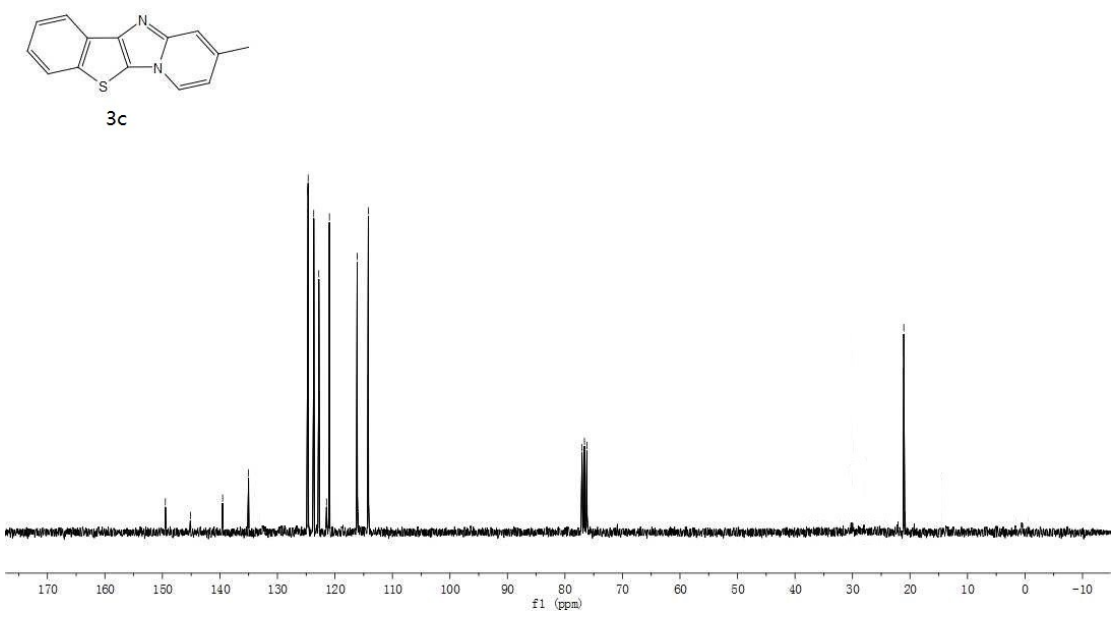
3b


149.53
144.85
139.56
128.75
127.83
124.73
124.71
123.69
122.76
122.58
121.53
121.19
111.53
77.01
76.59
76.16
17.03
f1 (ppm)

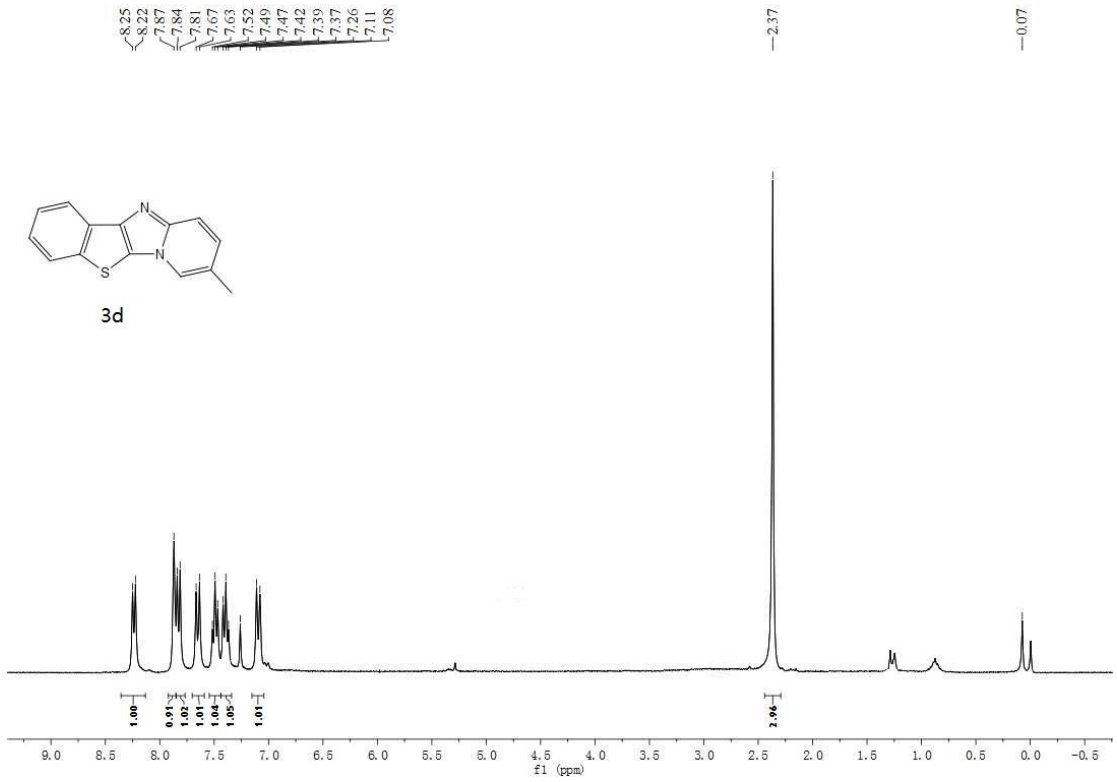
3b


8.24
8.21
7.99
7.96
7.84
7.82
7.52
7.49
7.47
7.42
7.39
6.72
6.70
6.70
2.44
0.07
0.95
0.96
0.92
2.01
1.06
0.96
2.81
f1 (ppm)

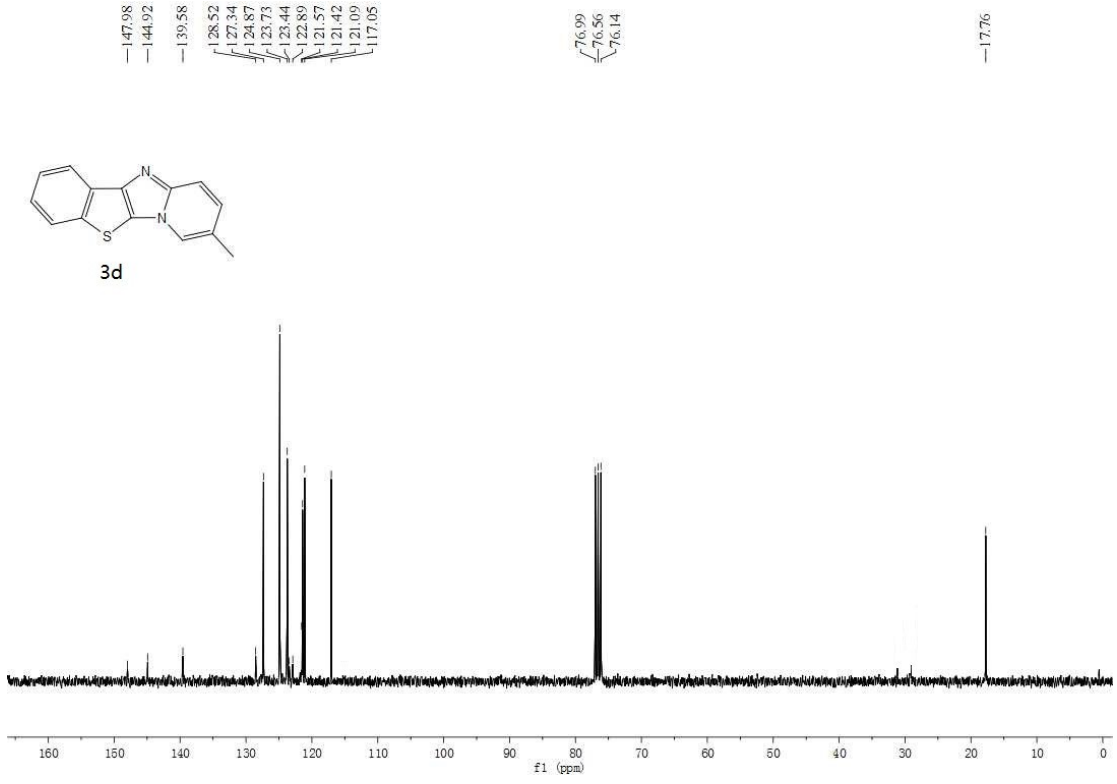
3c


149.48
145.14
139.53
135.02
129.54
124.75
124.65
123.69
122.80
121.46
120.95
116.13
114.19
77.03
76.61
76.18
21.08
f1 (ppm)

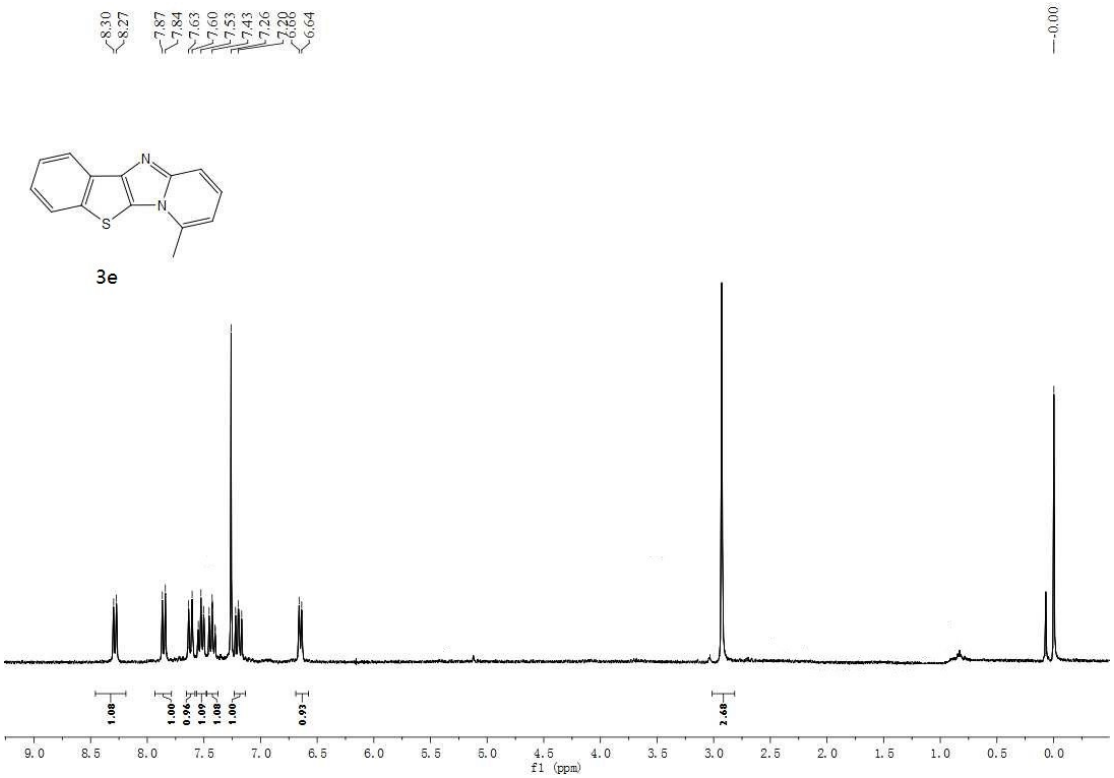
3c

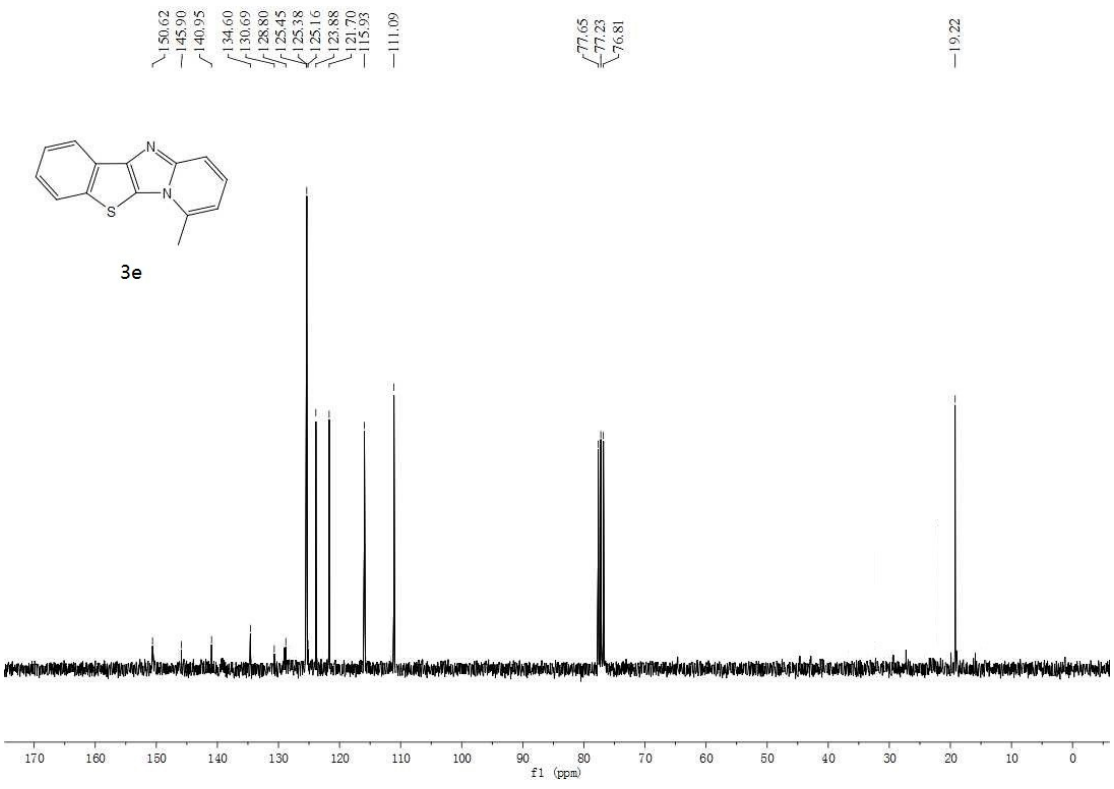

8.25
8.22
7.87
7.84
7.81
7.67
7.63
7.52
7.49
7.47
7.42
7.39
7.37
7.26
7.11
7.08
2.37
0.07
1.00
0.91
1.02
1.01
1.04
1.05
1.01
2.96
f1 (ppm)

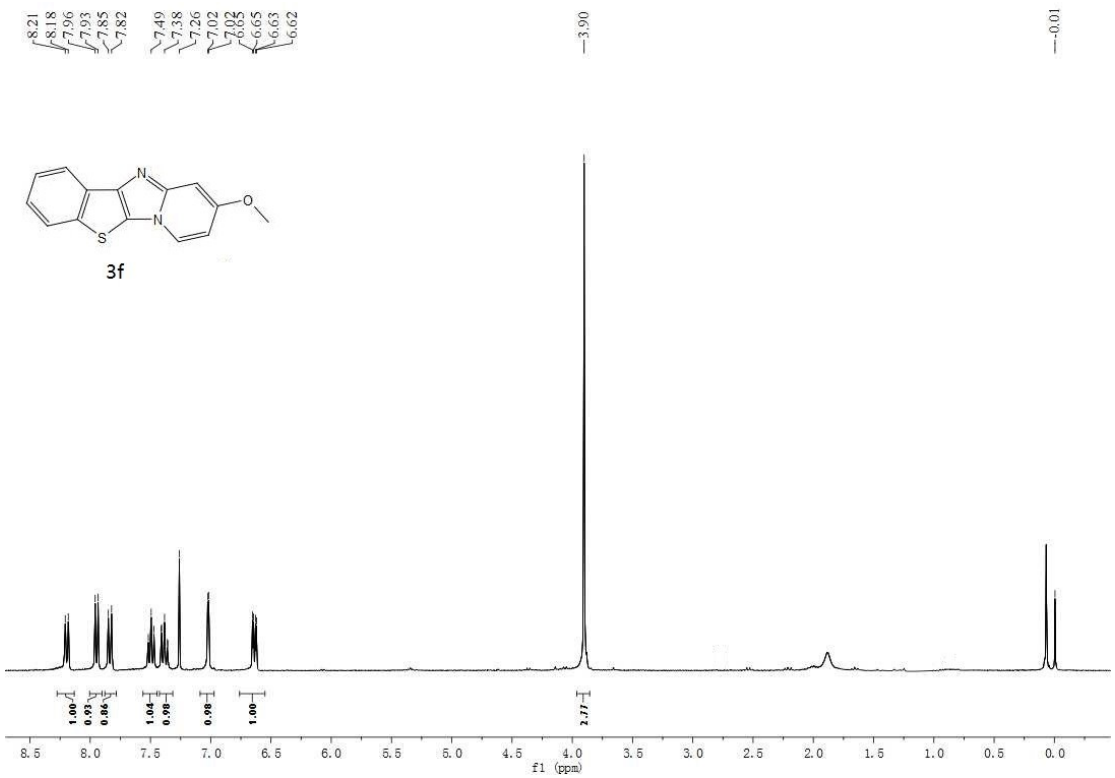
3d


147.98
144.92
139.58
128.52
127.34
124.87
123.73
123.44
122.89
121.57
121.42
121.09
117.05
76.99
76.56
76.14
17.76
f1 (ppm)

