Supporting Information

Micelle-Mediated Multicomponent Cross-Coupling in Water: General Construction of 3-Chalcogenylindoles

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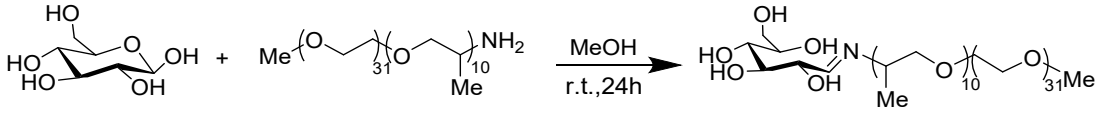
1. General Information

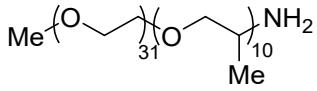
Unless otherwise noted, all reactions were carried out in oven-dried glassware under an atmosphere of air. Reaction temperatures are reported as the temperature of the oil bath surrounding the vessel. The M2070 (Polyether amine is a monoamine based on a copolymer backbone with a dispersity of M_w/M_n=1.14. The mean amount of ethylene oxide (EO) and propylene oxide (PO) are 31 and 10.[1, 2]) was purchased from Hengyu Trading (Guangzhou, China) Co., Ltd. Commercially available chemicals were obtained from Greagent, Adamas, Energy Chemical and Sinopharm and used as received unless otherwise stated. ^{1}H NMR spectra were recorded on Bruker DRX (400/600 MHz) and ^{13}C NMR spectra on Bruker DRX (100/150 MHz) spectrometer. Melting points were determined on an X4-Data microscopic melting point apparatus and were uncorrected. Mass spectra were recorded on a Finnigan TSQ Quantum-MS instrument in the electrospray ionization (ESI) mode. X-ray diffraction (XRD) pattern was recorded with a diffractometer (Bruker D8 Advance) using Cu Ka radiation at a range of 5-85° on 2θ. Crystallographic data were collected using a D8 VENTURE CMOS (Bruker) diffractometer with graphite-monochromated Mo−Kα (λ = 1.54178 Å) radiation. The transmission electron microscopy (TEM) was performed on JEM-2100plus at an acceleration voltage of 200 kV. Inductively coupled plasma optical emission spectrometer (ICP-OES) was performed on Aglient 5110 at the RF power of 1150w. Gel permeation chromatography (GPC) was performed on HLC-8320GPC EcoSEC with pure water as mobile phase. For the React-IR experiments, the reaction spectra were recorded using a React-IR 15 from Mettler-Toledo Auto-Chem. Data manipulation was carried out using the iC IR software, version 4.3.

2. The synthesis of sugar-based surfactants

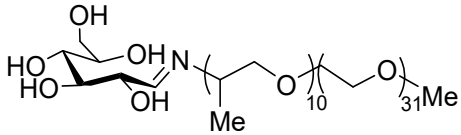
Preparation of N-polyoxyalkyl glucosamine (GluM)



A solution of glucose (1.80 g, 10 mmol), and polyether amine M2070 (20 g, 10 mmol) in methanol (100 mL) was mechanical stirred for 24 h at room temperature. Then the final mixture was placed at -15 °C for 5 times of recrystallization, and the supernatant liquid was removed the solvent by vacuum distillation to give yellow liquid in 85% yield. The dispersity of GluM is the same as that of M2070 and the mean amount of EO and PO are 31 and 10.



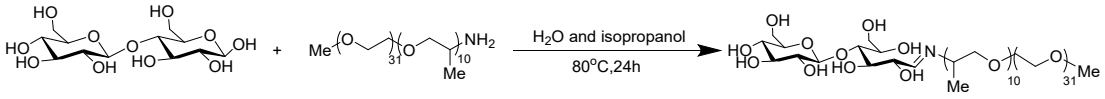
M2070. ^{1}H NMR (400 MHz, D_2O) δ 3.86 – 3.80 (m, 13H), 3.75 (s, 124H), 3.65 – 3.52 (m, 19H), 3.43 (s, 3H), 1.21 (d, *J* = 6.3 Hz, 30H). **^{13}C NMR (100 MHz, D_2O)** δ 178.48, 178.42, 75.16, 75.03, 74.85, 74.07, 74.05, 72.60, 72.21, 71.86, 71.25, 71.04, 70.97, 70.27, 70.01, 69.92, 69.64, 69.49, 67.55, 62.68, 58.11, 41.12, 15.96, 15.87, 15.77. **MS (MALDI-TOF):** Anal. Calced for $C_{93}H_{189}NO_{41}$: $[M+H]^+$ 1977.5. C, 56.49, H, 9.63, N, 0.71. Found: $[M+H]^+$ 1977.0. C, 55.99, H, 9.41, N, 0.76.



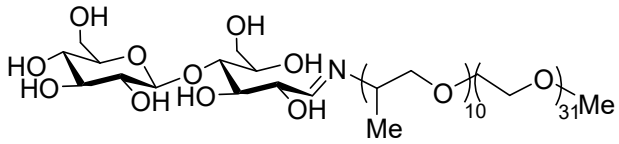
GluM. ^{1}H NMR (400 MHz, D_2O) δ 5.25 (d, *J* = 2.6 Hz, 1H), 4.67 (dd, *J* = 7.9, 0.9 Hz, 1H), 3.81 (dd, *J* = 8.5, 3.8 Hz, 13H), 3.74 (s, 124H), 3.58 (dd, *J* = 17.2, 7.0 Hz, 23H), 3.42 (s, 4H), 1.20 (d, *J*

= 6.1 Hz, 30H), 1.09 (d, *J* = 6.1 Hz, 2H). **MS (MALDI-TOF):** Anal. Calced for $C_{99}H_{199}NO_{46}$: $[M+H]^+$ 2139.6. C, 55.57, H, 9.38, N, 0.65. Found: $[M+H]^+$ 2139.4. C, 54.81; H, 8.96; N, 0.94.

Preparation of N-polyoxyalkyl lactosamine (LacM)

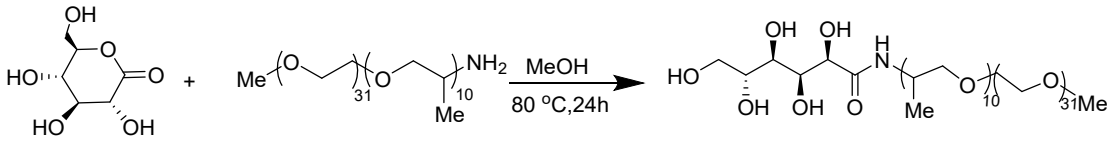


Lactose monohydrate (3.80 g, 10 mmol) was dissolved in 60 mL of ultrapure water, and polyether amine r M2070 (20 g, 10 mmol) was dissolved in 100 mL of isopropanol. The two solutions were mixed and stirred at 80 °C for 24 h. The final mixture was removed the solvent by vacuum distillation. Then recrystallized with ethanol at -15 °C for 5 times to give brown liquid in 80% yield. The dispersity of LacM is the same as that of M2070 and the mean amount of EO and PO are 31 and 10.

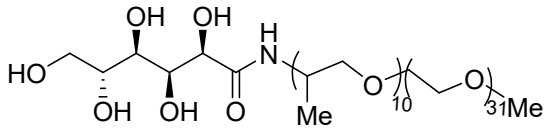


LacM. ^{1}H NMR (400 MHz, DMSO) δ 3.56 – 3.53 (m, 16H), 3.52 – 3.49 (m, 124H), 3.48 – 3.46 (m, 10H), 3.44 (d, *J* = 7.0 Hz, 8H), 3.38 (d, *J* = 5.8 Hz`, 6H), 3.31 (d, *J* = 4.8 Hz, 6H), 3.29 (d, *J* = 4.8 Hz, 4H), 3.24 (s, 2H), 1.05 – 1.03 (m, 30H), 0.96 (d, *J* = 6.5 Hz, 2H). **MS (MALDI-TOF):** Anal. Calced for $C_{105}H_{209}NO_{51}$: $[M+H]^+$ 2301.7. C, 54.79, H, 9.15, N, 0.61. Found: $[M+H]^+$ 2301.1. C, 55.01; H, 9.42; N, 0.85.

Preparation of N-polyoxyalkyl-D-glucamide (GluLM)

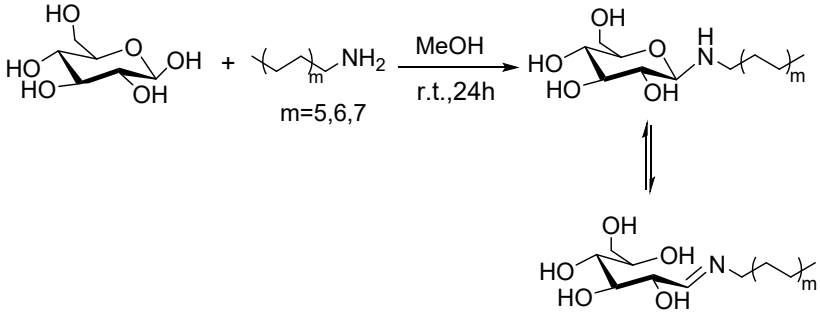


To a solution of the gluconolactone (1.78 g, 10 mmol) in methanol (100 mL) was slowly added polyether amine M2070 (20 g, 10 mmol). The resulting mixture was heated at 80°C for 24 h Then the final mixture was placed at -15 °C for 5 times of recrystallization, and the supernatant liquid was removed the solvent by vacuum distillation to give yellow liquid in 82% yield. The dispersity of GluLM is the same as that of M2070 and the mean amount of EO and PO are 31 and 10.

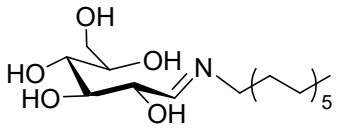


GluLM. ^{1}H NMR (400 MHz, DMSO) δ 3.55 (dd, *J* = 5.4, 3.5 Hz, 16H), 3.50 (d, *J* = 6.5 Hz, 124H), 3.48 – 3.46 (m, 9H), 3.40 (d, *J* = 5.8 Hz, 4H), 3.38 (d, *J* = 5.7 Hz, 4H), 3.31 (d, *J* = 4.6 Hz, 10H), 3.24 (s, 2H), 1.04 (d, *J* = 6.3 Hz, 30H). **MS (MALDI-TOF):** Anal. Calced for $C_{99}H_{199}NO_{47}$: $[M+H]^+$ 2155.6. C, 55.16, H, 9.31, N, 0.65. Found: $[M+H]^+$ 2155.2. C, 55.74; H, 9.48; N, 0.87.

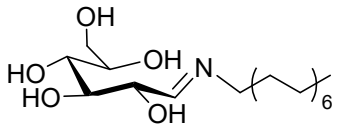
Preparation of N-alkyl glucosamine (AGA12, AGA14, AGA16)



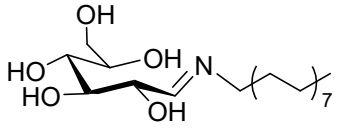
A solution of glucose (9.00 g, 50 mmol), and N-alkylamine (50 mmol) in methanol (100 mL) was mechanical stirred for 24 h at room temperature. Then the final mixture was suction filtered to remove solvent methanol, washed the filter cake three times with cyclohexane, once with water, twice with ethanol, recrystallized twice with ethanol, and dried in vacuum to give solid powder. The yields of AGA12, AGA14, AGA16 were respectively 87%, 78%, 58%.



AGA12. ^{1}H NMR (400 MHz, MeOD) δ 3.91 – 3.80 (m, 2H), 3.67 (dd, *J* = 11.6, 5.6 Hz, 1H), 3.38 (d, *J* = 8.4 Hz, 1H), 3.29 (dd, *J* = 8.8, 5.6 Hz, 1H), 3.27 – 3.21 (m, 1H), 3.08 (t, *J* = 8.8 Hz, 1H), 2.97 – 2.88 (m, 1H), 2.69 – 2.61 (m, 1H), 1.52 (m, 2H), 1.33 (d, *J* = 10.4 Hz, 18H), 0.92 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR (100 MHz, DMSO)** δ 91.29, 78.03 (d, *J* = 15.3 Hz), 74.01, 71.07, 61.91, 46.03, 31.76, 30.48, 29.51 (d, *J* = 5.5 Hz), 29.18, 27.32, 22.56, 14.42.

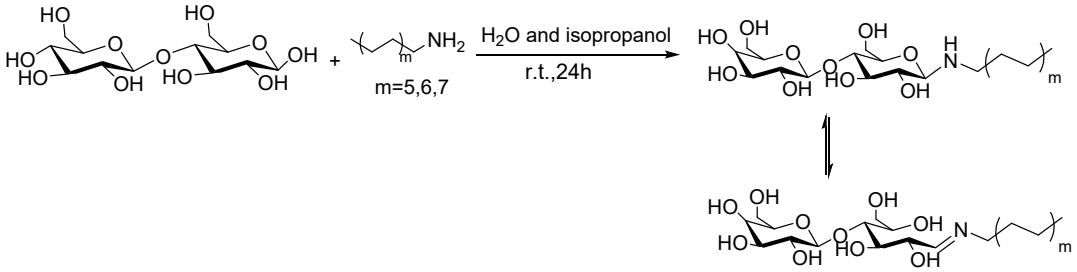


AGA14. ^{1}H NMR (400 MHz, MeOD) δ 3.88 – 3.82 (m, 2H), 3.67 (dd, *J* = 8.0, 3.6 Hz, 1H), 3.39 – 3.34 (m, 1H), 3.31 – 3.27 (m, 1H), 3.24 (m, 1H), 3.08 (t, *J* = 6.0 Hz, 1H), 2.93 (m, 1H), 2.65 (m, 1H), 1.57 – 1.48 (m, 2H), 1.37 – 1.28 (m, 22H), 0.92 (t, *J* = 4.6 Hz, 3H). **^{13}C NMR (100 MHz, MeOD)** δ 90.45, 77.57, 73.57, 70.47, 61.56, 45.83, 31.67, 29.66, 29.36 (d, *J* = 3.5 Hz), 29.07, 27.01, 22.33, 13.02.

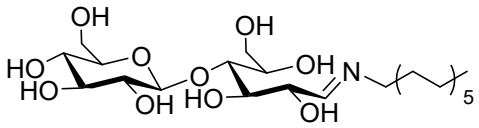


AGA16. ^{1}H NMR (400 MHz, DMSO) δ 4.90 – 4.66 (m, 2H), 4.45 (d, *J* = 3.6 Hz, 1H), 4.39 – 4.26 (m, 1H), 3.70 – 2.97 (m, 7H), 2.86 (td, *J* = 8.4, 2.8 Hz, 1H), 2.78 (dt, *J* = 11.6, 6.8 Hz, 1H), 1.37(m, 2H), 1.24 (s, 26H), 0.86 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR (100 MHz, DMSO)** δ 91.29, 78.02 (d, *J* = 14.8 Hz), 74.01, 71.06, 61.90, 46.04, 31.77, 30.49, 29.50 (d, J = 4.3 Hz), 29.18, 27.34, 22.56, 14.40.

