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Supporting Information

Using SeO_2 as a Selenium Source to Make RSe-Substituted Aniline and Imidazo[1,2-*a*]pyridine Derivatives

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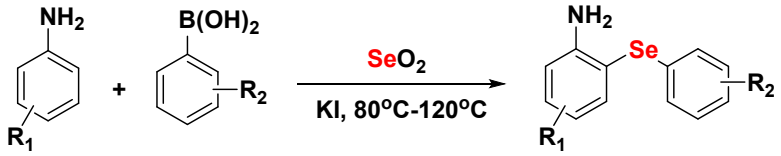
General Information

All reactions were carried out in round-bottom flasks; stirring was achieved with an oven-dried magnetic stirring bar. Solvents were purified by standard methods unless otherwise noted. Commercially available reagents were purchased from Aladdin Company in China and used throughout without further purification other than those detailed below. Flash column chromatography was performed on silica gel (200-300 mesh). All reactions were monitored by TLC analysis. Deuterated solvents were purchased from Cambridge Isotope laboratories. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz respectively. HRMS spectrometry (LC-HRMS) was recorded on a LXQ Spectrometer (Thermo Scientific) operating on ESI-TOF (MeOH as a solvent).

Experimental Procedure

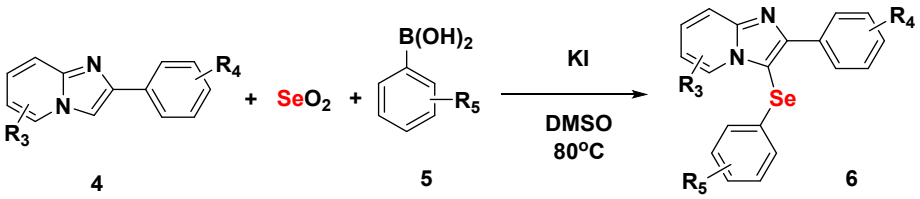
General procedure for the syntheses of compounds 3a-3o



1 2 3

Arylaniline (0.5 mmol, 1.0 equiv.), SeO_2 (1.2 equiv.), phenylboronic acid (1.2 equiv.) and KI (1.0 equiv.) were added to a round bottom flask with DMSO (0.5 mL). The mixture was stirred at 80℃or 120℃under reflux. After 12 hrs, the reaction was cooled to room temperature, extracted with ethyl acetate, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by silica gel flash chromatography (petroleum ether : EtOAc = 100: 1) to give product **3**.

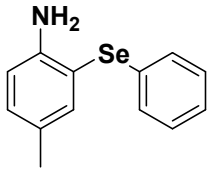
General procedure for the syntheses of compounds 6a-6i



Imidazo[1,2-a]pyridine (0.5 mmol, 1.0 equiv.), SeO_2 (1.2 equiv.), phenylboronic acid (1.2 equiv.) and KI (1.0 equiv.) were added to a round bottom flask with DMSO (0.5 mL). The mixture was stirred at 80℃under reflux. After 12 hrs, the reaction was cooled to room temperature, extracted with ethyl acetate, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by silica gel flash chromatography (petroleum ether : EtOAc = 15:1) to give product **6**.

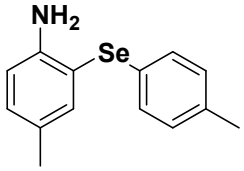
Characterization data of the products

4-Methyl-2-(phenylselanyl)aniline (3a)



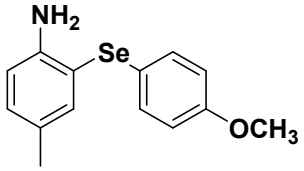
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 2.1 Hz, 1H), 7.32 - 7.15 (m, 5H), 7.07 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.76 (d, *J* = 8.1 Hz, 1H), 4.17 (s, 2H), 2.26 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 146.18, 138.64, 131.85, 131.78, 129.28, 129.23, 128.18, 126.11, 115.11, 112.72, 20.15. **IR**: 3452, 2918, 1620, 1491, 1145, 814, 738 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{13}H_{14}NSe^{+}$ 264.0286 $(M+H)^{+}$, found 264.0282.

4-Methyl-2-(p-tolylselanyl)aniline (3b)



^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 2.1 Hz, 1H), 7.23 (d, *J* = 8.2 Hz, 2H), 7.08 (dd, *J* = 8.2, 2.6 Hz, 3H), 6.76 (d, *J* = 8.1 Hz, 1H), 4.16 (s, 2H), 2.34 (s, 3H), 2.29 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 146.00, 138.34, 136.13, 131.53, 130.08, 129.82, 128.12, 127.84, 115.11, 113.41, 21.02 , 20.19. **IR**: 3452, 3061, 2971, 1748, 1608, 1448, 1259, 1071, 814, 710 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_{16}NSe^{+}$ 278.0442 $(M+H)^{+}$, found 278.0435.

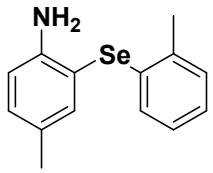
2-((4-Methoxyphenyl)selanyl)-4-methylaniline (3c)



^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.40 (dd, *J* = 2.0, 0.9 Hz, 1H), 7.34 - 7.26 (m, 2H), 7.03 (ddd, *J* = 8.0, 2.1, 0.8 Hz, 1H), 6.85 - 6.77 (m, 2H), 6.72 (d, *J* = 8.1 Hz, 1H), 4.16 (s, 2H), 3.79 (s, 3H), 2.26 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 158.78,

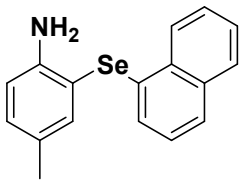
145.66, 137.76, 132.14, 131.24, 128.14, 121.38, 115.15, 115.07, 114.45, 55.29, 20.20. **IR:** 3467, 2915, 1548, 1469, 1217, 1142, 814, 778 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_{15}NNaOSe^+$ 316.0211 $(M+Na)^+$, found 316.0208.

4-Methyl-2-(o-tolylselanyl)aniline (3d)



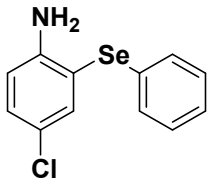
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.40 (dd, *J* = 2.0, 0.9 Hz, 1H), 7.18 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.15 - 7.05 (m, 2H), 7.04 - 6.97 (m, 1H), 6.91 (dd, *J* = 7.8, 1.3 Hz, 1H), 6.78 (d, *J* = 8.1 Hz, 1H), 4.13 (s, 2H), 2.44 (s, 3H), 2.27 (s, 3H).**^{13}C-NMR** (101 MHz, Chloroform-d) δ 146.45, 138.78, 136.87, 132.37, 131.78, 130.10, 128.33, 128.21, 126.70, 125.96, 115.12, 111.96, 21.50, 20.15. **IR:** 3436, 3014, 2945, 1579, 1492, 1234, 1045, 834, 747 cm^{-1} **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_{16}NSe^+$ 278.0442 $(M+H)^+$, found 278.0430.

4-Methyl-2-(naphthalen-1-ylselanyl)aniline (3e)



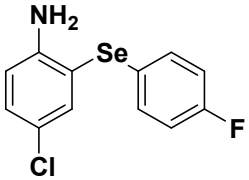
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.22 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.87 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.71 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.57 (dddd, *J* = 20.5, 8.1, 6.9, 1.4 Hz, 2H), 7.46 (d, *J* = 2.1 Hz, 1H), 7.34 - 7.25 (m, 1H), 7.21 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.10 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.78 (d, *J* = 8.1 Hz, 1H), 4.16 (s, 2H), 2.27 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 146.35, 138.70, 134.05, 132.59, 131.84, 130.53, 128.67, 128.40, 127.01, 126.79, 126.38, 126.19, 125.77, 115.26, 112.16, 20.22. **IR**: 3481, 3087, 2859, 1788, 1564, 1482, 1236, 972, 837, 743 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{17}H_{15}NNaSe^+$ 336.0262 $(M+Na)^+$, found 336.0259.

4-Chloro-2-(p-tolylselanyl)aniline (3f)



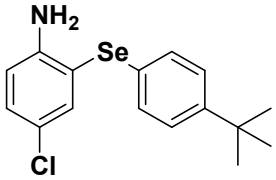
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, *J* = 2.4 Hz, 1H), 7.33 - 7.16 (m, 6H), 6.75 (d, *J* = 8.6 Hz, 1H), 4.30 (s, 2H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 147.06, 137.17, 130.80, 130.77, 129.82, 129.40, 126.67, 122.53, 115.85, 113.97. **IR**: 3487, 2948, 1769, 1575, 1488, 1230, 841, 735, 708 cm^{-1}.

4-Chloro-2-((4-fluorophenyl)selanyl)aniline (3g)



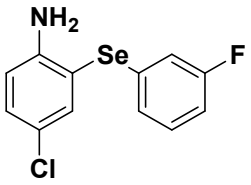
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 2.5 Hz, 1H), 7.36 - 7.25 (m, 2H), 7.18 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.03 - 6.93 (m, 2H), 6.74 (d, *J* = 8.6 Hz, 1H), 4.30 (s, 2H).**^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 163.35, 160.90, 146.80, 136.79, 132.23, 132.15, 130.76, 125.09, 125.05, 122.64, 116.69, 116.48, 115.93, 114.50. **^{19}F-NMR** (376 MHz, Chloroform-*d*) δ -115.26. **IR**: 3423, 2977, 1751, 1593, 1497, 1221, 1141, 835, 733, 715 cm^{-1}.

2-((4-(tert-Butyl)phenyl)selanyl)-4-chloroaniline (3h)



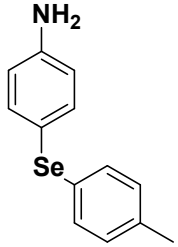
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 2.5 Hz, 1H), 7.42 - 7.03 (m, 5H), 6.74 (d, *J* = 8.6 Hz, 1H), 4.32 (s, 2H), 1.31 (s, 9H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 149.96, 147.00, 137.05, 130.57, 129.80, 127.08, 126.54, 122.51, 115.79, 114.39, 34.49, 31.25. **IR**: 3477, 3098, 2957, 1747, 1582, 1493, 1228, 1076, 840, 737, 715 cm^{-1}.

4-Chloro-2-((3-fluorophenyl)selanyl)aniline (3i)



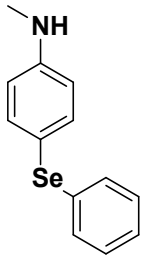
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 2.4 Hz, 1H), 7.27 - 7.15 (m, 2H), 7.05 (ddd, *J* = 7.9, 1.6, 1.0 Hz, 1H), 6.92 (dddd, *J* = 17.9, 8.6, 2.5, 1.3 Hz, 2H), 6.77 (d, *J* = 8.6 Hz, 1H), 4.32 (s, 2H).**^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 164.34, 161.86, 147.23, 137.47, 133.00, 132.93, 131.31, 130.57, 130.49, 124.95, 124.92, 122.60, 116.41, 116.18, 115.99, 113.66, 113.44, 112.87. **^{19}F-NMR** (376 MHz, Chloroform-*d*) δ -111.50. **IR:** 3421, 2956, 1737, 1564, 1482, 1225, 1123, 826, 745, 704 cm^{-1}.

4-(p-Tolylselanyl)aniline (3j)



^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.45 - 7.37 (m, 2H), 7.30 - 7.24 (m, 2H), 7.08 - 7.02 (m, 2H), 6.67 - 6.61 (m, 2H), 3.76 (s, 2H), 2.31 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 146.54, 136.46, 136.17, 133.99, 130.95, 129.88, 117.36, 115.99, 21.01. **IR:** 3459, 2919, 1544, 1482, 1287, 817, 792 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{13}H_{14}NSe^{+}$ 264.0286 $(M+H)^{+}$, found 264.0280.

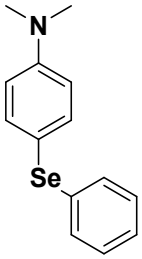
N-Methyl-4-(phenylselanyl)aniline (3k)



^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.54 - 7.44 (m, 2H), 7.35 - 7.27 (m, 2H), 7.25 - 7.15 (m, 3H), 6.64 - 6.56 (m, 2H), 3.88 (s, 1H), 2.88 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 149.58, 137.32, 134.57, 134.30, 129.80, 129.00, 125.84, 113.27,

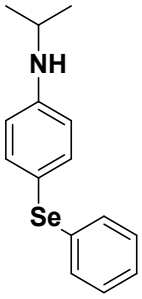
30.49. **IR**: 3428, 2892, 1607, 1532, 1188, 825, 737, 697 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{13}H_{14}NSe^+$ 284.0286 $(M+H)^+$, found 264.0277.

N,N-dimethyl-4-(phenylselanyl)aniline (3l)



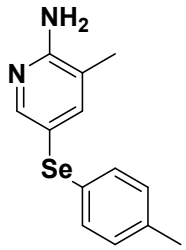
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.57 - 7.50 (m, 2H), 7.37 - 7.30 (m, 2H), 7.26 - 7.14 (m, 3H), 6.74 – 6.67 (m, 2H), 3.01 (s, 6H).**^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 150.55, 137.10, 134.60, 129.86, 129.00, 125.84, 113.82, 113.21, 40.31. **IR:** 3013, 2876, 1594, 1509, 1189, 824, 745, 703 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_{16}NSe^+$ 278.0442 $(M+H)^+$, found 278.0439.

N-isopropyl-4-(phenylselanyl)aniline (3m)



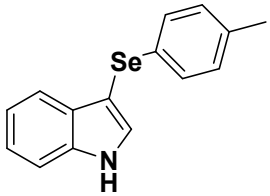
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.51 - 7.42 (m, 2H), 7.36 - 7.29 (m, 2H), 7.26 - 7.13 (m, 3H), 6.57 (d, J = 8.6 Hz, 2H), 3.67 (p, J = 6.3 Hz, 2H), 1.26 (d, J = 6.3 Hz, 6H).**^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 147.82, 137.40, 134.61, 129.82, 128.98, 125.83, 114.11, 113.97, 44.13, 22.94. **IR:** 3426, 2910, 1607, 1510, 1228, 828, 750, 708 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{15}H_{18}NSe^+$ 292.0599 $(M+H)^+$, found 292.0609.

3-Methyl-5-(p-tolylselanyl)pyridin-2-amine (3n)



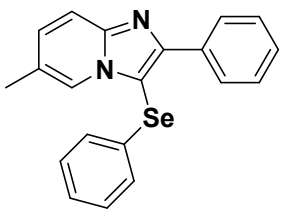
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.19 (d, *J* = 2.1 Hz, 1H), 7.51 (dd, *J* = 2.1, 1.0 Hz, 1H), 7.32 - 7.21 (m, 2H), 7.05 (d, *J* = 7.8 Hz, 2H), 4.61 (s, 2H), 2.31 (s, 3H), 2.11 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 156.97, 151.55, 144.47, 136.49, 130.91, 129.96, 129.14, 117.64, 114.49, 21.00, 16.98. **IR:** 3468, 2960, 1752, 1665, 1490, 1204, 831, 747 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{13}H_{15}N_2Se^+$ 279.0395 $(M+H)^+$, found 279.0403.

3-(p-Tolylselanyl)-1H-indole (3o)



^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.41 (s, 1H), 7.67 (dq, *J* = 7.9, 0.9 Hz, 1H), 7.51 - 7.42 (m, 2H), 7.29 (td, *J* = 7.4, 1.2 Hz, 1H), 7.26 - 7.13 (m, 3H), 7.02 - 6.91 (m, 2H), 2.27 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 136.38, 135.49, 130.95, 129.99, 129.76, 129.09, 122.87, 120.79, 120.41, 111.30, 98.72, 20.93. **IR:** 3482, 2985, 1762, 1560, 1497, 1225, 844, 713 cm^{-1}. **HRMS** (ESI-TOF) m/z calculated for $C_{15}H_{13}NNaSe^+$ 310.0105 $(M+H)^+$, found 310.0102.

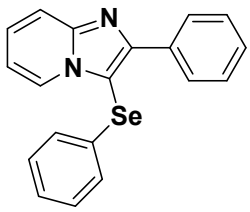
6-Methyl-2-phenyl-3-(phenylselanyl)imidazo[1,2-a]pyridine (6a)



^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.23 - 8.09 (m, 3H), 7.64 (dd, *J* = 9.1, 1.0 Hz, 1H), 7.51 - 7.41 (m, 2H), 7.41 - 7.35 (m, 1H), 7.25 - 7.15 (m, 4H), 7.16 - 7.06 (m, 2H), 2.35 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 151.70, 146.81, 133.93, 131.30, 129.66, 129.57, 128.65, 128.30, 128.25, 128.04, 126.54, 123.31, 122.77, 116.88,

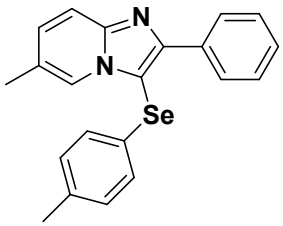
102.29, 18.40. **IR:** 3068, 2362, 1797, 1577, 1444, 1328, 1249, 819, 641 cm^{-1}; **HRMS** (ESI-TOF) m/z calculated for $C_{20}H_{17}N_2Se^+$ 365.0551 $(M+H)^+$, found 365.0550.

2-Phenyl-3-(phenylselanyl)imidazo[1,2-a]pyridine (6b)



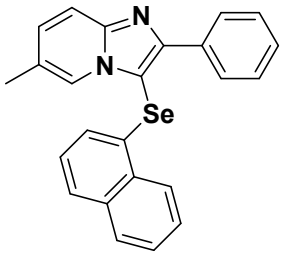
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.37 (dt, *J* = 6.8, 1.2 Hz, 1H), 8.24 - 8.13 (m, 2H), 7.74 (dt, *J* = 9.0, 1.1 Hz, 1H), 7.52 - 7.43 (m, 2H), 7.44 - 7.37 (m, 1H), 7.33 (ddd, *J* = 9.0, 6.7, 1.3 Hz, 1H), 7.20 (qd, *J* = 4.4, 1.5 Hz, 3H), 7.17 - 7.07 (m, 2H), 6.87 (td, *J* = 6.8, 1.2 Hz, 1H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 151.85, 147.76, 133.79, 130.91, 129.68, 128.76, 128.45, 128.31, 128.23, 126.68, 126.44, 125.62, 117.54, 112.99, 102.85. **IR:** 2932, 2362, 1645, 1578, 1441, 1349, 1228, 741, 690 cm^{-1}; **HRMS** (ESI-TOF) m/z calculated for $C_{19}H_{15}N_2Se^+$ 351.0395 $(M+H)^+$, found 351.0397.

6-Methyl-2-phenyl-3-(p-tolylselanyl)imidazo[1,2-a]pyridine (6c)



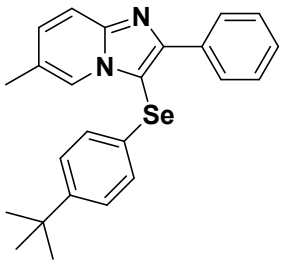
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.17 (dt, *J* = 8.1, 1.5 Hz, 3H), 7.63 (dd, *J* = 9.1, 0.9 Hz, 1H), 7.49 - 7.41 (m, 2H), 7.42 - 7.32 (m, 1H), 7.17 (dd, *J* = 9.1, 1.8 Hz, 1H), 7.10 - 6.95 (m, 4H), 2.34 (s, 3H), 2.28 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 151.47, 146.72, 136.52, 134.00, 130.44, 129.47, 128.66, 128.28, 128.23, 127.36, 123.34, 122.67, 116.83, 102.68, 20.94, 18.41. **IR:** 2928, 2854, 1623, 1576, 1474, 1340, 1188, 803, 737 cm^{-1}; **HRMS** (ESI-TOF) m/z calculated for $C_{20}H_{16}N_2OSe^+$ 379.0708 $(M+H)^+$, found 379.0712.

6-Methyl-3-(naphthalen-1-ylselanyl)-2-phenylimidazo[1,2-a]pyridine (6d)



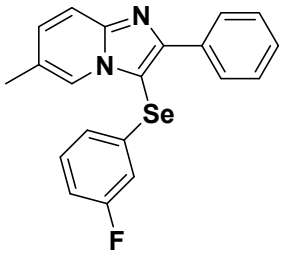
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.24 - 8.07 (m, 4H), 7.89 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.74 - 7.65 (m, 2H), 7.60 (dddd, *J* = 17.9, 8.1, 6.9, 1.4 Hz, 2H), 7.48 - 7.33 (m, 3H), 7.23 - 7.12 (m, 2H), 6.89 (dd, *J* = 7.4, 1.1 Hz, 1H), 2.28 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 152.41, 147.17, 134.29, 133.90, 132.17, 129.66, 129.59, 128.80, 128.66, 128.38, 128.31, 127.00, 126.58, 126.44, 126.37, 125.19, 125.07, 123.44, 122.87, 116.93, 100.89, 18.34. **IR:** 3058, 1827, 1501, 1379, 1242, 1064, 771, 693, 602 cm^{-1}; **HRMS** (ESI-TOF) m/z calculated for $C_{24}H_{19}N_2Se^+$ 415.0708 $(M+H)^+$, found 415.0710.