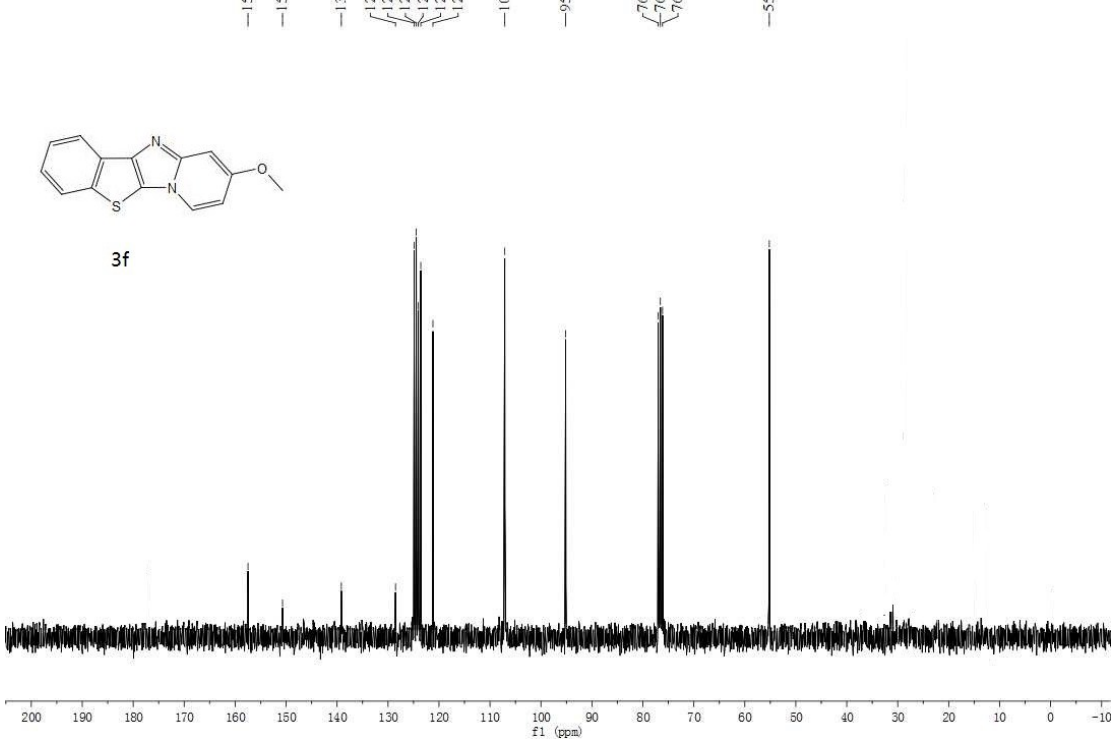
3d


8.30
8.27
7.87
7.84
7.63
7.60
7.53
7.43
7.26
7.20
6.68
6.64
0.00
3e
1.08
1.00
0.96
1.09
1.08
1.00
0.93
2.68
f1 (ppm)

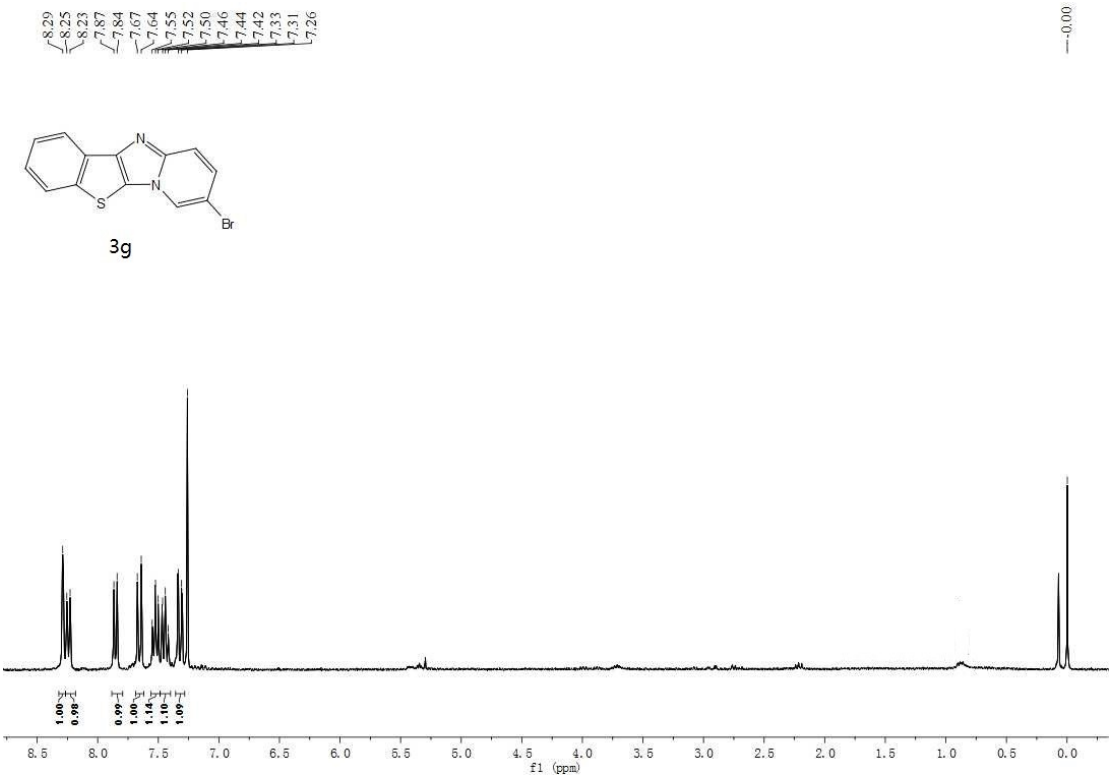

150.62
145.90
140.95
134.60
130.69
128.80
125.45
125.38
125.16
123.88
121.70
115.93
111.09
77.65
77.23
76.81
19.22
3e
f1 (ppm)

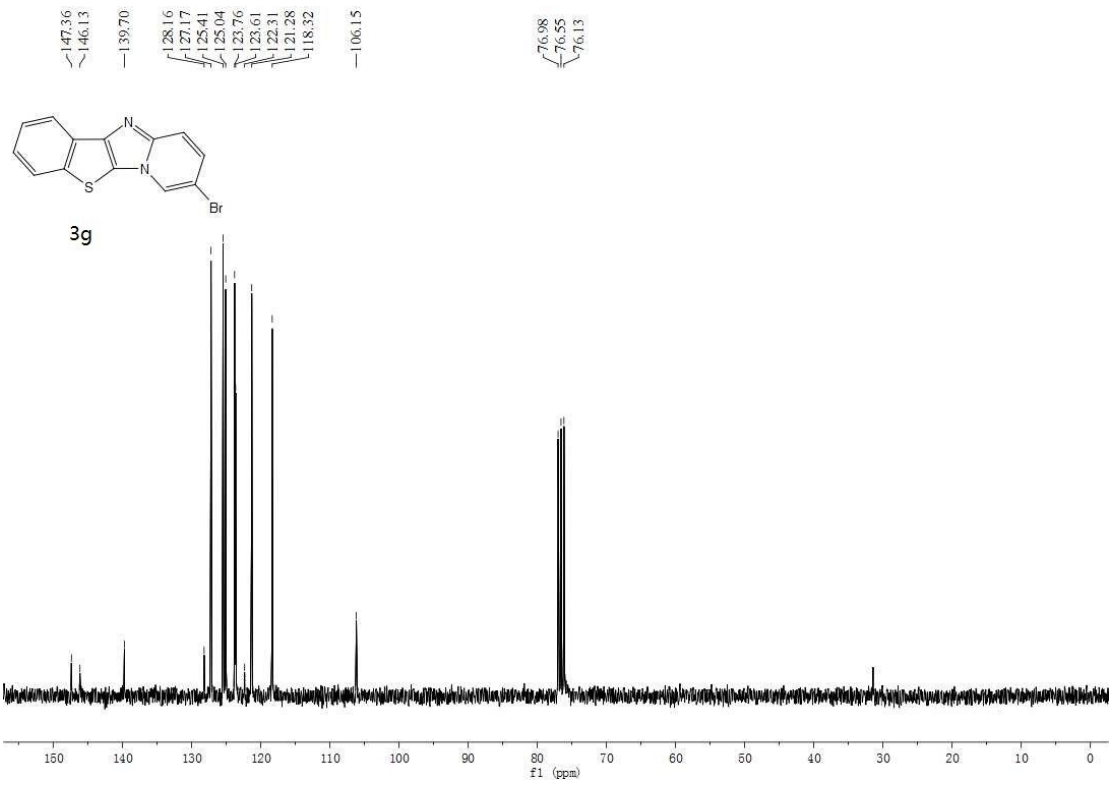

8.21
8.18
7.96
7.93
7.85
7.82
7.49
7.38
7.26
7.02
7.02
6.65
6.63
6.62
3.90
-0.01
1.00
0.93
0.86
1.04
0.98
0.98
1.00
2.17
f1 (ppm)

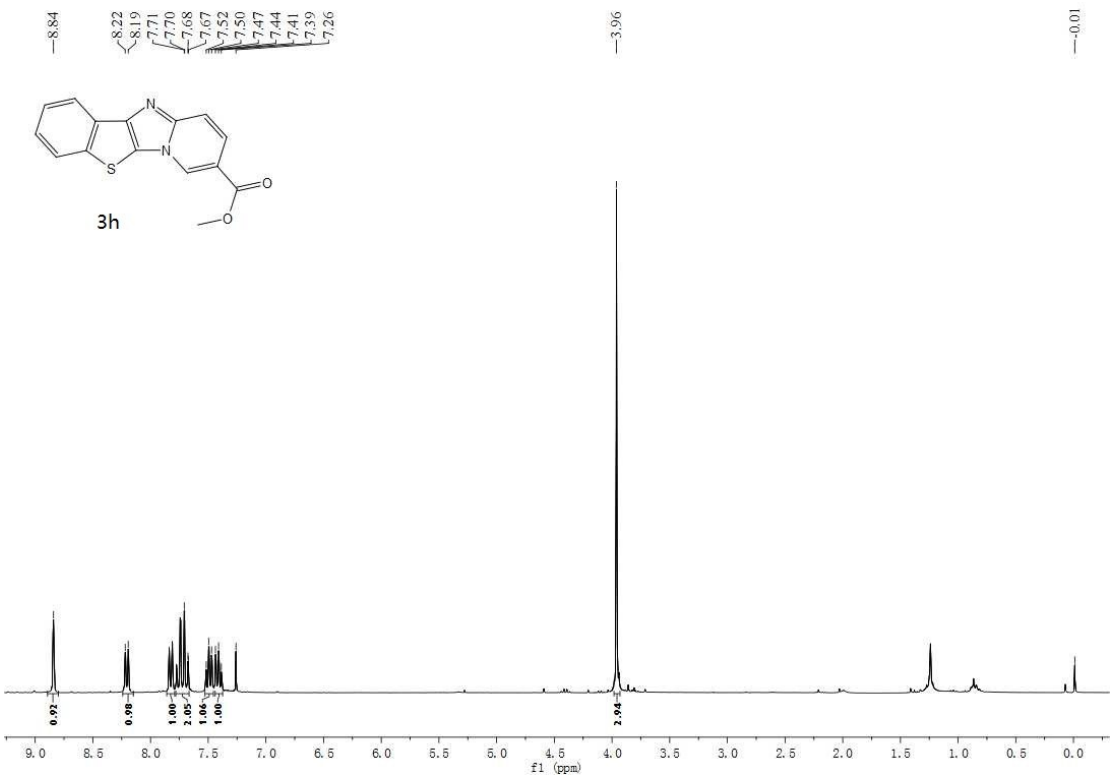
3f

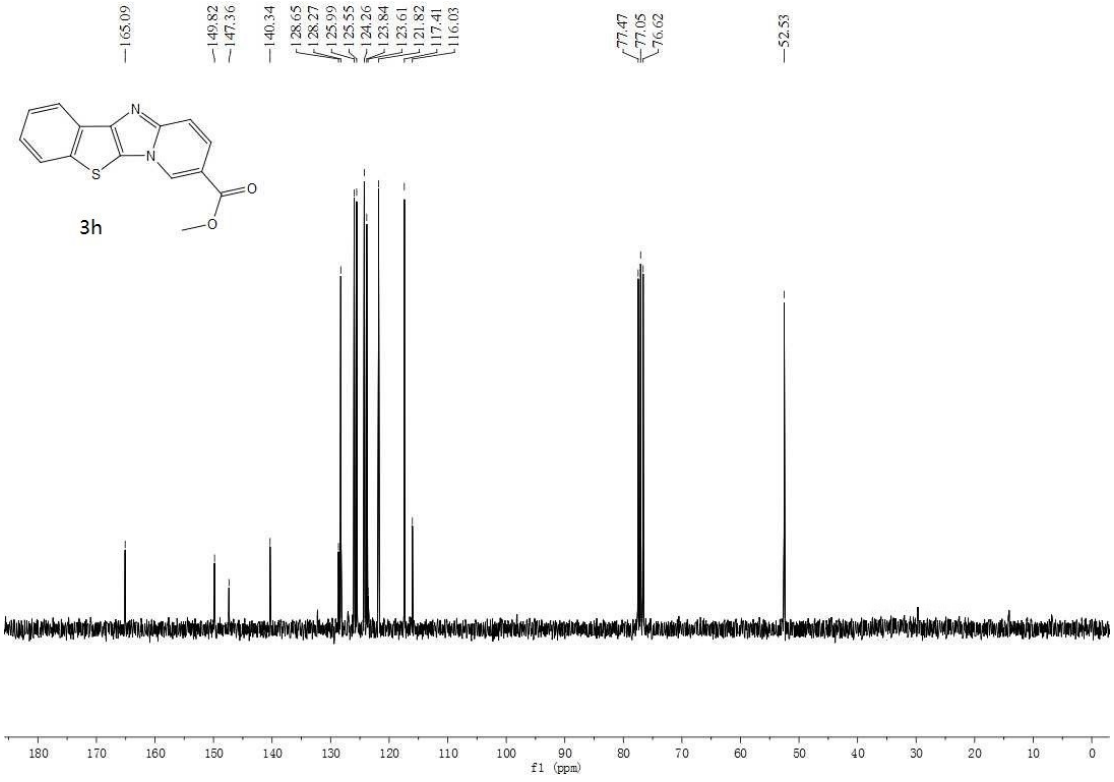

157.48
150.70
139.16
128.53
124.87
124.46
124.08
123.57
121.20
107.10
95.14
76.99
76.57
76.14
55.19
f1 (ppm)

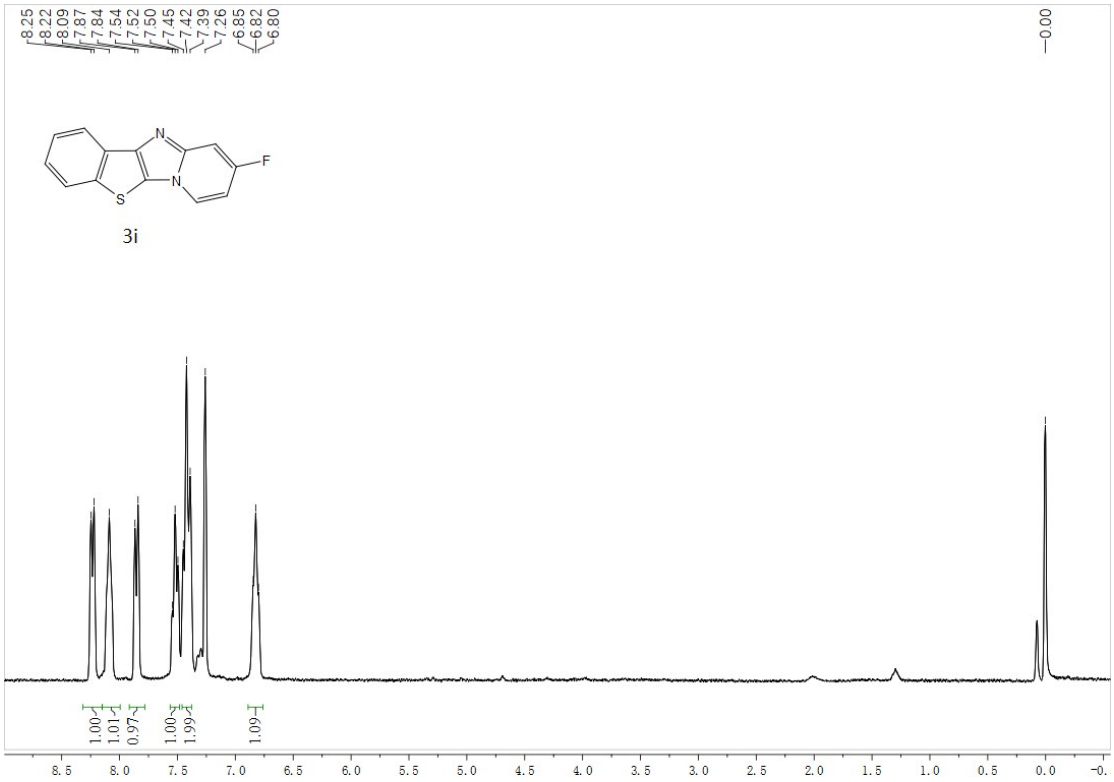
3f

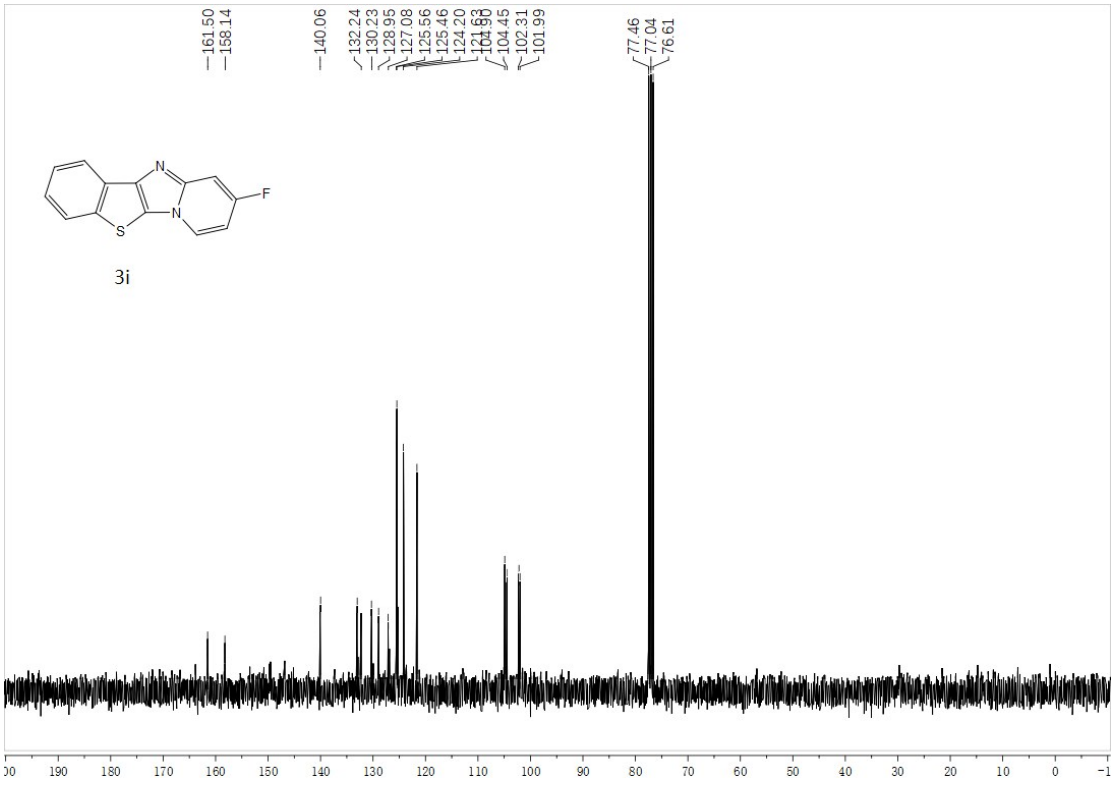

8.29
8.25
8.23
7.87
7.84
7.67
7.64
7.55
7.52
7.50
7.46
7.44
7.42
7.33
7.31
7.26
0.00
N
N
S
Br
3g
1.00
0.98
0.99
1.00
1.14
1.10
1.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