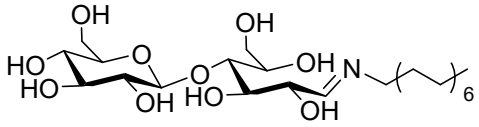
Preparation of N-alkyl lactosamine (ALA12, ALA14, ALA16)



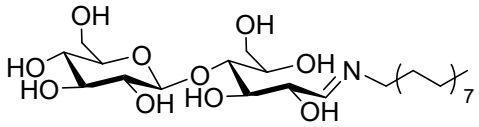
Lactose monohydrate (6.48 g, 18 mmol) was dissolved in 60 mL of ultrapure water, and N-alkylamine (30 mmol) was dissolved in 100 mL of isopropanol. The two solutions were mixed and mechanical stirred at room temperature for 24 hours, then transfer to a 60 ºC water bath for 30 minutes. The final mixture was suction filtered to remove solvent and the filter cake were rinsed three times with ethanol, recrystallized with ethanol, and dried in vacuum to give white solid powder. The yields of ALA12, ALA14, ALA16 were respectively 75%, 86%, 65%.



ALA12. ^{1}H NMR (400 MHz, MeOD) δ 4.38 (d, *J* = 3.2 Hz, 1H), 3.89 – 3.77 (m, 5H), 3.72 (dd, *J* = 7.6, 3.2 Hz, 1H), 3.62 – 3.48 (m, 5H), 3.40 – 3.35 (m, 1H), 3.15 (t, *J* = 6.0 Hz, 1H), 2.91 (m, 1H), 2.65 (m, 1H), 1.58 – 1.46 (m, 2H), 1.33 (d, *J* = 12.8 Hz, 18H), 0.92 (t, *J* = 4.8 Hz, 3H). **^{13}C NMR (100 MHz, MeOD)** δ 103.72, 90.37, 79.57, 76.10, 75.87, 75.69, 73.45, 73.25, 71.19, 68.91, 61.10, 60.75, 31.67, 29.65, 29.31 (d, *J* = 7.0 Hz), 29.07, 27.00, 22.33, 13.02.

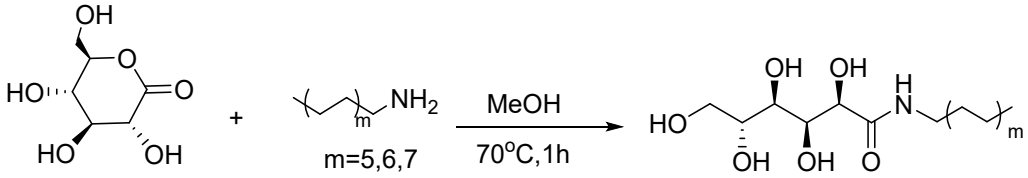


ALA14. ^{1}H NMR (400 MHz, DMSO) δ 5.12 (s, 1H), 4.80 (s, 1H), 4.64 (s, 2H), 4.49 (d, *J* = 29.6 Hz, 2H), 4.19 (dd, *J* = 12.4, 7.6 Hz, 1H), 3.76 – 3.15 (m, 14H), 2.93 (t, *J* = 8.4 Hz, 1H), 2.77 (dt, *J* = 11.2, 7.2 Hz, 1H), 1.37 (d, *J* = 6.4 Hz, 2H), 1.24 (s, 22H), 0.86 (t, *J* = 6.4 Hz, 3H).**^{13}C NMR (100 MHz, MeOD)** δ 103.72, 90.38, 79.58, 76.10, 75.87, 75.69, 73.45, 73.25, 71.19, 68.91, 61.10, 60.75, 40.92, 31.67, 29.21 (d, *J* = 11.0 Hz), 29.07, 27.01, 26.57, 22.33, 13.02.

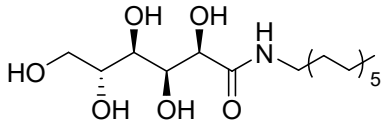


ALA16. ^{1}H NMR (400 MHz, DMSO) δ 5.12 (s, 1H), 4.80 (s, 1H), 4.64 (s, 2H), 4.49 (d, *J* = 25.6 Hz, 2H), 4.19 (dd, *J* = 12.4, 7.6 Hz, 1H), 3.76 – 3.15 (m, 14H), 2.93 (t, *J* = 8.4 Hz, 1H), 2.77 (dt, *J* = 11.2, 7.2 Hz, 1H), 1.37 (m, 2H), 1.24 (s, 22H), 0.86 (t, *J* = 6.4 Hz, 3H).**^{13}C NMR (100 MHz, MeOD)** δ 103.71, 90.37, 79.56, 76.10, 75.86, 75.68, 73.44, 73.24, 71.18, 68.91, 61.09, 60.74, 40.66, 31.67, 29.37, 29.06, 27.00, 26.48, 22.33, 13.02.

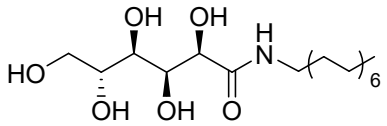
Preparation of N-alkyl-D-glucamide (C12NG, C14NG, C16NG)



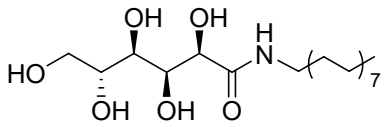
A mixture of gluconolactone (3.92 g, 22 mmol) and N-alkylamine (23 mmol) in CH_3OH (25 mL) were stirred for 1 hour at 70 °C. Then the final mixture was suction filtered to remove solvent CH_3OH, and the filter cake were rinsed three times with ethanol, recrystallized twice with methanol, and dried in vacuum to give solid powder. The yields of C12NG, C14NG, C16NG are respectively 92%, 93%, 90%.



C12NG. ^{1}H NMR (400 MHz, DMSO) δ 7.59 (t, *J* = 5.9 Hz, 1H), 5.34 (d, *J* = 5.1 Hz, 1H), 4.55 – 4.51 (m, 1H), 4.49 – 4.44 (m, 1H), 4.38 (d, *J* = 7.2 Hz, 1H), 4.33 (t, *J* = 5.7 Hz, 1H), 3.97 (dd, *J* = 5.0, 3.9 Hz, 1H), 3.90 (ddd, *J* = 7.1, 3.7, 2.1 Hz, 1H), 3.58 (ddd, *J* = 10.9, 5.8, 2.7 Hz, 1H), 3.52 – 3.44 (m, 2H), 3.41 – 3.34 (m, 1H), 3.15 – 2.98 (m, 2H), 1.44 – 1.36 (m, 2H), 1.26 (d, *J* = 13.8 Hz, 18H), 0.86 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR (100 MHz, DMSO)** δ 172.68, 74.10, 72.89, 71.96, 70.58, 63.85, 38.72, 31.78, 29.78 – 29.41, 29.25, 26.86, 22.57, 14.42.



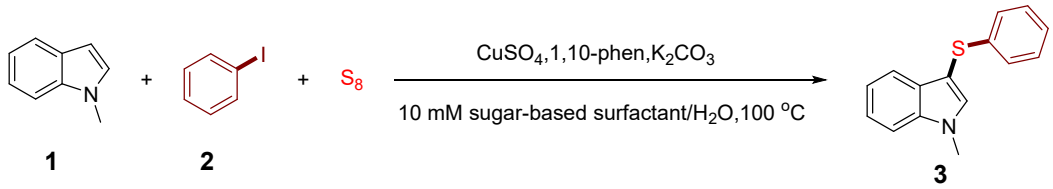
C14NG. ^{1}H NMR (400 MHz, DMSO) δ 7.59 (t, *J* = 5.9 Hz, 1H), 5.34 (d, *J* = 5.1 Hz, 1H), 4.55 – 4.51 (m, 1H), 4.49 – 4.44 (m, 1H), 4.38 (d, *J* = 7.2 Hz, 1H), 4.33 (t, *J* = 5.7 Hz, 1H), 3.97 (dd, *J* = 5.0, 3.9 Hz, 1H), 3.90 (ddd, *J* = 7.1, 3.7, 2.1 Hz, 1H), 3.58 (ddd, *J* = 10.9, 5.8, 2.7 Hz, 1H), 3.52 – 3.44 (m, 2H), 3.41 – 3.34 (m, 1H), 3.15 – 2.98 (m, 2H), 1.44 – 1.36 (m, 2H), 1.26 (d, *J* = 13.8 Hz, 18H), 0.86 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR (100 MHz, DMSO)** δ 172.68, 74.10, 72.89, 71.96, 70.59, 63.86, 38.72, 31.77, 29.55, 29.24, 26.86, 22.57, 14.42.



C16NG. ^{1}H NMR (400 MHz, DMSO) δ 7.59 (t, *J* = 5.9 Hz, 1H), 5.34 (d, *J* = 5.1 Hz, 1H), 4.53 (d, *J* = 5.1 Hz, 1H), 4.46 (d, *J* = 5.5 Hz, 1H), 4.38 (d, *J* = 7.2 Hz, 1H), 4.33 (t, *J* = 5.7 Hz, 1H), 3.97 (dd, *J* = 5.0, 3.9 Hz, 1H), 3.90 (ddd, *J* = 7.0, 3.7, 2.1 Hz, 1H), 3.58 (ddd, *J* = 10.9, 5.7, 2.7 Hz, 1H), 3.51 – 3.44 (m, 2H), 3.40 – 3.34 (m, 1H), 3.07 (qd, *J* = 13.0, 6.0 Hz, 2H), 1.44 – 1.36 (m, 2H), 1.24 (s, 26H), 0.86 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR (100 MHz, DMSO)** δ 172.68, 74.10, 72.89, 71.96, 70.59, 63.86, 38.72, 31.76, 29.87 – 29.07, 26.86, 22.56, 14.42.

3. Optimization of reaction conditions

Table S1 Screening of sugar-based surfactant [a]

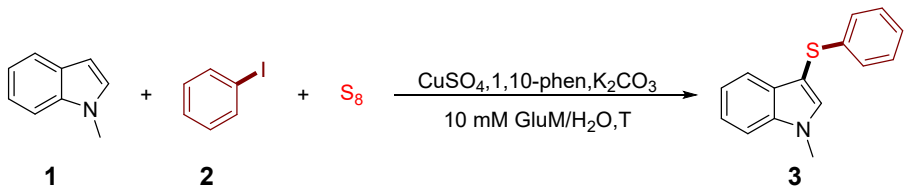


1 2 3

Entry	Surfactant	Conversion/%	Yield/% [b]
1	**GluM**	**97**	**92**
2	LacM	92	87
3	GluLM	94	88
4	AGA12	88	84
5	AGA14	86	85
6	AGA16	85	80
7	ALA12	88	81
8	ALA14	85	82
9	ALA16	83	77
10	C12NG	77	71
11	C14NG	80	76
12	C16NG	77	73

[a] Reaction conditions: indole 1 (1.0 mmol), iodobenzene 2 (1.2 mmol), sulfur (2.5 mmol), $CuSO_4$, 1,10-phen (0.1 mmol), K_2CO_3 (0.6 mmol), 10 mM sugar-based surfactant/H_2O (10 mL) under air at 100 °C for 12 h; [b] Isolated yield.

Table S2 Screening of reaction temperature [a]



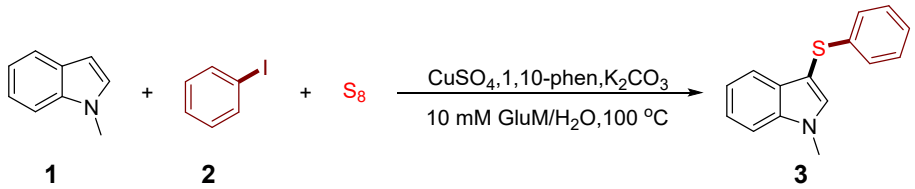
1 2 3

Entry	Temperature/°C	Conversion/%	Yield/% [b]
1	60	60	57
2	80	76	74
3	**100**	**97**	**92**

4	110	97	92

[a] Reaction conditions: indole 1 (1.0 mmol), iodobenzene 2 (1.2 mmol), sulfur (2.5 mmol), $CuSO_4$, 1,10-phen (0.1 mmol), K_2CO_3 (0.6 mmol), 10 mM GluM/H_2O (10 mL) under air for 12 h; [b] Isolated yield.

Table S3 Screening of surfactant equivalence [a]

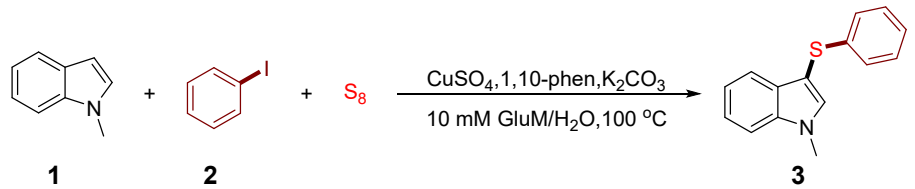


1 **2** **3**

Entry	GluM(equiv.)	Conversion/%	Yield/% [b]
1	0.025	80	56
2	0.05	85	63
3	0.075	90	76
4	**0.1**	**97**	**92**
5	0.15	90	90

[a] Reaction conditions: indole 1 (1.0 mmol), iodobenzene 2 (1.2 mmol), sulfur (2.5 mmol), $CuSO_4$ (0.1 mmol), 1,10-phen (0.1 mmol), K_2CO_3 (0.6 mmol), GluM/H_2O (10 mL) under air at 100 °C for 12 h; [b] Isolated yield.

Table S4 Screening of copper salt equivalence [a]



1 **2** **3**

Entry	$CuSO_4$(equiv.)	Conversion/%	Yield/% [b]
1	0.05	80	76
2	**0.1**	**97**	**92**
3	0.2	92	90

[a] Reaction conditions: indole 1 (1.0 mmol), iodobenzene 2 (1.2 mmol), sulfur (2.5 mmol), $CuSO_4$, 1,10-phen (0.1 mmol), K_2CO_3 (0.6 mmol), 10 mM GluM/H_2O (10 mL) under air at 100 °C for 12 h; [b] Isolated yield.