3-((4-(tert-Butyl)phenyl)selanyl)-6-methyl-2-phenylimidazo[1,2-a]pyridine (6e)



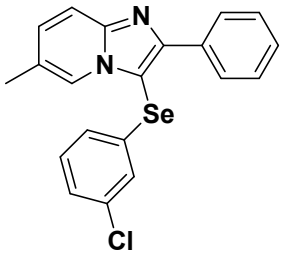
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.24 - 8.14 (m, 3H), 7.63 (dd, *J* = 9.0, 0.9 Hz, 1H), 7.48 - 7.42 (m, 2H), 7.39 (d, *J* = 7.3 Hz, 1H), 7.26 - 7.20 (m, 2H), 7.18 (dd, *J* = 9.1, 1.8 Hz, 1H), 7.10 - 7.03 (m, 2H), 2.35 (s, 3H), 1.27 (s, 9H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 151.49, 149.78, 146.73, 134.01, 129.48, 128.68, 128.45, 128.23, 127.94, 127.64, 126.76, 123.42, 122.65, 116.83, 102.61, 34.45, 31.22, 18.41. **IR**: 3052, 2930, 1488, 1346, 1279, 1082, 937, 789, 697 cm^{-1}; **HRMS (**ESI-TOF) m/z calculated for $C_{21}H_{19}N_2Se^+$ 421.1177 $(M+H)^+$, found 421.1173.

3-((3-Fluorophenyl)selanyl)-6-methyl-2-phenylimidazo[1,2-a]pyridine (6f)



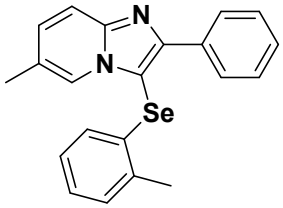
^{1}H-NMR (400 MHz, Chloroform-d) δ 8.20 - 8.03 (m, 3H), 7.66 (dd, J = 9.0, 0.9 Hz, 1H), 7.51 - 7.42 (m, 2H), 7.42 - 7.35 (m, 1H), 7.26 - 7.07 (m, 2H), 6.94 - 6.84 (m, 2H), 6.81 (ddd, J = 8.7, 2.5, 1.6 Hz, 1H), 2.35 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-d) δ 164.55, 162.07, 152.04, 146.97, 133.73, 133.43, 133.37, 130.93, 130.85, 129.82, 128.63, 128.45, 128.32, 123.47, 123.44, 123.15, 123.06, 117.01, 115.02, 114.79, 113.74, 113.53, 101.53, 18.42. **^{19}F-NMR** (376 MHz, Chloroform-*d*) δ -110.94 .**IR**: 2929, 1507, 1469, 1462, 1337, 1282, 1077, 812, 679 cm^{-1}; **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{16}BrN_2Se^+$ 383.0457 $(M+H)^+$, found 383.0461.

3-((3-Chlorophenyl)selanyl)-6-methyl-2-phenylimidazo[1,2-a]pyridine (6g)



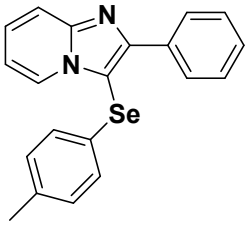
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.12 (dt, *J* = 8.2, 1.4 Hz, 3H), 7.66 (dd, *J* = 9.1, 0.9 Hz, 1H), 7.51 - 7.43 (m, 2H), 7.42 - 7.35 (m, 1H), 7.25 - 7.05 (m, 4H), 6.94 (dt, *J* = 7.6, 1.4 Hz, 1H), 2.35 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 152.10, 146.98, 135.52, 133.70, 133.20, 130.63, 129.86, 128.62, 128.47, 128.33, 127.62, 126.83, 125.89, 123.15, 123.09, 117.00, 101.42, 18.42.**IR**: 2379, 1682, 1567, 1470, 1345, 1218, 1034, 829, 693 cm^{-1}; **HRMS (**ESI-TOF) m/z calculated for $C_{19}H_{14}ClN_2Se^+$ 399.0162 $(M+H)^+$, found 399.0159.

6-Methyl-2-phenyl-3-(o-tolylselanyl)imidazo[1,2-a]pyridine (6h)



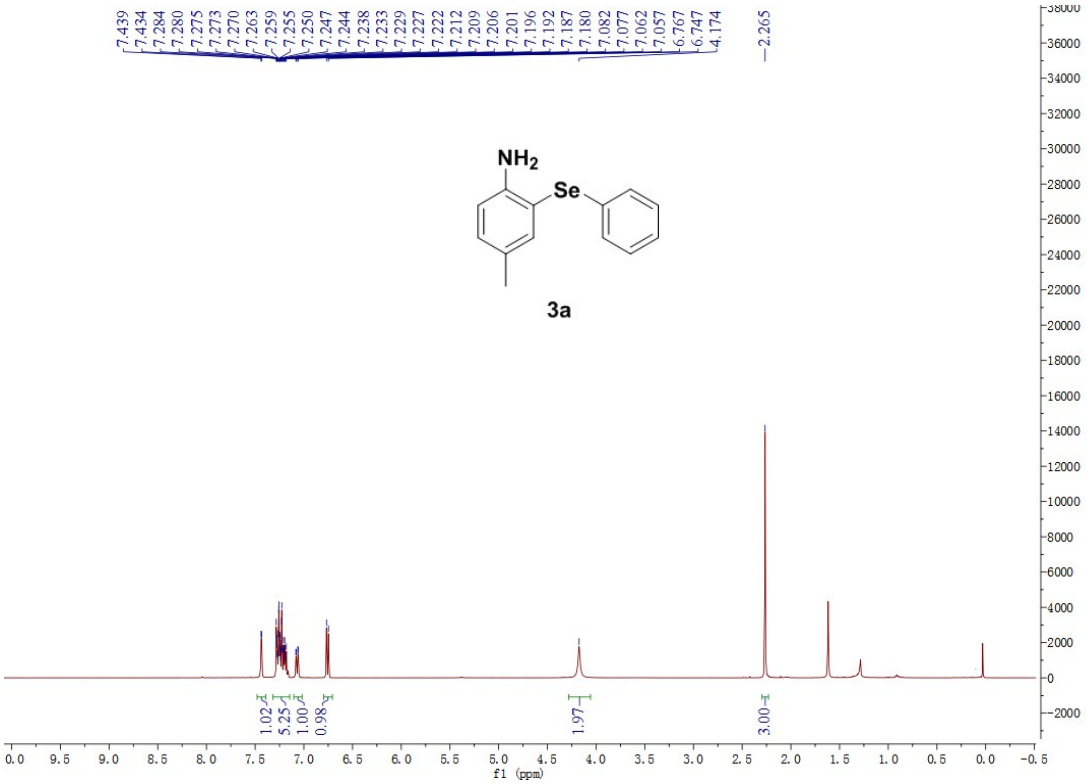
^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.11 (dt, *J* = 6.2, 1.4 Hz, 3H), 7.66 (dd, *J* = 9.0, 0.9 Hz, 1H), 7.50 - 7.41 (m, 2H), 7.41 - 7.33 (m, 1H), 7.21 (td, *J* = 9.1, 8.7, 1.6 Hz, 2H), 7.11 (td, *J* = 7.4, 1.3 Hz, 1H), 6.91 (td, *J* = 7.6, 1.4 Hz, 1H), 6.57 (dd, *J* = 7.9, 1.2 Hz, 1H), 2.51 (s, 3H), 2.34 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 152.21, 147.06, 136.35, 133.93, 131.82, 130.61, 129.60, 128.63, 128.30, 128.25, 127.17, 126.67, 126.29, 123.35, 122.80, 116.90, 101.22, 21.10, 18.41. **IR:** 2978, 2382, 2369, 1448, 1367, 1246, 1039, 779, 705 cm^{-1}; **HRMS** (ESI-TOF) m/z calculated for $C_{20}H_{17}N_2OSe^+$ 379.0708 $(M+H)^+$, found 379.0715.

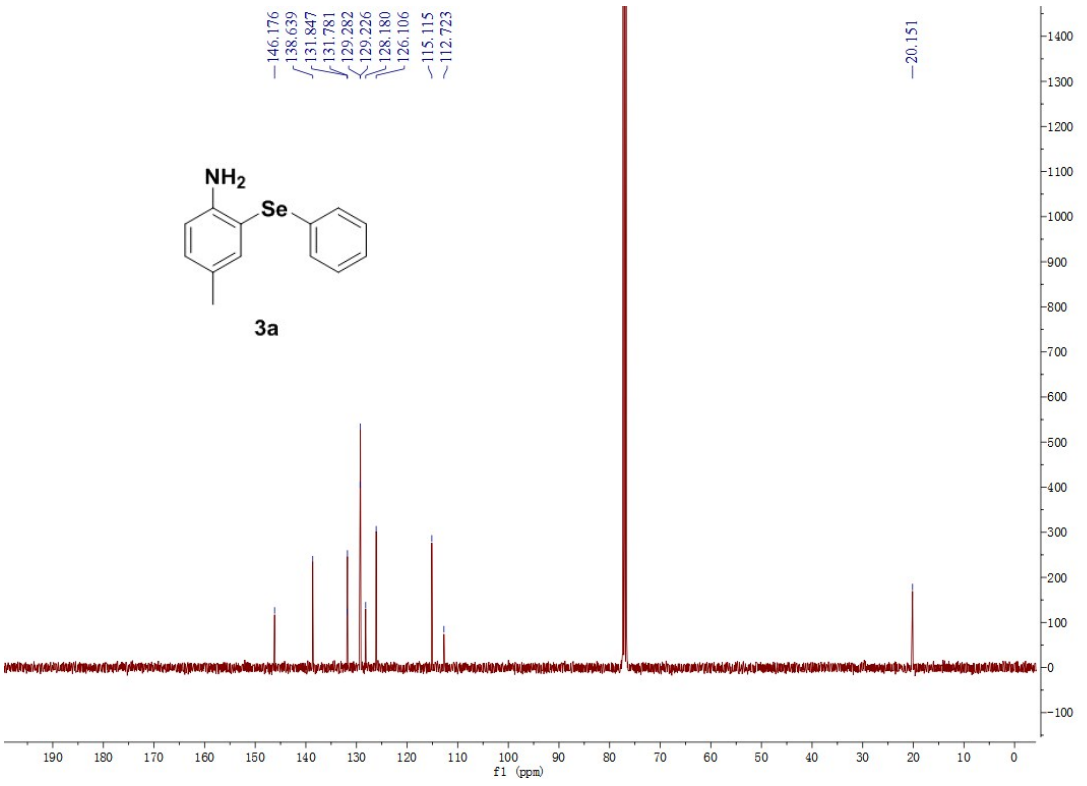
2-Phenyl-3-(p-tolylselanyl)imidazo[1,2-a]pyridine (6i)

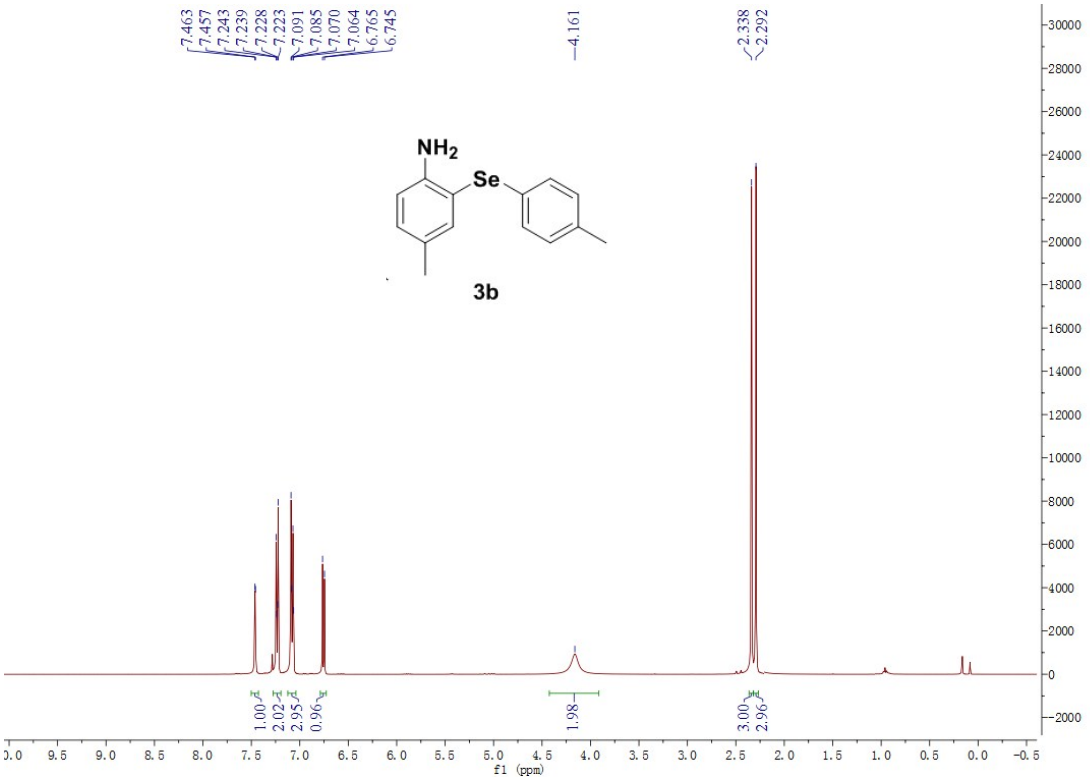


^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.38 (dt, *J* = 6.9, 1.2 Hz, 1H), 8.24 - 8.14 (m, 2H), 7.73 (dt, *J* = 9.0, 1.1 Hz, 1H), 7.51 - 7.44 (m, 2H), 7.44 - 7.38 (m, 1H), 7.36 - 7.30 (m, 1H), 7.09 - 6.99 (m, 4H), 6.87 (td, *J* = 6.8, 1.2 Hz, 1H), 2.27 (s, 3H). **^{13}C-NMR** (101 MHz, Chloroform-*d*) δ 151.61, 147.67, 136.68, 133.86, 130.46, 128.76, 128.54, 128.50, 128.28, 126.96, 126.32, 125.64, 117.50, 112.91, 103.23, 20.94. **IR:** 3072, 2945, 2367, 1467, 1324, 1227, 1015, 757, 681 cm^{-1}; **HRMS** (ESI-TOF) m/z calculated for $C_{19}H_{14}BrN_2Se^+$ 365.0051 $(M+H)^+$, found 365.0058.

^{1}H NMR and ^{13}C NMR spectra



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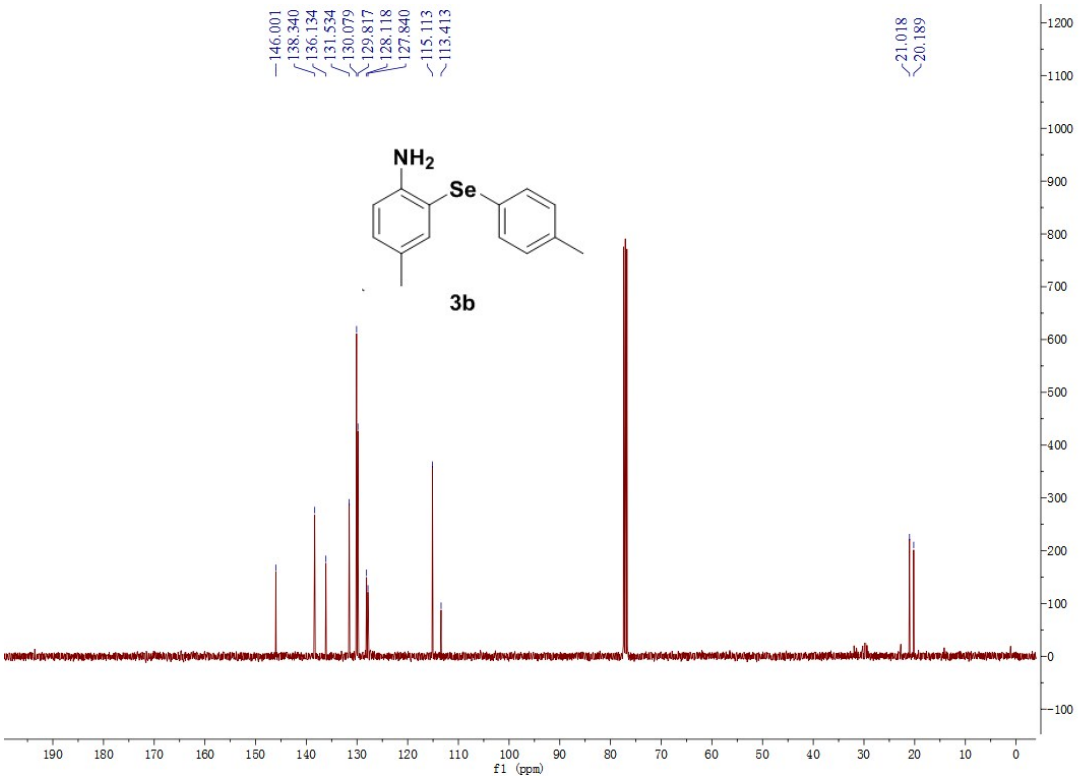
7.243
7.239
7.228
7.223
7.091
7.085
7.070
7.064
6.765
6.745
4.161
2.338
2.292
NH2
Se
3b
1.00
2.02
2.95
0.96
1.98
3.00
2.96
f1 (ppm)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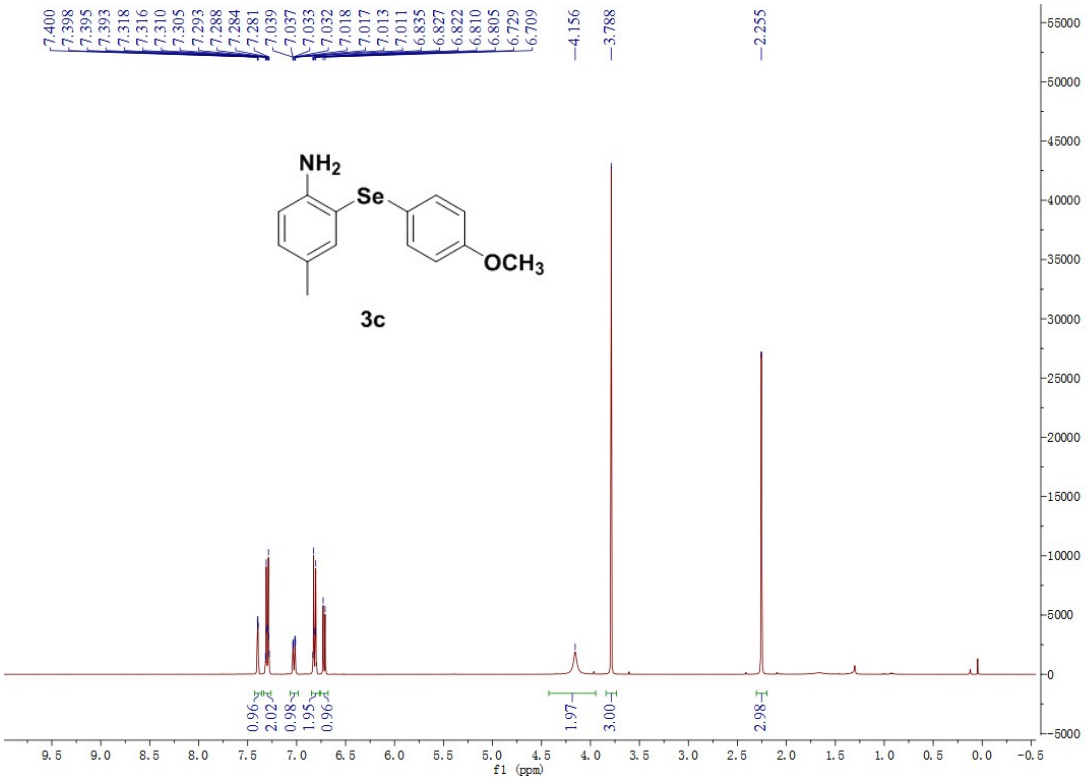
131.534
130.079
129.817
128.118
127.840
115.113
113.413
21.018
20.189
NH2
Se
3b
f1 (ppm)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7.393
7.318
7.316
7.310
7.305
7.293
7.288
7.284
7.281
7.039
7.037
7.033
7.032
7.018
7.017
7.013
7.011
6.835
6.827
6.822
6.810
6.805
6.729
6.709
4.156
3.788
2.255
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Se
OCH3
3c
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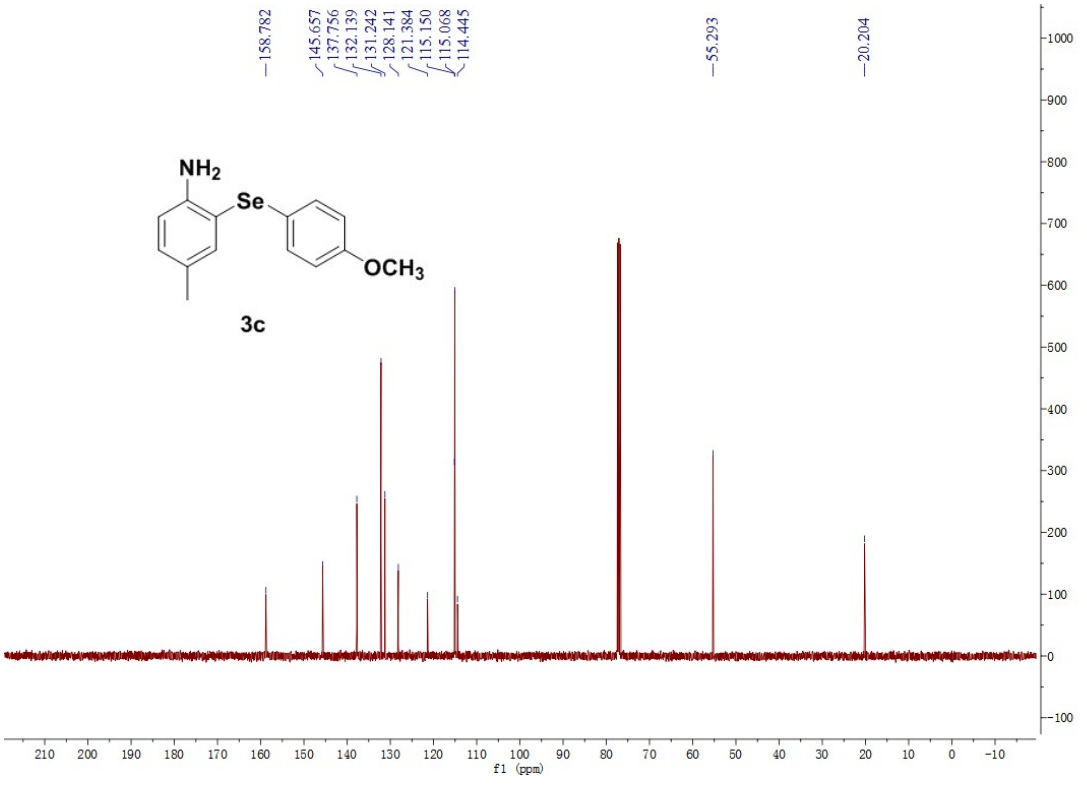
2.02
0.98
1.95
0.96
1.97
3.00
2.98
f1 (ppm)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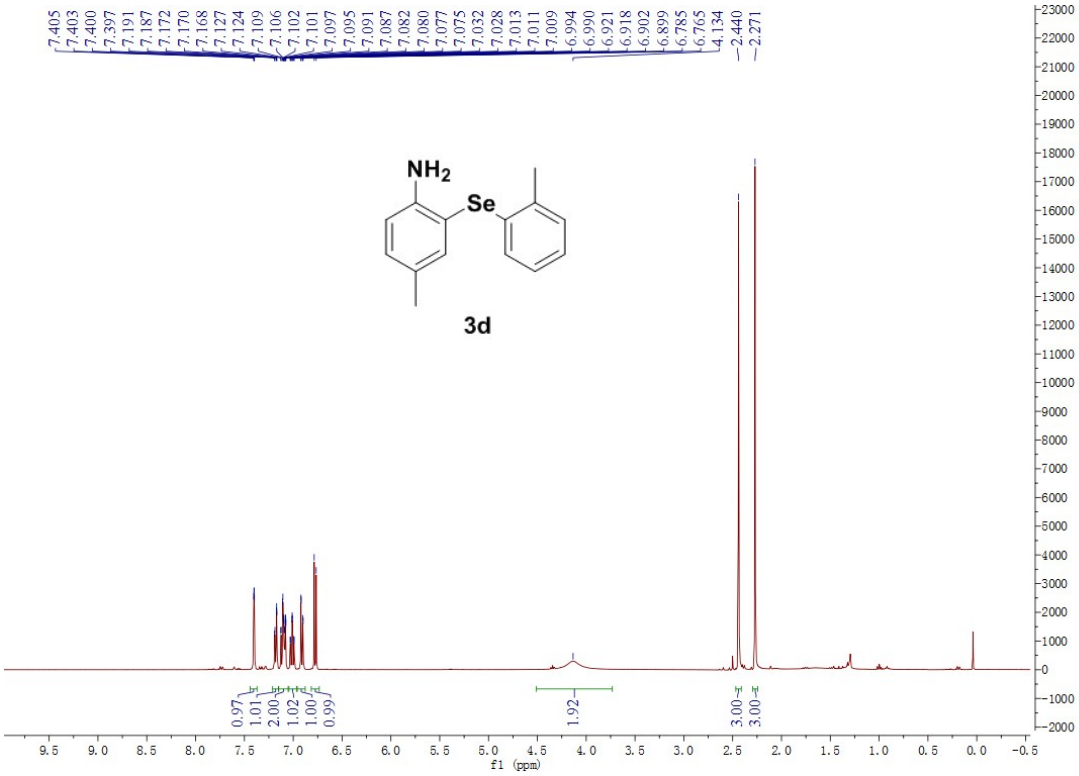
137.756
132.139
131.242
128.141
121.384
115.150
115.068
114.445
55.293
20.204
NH2
Se
OCH3
3c
f1 (ppm)