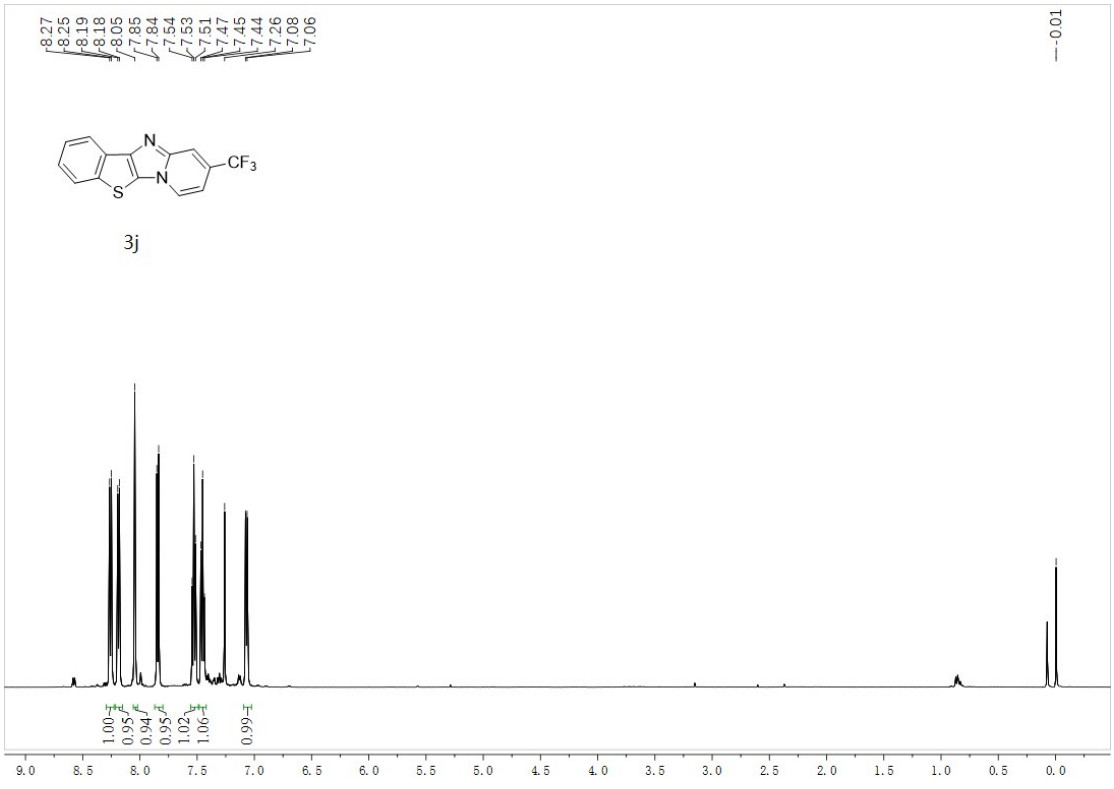

147.36
146.13
139.70
128.16
127.17
125.41
125.04
123.76
123.61
122.31
121.28
118.32
106.15
76.98
76.55
76.13
N
N
S
Br
3g
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

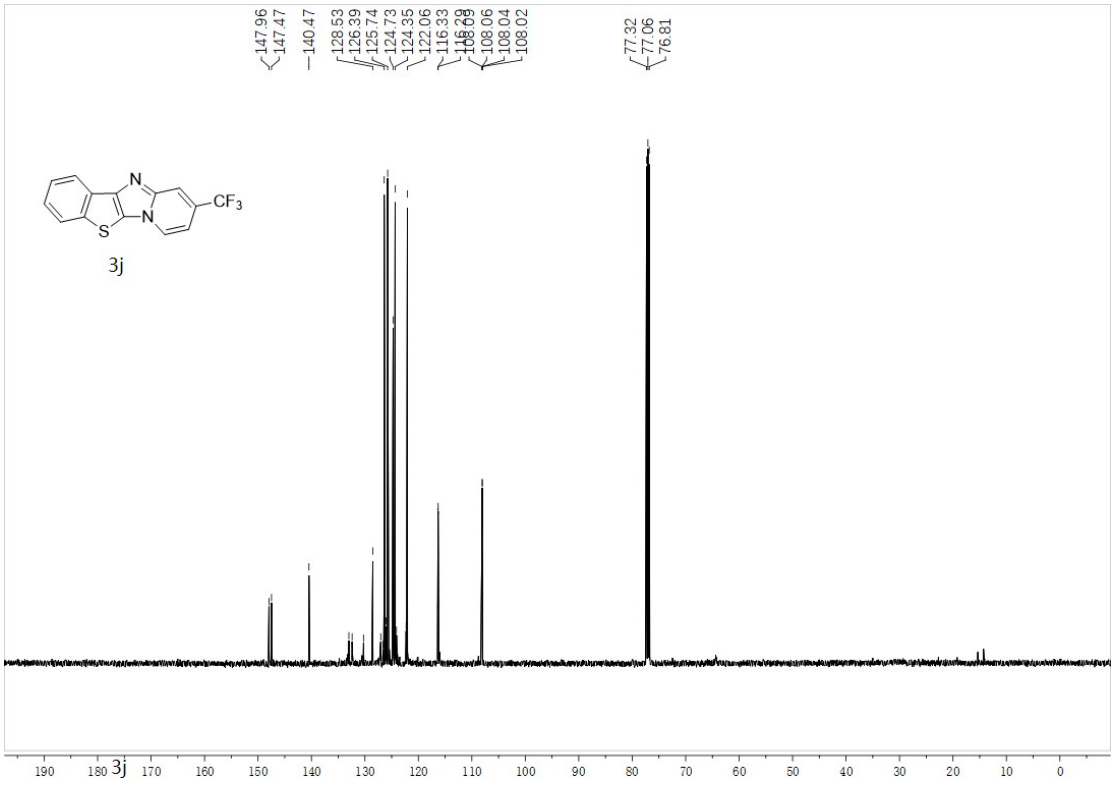

8.84
8.22
8.19
7.71
7.70
7.68
7.67
7.52
7.50
7.47
7.44
7.41
7.39
7.26
3.96
-0.01
3h
0.92
0.98
1.00
2.05
1.06
1.00
2.94
f1 (ppm)


165.09
149.82
147.36
140.34
128.65
128.27
125.99
125.55
124.26
123.84
123.61
121.82
117.41
116.03
77.47
77.05
76.62
52.53
3h
f1 (ppm)

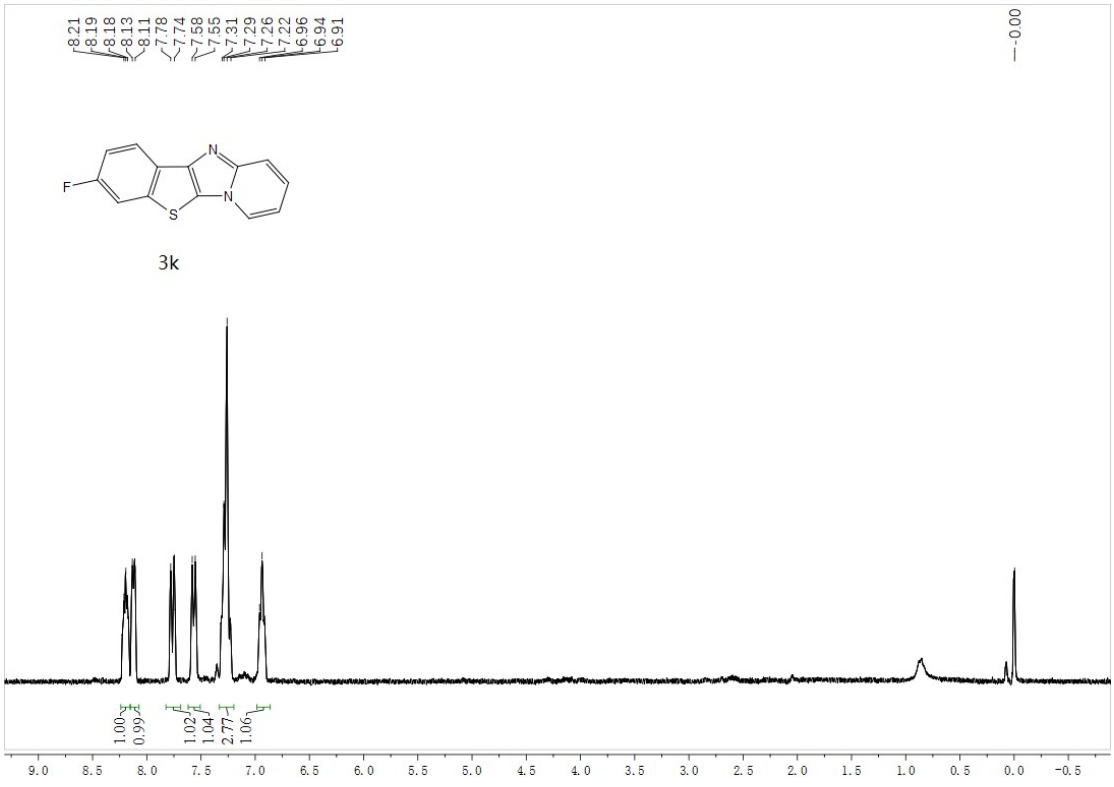

8.25
8.22
8.09
7.87
7.84
7.54
7.52
7.50
7.45
7.42
7.39
7.26
6.85
6.82
6.80
0.00
N
F
S
N
3i
1.00
1.01
0.97
1.00
1.99
1.09

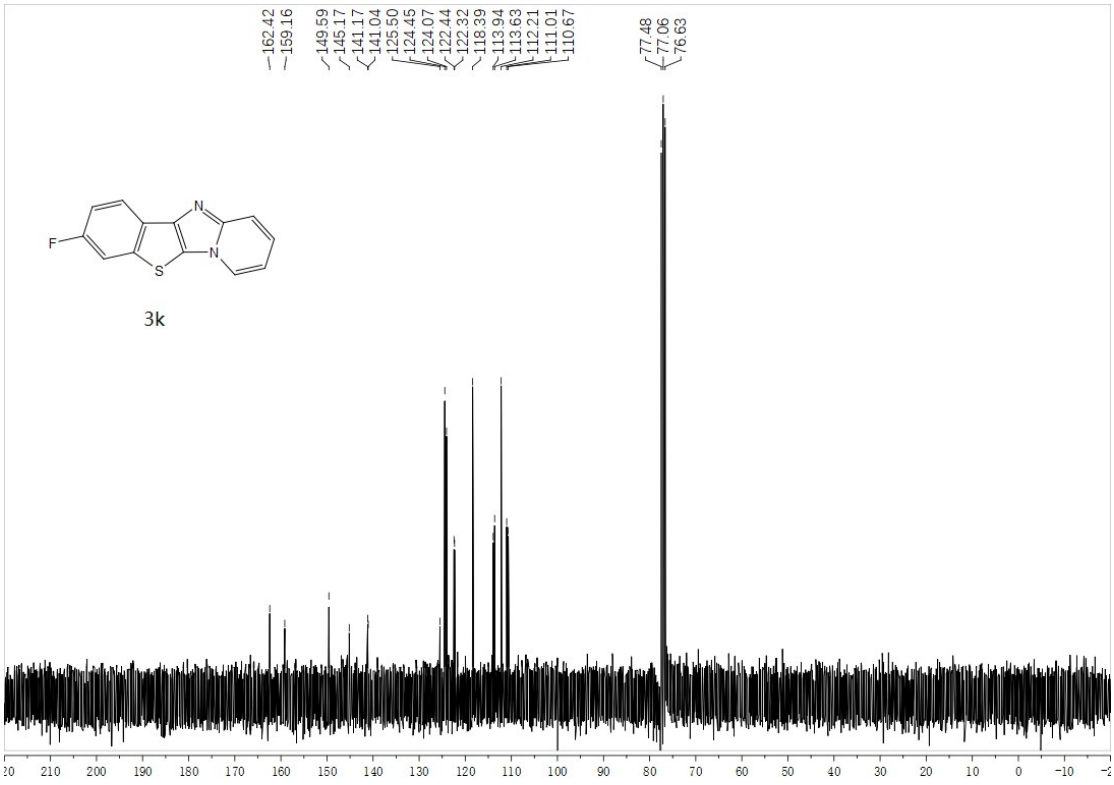

161.50
158.14
140.06
132.24
130.23
128.95
127.08
125.56
125.46
124.20
121.63
104.45
102.31
101.99
77.46
77.04
76.61
N
F
S
N
3i


8.27
8.25
8.19
8.18
8.05
7.85
7.84
7.54
7.53
7.51
7.47
7.45
7.44
7.26
7.08
7.06
0.01
N
S
N
CF3
3j
1.00
0.95
0.94
0.95
1.02
1.06
0.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


147.96
147.47
140.47
128.53
126.39
125.74
124.73
124.35
122.06
116.33
108.06
108.04
108.02
77.32
77.06
76.81
N
S
N
CF3
3j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

3j

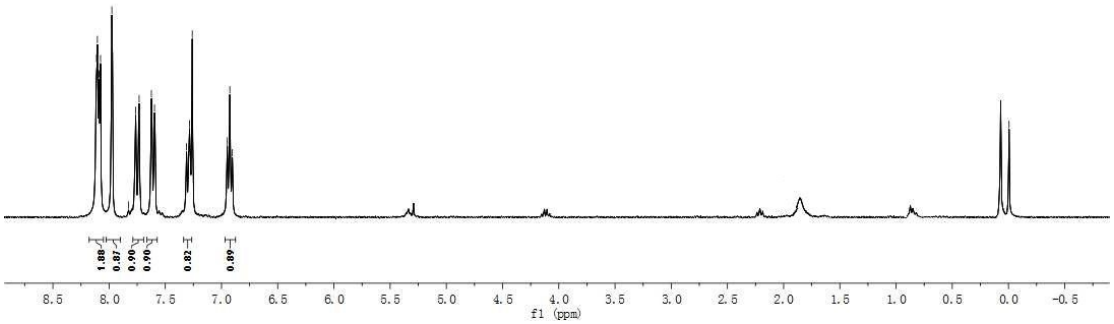

8.21
8.19
8.18
8.13
8.11
7.78
7.74
7.58
7.55
7.31
7.29
7.26
7.22
6.96
6.94
6.91
-0.00
F
N
S
N
3k
1.00
0.99
1.02
1.04
2.77
1.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


162.42
159.16
149.59
145.17
141.17
141.04
125.50
124.45
124.07
122.44
122.32
118.39
113.94
113.63
112.21
111.01
110.67
77.48
77.06
76.63
F
N
S
N
3k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

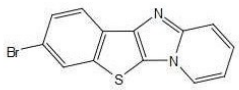

8.11
8.10
8.09
8.08
7.98
7.83
7.76
7.73
7.62
7.60
7.31
7.28
7.26
6.95
6.93
6.90
-0.01

Br
N
N
S

3l

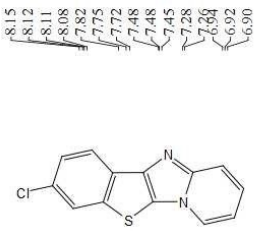

1.00
0.87
0.90
0.90
0.82
0.89
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


149.77
145.25
141.44
128.76
127.87
127.56
126.75
124.78
124.22
122.59
118.60
118.53
112.37
77.45
77.03
76.61

