Supporting Information

An Efficient *t*-BuOK Promoted C3-Chalcogenylation of Indoles with Dichalcogenides

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General information and materials:

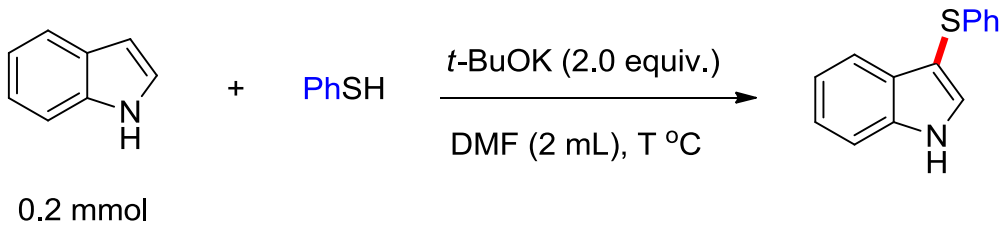
Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were technical grade. Column chromatography was performed using silica gel Merck 60 (particle size 0.040-0.063 mm). Solvent mixtures are understood as volume/volume.

^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR were recorded on a *Bruker DRX500 (500 MHz)* spectrometer in $CDCl_3$ (δ = 7.26 ppm for ^{1}H, δ = 77.00 ppm for ^{13}C) and in DMSO-d_6 (δ = 2.50 ppm for ^{1}H, δ = 39.43 ppm for ^{13}C). Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); coupling constants (*J*) are given in Hertz (Hz). High resolution mass spectra were recorded on a ESI-Q-TOF mass spectrometer. Chemical yields refer to isolated pure substances.

General procedure for product synthesis:

A mixture of indole **1** (0.2 mmol), dichalcogenide **2** (0.22 mmol), *t*-BuOK (0.4 mmol), and DMF (2 mL) were added in a 5 mL glass tube, which was stirred at room temperature for 0.5−12 h. When the reaction was completed, it was mixed with water and ethyl acetate. The reaction mixture was extracted three times with ethyl acetate or dichloromethane. The combined organic layer was washed two times with a little amount of water, dried over anhydrous magnesium sulfate and filtered. The filtrate was evaporated under vacuum and the residue was purified by flash column chromatography on silica gel (elutig with petroleum ether-ethyl acetate) to provide the desired product **3**.

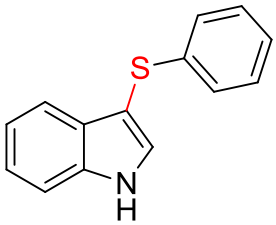
Sulfenylation of indole with thiophenol:



0.2 mmol

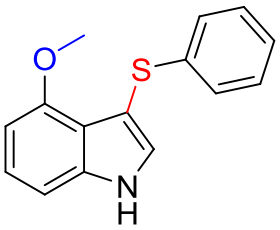
Entry	Amount of PhSH (equiv.)	T (^{o}C)	Reaction Time (h)	Yield (%)
1	1.1	rt	12	trace
2	2.2	rt	12	28
3	2.0	70	2	85

Characterization of product 3



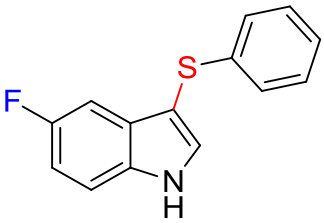
3-(Phenylthio)-1*H*-indole (3a)

Brick red solid; mp 131–132 ^{o}C; R_f = 0.4 (9% EtOAc in petroleum ether);^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (brs, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.49 (d, *J* = 2.1 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.20 – 7.16 (m, 3H), 7.13 – 7.11 (m, 2H), 7.07 (t, *J* = 7.2 Hz, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.20, 136.47, 130.63, 129.08, 128.67, 125.85, 124.76, 123.03, 120.89, 119.65, 111.54, 102.87 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{11}NS$: 226.0685, found: 226.0685.



4-Methoxy-3-(phenylthio)-1*H*-indole (3b)

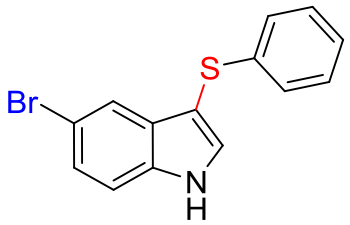
Black oil; R_f = 0.2 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.61 (brs, 1H), 7.53 (d, *J* = 2.2 Hz, 1H), 7.19 – 7.16 (m, 2H), 7.07 (d, *J* = 4.1 Hz, 2H), 7.04 – 7.02 (m, 3H), 6.51 (t, *J* = 4.2 Hz, 1H), 3.61 (s, 3H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 153.85, 141.09, 138.53, 131.15, 128.38, 125.44, 124.24, 122.93, 118.03, 105.31, 100.82, 98.96, 55.08 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NOS$: 256.0791, found: 256.0791.



5-Fluoro-3-(phenylthio)-1*H*-indole (3c)

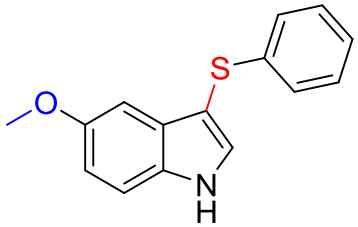
Yellow solid; mp 164–166 ^{o}C; R_f = 0.3 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.84 (brs, 1H), 7.86 (s, 1H), 7.51 (dd, *J* = 7.8, 3.7 Hz, 1H), 7.21 – 7.18 (m, 2H), 7.08 – 7.06 (m, 2H), 7.03 – 7.01(m, 3H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.65 (d, *J* = 233.9 Hz), 138.76, 134.40, 133.31, 129.38 (d, *J* = 10.0 Hz), 128.87, 125.44 , 124.92, 113.63 (d, *J* = 9.7 Hz), 110.43 (d, *J* = 26.0 Hz), 102.89 (d, *J* = 23.8 Hz), 99.62 (d, *J* = 4.7 Hz) ppm; ^{19}F NMR (471 MHz,

DMSO-d_6) δ -123.19 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}FNS$: 244.0591, found: 244.0591.



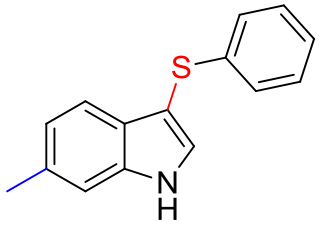
5-Bromo-3-(phenylthio)-1*H*-indole (3d)

Light yellow solid; mp 118–119 °C; R_f = 0.35 (9% EtOAc in petroleum ether);^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (brs, 1H), 7.76 (s, 1H), 7.48 (d, *J* = 2.5 Hz, 1H), 7.34 (td, *J* = 8.6, 1.6 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 1H), 7.20 – 7.17 (m, 2H), 7.10 – 7.07 (m, 3H) ppm;^{13}C NMR (126 MHz, $CDCl_3$) δ 138.67, 135.11, 131.82, 130.98, 128.80, 126.10, 125.90, 125.03, 122.23, 114.47, 113.04, 102.82 ppm; HRMS: calc. for $[M+Na]^+$ $C_{14}H_{10}BrNS$: 325.9615, found: 325.9613.



5-Methoxy-3-(phenylthio)-1*H*-indole (3e)

Dark green oil; R_f = 0.2 (9% EtOAc in petroleum ether);^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (brs, 1H), 7.43 (d, *J* = 2.5 Hz, 1H), 7.32 (d, *J* = 8.8 Hz, 1H), 7.19 – 7.16 (m, 2H), 7.12 – 7.10 (m, 2H), 7.08 – 7.06 (m, 2H), 6.93 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.79 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.12, 139.32, 131.38, 131.31, 129.95, 128.68, 125.69, 124.70, 113.55, 112.40, 102.18, 100.86, 55.77 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NOS$: 256.0791, found: 256.0791.

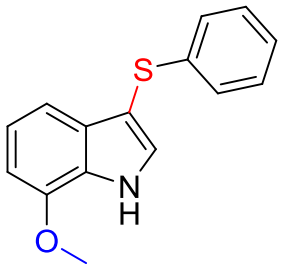


6-Methyl-3-(phenylthio)-1*H*-indole (3f)

Brown black solid; mp 131–132 °C; R_f = 0.4 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (brs, 1H), 7.50 (d, *J* = 8.1 Hz, 1H), 7.39 (s, 1H), 7.22 (s, 1H), 7.19 – 7.16 (m, 2H), 7.13 – 7.11 (m, 2H), 7.07 (t, *J* = 7.2 Hz, 1H), 7.02 (d, *J* = 8.1 Hz, 1H), 2.49 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.37, 136.94, 132.95, 130.05, 128.64, 126.90, 125.78, 124.67, 122.65, 119.24, 111.52, 102.49, 21.65 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NS$: 240.0842, found: 240.0841.

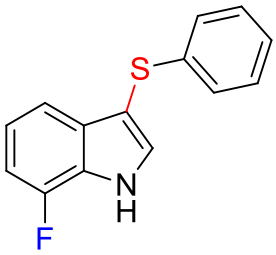
3-(Phenylthio)-1*H*-indol-6-amine (3g)

Dark brown solid; mp 120–121 ^{o}C; R_f = 0.4 (50% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.07 (brs, 1H), 7.39 (d, *J* = 1.7 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 2H), 7.05 – 7.00 (m, 4H), 6.64 (s, 1H), 6.44 (d, *J* = 8.3 Hz, 1H), 4.90 (brs, 2H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 144.76, 139.64, 138.37, 128.88, 128.61, 125.07, 124.43, 120.07, 118.38, 110.72, 98.79, 95.55 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{12}N_2S$: 241.0794, found: 241.0794.



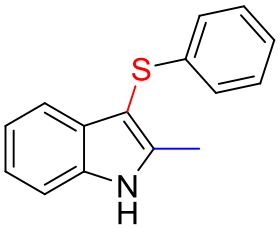
7-Methoxy-3-(phenylthio)-1*H*-indole (3h)

Amorphous; R_f = 0.3 (6% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (brs, 1H), 7.45 (d, *J* = 2.5 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.18 – 7.15 (m, 2H), 7.12 – 7.04 (m, 4H), 6.71 (d, *J* = 7.7 Hz, 1H), 3.99 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.29, 139.35, 130.56, 130.14, 128.63, 127.06, 125.84, 124.68, 121.28, 112.20, 103.12, 102.77, 55.40 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NOS$: 256.0791, found: 256.0791.



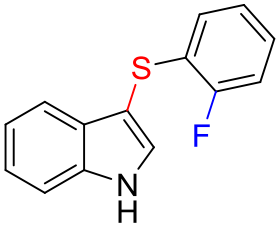
7-Fluoro-3-(phenylthio)-1*H*-indole (3i)

Gray solid; mp 91–92 ^{o}C; R_f = 0.4 (6% EtOAc in petroleum ether); ^{1}H NMR (500 MHz,$CDCl_3$) δ 8.70 (brs, 1H), 7.50 (d, *J* = 2.5 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.20 – 7.16 (m, 2H), 7.12 – 7.05 (m, 4H), 6.98 (dd, *J* = 11.0, 7.8 Hz, 1H) ppm; ^{13}C NMR (126 MHz,$CDCl_3$) δ 149.56 (d, *J* = 245.2 Hz), 138.69, 132.63 (d, *J* = 4.4 Hz), 131.15, 128.73, 126.06, 124.99, 124.90 (d, *J* = 13.9 Hz), 121.14 (d, *J* = 6.2 Hz), 115.41 (d, *J* = 3.6 Hz), 107.88 (d, *J* = 16.1 Hz), 104.13 ppm; ^{19}F NMR (471 MHz,$CDCl_3$) δ -135.15 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}FNS$: 244.0591, found: 244.0609.



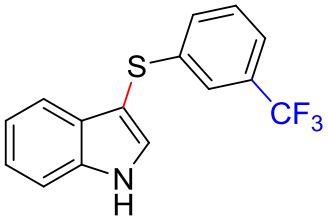
2-Methyl-3-(phenylthio)-1*H*-indole (3j)

Red solid; mp 115–117 °C; R_f = 0.5 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz,$CDCl_3$) δ 8.21 (brs, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.18 – 7.07 (m, 4H), 7.01 – 6.98 (m, 3H), 2.42 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.13, 139.32, 135.42, 130.25, 128.64, 125.47, 124.47, 122.10, 120.62, 118.90, 110.65, 99.21, 12.06 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NS$: 240.0842, found: 240.0841.



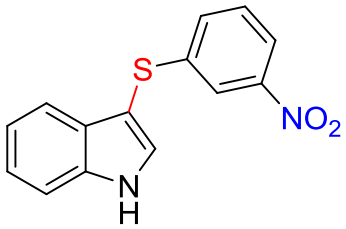
3-(2-Fluorophenylthio)-1*H*-indole (3k)

Gray solid; mp 132–133 °C; R_f = 0.3 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (brs, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.51 (d, *J* = 2.5 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.07 – 7.01 (m, 2H), 6.87 – 6.84 (m, 1H), 6.79 (td, J = 7.8, 1.1 Hz, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.14 (d, *J* = 243.6 Hz), 136.52, 131.10, 129.11, 128.16 (d, *J* = 1.5 Hz), 126.45 (d, *J* = 16.5 Hz), 126.27 (d, *J* = 7.4 Hz), 124.30 (d, *J* = 3.2 Hz), 123.16, 121.03, 119.54, 115.08 (d, *J* = 21.3 Hz), 111.64, 100.94 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}FNS$: 244.0591, found: 244.0591.



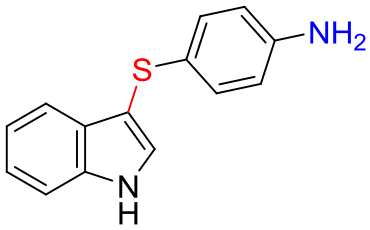
4-(3-(Trifluoromethyl)phenylthio)-1*H*-indole (3l)

Gray solid; mp 69–70 °C; R_f = 0.15 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (brs, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.57 (s, 1H), 7.51 (s, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.36 – 7.29 (m, 3H), 7.23 – 7.19 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.43, 135.23, 131.77, 131.46, 131.13 (q, *J* = 32.1 Hz), 129.64, 129.17, 125.11 (q, *J* = 3.8 Hz), 124.88, 123.18, 122.38 (q, *J* = 3.6 Hz), 121.10, 120.09, 111.49, 97.30 ppm; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.70 ppm; HRMS: calc. for $[M+Na]^+$ $C_{15}H_{10}F_3NS$: 316.0384, found: 316.0378 .



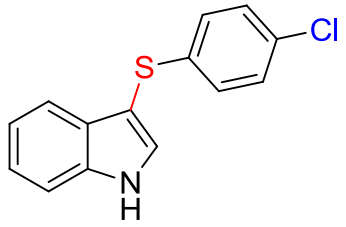
3-(3-Nitrophenylthio)-1*H*-indole (3m)

Orange solid; mp 124–126 °C; R_f = 0.3 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (brs, 1H), 7.92 (s, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.55 (s, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.19 (t, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.62, 142.57, 136.59, 131.30, 131.23, 129.28, 128.48, 123.44, 121.30, 120.23, 119.62, 119.14, 111.89, 100.82 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}N_2O_2S$: 271.0536, found: 271.0526.



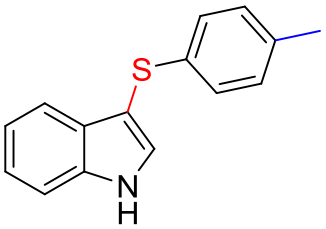
4-(1*H*-Indol-3-ylthio)aniline (3n)

Brown solid; mp 108–109 °C; R_f = 0.45 (50% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.46 (brs, 1H), 7.63 (s, 1H), 7.48 (d, *J* = 7.4 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 7.4 Hz, 1H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.98 – 6.96 (m, 2H), 6.47 – 6.45 (m, 2H), 5.24 (brs, 2H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 146.75, 136.37, 130.57, 129.82, 128.53, 122.69, 121.66, 119.52, 118.40, 114.52, 111.92, 103.51 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{12}N_2S$: 241.0794, found: 241.0794.



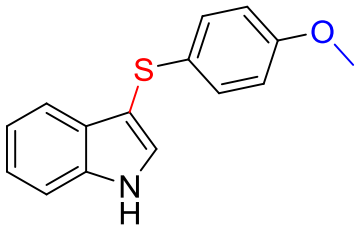
3-(4-Chlorophenylthio)-1*H*-indole (3o)

Yellow solid; mp 124–125 °C; R_f = 0.4 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (brs, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.48 (s, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.12 (d, *J* = 8.5 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.82, 136.52, 130.68, 130.54, 128.80, 128.73, 127.12, 123.18, 121.03, 119.48, 111.65, 102.46 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}ClNS$: 260.0295, found: 260.0278.



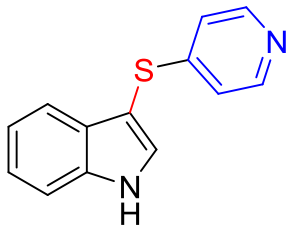
3-(*p*-Tolylthio)-1*H*-indole (3p)

Brown solid; mp 116–117 ^{o}C; R_f = 0.4 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (brs, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.46 (d, *J* = 2.5 Hz, 1H), 7.43 (d, *J* = 8.2 Hz, 1H), 7.29 – 7.26 (m, 1H),7.19 – 7.16 (m, 1H), 7.06 – 7.04 (m, 2H), 7.00 – 6.98 (m, 2H), 2.26 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.47, 135.47, 134.64, 130.36, 129.46, 129.12, 126.30, 122.95, 120.81, 119.69, 111.49, 103.60, 20.82 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NS$: 240.0842, found: 240.0835.



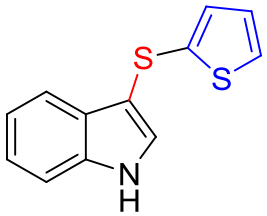
3-(4-Methoxyphenylthio)-1*H*-indole (3q)

Brown solid; mp 96–98 ^{o}C; R_f = 0.3 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (brs, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.45 (d, *J* = 2.4 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.27 – 7.24 (m, 1H), 7.18 – 7.13 (m, 3H), 6.74 (d, *J* = 8.8 Hz, 2H), 3.73 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.79, 136.46, 129.98, 129.52, 129.00, 128.58, 122.90, 120.74, 119.62, 114.48, 111.49, 104.64, 55.31 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NOS$: 256.0791, found: 256.0784.



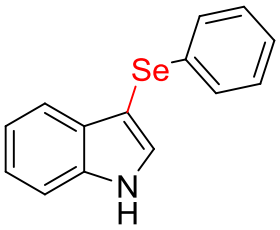
3-(Pyridin-4-ylthio)-1*H*-indole (3r)

Light yellow solid; mp 172–173 ^{o}C; R_f = 0.3 (33% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.88 (brs, 1H), 8.26 (d, *J* = 5.0 Hz, 2H), 7.84 (d, *J* = 1.6 Hz, 1H), 7.54 (d, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.93 (d, *J* = 5.0 Hz, 2H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 150.70, 149.05, 136.69, 132.98, 128.15, 122.28, 120.34, 119.38, 117.90, 112.46, 95.97 ppm; HRMS: calc. for $[M+H]^+$ $C_{13}H_{10}N_2S$: 227.0638, found: 227.0637.



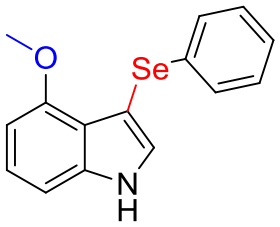
3-(Thiophen-2-ylthio)-1*H*-indole (3s)

Tan solid; mp 84–85 ^{o}C; R_f = 0.4 (9% EtOAc in petroleum ether);^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (brs, 1H), 7.75 (d, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 2.6 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.19 – 7.13 (m, 2H), 7.09 (dd, *J* = 5.3, 0.9 Hz, 1H), 7.05 (dd, *J* = 3.5, 1.0 Hz, 1H), 6.82 – 6.80 (m, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.91, 136.10, 129.77, 129.23, 128.45, 127.26, 127.20, 122.91, 120.77, 119.36, 111.52, 106.60 ppm; HRMS: calc. for $[M+Na]^+$ $C_{12}H_9NS_2$: 254.0074, found: 254.0066.



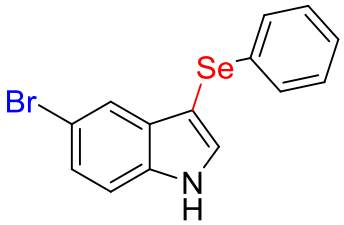
3-(Phenylselanyl)-1*H*-indole (3t)

Brown solid; mp 113–114 ^{o}C; R_f = 0.15 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz,$CDCl_3$) δ 8.45 (brs, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.47 (d, *J* = 2.5 Hz, 1H), 7.44 (d, *J* = 8.2 Hz, 1H), 7.29 – 7.24 (m, 3H), 7.20 – 7.17 (m, 1H), 7.16 – 7.09 (m, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.40, 133.78, 131.18, 129.97, 128.92, 128.70, 125.58, 122.91, 120.83, 120.35, 111.34, 98.21 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{11}NSe$: 274.0130, found: 274.0153.



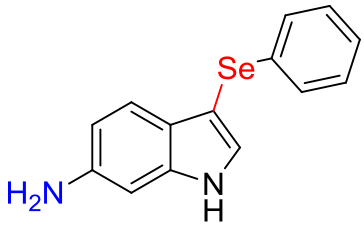
4-Methoxy-3-(phenylselanyl)-1*H*-indole (3u)

White solid; mp 82–83 ^{o}C; R_f = 0.35 (11% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (brs, 1H), 7.39 (d, *J* = 7.2 Hz, 2H), 7.20 – 7.13 (m, 5H), 7.02 (d, *J* = 8.1 Hz, 1H), 6.55 (d, *J* = 7.8 Hz, 1H), 3.77 (s, 3H) ppm; ^{13}C NMR (126 MHz,$CDCl_3$) δ 154.59, 138.35, 134.62, 130.01, 128.99, 128.73, 125.72, 123.66, 118.97, 104.57, 101.15, 97.01, 55.41 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NOSe$: 304.0235, found: 304.0230.



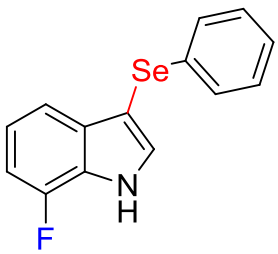
5-Bromo-3-(phenylselanyl)-1*H*-indole (3v)

Pink solid; mp 101–102 ^{o}C; R_f = 0.25 (11% EtOAc in petroleum ether);^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (brs, 1H), 7.76 (s, 1H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.32 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.23 (d, *J* = 9.1 Hz, 1H), 7.21 – 7.19 (m, 2H), 7.14 – 7.10 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.00, 133.29, 132.34, 131.84, 129.05, 128.73, 125.94, 125.83, 122.92, 114.35, 112.83, 97.92 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}BrNSe$: 351.9235, found: 351.9233.



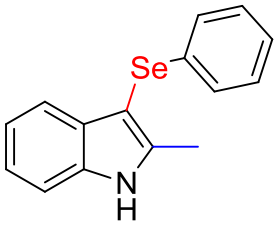
3-(Phenylselanyl)-1*H*-indol-6-amine (3w)

Black solid; mp 167–169 ^{o}C; R_f = 0.3 (50% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.06 (brs, 1H), 7.35 (s, 1H), 7.16 – 7.15 (m, 4H), 7.11 – 7.07 (m, 1H), 7.06 – 7.03 (m, 1H), 6.64 (d, *J* = 4.4 Hz, 1H), 6.46 – 6.43 (m, 1H), 4.87 (brs, 2H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 144.65, 138.21, 134.08, 129.22, 128.82, 127.85, 125.24, 121.02, 119.04, 110.67, 95.30, 94.64 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{12}N_2Se$: 289.0239, found: 289.0267.



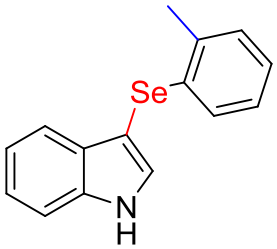
7-Fluoro-3-(phenylselanyl)-1*H*-indole (3x)

White solid; mp 91–92 ^{o}C; R_f = 0.45 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (brs, 1H), 7.50 (s, 1H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.25 (d, *J* = 9.0 Hz, 2H), 7.17 – 7.07 (m, 4H), 7.01 – 6.97 (m, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.42 (d, *J* = 245.2 Hz), 133.52 (d, *J* = 4.4 Hz), 133.29 , 131.64, 129.00, 128.86, 125.80, 124.78 (d, *J* = 13.3 Hz), 121.03 (d, *J* = 6.2 Hz), 116.13 (d, *J* = 3.5 Hz), 107.74 (d, *J* = 15.9 Hz), 99.22 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}FNSe$: 292.0035, found: 292.0064.



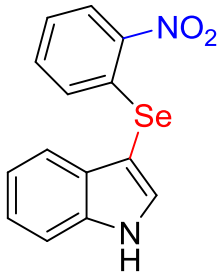
2-Methyl-3-(phenylselanyl)-1*H*-indole (3y)

Red solid; mp 89–91 ^{o}C; R_f = 0.25 (9% EtOAc in petroleum ether);^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.19 – 7.06 (m, 7H), 2.47 (s, 3H) ppm; ^{13}C NMR (126 MHz,$CDCl_3$) δ 140.80, 135.72, 133.88, 131.18, 128.90, 128.31, 125.33, 122.04, 120.58, 119.69, 110.48, 96.17, 13.06 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NSe$: 288.0286, found: 288.0290.



3-(*o*-Tolylselanyl)-1*H*-indole (3z)

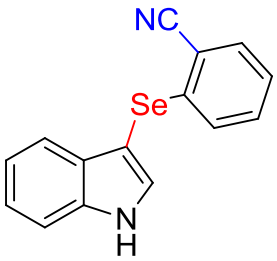
Brown solid; mp 83–85 ^{o}C; R_f = 0.4 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.69 (brs, 1H), 7.71 (s, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.38 (d, *J* = 6.7 Hz, 1H), 7.20 – 7.15 (m, 2H), 7.06 (t, *J* = 7.4 Hz, 1H), 7.01 (t, *J* = 7.2 Hz, 1H), 6.87 (t, *J* = 7.5 Hz, 1H), 6.70 – 6.69 (m, 1H), 2.40 (s, 3H) ppm;^{13}C NMR (126 MHz, DMSO-d_6) δ 136.64, 135.34, 134.17, 132.91, 129.70, 129.53, 127.20, 126.34, 125.23, 121.91, 119.92, 118.87, 112.04, 93.97, 20.68 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NSe$: 288.0286, found: 288.0291.