7.405
7.403
7.400
7.397
7.191
7.187
7.172
7.170
7.168
7.127
7.124
7.109
7.106
7.102
7.101
7.097
7.095
7.091
7.087
7.082
7.080
7.077
7.075
7.032
7.028
7.013
7.011
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6.990
6.921
6.918
6.902
6.899
6.785
6.765
4.134
2.440
2.271
NH2
Se
3d
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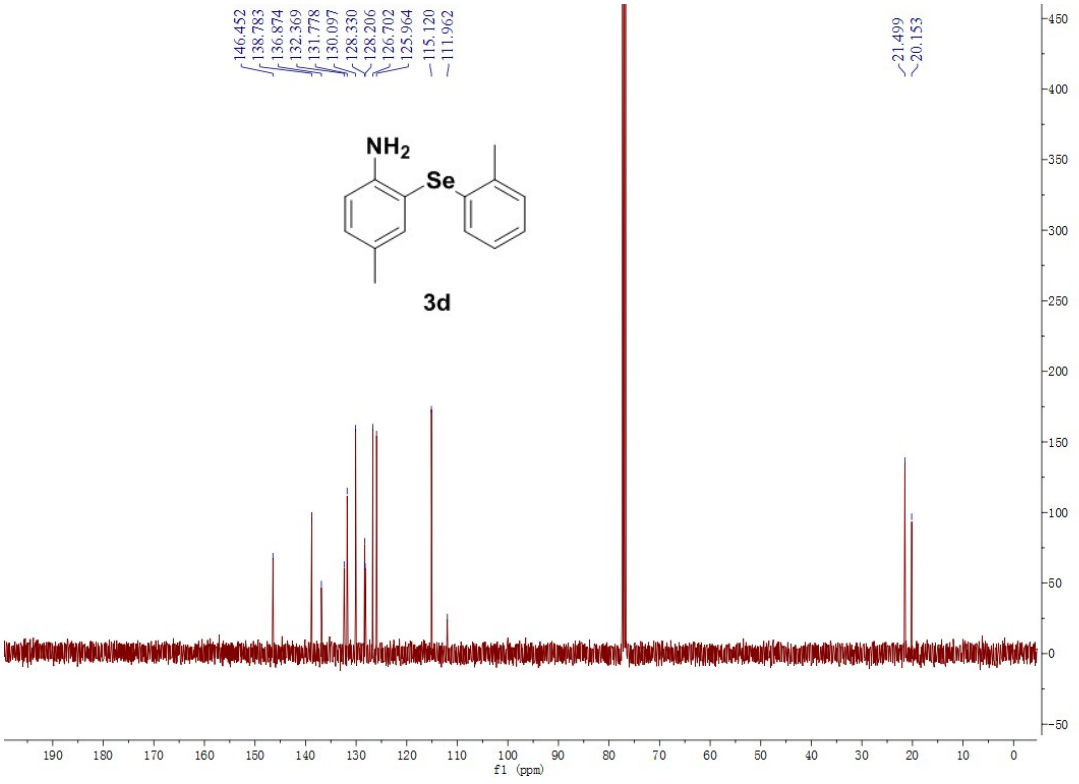
1.01
2.00
1.02
1.00
0.99
1.92
3.00
3.00
f1 (ppm)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130.097
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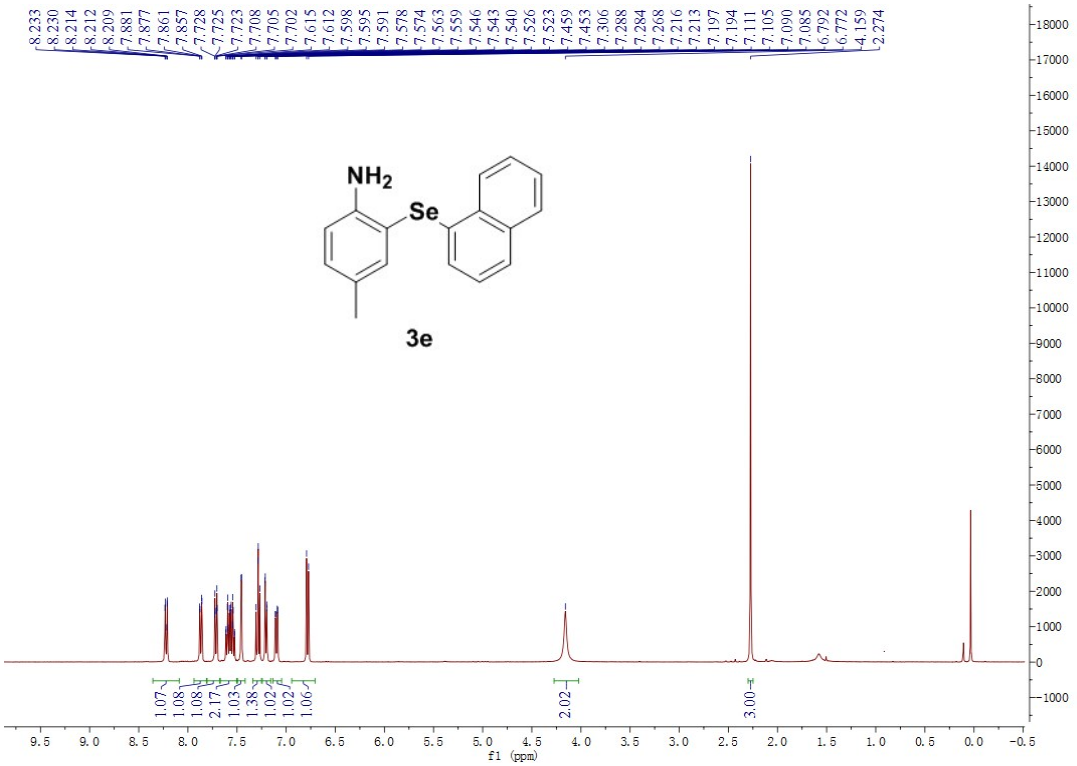
128.206
126.702
125.964
115.120
111.962
21.499
20.153
NH2
Se
3d
f1 (ppm)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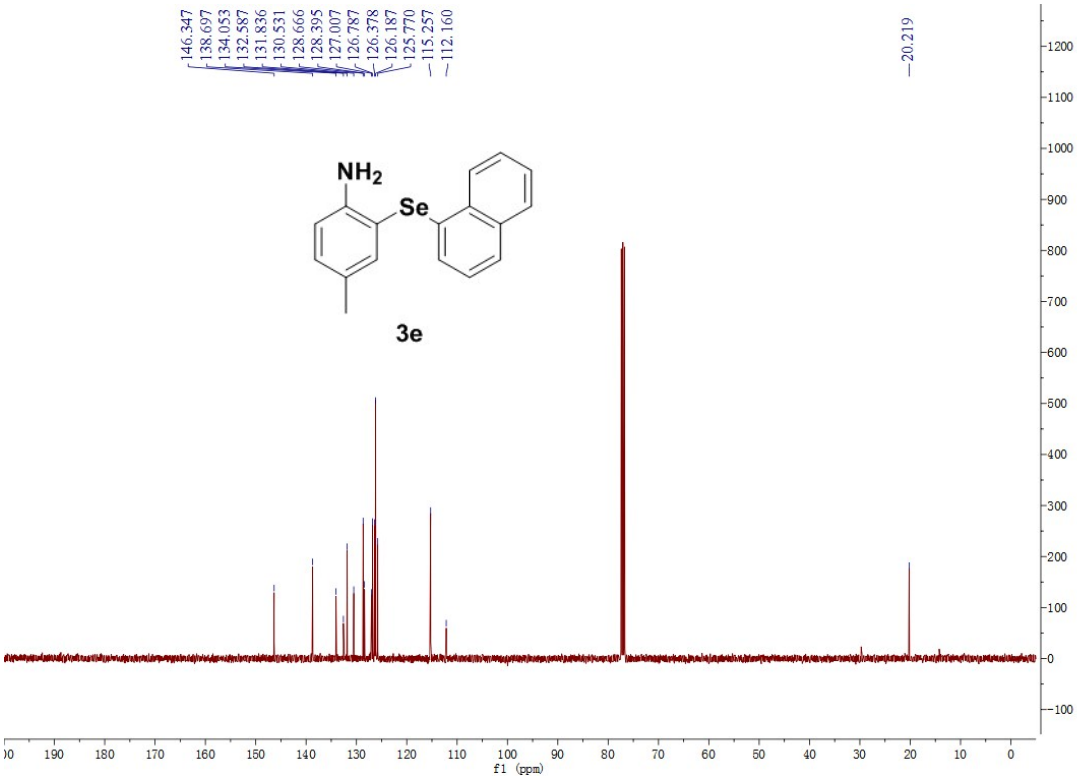
8.214
8.212
8.209
7.881
7.877
7.861
7.857
7.728
7.725
7.723
7.708
7.705
7.702
7.615
7.612
7.598
7.595
7.591
7.578
7.574
7.563
7.559
7.546
7.543
7.540
7.526
7.523
7.459
7.453
7.306
7.288
7.284
7.268
7.216
7.213
7.197
7.194
7.111
7.105
7.090
7.085
6.792
6.772
4.159
2.274
NH2
Se
3e
1.07
1.08
1.08
2.17
1.03
1.38
1.02
1.02
1.06
2.02
3.00
f1 (ppm)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134.053
132.587
131.836
130.531
128.666
128.395
127.007
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126.378
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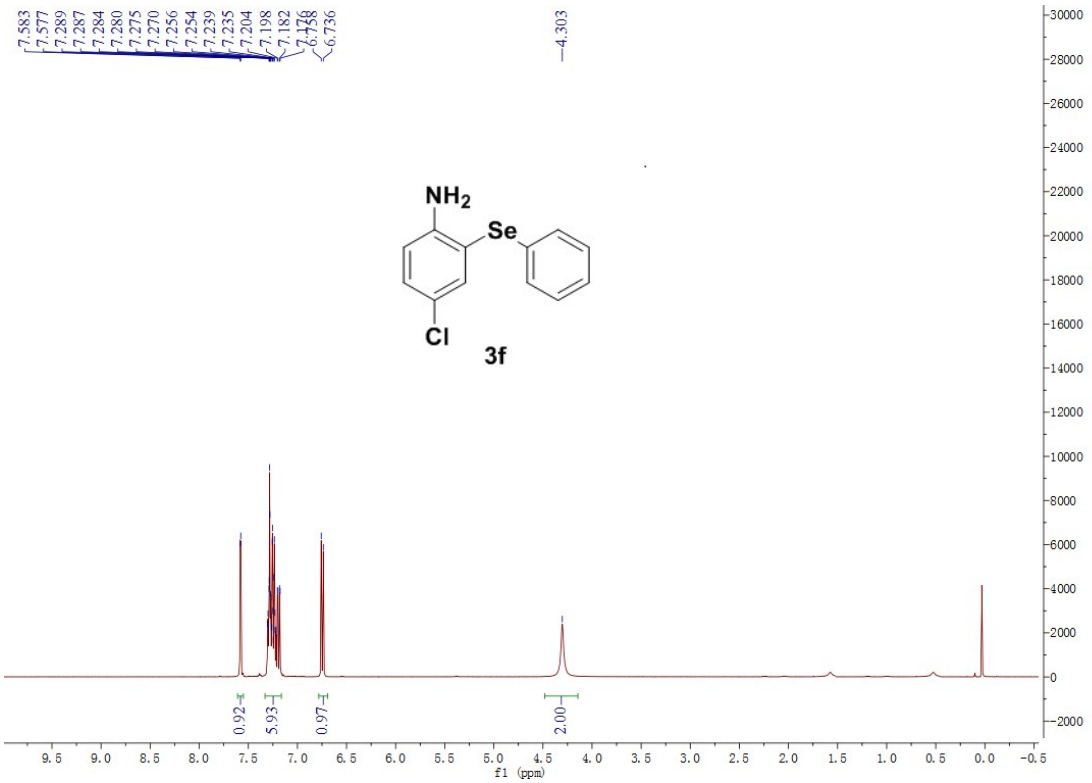
112.160
20.219
NH2
Se
3e
f1 (ppm)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7.289
7.287
7.284
7.280
7.275
7.270
7.256
7.254
7.239
7.235
7.204
7.198
7.182
6.758
6.736
4.303
NH2
Se
Cl
3f
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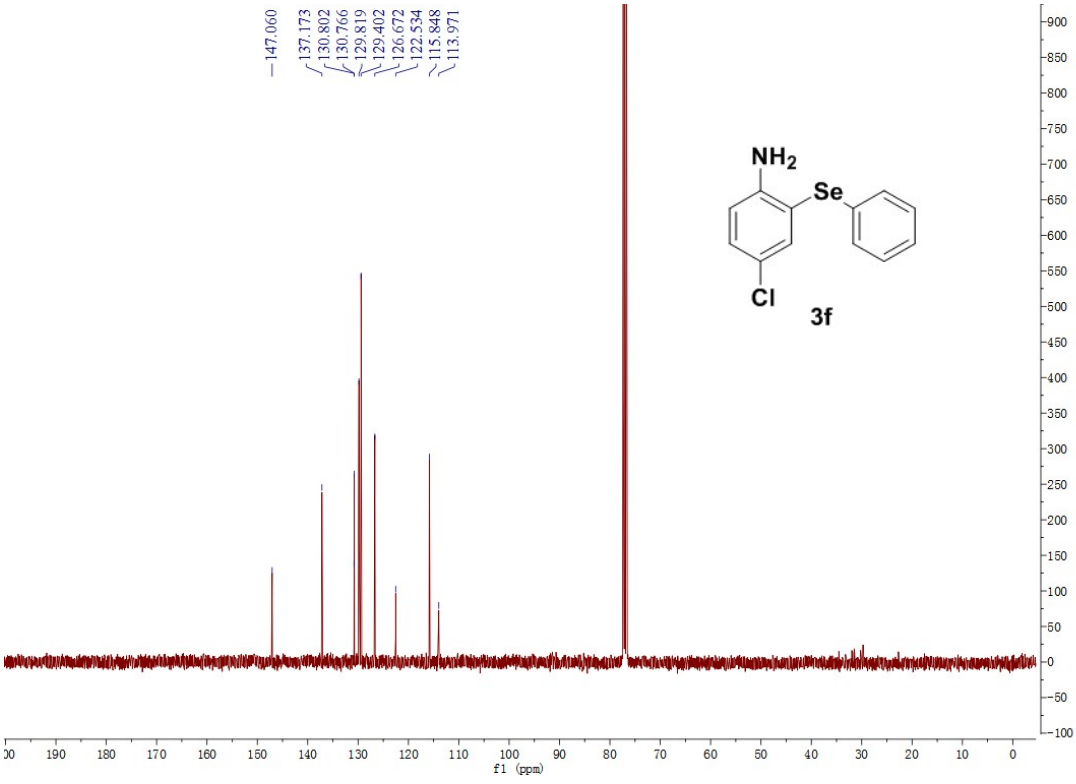
0.97
2.00
f1 (ppm)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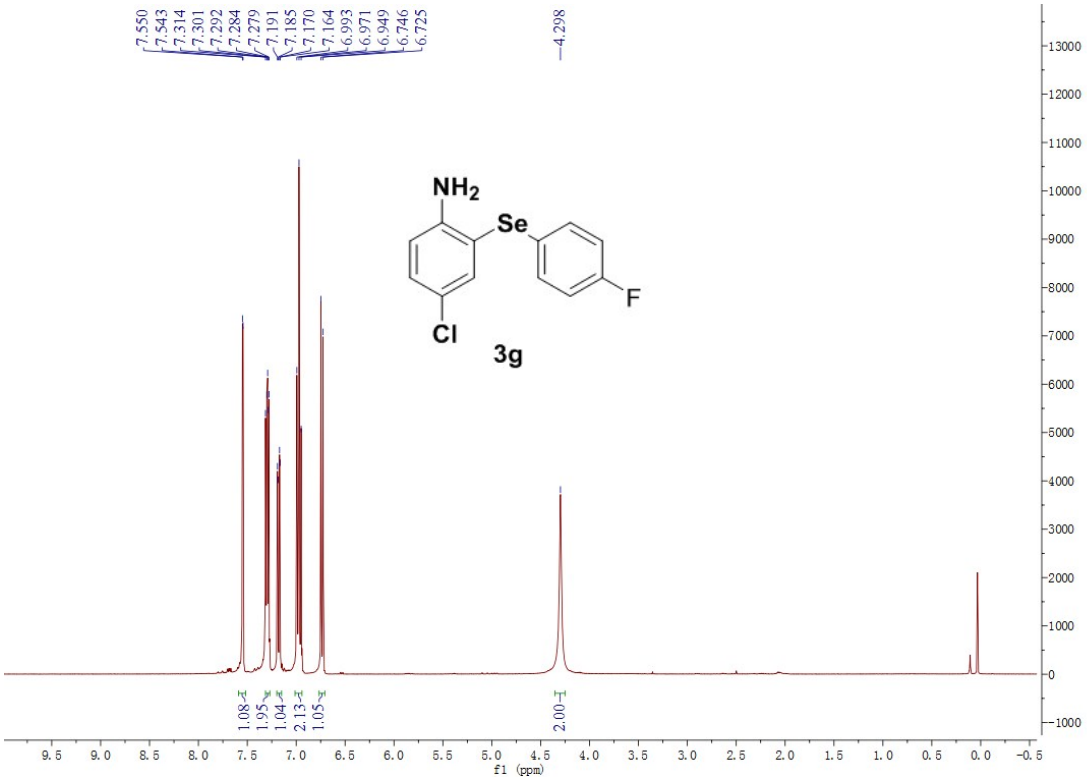
Cl
3f
f1 (ppm)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6.971
6.949
6.746
6.725
4.298
NH2
Se
F
Cl
3g
1.08
1.95
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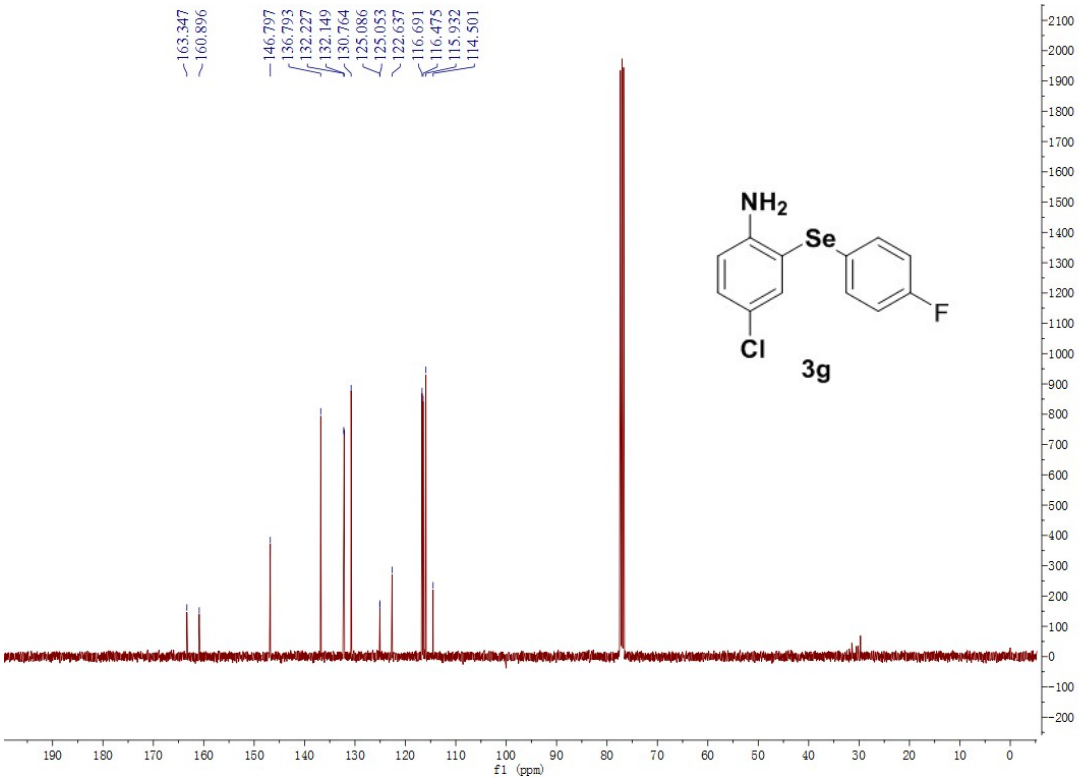
2.13
1.05
2.00
f1 (ppm)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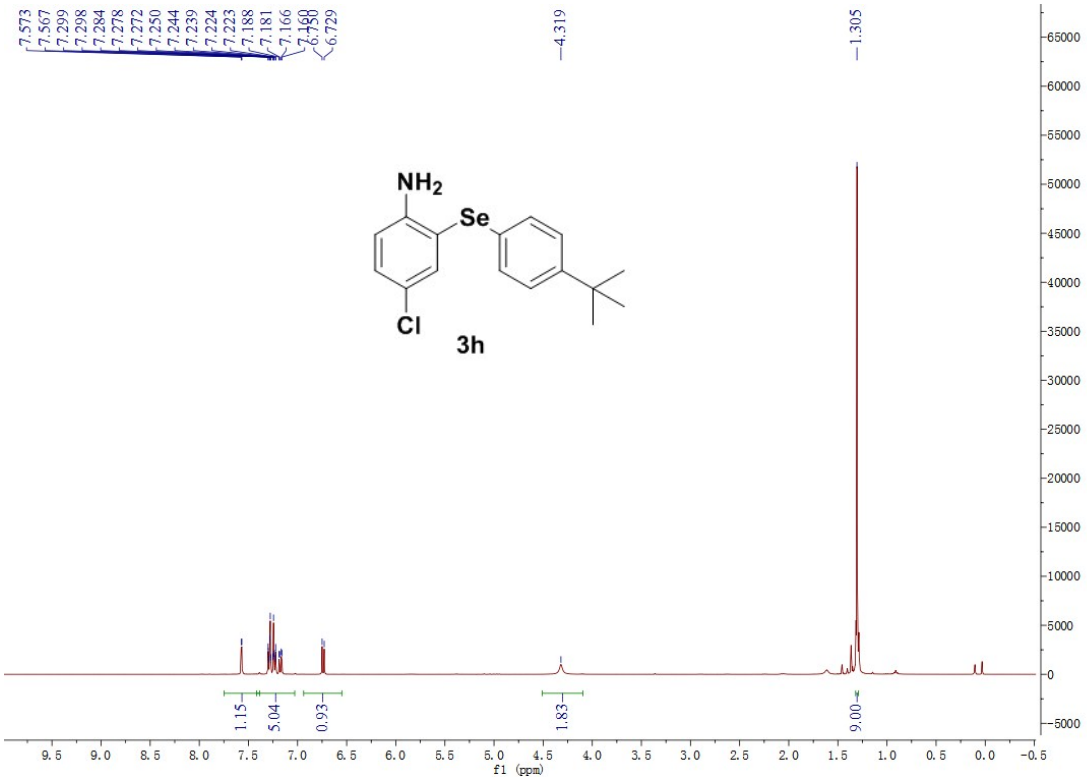
114.501
NH2
Se
F
Cl
3g
f1 (ppm)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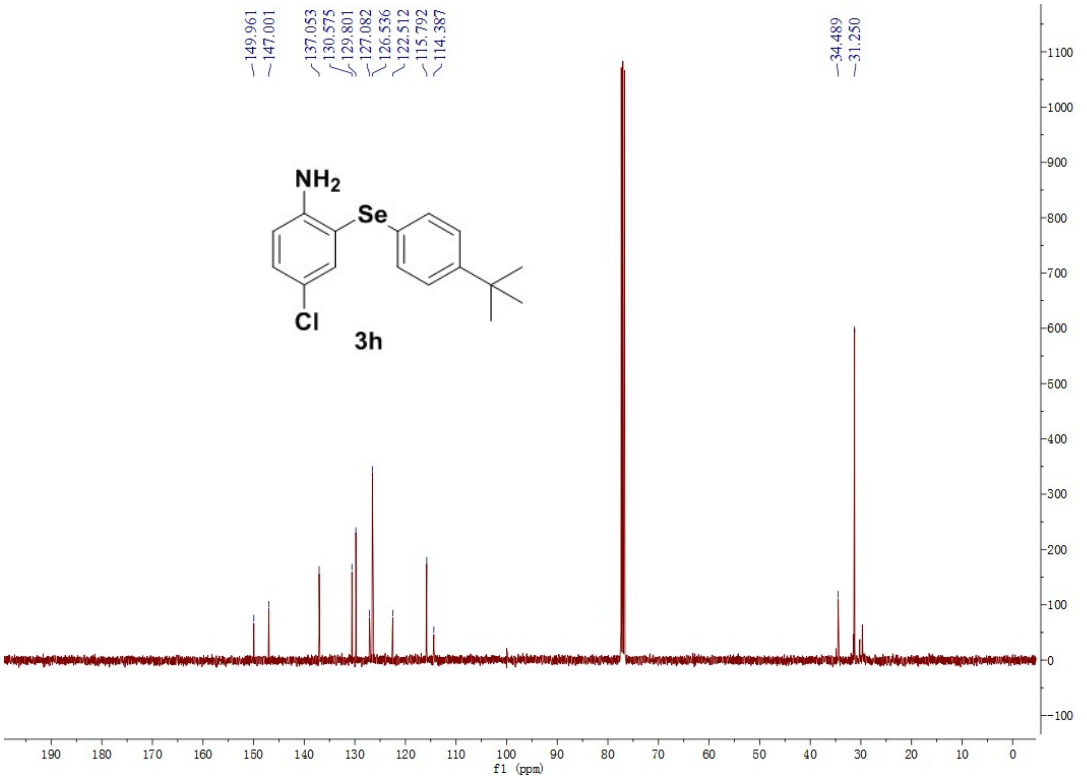
7.250
7.244
7.239
7.224
7.223
7.188
7.181
7.166
7.160
6.750
6.729
4.319
1.305
NH2
Se
Cl
3h
1.15
5.04
0.93
1.83
9.00
f1 (ppm)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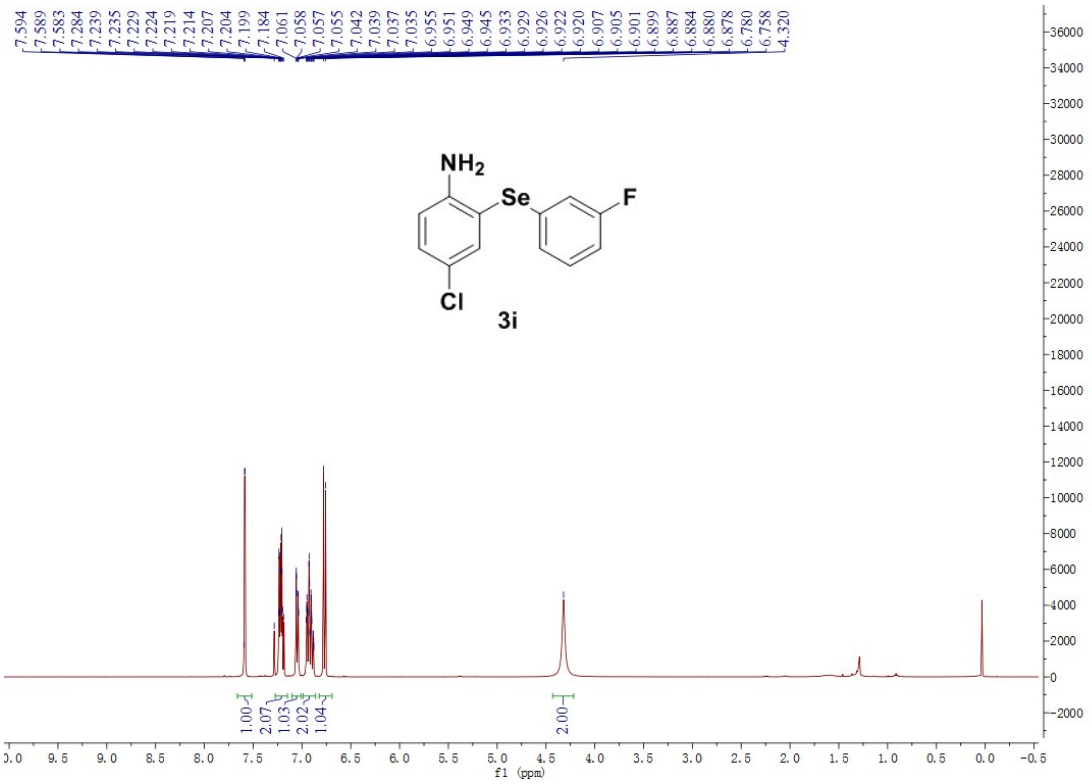
126.536
122.512
115.792
114.387
34.489
31.250
NH2
Se
Cl
3h
f1 (ppm)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7.057
7.055
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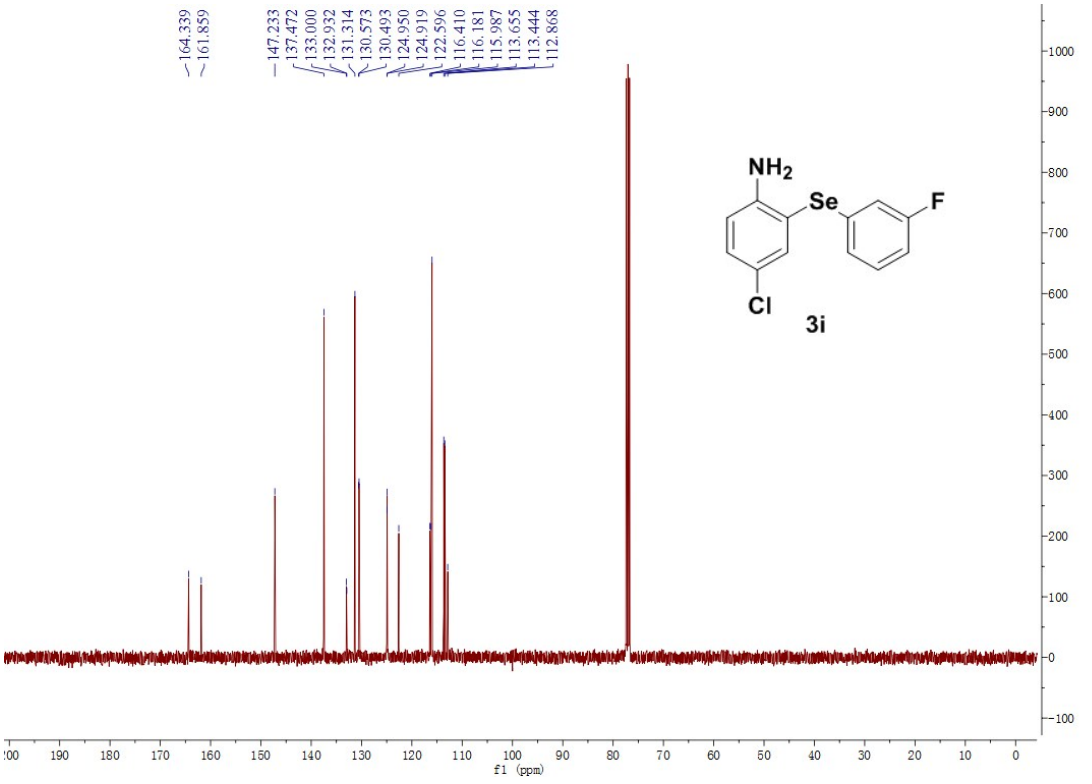
7.037
7.035
6.955
6.951
6.949
6.945
6.933
6.929
6.926
6.922
6.920
6.907
6.905
6.901
6.899
6.887
6.884
6.880
6.878
6.780
6.758
4.320
NH2
Se
F
Cl
3i
1.00
2.07
1.03
2.02
1.04
2.00
f1 (ppm)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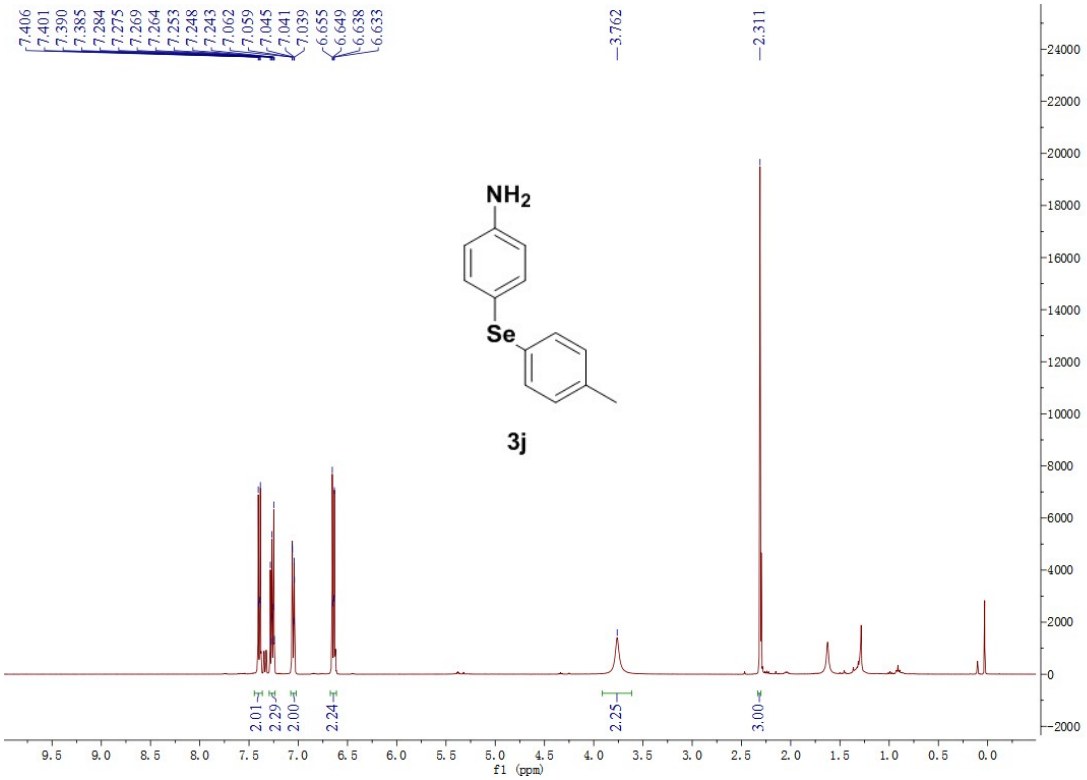
124.919
122.596
116.410
116.181
115.987
113.655
113.444
112.868
NH2
Se
F
Cl
3i
f1 (ppm)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7.390
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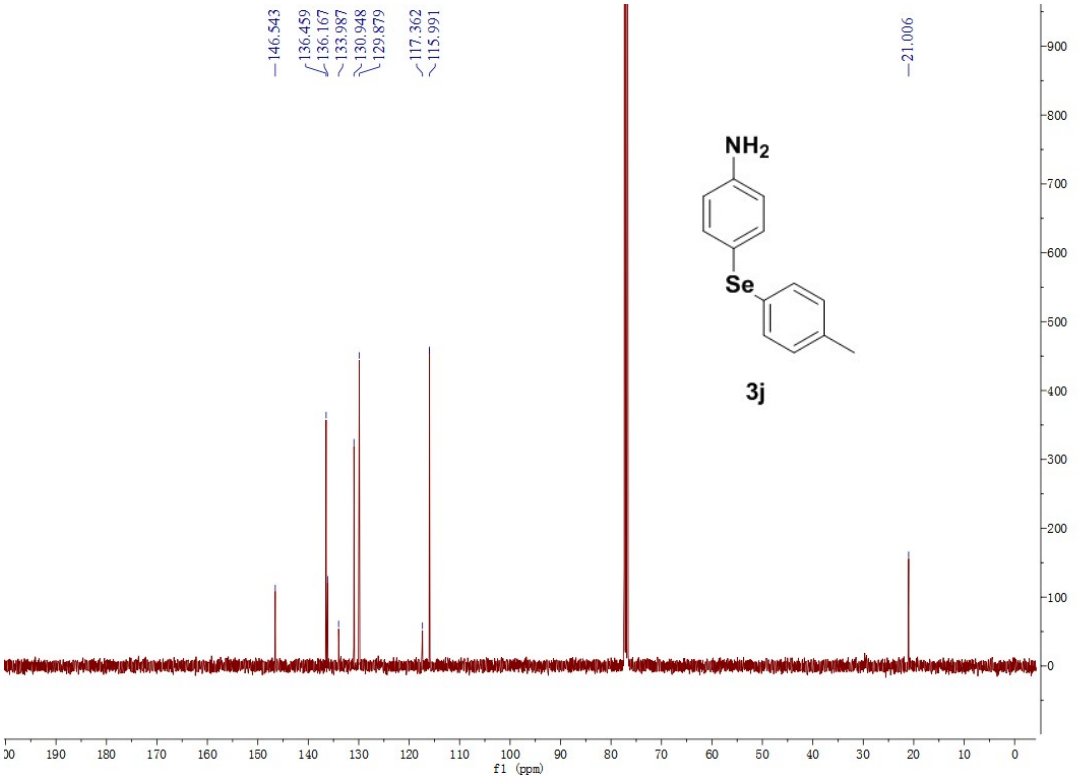
7.275
7.269
7.264
7.253
7.248
7.243
7.062
7.059
7.045
7.041
7.039
6.655
6.649
6.638
6.633
3.762
2.311
NH2
Se
3j
2.01
2.29
2.00
2.24
2.25
3.00
f1 (ppm)