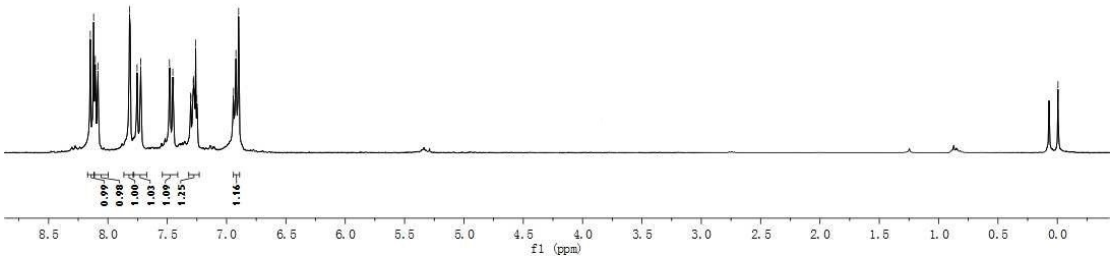

Br
N
N
S

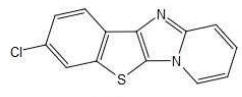
3l

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

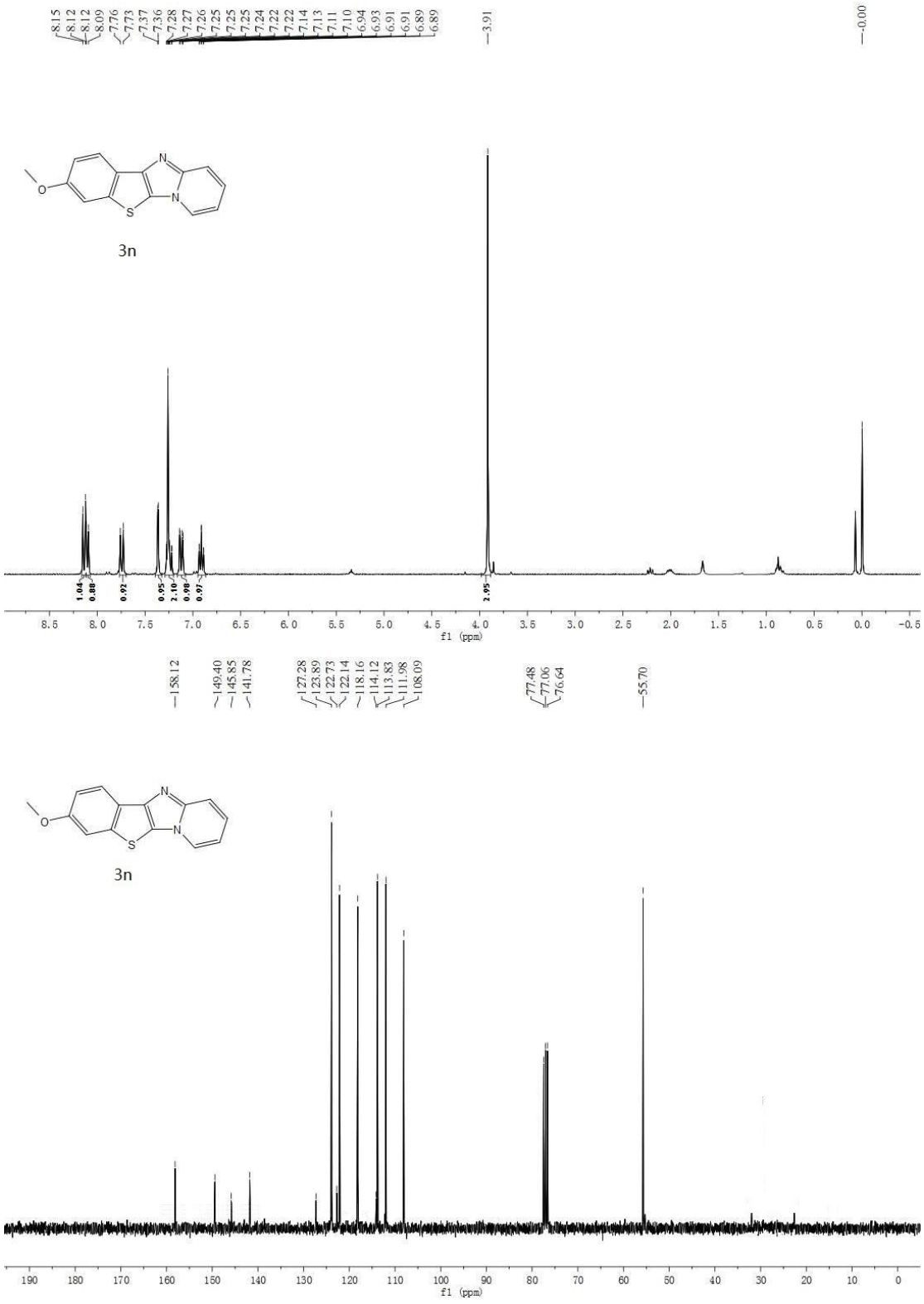


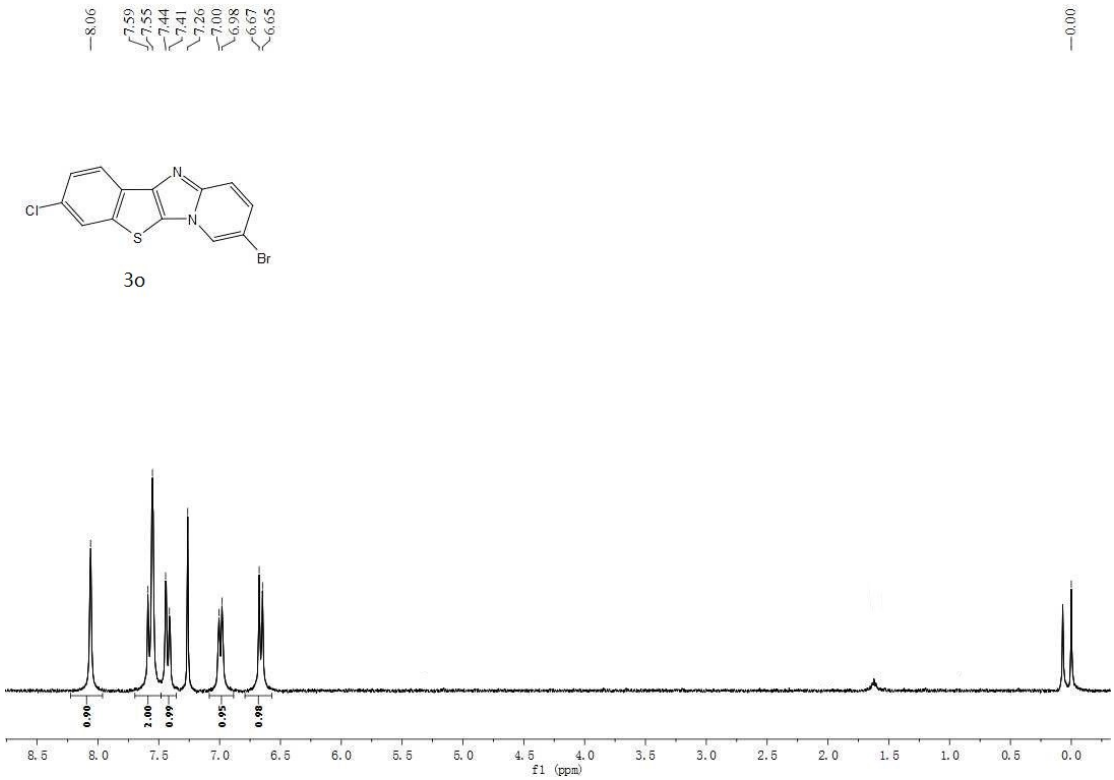
3m

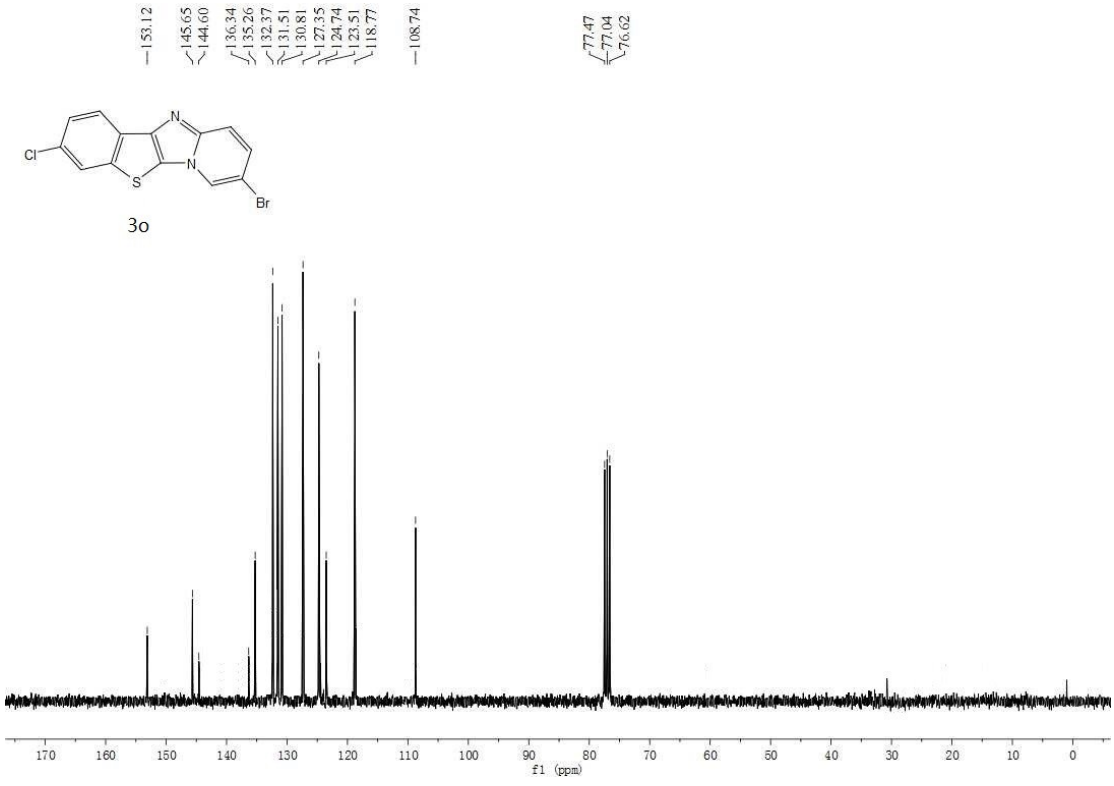


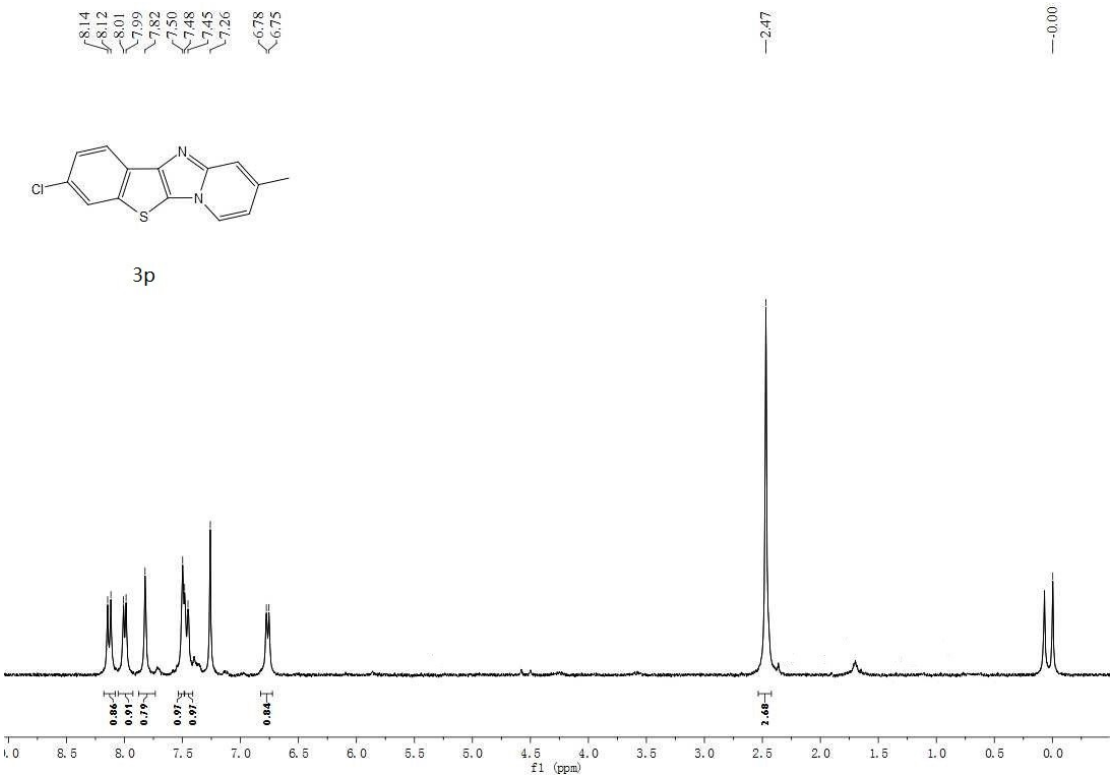


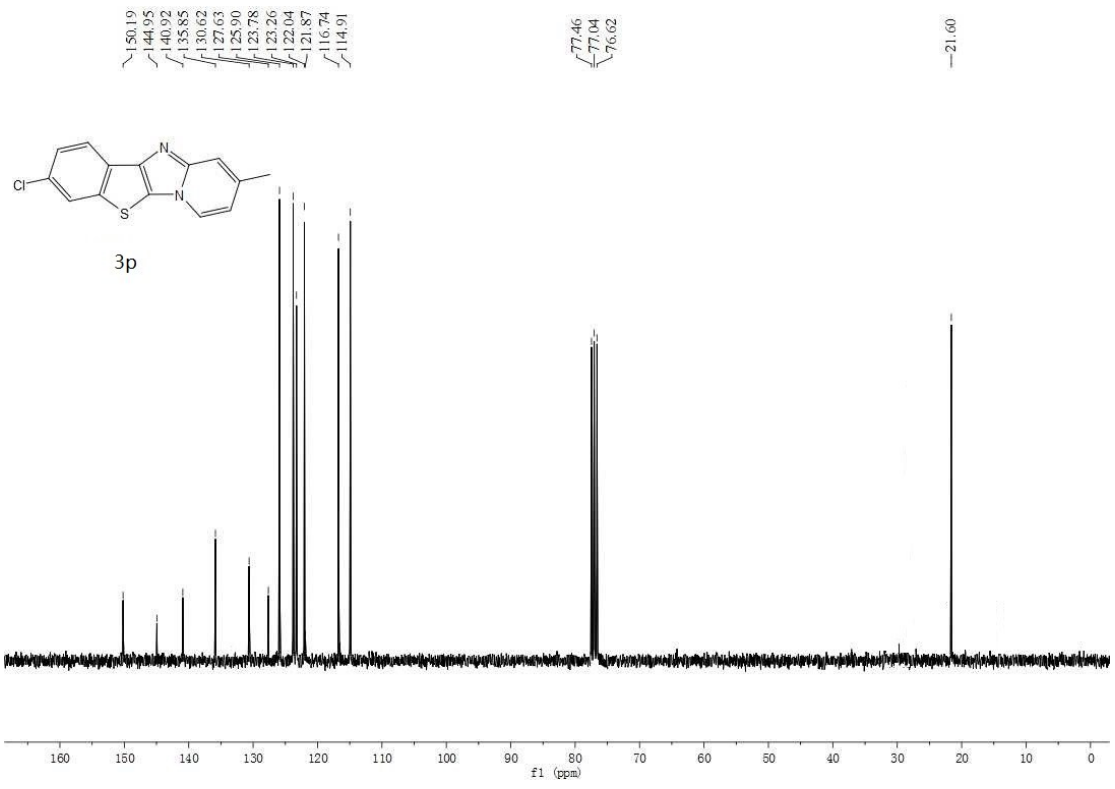
3m

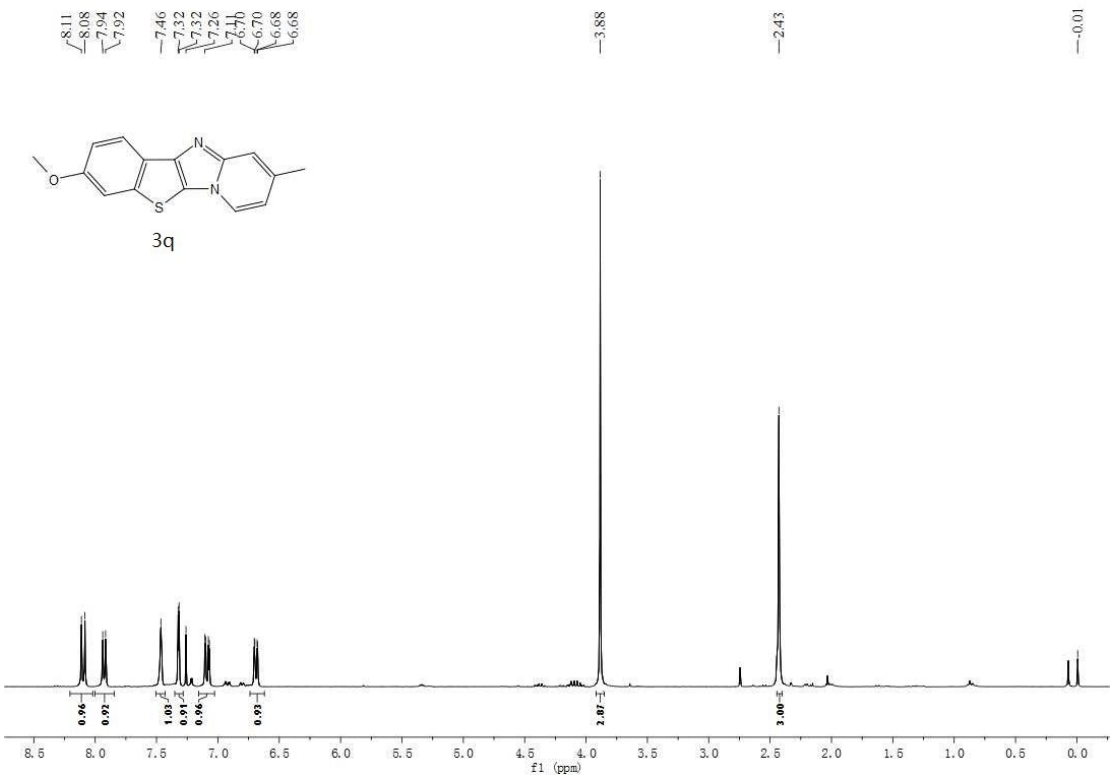

8.15
8.12
8.12
8.09
7.76
7.73
7.37
7.36
7.28
7.27
7.26
7.25
7.25
7.25
7.24
7.22
7.22
7.14
7.13
7.11
7.10
6.94
6.93
6.91
6.91
6.89
6.89
3.91
0.00
3n
1.04
0.88
0.92
0.95
2.10
0.98
0.97
2.95
f1 (ppm)
158.12
149.40
145.85
141.78
127.28
123.89
122.73
122.14
118.16
114.12
113.83
111.98
108.09
77.48
77.06
76.64
55.70
3n
f1 (ppm)