3-(2-Nitrophenylselanyl)-1*H*-indole (3aa)

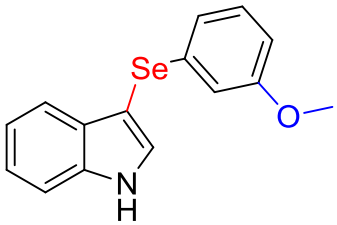
Yellow amorphous; R_f = 0.15 (17% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.89 (brs, 1H), 8.33 (d, *J* = 7.9 Hz, 1H), 7.83 (d, *J* = 2.2 Hz, 1H), 7.55 (d, *J* = 8.2 Hz, 1H), 7.44 – 7.37 (m, 2H), 7.34 (d, *J* = 7.9 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.08 (t, *J* = 7.4 Hz, 1H), 6.96 (d, *J* = 7.8 Hz, 1H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 145.26, 136.84, 135.19, 134.18, 133.90, 129.43, 129.25, 126.23, 126.02, 122.23, 120.33, 118.73, 112.25, 95.24 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}N_2O_2Se$:

318.9980, found: 319.0005.



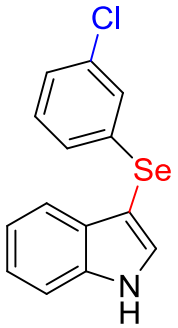
2-(1*H*-Indol-3-ylselanyl)benzonitrile (3ab)

Gray solid; mp 101–102 °C; R_f = 0.2 (25% EtOAc in petroleum ether); ^{1}H NMR (500 MHz,$CDCl_3$) δ 8.67 (brs, 1H), 7.61 – 7.56 (m, 3H), 7.49 (d, *J* = 8.2 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.22 – 7.14 (m, 3H), 7.02 (d, *J* = 7.8 Hz, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.60, 136.48, 133.35, 132.77, 132.05, 129.66, 129.59, 125.76, 123.26, 121.22, 120.04, 117.60, 112.25, 111.60, 96.43 ppm; HRMS: calc. for $[M+Na]^+$ $C_{15}H_{10}N_2S$: 320.2031, found: 320.2059.



3-(3-Methoxyphenylselanyl)-1*H*-indole (3ac)

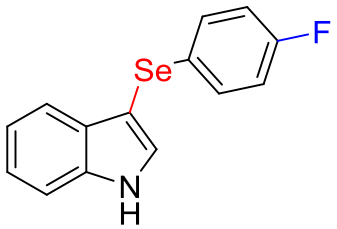
Amorphous; R_f = 0.2 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (brs, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.45 (s, 1H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.26 (t, *J* = 7.4 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.06 (t, *J* = 7.9 Hz, 1H), 6.85 – 6.81 (m, 2H), 6.65 (d, *J* = 8.1 Hz, 1H), 3.67 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.95, 136.43, 135.09, 131.24, 129.99, 129.65, 122.92, 121.09, 120.85, 120.34, 114.41, 111.34, 111.29, 98.14, 55.10 ppm; HRMS: calc. for $[M+H]^+$ $C_{15}H_{13}NOSe$: 304.0235, found: 304.0230.



3-(3-Chlorophenylselanyl)-1*H*-indole (3ad)

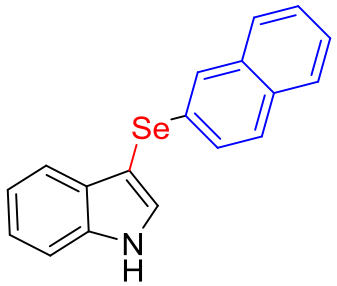
White solid; mp 95–97 °C; R_f = 0.4 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (brs, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.48 (d, *J* = 2.3 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.30

(t, *J* = 7.6 Hz, 1H), 7.23 – 7.20 (m, 2H), 7.12 – 7.03 (m, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.39, 135.80, 134.79, 131.43, 129.85, 129.73, 128.21, 126.65, 125.76, 123.11, 121.05, 120.17, 111.44, 97.52 ppm; HRMS: calc. for $[M+Na]^+$ $C_{14}H_{10}ClNSe$: 329.9865, found: 329.9862.



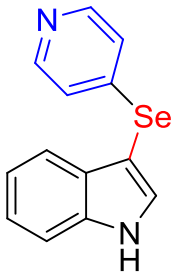
3-(4-Fluorophenylselanyl)-1*H*-indole (3ae)

Brown solid; mp 105–106 °C; R_f = 0.3 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (brs, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.40 – 7.37 (m, 2H),7.26 (t, *J* = 7.6 Hz, 1H), 7.23 – 7.17 (m, 3H), 6.83 (t, *J* = 8.5 Hz, 2H) ppm; ^{13}CNMR (126 MHz, $CDCl_3$) δ 161.48 (d, *J* = 244.7 Hz), 136.31 , 130.99, 130.71 (d, *J* = 7.6 Hz), 129.67, 127.86 (d, *J* = 3.3 Hz), 122.96, 120.88 , 120.13 ,115.98 (d, *J* = 21.7 Hz) , 111.40 , 98.51 ppm; ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.02 ppm; HRMS: calc. for $[M+H]^+$ $C_{14}H_{10}FNSe$: 292.0035, found: 292.0040.



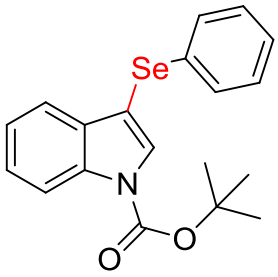
3-(Naphthalen-2-ylselanyl)-1*H*-indole (3af)

Yellow solid; mp 152–154 °C; R_f = 0.15 (9% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.75 (brs, 1H), 7.82 (d, *J* = 2.5 Hz, 1H), 7.80 – 7.78 (m, 1H), 7.72 – 7.70 (m, 2H), 7.66 – 7.64 (m, 1H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.44 – 7.39 (m, 3H), 7.29 (dd, *J* = 8.6, 1.3 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 136.58, 133.37, 132.72, 131.23, 131.13, 129.43, 128.20, 127.51, 126.58, 126.49, 126.41, 126.05, 125.33, 121.92, 119.94, 118.89, 112.04, 94.95 ppm; HRMS: calc. for $[M+H]^+$ $C_{18}H_{13}NSe$: 324.0286, found: 324.0299.



3-(Pyridin-4-ylselanyl)-1*H*-indole (3ag)

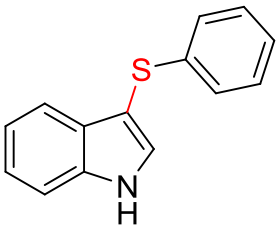
Light yellow oil; R_f = 0.3 (33% EtOAc in petroleum ether); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.85 (brs, 1H), 8.22 (d, *J* = 5.5 Hz, 2H), 7.80 (d, *J* = 2.5 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.11 – 7.07 (m, 3H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 149.12, 146.22, 136.64, 133.34, 129.10, 122.41, 122.14, 120.24, 118.64, 112.21, 92.47 ppm; HRMS: calc. for $[M+H]^+$ $C_{13}H_{10}N_2Se$: 275.0082, found: 275.0060.



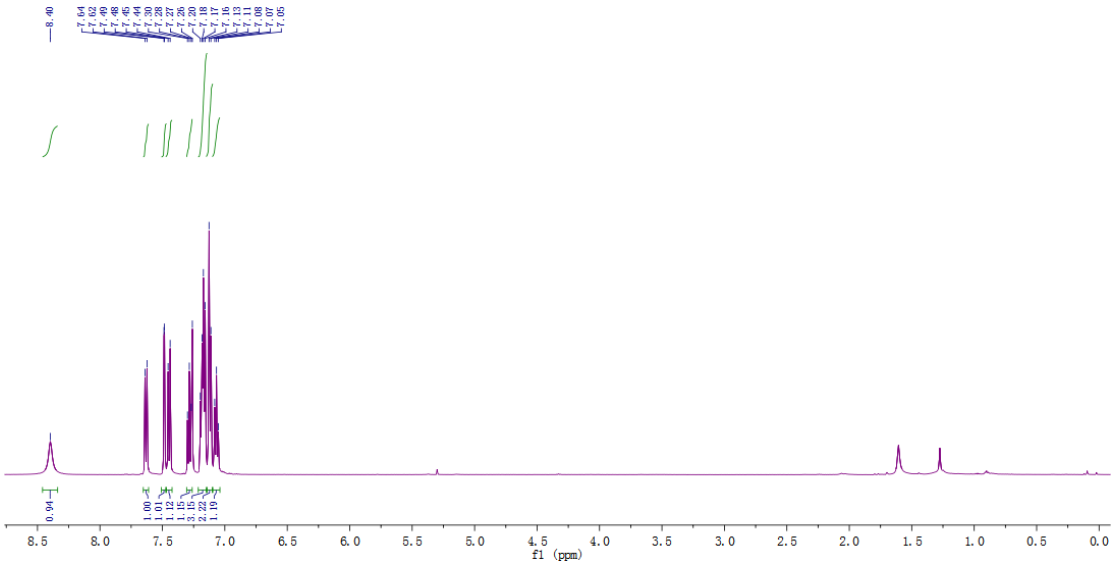
***Tert*-butyl 3-(phenylselanyl)-1H-indole-1-carboxylate (3ah)**

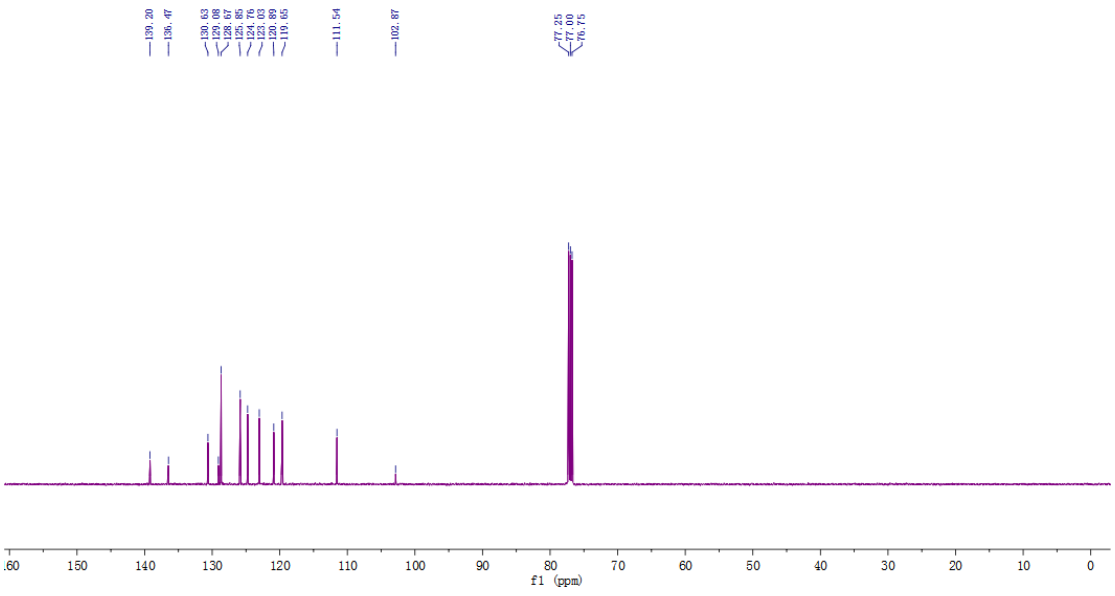
Colorless oil; R_f = 0.3 (100% petroleum ether); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 7.8 Hz, 1H) , 7.90 (s, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.33 – 7.32 (m, 2H), 7.26 (t, *J* = 7.5 Hz, 1H), 7.20 – 7.15 (m, 3H), 1.70 (s, 9H) ppm; ^{13}CNMR (126 MHz, $CDCl_3$) δ 149.07, 135.72, 131.85, 129.64, 129.09, 126.20, 124.98, 123.24, 120.72, 115.20, 104.58, 84.29, 28.15 ppm; HRMS: calc. for $[M+H]^+$ $C_{19}H_{19}NO_2Se$: 374.0654, found: 374.0645.

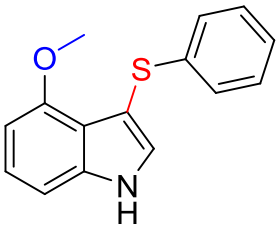
Copies of ^{1}H, ^{13}C and F^{19} NMR spectrum of products



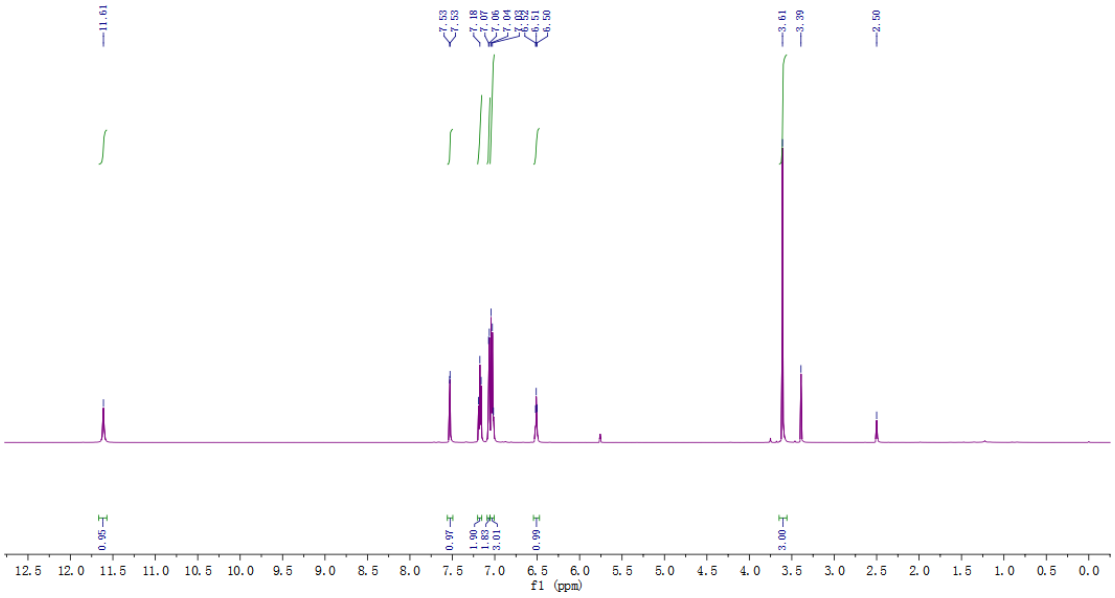
3a

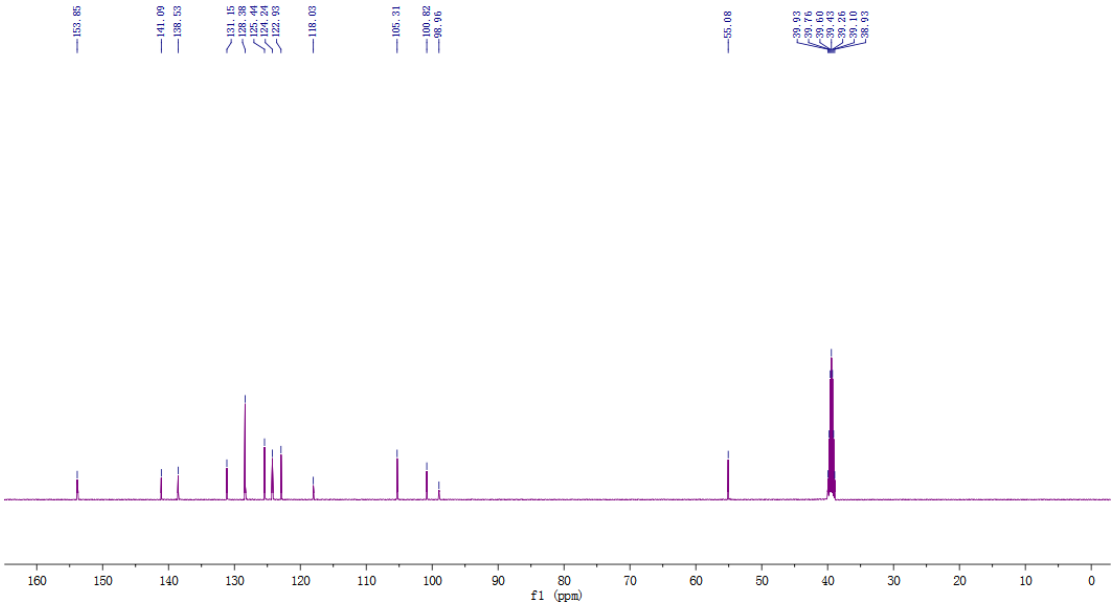


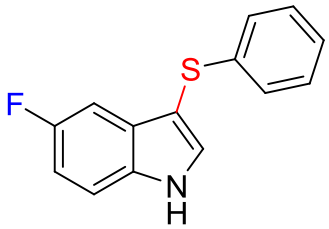



O
S
N
H

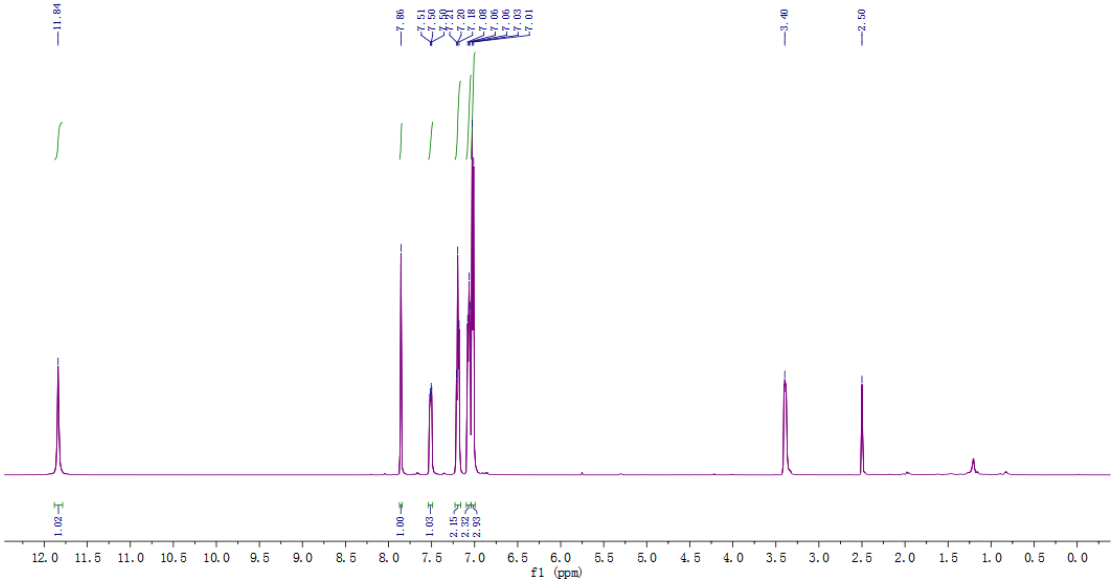
3b

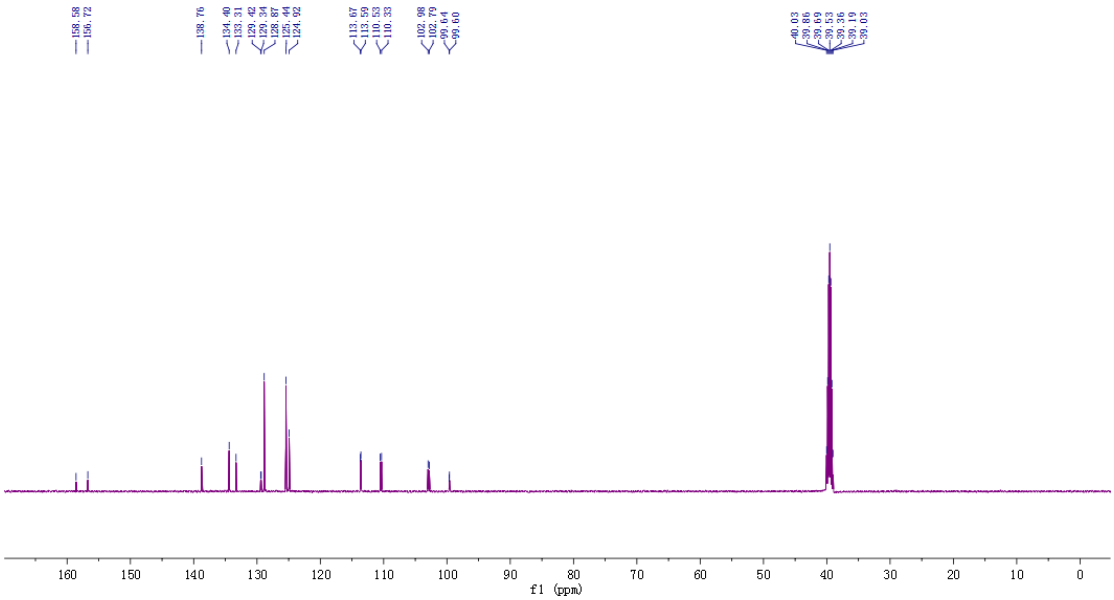

11.61
7.53
7.53
7.18
7.07
7.06
7.04
6.52
6.51
6.50
3.61
3.39
2.50
0.95
0.97
1.90
1.83
3.01
0.99
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

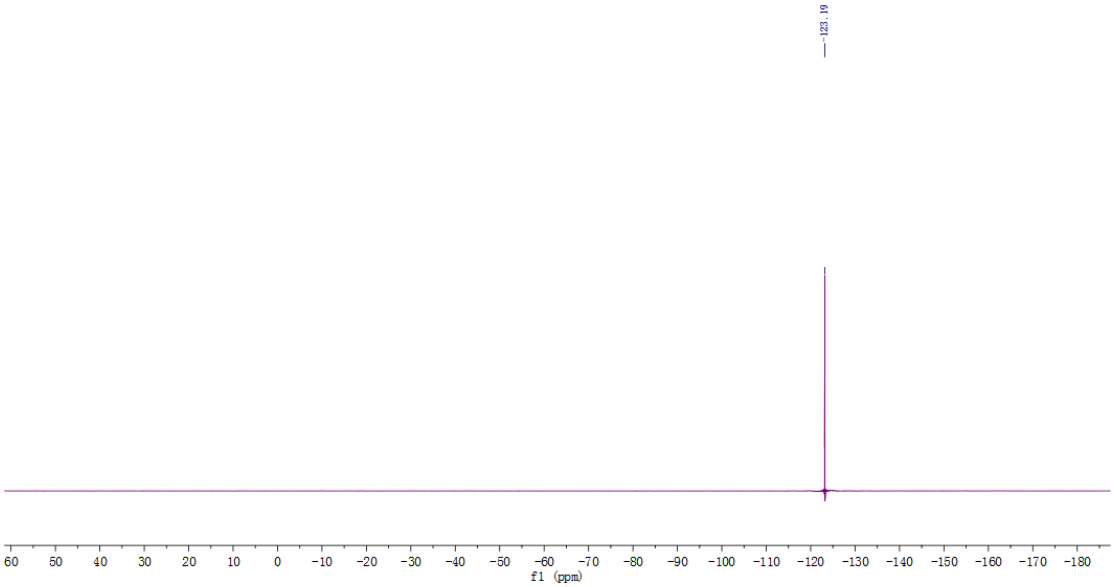

153.85
141.09
138.53
131.15
128.38
125.44
124.24
122.93
118.03
105.31
100.82
98.96
55.08
39.93
39.76
39.60
39.43
39.26
39.10
38.93
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

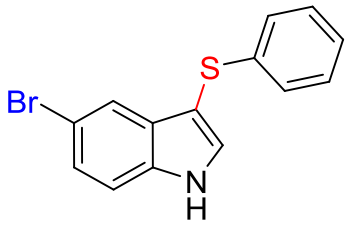

S
F
N
H

3c

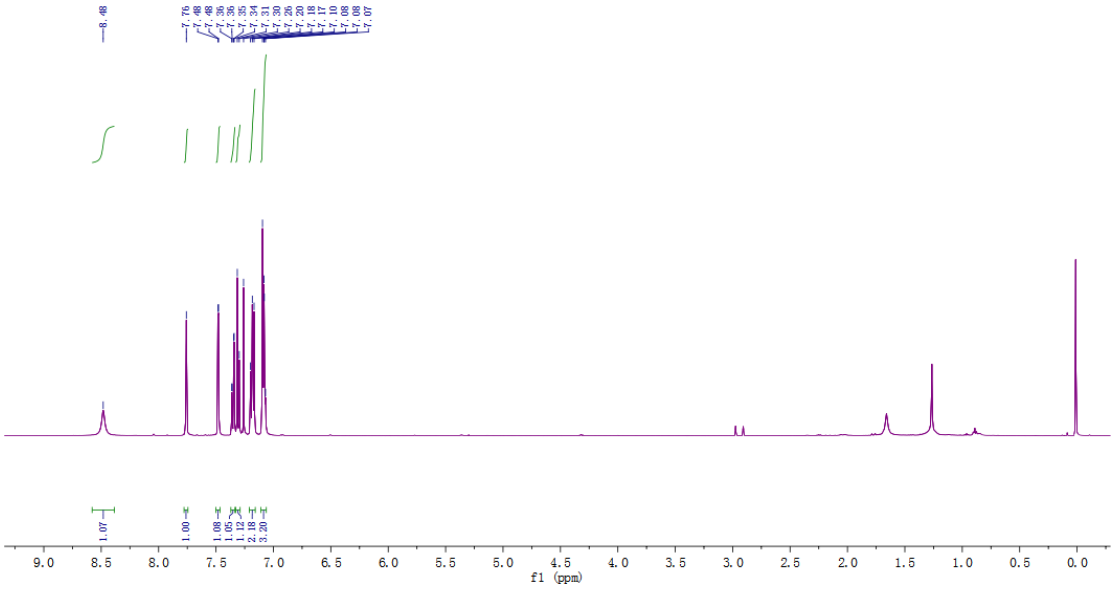

11.84
7.86
7.51
7.50
7.50
7.20
7.18
7.08
7.06
7.06
7.05
7.01
3.40
2.50
1.02
1.00
1.03
2.15
2.32
2.93
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