146.543
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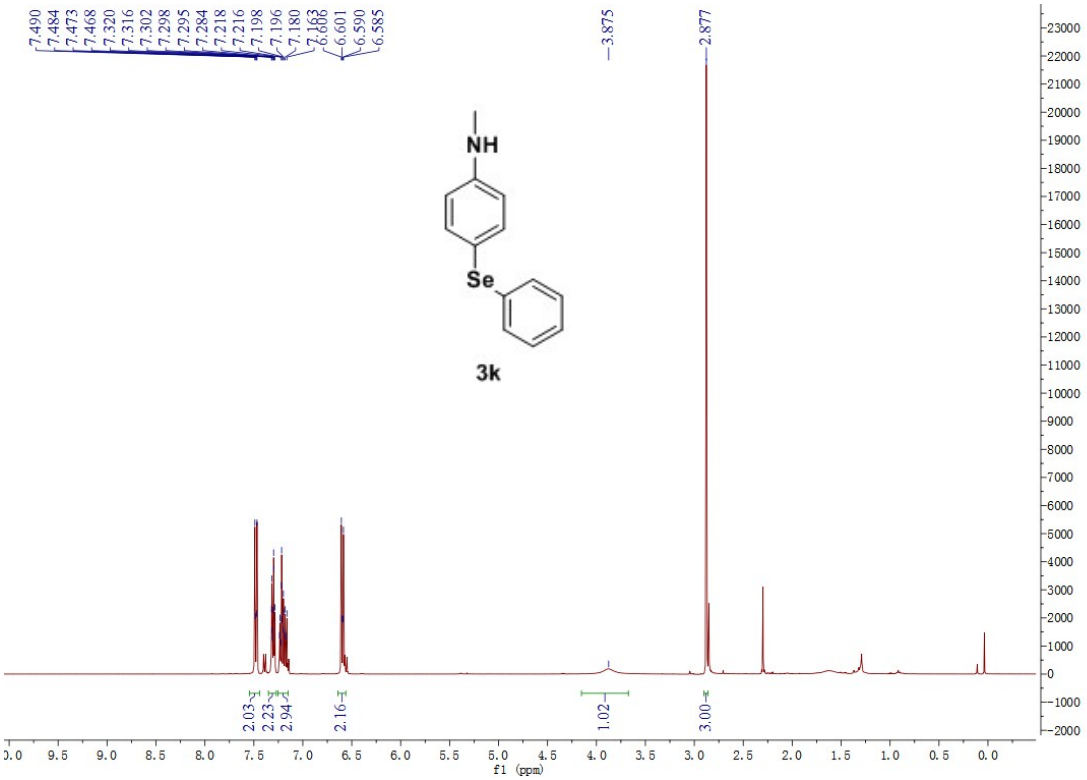
136.167
133.987
130.948
129.879
117.362
115.991
21.006
NH2
Se
3j
f1 (ppm)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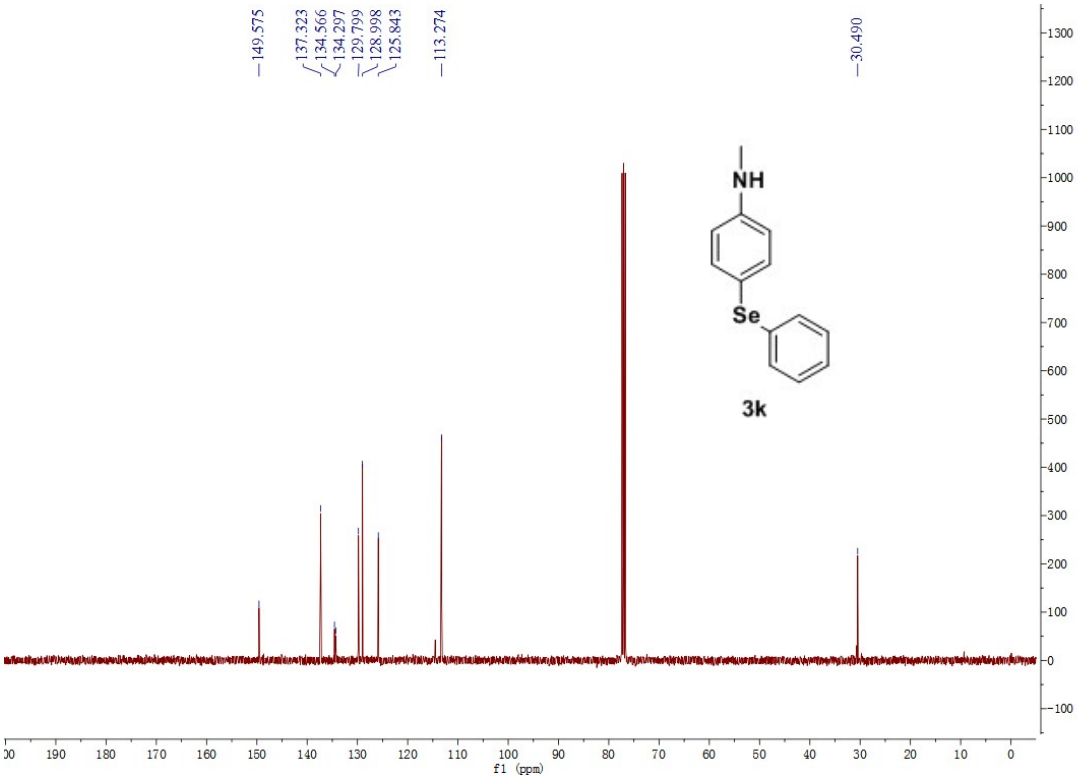
7.484
7.473
7.468
7.320
7.316
7.302
7.298
7.295
7.284
7.218
7.216
7.198
7.196
7.180
6.601
6.590
6.585
3.875
2.877
NH
Se
3k
2.03
2.23
2.94
2.16
1.02
3.00
f1 (ppm)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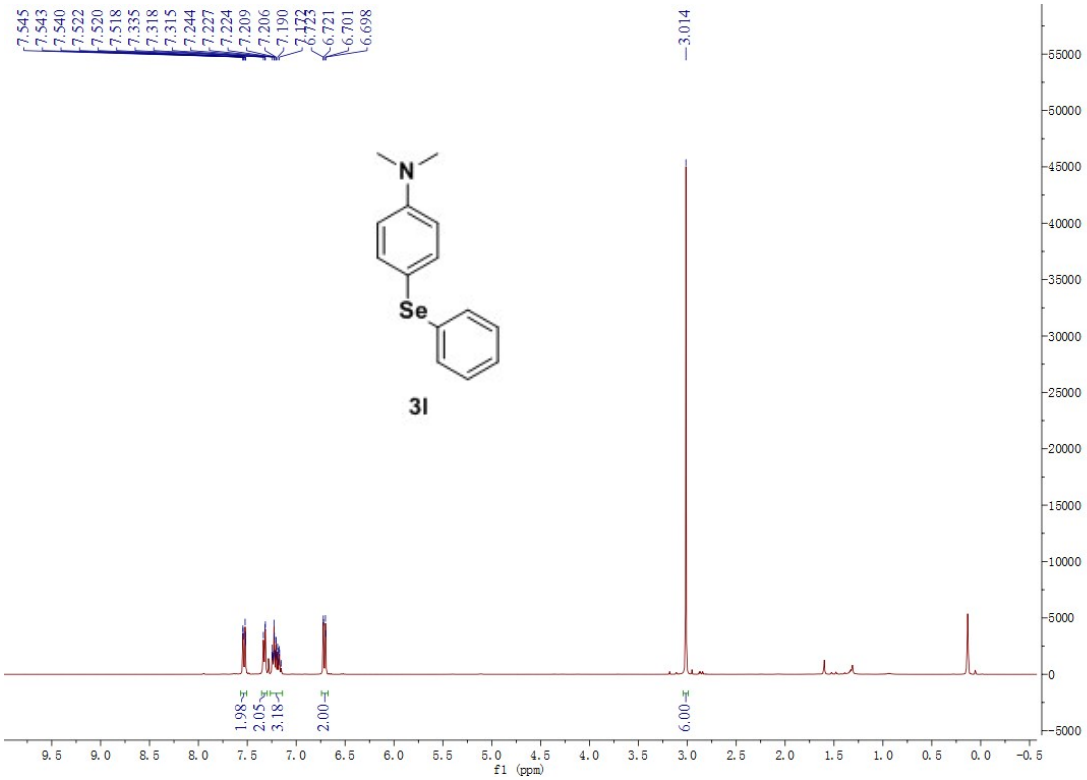
125.843
113.274
30.490
NH
Se
3k
f1 (ppm)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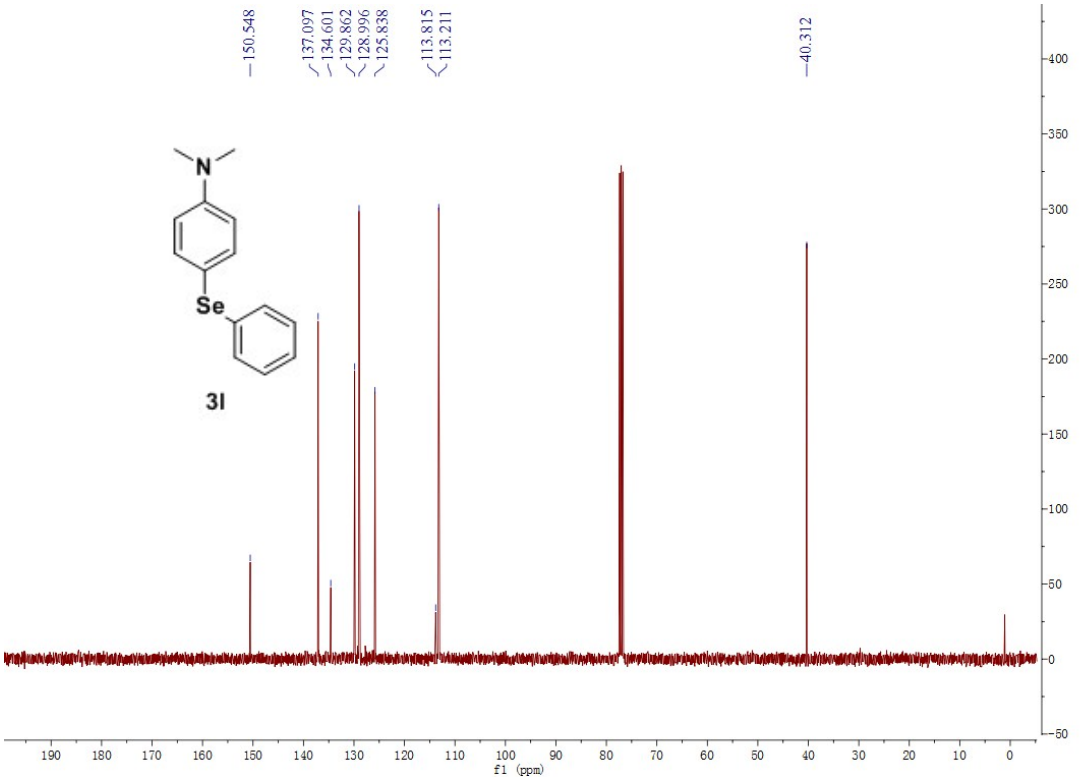
7.518
7.335
7.318
7.315
7.244
7.227
7.224
7.209
7.206
7.190
6.723
6.721
6.701
6.698
3.014
N
Se
3l
1.98
2.05
3.18
2.00
6.00
f1 (ppm)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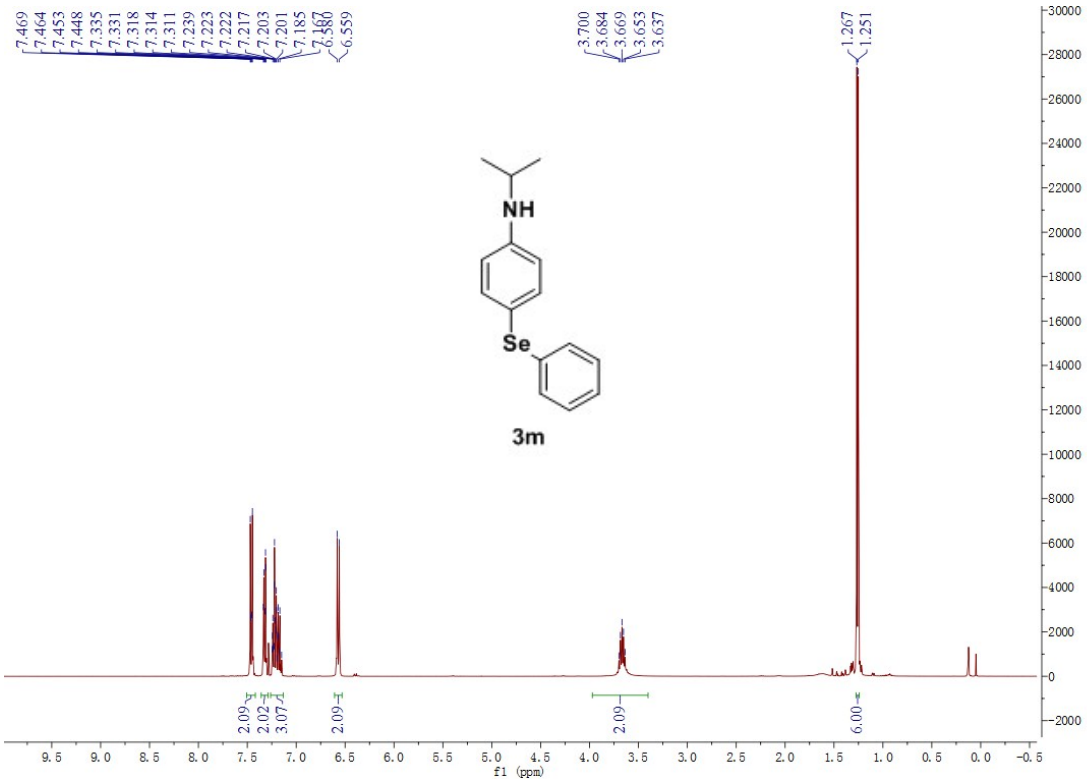
128.996
125.838
113.815
113.211
40.312
N
Se
3l
f1 (ppm)