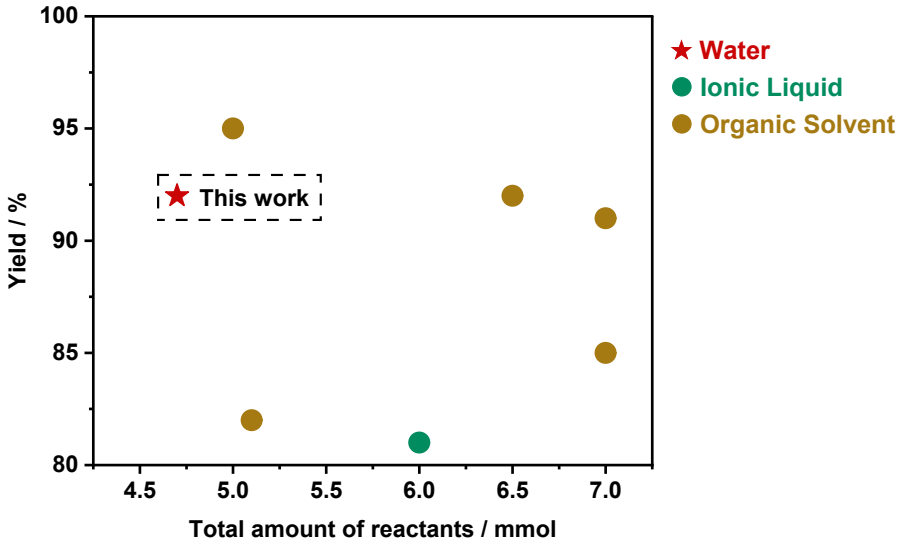


Fig. S1 Comparison of total amount of reactants and yields in different catalytic systems. [a]

[a] The total amount of reactants was calculated by the equation

$$n(total) = \frac{n(Heterocycle) + n(Iodobenzen\ /\ Phenyloronic\ acid) + n(S/Se\ source)}{n(minimum)}$$

Where *n(minimum)* is the minimum amount of reactants. All data are adapted from Table S5.

Table S5 Summary on the multicomponent chalcogenization of elemental S/Se

Entry	Heterocycle	Iodobenzen/ Phenyloronic acid	S/Se source	Yield/%	Solvent	Ref
1 [a]	**1**	**1.2**	**2.5**	**92**	**Water**	**This work**
2 [a]	1	2	3	81	[Bmim]Cl	Jiang's work[3]
3 [a]	1	1.5	2.6	82	DMSO	Golzar's work[4]
4 [a]	1	3	3	91	DMF	Ravi's work[5]
5 [b]	2.5	1	3	92	DMSO	Wu's work[6]
6 [a]	1	3	3	85	DMF	Hu' work[7]
7 [a]	1	2	2	95	DMF	Our previous work[8]

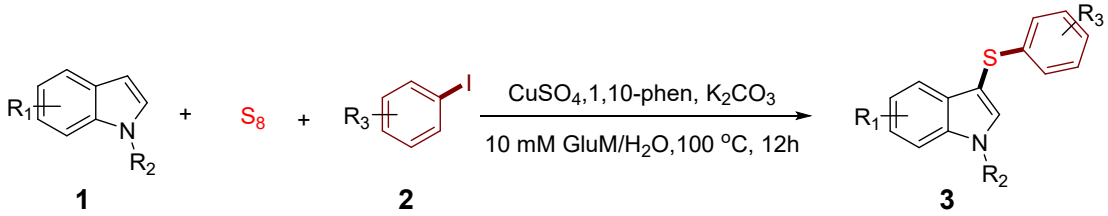
[a] Considering the amount of heterocycle as an equivalent. [b] Considering the amount of iodobenzen as an equivalent.

4. Experimental and characterization of reaction products

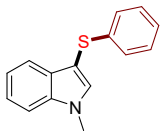
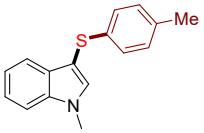
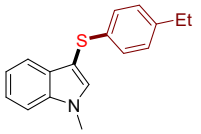
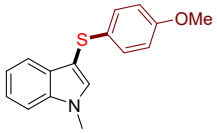
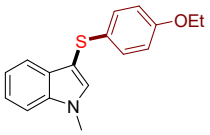
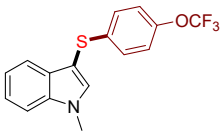
General procedure of C-S coupling in aqueous solution of GluM

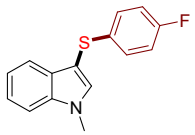
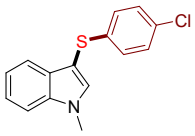
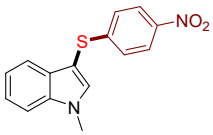
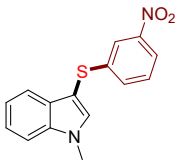
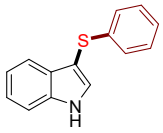
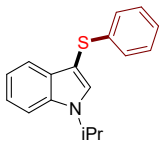
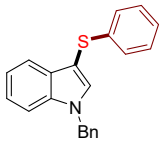
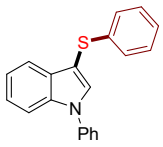
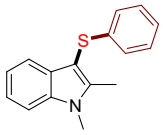
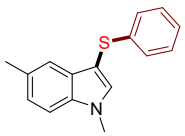
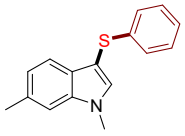
The copper salt catalyst, 1,10-phen (0.1 mmol), base (0.6 mmol), indole (1.0 mmol), aryl halide or its derivatives (1.2 mmol) and sulfur powder (2.5 mmol) were added to a micellar aqueous solution of surfactant (10 mL). The micelle solution mixture was then heated and stirred at 100 °C for 12 h. At the end of the reaction, the organic phase was extracted with ethyl acetate (1 mL×3) and dried with anhydrous Na_2SO_4, and the crude product was obtained by vacuum concentration. Crude products were purified by silica gel column chromatography (eluent: ethyl acetate/petroleum ether) to obtain the corresponding pure products, and characterized by ^1H NMR and ^{13}C NMR.

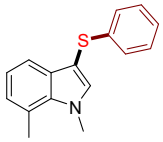
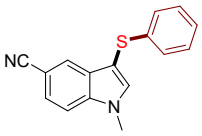
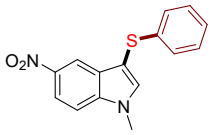
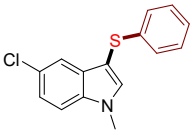
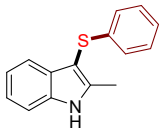
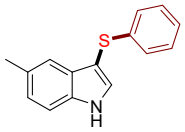
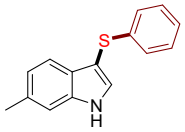
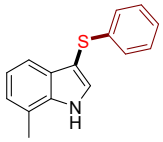
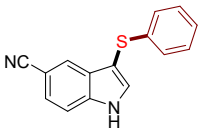
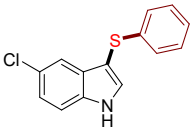
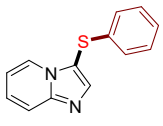
Table S6 Substrate scope of C-S coupling in aqueous solution of GluM [a]

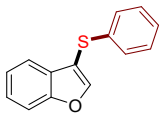
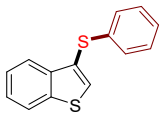


1 **2** **3**

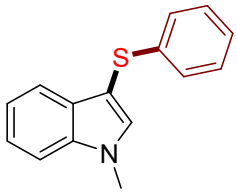
Entry	Target product	Conversion/%	Yield/% [b]
3a		97	92
3b		67	60
3c		56	53
3d		89	85
3e		77	73
3f		81	75

3g		88	82
3h		97	91
3i		97	94
3j		87	84
3k		80	76
3l		79	75
3m		67	64
3n		91	87
3o		85	80
3p		66	60
3q		80	76

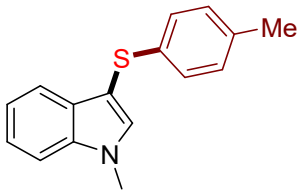
3r		89	85
3s		88	84
3t		92	86
3u		89	83
3v		66	60
3w		56	50
3x		61	55
3y		77	70
3z		94	88
3aa		94	90
3ab		91	87

3ac		n.d.	n.d.
3ad		n.d.	n.d.

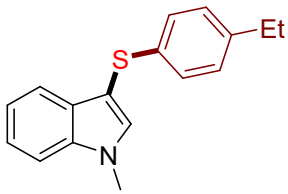
[a] Standard conditions: indole derivatives **1** (1.0 mmol), aryl iodides **2** (1.2 mmol), sulfur (2.5 mmol), $CuSO_4$ (0.1 mmol), 1,10-phen (0.1 mmol), K_2CO_3 (0.6 mmol), 10 mM GluM/H_2O (10 mL) under air at 100 °C for 12 h; [b] Isolated yield.



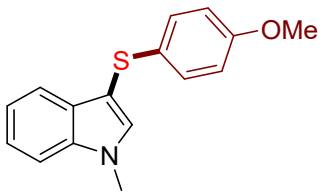
1-methyl-3-(phenylthio)-1H-indole 3a (0.219 g, 92% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.37 (s, 1H), 7.36–7.29 (m, 1H), 7.23–7.15 (m, 3H), 7.15–7.10 (m, 2H), 7.10 – 7.03 (m, 1H), 3.88 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.68, 137.58, 135.03, 129.86, 128.64, 125.78, 124.67, 122.57, 120.49, 119.75, 109.70, 100.64, 30.89.



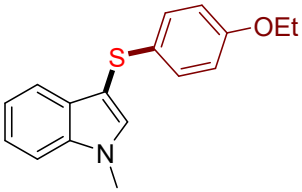
1-methyl-3-(p-tolylthio)-1*H*-indole 3b (0.152 g, 60% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (m, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.36–7.30 (m, 2H), 7.20 (m, 1H), 7.10–7.04 (m, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 3.86 (s, 3H), 2.29 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 136.46, 134.90, 133.80, 133.47, 128.79, 128.40, 125.07, 121.44, 119.37, 118.72, 108.62, 100.13, 32.07, 19.82.



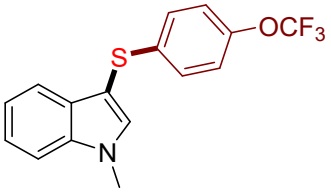
3-((4-ethylphenyl)thio)-1-methyl-1H-indole 3c (0.141 g, 53% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.64 (m, 1H), 7.50 – 7.45 (d, *J* = 8.4 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.23 – 7.18 (m, 2H), 7.11 – 7.05 (d, *J* = 8.4 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 3.87 (s, 3H), 2.58 (q, *J* = 7.6 Hz, 2H), 1.20 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.98, 134.88, 130.87, 129.94, 128.48, 128.27, 126.17, 122.51, 120.43, 119.81, 109.67, 101.27, 33.11, 28.30, 15.57.



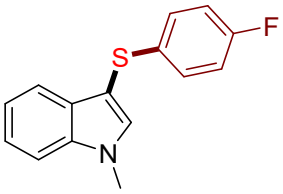
3-((4-methoxyphenyl)thio)-1-methyl-1*H*-indole 3d (0.228 g, 85% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.39–7.31 (m, 2H), 7.29–7.16 (m, 3H), 6.83–6.77 (m, 2H), 3.83 (s, 3H), 3.78 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.83, 137.57, 134.59, 130.09, 129.83, 128.53, 122.55, 120.45, 119.76, 114.55, 109.77, 102.39, 55.38, 33.07.



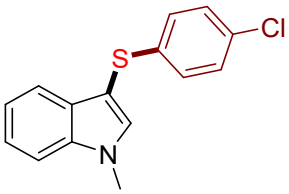
3-((4-ethoxyphenyl)thio)-1-methyl-1*H*-indole 3e (0.206 g, 73% isolated yield). ^{1}H NMR (400 MHz, DMSO) δ 7.73 (s, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.28–7.19 (m, 1H), 7.16–7.03 (m, 3H), 6.86–6.72 (m, 2H), 3.92 (q, *J* = 7.0 Hz, 2H), 3.84 (s, 3H), 1.27 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR (100 MHz, DMSO)** δ 157.24, 137.66, 135.99, 129.47, 128.79, 122.55, 120.59, 119.01, 115.60, 111.00, 100.89, 63.56, 33.21, 15.05.



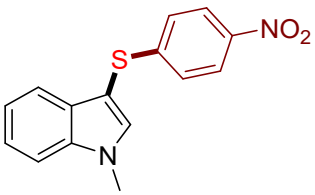
1-methyl-3-((4-(trifluoromethoxy)phenyl)thio)-1*H*-indole 3f (0.242 g, 75% isolated yield). ^{1}H NMR (400 MHz, DMSO) δ 7.81 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.25 (m, 1H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.18 – 7.05 (m, 3H), 3.88 (s, 3H). **^{13}C NMR (100 MHz, DMSO)** δ 146.21, 139.30, 137.83, 136.91, 129.32, 127.24, 122.82, 122.22, 120.99, 120.5, 118.79, 111.25, 98.09, 33.34.



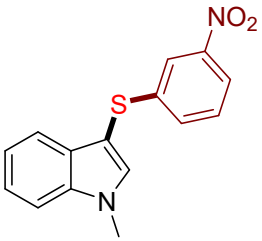
3-((4-fluorophenyl)thio)-1-methyl-1*H*-indole 3g (0.210 g, 82% isolated yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.36 (s, 1H), 7.35–7.29 (m, 1H), 7.23–7.17 (m, 1H), 7.15–7.07 (m, 2H), 6.92–6.85 (m, 2H), 3.87 (s, 3H). **^{13}C NMR (150 MHz, $CDCl_3$)** δ 160.84, 139.15, 136.19, 131.63, 128.79, 125.69, 124.93, 122.29, 119.42, 114.28, 111.29, 100.33, 33.37.



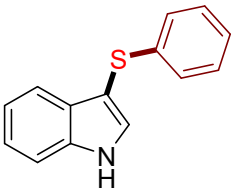
3-((4-chlorophenyl)thio)-1-methyl-1*H*-indole 3h (0.221 g, 91% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.39–7.31 (m, 2H), 7.25-7.17 (m, 1H), 7.17–7.11 (m, 2H), 7.09–6.99 (m, 2H), 3.88 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.32, 137.62, 135.05, 130.46, 129.58, 128.72, 127.04, 122.74, 120.67, 119.60, 109.82, 100.21, 33.16.



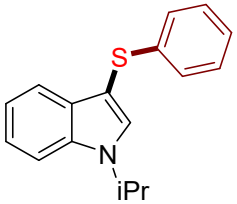
1-methyl-3-((4-nitrophenyl)thio)-1*H*-indole 3i (0.267 g, 94% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.96 (m, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.43 – 7.34 (m, 2H), 7.26 – 7.20 (m, 1H), 7.18 – 7.10 (m, 2H), 3.92 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.23, 144.91, 137.73, 135.43, 129.22, 125.03, 123.83, 123.10, 121.07, 119.31, 110.14, 97.90, 33.33.