8.06
7.59
7.55
7.44
7.41
7.26
7.00
6.98
6.67
6.65
0.00
Cl
N
S
N
Br
3o
0.90
2.00
0.99
0.95
0.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

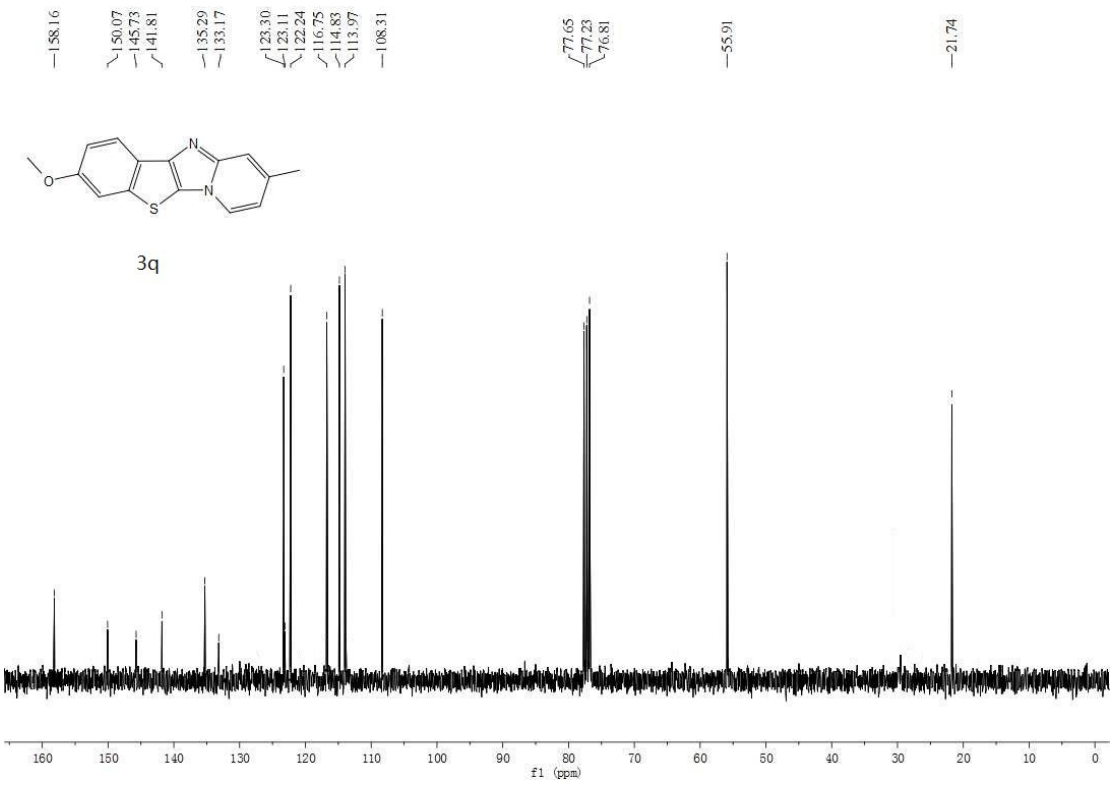

153.12
145.65
144.60
136.34
135.26
132.37
131.51
130.81
127.35
124.74
123.51
118.77
108.74
77.47
77.04
76.62
Cl
N
S
N
Br
3o
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.14
8.12
8.01
7.99
7.82
7.50
7.48
7.45
7.26
6.78
6.75
2.47
0.00
Cl
N
S
N
3p
0.86
0.91
0.79
0.97
0.97
0.84
2.68
f1 (ppm)


150.19
144.95
140.92
135.85
130.62
127.63
125.90
123.78
123.26
122.04
121.87
116.74
114.91
77.46
77.04
76.62
21.60
Cl
N
S
N
3p
f1 (ppm)

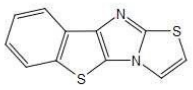

8.11
8.08
7.94
7.92
7.46
7.32
7.32
7.26
7.11
6.70
6.68
6.68
3.88
2.43
-0.01
0.96
0.92
1.03
0.91
0.96
0.93
2.07
3.00
f1 (ppm)

3q

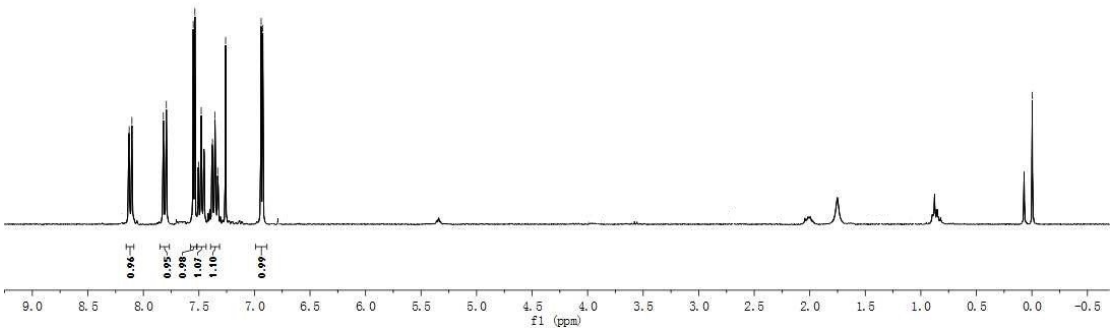

158.16
150.07
145.73
141.81
135.29
133.17
123.30
123.11
122.24
116.75
114.83
113.97
108.31
77.65
77.23
76.81
55.91
21.74
f1 (ppm)

3q

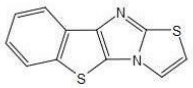

8.13
8.10
7.82
7.79
7.55
7.54
7.50
7.48
7.45
7.38
7.36
7.33
7.26
6.94
6.92
0.00


N
S
S
N

3r


0.96
0.95
0.98
1.07
1.10
0.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

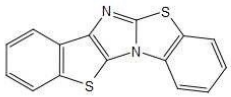

152.91
147.19
138.09
131.83
128.73
124.80
123.94
123.52
120.17
116.73
111.63
76.97
76.54
76.12


N
S
S
N

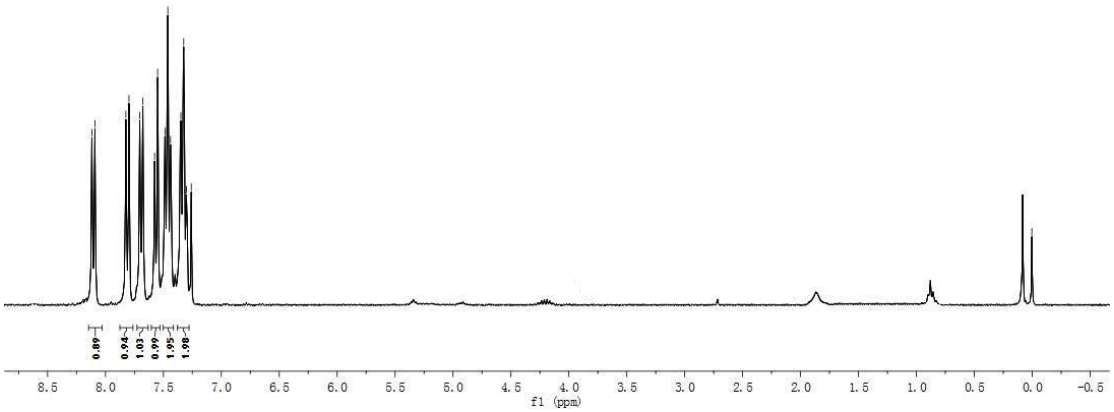
3r

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

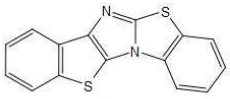

8.12
8.09
7.82
7.80
7.70
7.68
7.58
7.55
7.49
7.46
7.44
7.35
7.32
7.30
7.26
0.00


N
S
N
S

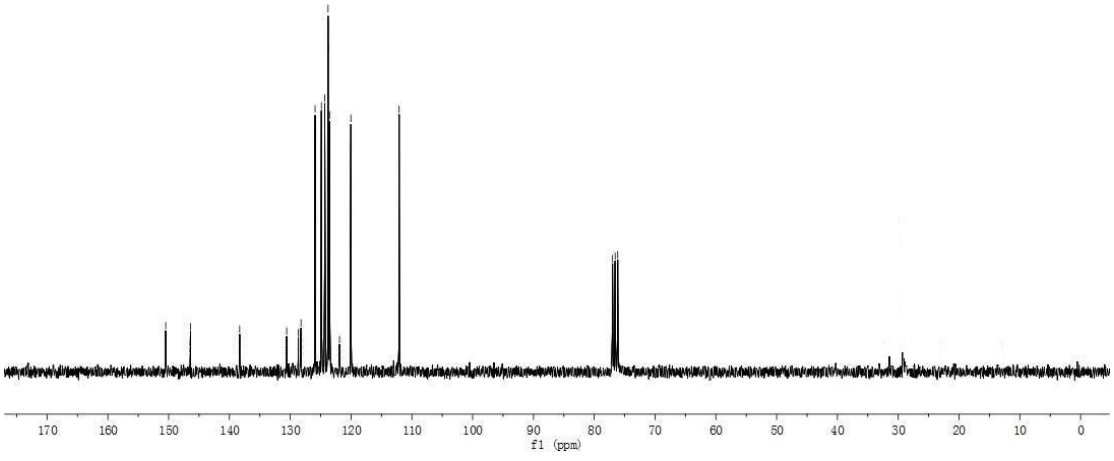
3s


0.89
0.94
1.03
0.99
1.95
1.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

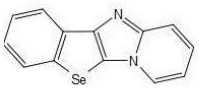

150.48
146.41
138.32
128.23
125.91
124.88
124.33
123.78
123.76
123.53
120.03
112.08
76.99
76.57
76.14


N
S
N
S

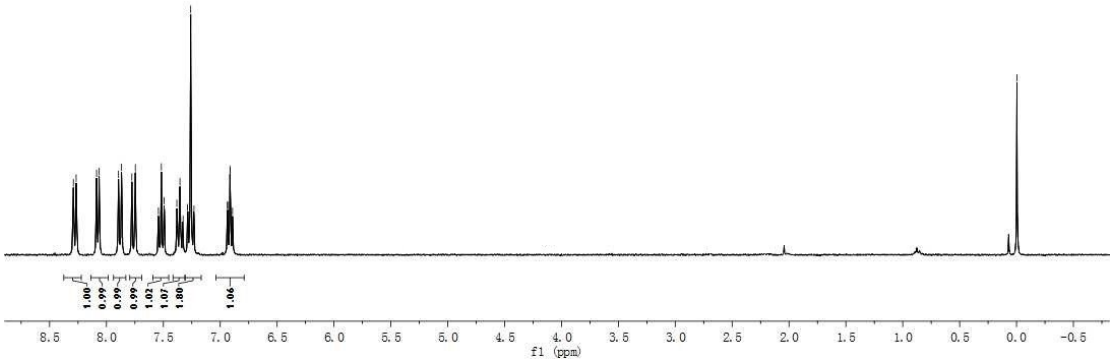
3s


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

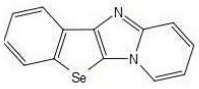

8.29
8.27
8.09
8.06
7.89
7.87
7.78
7.75
7.54
7.52
7.49
7.38
7.35
7.33
7.29
7.26
7.23
6.94
6.93
6.91
6.91
6.89
-0.00


N
N
Se

4a

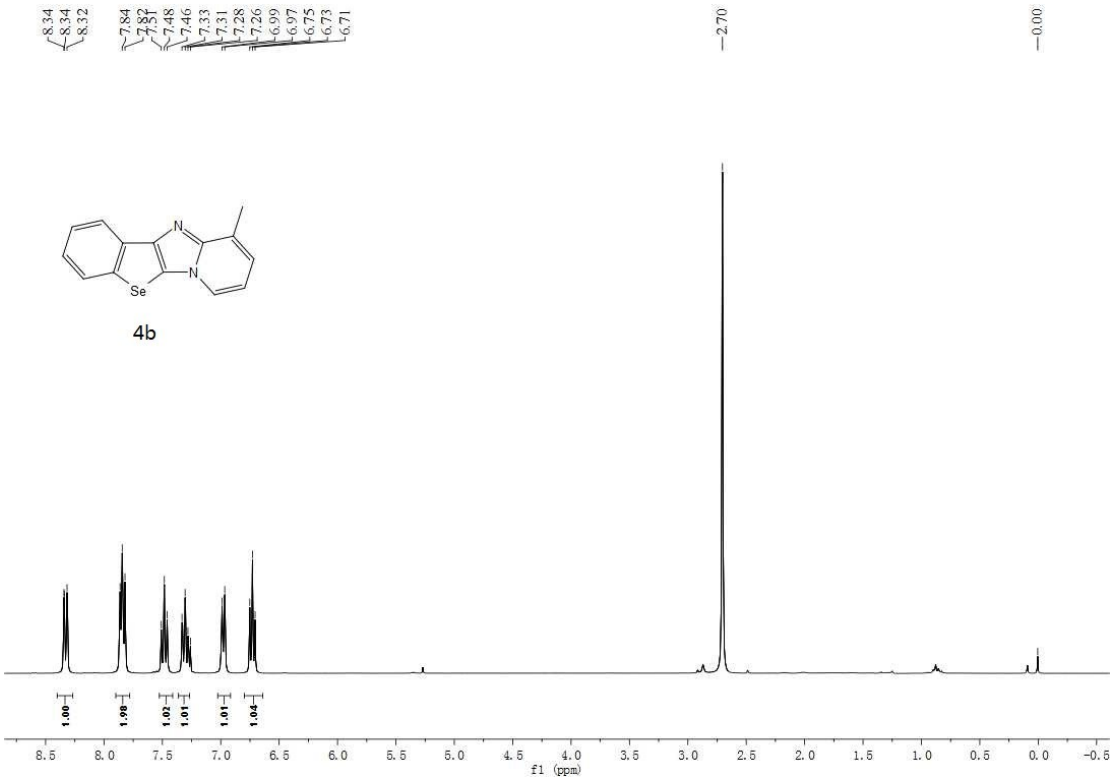

1.00
0.99
0.99
0.99
1.02
1.07
1.80
1.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

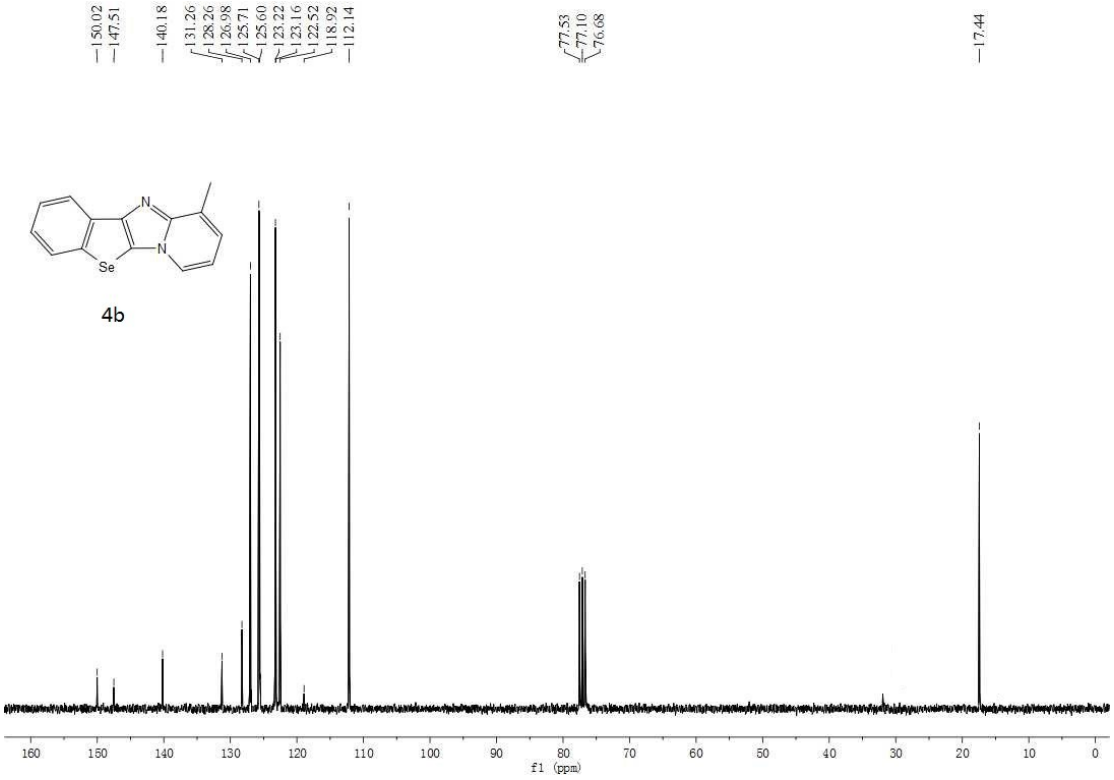

149.01
147.56
139.78
130.52
126.53
125.40
125.37
124.18
123.90
122.57
117.82
111.74
77.01
76.59
76.17