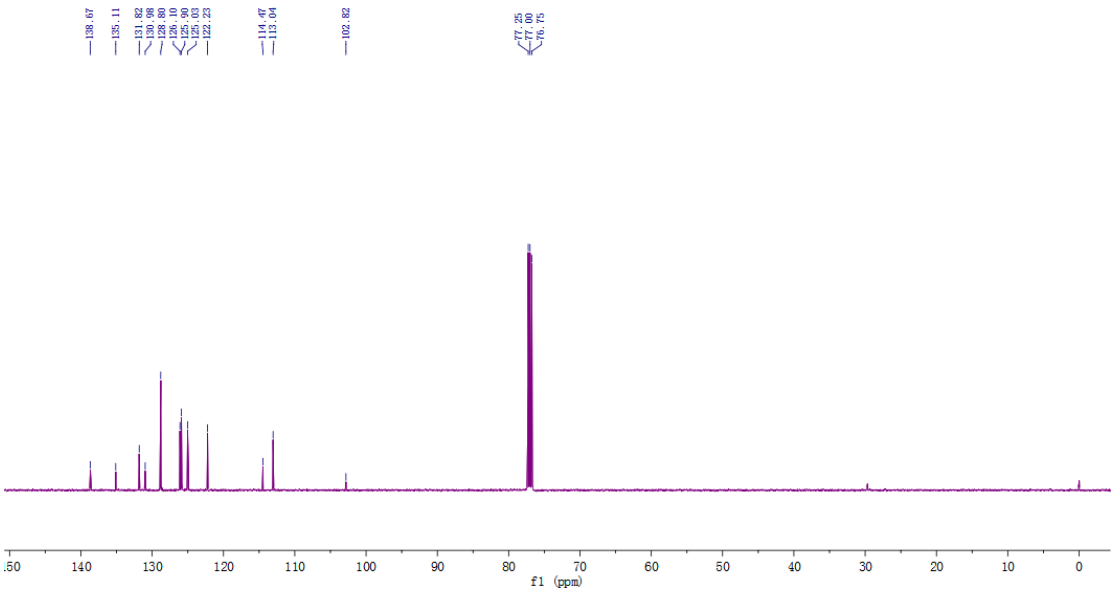

158.58
156.72
138.76
134.40
133.31
129.42
129.34
128.87
125.44
124.92
113.67
113.59
110.53
110.33
102.98
102.79
99.64
99.60
40.03
39.86
39.69
39.53
39.36
39.19
39.03
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

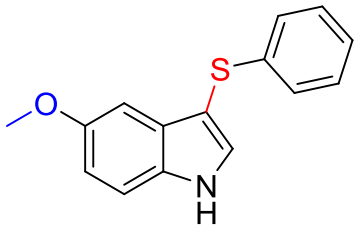

-123.19
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)


Br
S
N
H

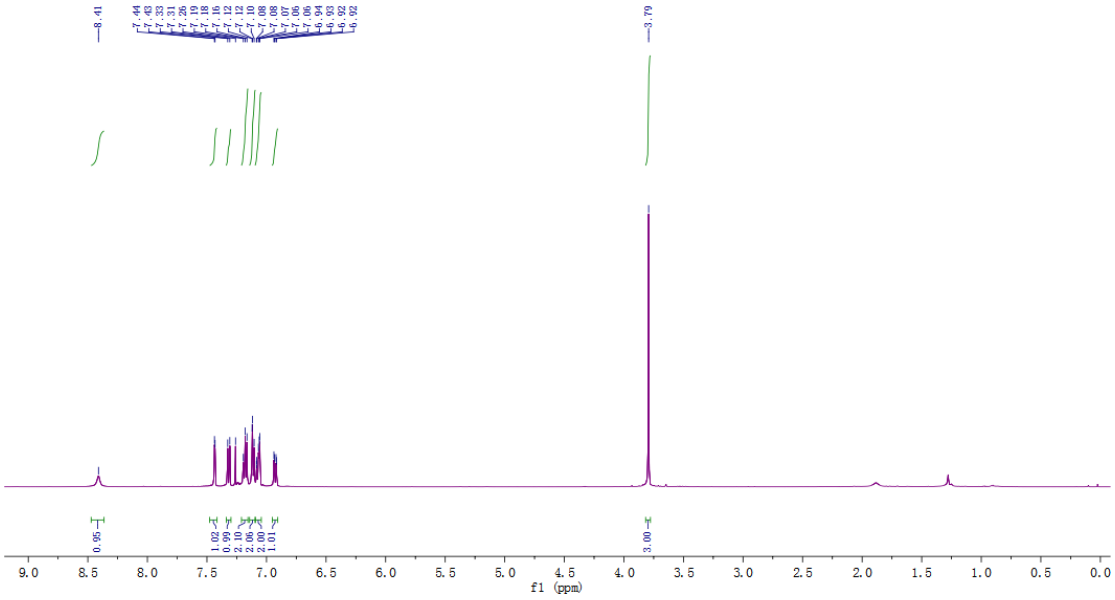
3d

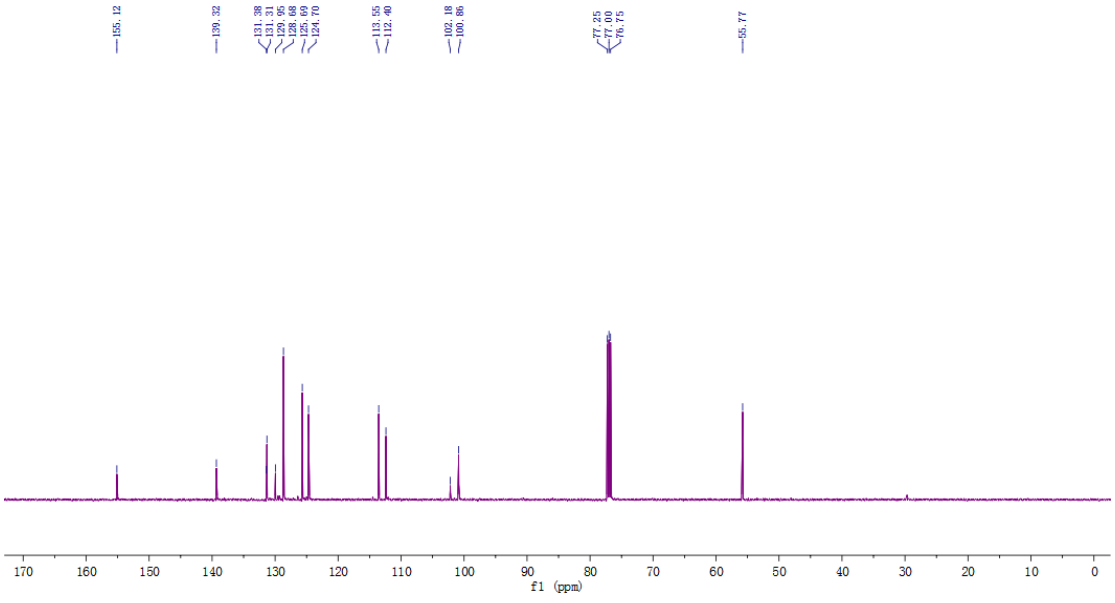

8.48
7.76
7.48
7.36
7.35
7.34
7.31
7.30
7.26
7.20
7.18
7.17
7.10
7.08
7.08
7.07
1.07
1.00
1.08
1.05
1.12
1.18
2.18
3.20
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

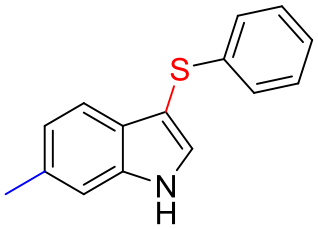

138.67
135.11
131.82
130.98
128.80
126.10
125.89
125.03
122.23
114.47
113.04
102.82
77.25
77.00
76.75
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


S
O
N
H

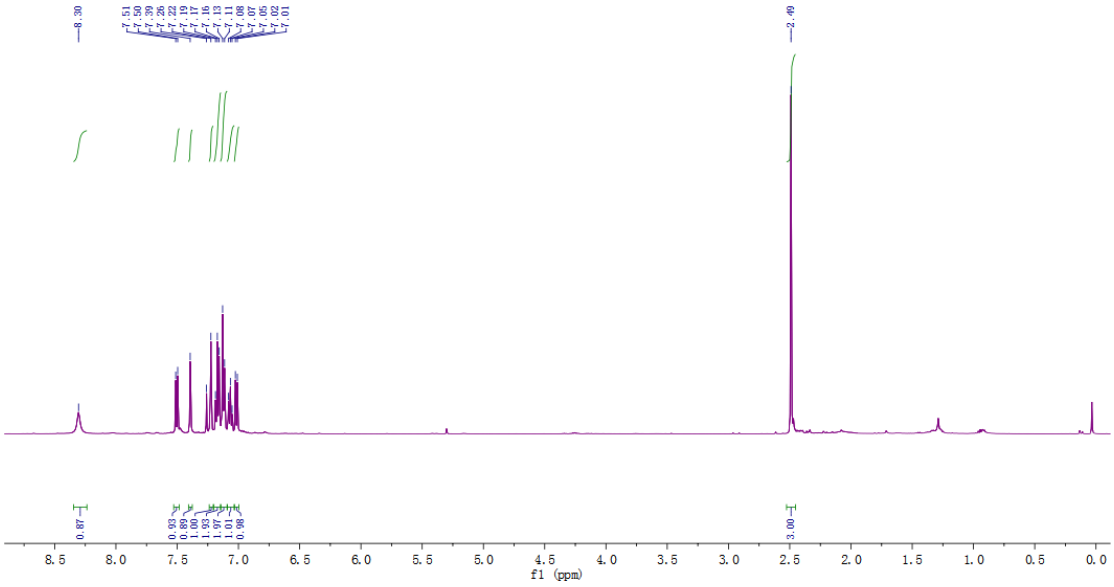
3e

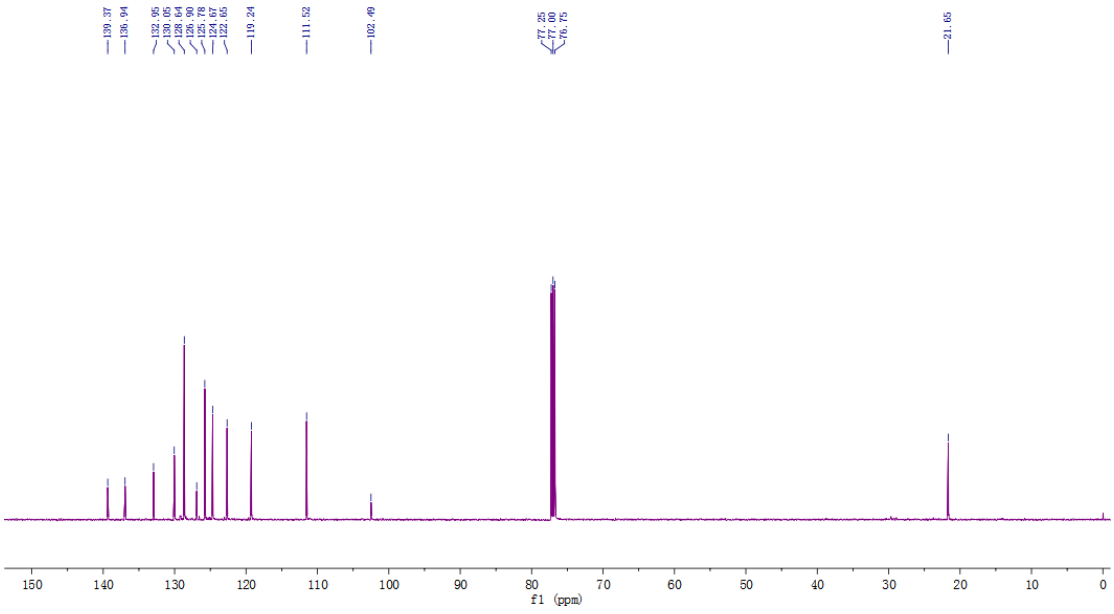

8.41
7.44
7.43
7.33
7.31
7.26
7.19
7.18
7.16
7.12
7.12
7.12
7.10
7.08
7.08
7.07
7.06
7.06
6.94
6.93
6.92
6.92
3.79
0.95
1.02
0.99
2.10
2.06
2.00
1.01
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

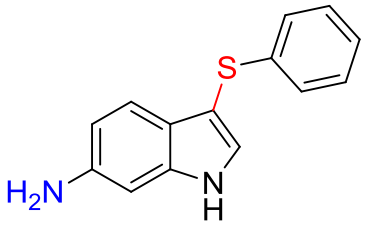

155.12
139.32
131.38
131.31
129.95
128.68
125.69
124.70
113.55
112.40
102.18
100.86
77.25
77.00
76.75
55.77
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


S
N
H

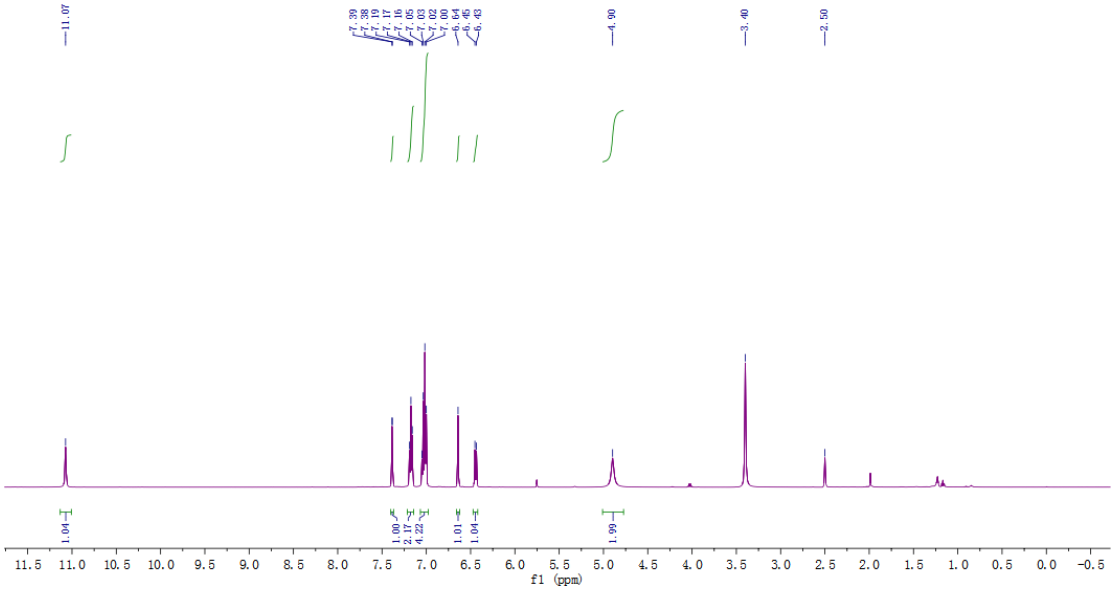
3f

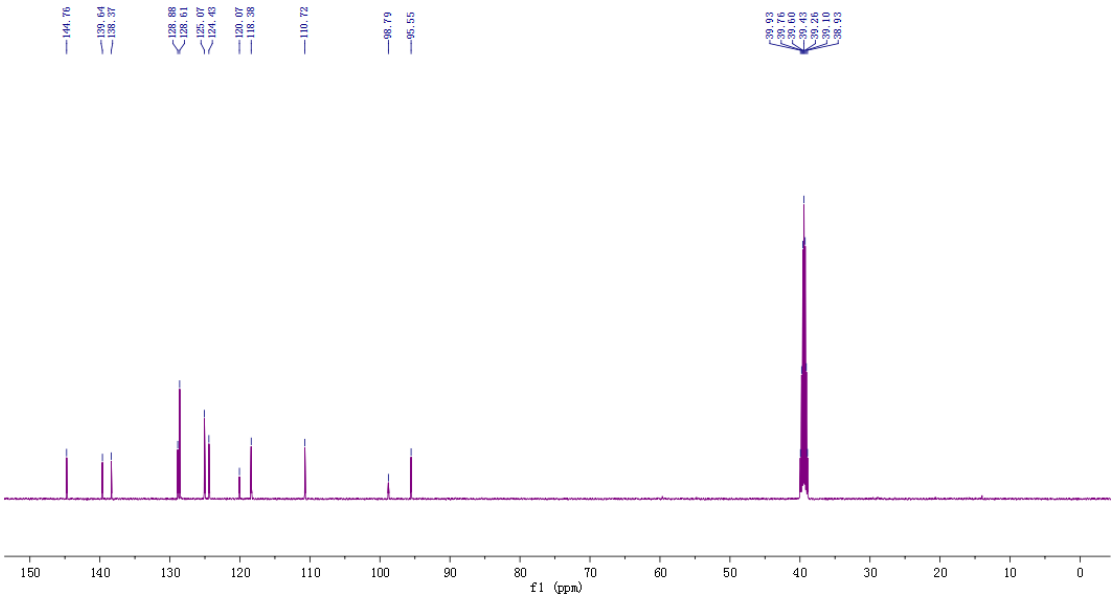

8.30
7.51
7.50
7.39
7.26
7.22
7.19
7.17
7.16
7.13
7.11
7.08
7.07
7.05
7.02
7.01
2.49
0.87
0.93
0.89
1.00
1.93
1.97
1.01
0.98
3.00
f1 (ppm)

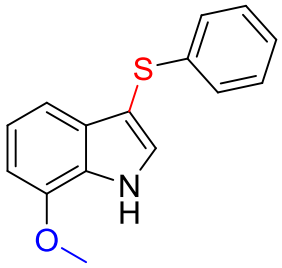

139.37
136.94
132.95
130.05
128.64
126.90
125.78
124.67
122.65
119.24
111.52
102.49
77.25
77.00
76.75
21.65
f1 (ppm)


S
H2N
N
H

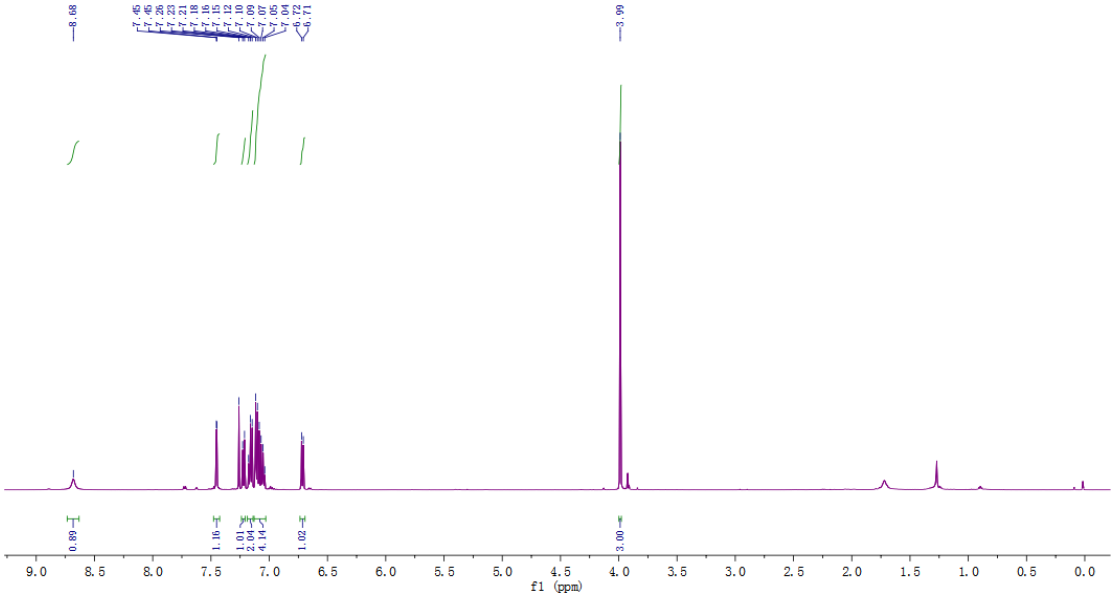
3g

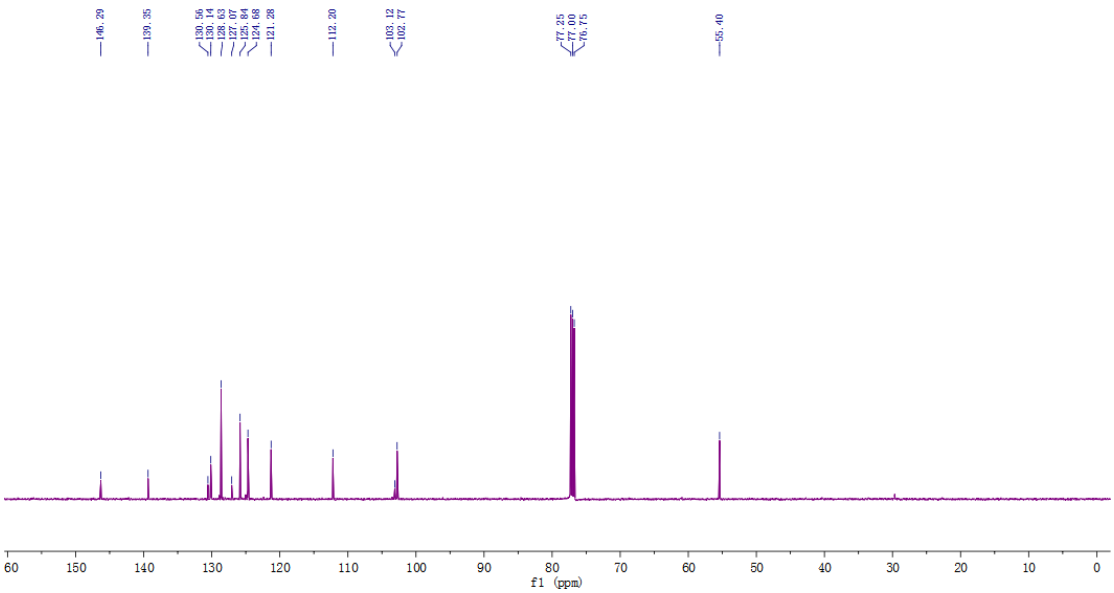

11.07
7.39
7.38
7.19
7.17
7.16
7.05
7.03
7.02
7.00
6.64
6.45
6.43
4.90
3.40
2.50
1.04
1.00
2.17
4.22
1.01
1.04
1.99
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

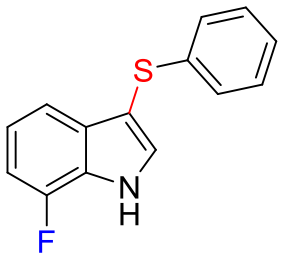

144.76
139.64
138.97
128.88
128.61
125.07
124.43
120.07
118.38
110.72
98.79
95.55
39.93
39.76
39.60
39.43
39.26
39.10
38.93
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


S
N
H
O

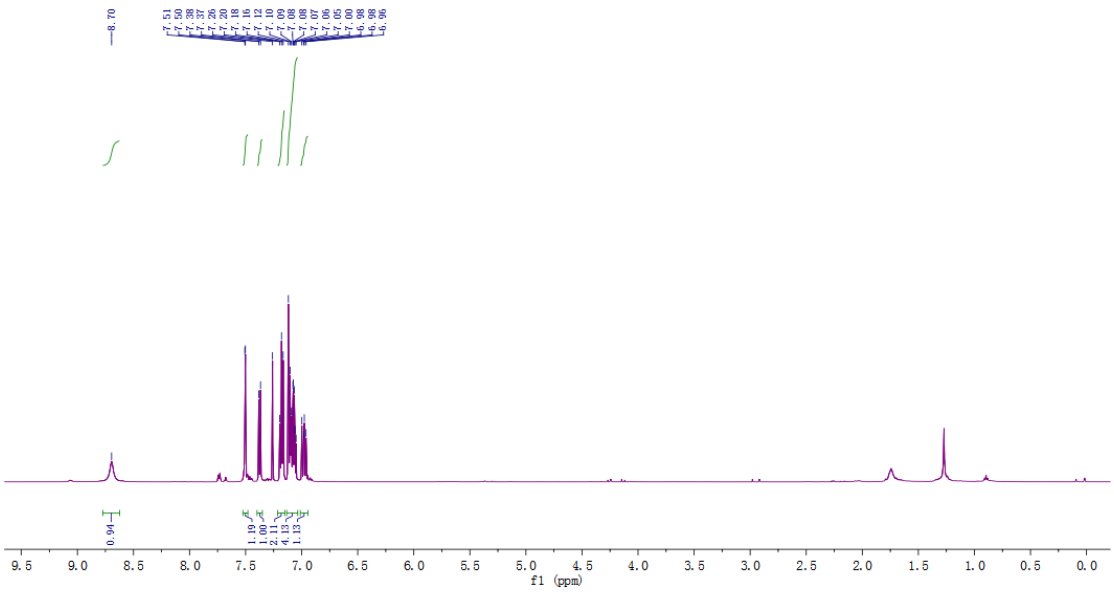
3h

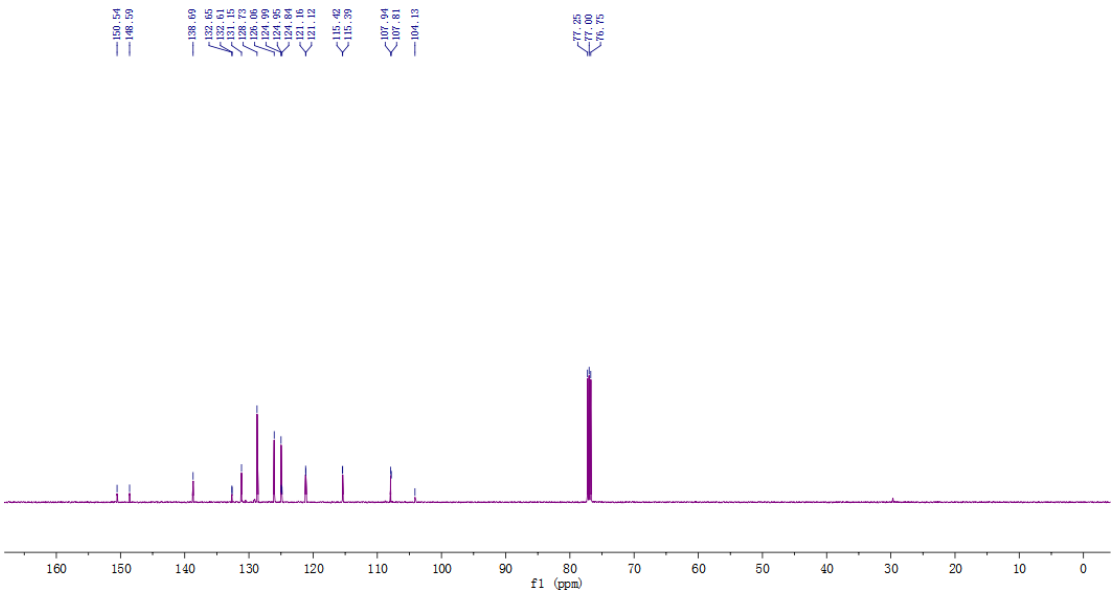

8.68
7.45
7.45
7.26
7.23
7.21
7.18
7.16
7.15
7.12
7.10
7.09
7.07
7.05
7.04
6.72
6.71
3.99
0.89
1.16
1.01
2.04
4.14
1.02
3.00
f1 (ppm)