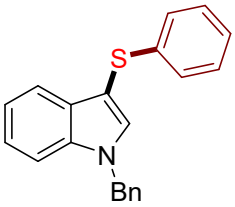
1-methyl-3-((3-nitrophenyl)thio)-1*H*-indole 3j (0.188 g, 84% isolated yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (t, *J* = 2.0 Hz, 1H), 7.90 (m, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.42 (s, 1H), 7.40 – 7.36 (m, 1H), 7.36 – 7.30 (m, 2H), 7.21 (t, *J* = 7.4 Hz, 1H), 3.92 (s, 3H). **^{13}C NMR (150 MHz, $CDCl_3$)** δ 148.72, 143.00, 137.70, 135.48, 131.18, 129.26, 122.99, 120.96, 120.15, 119.56, 119.27, 110.07, 98.46, 33.35.



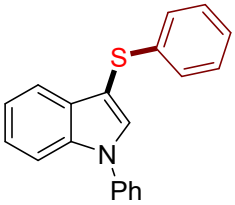
3-(phenylthio)-1*H*-indole 3k (0.171 g, 76% isolated yield). ^{1}H NMR (400 MHz, DMSO) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.40 (d, *J* = 2.6 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.22 - 7.14 (m, 1H), 7.13 - 7.05 (m, 3H), 7.03 (t, *J* = 4.2 Hz, 2H), 6.97 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.19, 135.47, 129.66, 128.07, 127.66, 124.82, 123.74, 122.01, 119.87, 118.64, 110.55, 101.78.



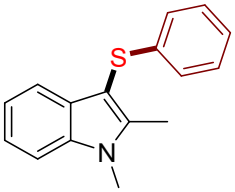
1-isopropyl-3-(phenylthio)-1*H*-indole 3l (0.200 g, 75% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 1H), 7.56 (s, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.20 (m, 3H), 7.17 – 7.12 (m, 2H), 7.09 (m, 1H), 4.77 (m, *J* =6.8 Hz, 1H), 1.62 (d, *J* = 6.8 Hz, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.97, 136.63, 130.43, 130.13, 128.79, 125.79, 124.74, 122.46, 120.63, 119.99, 110.19, 100.75, 47.77.



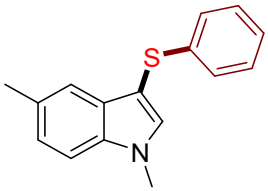
benzyl-3-(phenylthio)-1*H*-indole 3m (0.202 g, 64% isolated yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.8 Hz, 1H), 7.44 (s, 1H), 7.40 – 7.35 (m, 3H), 7.35 – 7.31 (m, 1H), 7.30 – 7.27 (m, 1H), 7.20 (m, 4H), 7.18 (s, 1H), 7.15 (d, *J* = 1.2 Hz, 1H), 7.14 (d, *J* = 1.2 Hz, 1H), 7.10 – 7.06 (m, 1H), 5.39 (s, 2H). **^{13}C NMR (150 MHz, $CDCl_3$)** δ 139.51, 137.19, 136.64, 134.47, 130.05, 128.96, 128.71, 127.99, 127.01, 125.76, 124.72, 122.79, 120.75, 119.92, 110.27, 101.45, 50.49.



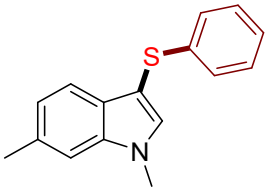
phenyl-3-(phenylthio)-1*H*-indole 3n (0.262 g, 87% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.62 (m, 3H), 7.62 – 7.56 (m, 4H), 7.49 – 7.42 (m, 1H), 7.33 (dd, *J* = 8.0, 7.2 Hz, 1H), 7.30 – 7.19 (m, 5H), 7.17 – 7.09 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 137.94, 137.84, 135.75, 132.82, 129.22, 128.77, 127.73, 126.12, 125.07, 123.91, 123.43, 122.33, 120.34, 119.03, 109.97, 102.87.



1,2-dimethyl-3-(phenylthio)-1*H*-indole 3o (0.202 g, 80% isolated yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.69 – 7.55 (m, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.33 – 7.24 (m, 1H), 7.23 – 7.14 (m, 3H), 7.14 – 7.02 (m, 3H), 3.80 (s, 3H), 2.56 (s, 3H). **^{13}C NMR (150 MHz, $CDCl_3$)** δ 142.87, 139.79, 137.10, 129.77, 128.64, 125.38, 124.39, 121.75, 120.45, 118.98, 109.01, 98.04, 30.36, 10.90.

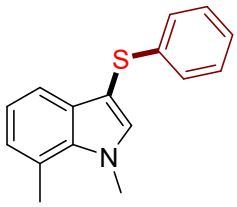


1,5-dimethyl-3-(phenylthio)-1*H*-indole 3p (0.152 g, 60% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.23 – 7.10 (m, 5H), 7.10 – 7.05 (m, 1H), 3.85 (s, 3H), 2.46 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.98, 135.99, 135.21, 130.16, 130.01, 128.66, 125.56, 124.56, 124.24, 119.28, 109.43, 99.64, 33.17, 21.42.

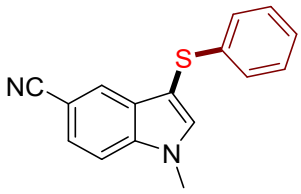


1,6-dimethyl-3-(phenylthio)-1*H*-indole 3q (0.192 g, 76% isolated yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.4 Hz, 1H), 7.29 (s, 1H), 7.21 (s, 1H), 7.19 – 7.14 (m, 2H), 7.13-7.10 (m,

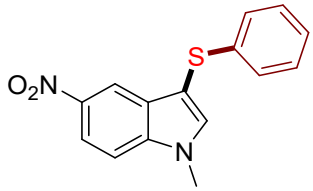
2H), 7.08 – 7.04 (m, 1H), 7.04-7.01 (m, 1H), 3.84 (s, 3H), 2.54 (s, 3H). **^{13}C NMR (150 MHz, $CDCl_3$)** δ 139.82, 137.95, 134.50, 132.54, 128.62, 127.66, 125.63, 124.56, 122.26, 119.41, 109.71, 99.99, 33.06, 21.87.



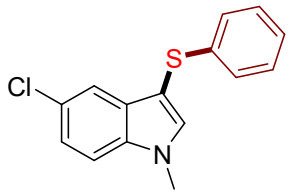
1,7-dimethyl-3-(phenylthio)-1*H*-indole 3r (0.215 g, 85% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.6 Hz, 1H), 7.25 (s, 1H), 7.21-7.15 (m, 2H), 7.15-7.10 (m, 2H), 7.10 – 6.98 (m, 3H), 4.13 (s, 3H), 2.83 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.62, 135.57, 135.20, 129.92, 127.60, 124.61, 124.21, 123.56, 120.71, 119.69, 116.87, 99.09, 36.10, 18.61.



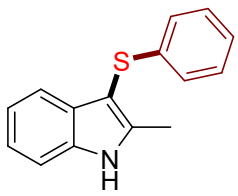
1-methyl-5-nitrile-3-(phenylthio)-1*H*-indole 3s (0.222 g, 84% isolated yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 (s, 1H), 7.55-7.50 (m, 1H), 7.49–7.43 (m, 2H), 7.25–7.19 (m, 2H), 7.15–7.08 (m, 3H), 3.91 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.09, 138.22, 137.03, 129.61, 128.91, 126.30, 125.57, 125.42, 125.32, 120.27, 110.77, 103.82, 103.07, 33.42.



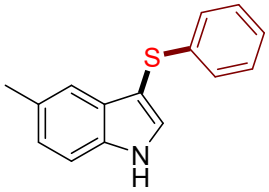
1-methyl-5-nitro-3-(phenylthio)-1*H*-indole 3t (0.244 g, 86% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 2.2 Hz, 1H), 8.20 (dd, *J* = 9.2, 2.0 Hz, 1H), 7.51 (s, 1H), 7.43 (d, *J* = 9.2 Hz, 1H), 7.24 – 7.17 (m, 2H), 7.16 – 7.09 (m, 3H), 3.93 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 141.48, 139.24, 137.13, 137.05, 128.28, 127.89, 125.27, 124.42, 117.21, 115.86, 109.00, 103.67, 32.64.



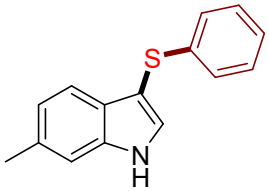
1-methyl-5-chloro-3-(phenylthio)-1*H*-indole 3u (0.226 g, 83% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 2.0 Hz, 1H), 7.35 (s, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 2.0 Hz, 1H), 7.20 (m, 2H), 7.12 (m, 3H), 3.83 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.20, 136.40, 135.98, 131.04, 128.82, 126.69, 125.82, 124.97, 123.04, 119.15, 110.97, 100.45, 33.36.



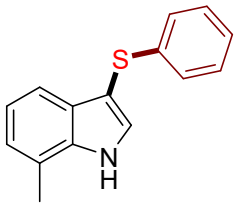
2-methyl-3-(phenylthio)-1*H*-indole 3v (0.143 g, 60% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.47 (d, *J* = 8.2 Hz, 1H), 7.27 (d, *J* = 8.1 Hz, 1H), 7.15 – 7.09 (m, 1H), 7.08 – 7.03 (m, 3H), 6.94-6.99 (m, 3H), 2.44 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.68, 137.56, 135.05, 129.85, 128.65, 125.74, 124.67, 122.57, 120.50, 119.76, 109.71, 100.57, 33.15.



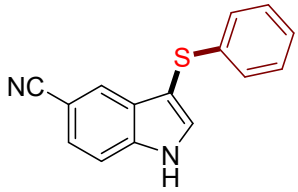
5-methyl-3-(phenylthio)-1*H*-indole 3w (0.119 g, 50% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.38-7.31 (m, 2H), 7.24 (d, *J* = 8.3 Hz, 1H), 7.12-7.05 (m, 2H), 7.04-6.98 (m, 3H), 6.99-6.93 (m, 1H), 2.33 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.47, 133.74, 129.87, 129.38, 128.37, 127.66, 124.60, 123.68, 123.62, 118.12, 110.20, 100.91, 20.41.



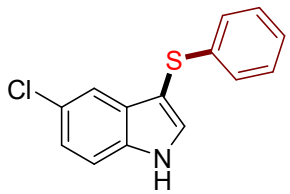
6-methyl-3-(phenylthio)-1*H*-indole 3x (0.132 g, 55% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.40 (d, *J* = 8.1 Hz, 1H), 7.31 (d, *J* = 2.6 Hz, 1H), 7.14 (s, 1H), 7.07 (dd, *J* = 10.1, 4.9 Hz, 2H), 7.02 (dd, *J* = 5.4, 3.2 Hz, 2H), 6.99 - 6.94 (m, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 2.39 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.33, 135.91, 131.98, 129.02, 127.64, 125.88, 124.73, 123.65, 121.66, 118.26, 110.48, 101.51, 20.67.



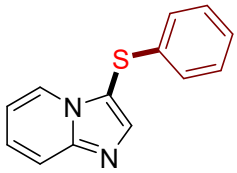
7-methyl-3-(phenylthio)-1*H*-indole 3y (0.167 g, 70% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.56 – 7.46 (m, 2H), 7.25 – 7.00 (m, 7H), 2.56 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.35, 136.10, 130.42, 128.74, 128.71, 125.87, 124.76, 123.61, 121.09, 120.80, 117.39, 103.23, 16.46.



5-nitrile-3-(phenylthio)-1*H*-indole 3z (0.220 g, 88% isolated yield). ^{1}H NMR (400 MHz, DMSO) δ 12.25 (s, 1H), 8.00 (s, 1H), 7.82 (d, *J* = 0.9 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.54 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.09 (s, 1H), 7.07 – 7.01 (m, 2H). **^{13}C NMR (100 MHz, DMSO)** δ 139.08, 138.59, 135.60, 129.47, 129.03, 126.34, 125.76, 125.47, 124.04, 120.61, 114.32, 102.90, 101.76.



5-chloro-3-(phenylthio)-1*H*-indole 3aa (0.233 g, 90% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 7.62 (d, *J* = 2.0 Hz, 1H), 7.52 (d, *J* = 2.6 Hz, 1H), 7.37 (d, *J* = 8.6 Hz, 1H), 7.26 (dd, *J* = 10.9, 8.9 Hz, 1H), 7.23 – 7.17 (m, 2H), 7.14 – 7.09 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.71, 134.84, 131.99, 130.42, 128.82, 126.95, 125.97, 125.06, 123.56, 119.17, 112.67, 102.97.

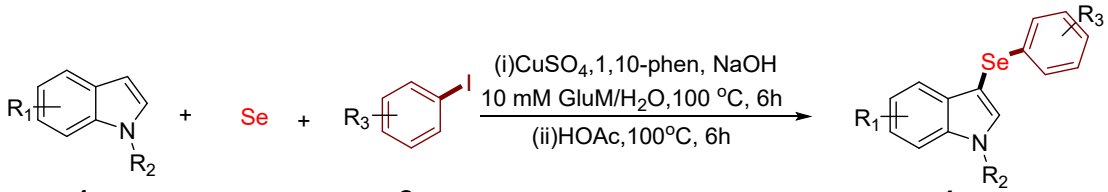


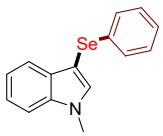
3-(Phenylthio)imidazo[1,2-*a*]pyridine 3ab (0.197 g, 87% isolated yield)^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 6.8 Hz, 1H), 7.98 (s, 1H), 7.68 (d, *J* = 9.0 Hz, 1H), 7.28 (t, *J* = 7.7 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 2H), 7.10 (t, *J* = 7.3 Hz, 1H), 6.97 (d, *J* = 7.4 Hz, 2H), 6.84 (t, *J* = 6.8 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 142.63, 135.38, 129.44, 126.34, 126.12, 124.49, 118.33, 113.31.