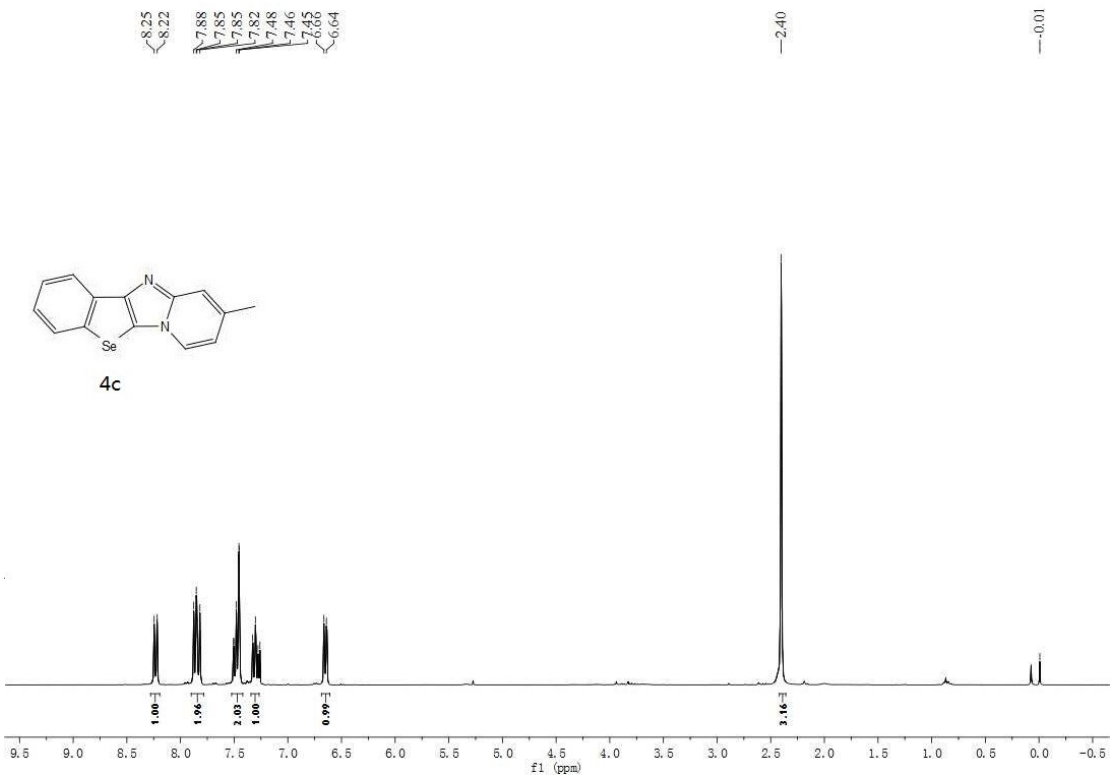

N
N
Se

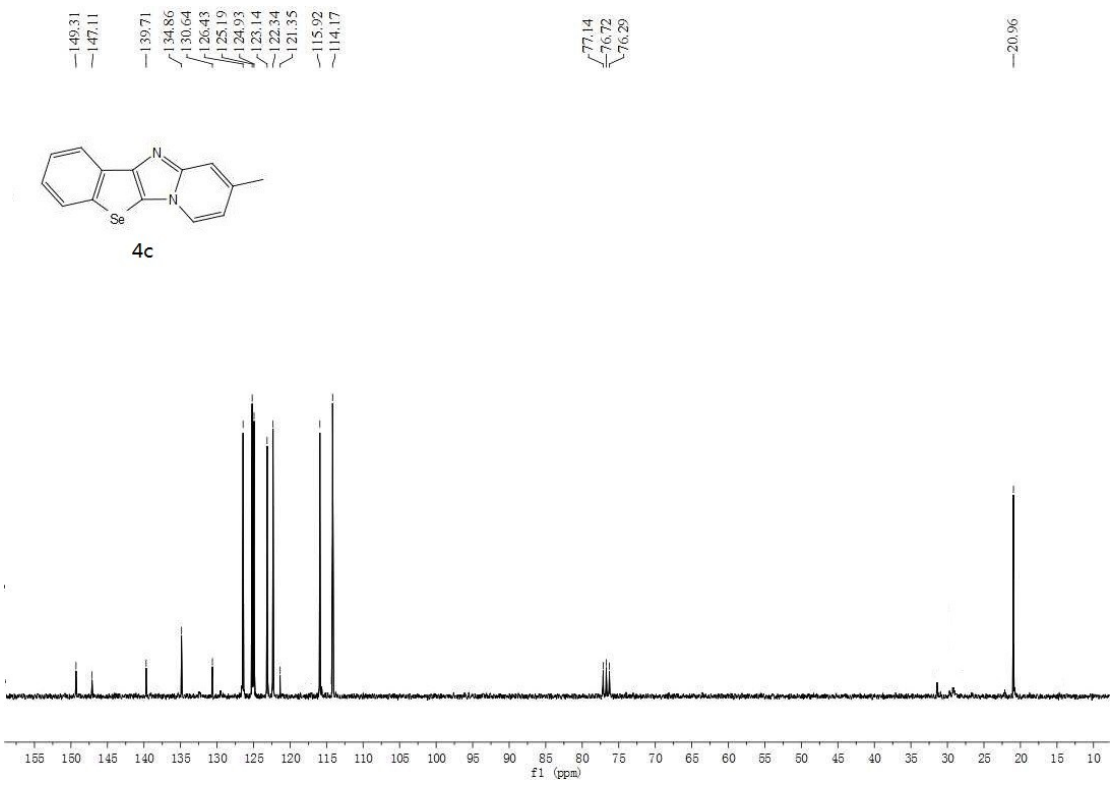
4a

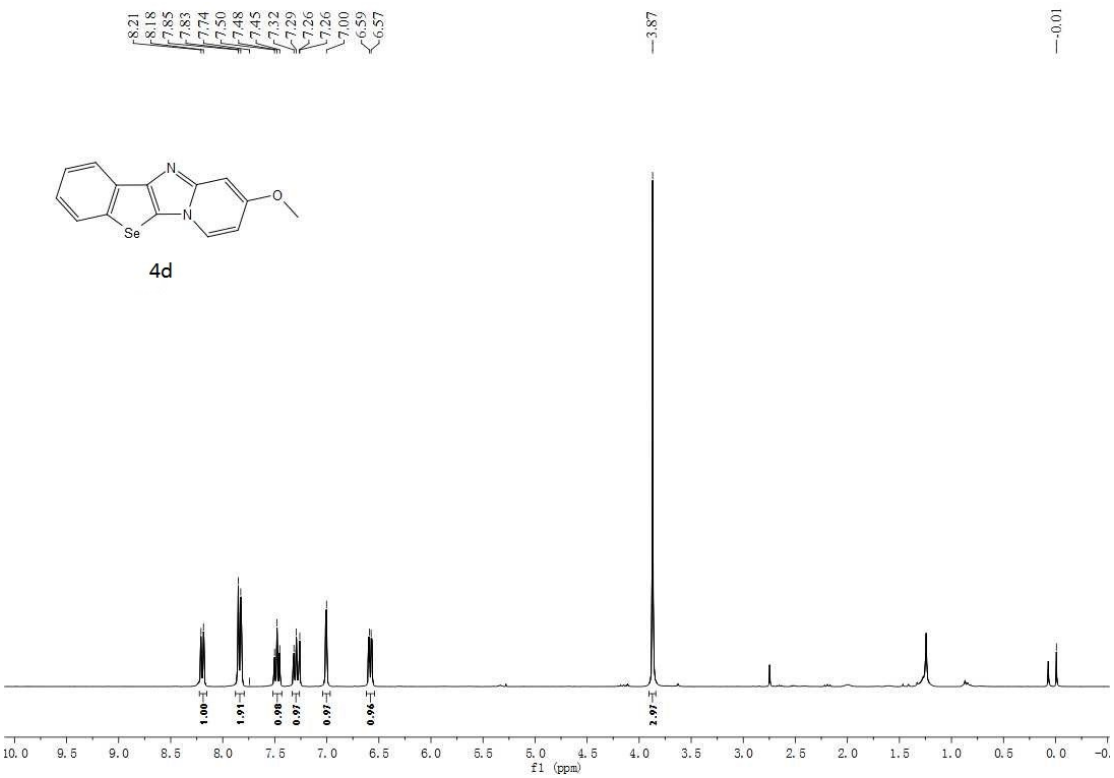
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

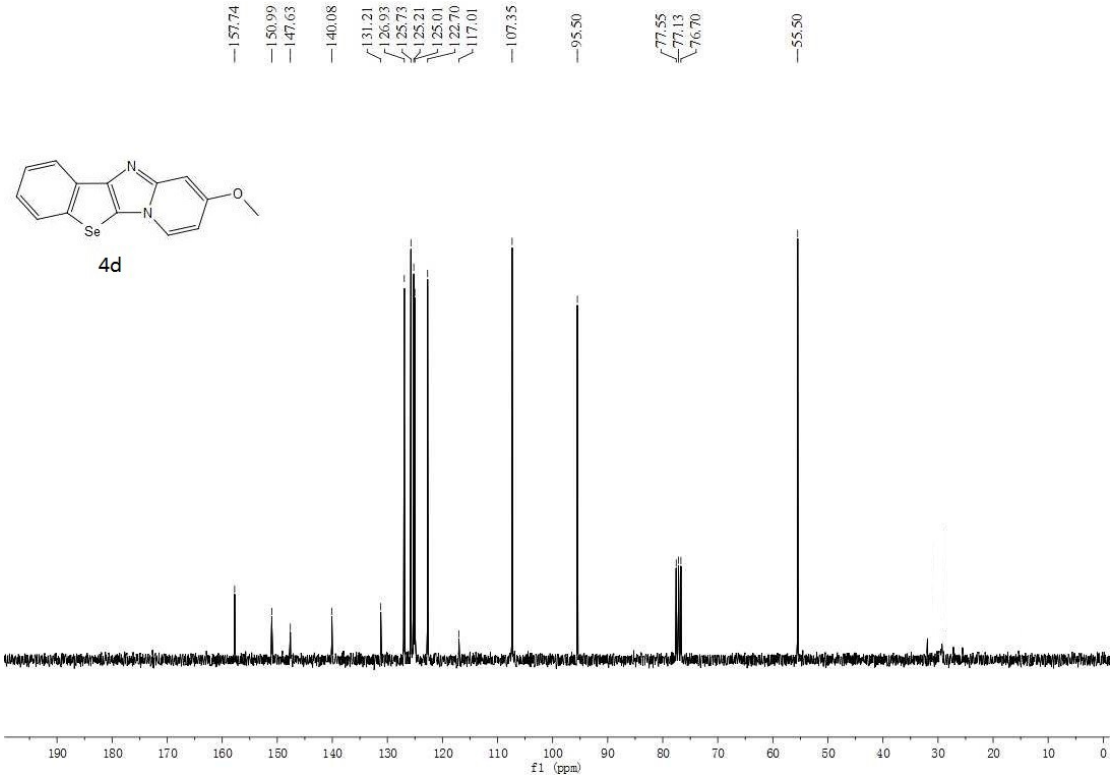

8.34
8.34
8.32
7.84
7.82
7.81
7.48
7.46
7.33
7.31
7.28
7.26
6.99
6.97
6.75
6.73
6.71
2.70
0.00
N
N
Se
4b
1.00
1.98
1.02
1.01
1.01
1.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


150.02
147.51
140.18
131.26
128.26
126.98
125.71
125.60
123.22
123.16
122.52
118.92
112.14
77.53
77.10
76.68
17.44
N
N
Se
4b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

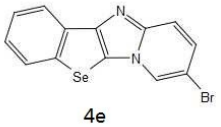

8.25
8.22
7.88
7.85
7.85
7.82
7.48
7.46
7.45
6.66
6.64
2.40
-0.01
Se
N
N
4c
1.00
1.96
2.03
1.00
0.99
3.16
f1 (ppm)


149.31
147.11
139.71
134.86
130.64
126.43
125.19
124.93
123.14
122.34
121.35
115.92
114.17
77.14
76.72
76.29
20.96
Se
N
N
4c
f1 (ppm)

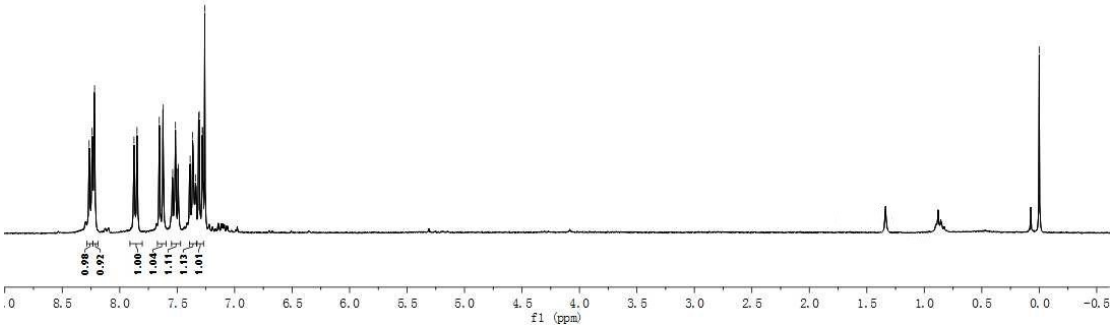

8.21
8.18
7.85
7.83
7.74
7.50
7.48
7.45
7.32
7.29
7.26
7.26
7.00
6.59
6.57
3.87
-0.01
Se
N
N
O
4d
1.00
1.91
0.98
0.97
0.97
0.96
2.97
f1 (ppm)

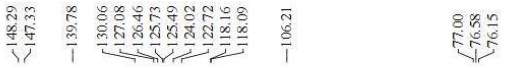

157.74
150.99
147.63
140.08
131.21
126.93
125.73
125.21
125.01
122.70
117.01
107.35
95.50
77.55
77.13
76.70
55.50
Se
N
N
O
4d
f1 (ppm)

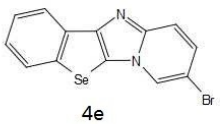

8.27
8.24
8.22
7.88
7.85
7.66
7.62
7.54
7.51
7.49
7.39
7.36
7.34
7.31
7.31
7.28
7.28
7.26
0.00


N
N
Se
Br

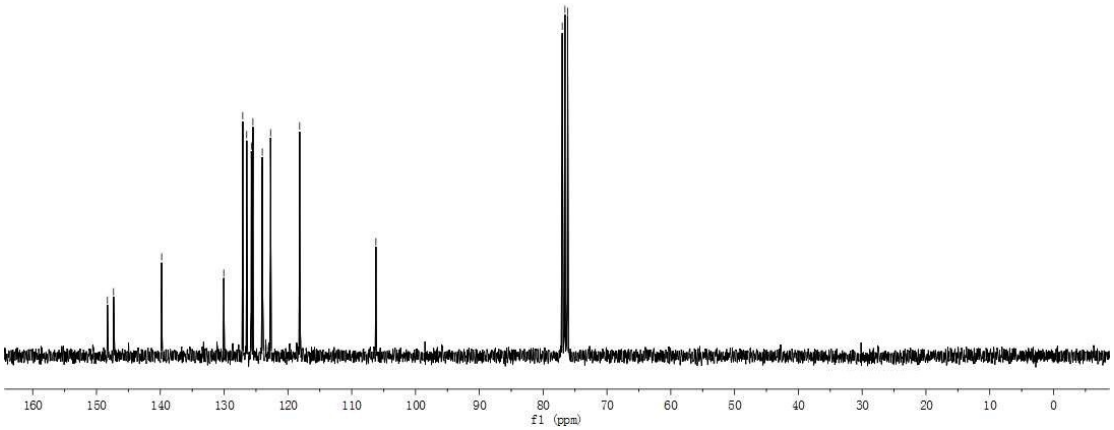
4e

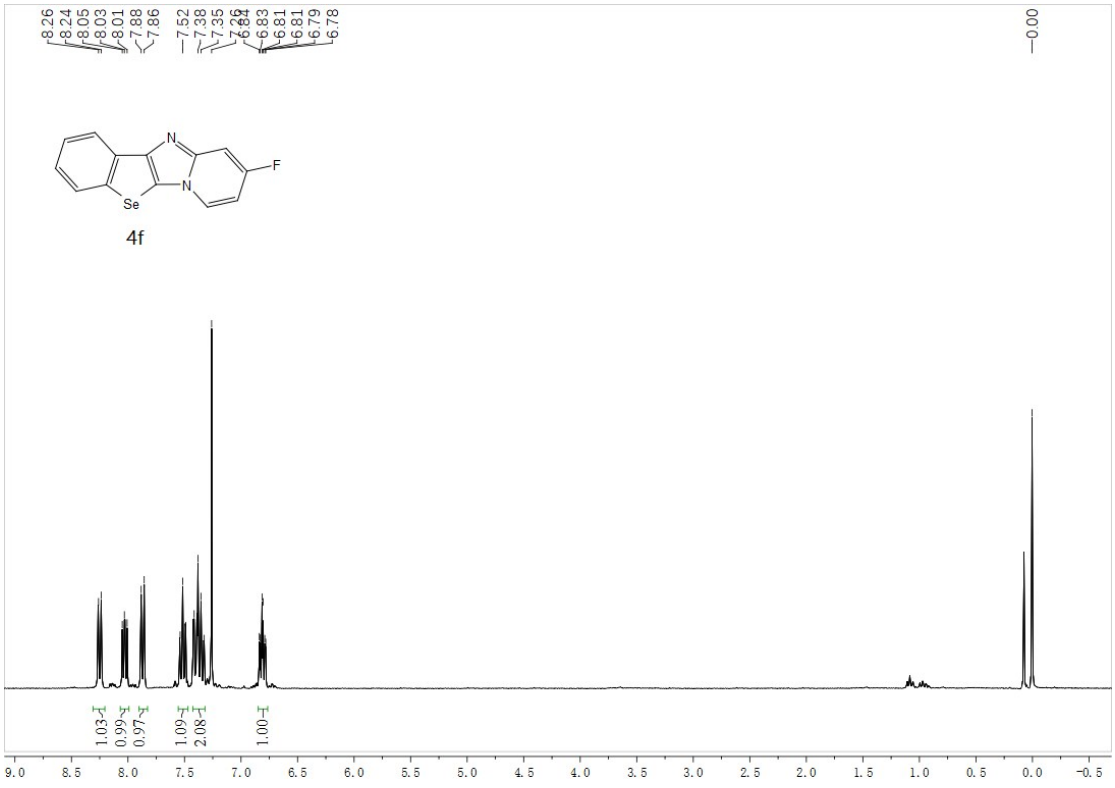

0.98
0.92
1.00
1.04
1.11
1.13
1.01
f1 (ppm)