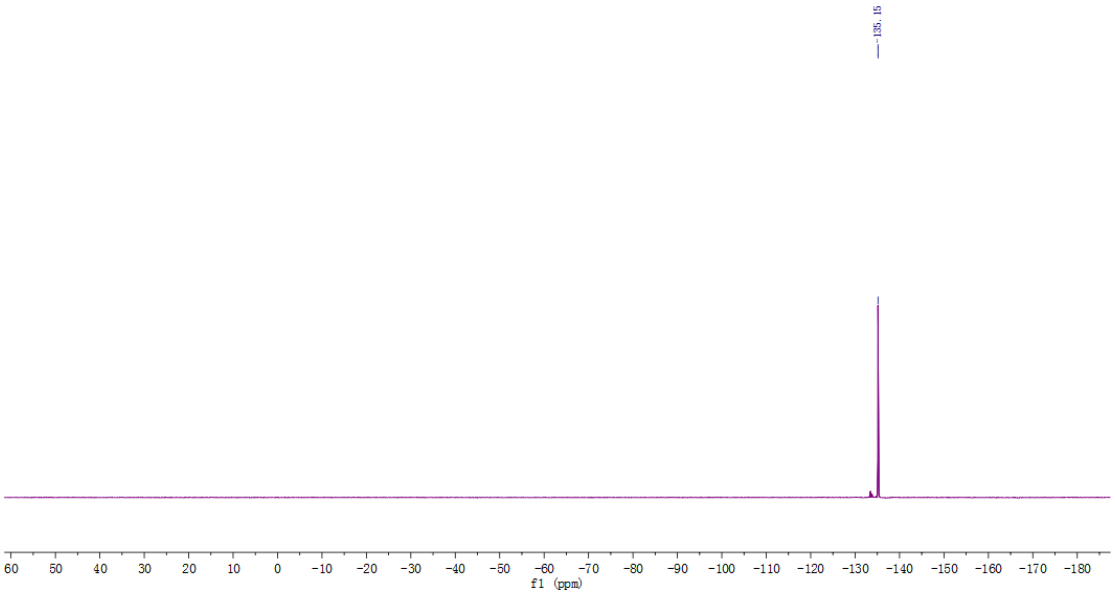

146.29
139.35
130.56
130.14
128.63
127.07
125.84
124.68
121.28
112.20
103.12
102.77
77.25
77.00
76.75
55.40
f1 (ppm)

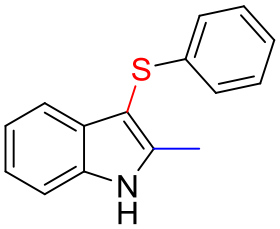

S
N
H
F

3i

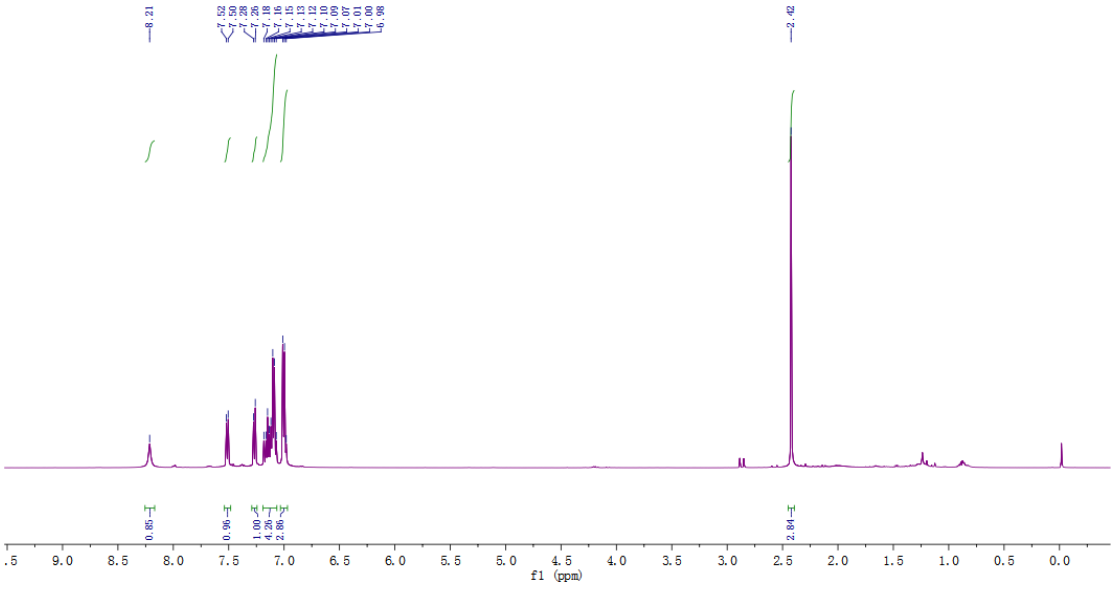

8.70
7.51
7.50
7.38
7.37
7.36
7.20
7.18
7.16
7.12
7.10
7.09
7.08
7.08
7.07
7.06
7.05
7.00
6.98
6.96
0.94
1.19
1.00
2.11
4.13
1.13
f1 (ppm)

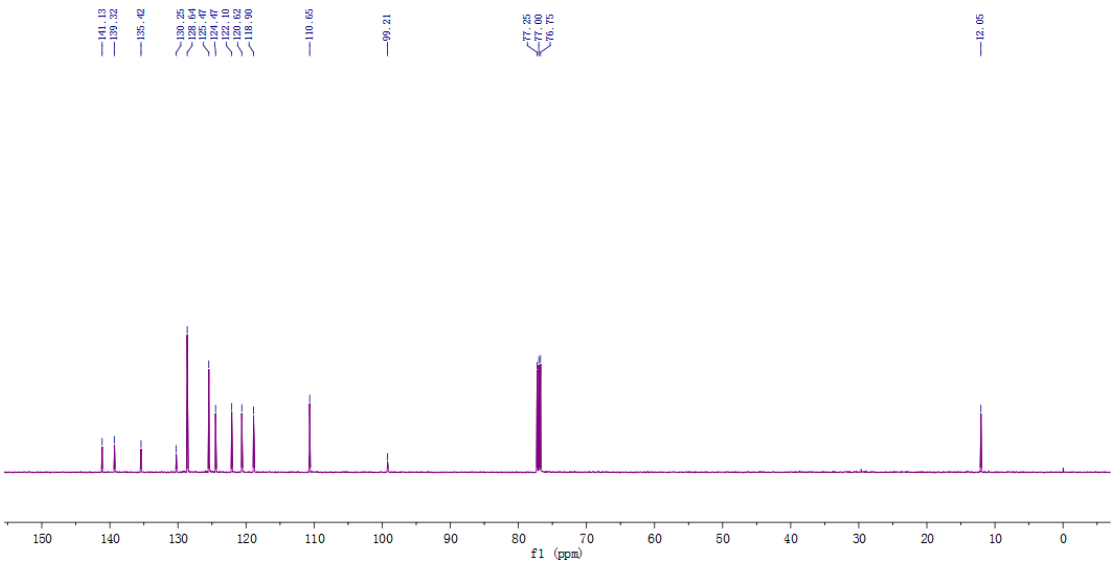

150.54
146.59
138.69
132.65
132.61
131.15
128.73
126.96
124.99
124.95
124.84
121.16
121.12
115.42
115.39
107.94
107.81
104.13
77.25
77.00
76.75
f1 (ppm)

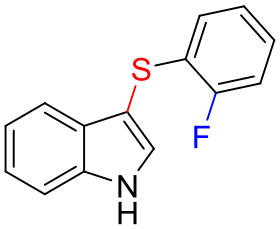

135.15
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)


S
N
H

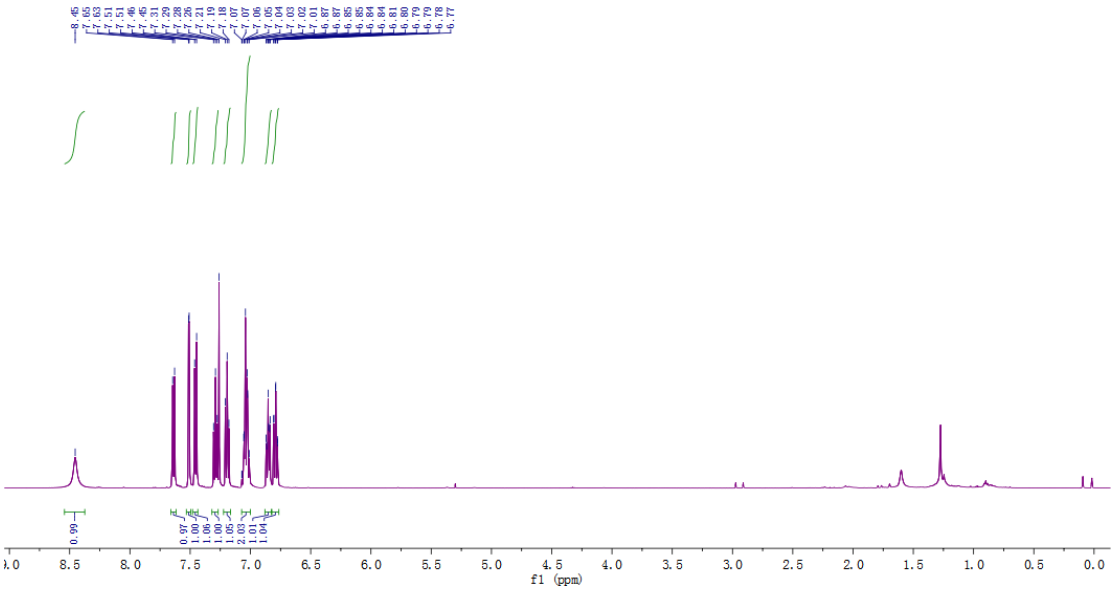
3j

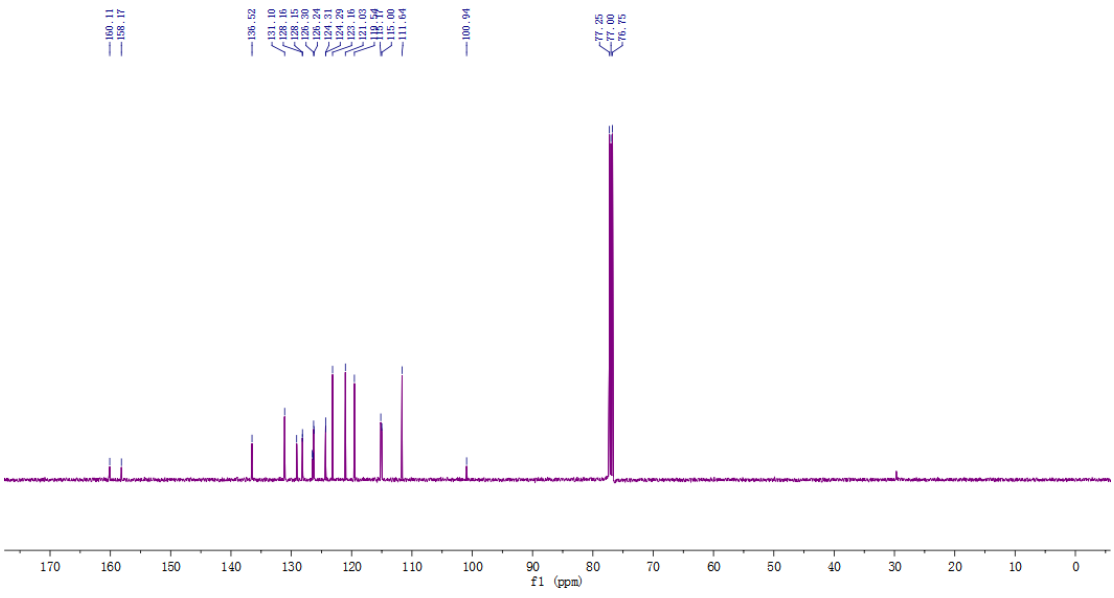

8.21
7.52
7.50
7.28
7.26
7.18
7.16
7.15
7.13
7.12
7.10
7.09
7.07
7.01
7.00
6.98
2.42
0.85
0.96
1.00
4.26
2.86
2.84
f1 (ppm)

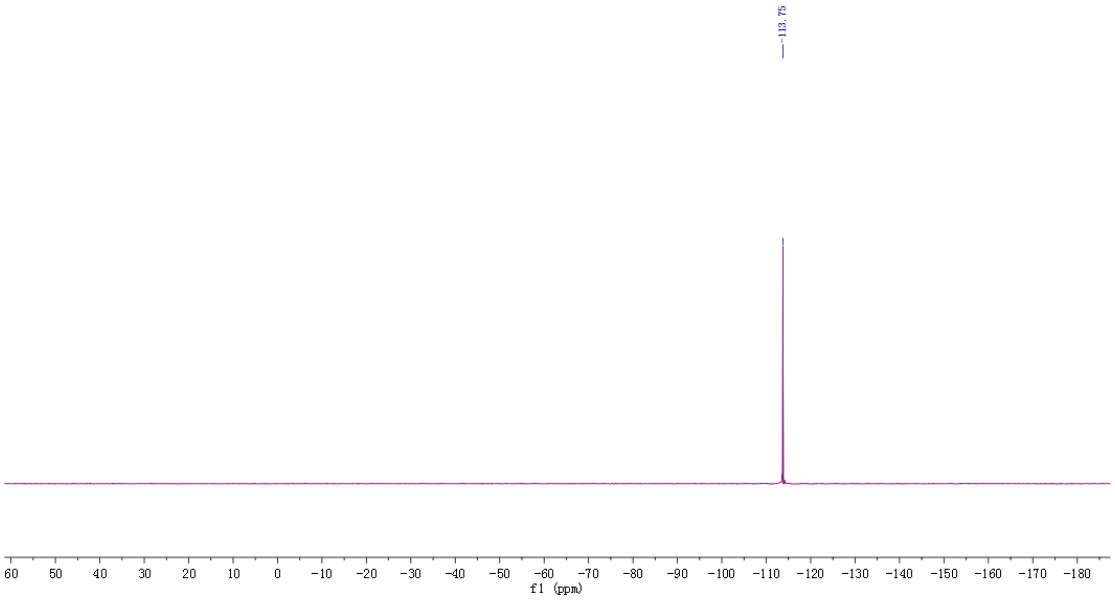

141.13
139.32
135.42
130.25
128.64
125.47
124.47
122.10
120.62
118.90
110.65
99.21
77.25
77.00
76.75
12.05
f1 (ppm)



3k






113.75
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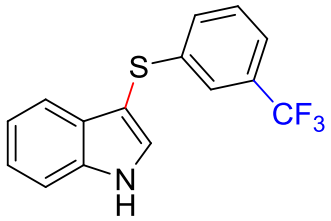
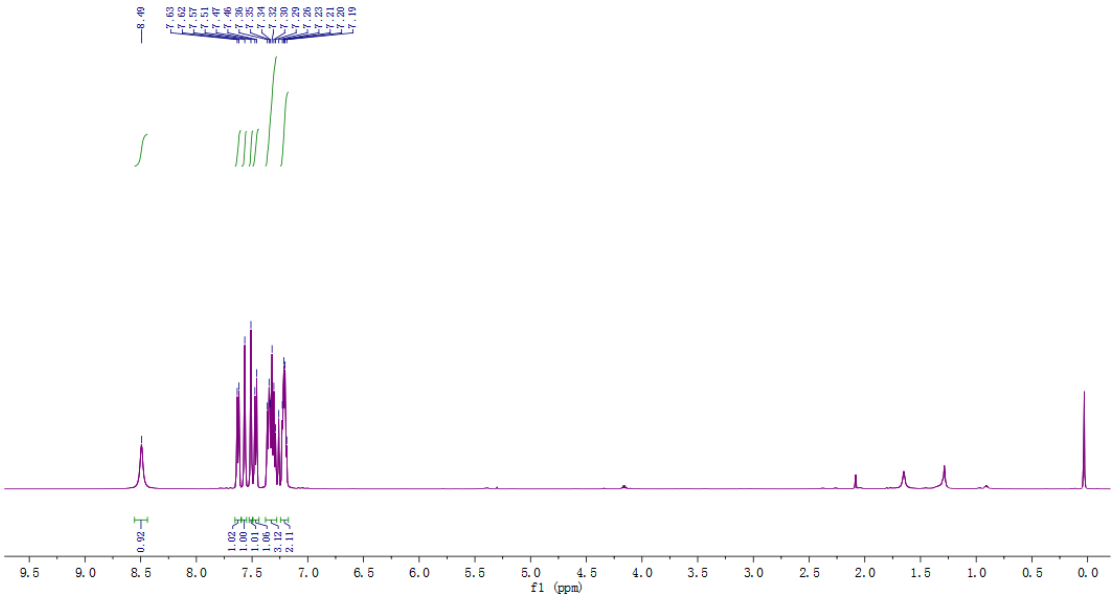
f1 (ppm)


S
CF3
N
H

3l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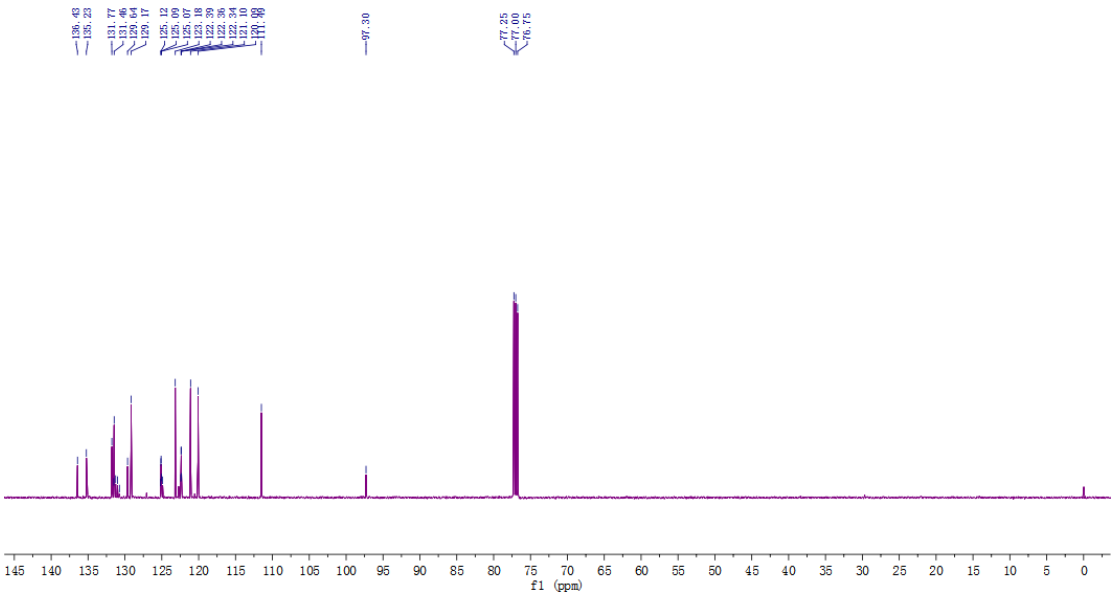
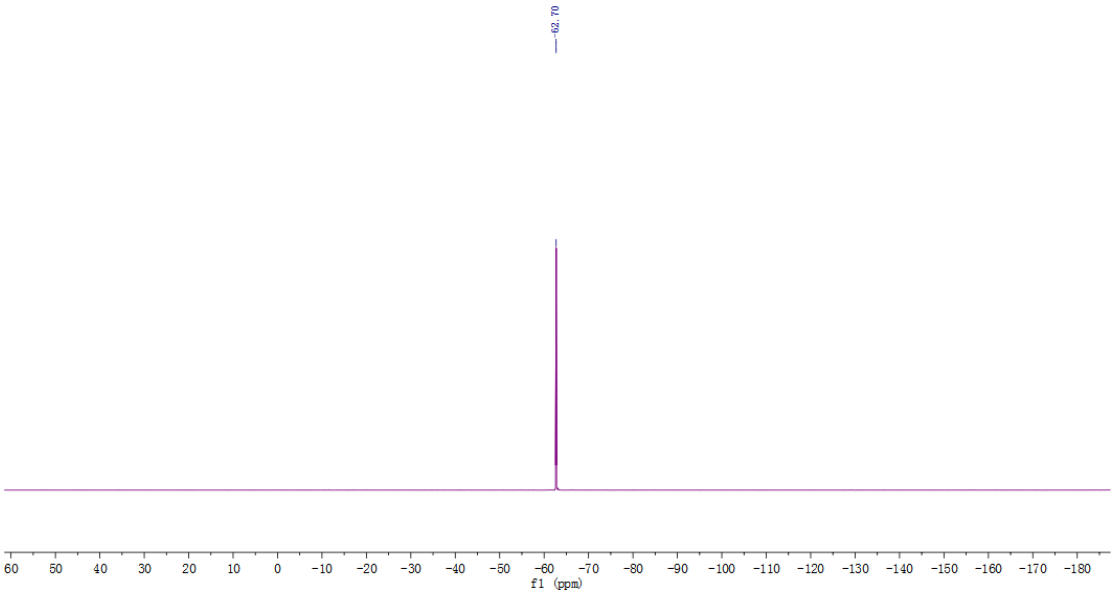
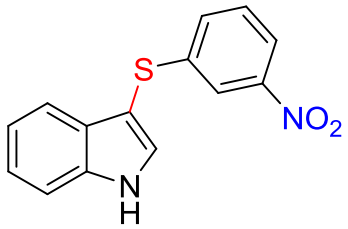
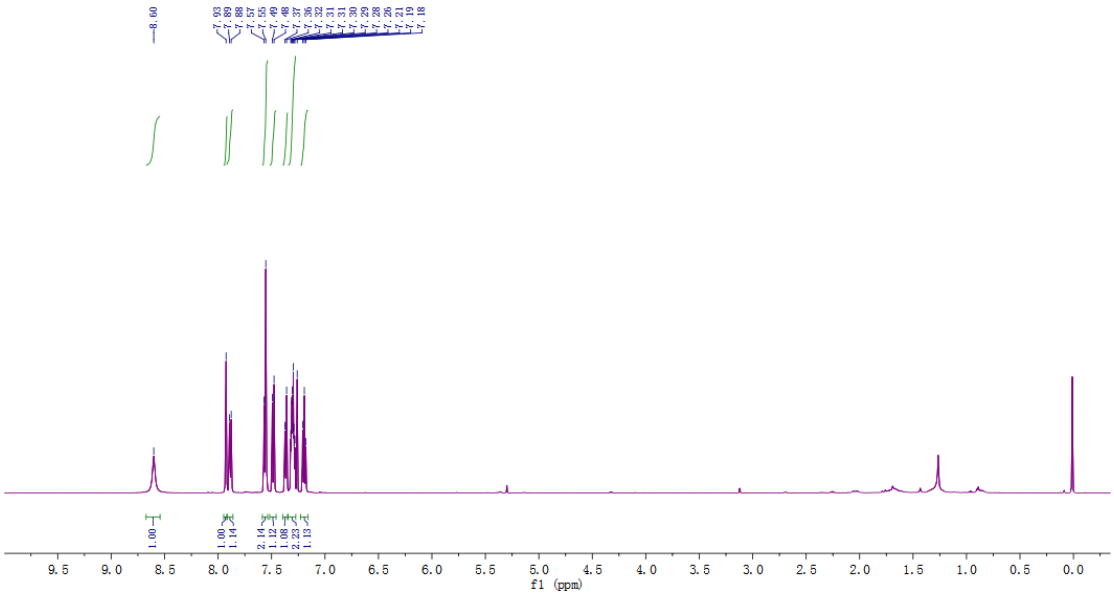
7.62
7.57
7.51
7.47
7.46
7.35
7.34
7.32
7.30
7.29
7.26
7.23
7.21
7.20
7.19
0.92
1.02
1.00
1.01
1.06
3.12
2.11
f1 (ppm)


136.43
135.23
131.77
131.46
129.64
129.17
125.12
125.09
125.07
123.38
122.38
122.36
122.34
121.10
97.30
77.25
77.00
76.75
f1 (ppm)


-62.70
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)


S
NO2
N
H

3m


8.60
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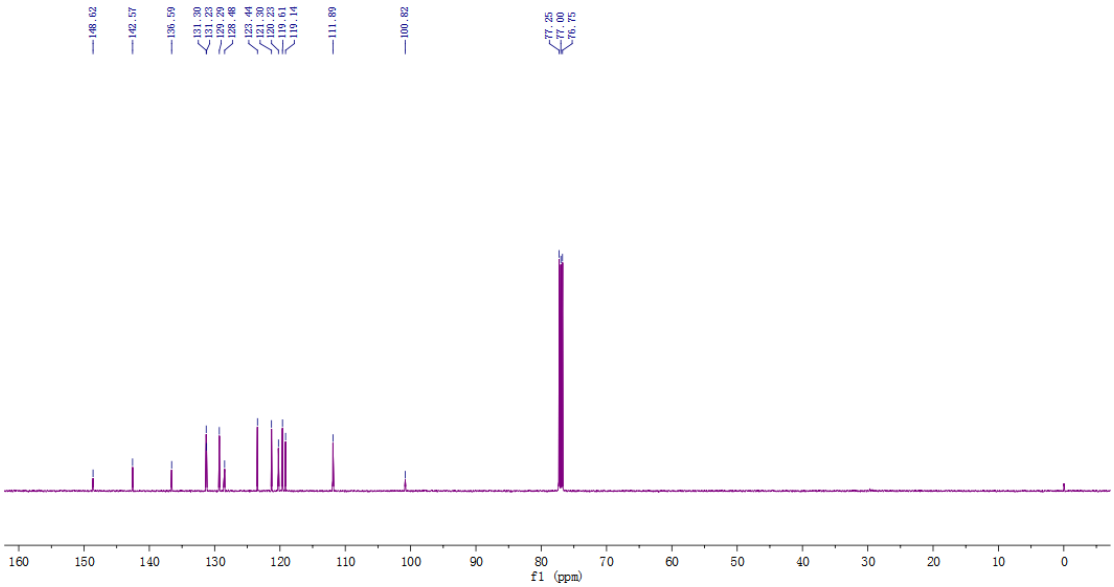
7.88
7.57
7.55
7.49
7.48
7.37
7.36
7.32
7.31
7.30
7.29
7.28
7.26
7.21
7.19
7.18
1.00
1.00
1.14
2.14
1.12
1.08
2.23
1.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