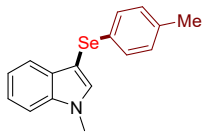
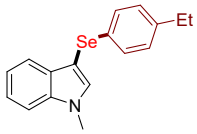
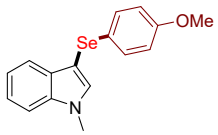
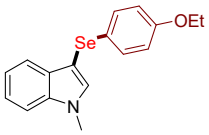
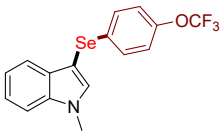
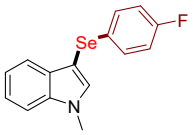
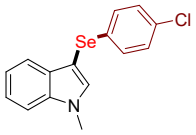
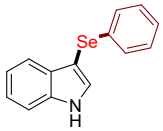
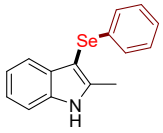
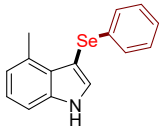
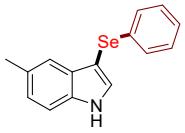
General procedure of C-Se coupling in aqueous solution of GluM

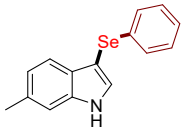
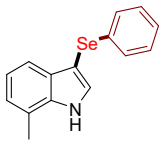
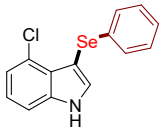
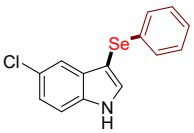
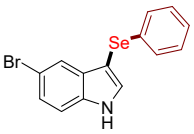
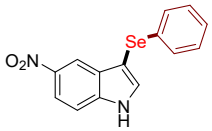
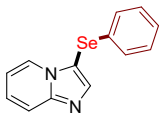
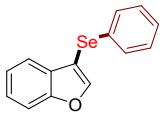
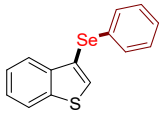
The copper salt catalyst (0.1 mmol), 1,10-phen (0.1 mmol), base (3.0 mmol), indole (1.0 mmol), aryl halide or its derivatives (1.2 mmol) and selenium powder (2.5 mmol) were added to a micellar aqueous solution of glycosyl polyether surfactant and H_2O (10 mM, 10 mL). The micelle solution mixture was then heated and stirred at 100 °C for 6 h. Then, the micelle solution mixture was added acetic acid (3.0 mmol) and heated and stirred at 100 °C for 6 h. At the end of the reaction, the organic phase was extracted with ethyl acetate (1 mL×3) and dried with anhydrous Na_2SO_4, and the crude product was obtained by vacuum concentration. Crude products were purified by silica gel column chromatography (eluent: ethyl acetate/petroleum ether) to obtain the corresponding pure products, and characterized by ^{1}H NMR and ^{13}C NMR.

Table S7 Substrate scope of C-Se coupling in aqueous solution of GluM [a]

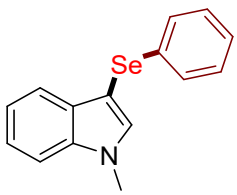


Entry	Target product	Conversion/%	Yield/% [b]
4a		81	75

4b		63	55
4c		53	48
4d		77	73
4e		74	70
4f		66	60
4g		77	72
4h		86	79
4i		77	73
4j		73	67
4k		64	58
4l		75	68

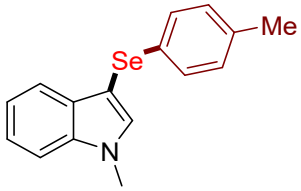
4m		74	71
4n		74	67
4o		73	68
4p		90	85
4q		80	76
4r		86	79
4s		82	76
4g		n.d.	n.d.
4h		n.d.	n.d.

[a] Standard conditions: (i) indole derivatives **1** (1.0 mmol), aryl iodides **2** (1.2 mmol), selenium (2.5 mmol), $CuSO_4$ (0.1 mmol), 1,10-phen (0.1 mmol), NaOH (3.0 mmol), 10 mM GluM/H_2O (10 mL) under air at 100 °C for 6 h, (ii) HOAc (3.0 mmol) under air at 100 °C for 6 h; [b] Isolated yield.

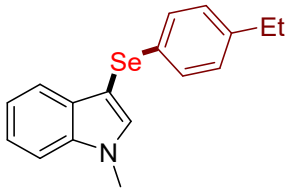


1-methyl-3-(phenylseleno)-1*H*-indole 4a (0.215 g, 75% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.30 (d, *J* = 2.3 Hz, 1H), 7.27 (dd, *J* =

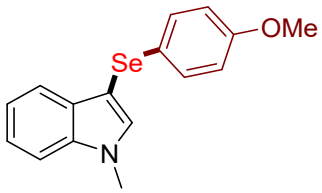
8.2, 1.0 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.19 – 7.14 (m, 1H), 7.13 – 7.04 (m, 3H), 3.80 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 137.66, 135.81, 134.40, 130.89, 129.10, 128.76, 125.69, 122.62, 120.65, 109.72, 96.12, 33.21.



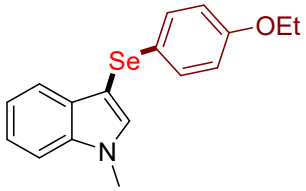
1-methyl-3-[(4-methylphenyl)seleno]-1*H*-indole 4b (0.165 g, 55% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.30 (dt, *J* = 8.2, 1.9 Hz, 2H), 7.21 – 7.16 (m, 3H), 6.96 (d, *J* = 7.9 Hz, 2H), 3.82 (s, 3H), 2.25 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 137.64, 135.58 135.56, 130.90, 130.40, 129.91, 129.19, 122.55, 120.68, 120.53, 109.67, 96.66, 33.18, 21.10.



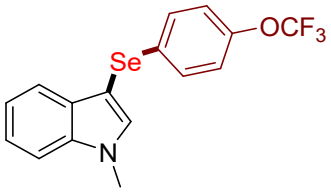
1-methyl-3-[(4-ethylphenyl)seleno]-1*H*-indole 4c (0.151 g, 48% isolated yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.66 (d, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.18 (dd, *J* = 11.5, 4.8 Hz, 3H), 6.97 (d, *J* = 8.2 Hz, 2H), 3.82 (s, 3H), 2.54 (q, *J* = 7.6 Hz, 2H), 1.16 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 142.00, 137.64, 135.64, 130.97, 130.75, 129.19, 128.75, 122.56, 120.72, 120.54, 109.67, 96.66, 33.21, 28.54, 15.73.



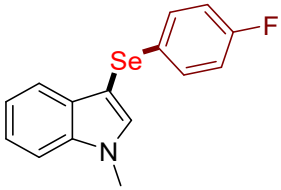
1-methyl-3-[(4-methoxyphenyl)selanyl]-1*H*-indole 4d (0.231 g, 73% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.21 (ddd, *J* = 6.3, 3.8, 1.6 Hz, 3H), 7.14 – 7.08 (m, 1H), 6.69 – 6.62 (m, 2H), 3.75 (s, 3H), 3.66 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.50, 137.60, 131.34, 130.80, 124.01, 122.52, 120.55, 114.92, 109.66, 97.52, 55.43, 33.17.



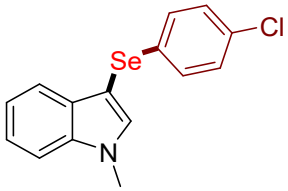
1-methyl-3-[(4-ethylphenyl)selanyl]-1*H*-indole 4e (0.232 g, 70% isolated yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.62 (d, *J* = 7.9 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.21 (td, *J* = 4.4, 1.7 Hz, 2H), 7.19 (t, *J* = 2.1 Hz, 1H), 7.15 – 7.09 (m, 1H), 6.67 – 6.62 (m, 2H), 3.88 (q, *J* = 7.0 Hz, 2H), 3.75 (s, 3H), 1.30 (dd, *J* = 8.3, 5.6 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.85, 137.58, 135.24, 131.34, 130.81, 123.79, 122.50, 120.64, 120.46, 115.50, 109.65, 97.55, 63.62, 33.16, 14.97.



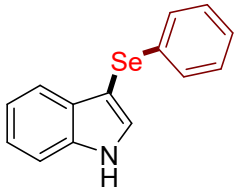
1-methyl-3-((4-(trifluoromethoxy) seleno)-1*H*-indole 4f (0.223 g, 60% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.36 – 7.30 (m, 2H), 7.26 (t, *J* = 2.4 Hz, 1H), 7.24 – 7.19 (m, 2H), 6.99 (dd, *J* = 8.8, 0.8 Hz, 2H), 3.86 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.56, 137.73, 135.93, 132.98, 130.69, 129.91, 122.84, 121.86, 120.84 120.48, 109.87, 95.82, 33.28.



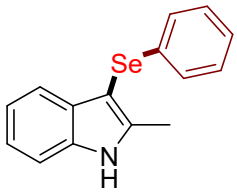
1*H*-Indole, 3-[(4-fluorophenyl)seleno] -1-methyl-1*H*-indole 4g (0.220 g, 72% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.32 (s, 1H), 7.31 – 7.26 (m, 1H), 7.23 – 7.15 (m, 3H), 6.87 – 6.79 (m, 2H), 3.83 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.50, 137.69, 135.65, 130.98, 130.60, 128.54, 122.73, 120.62, 116.30, 116.08, 109.79, 96.64, 33.27.



3-[(4-Chlorophenyl)seleno]-1-methyl-1*H*-indole 4h (0.253 g, 79% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.33 – 7.25 (m, 2H), 7.20 – 7.10 (m, 3H), 7.09 – 7.03 (m, 2H), 3.83 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 137.69, 135.81, 132.66, 131.64, 130.61, 130.04, 129.12, 122.75, 120.74, 120.45, 109.81, 95.8, 33.26.

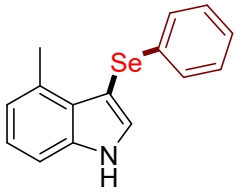


3-(phenylseleno)-1*H*-indole 4i (0.199 g, 73% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.39 (dd, *J* = 11.8, 5.3 Hz, 2H), 7.23 – 7.17 (m, 3H), 7.14 (d, *J* = 7.8 Hz, 1H), 7.09 (dt, *J* = 15.1, 5.3 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 136.59, 134.00, 131.42, 130.17, 129.16, 128.87, 125.80, 123.14, 121.06, 120.57, 111.56, 98.36.

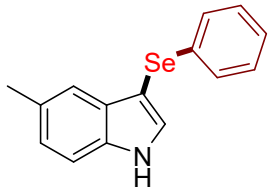


2-methyl-3-(phenylseleno)-1*H*-indole 4j (0.192 g, 67% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 7.22 – 7.05 (m, 7H), 2.53

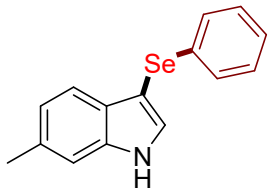
(s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 141.03, 135.96, 134.12, 131.43, 129.13, 128.52, 125.55, 122.29, 120.83, 119.96, 110.68, 96.43, 13.35.



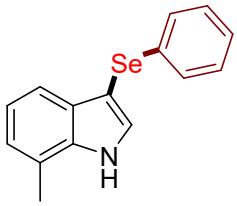
4-methyl-3-(phenylseleno)-1*H*-indole 4k (0.166 g, 58% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.42 (d, *J* = 2.5 Hz, 1H), 7.28 (d, *J* = 8.2 Hz, 1H), 7.23 – 7.18 (m, 2H), 7.11 (d, *J* = 9.6, 7.1, 5.5, 1.6 Hz, 4H), 6.90 (d, *J* = 7.1 Hz, 1H), 2.71 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 137.09, 136.31, 132.65, 132.43, 129.24, 128.26, 125.57, 123.15, 122.63, 109.55, 97.09, 19.03



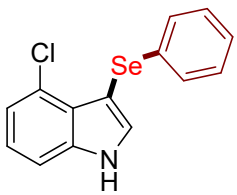
5-methyl-3-(phenylseleno)-1*H*-indole 4l (0.195 g, 68% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 7.36 (s, 1H), 7.33 (d, *J* = 2.5 Hz, 1H), 7.22 (s, 1H), 7.18 – 7.13 (m, 2H), 7.08 – 6.99 (m, 4H), 2.35 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 134.88, 134.27, 131.68, 130.45, 129.15, 128.64, 125.68, 124.75, 120.04, 111.09, 97.48, 21.63.



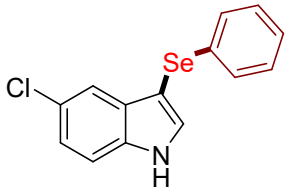
6-methyl-3-(phenylseleno)-1*H*-indole 4m (0.201 g, 71% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.50 (d, *J* = 8.1 Hz, 1H), 7.36 (d, *J* = 2.5 Hz, 1H), 7.23 (d, *J* = 2.2 Hz, 1H), 7.23 – 7.21 (m, 1H), 7.20 (s, 1H), 7.15 – 7.05 (m, 3H), 7.00 (dd, *J* = 8.1, 0.8 Hz, 1H), 2.45 (d, *J* = 18.3 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 137.03, 134.15, 133.04, 130.83, 129.13, 128.76, 128.00, 125.71, 122.83, 120.14, 111.51, 21.87.



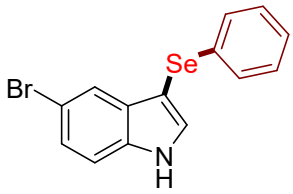
7-methyl-3-(phenylseleno)-1*H*-indole 4n (0.192 g, 67% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 2.5 Hz, 1H), 7.24 – 7.20 (m, 2H), 7.15 – 7.03 (m, 5H), 2.51 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 136.16, 134.09, 131.11, 129.76, 129.13, 128.85, 125.75, 123.65, 121.20, 120.74, 118.28, 98.78, 16.67.



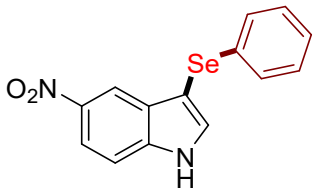
4-chloro-3-(phenylseleno)-1*H*-indole 4o (0.209 g, 68% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.39 (d, *J* = 2.6 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.19 – 7.09 (m, 5H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.05, 135.30, 132.90, 129.49, 129.17, 127.49, 126.00, 125.67, 123.61, 122.28, 110.49, 97.89.



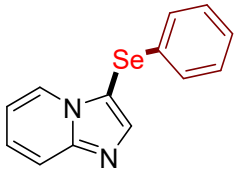
5-chloro-3-(phenylseleno)-1*H*-indole 4p (0.261 g, 85% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 7.61 (d, *J* = 1.9 Hz, 1H), 7.46 (d, *J* = 2.5 Hz, 1H), 7.32 (d, *J* = 8.6 Hz, 1H), 7.23 – 7.21 (m, 1H), 7.21 – 7.17 (m, 2H), 7.17 – 7.09 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 134.95, 133.54, 132.74, 131.48, 129.27, 128.94, 127.03, 126.04, 123.61, 120.07, 112.66, 98.22.