7.469
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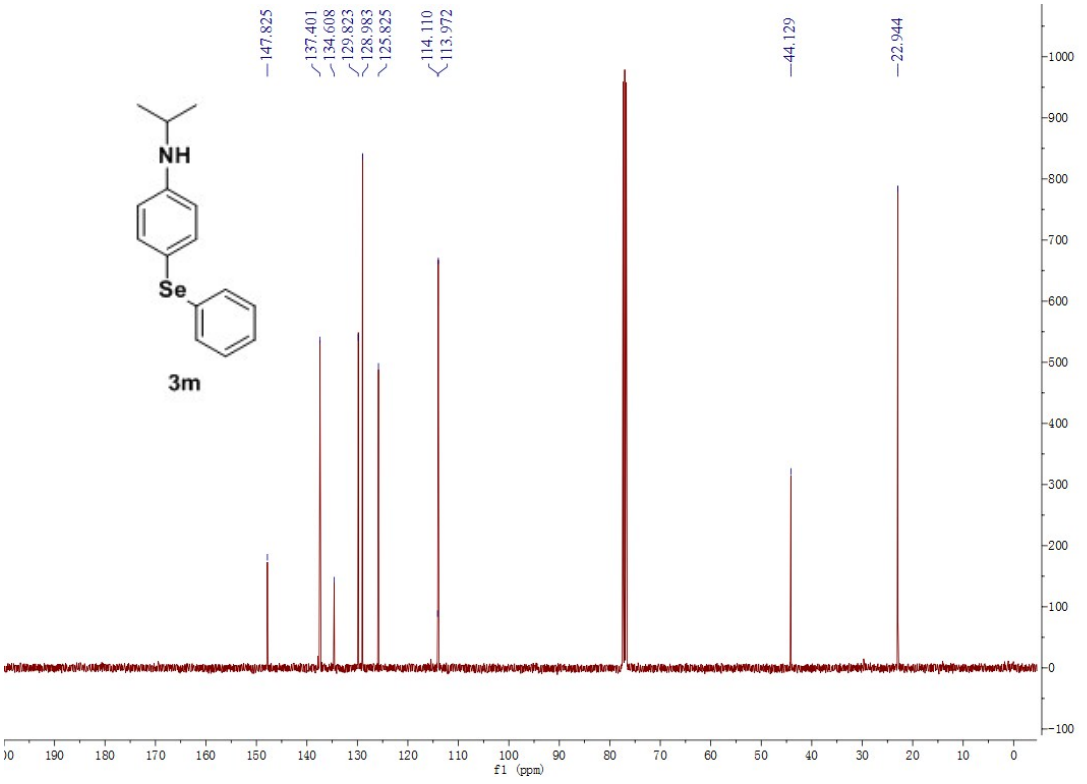
7.318
7.314
7.311
7.239
7.223
7.222
7.217
7.203
7.201
7.185
7.167
6.580
6.559
3.700
3.684
3.669
3.653
3.637
1.267
1.251
NH
Se
3m
2.09
2.02
3.07
2.09
2.09
6.00
f1 (ppm)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137.401
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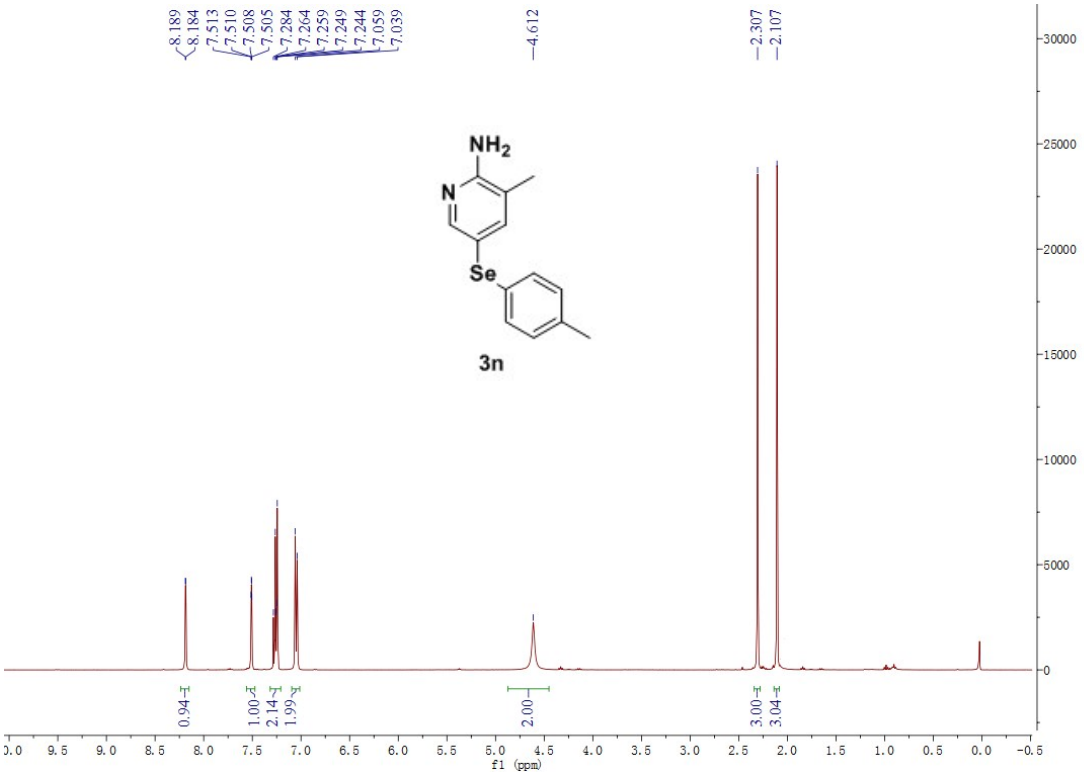
129.823
128.983
125.825
114.110
113.972
44.129
22.944
NH
Se
3m
f1 (ppm)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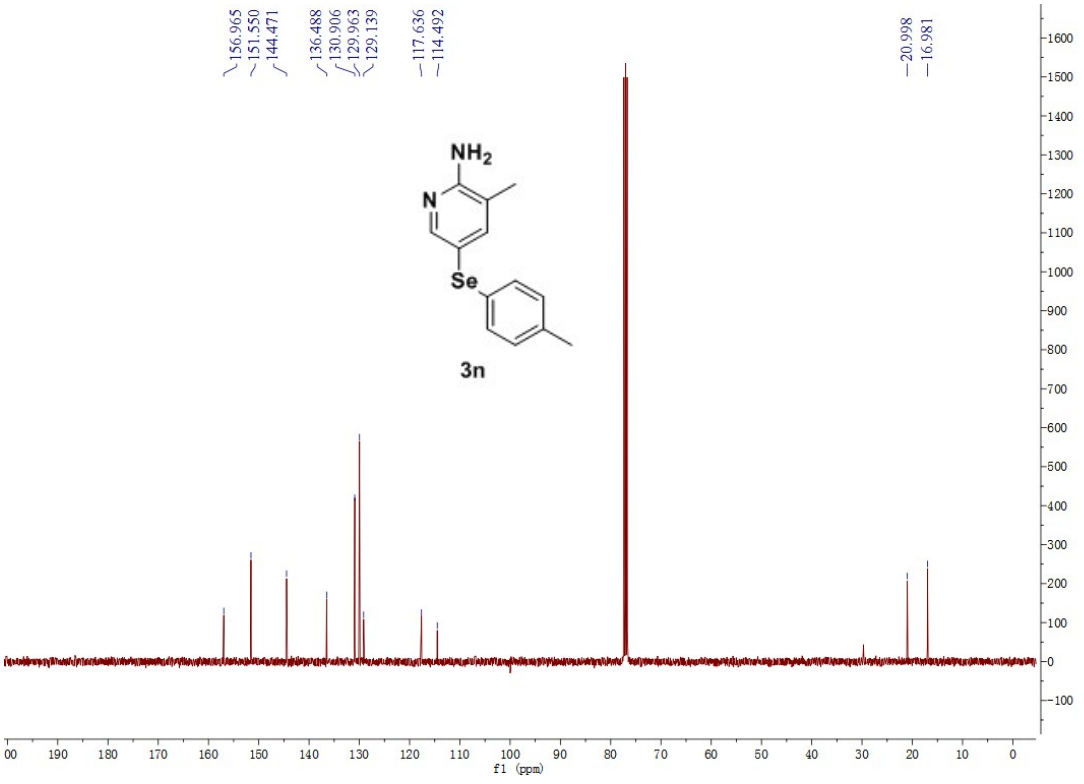
8.184
7.513
7.510
7.508
7.505
7.284
7.264
7.259
7.249
7.244
7.059
7.039
4.612
2.307
2.107
NH2
N
Se
3n
0.94
1.00
2.14
1.99
2.00
3.00
3.04
f1 (ppm)