148.62
142.57
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131.30
131.23
129.29
128.48
123.44
121.30
120.23
119.51
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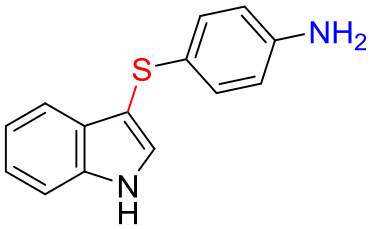
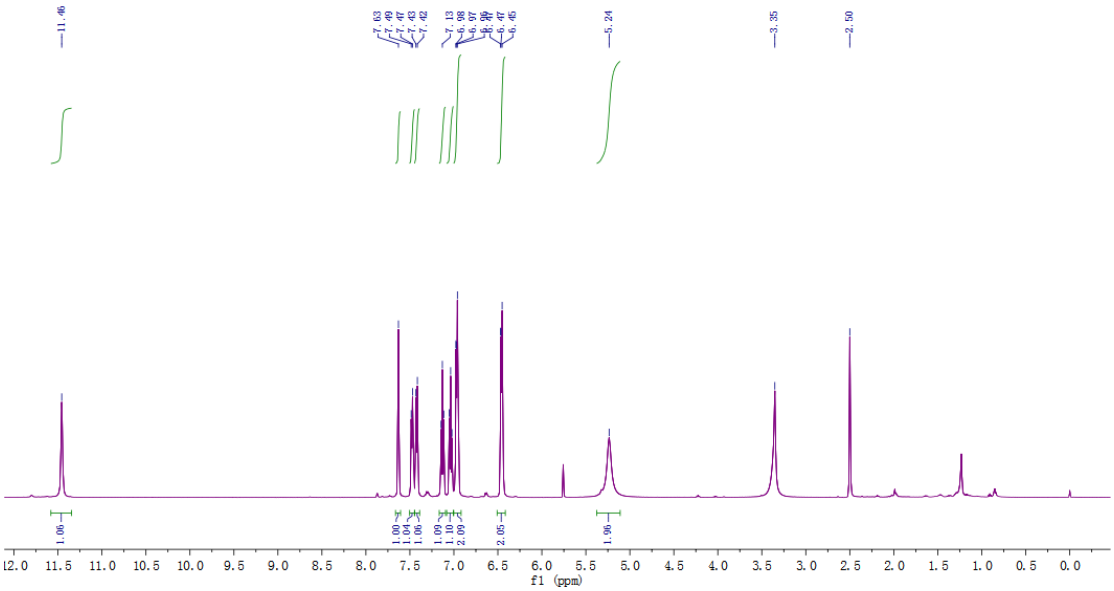
100.82
77.25
77.00
76.75
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


NH2
S
N
H

3n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6.47
6.45
5.24
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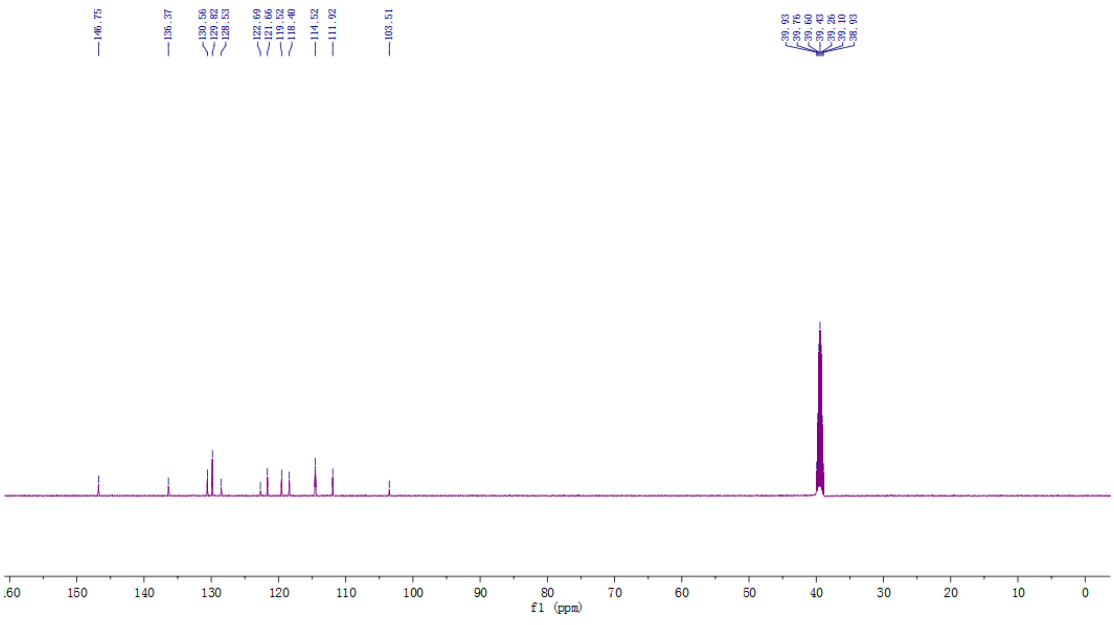
1.00
1.04
1.06
1.09
1.10
2.09
2.05
1.96
f1 (ppm)


146.75
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122.69
121.66
119.52
118.40
114.52
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103.51
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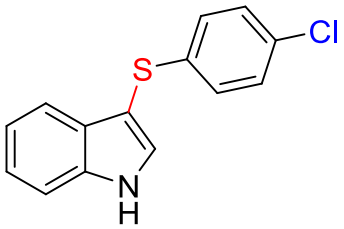
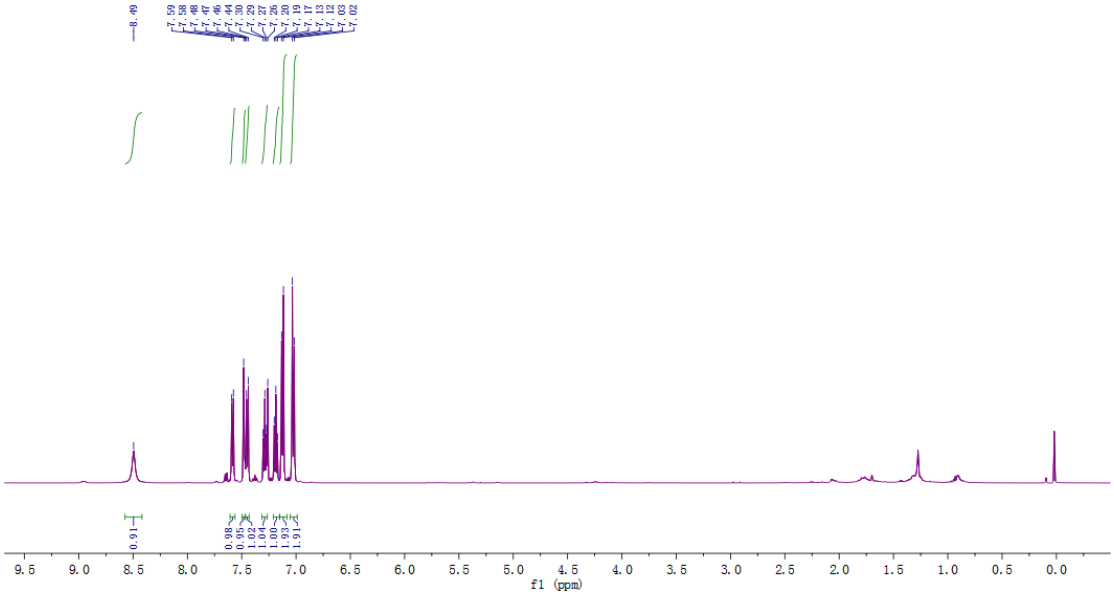
39.43
39.26
39.10
38.93
f1 (ppm)


Cl
S
N
H

3o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7.30
7.29
7.27
7.26
7.20
7.19
7.17
7.13
7.12
7.03
7.02
0.91
0.98
0.95
1.02
1.04
1.00
1.93
1.91
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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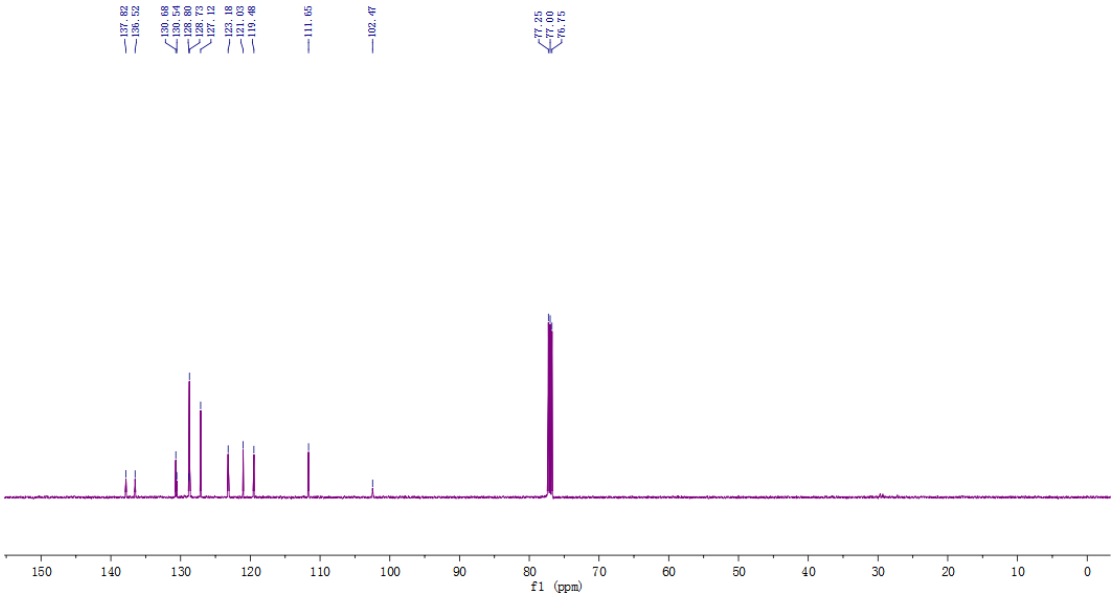
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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123.18
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119.48
111.65
102.47
77.25
77.00
76.75
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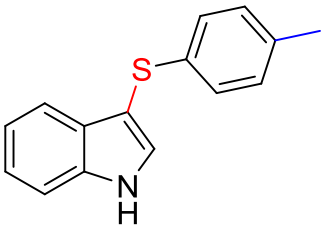
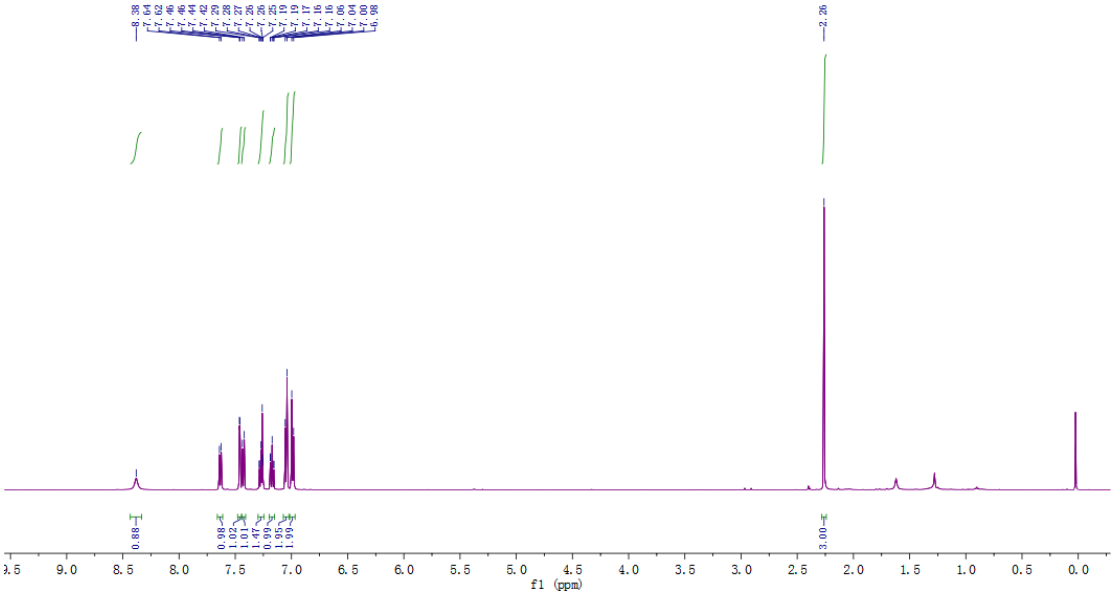
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


S
N
H

3p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7.46
7.44
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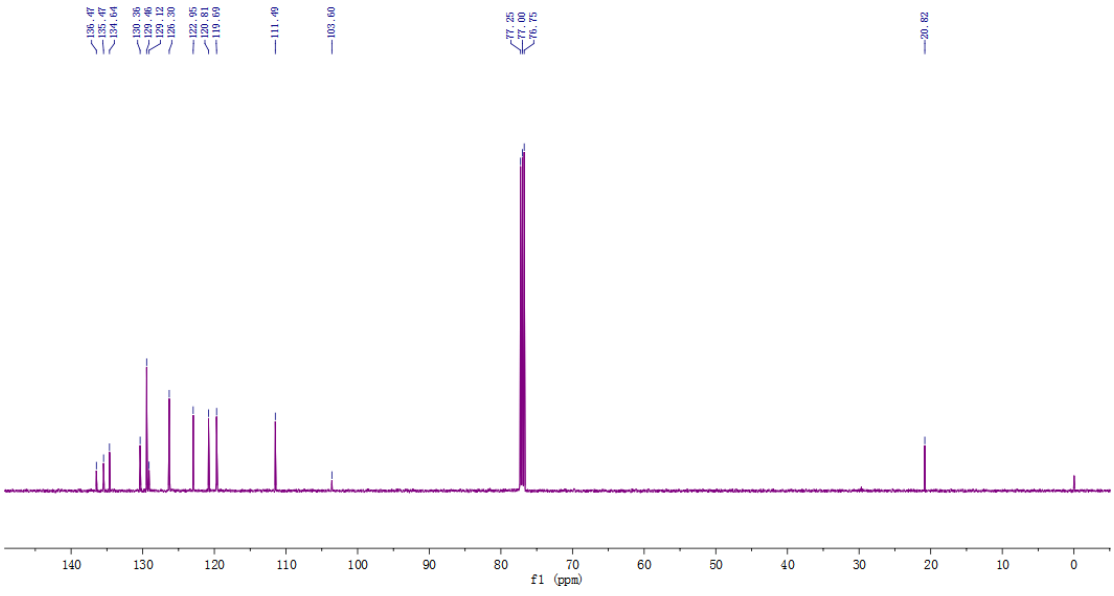
7.29
7.28
7.27
7.26
7.25
7.19
7.19
7.17
7.16
7.06
7.04
7.00
6.98
2.26
0.88
0.98
1.02
1.01
1.47
0.99
1.95
1.99
3.00
f1 (ppm)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135.47
134.64
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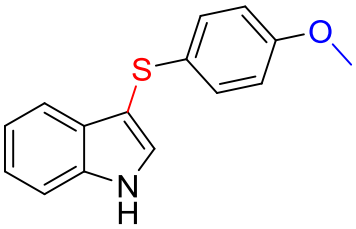
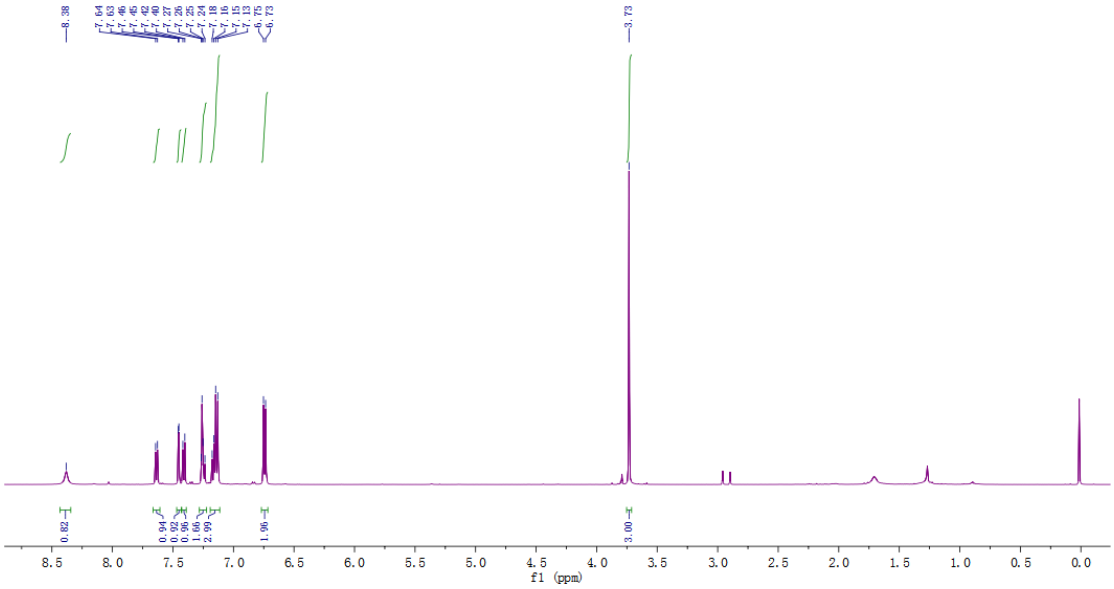
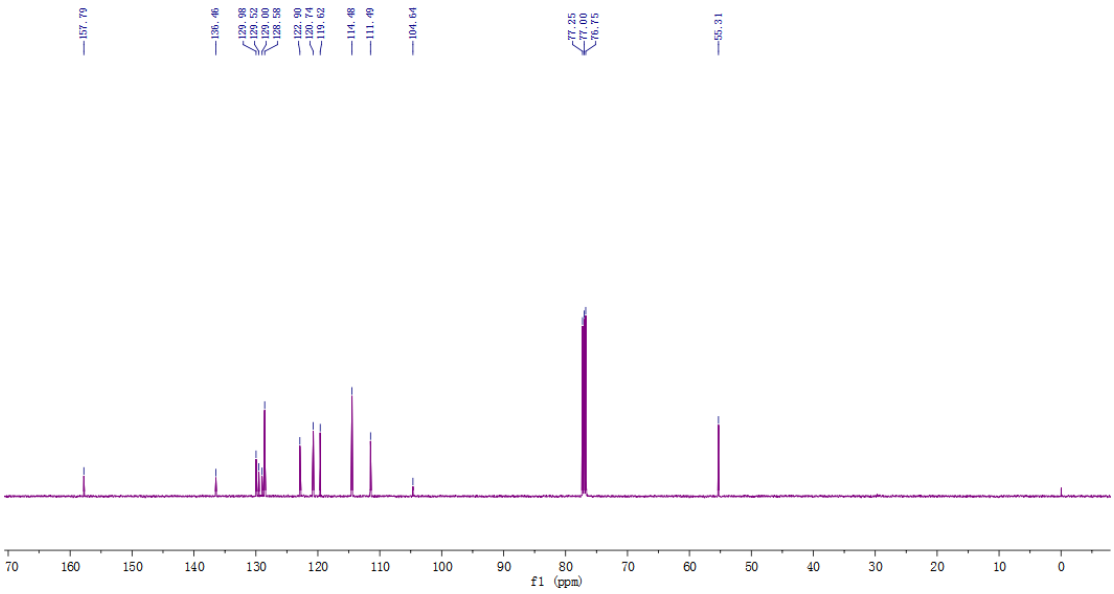
129.46
129.12
126.30
122.95
120.81
119.69
111.49
103.60
77.25
77.00
76.75
20.82
f1 (ppm)


S
O
N
H

3q


8.38
7.64
7.63
7.46
7.45
7.42
7.40
7.27
7.26
7.25
7.24
7.18
7.16
7.15
7.13
6.75
6.73
3.73
0.82
0.94
0.92
0.96
1.96
2.99
1.96
3.00
f1 (ppm)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129.88
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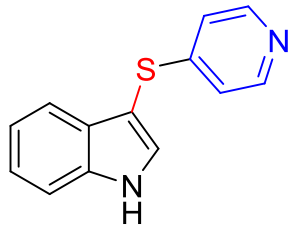
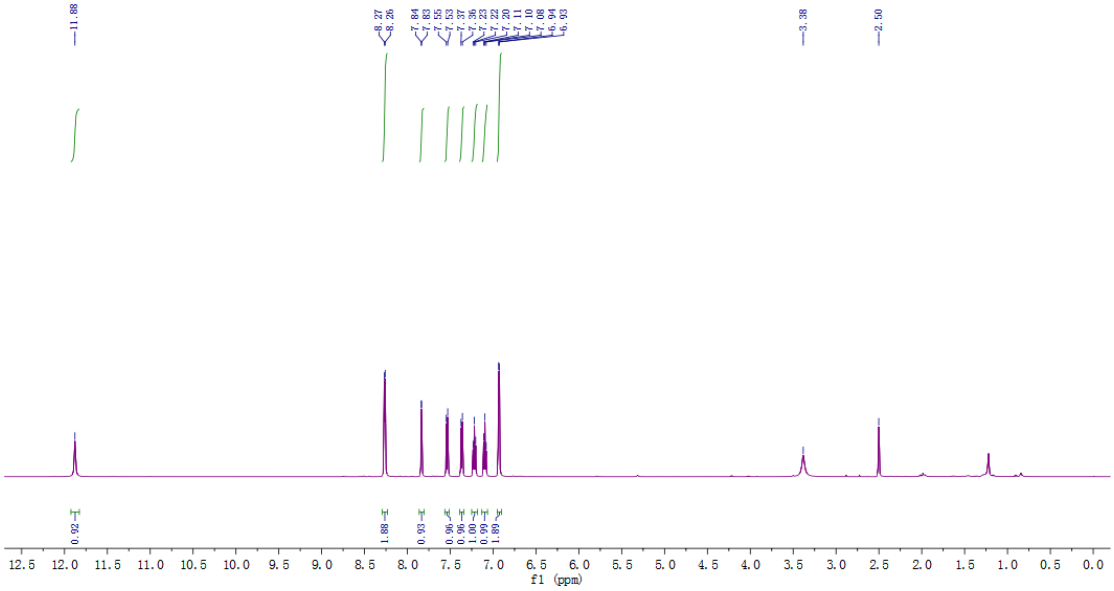
129.00
128.58
122.90
120.74
119.62
114.48
111.49
104.64
77.25
77.00
76.75
55.31
f1 (ppm)


S
N
N
H

3r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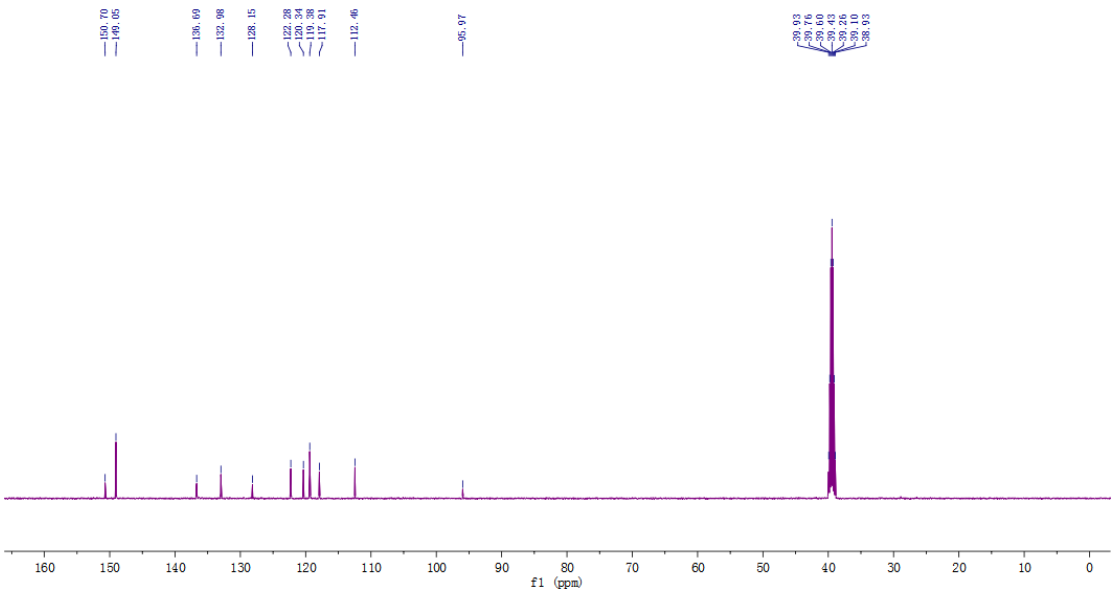
7.83
7.55
7.53
7.37
7.36
7.23
7.22
7.20
7.11
7.10
7.08
6.94
6.93
3.38
2.50
0.92
1.88
0.93
0.96
0.96
1.00
0.99
1.89
f1 (ppm)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128.15
122.28
120.34
119.38
117.91
112.46
95.97
39.93
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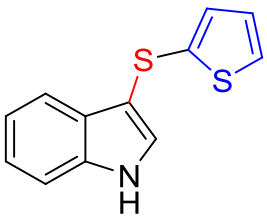
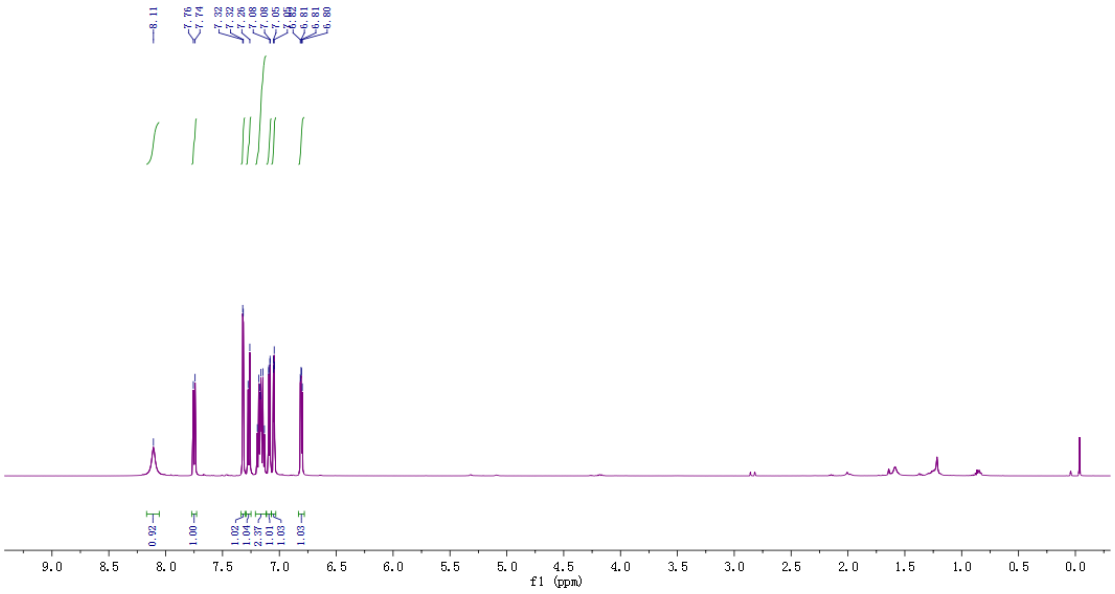
39.60
39.43
39.26
39.10
38.93
f1 (ppm)