5-bromo-3-(phenylseleno)-1*H*-indole 4q (0.277 g, 76% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.77 (d, *J* = 1.8 Hz, 1H), 7.44 (d, *J* = 2.5 Hz, 1H), 7.33 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.27 (d, *J* = 8.6 Hz, 1H), 7.21 (dt, *J* = 8.5, 2.3 Hz, 2H), 7.17 – 7.10 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 135.23, 133.54, 132.60, 132.06 129.28, 128.91, 126.10, 123.14, 114.57, 113.07, 98.08.



5-nitro-3-(phenylseleno)-1*H*-indole 4r (0.262 g, 79% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 (s, 1H), 8.56 (d, *J* = 2.2 Hz, 1H), 8.13 (dd, *J* = 9.0, 2.2 Hz, 1H), 7.62 (d, *J* = 2.4 Hz, 1H), 7.46 (d, *J* = 9.0 Hz, 1H), 7.24 – 7.21 (m, 2H), 7.16 – 7.10 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 143.06, 139.69, 134.33, 132.72, 130.01, 129.46, 126.52, 118.82, 117.90, 111.88, 101.70.



3-(Phenylseleno)imidazo[1,2-*a*]pyridine 4s (0.208 g, 76% isolated yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 6.8 Hz, 1H), 7.95 (s, 1H), 7.66 (d, *J* = 9.0 Hz, 1H), 7.29 – 7.21 (m, 1H), 7.19 – 7.07 (m, 5H), 6.82 (t, *J* = 6.8 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 143.19, 130.71, 129.68, 129.15, 127.03, 125.94, 125.39, 118.08, 113.23, 106.64.

Procedure of gram-scale synthesis of 3-chalcogenylindoles in aqueous solution of GluM

The copper salt catalyst (1.0 mmol), 1,10-phen (1.0 mmol), base (6.0 mmol), indole (10.0 mmol), aryl halide (12.0 mmol) and sulfur powder (25.0 mmol) were added to a micellar aqueous solution

of glycosyl polyether surfactant (10 mM, 100 mL). The mixture was then heated and stirred at 100 °C for 12 h. At the end of the reaction, the organic phase (10 mL×3) was extracted with ethyl acetate and dried with anhydrous Na_2SO_4, and the crude product was obtained via vacuum concentration. Crude products were purified by silica gel column chromatography (eluent: ethyl acetate/petroleum ether) to obtain the corresponding pure products.

Procedure of recycling and reuse of GluM aqueous solution

Once the reaction was finished, the reaction mixture was cooled naturally and extracted with ethyl acetate (1 mL×3) to remove the product. After removing the organic phase, the substrates (1.0 mmol indole, 1.2 mmol aryl halide and 2.5 mmol sulfur powder) and base (0.6 mmol) were again added to the obtained aqueous solution containing Cu-(1,10-phen) complex and GluM for the next catalytic cycle.

5. Mechanistic investigation

TEM and DLS analysis of micelles at 25 °C

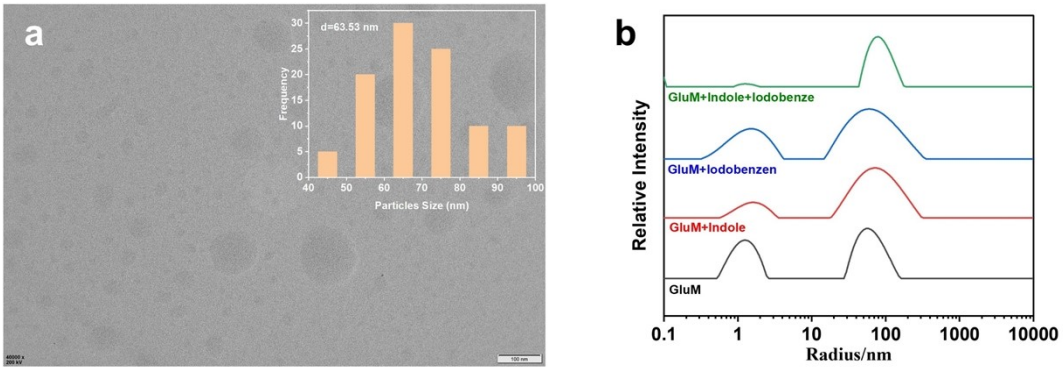


Fig. S2 (a) TEM images of 10 mM GluM aqueous sample as 25 °C (b) The particle size distribution of GluM aqueous solution before and after adding organic substrates at 25 °C.

Following a modified procedure from the literature[9], samples for TEM were stained with an equal volume of aqueous phosphomolybdic acid at a concentration of 1 g/L and diluted to the concentration of 10 mM. Dilute solutions in the presence of the staining agent (volume: 5 μL) were deposited on copper grids coated either with carbon or a formvar-supported carbon and allowed to air-dry. (The sample of $CuSO_4$ and 1,10-phen addition to 10 mM GluM aqueous for TEM was prepared followed the above procedure without phosphomolybdic acid at 100 °C.)

Dynamic light scattering (DLS) was used to study the size changes of the GluM micelles after dissolving substrates at 25 °C. Before measurement, 0.22 μm hydrophilic polyvinyl fluoride (PVDF) membrane was used to remove the present impurities. The size and distribution of the micelle were measured at 90° by an AlV/DLS/LS-5022F laser scattering system (He-Ne laser (λ= 632.8 nm)). ALV-V3.0 software was used to analyze and process the experimental data.

XRD parttern and crystal structure of complex

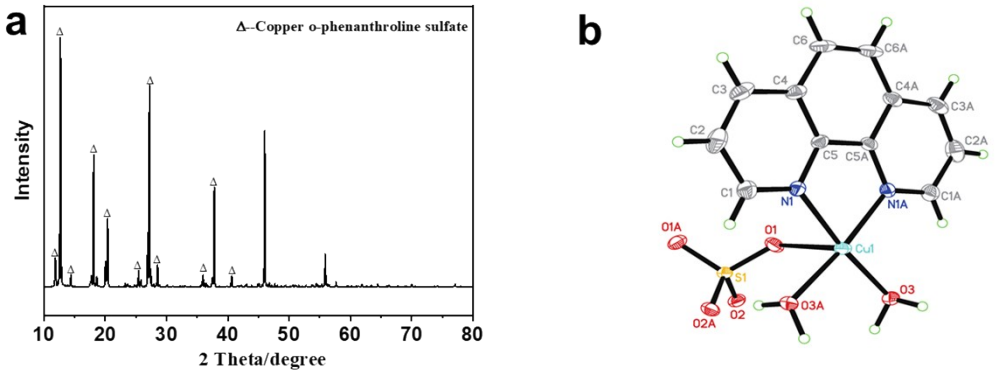


Fig. S3 (a) XRD pattern for complex. (b) Molecular structure of complex.

Investigation for the synergistic effect beween $CuSO_4$ and GluM

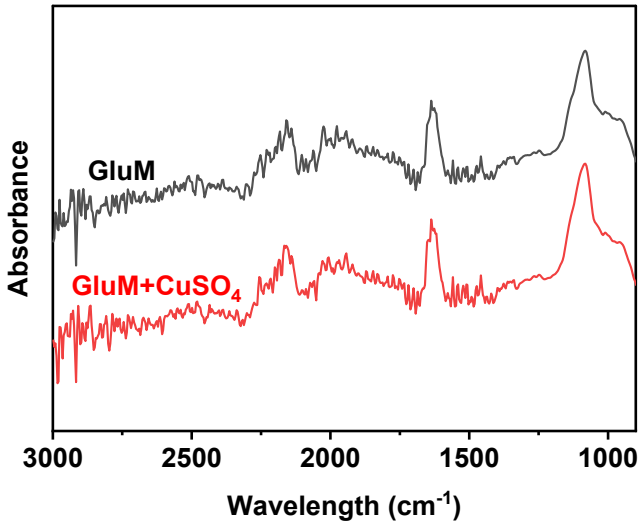
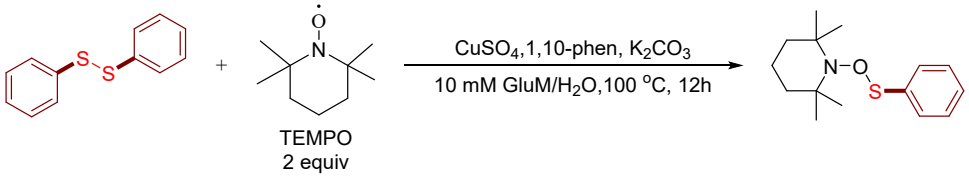
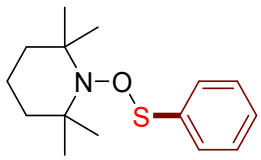


Fig. S4 *in-situ* ConcIRT spectra of $CuSO_4$ added into GluM aqueous solution.

Radical trapping experiment



The copper salt catalyst, 1,10-phen, base, diphenyl disulfide (1 mmol) and TEMPO (2 mmol) were added to a micellar solution of glycosyl polyether surfactant and H_2O (10 mL). The micelle solution mixture was then heated and stirred at 100 °C for 12 h. At the end of the reaction, the organic phase was extracted with ethyl acetate and dried with anhydrous Na_2SO_4, and the crude product was obtained by vacuum concentration. Crude product was purified by silica gel column chromatography (eluent: ethyl acetate/petroleum ether) to obtain the corresponding pure products, and characterized by ^1H NMR and ^{13}C NMR.



2,2,6,6-Tetramethyl-1-piperidinyl benzenesulfenate. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.1 Hz, 2H), 7.42 (t, *J* = 7.9 Hz, 2H), 7.37 (d, *J* = 7.1 Hz, 1H), 1.67 (d, *J* = 23.1 Hz, 6H), 1.51 (d, *J* = 26.3 Hz, 9H), 0.88 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.00, 130.03, 129.25, 126.73, 62.02, 59.59, 44.22, 42.14, 36.39, 33.34, 32.16, 30.62, 29.97, 28.73, 18.03.

DFT calculations

Computational Details

The structural optimization and frequency analysis were performed using the Gaussian 09[10] program. The structures were obtained with the PBE[11] functional with D3(BJ)[12, 13] correction; the 6-31+g(d) basis set was used for the S, C, N and H atoms while MWB10 pseudopotential and the associated basis set for Cu (BSI). More accurate single-point energies were obtained at the B2GP-PLYP[14]-D3(BJ)[12, 13]/def2-TZVP[15] level of theory using ORCA 4.2 package[16]. Stationary points were optimized without symmetry constraint, and their nature was confirmed by vibrational frequency analysis. Intrinsic reaction coordinate (IRC)[17-19] calculations were also performed to link transition structures with the respective intermediates. Unscaled vibrational frequencies were used to correct the relative energies for zero-point vibrational energy (ZPVE) contributions. The gas-phase models were used for all calculations as a rational solvation model for the current system is premature.

The MECP was searched and optimized on the PES using the SurfCrossOpt strategy in ORCA. The complete active space self-consistent field (CASSCF(12,12)) wave function was used to calculate the spin-orbit coupling (SOC) constant at the minimum energy crossing point (MECP).[20]

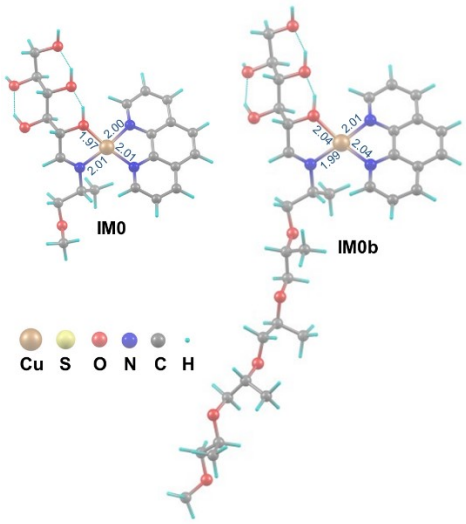


Fig. S5 Selected structural information for the optimized structures of the $CuC_{22}N_3H_{29}O_6$ and the $CuC_{34}N_3H_{53}O_{10}$ species.

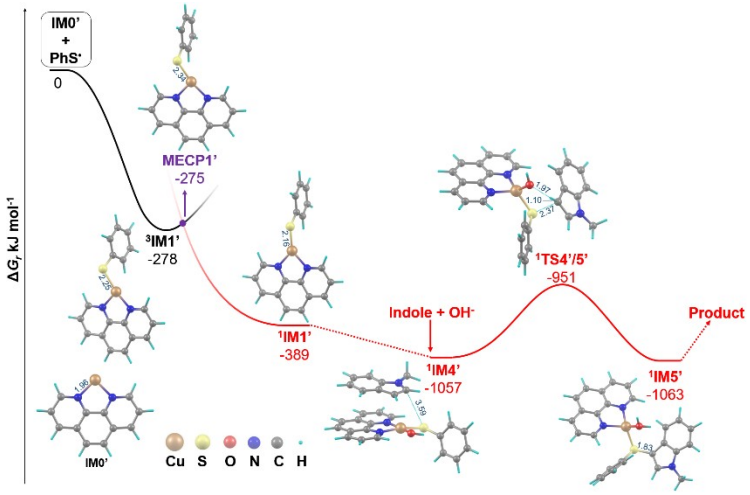


Fig. S6 Simplified PES and selected structural information for the Cu-catalyzed reaction of PhS• radical and 1-methyl-indole to generate 1-methyl-3-phenyl-indole without the surfactant ligand as calculated at the B2GP-PLYP-D3(BJ)/def2-TZVP//PBE-D3(BJ)/BSI level of theory. Bond lengths are given in Å.

Similar to the GluM participated reaction, the two-state reactivity may prevail as well for the Cu-phenanthroline complex mediated C-S coupling process. As shown in Fig. S6, upon complexation with PhS•, the intermediate **^{3}IM1'** forms and may flip into the singlet state via **MECP1'**, generating **^{1}IM1'**. Next, without the GluM moiety, the OH^- group from the reaction media serves directly as the hydrogen acceptor. Thus, by surmounting a barrier ~100 kJ/mol the C-S coupling takes place upon transfer of a hydrogen atom from 1-methyl-indole to OH^-; a water and a 1-methyl-3-phenyl-indole ligands form synergistically. Here, the barrier is obviously higher than that in the GluM participated reaction. Moreover, the SOC constant at **MECP1'** amounts to 21 cm^{-1}, suggesting a relatively low ISC probability. As to the S-C coupling step on the triplet surface, here, the barrier amounts to ~120 kJ/mol. Thus, for the reaction of iodobenzene and 1-methyl-indole, the GluM species do not only serve as the reaction media, but also mediate an efficient intersystem crossing and lowering of the reaction barrier for the C-S coupling step.