156.965
151.550
144.471
136.488
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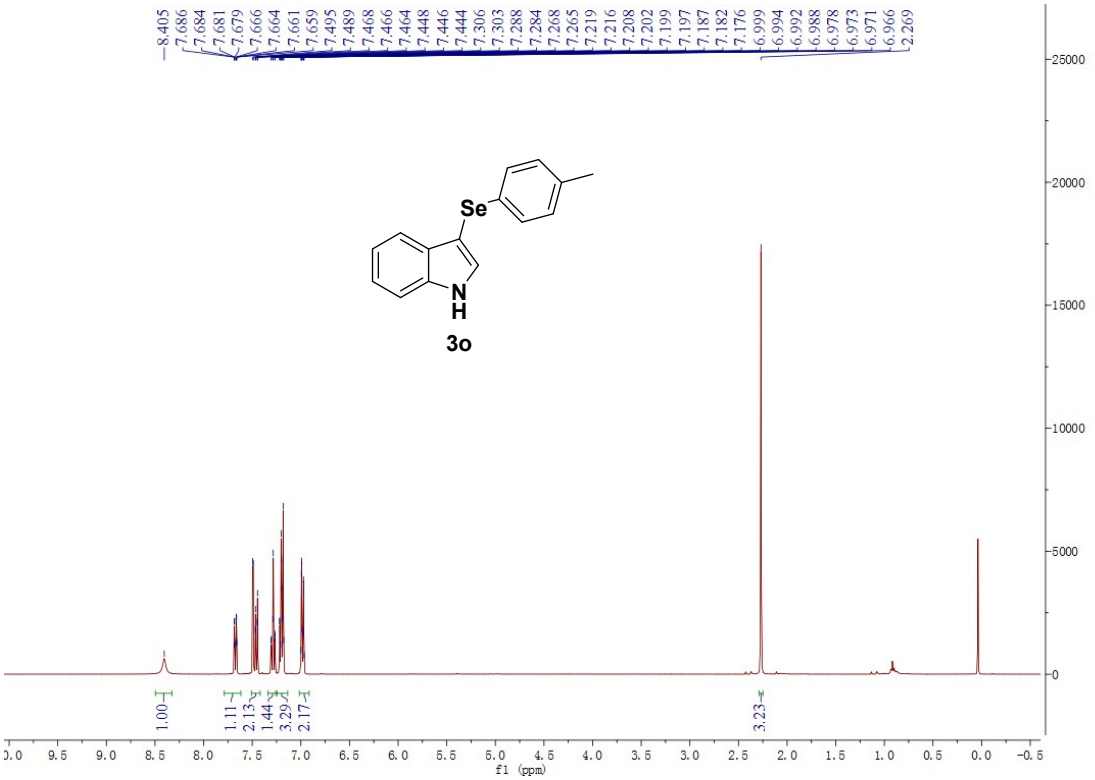
129.963
129.139
117.636
114.492
20.998
16.981
NH2
N
Se
3n
f1 (ppm)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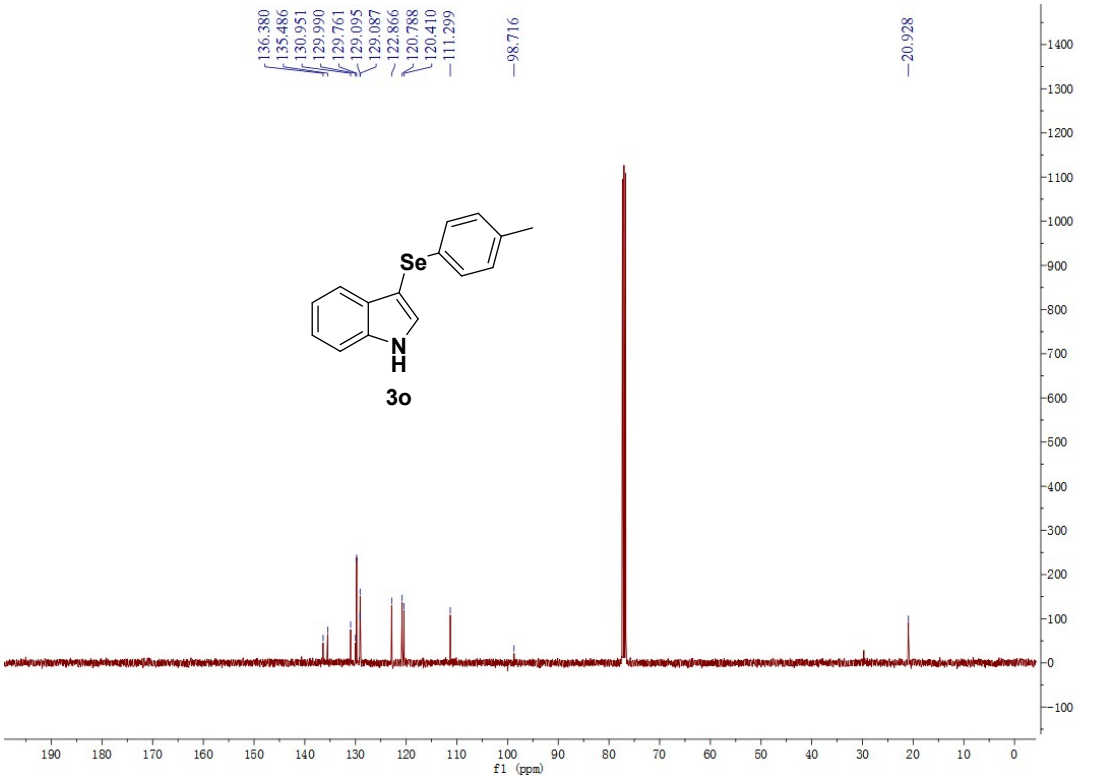
7.686
7.684
7.681
7.679
7.666
7.664
7.661
7.659
7.495
7.489
7.468
7.466
7.464
7.448
7.446
7.444
7.306
7.303
7.288
7.284
7.268
7.265
7.219
7.216
7.208
7.202
7.199
7.197
7.187
7.182
7.176
6.999
6.994
6.992
6.988
6.978
6.973
6.971
6.966
2.269
Se
N
H
3o
1.00
1.11
2.13
1.44
3.29
2.17
3.23
f1 (ppm)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130.951
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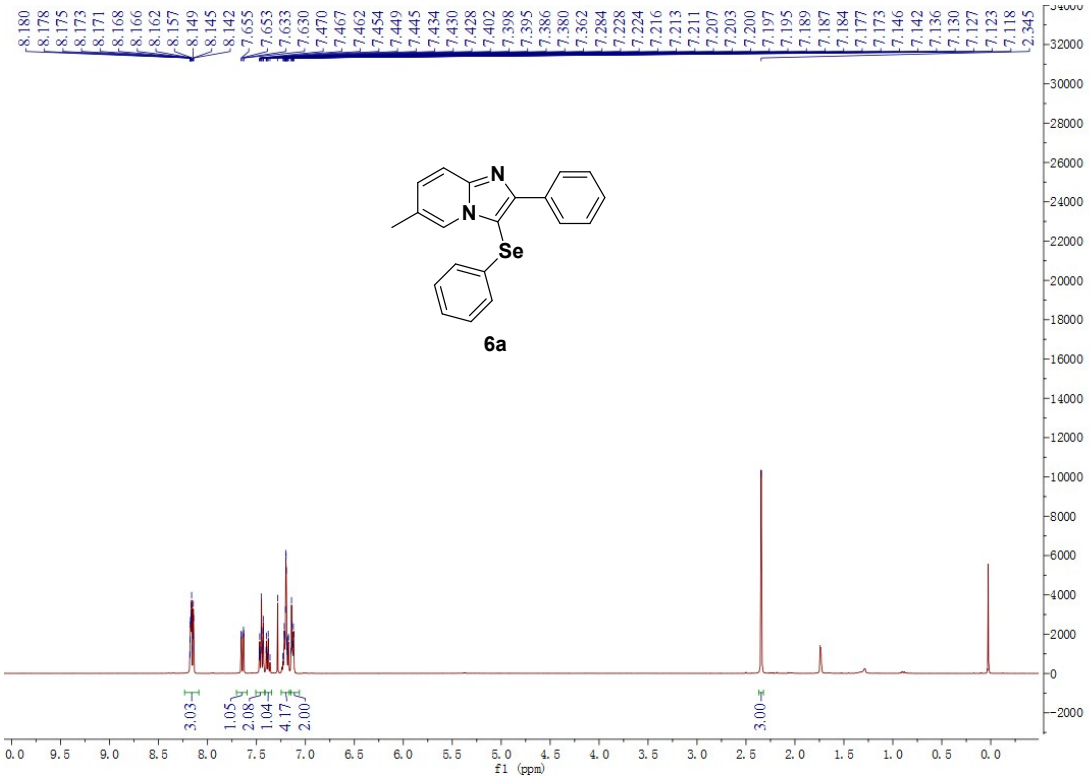
111.299
98.716
20.928
Se
N
H
3o
f1 (ppm)