S
S
N
H

3s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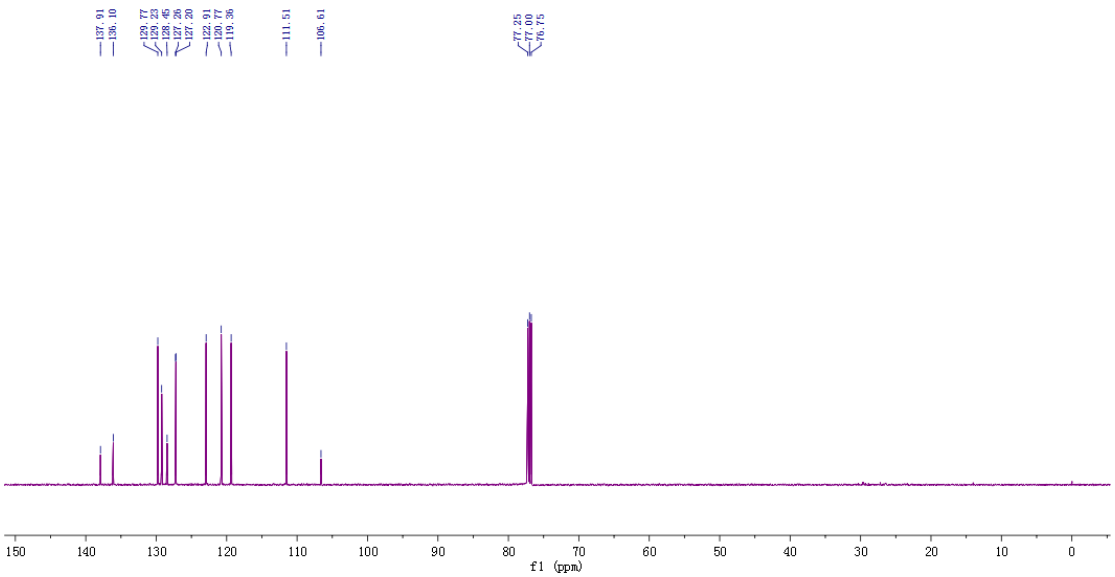
7.76
7.74
7.32
7.32
7.26
7.08
7.08
7.05
6.82
6.81
6.81
6.80
0.92
1.00
1.02
1.04
2.37
1.01
1.03
1.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.22
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127.26
127.20
122.91
120.77
119.36
111.51
106.61
77.25
77.00
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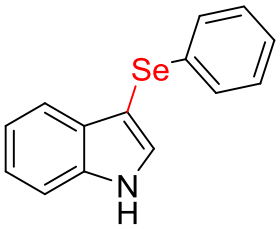
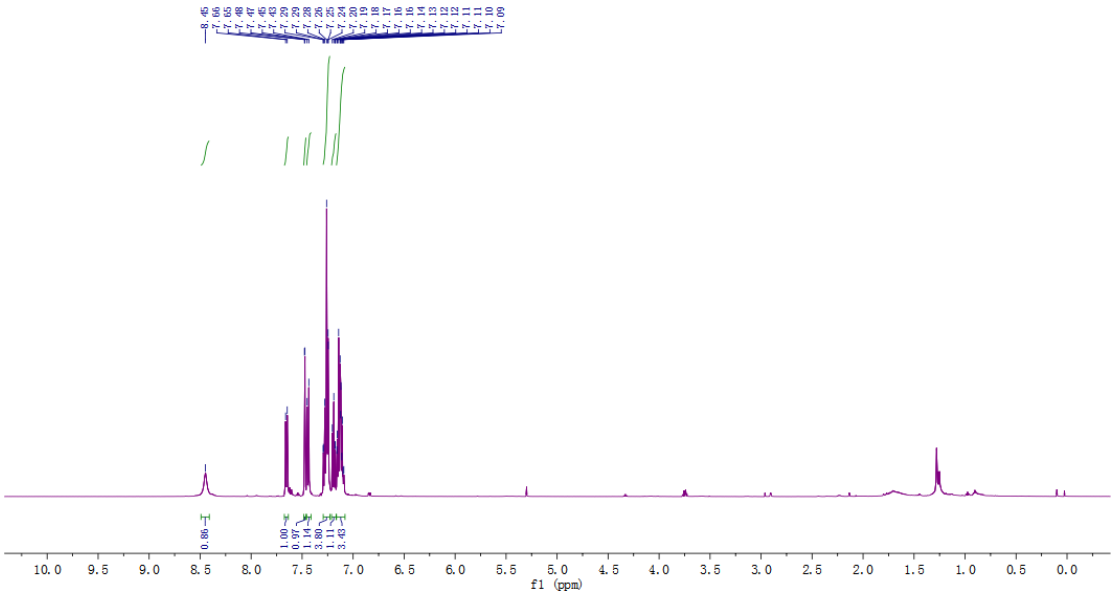
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Se
N
H

3t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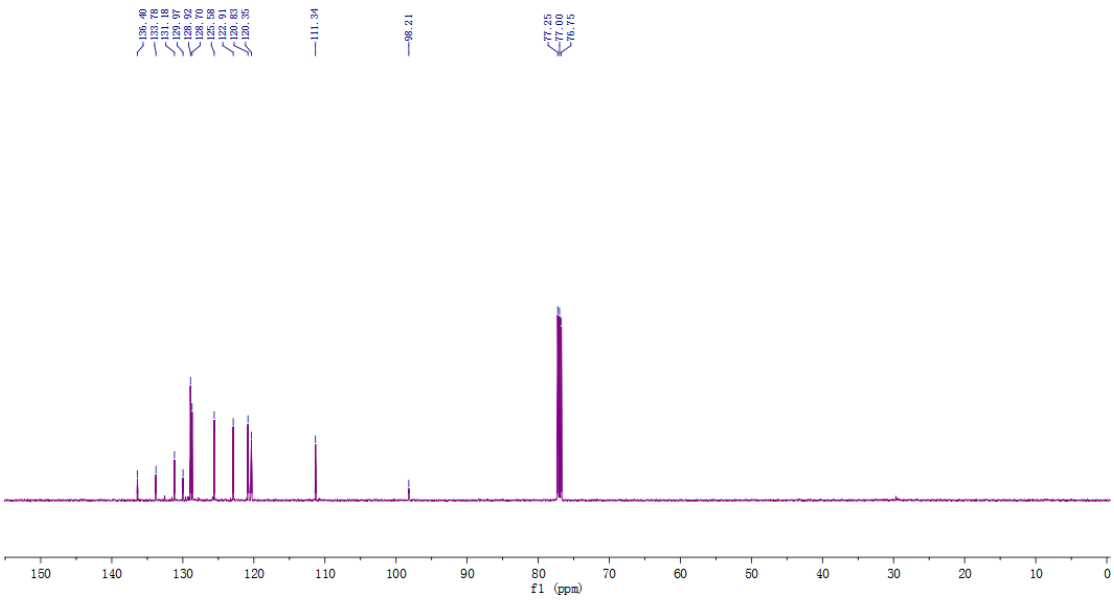
7.28
7.26
7.25
7.24
7.20
7.19
7.18
7.17
7.16
7.16
7.14
7.13
7.12
7.12
7.11
7.11
7.10
7.09
0.86
1.00
0.97
1.14
3.80
1.11
3.43
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.97
128.92
128.70
125.58
122.91
120.83
120.35
111.34
98.21
77.25
77.00
76.75
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110
100
90
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70
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50
40
30
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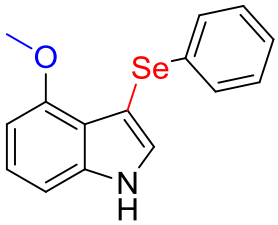
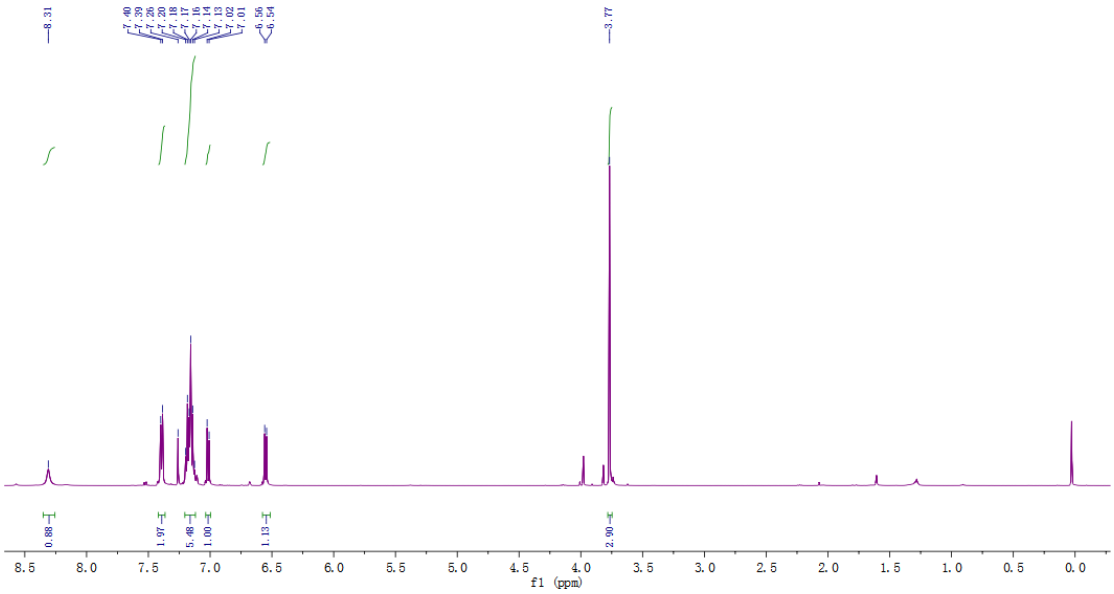
10
0
f1 (ppm)


O
Se
N
H

3u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7.26
7.20
7.18
7.17
7.16
7.14
7.13
7.02
7.01
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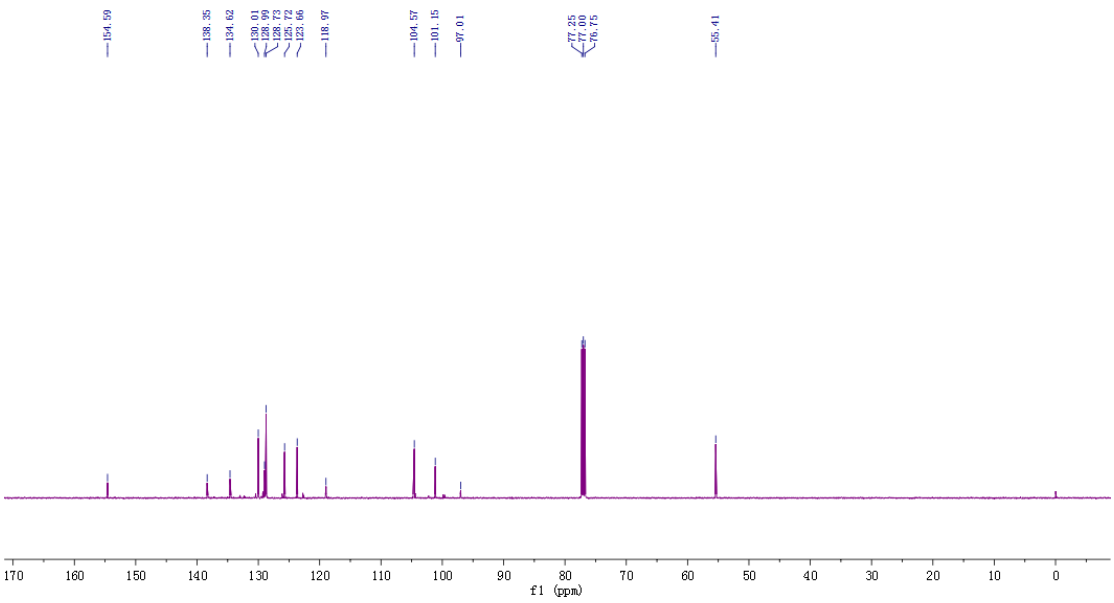
6.54
3.77
0.88
1.97
5.48
1.00
1.13
2.90
f1 (ppm)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128.99
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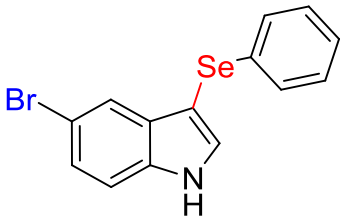
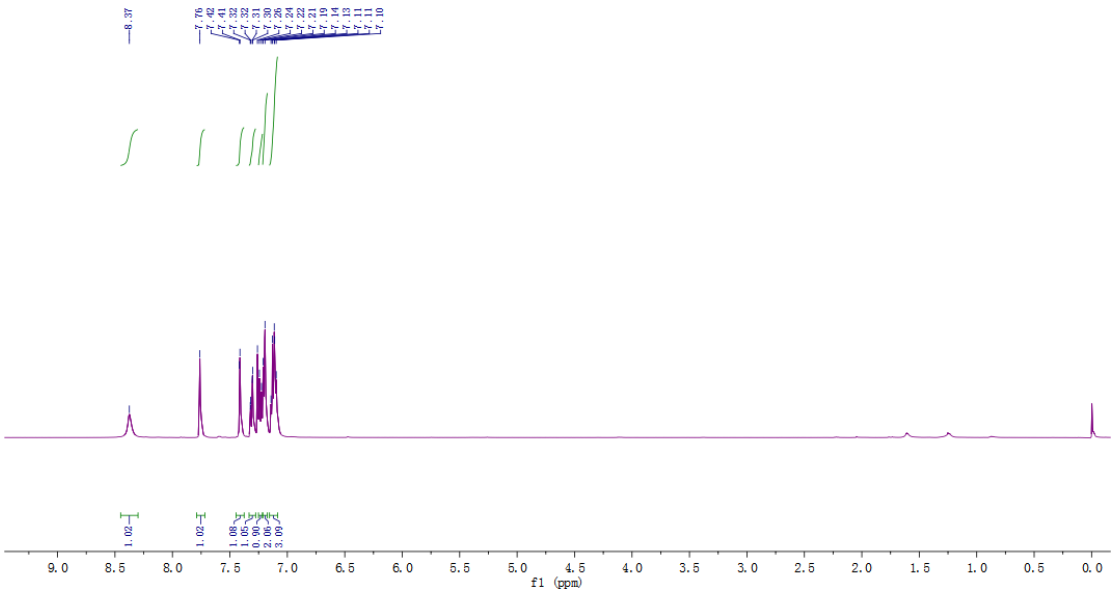
118.97
104.57
101.15
97.01
77.25
77.00
76.75
55.41
f1 (ppm)


Br
Se
N
H

3v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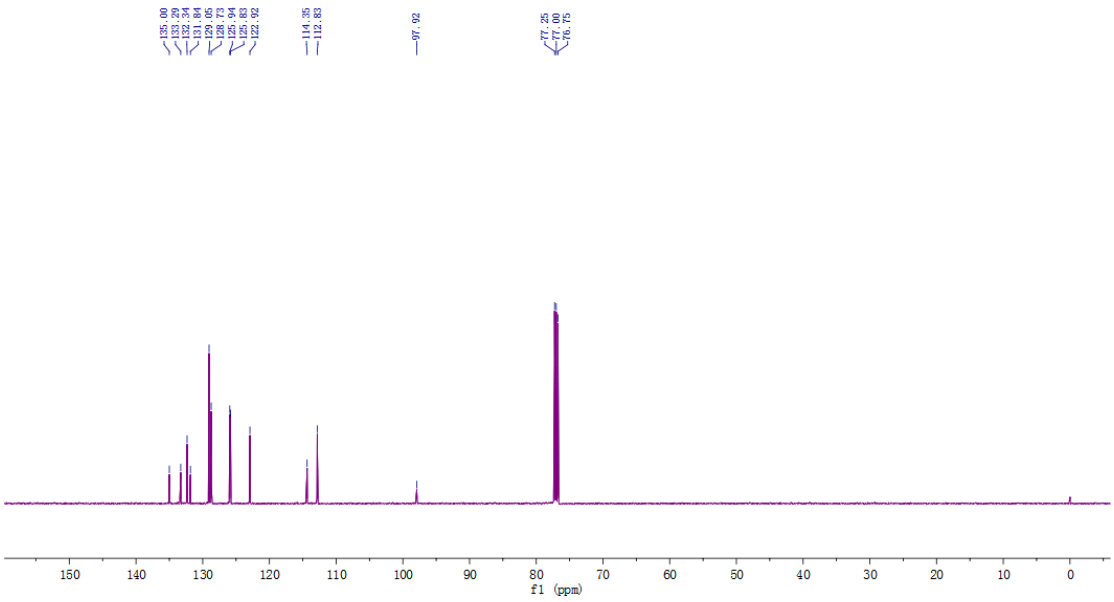
7.26
7.24
7.22
7.21
7.19
7.14
7.13
7.11
7.11
7.10
1.02
1.02
1.08
1.05
0.90
0.86
3.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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125.94
125.83
122.92
114.35
112.83
97.92
77.25
77.00
76.75
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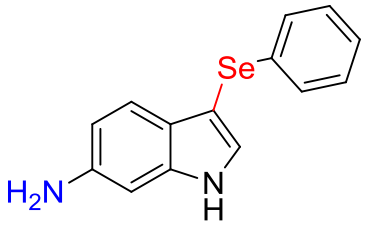
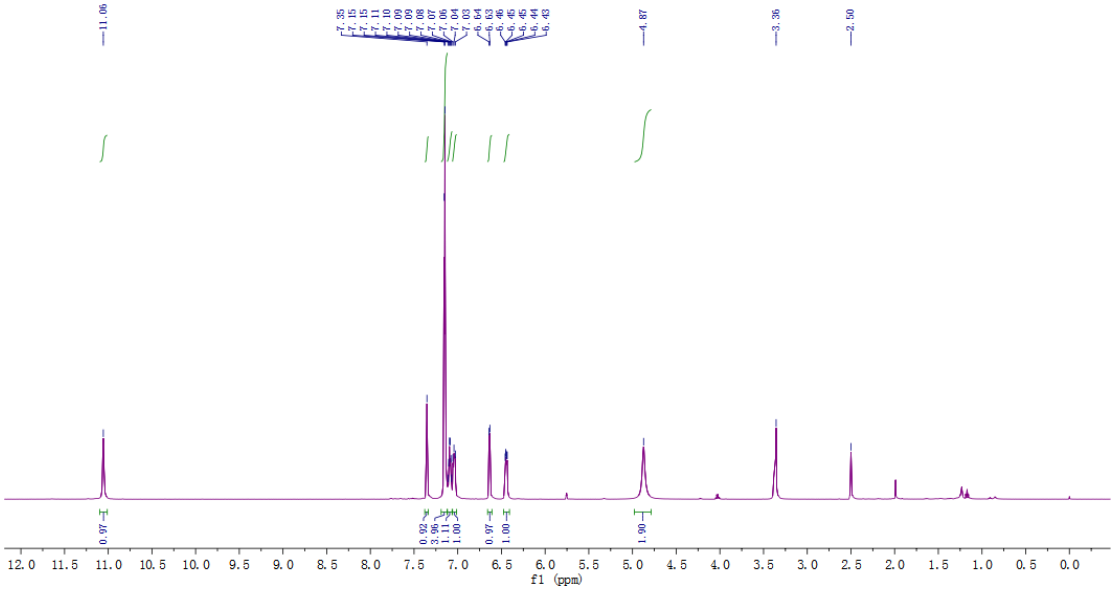
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Se
H2N
N
H

3w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7.06
7.04
7.03
6.54
6.53
6.46
6.45
6.44
6.43
4.87
3.36
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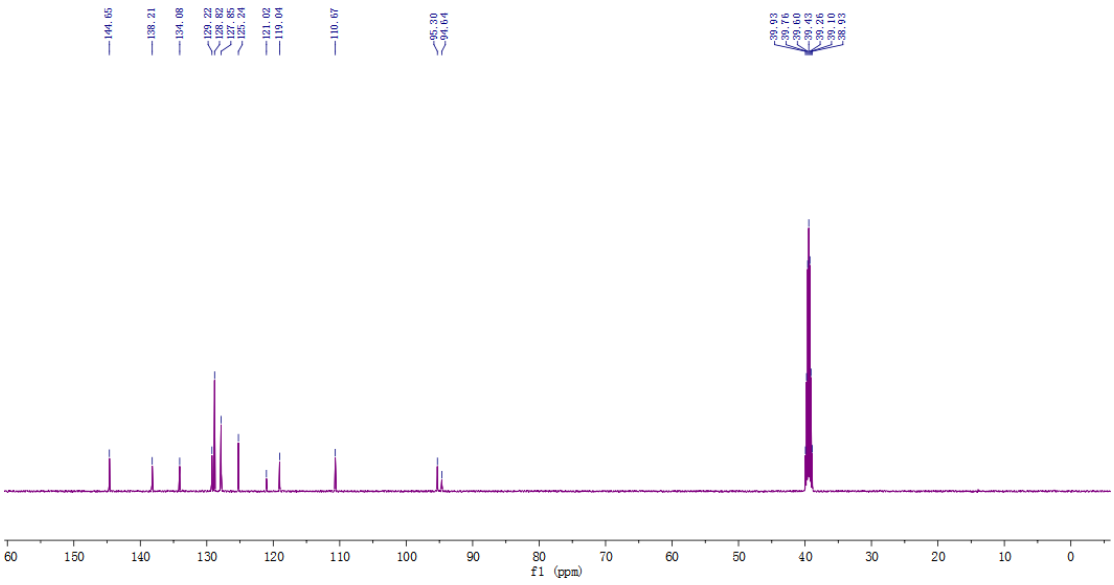
0.97
0.92
3.06
1.11
1.00
0.97
1.00
1.90
f1 (ppm)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138.21
134.08
129.22
128.82
127.85
125.24
121.02
119.04
110.67
95.30
94.64
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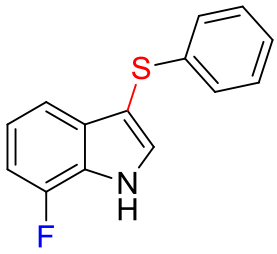
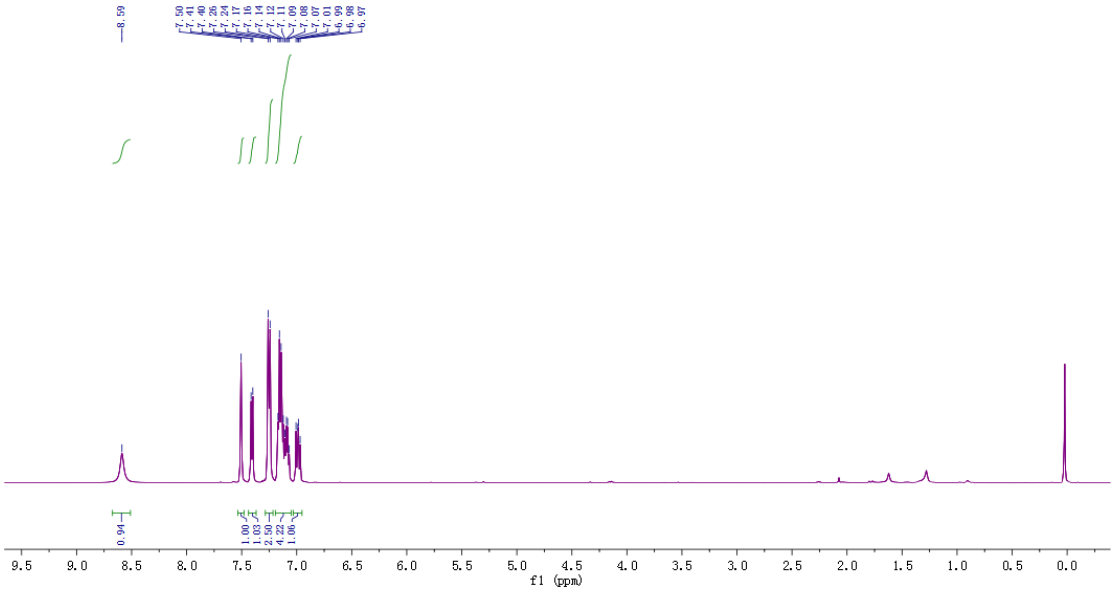
39.60
39.43
39.26
39.10
38.93
f1 (ppm)