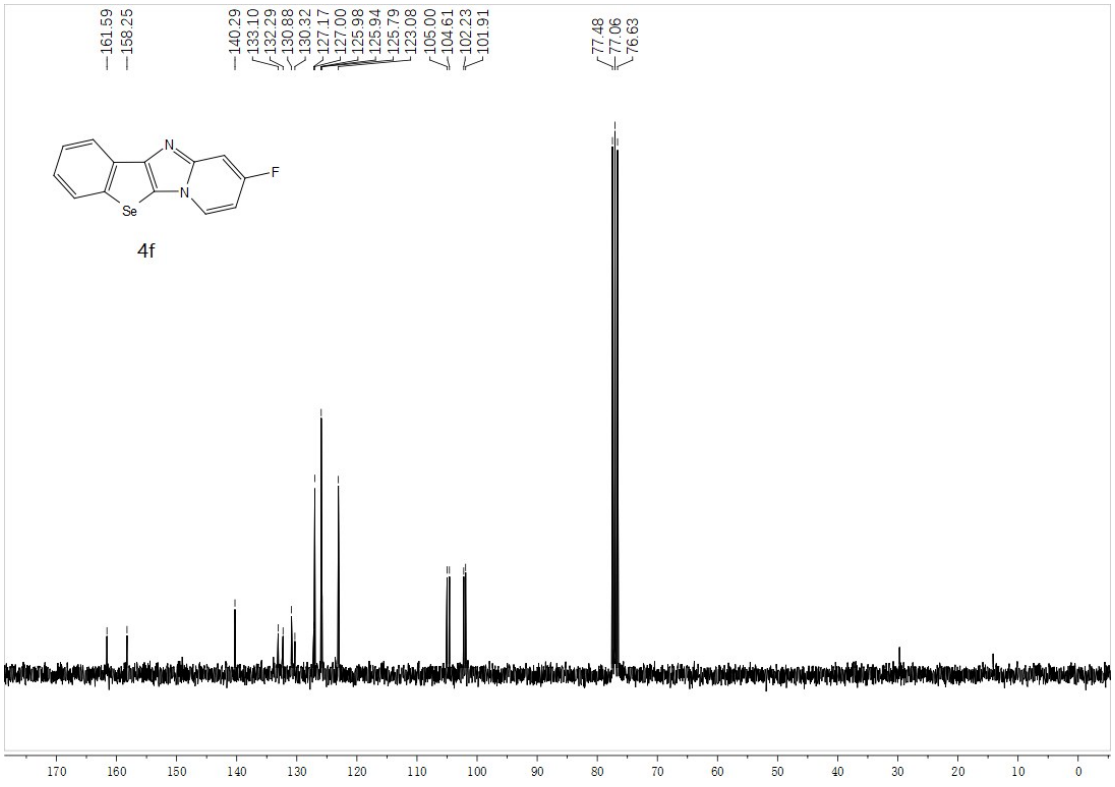

148.29
147.33
139.78
130.06
127.08
126.46
125.73
125.49
124.02
122.72
118.16
118.09
106.21
77.00
76.58
76.15

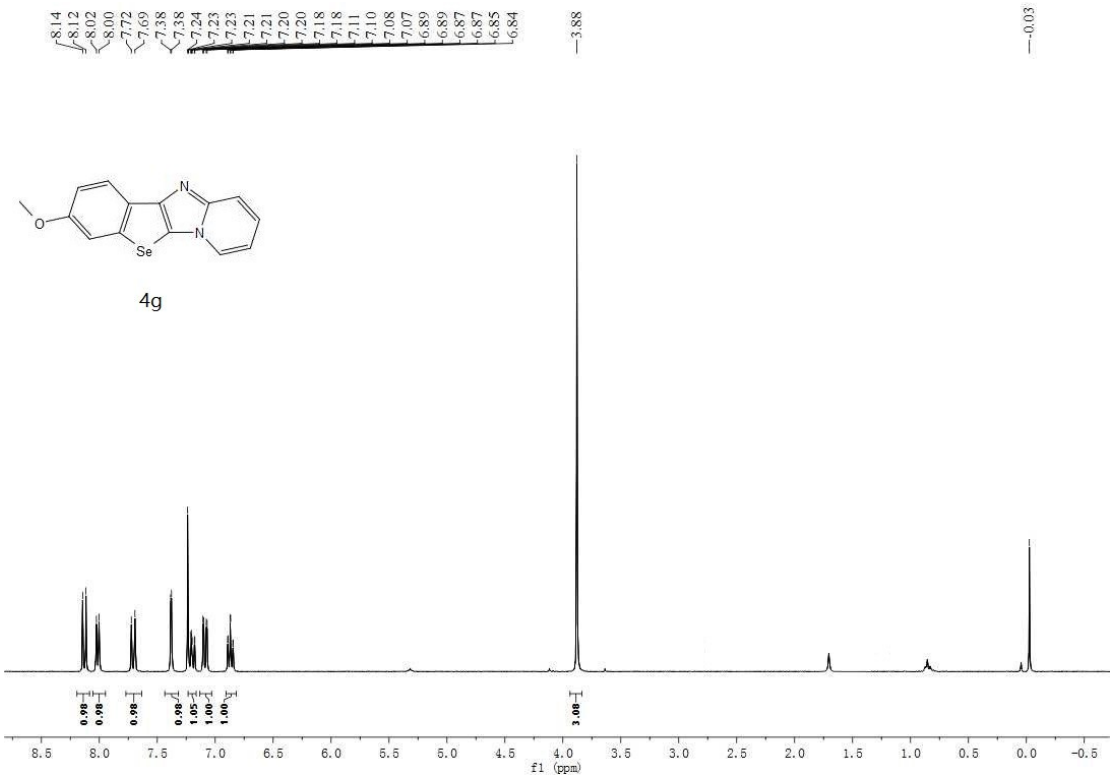

N
N
Se
Br

4e

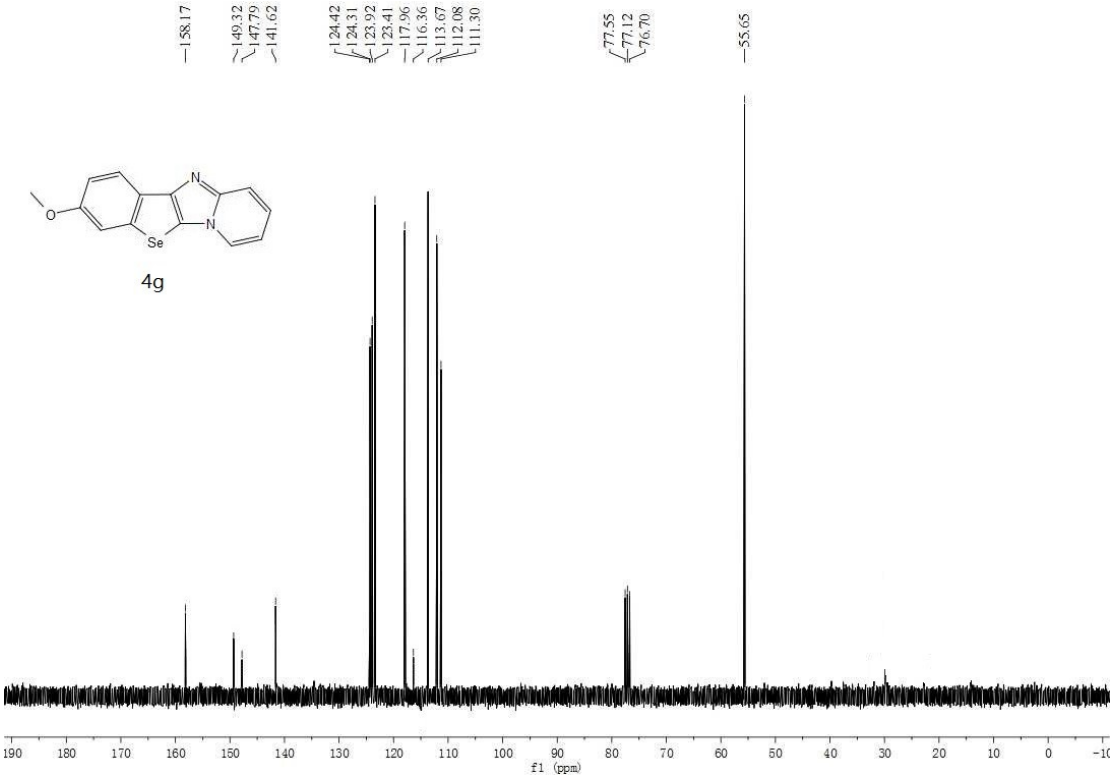

f1 (ppm)


8.26
8.24
8.05
8.03
8.01
7.88
7.86
7.52
7.38
7.35
7.26
6.84
6.83
6.81
6.81
6.79
6.78
0.00
N
F
Se
N
4f
1.03
0.99
0.97
1.09
2.08
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

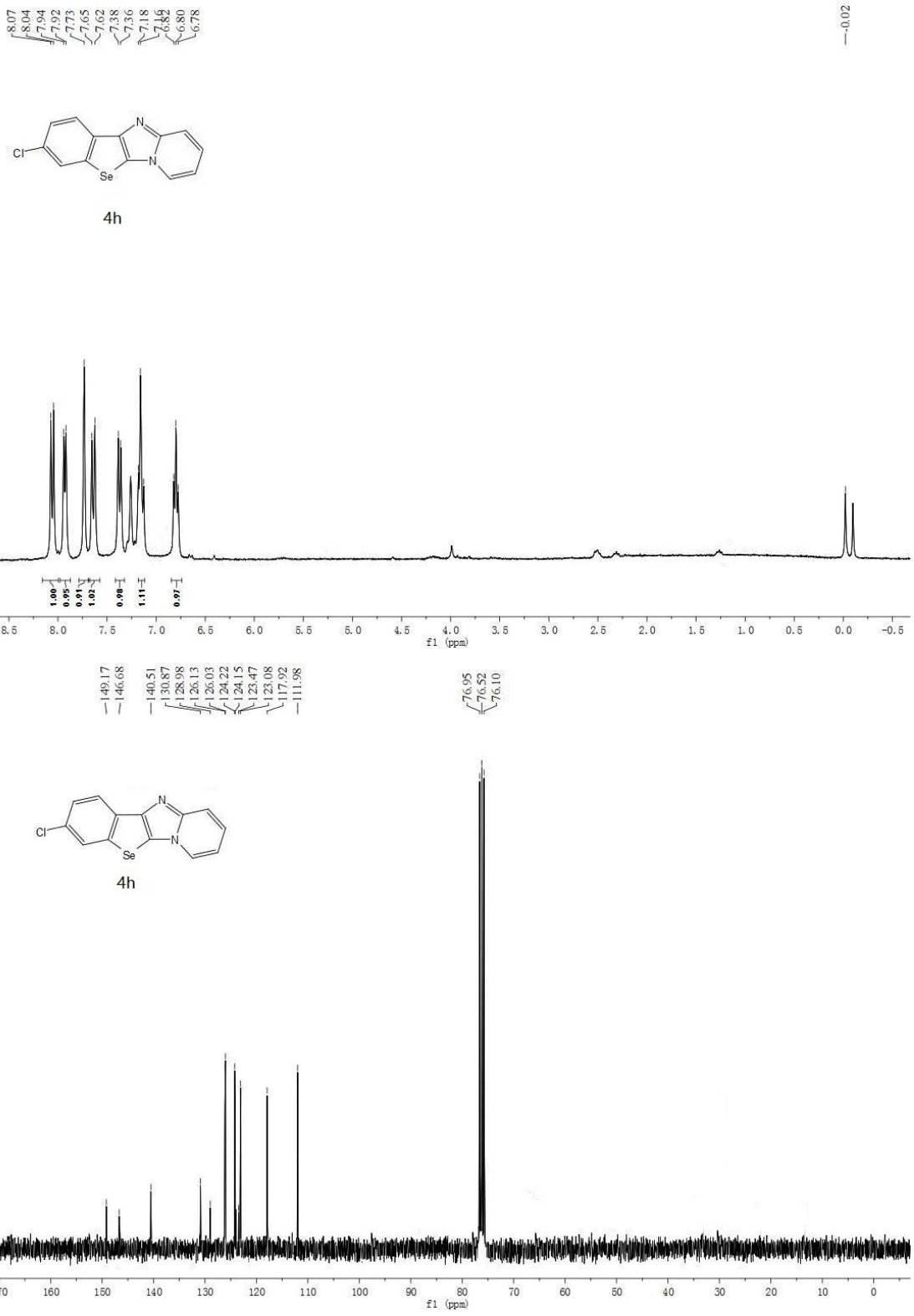

161.59
158.25
140.29
133.10
132.29
130.88
130.32
127.17
127.00
125.98
125.94
125.79
123.08
105.00
104.61
102.23
101.91
77.48
77.06
76.63
N
F
Se
N
4f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

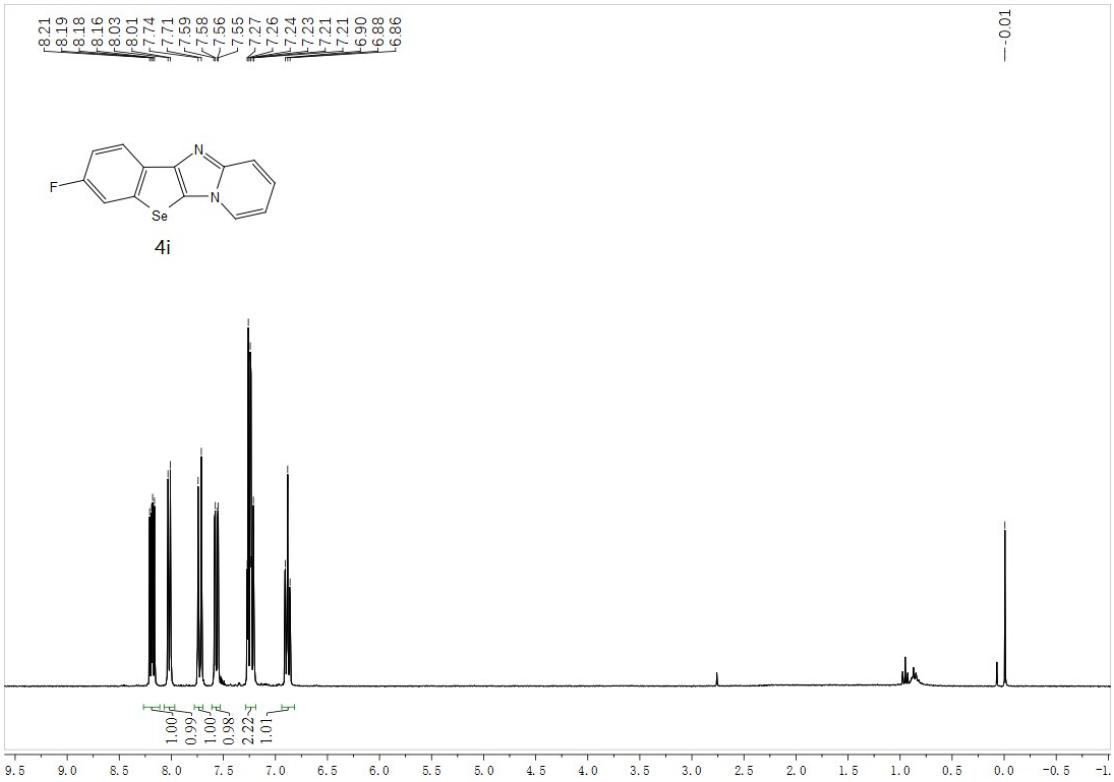

8.14
8.12
8.02
8.00
7.72
7.69
7.38
7.38
7.24
7.23
7.23
7.21
7.21
7.20
7.20
7.18
7.18
7.11
7.10
7.08
7.07
6.89
6.89
6.87
6.87
6.85
6.84
3.88
-0.03
O
N
N
Se
0.98
0.98
0.98
0.98
1.05
1.00
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