8.180
8.178
8.175
8.173
8.171
8.168
8.166
8.162
8.157
8.149
8.145
8.142
7.655
7.653
7.633
7.630
7.470
7.467
7.462
7.454
7.449
7.445
7.434
7.430
7.428
7.402
7.398
7.395
7.386
7.380
7.362
7.284
7.228
7.224
7.216
7.213
7.211
7.207
7.203
7.200
7.197
7.195
7.189
7.187
7.184
7.177
7.173
7.146
7.142
7.136
7.130
7.127
7.123
7.118
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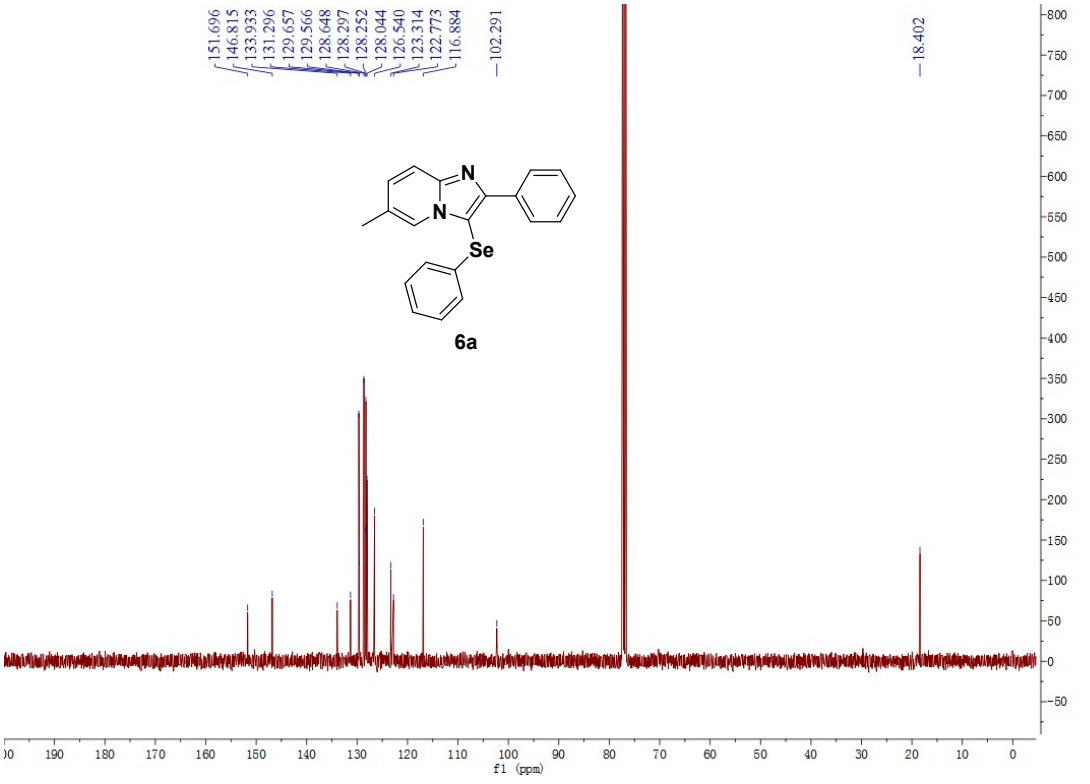
N
N
Se
6a
3.03
1.05
2.08
1.04
4.17
2.00
3.00
f1 (ppm)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128.297
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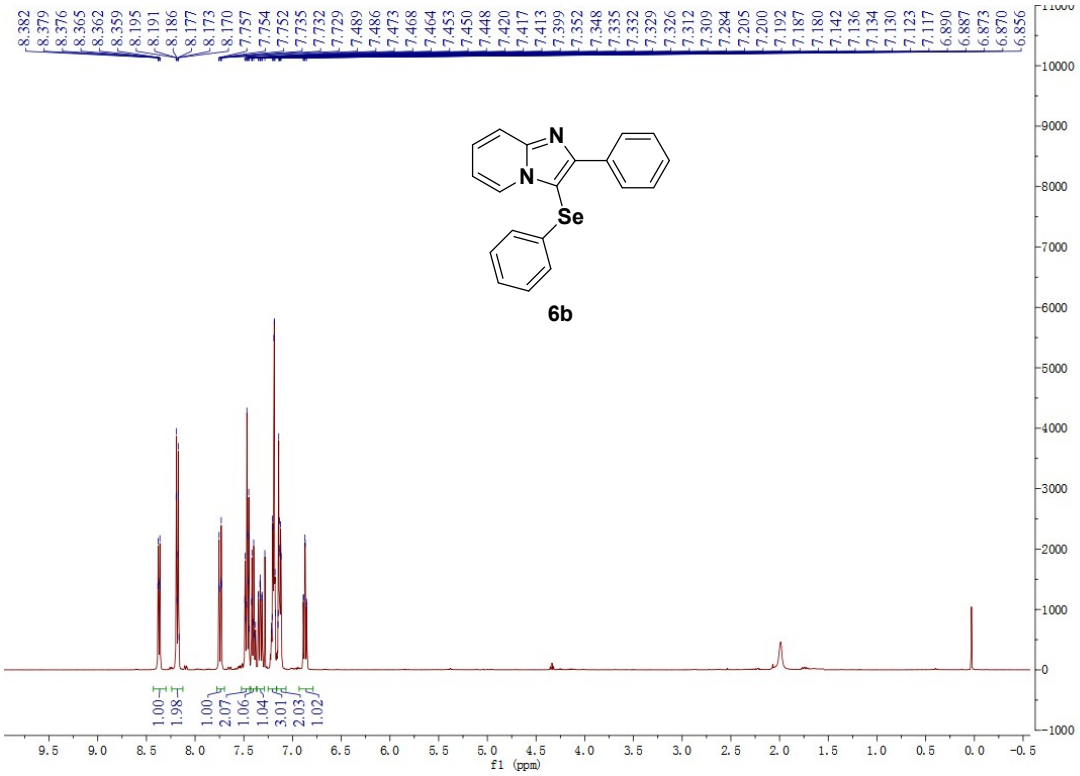
123.314
122.773
116.884
102.291
18.402
N
N
Se
6a
f1 (ppm)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8.359
8.195
8.191
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8.177
8.173
8.170
7.757
7.754
7.752
7.735
7.732
7.729
7.489
7.486
7.473
7.468
7.464
7.453
7.450
7.448
7.420
7.417
7.413
7.399
7.352
7.348
7.335
7.332
7.329
7.326
7.312
7.309
7.284
7.205
7.200
7.192
7.187
7.180
7.142
7.136
7.134
7.130
7.123
7.117
6.890
6.887
6.873
6.870
6.856
N
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Se
6b
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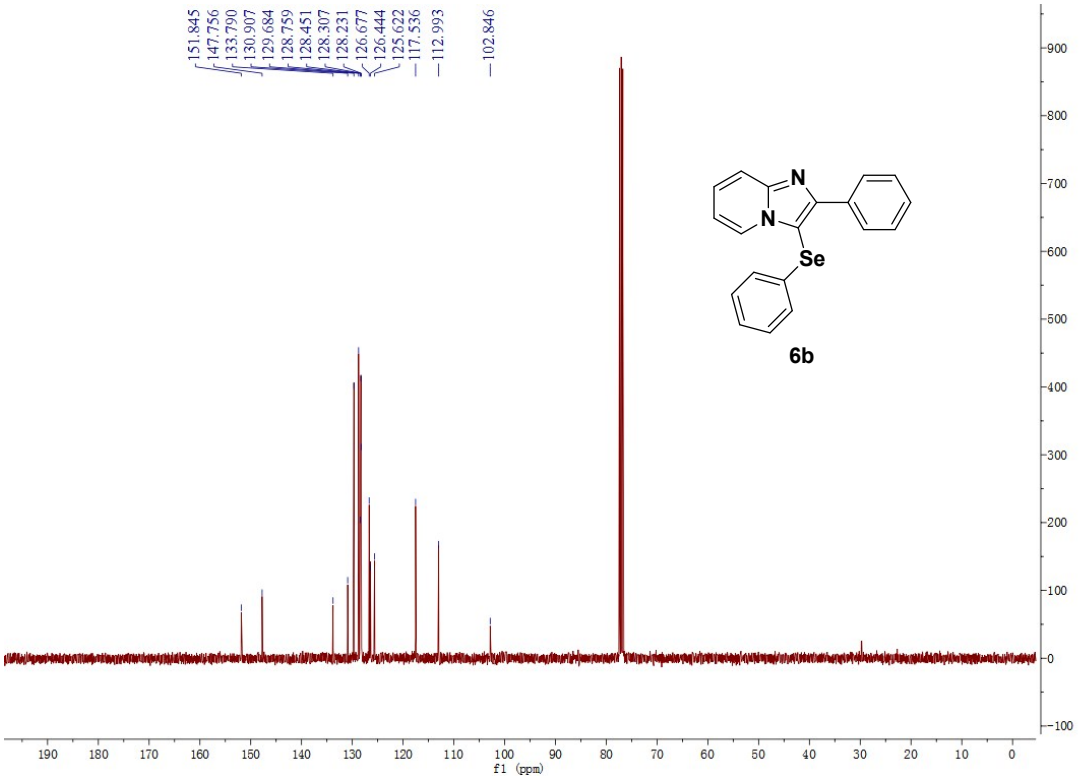
1.98
1.00
2.07
1.06
1.04
3.01
2.03
1.02
f1 (ppm)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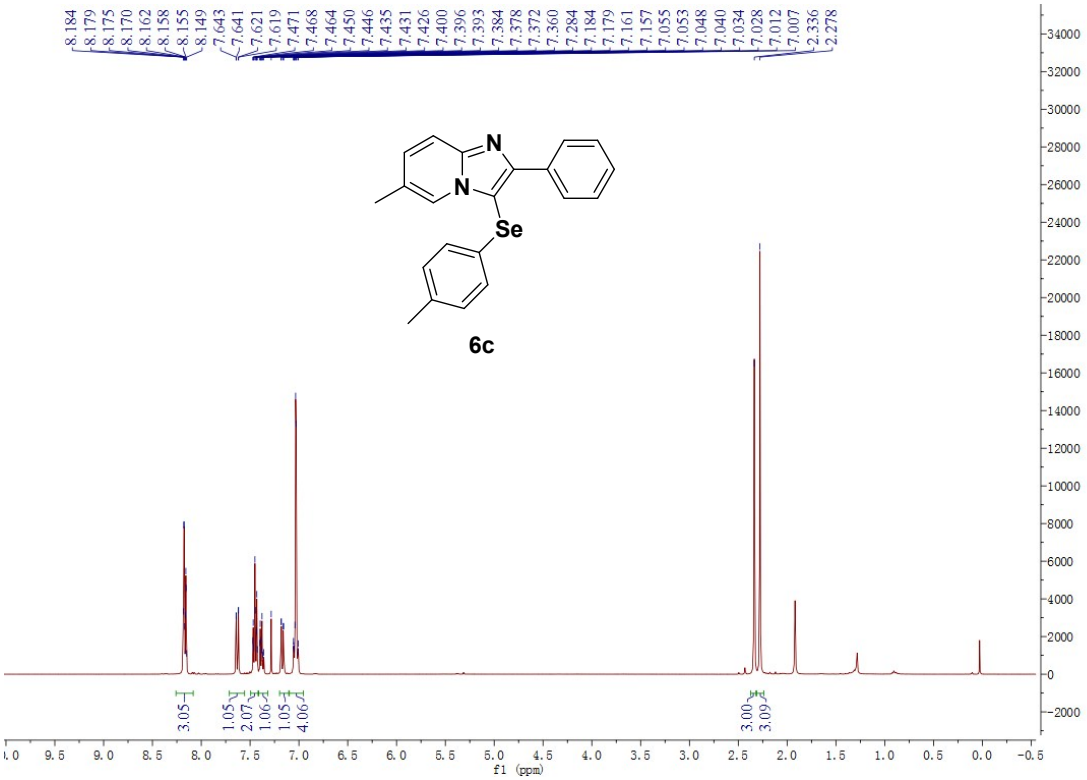
128.759
128.451
128.307
128.231
126.677
126.444
125.622
117.536
112.993
102.846
N
N
Se
6b
f1 (ppm)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8.162
8.158
8.155
8.149
7.643
7.641
7.621
7.619
7.471
7.468
7.464
7.450
7.446
7.435
7.431
7.426
7.400
7.396
7.393
7.384
7.378
7.372
7.360
7.284
7.184
7.179
7.161
7.157
7.055
7.053
7.048
7.040
7.034
7.028
7.012
7.007
2.336
2.278
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N
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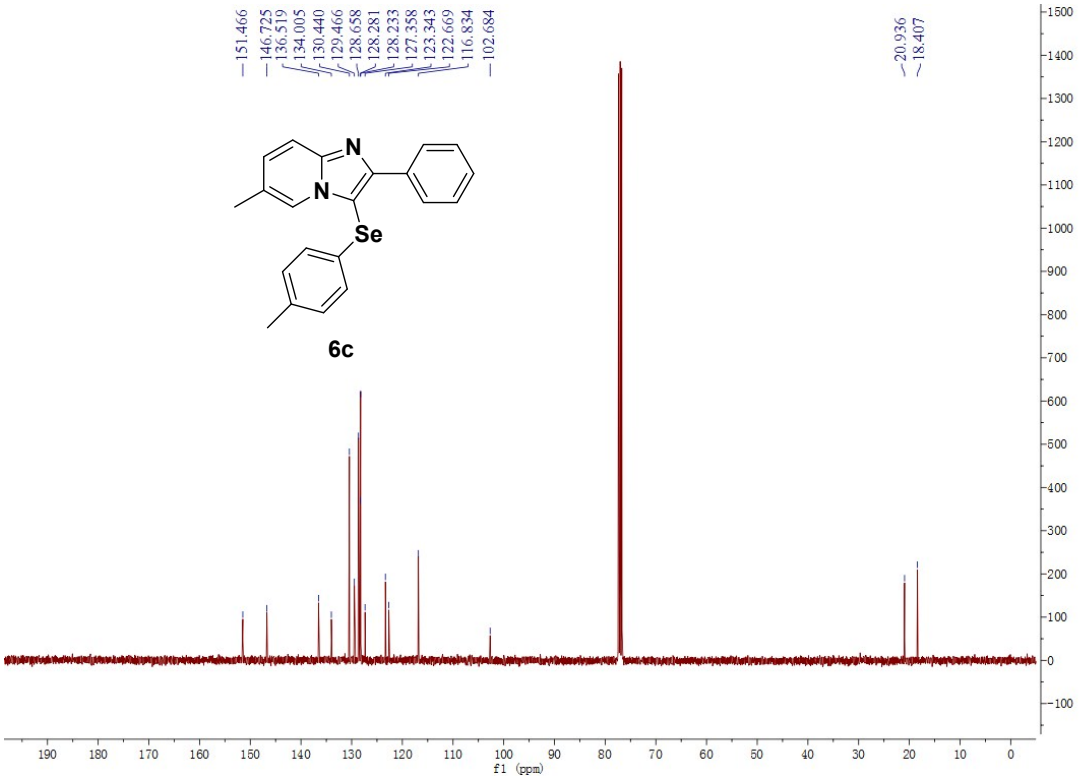
6c
3.05
1.05
2.07
1.06
1.05
4.06
3.00
3.09
f1 (ppm)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128.281
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122.669
116.834
102.684
20.936
18.407
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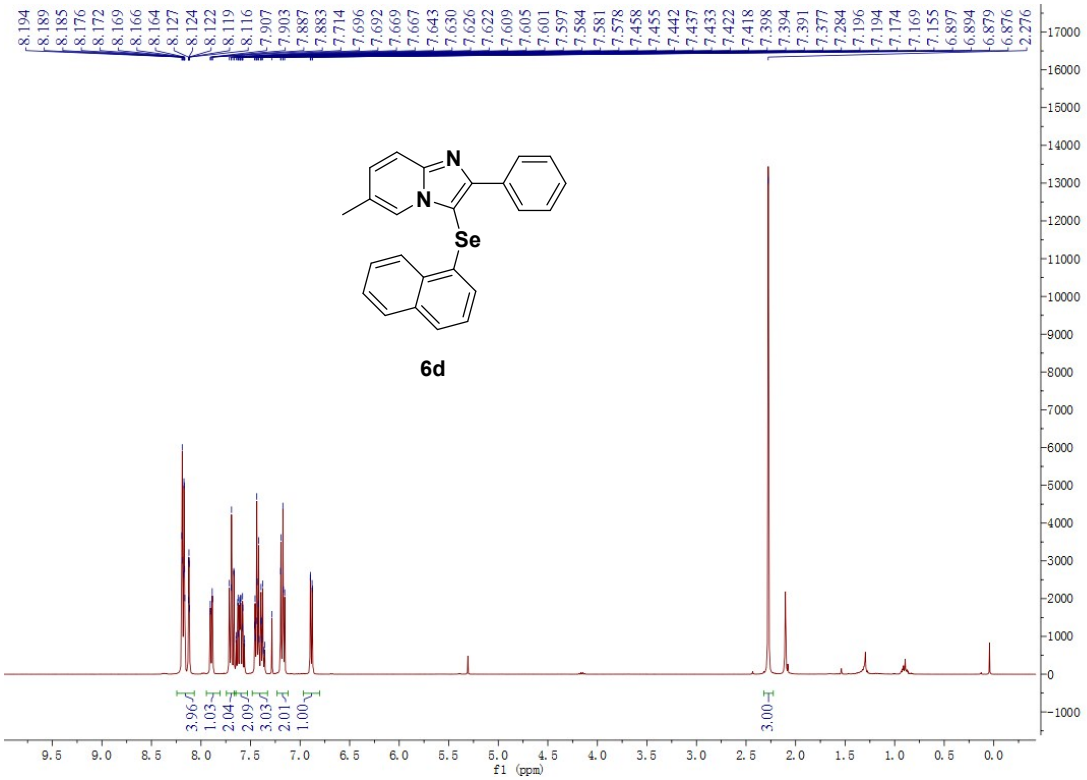
N
Se
6c
f1 (ppm)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8.122
8.119
8.116
7.907
7.903
7.887
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7.714
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7.643
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7.626
7.622
7.609
7.605
7.601
7.597
7.584
7.581
7.578
7.458
7.455
7.442
7.437
7.433
7.422
7.418
7.398
7.394
7.391
7.377
7.284
7.196
7.194
7.174
7.169
7.155
6.897
6.894
6.879
6.876
2.276
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N
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6d
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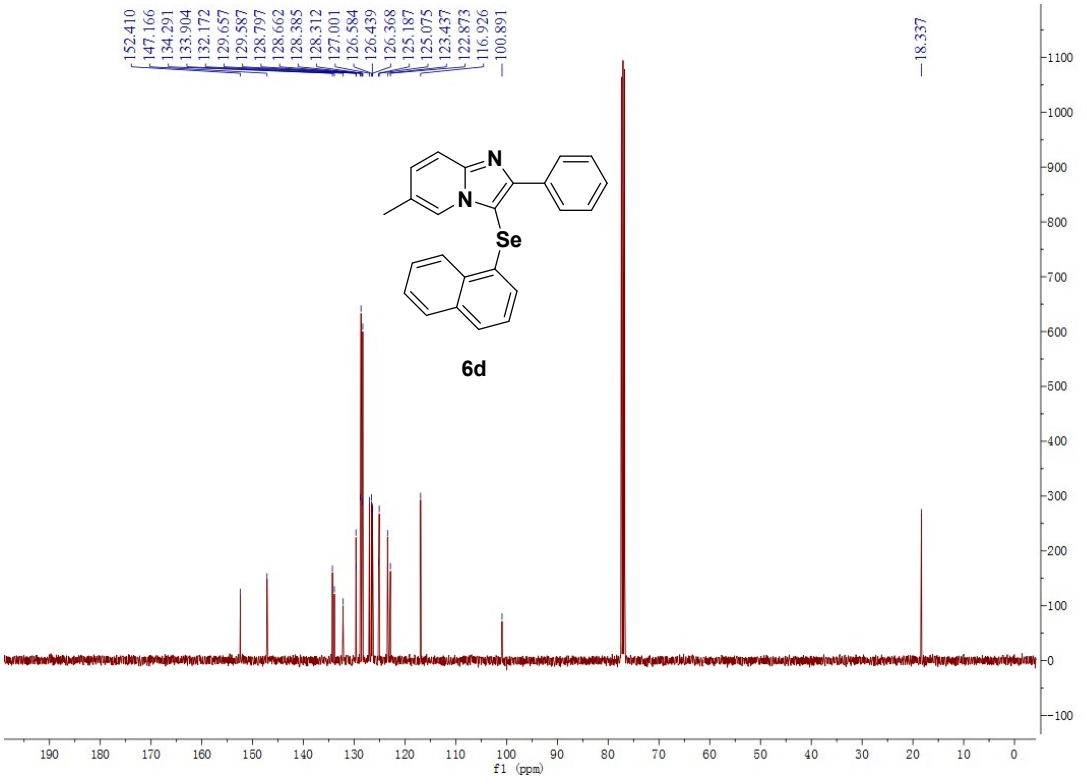
2.04
2.09
3.03
2.01
1.00
3.00
f1 (ppm)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127.001
126.584
126.439
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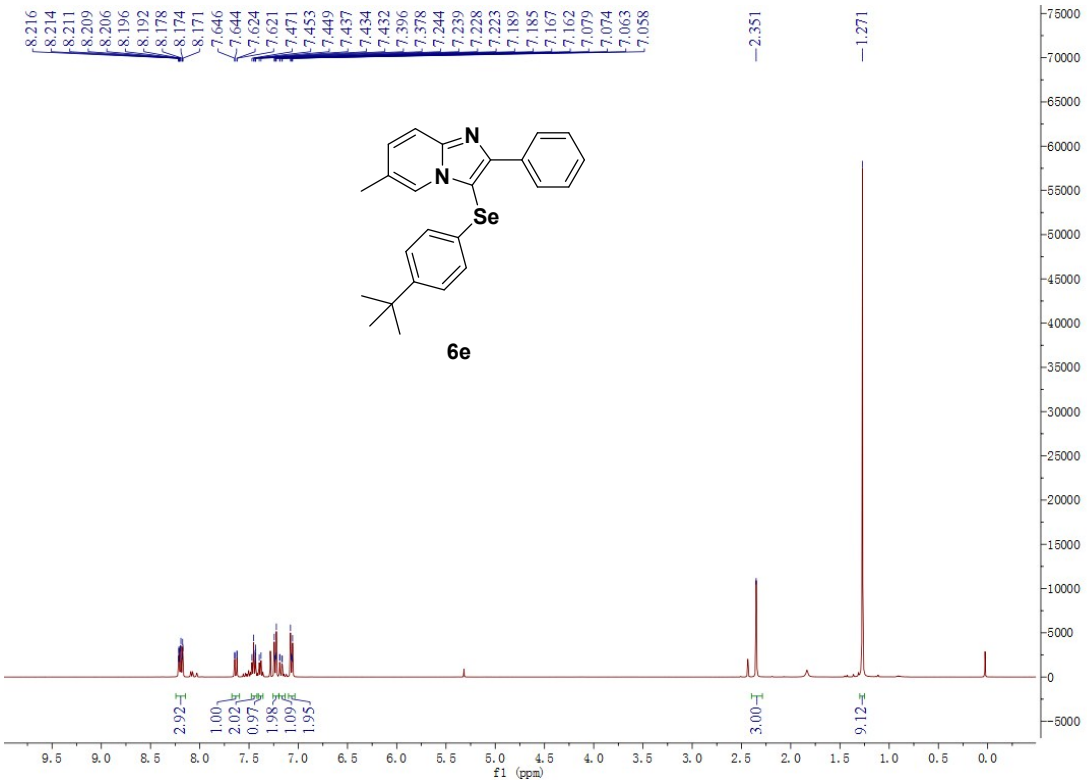
18.337
N
N
Se
6d
f1 (ppm)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7.432
7.396
7.378
7.244
7.239
7.228
7.223
7.189
7.185
7.167
7.162
7.079
7.074
7.063
7.058
2.351
1.271
N
N
Se
6e
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1.00
2.02
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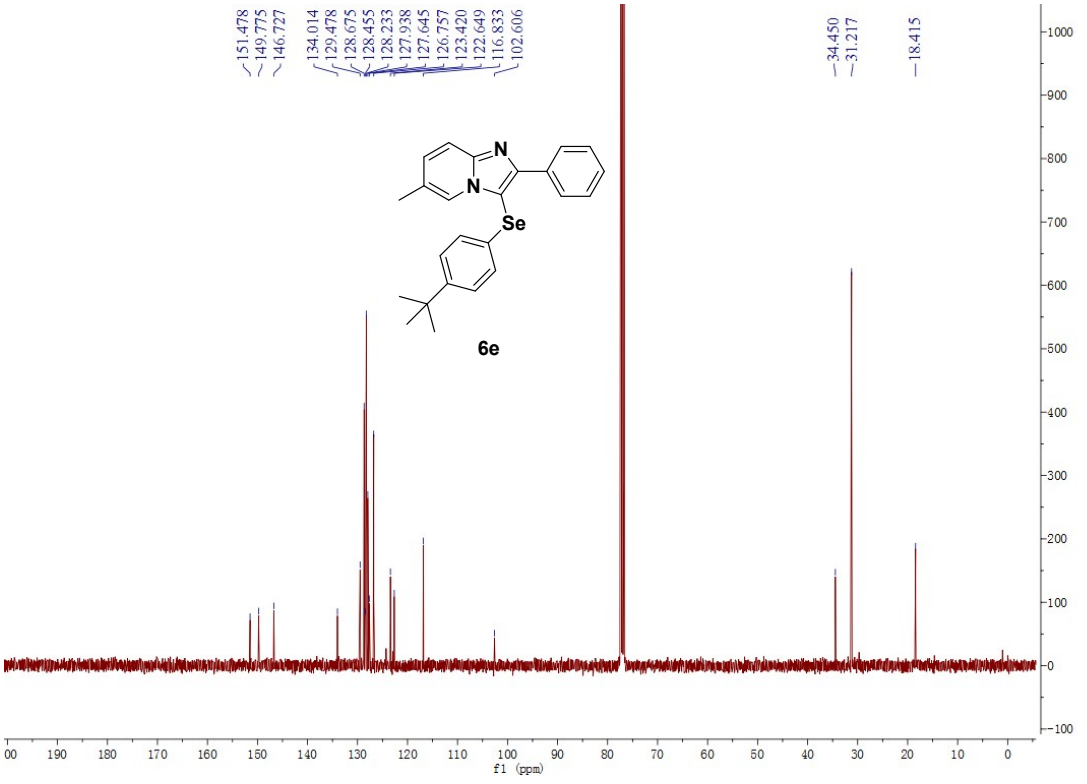
1.98
1.09
1.95
3.00
9.12
f1 (ppm)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18.415
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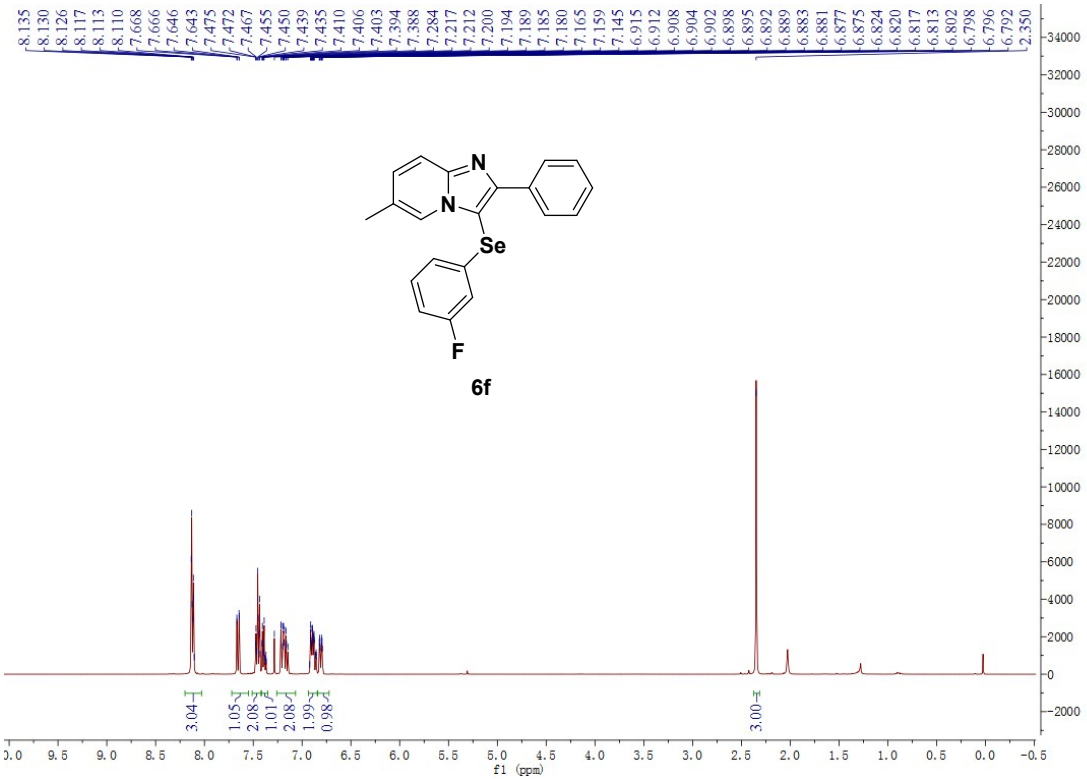
Se
6e
f1 (ppm)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7.475
7.472
7.467
7.455
7.450
7.439
7.435
7.410
7.406
7.403
7.394
7.388
7.284
7.217
7.212
7.200
7.194
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7.185
7.180
7.165
7.159
7.145
6.915
6.912
6.908
6.904
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6.895
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6.877
6.875
6.824
6.820
6.817
6.813
6.802
6.798
6.796
6.792
2.350
N
N
Se
F
6f
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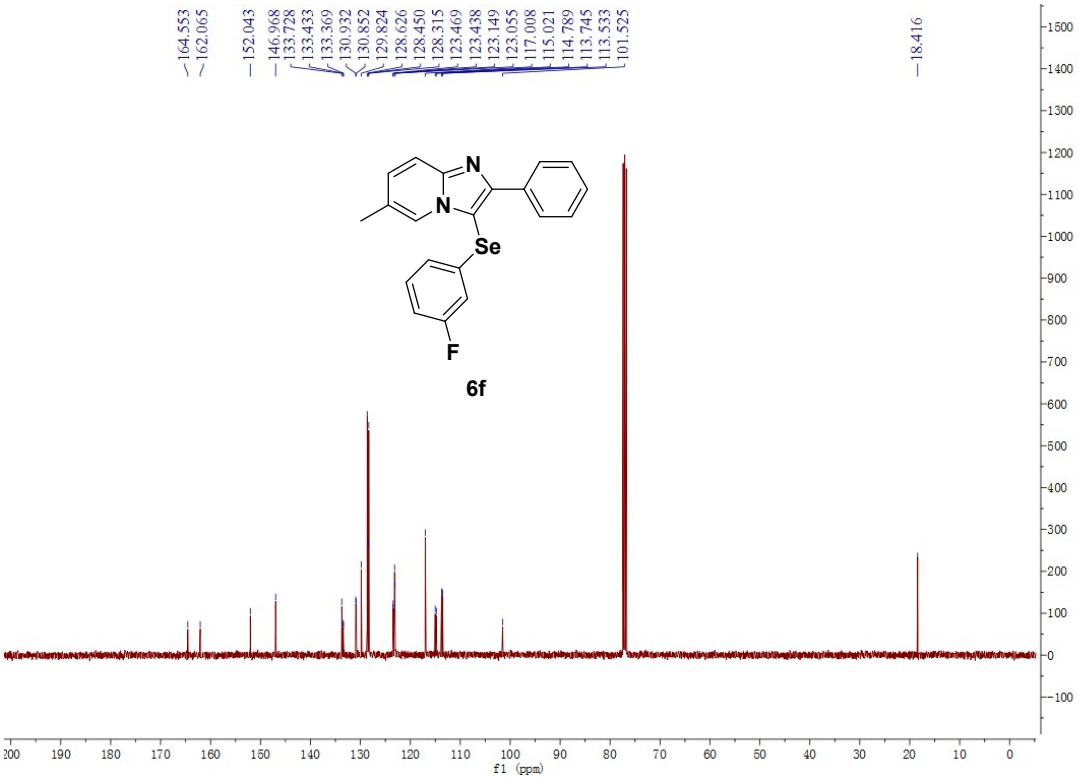
1.05
2.08
1.01
2.08
1.99
0.98
3.00
f1 (ppm)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123.149
123.055
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114.789
113.745
113.533
101.525
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N
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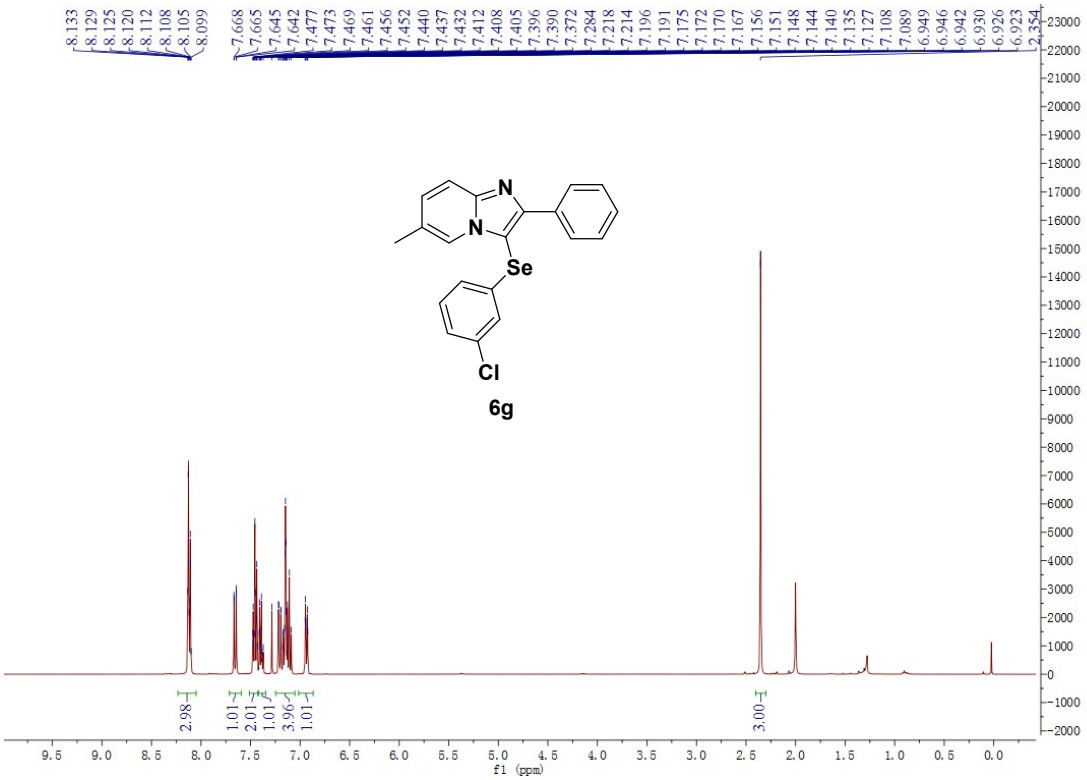
Se
F
6f
f1 (ppm)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7.477
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7.452
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7.408
7.405
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7.390
7.372
7.284
7.218
7.214
7.196
7.191
7.175
7.172
7.170
7.167
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7.151
7.148
7.144
7.140
7.135
7.127
7.108
7.089
6.949
6.946
6.942
6.930
6.926
6.923
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N
Se
Cl
6g
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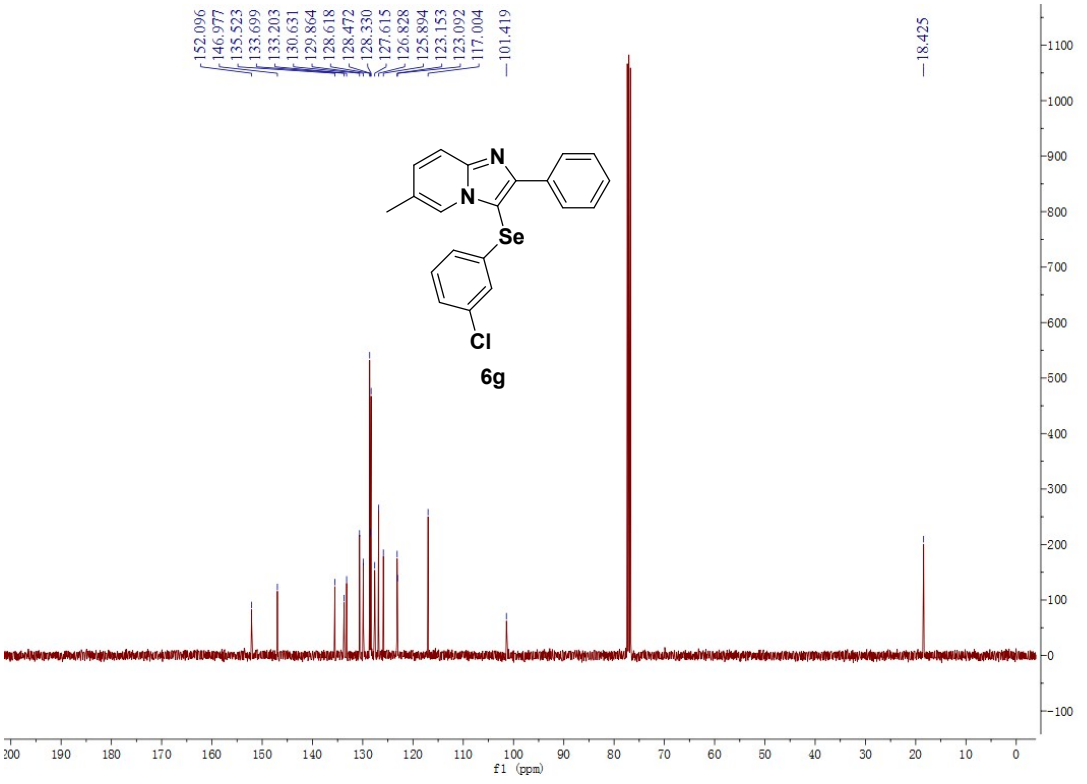
3.00
f1 (ppm)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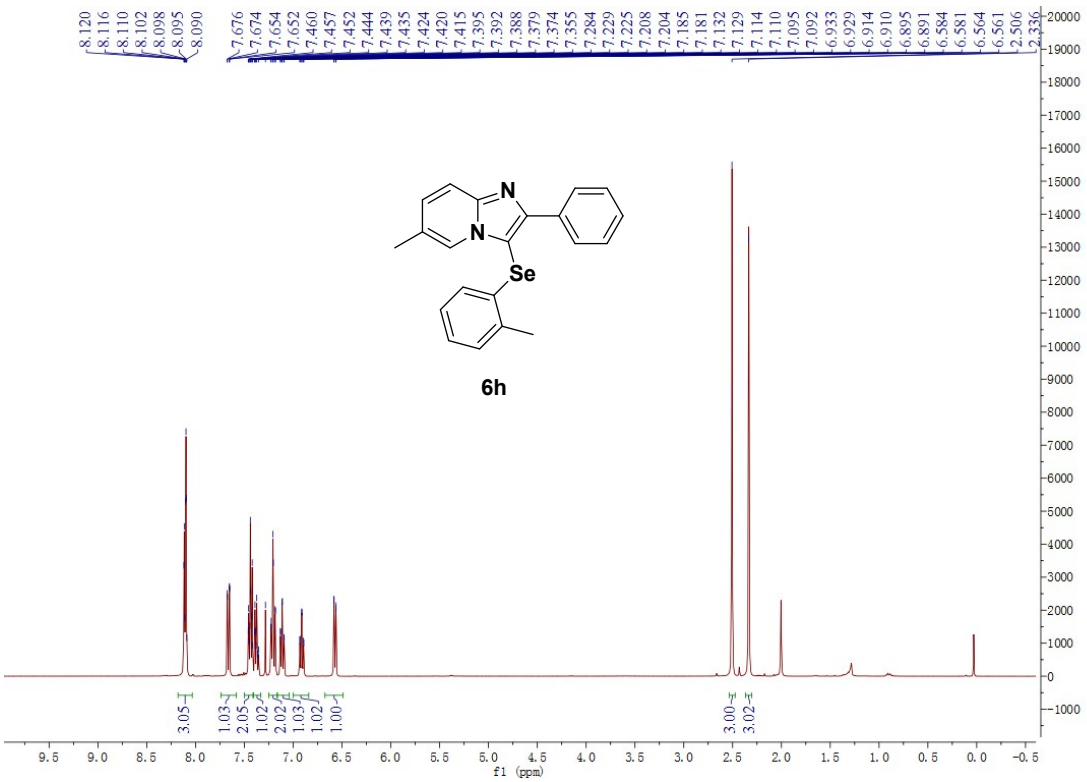
101.419
18.425
N
N
Se
Cl
6g
f1 (ppm)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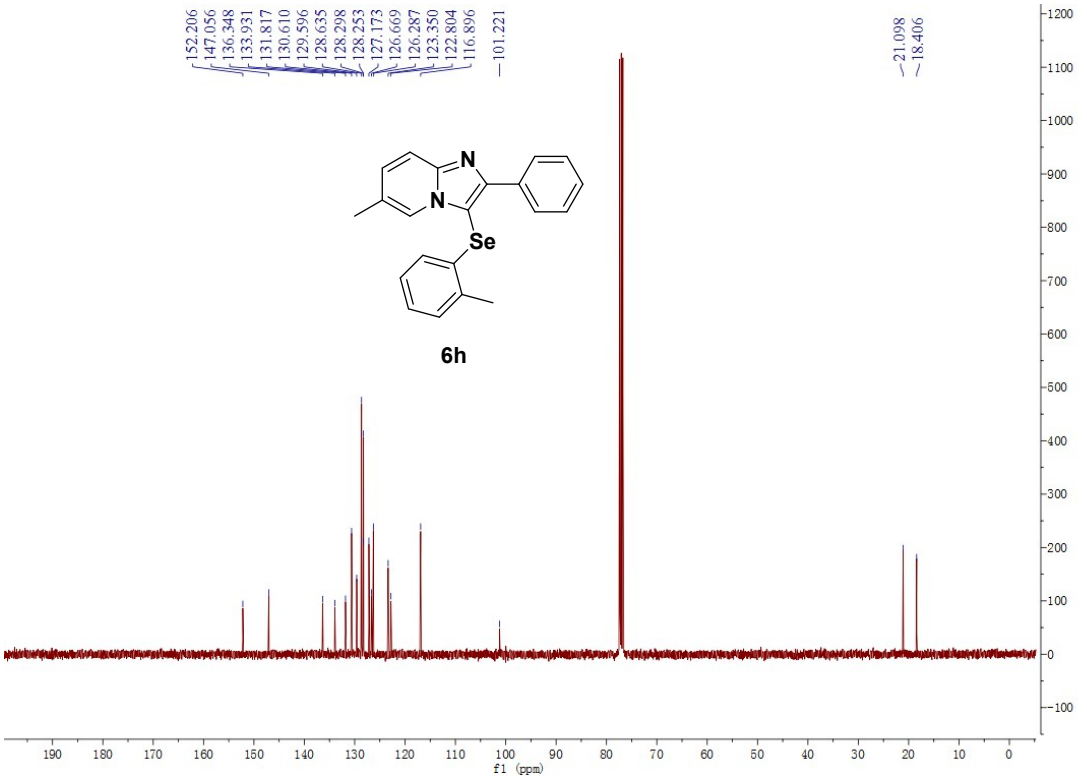
6.891
6.584
6.581
6.564
6.561
2.506
2.336
N
N
Se
6h
3.05
1.03
2.05
1.02
2.02
1.03
1.02
1.00
3.00
3.02
f1 (ppm)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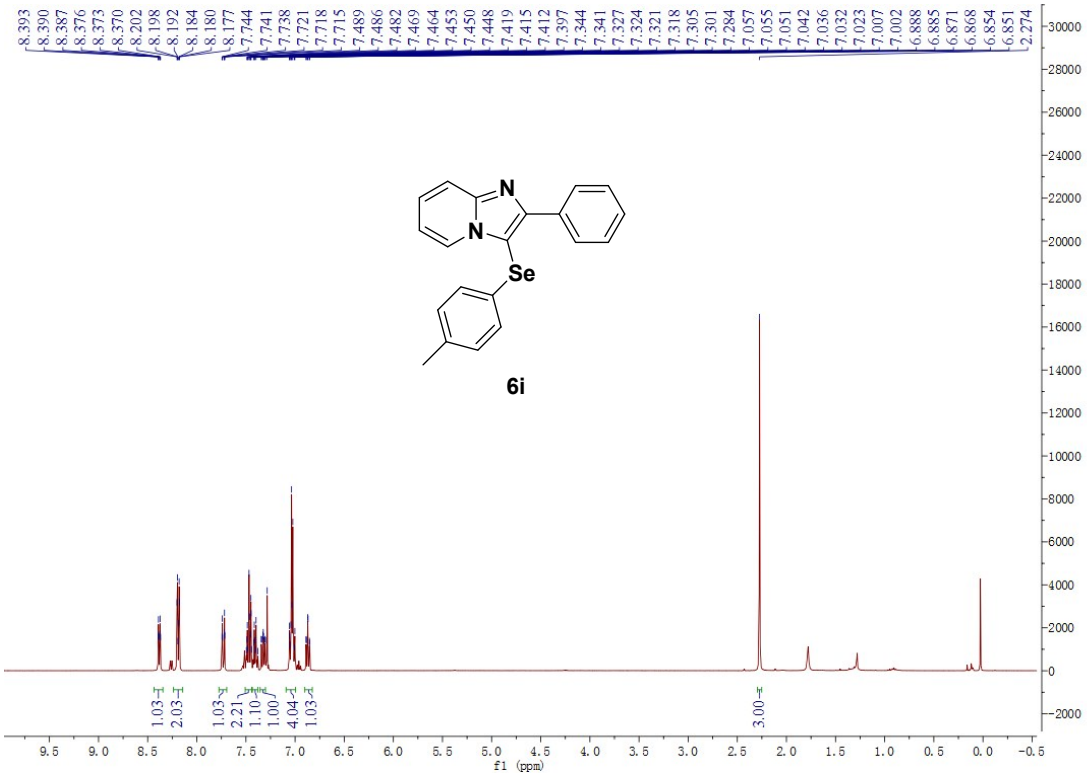
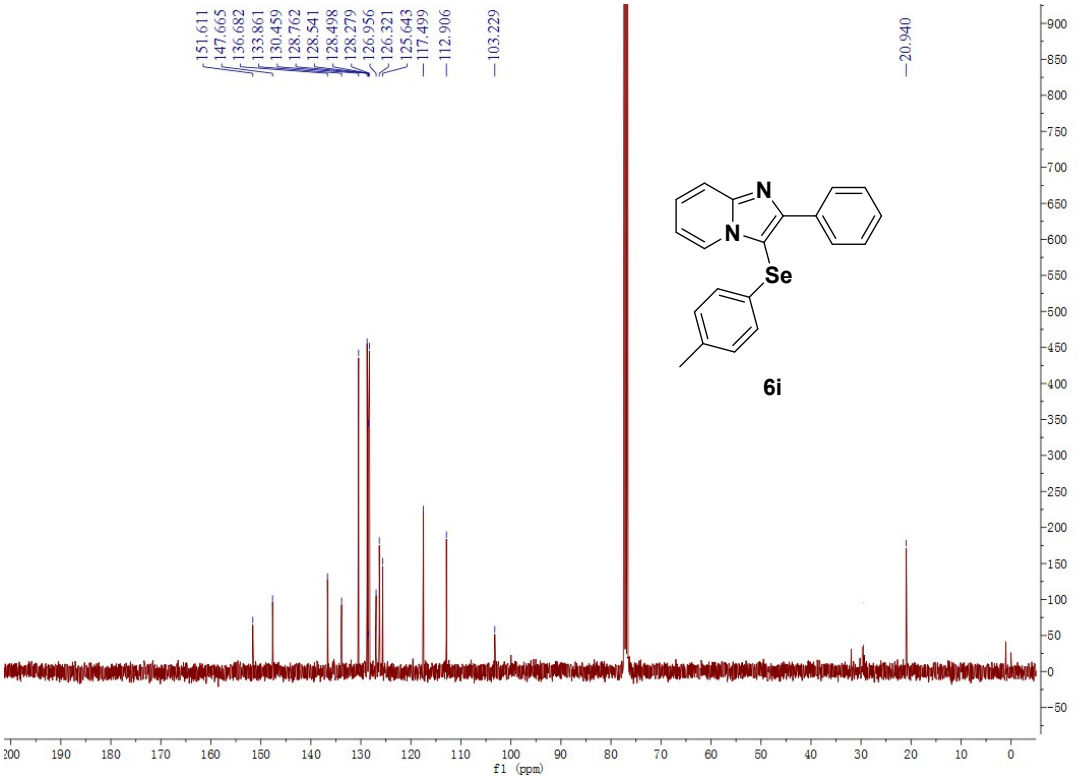
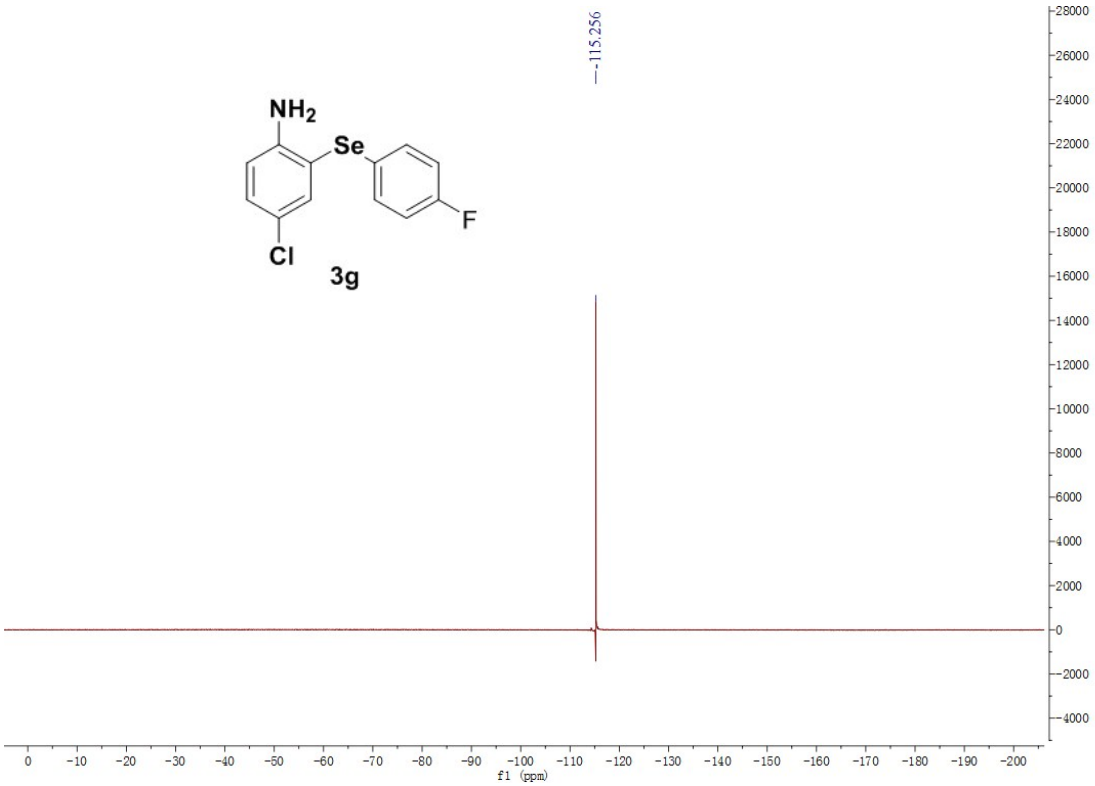
147.056
136.348
133.931
131.817
130.610
129.596
128.635
128.298
128.253
127.173
126.669
126.287
123.350
122.804
116.896
101.221
21.098
18.406
N
N
Se
6h
f1 (ppm)