S
N
H
F

3x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7.26
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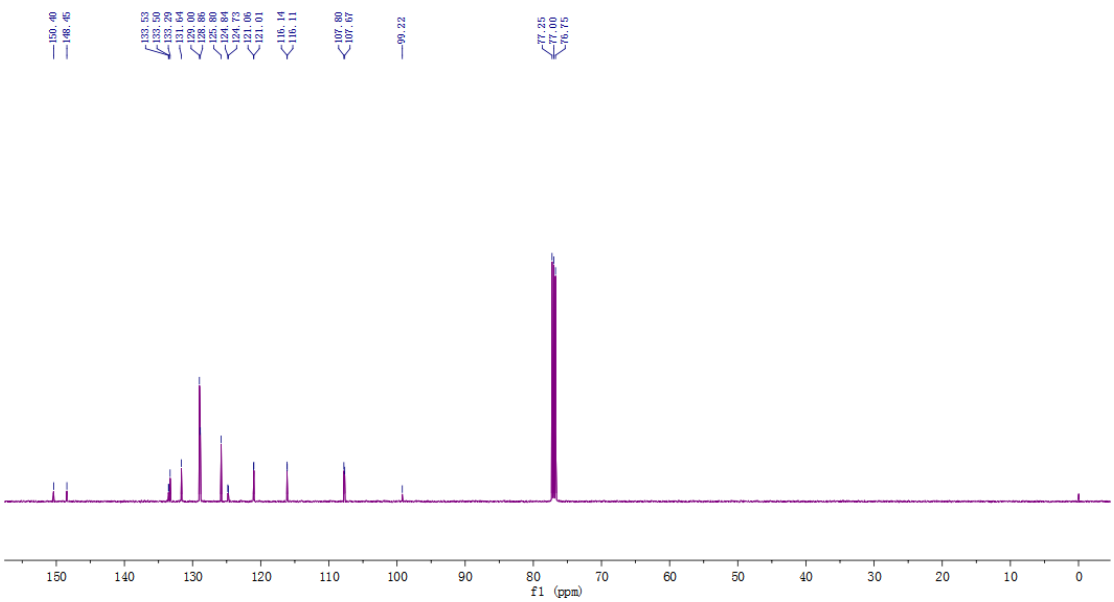
7.17
7.16
7.14
7.12
7.11
7.09
7.08
7.07
7.01
6.99
6.98
6.97
0.94
1.00
1.03
2.59
4.47
1.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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124.84
124.73
121.06
121.01
116.14
116.11
107.80
107.67
99.22
77.25
77.00
76.75
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130
120
110
100
90
80
70
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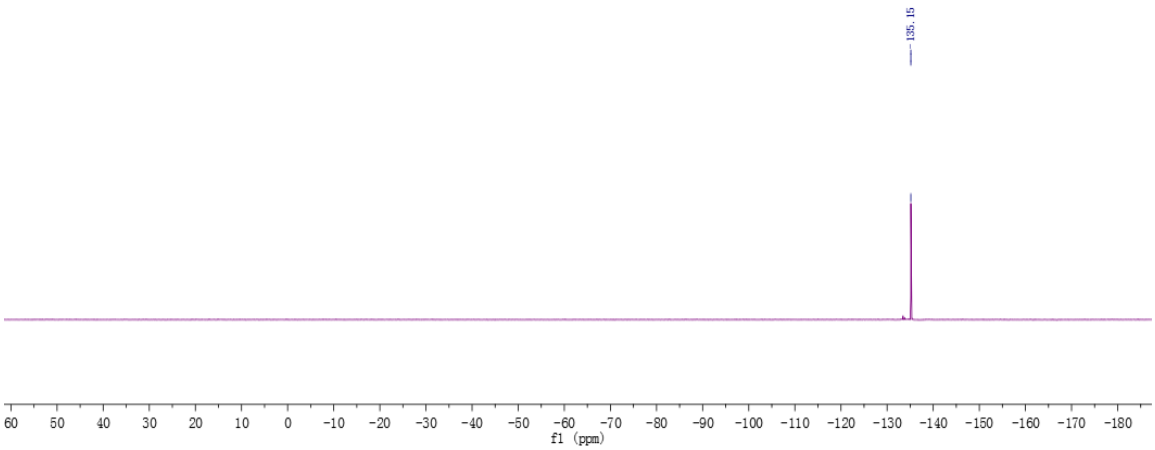
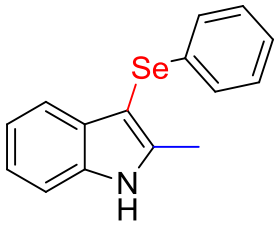
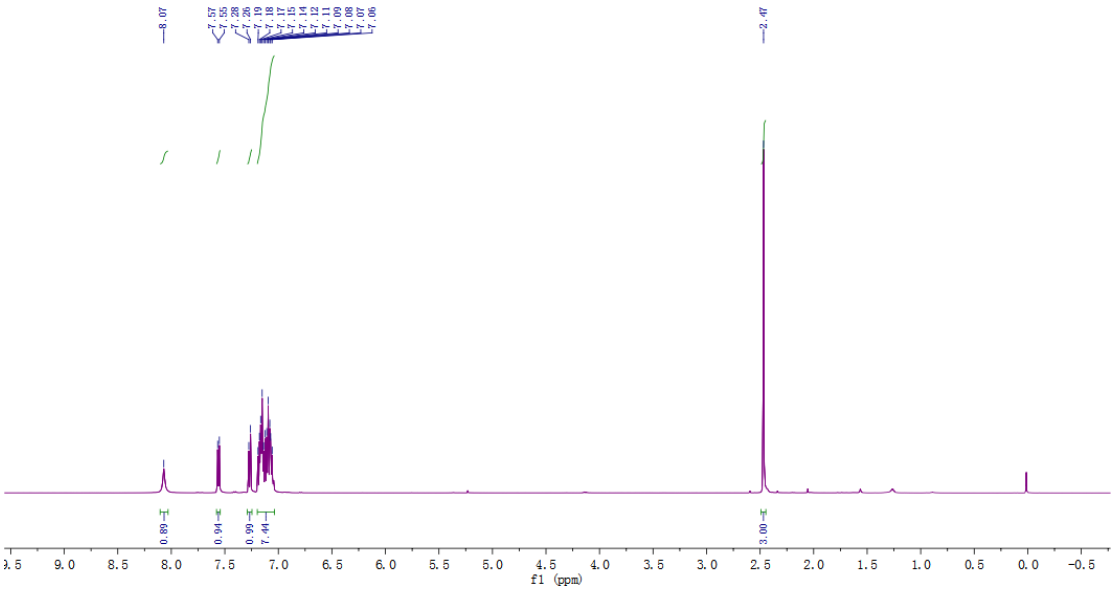
50
40
30
20
10
0
f1 (ppm)


135.15
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)


Se
N
H

3y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7.14
7.12
7.11
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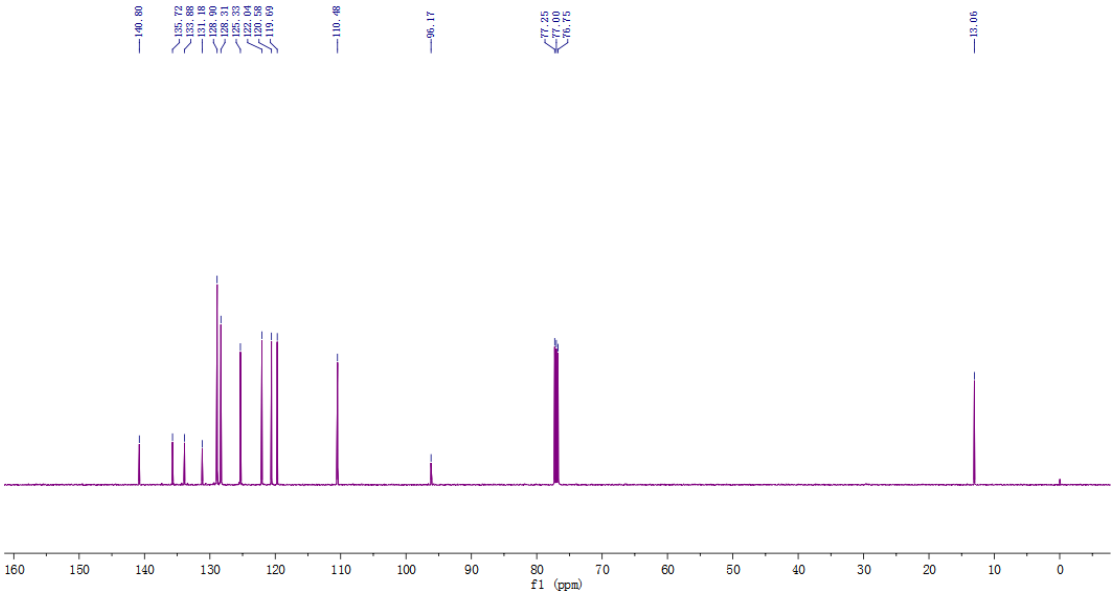
7.08
7.07
7.06
2.47
0.89
0.94
0.99
7.44
3.00
f1 (ppm)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128.90
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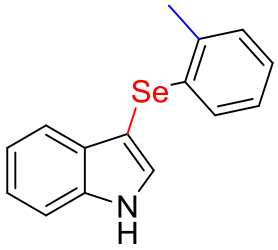
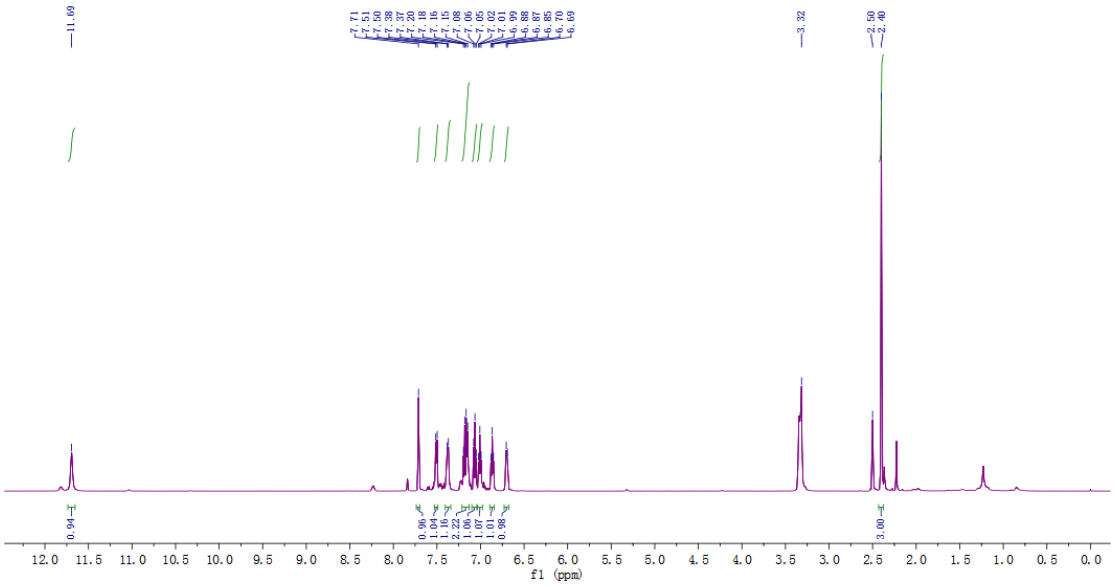
120.58
119.69
110.48
96.17
77.25
77.00
76.75
13.06
f1 (ppm)


Se
N
H

3z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7.37
7.20
7.18
7.16
7.15
7.08
7.06
7.05
7.02
7.01
6.99
6.88
6.87
6.85
6.70
6.69
3.32
2.50
2.49
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0.96
1.04
1.16
2.22
1.06
1.07
1.01
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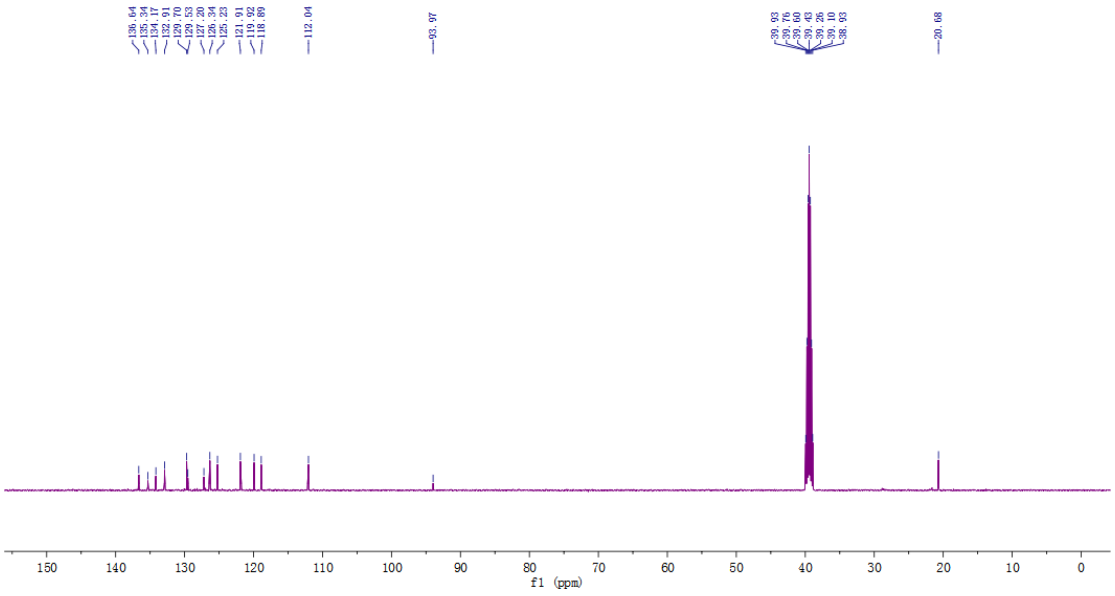
3.00
f1 (ppm)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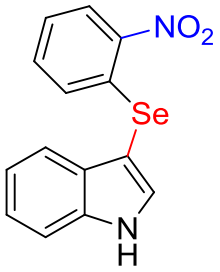
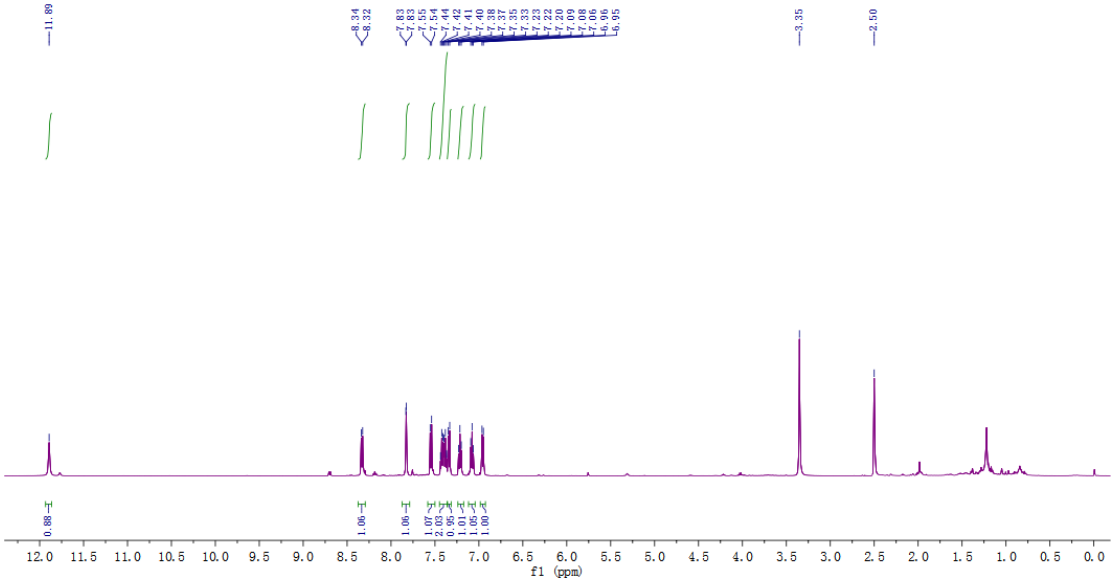
127.20
126.34
125.23
121.91
119.92
118.89
112.04
93.97
39.93
39.76
39.60
39.43
39.26
39.10
38.93
20.68
f1 (ppm)


NO2
Se
N
H

3aa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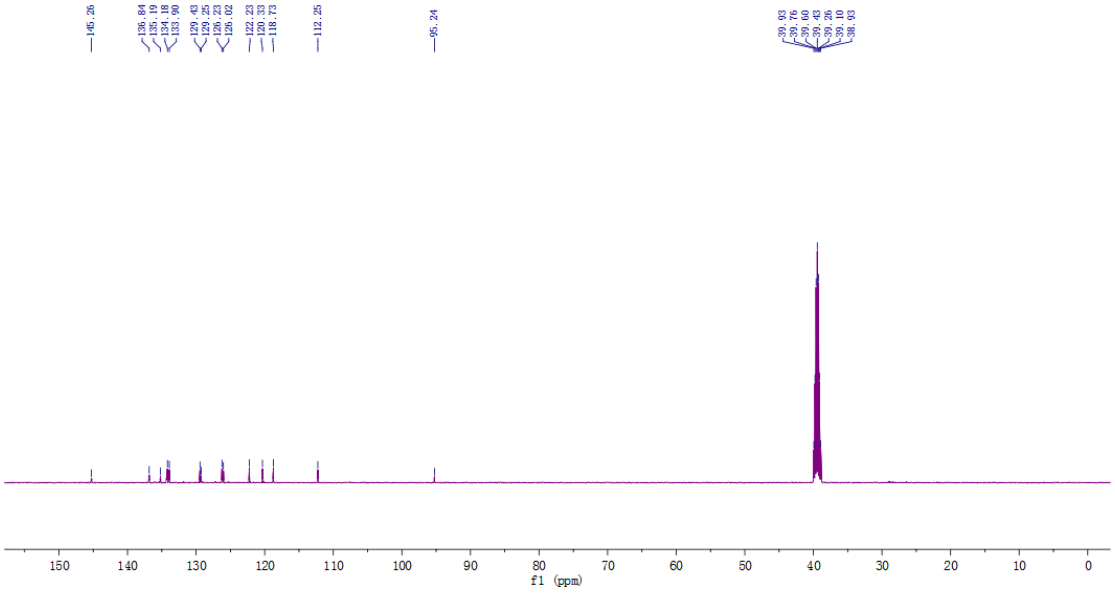
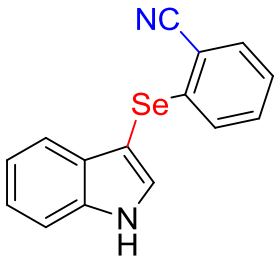
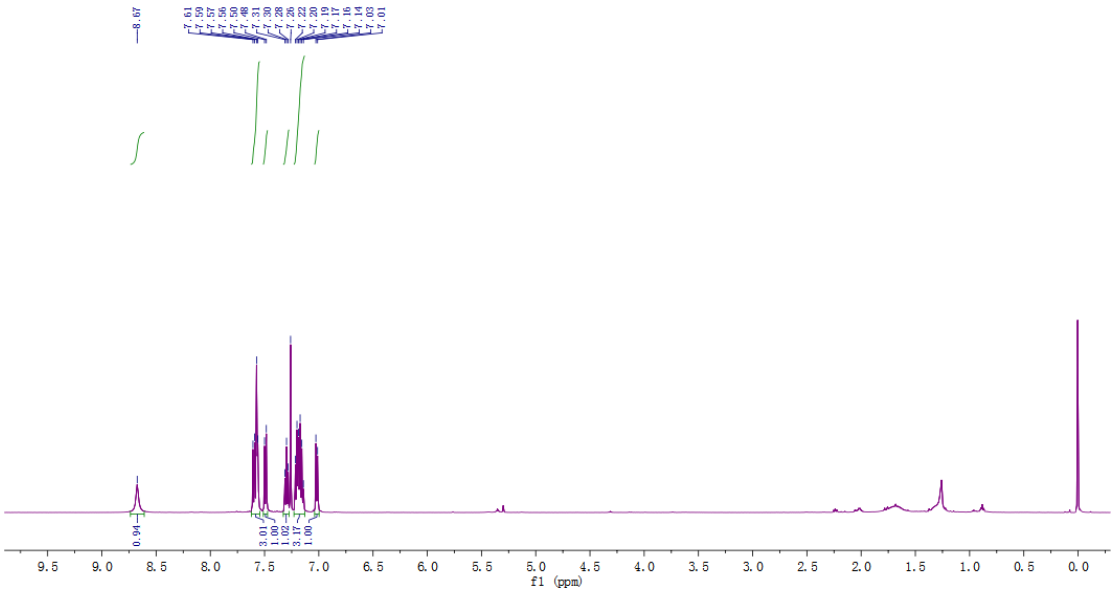
7.55
7.54
7.44
7.42
7.41
7.40
7.38
7.37
7.35
7.33
7.23
7.22
7.20
7.09
7.08
7.06
6.96
6.95
3.35
2.50
0.88
1.06
1.06
1.07
2.03
0.85
1.03
1.05
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


145.26
136.84
135.19
134.18
133.90
120.43
129.25
126.23
126.02
122.23
120.33
118.73
112.25
95.24
39.93
39.76
39.60
39.43
39.26
39.10
38.93
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


NC
Se
N
H

3ab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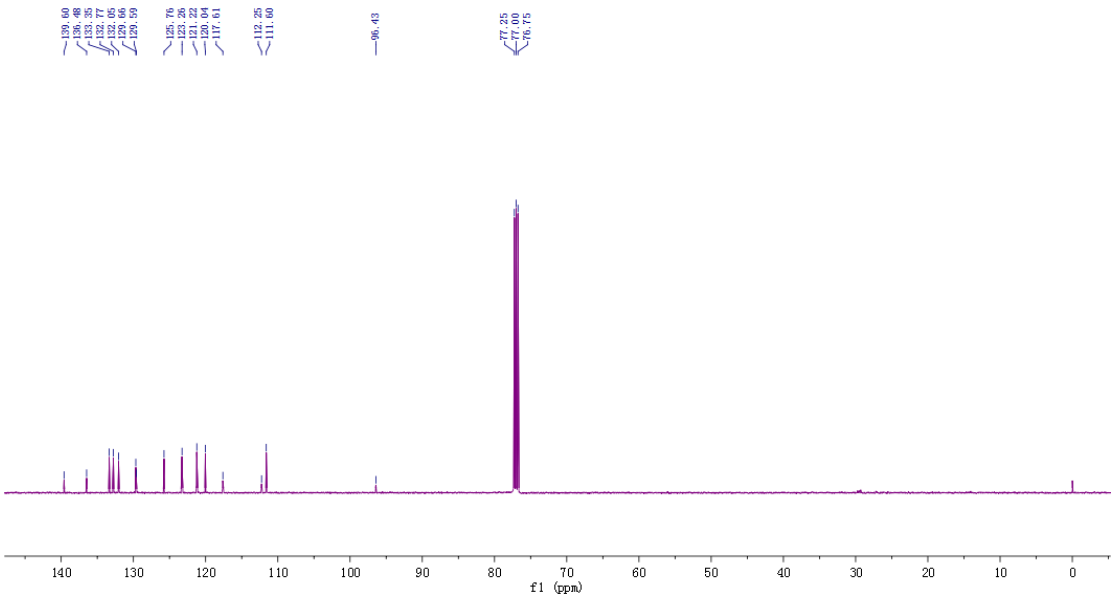
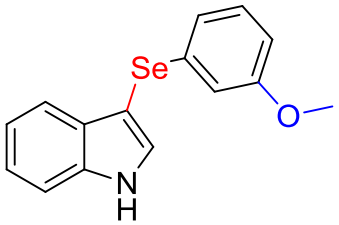
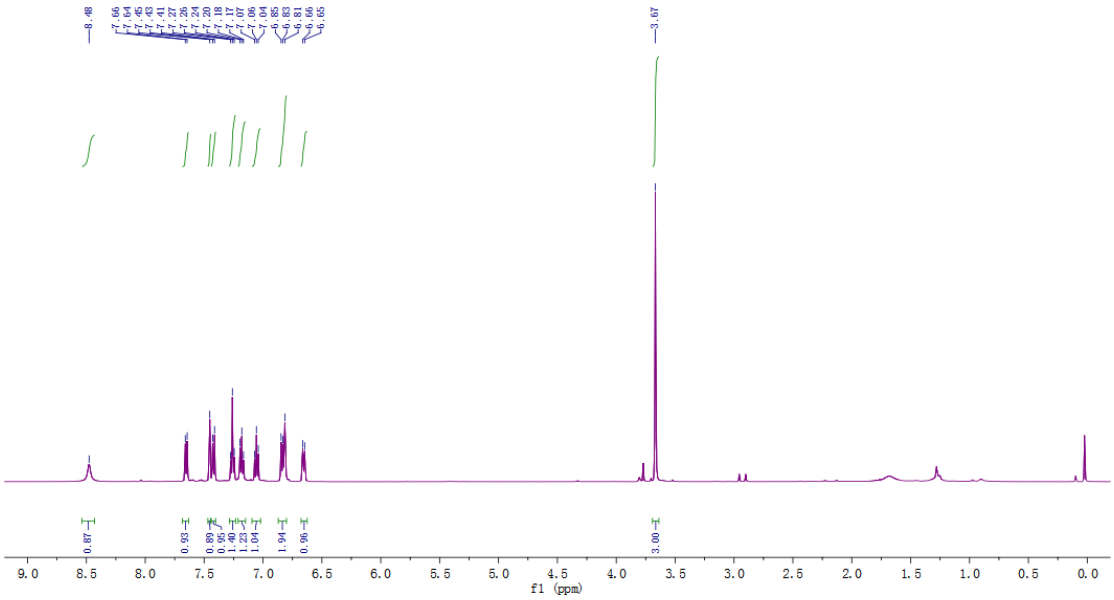
7.61
7.59
7.57
7.56
7.50
7.48
7.31
7.30
7.28
7.26
7.22
7.20
7.19
7.17
7.16
7.14
7.03
7.01
0.94
3.01
1.00
1.02
3.17
1.00
f1 (ppm)


139.60
136.48
133.35
132.77
132.05
129.66
129.59
125.76
123.26
121.22
120.04
117.61
112.25
111.60
96.43
77.25
77.00
76.75
f1 (ppm)


Se
O
N
H

3ac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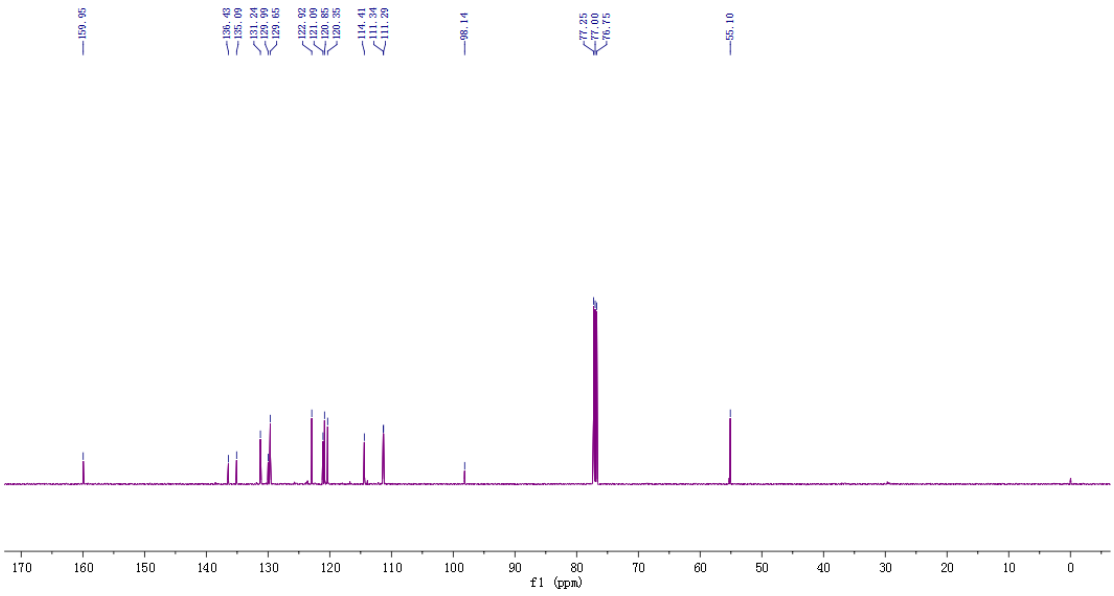
7.64
7.45
7.43
7.41
7.27
7.26
7.24
7.20
7.18
7.17
7.07
7.06
7.04
6.85
6.83
6.81
6.66
6.65
3.67
0.87
0.93
0.89
0.95
1.40
1.23
1.04
1.94
0.96
3.00
f1 (ppm)