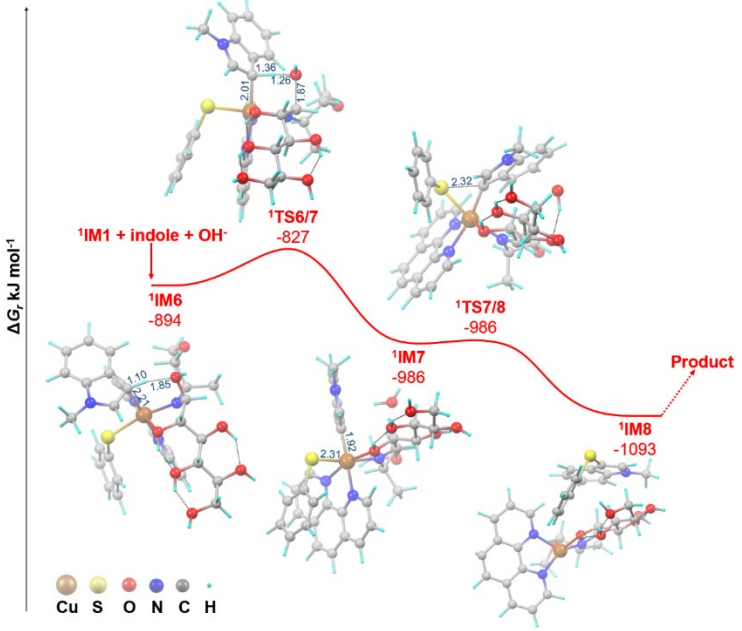


Fig. S7. Simplified PES and selected structural information of the stepwise route for the Cu-catalyzed reaction of PhS• radical and 1-methyl-indole to generate 1-methyl-3-phenyl-indole without the surfactant ligand as calculated at the B2GP-PLYP-D3(BJ)/def2-TZVP//PBE-D3(BJ)/BSI level of theory. Bond lengths are given in Å.

As shown in Fig. S7, by introducing a hydroxyl anion into the reaction complex, **^{1}IM6** forms by addition of OH to the C=N bond, concomitantly generating a covalent Cu-N bond. Next, via **^{1}TS6/7**, the 1-methyl-indole transfers a hydrogen to the incoming OH to produce an intact water molecule and, makes a C-Cu bond; meanwhile, the C=N bond re-forms. Further C-S coupling proceeds almost barrierlessly via **^{1}TS7/8** to afford the 1-methyl-3-phenyl-indole molecule, generating **^{1}IM8**. This pathway is, less favorable as compared to the one-step, concerted C-H activation and C-S coupling process both energetically and entropically.

Optimized Coordinates of Key Structures

IM0

2 2

C	0.32194600	-3.97750100	1.18143600
C	1.66713100	-4.35064700	1.18813400
C	2.65432300	-3.44233300	0.71243000
C	2.19760000	-2.17345400	0.25630500
C	-0.05503100	-2.70282000	0.69956400
C	4.06683900	-3.72474600	0.65757600
C	3.12470200	-1.20316300	-0.23895500
C	4.51384800	-1.50936700	-0.30849700
C	4.95931800	-2.79749000	0.16243500
C	5.37108800	-0.51412500	-0.85579200
H	6.44460900	-0.70378600	-0.93012700
C	4.83090100	0.69223400	-1.30378900
C	3.44206500	0.92613800	-1.18861000
H	4.42017600	-4.69616500	1.01091000
H	-0.44863300	-4.66064900	1.54124400
H	1.96835700	-5.33591600	1.55218500
H	-1.09984000	-2.38577300	0.66775200
H	6.02582500	-3.02929900	0.11550200
H	5.46641800	1.46215500	-1.74339200
H	2.99444800	1.85859900	-1.53364200
N	2.60830200	0.00499300	-0.65667600
N	0.86765600	-1.82310000	0.25006600
Cu	0.61516100	0.05395900	-0.39714700
C	-2.04578400	1.08825600	-0.95079200
C	-5.23486100	-0.73727200	0.45333100
C	-3.23149400	0.82420000	0.01842300
H	-2.46374100	1.35088100	-1.94234300
C	-4.10230300	-0.33255100	-0.51019500
H	-4.78143600	-1.13822500	1.38065200
H	-2.81910100	0.53473200	1.01038100
H	-4.53540400	-0.03509200	-1.48552100

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H	-4.87080700	1.86987700	0.41249300
O	-3.21323000	-1.49888700	-0.68585100
H	-3.81945500	-2.31083800	-0.83552400
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O	-1.22479400	-0.12252200	-1.07156900
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O	-5.98293600	0.49242700	0.71799500
H	-6.65559600	0.37191200	1.42963400
C	-6.16279800	-1.78556000	-0.18332100
H	-6.91068800	-2.14131400	0.54727000
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O	-5.29316700	-2.89890800	-0.60600800
H	-5.79941100	-3.63874400	-1.01099100
C	0.95613000	2.99256100	0.44375900
H	1.80627600	3.11805600	-0.25288000
C	0.28594100	4.38453600	0.61821200
H	-0.11625000	4.76028500	-0.34352700
H	-0.52741400	4.32484400	1.36177300
C	1.47570800	2.45746300	1.78793000
H	0.63498300	2.24338800	2.46978000
H	2.07313500	1.54008700	1.65724700
H	2.10664300	3.23098000	2.25205400
O	1.26242600	5.30119600	1.16606400
C	2.00659200	6.07909900	0.16365500
H	1.31485900	6.68379000	-0.44884100
H	2.66923800	6.73568400	0.74016400
H	2.61114500	5.42537800	-0.49336200

IM0b

2 2

C	-8.08825800	-1.70597800	1.22869600
C	-7.95786000	-3.09478100	1.26820900
C	-6.76684000	-3.70473700	0.78520600
C	-5.75019900	-2.83995800	0.28645900
C	-7.03287400	-0.91526200	0.71940200
C	-6.53476400	-5.12704500	0.76868200
C	-4.52902400	-3.38384900	-0.23599900
C	-4.32561700	-4.79442500	-0.25201900
C	-5.36066700	-5.65020200	0.27186800
C	-3.10254800	-5.26922000	-0.80168100
H	-2.90481900	-6.34342500	-0.83389300
C	-2.17240300	-4.35860500	-1.30333000
C	-2.45063100	-2.97388300	-1.25217500

H	-7.31341000	-5.78804200	1.15674400
H	-8.99611300	-1.21966900	1.58866400
H	-8.76360900	-3.71927400	1.66178600
H	-7.10383200	0.17354700	0.66255300
H	-5.19855100	-6.73068200	0.26146300
H	-1.23339000	-4.69992000	-1.74150400
H	-1.74700700	-2.23921100	-1.64703500
N	-3.59899300	-2.49304300	-0.72634700
N	-5.88663300	-1.47123100	0.26726300
Cu	-4.22810600	-0.57547300	-0.43818500
C	-4.23947100	2.31667700	-1.00257400
C	-7.16908800	4.52130900	0.45174100
C	-4.96805300	3.25531200	-0.00162800
H	-4.09924200	2.87213000	-1.95029400
C	-6.35052000	3.67151100	-0.54156600
H	-7.40351600	3.89442600	1.33406900
H	-5.11302100	2.70246900	0.95295300
H	-6.20743900	4.23985600	-1.48235500
O	-4.08896700	4.38845100	0.14803100
H	-4.63137000	5.13648700	0.53723500
O	-7.10653000	2.43338100	-0.80143700
H	-8.07363600	2.70356400	-0.96398500
C	-2.90670300	1.90602100	-0.45347900
H	-2.18336400	2.71200300	-0.28786800
N	-2.69153900	0.66071700	-0.15116500
O	-5.03753500	1.11391500	-1.24411300
H	-6.02843300	1.40145200	-1.24031500
O	-6.31960000	5.65680100	0.82245800
H	-6.70006700	6.16393600	1.57828500
C	-8.46374200	5.04858600	-0.18758900
H	-9.07351100	5.58769700	0.56000600
H	-8.20415800	5.73657500	-1.01257600
O	-9.19225300	3.87083200	-0.68823900
H	-10.04000100	4.11610300	-1.12325800
C	-1.42111700	0.18824000	0.46914100
H	-1.07649000	-0.65191400	-0.16036600
C	-0.29229600	1.24001800	0.49843100
H	-0.10401100	1.64747800	-0.51457500
H	-0.55545200	2.07417600	1.17495000
C	-1.72795800	-0.34801000	1.87696500
H	-2.13912400	0.45395400	2.51394700
H	-2.45259000	-1.17887900	1.84003600
H	-0.78838600	-0.70541000	2.32509500
O	0.90351100	0.61315900	1.03904000
C	2.00070100	0.38836400	0.06740100
H	2.20300400	1.33906900	-0.46479200

C	1.68326200	-0.72108400	-0.93289800
H	0.86507900	-0.43628000	-1.61813800
H	2.58262900	-0.92428700	-1.53629300
H	1.40698900	-1.64573800	-0.39603500
C	3.20026500	0.05639100	0.95508700
H	3.37409000	0.87917900	1.67547800
H	2.99578100	-0.87126500	1.52441200
O	4.33596900	-0.10098400	0.05803000
C	5.62964200	-0.27119400	0.74554800
H	5.74824100	0.53941000	1.49419300
C	6.65356800	-0.06207000	-0.37041400
H	6.49072000	0.91770300	-0.85874300
H	6.54856500	-0.85977400	-1.13184900
C	5.75703100	-1.63752100	1.41551700
H	5.06364400	-1.74700100	2.26539500
H	5.55024300	-2.43647500	0.68289500
H	6.78473000	-1.76315400	1.79215600
O	7.97131600	-0.11321900	0.25819600
C	9.10121000	-0.01884200	-0.67717600
H	8.80171600	0.57157600	-1.56539500
C	9.56634700	-1.41307300	-1.09011700
H	8.76351800	-1.95164000	-1.62021200
H	10.43151500	-1.33565700	-1.76968000
H	9.85303400	-2.00304900	-0.20352400
C	10.16762300	0.77256500	0.10846000
H	9.76493800	1.75992800	0.38395000
H	10.43820400	0.21533700	1.02416100
O	11.33045000	0.98946800	-0.75266800
C	12.57302000	0.32131200	-0.35170500
H	12.34081600	-0.63671000	0.15162000
C	13.26830500	1.25882500	0.68209700
H	13.47277300	2.23612600	0.20988600
H	12.60177300	1.39743800	1.55078900
C	13.40040800	0.09701300	-1.60682800
H	12.86540400	-0.56388200	-2.30709700
H	13.60079400	1.05267600	-2.11910200
H	14.35735300	-0.38064600	-1.34153700
O	14.47735600	0.61852800	1.16616400
C	15.73359600	1.26666400	0.77314600
H	15.78087000	2.29321100	1.17801500
H	16.53128000	0.65086900	1.20632900
H	15.83626100	1.30012800	-0.32648700

MECP1

C	-0.51154847186223	-2.28099320619922	3.05183858147715
C	0.77203152567078	-2.26926028277976	3.58834477707429

C	1.80898441330593	-1.57354956501610	2.90953549734285
C	1.45452549650702	-0.90507864399483	1.70035647370618
C	-0.76352343085067	-1.59008940341201	1.84327414331267
C	3.17043573385254	-1.51776137144397	3.37146779073662
C	2.46657467533191	-0.19438787805615	0.95578677407331
C	3.81177315686240	-0.16080930450308	1.43369814399735
C	4.13304531875674	-0.83871802156145	2.66104020879209
C	4.76154226681446	0.55927824965355	0.66180687650219
H	5.80860191203135	0.60866274010460	0.99736550102523
C	4.36139377578002	1.19440744067385	-0.51020528456730
C	3.01270083422374	1.10871554276489	-0.91452458772359
H	3.43051584963230	-2.02893922976837	4.31007121437260
H	-1.33018555083300	-2.81732385328625	3.55192119663062
H	0.99476540873823	-2.79419670274034	4.52955731628029
H	-1.76709957846883	-1.59143680987269	1.38378259088533
H	5.17027694868216	-0.79890566340449	3.02598934942771
H	5.07562958173559	1.75523126432789	-1.12940254134438
H	2.66485068598227	1.57717242232675	-1.84789654991610
N	2.10257315118699	0.43825851176313	-0.19687893046900
N	0.19051461209529	-0.91693102676691	1.19441612306474
Cu	0.16833603302277	0.23094840555806	-0.63870162700688
C	-2.61414548658329	1.14561582714248	-0.95290037252187
C	-5.58270421839056	-0.78590010887102	0.78791616776114
C	-3.69804275959024	0.84545562321982	0.12560569934369
H	-3.16234505558320	1.43355431779090	-1.88090088160699
C	-4.49632114976038	-0.42195106141131	-0.24372644182099
H	-5.06356005990624	-1.03250217902896	1.74582007438374
H	-3.16136765518506	0.62758557901218	1.08807053914327
H	-4.99321687478245	-0.24557693551000	-1.22863064427501
O	-4.48185651329794	1.99948097885454	0.18859242105244
H	-5.35286431520508	1.73305214965560	0.57382020336318
O	-3.54911234848508	-1.49547354479686	-0.32894844112241
H	-4.07944452560235	-2.34681713907636	-0.36155799419605
C	-1.79063068325389	2.30652958928816	-0.50116131349318
H	-2.33919133309674	3.25290432905409	-0.33271558945669
N	-0.53398104688777	2.16171926382891	-0.26567989014396
O	-1.75951361731476	0.03116017867624	-1.21365073565150
H	-2.29523810796524	-0.81097196717885	-1.01263655988137
O	-6.43102898290898	0.34827082001649	0.92274523581929
H	-7.01834942531851	0.23510741784046	1.69416715277226
C	-6.40733520403634	-1.99895062713478	0.33153403040110
H	-7.15914092273372	-2.24693277573790	1.11543699786866
H	-6.95730342685873	-1.71990930886527	-0.59627473803064
O	-5.51070111564201	-3.09267655391015	0.11734292146483
H	-5.99207260255058	-3.84125261929133	-0.28191318147511
C	0.28830668593951	3.24083961969612	0.28153067501166