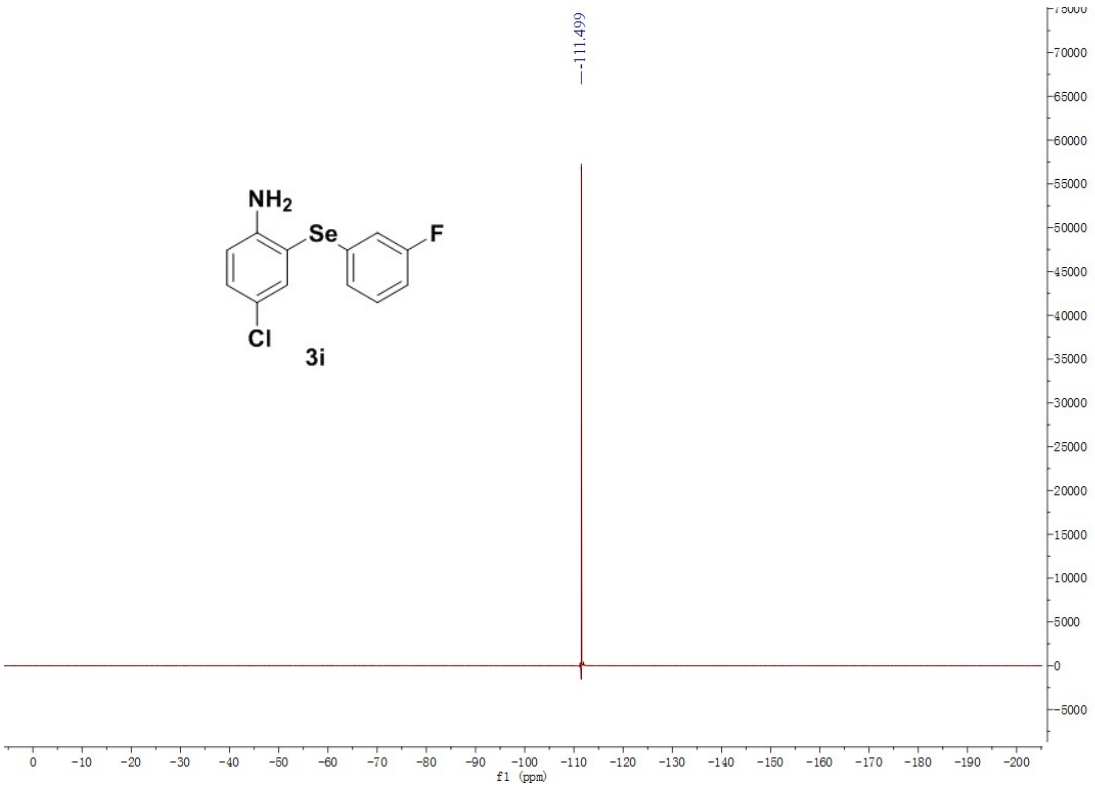

8.393
8.390
8.387
8.376
8.373
8.370
8.202
8.198
8.192
8.184
8.180
8.177
7.744
7.741
7.738
7.721
7.718
7.715
7.489
7.486
7.482
7.469
7.464
7.453
7.450
7.448
7.419
7.415
7.412
7.397
7.344
7.341
7.327
7.324
7.321
7.318
7.305
7.301
7.284
7.057
7.055
7.051
7.042
7.036
7.032
7.023
7.007
7.002
6.888
6.885
6.871
6.868
6.854
6.851
2.274
N
N
Se
6i
1.03
2.03
1.03
2.21
1.10
1.00
4.04
1.03
3.00
f1 (ppm)


151.611
147.665
136.682
133.861
130.459
128.762
128.541
128.498
128.279
126.956
126.321
125.643
117.499
112.906
103.229
20.940
N
N
Se
6i
f1 (ppm)

^{19}F NMR spectra



^{19}F NMR spectra



^{19}F NMR spectra