159.95
138.43
135.09
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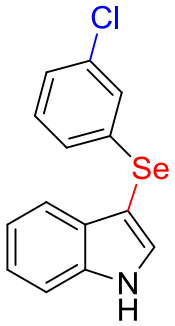
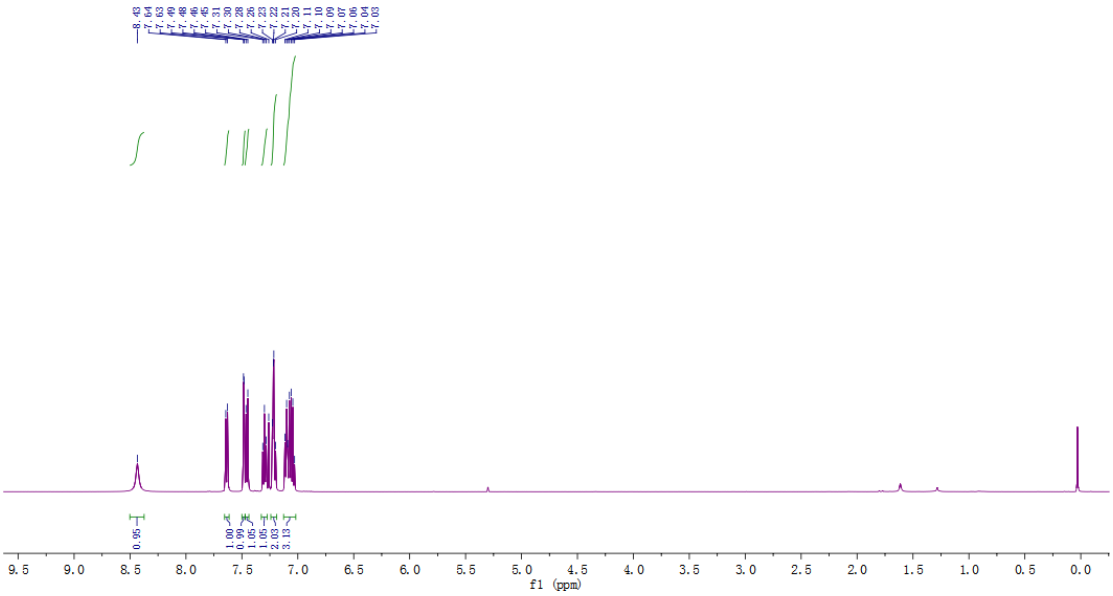
129.99
129.65
122.92
121.09
120.85
120.35
114.41
111.34
111.29
98.14
77.25
77.00
76.75
55.10
f1 (ppm)


Cl
Se
N
H

3ad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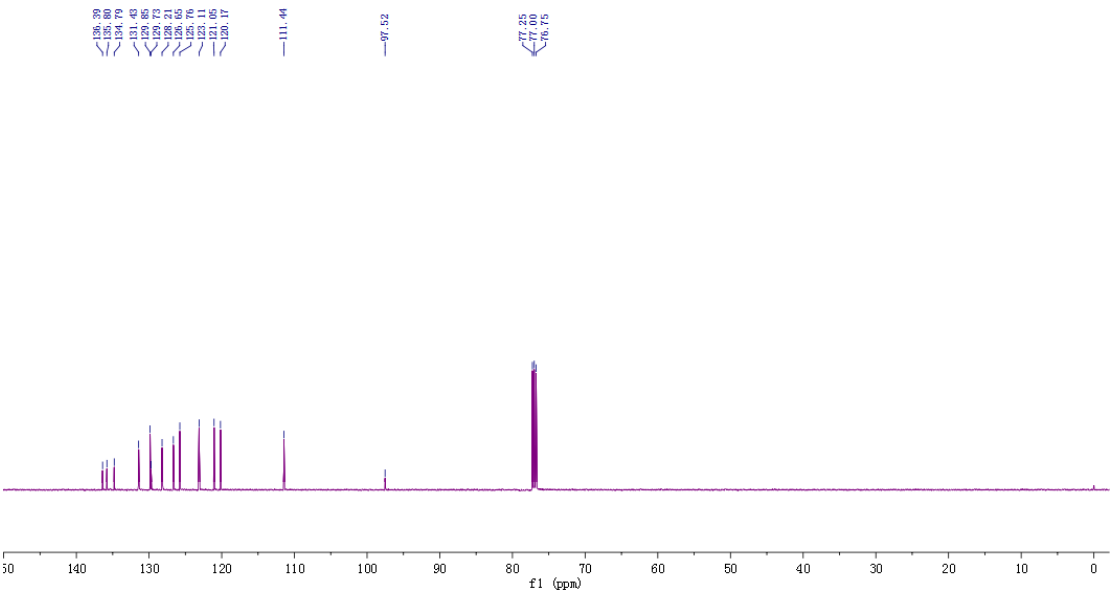
7.63
7.49
7.48
7.46
7.45
7.31
7.30
7.28
7.25
7.23
7.22
7.21
7.20
7.11
7.10
7.09
7.07
7.06
7.04
7.03
0.95
1.00
0.99
1.05
1.05
2.03
3.13
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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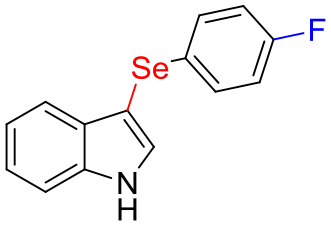
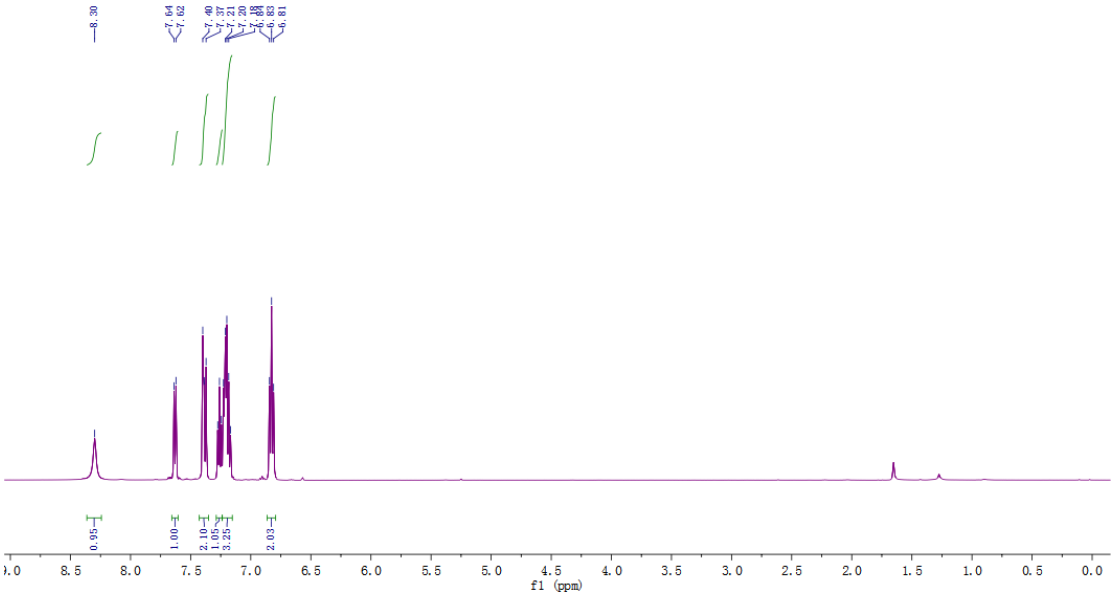
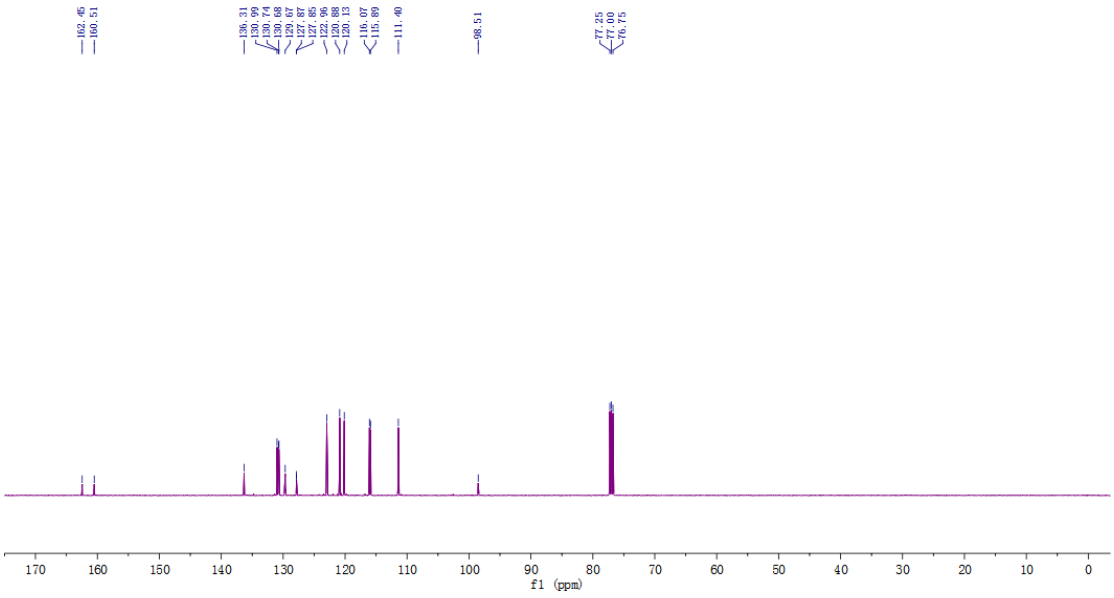
135.80
134.79
131.43
129.85
129.73
128.21
126.65
125.76
123.11
121.05
120.17
111.44
97.52
77.25
77.00
76.75
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


F
Se
N
H

3ae


8.39
7.64
7.62
7.40
7.37
7.21
7.20
6.84
6.83
6.81
0.95
1.00
2.10
1.05
3.25
2.03
f1 (ppm)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160.51
136.31
130.99
130.74
130.68
129.67
127.87
127.65
122.56
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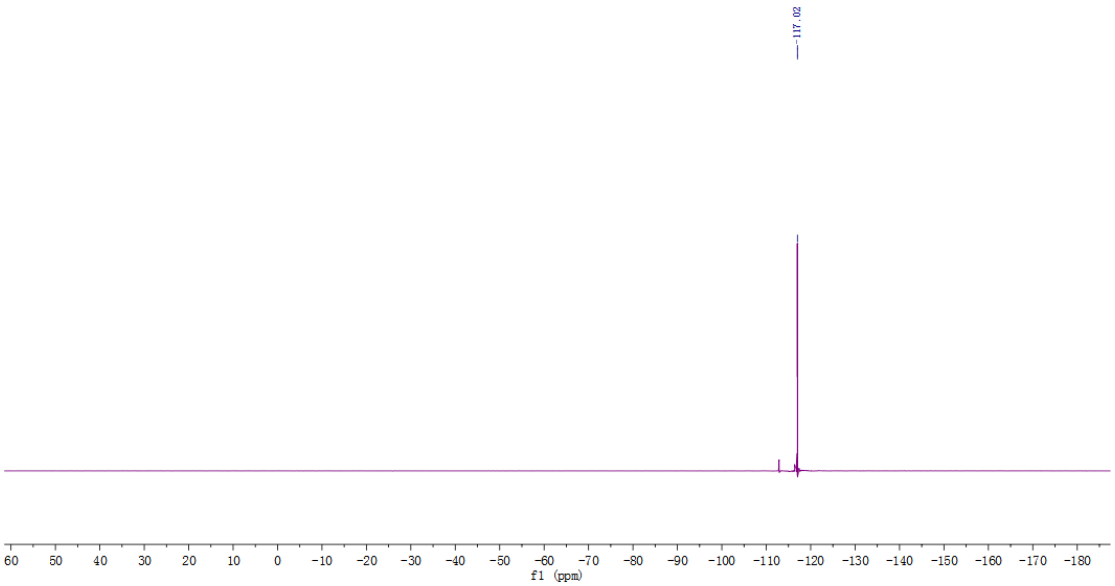
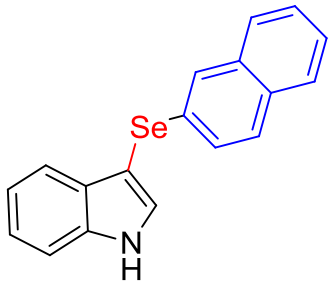
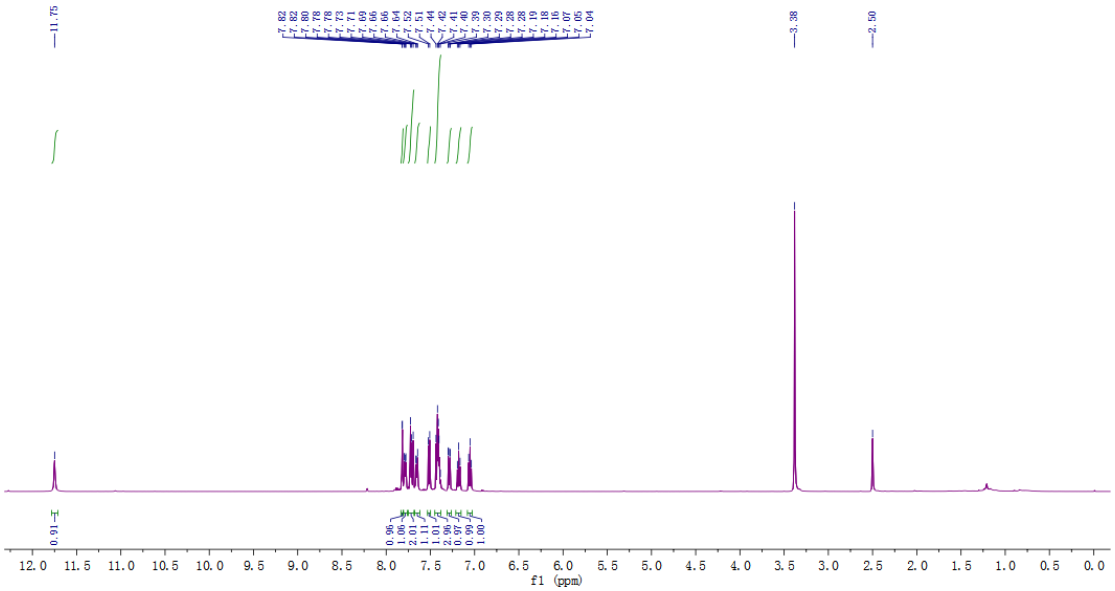
120.13
116.07
115.89
111.40
98.51
77.25
77.00
76.75
f1 (ppm)


-117.02
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)


Se
N
H

3af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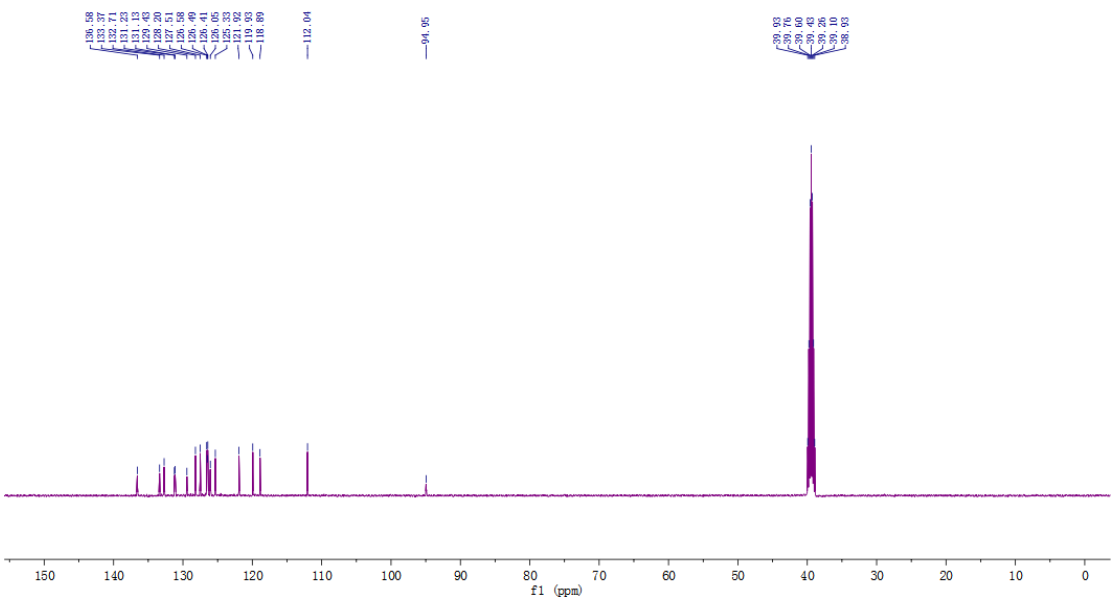
7.64
7.52
7.51
7.44
7.42
7.41
7.40
7.39
7.30
7.29
7.28
7.28
7.19
7.18
7.16
7.07
7.05
7.04
3.38
2.50
0.91
0.96
1.06
2.01
1.11
1.07
2.96
0.97
0.99
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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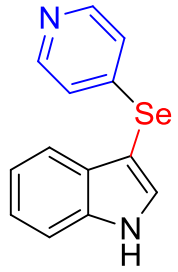
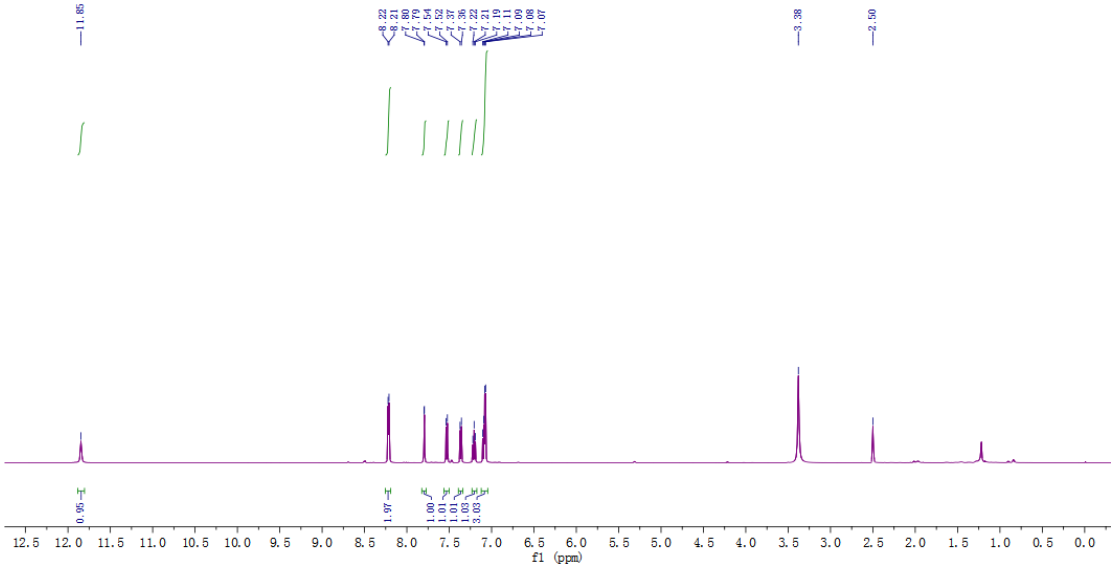
127.51
126.58
126.49
126.41
126.05
125.32
124.94
119.93
118.89
112.04
94.95
39.93
39.76
39.60
39.43
39.26
39.10
38.93
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


N
Se
N
H

3ag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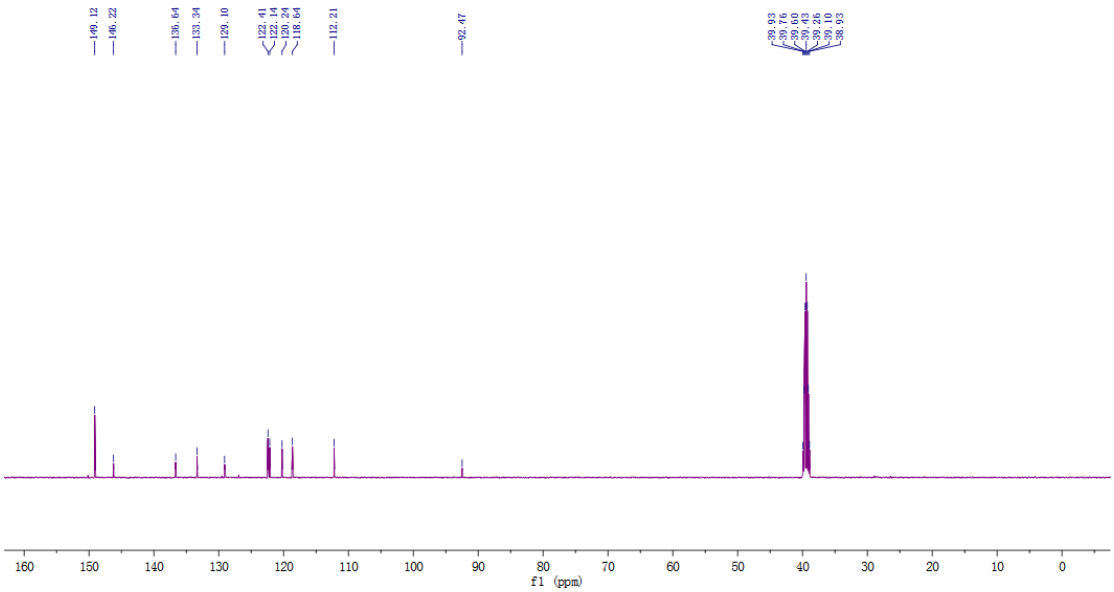
7.37
7.36
7.22
7.21
7.19
7.11
7.09
7.08
7.07
3.38
2.50
0.95
1.97
1.00
1.01
1.01
1.03
3.03
f1 (ppm)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146.22
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133.34
129.10
122.41
122.14
120.24
118.64
112.21
92.47
39.93
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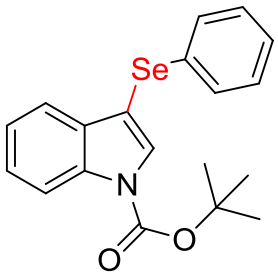
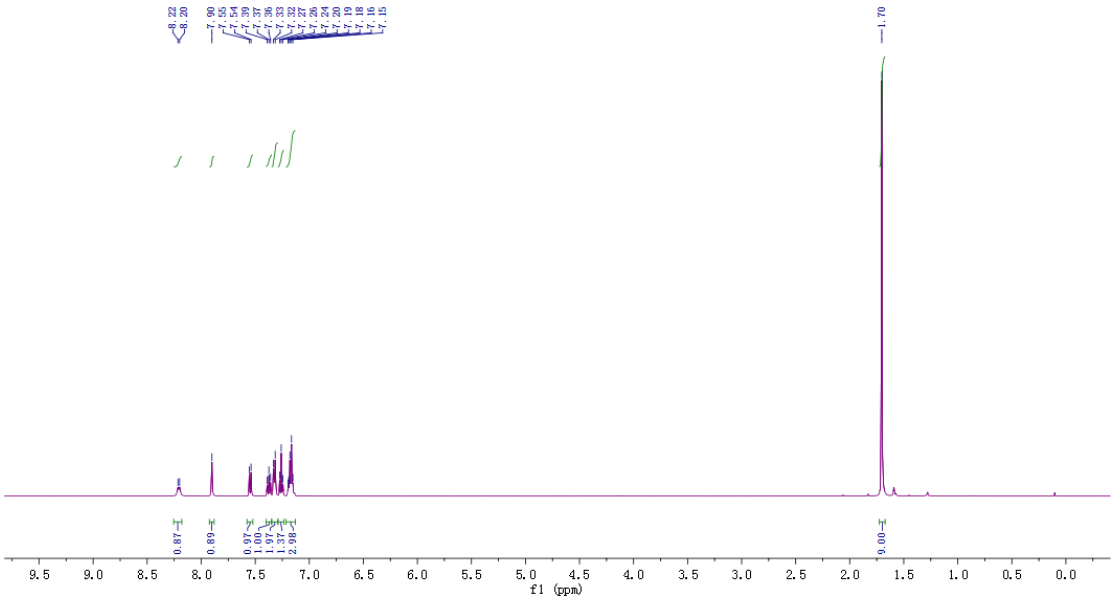
39.60
39.43
39.26
39.10
38.93
f1 (ppm)


Se
N
O
O

3ah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7.37
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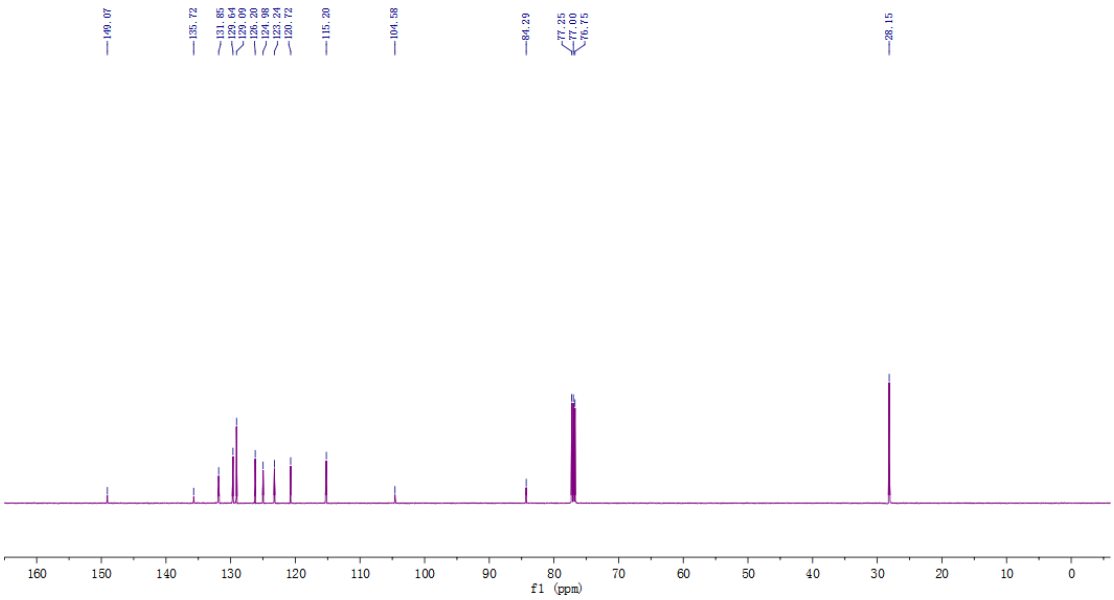
7.33
7.32
7.27
7.26
7.24
7.20
7.19
7.18
7.16
7.15
1.70
0.87
0.89
0.97
1.00
1.97
1.37
2.98
9.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.20
124.88
123.24
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115.20
104.58
84.29
77.25
77.00
76.75
28.15
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)