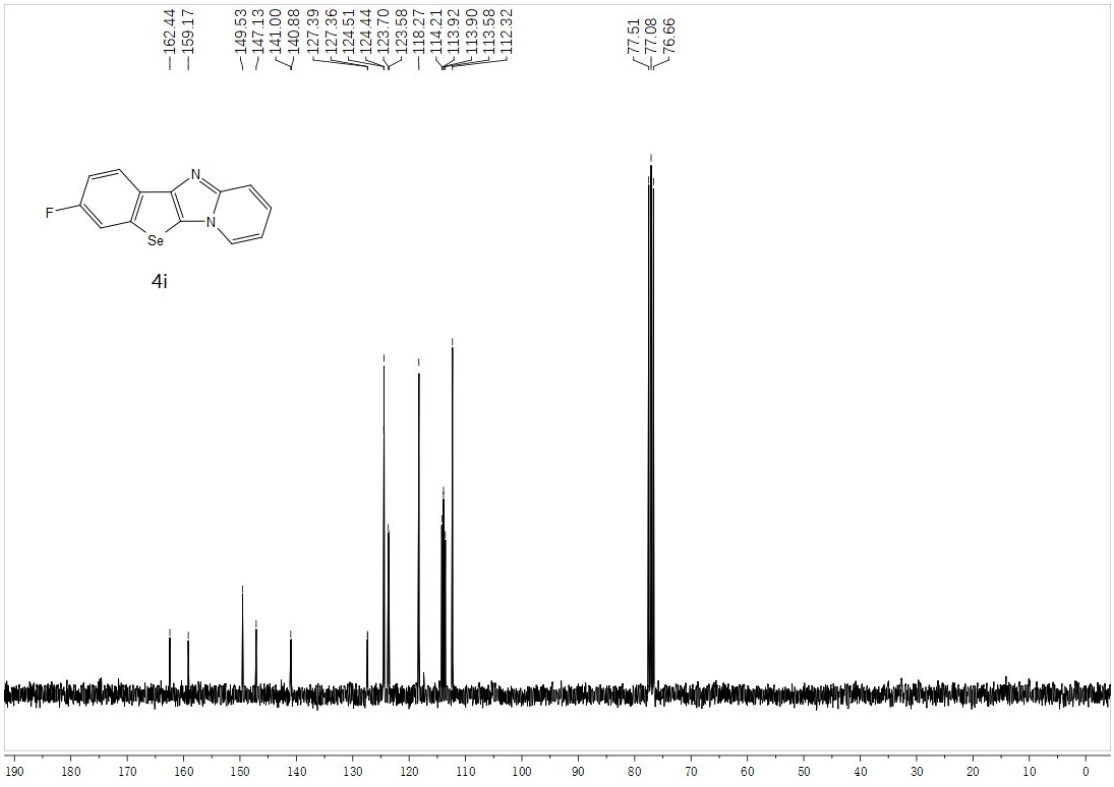
4g

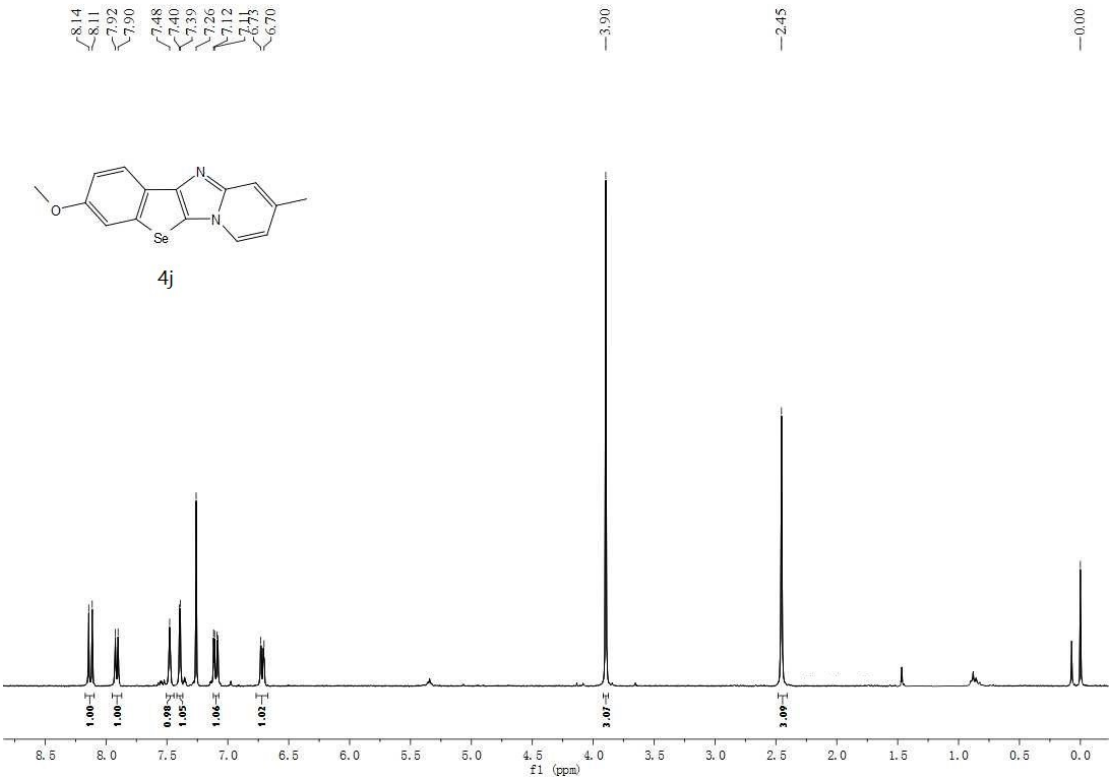

158.17
149.32
147.79
141.62
124.42
124.31
123.92
123.41
117.96
116.36
113.67
112.08
111.30
77.55
77.12
76.70
55.65
O
N
N
Se
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

4g

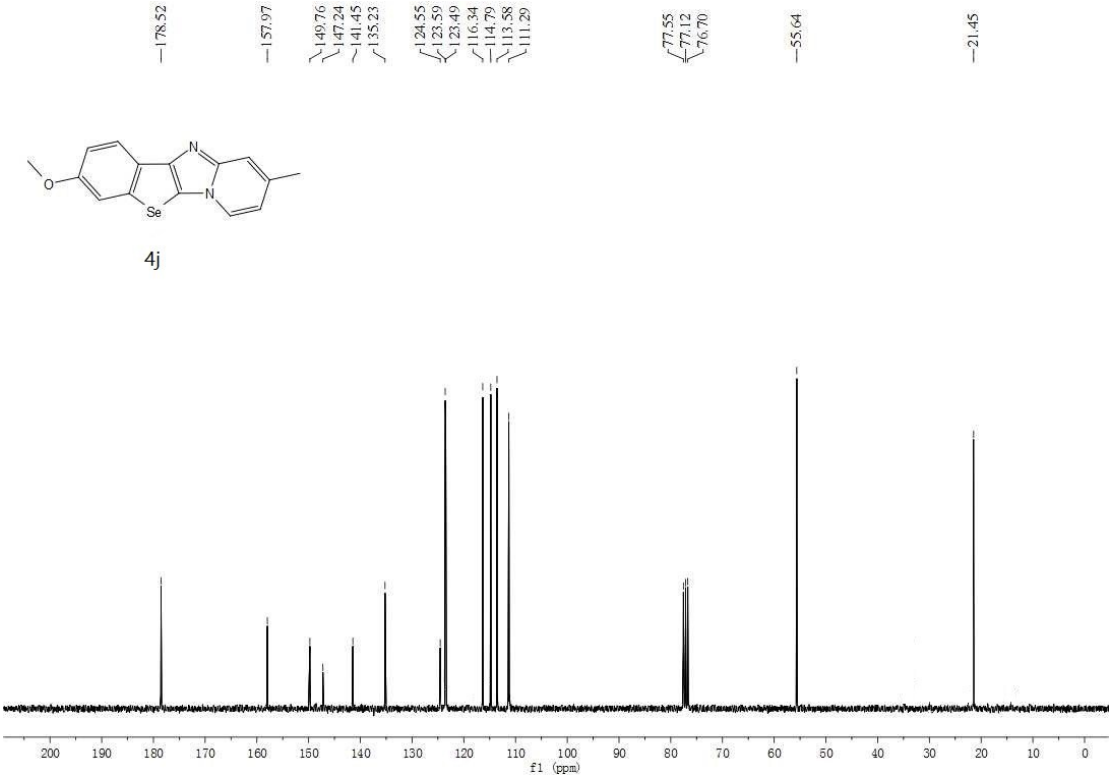

8.07
8.04
7.94
7.92
7.73
7.65
7.62
7.38
7.36
7.18
7.16
6.82
6.80
6.78
-0.02
Cl
N
N
Se
4h
1.00
0.95
0.91
1.02
0.98
1.11
0.97
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
149.17
146.68
140.51
130.87
128.98
126.13
126.03
124.22
124.15
123.47
123.08
117.92
111.98
76.95
76.52
76.10
Cl
N
N
Se
4h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.21
8.19
8.18
8.16
8.03
8.01
7.74
7.71
7.59
7.58
7.56
7.55
7.27
7.26
7.24
7.23
7.21
7.21
6.90
6.88
6.86
-0.01
F
N
N
Se
4i
1.00
0.99
1.00
0.98
2.22
1.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

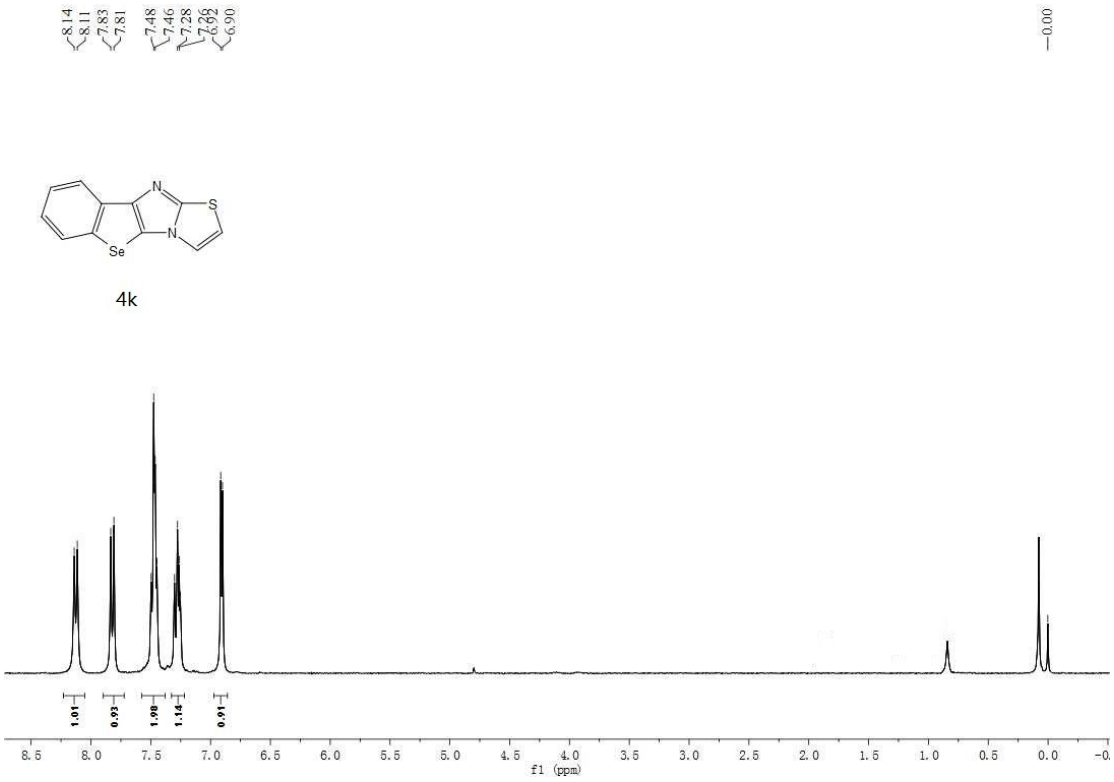

162.44
159.17
149.53
147.13
141.00
140.88
127.39
127.36
124.51
124.44
123.70
123.58
118.27
114.21
113.92
113.90
113.58
112.32
77.51
77.08
76.66
F
N
N
Se
4i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


8.14
8.11
7.92
7.90
7.48
7.40
7.39
7.26
7.12
7.11
6.73
6.70
3.90
2.45
0.00
O
N
N
Se
1.00
1.00
0.98
1.05
1.06
1.02
3.07
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

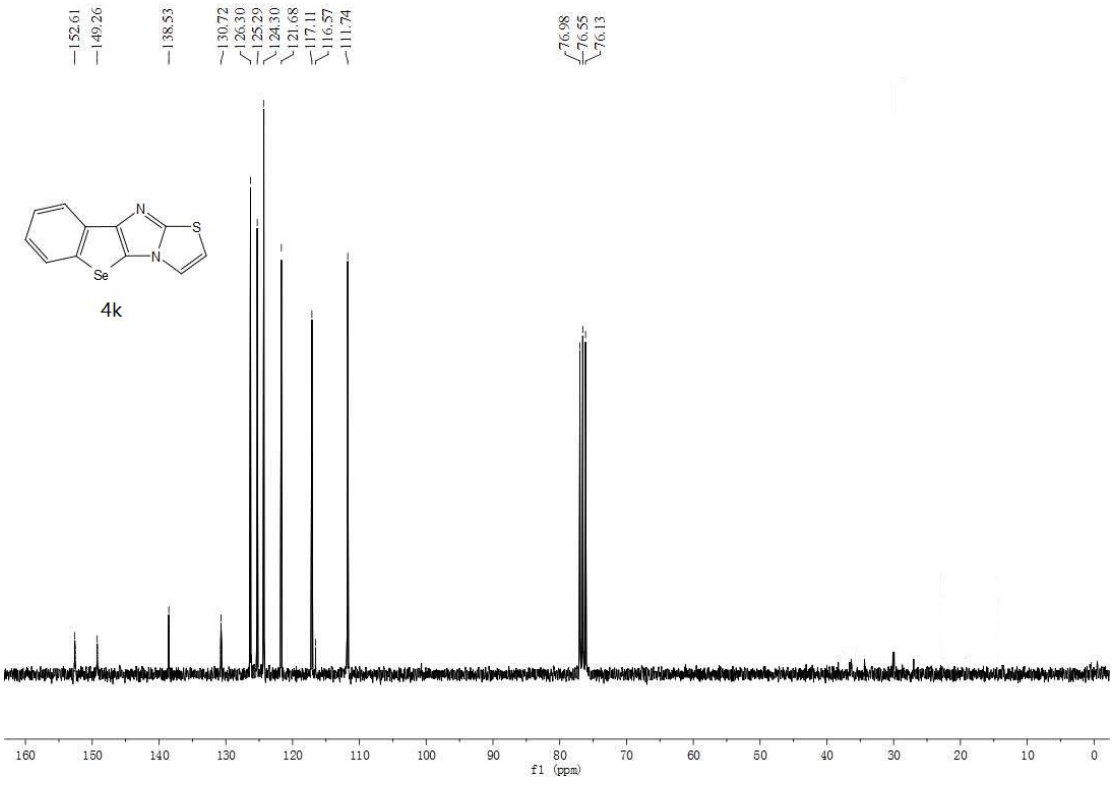
4j


178.52
157.97
149.76
147.24
141.45
135.23
124.55
123.59
123.49
116.34
114.79
113.58
111.29
77.55
77.12
76.70
55.64
21.45
O
N
N
Se
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

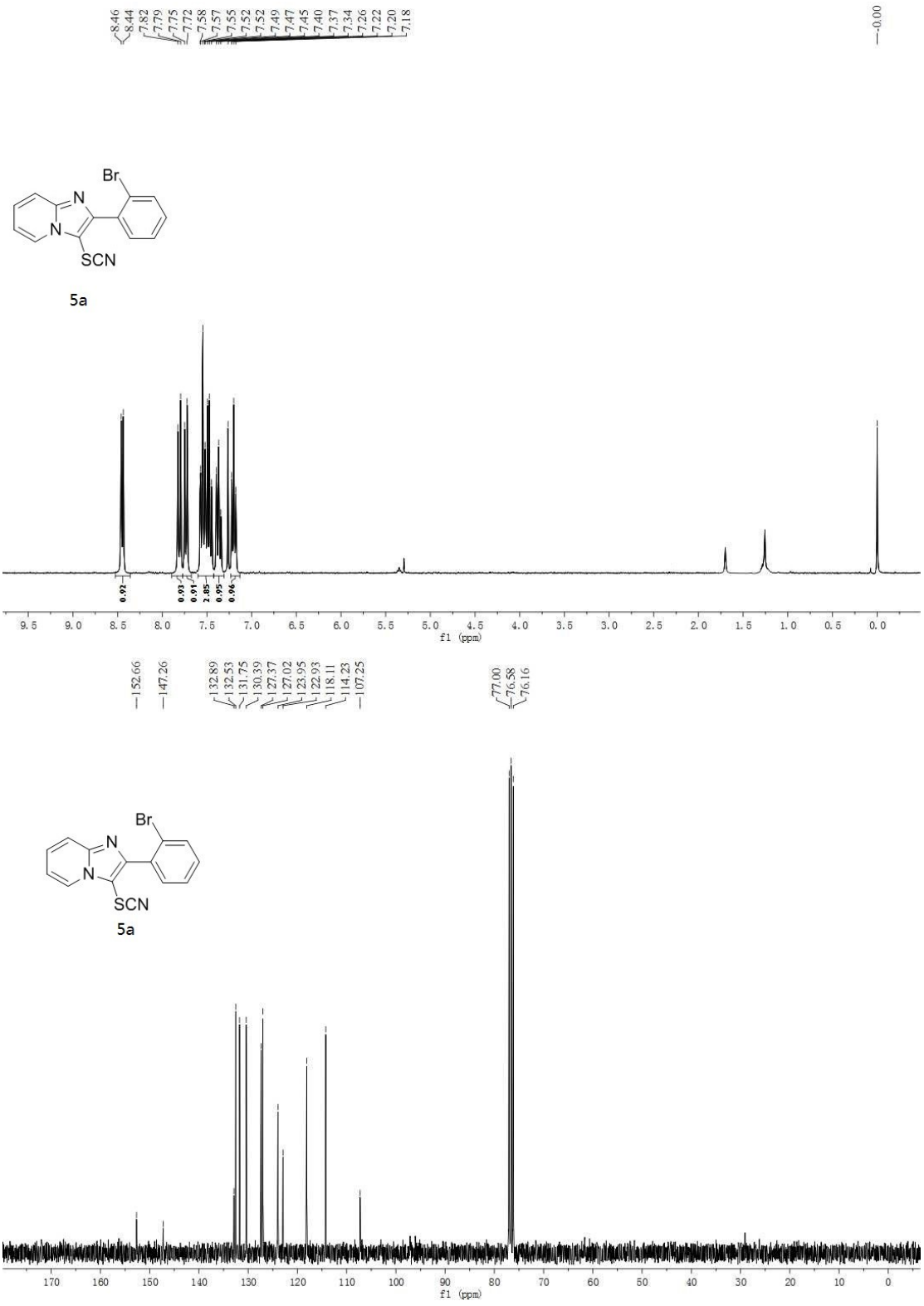
4j


8.14
8.11
7.83
7.81
7.48
7.46
7.28
6.92
6.90
0.00
N
S
N
Se
1.01
0.93
1.98
1.14
0.91
f1 (ppm)

4k


152.61
149.26
138.53
130.72
126.30
125.29
124.30
121.68
117.11
116.57
111.74
76.98
76.55
76.13
N
S
N
Se
f1 (ppm)

4k


8.46
8.44
7.82
7.79
7.75
7.72
7.58
7.57
7.55
7.52
7.52
7.49
7.47
7.45
7.40
7.37
7.34
7.26
7.22
7.20
7.18
0.00
Br
N
N
SCN
5a
0.92
0.93
0.91
2.85
0.95
0.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
152.66
147.26
132.89
132.53
131.75
130.39
127.37
127.02
123.95
122.93
118.11
114.23
107.25
77.00
76.58
76.16
Br
N
N
SCN
5a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)