H	1.24925538329691	3.20510591147644	-0.27663541418862
C	-0.29732093960308	4.66559832292482	0.07301385689466
H	-0.58874954598234	4.80346920384461	-0.99526426729928
H	-1.20436907214952	4.79079945265439	0.70298079298208
C	0.57119262821922	2.97332026508373	1.76257918422328
H	-0.37633295385027	2.95487520419343	2.33766153682842
H	1.09201267710719	2.00917056184937	1.91328860449731
O	0.62475028194136	5.63260131426102	0.49262315615490
C	1.52023675730950	6.09417598430521	-0.50553703387010
H	0.97326761110314	6.54653888777226	-1.36357666534840
H	2.16038137196581	6.86446192803579	-0.03760894272103
H	2.17513670292283	5.27952507957217	-0.89652802701993
H	1.20377561889564	3.78963421141406	2.15931844369312
S	0.77853240469376	-0.97809900213823	-2.57446215067437
C	2.06371498037330	-2.09062756076602	-2.25623188456535
C	2.07283969919278	-2.90894714174475	-1.08611561746497
C	3.11164186068190	-2.22588294420548	-3.21833253546428
C	3.10737647295838	-3.81905288394756	-0.88342324370368
H	1.24181524227422	-2.82485013556066	-0.37209623037020
C	4.13745290416701	-3.14596318870391	-3.00421509570212
H	3.09176128287809	-1.60247385744178	-4.12450523660543
C	4.14233302989117	-3.94007861165464	-1.83830431730077
H	3.11177669978645	-4.45712705678002	0.01314167371635
H	4.94137105949209	-3.25523228891544	-3.74765462441317
H	4.95171423923634	-4.66844114315908	-1.67680533466187

[1]TS2/3

2 1

C	-0.67012000	-4.19789900	-1.90244000
C	0.52340700	-4.89430400	-2.09055900
C	1.74856300	-4.30753100	-1.67299200
C	1.68815000	-3.02141300	-1.05418500
C	-0.64707300	-2.92747300	-1.28629900
C	3.03178100	-4.93348200	-1.86400200
C	2.90181000	-2.36304600	-0.64789800
C	4.16308800	-2.98833400	-0.88824500
C	4.19368100	-4.29659900	-1.49076100
C	5.33373700	-2.26578500	-0.52872300
H	6.31701900	-2.71215100	-0.69683500
C	5.21099300	-0.98937900	0.01856500
C	3.92504300	-0.44673200	0.23765300
H	3.06645600	-5.92285800	-2.32676300
H	-1.62116900	-4.61928700	-2.23319700
H	0.53043100	-5.87805600	-2.56635200
H	-1.56264200	-2.35173900	-1.14135800
H	5.16357900	-4.77287900	-1.65446400

H	6.09301300	-0.40292400	0.28161800
H	3.79992100	0.55410400	0.65265800
N	2.78981400	-1.11793200	-0.06494700
N	0.49941600	-2.34963300	-0.85819400
Cu	0.77439600	-0.60448600	0.16354400
C	-2.45998900	-0.09621400	1.30461000
C	-5.29727000	-2.65059900	0.27782400
C	-3.33365200	-1.38545000	1.34785900
H	-3.10263900	0.73680500	1.65367300
C	-4.51812700	-1.32278500	0.36190600
H	-4.60870500	-3.43618100	-0.09132800
H	-2.69102100	-2.25109800	1.07973400
H	-5.20260500	-0.50758700	0.66791400
O	-3.80036800	-1.44762300	2.71092600
H	-4.55805600	-2.10344500	2.73627500
O	-3.95722400	-1.04360900	-0.97308700
H	-4.65351900	-1.29842100	-1.68023100
C	-1.30238800	-0.24251500	2.25080000
H	-1.63238700	-0.30688300	3.29475800
N	-0.04790700	-0.37413800	1.92036700
O	-2.06681500	0.15918600	-0.09267600
H	-2.83071900	-0.24636200	-0.73765600
O	-5.74208200	-2.93349900	1.64250900
H	-6.12380000	-3.84000200	1.72327900
C	-6.51456700	-2.54069600	-0.65484200
H	-7.02296900	-3.51690900	-0.74667400
H	-7.22250900	-1.79420500	-0.25238100
O	-5.98545600	-2.11718100	-1.96397000
H	-6.67998100	-2.06890400	-2.65857500
C	0.96770700	-0.49376500	3.03441700
H	1.72617500	-1.19405300	2.64232500
C	1.62072600	0.90975900	3.18298700
H	2.02501700	1.24568400	2.20389700
H	0.84246000	1.61951900	3.52119000
C	0.44115800	-1.00373400	4.37576800
H	-0.24877400	-0.29101900	4.86008400
H	-0.06226800	-1.97912200	4.27191300
O	2.63248900	0.94090700	4.21257600
C	3.95031400	0.47320000	3.77685800
H	4.34612400	1.11662200	2.96741000
H	4.59597200	0.55604900	4.66018200
H	3.92909600	-0.57878400	3.43512100
H	1.29643100	-1.11855800	5.05886600
S	0.61977100	1.24397800	-1.35635600
C	2.23387000	2.18046000	-1.26491300
C	3.16559100	1.85165200	-2.26433100

C	2.55914200	3.06029600	-0.22313800
C	4.45595900	2.40935200	-2.20313600
H	2.89055400	1.17759600	-3.07926100
C	3.84910400	3.62314700	-0.18105000
H	1.82557100	3.32842500	0.54014500
C	4.79967300	3.29211000	-1.16377800
H	5.18359700	2.16420500	-2.98038900
H	4.10558000	4.32302700	0.61817400
H	5.79822100	3.73329100	-1.12806700
C	-2.66055100	5.42183200	-0.89128300
C	-1.86345000	4.33837700	-0.49523500
C	-3.00870600	5.48185700	-2.24919600
C	-1.43350600	3.32204000	-1.39679300
C	-2.57432800	4.49245900	-3.16590900
H	-3.61911100	6.31312500	-2.60778600
C	-1.79079800	3.40378200	-2.75243900
C	-0.67792000	2.33621800	-0.60189200
C	-0.58744100	2.89635400	0.71953400
H	-2.85087400	4.58690400	-4.21827800
H	-1.44747100	2.65142200	-3.46631900
H	-2.99172200	6.18953200	-0.18904000
N	-1.32432900	4.03399100	0.78392800
H	-0.09018100	2.48574400	1.59472000
C	-1.55553100	4.84826500	1.98552900
H	-2.62989100	4.87552400	2.22536100
H	-1.00412000	4.41532800	2.83075800
H	-1.19814900	5.87451700	1.80941500
H	-1.52555100	1.21843000	-0.31553800

^{1}TS2'/3'

1 1

C	-2.04591200	-3.87845200	0.85132100
C	-3.40174900	-3.58923400	1.00528600
C	-3.87586500	-2.28269100	0.70934700
C	-2.91806400	-1.32429900	0.26068000
C	-1.16368600	-2.87256500	0.39510600
C	-5.25380900	-1.88292200	0.84162800
C	-3.33735900	0.01773300	-0.03705400
C	-4.70641300	0.39281100	0.10504500
C	-5.65347000	-0.59779900	0.54962100
C	-5.05168700	1.73813200	-0.19706300
H	-6.09062200	2.06338000	-0.10114400
C	-4.05991500	2.62882300	-0.60954700
C	-2.72451800	2.18411100	-0.72657600
H	-5.98084800	-2.62425500	1.18315100
H	-1.65608800	-4.87286400	1.07588900

H	-4.10248200	-4.35295700	1.35203600
H	-0.09828000	-3.06905700	0.26042000
H	-6.70144600	-0.30599600	0.65521300
H	-4.30007100	3.66734600	-0.84281300
H	-1.91789100	2.85034000	-1.03675400
N	-2.37224800	0.90915400	-0.44790800
N	-1.58264100	-1.62136700	0.09963700
Cu	-0.55370900	0.11452200	-0.56624900
S	1.15995200	0.65963000	0.83200900
C	1.24564000	2.48361400	0.60297300
C	1.69006800	3.27348900	1.68421500
C	0.87675500	3.07217200	-0.62759600
C	1.73126800	4.67079700	1.54256100
H	1.98143100	2.79839800	2.62429500
C	0.94607800	4.46979800	-0.75932800
H	0.56992300	2.42691900	-1.46362300
C	1.36312000	5.26938500	0.32260200
H	2.05695900	5.29038800	2.38185300
H	0.67793500	4.93531700	-1.71175600
H	1.40913000	6.35578700	0.21333900
C	4.51224000	-2.94767800	0.29883800
C	4.08611100	-1.64759100	0.01137400
C	3.71274500	-3.99909500	-0.19252300
C	2.90559500	-1.37104500	-0.73526100
C	2.54565900	-3.74617900	-0.94946800
H	4.01188700	-5.03079600	0.00544300
C	2.12886800	-2.43021400	-1.22965700
C	2.76335900	0.08148800	-0.82115300
C	3.91980100	0.61581700	-0.16628700
H	1.96760100	-4.58998500	-1.33459000
H	1.23584700	-2.21669600	-1.82222200
H	5.42215900	-3.15242100	0.86698700
N	4.67988200	-0.39669000	0.33785900
H	4.18940200	1.65706600	-0.00834700
C	5.90704900	-0.24871100	1.12333400
H	5.76266400	-0.66701200	2.13254000
H	6.73724700	-0.77635200	0.62775900
H	6.15712200	0.81706400	1.20675700
H	2.14192300	0.55075100	-1.60465100
O	0.28419300	0.43954400	-2.24136600
H	-0.17512600	0.13822500	-3.06143200

^{3}TS2'/3'

1 3

C	-2.77151100	0.03209300	3.47027500

C	-4.09911800	-0.20980300	3.05572700
C	-4.37384500	-0.37911000	1.68188100
C	-3.27886800	-0.29589200	0.76456200
C	-1.74445100	0.12271800	2.52301200
C	-5.68564600	-0.62805400	1.13249300
C	-3.48110100	-0.45691100	-0.62185000
C	-4.78624800	-0.68768000	-1.15799800
C	-5.88341600	-0.77290500	-0.22311200
C	-4.91027300	-0.81013900	-2.55996900
H	-5.89050900	-0.98844400	-3.00765300
C	-3.76109500	-0.68788100	-3.37193300
C	-2.51012700	-0.45849500	-2.78689500
H	-6.53057200	-0.69604800	1.82274300
H	-2.53180800	0.16143800	4.52653100
H	-4.90980600	-0.26310600	3.78586300
H	-0.71538900	0.33017500	2.82040300
H	-6.88677100	-0.95395400	-0.61736900
H	-3.83576800	-0.76642100	-4.45752400
H	-1.60999800	-0.33265600	-3.39076700
N	-2.35358400	-0.35963200	-1.43456900
N	-1.97097900	-0.03590300	1.18683900
Cu	-0.73946300	-0.03078100	-0.34009300
S	1.23203000	0.64369500	0.95492200
C	1.46660000	2.40028400	0.38322000
C	1.95582600	3.31753600	1.32963200
C	1.15958100	2.78861000	-0.93340700
C	2.13316600	4.65941900	0.94681000
H	2.19046400	2.99082900	2.34525100
C	1.35071100	4.13235300	-1.30164300
H	0.78757500	2.05765000	-1.65664200
C	1.83223500	5.06616400	-0.36526800
H	2.50757600	5.38221100	1.67556200
H	1.11513200	4.44841600	-2.32092200
H	1.97003200	6.10978800	-0.65751600
C	4.95785700	-3.01912700	0.12201700
C	4.29252500	-1.79593400	-0.03766000
C	4.18636400	-4.11237000	0.55005600
C	2.89313100	-1.64614500	0.19509900
C	2.80084600	-3.98097400	0.80290400
H	4.66785300	-5.08233100	0.69202000
C	2.14144200	-2.75249400	0.62336800
C	2.54484400	-0.25580300	-0.16053300
C	3.79023400	0.38839700	-0.45667300
H	2.23574300	-4.85086700	1.14502700
H	1.07032100	-2.66088500	0.82659400
H	6.02706600	-3.12615900	-0.07302700

N	4.80272600	-0.53483600	-0.42817700
H	3.97584400	1.42932200	-0.70738700
C	6.20491200	-0.28604100	-0.77182800
H	6.49003000	-0.86014700	-1.66839100
H	6.34326200	0.78483800	-0.97134500
H	6.85408800	-0.58134200	0.06789800
H	1.62294500	-0.30726100	-1.22793700
O	0.56065200	-0.26917900	-1.77588000
H	0.40485100	-0.99636900	-2.42279300

MECP1'

C	-2.48436703271564	3.41678441738253	-0.13867251006003
C	-3.59760938763047	2.66820939599549	0.23570350538437
C	-3.49824598394787	1.25237565729842	0.33184684068104
C	-2.23278589180735	0.67474889139156	0.03351459953390
C	-1.26332848202497	2.76135288715073	-0.41355838429086
C	-4.58570161674796	0.38174174874415	0.69551827824520
C	-2.05824865046264	-0.74671757183931	0.09180464333217
C	-3.14894034429935	-1.59304125445157	0.44590634716579
C	-4.41685636265092	-0.98412206162455	0.75222673052168
C	-2.89637424640541	-2.99220140041556	0.47356289854972
H	-3.70854043172262	-3.68694596257346	0.73896815056724
C	-1.62878895172800	-3.47709593264502	0.15979561370171
C	-0.60123169392208	-2.57170678175604	-0.18907493590767
H	-5.56374612039530	0.82952798113709	0.92648913741700
H	-2.53573447800800	4.51192457332751	-0.22495848506767
H	-4.55563585407537	3.16428460323546	0.45592048467598
H	-0.36818693402549	3.33212173572108	-0.70794494424931
H	-5.25607086199571	-1.63615409307711	1.03749113714342
H	-1.40798755227768	-4.55454497990294	0.17076978979458
H	0.40637213425076	-2.92321426526632	-0.45985371069886
N	-0.82423887590330	-1.25353400242092	-0.20678741593488
N	-1.14907667186849	1.42825945255884	-0.32991715897037
Cu	0.39506038559056	0.25470684363772	-0.69815042656974
S	2.30559758577982	-0.63074514751666	-1.45727390721899
C	3.48142178639034	-0.17923049815251	-0.27078619123260
C	3.14137364885873	0.06409354712281	1.10216125693588
C	4.84556611595650	-0.07342068156219	-0.70508747327844
C	4.13445511557774	0.42770590346998	2.00038768733385
H	2.10052892304527	-0.06343881240640	1.44118862247836
C	5.82713596763421	0.28797126598297	0.21077977436319
H	5.09979468124395	-0.27502446978429	-1.75636491739699
C	5.48036009422505	0.54310466752906	1.56072876178473
H	3.88542731694438	0.61609533004016	3.05519700670273
H	6.87509898041954	0.37291698331574	-0.11338810464690
H	6.26394968869780	0.82630103035353	2.28058629921078

ICP-OES for the copper leaching

After purified via silica gel column chromatography, the pure product was mixed with nitric acid (10 mL), hydrofluoric acid (10 mL) and perchloric acid (10 mL). The mixture was heated and dissolved at the hot plate (230 °C) until the solid substance was completely dissolved for at least 4h. After the solvent was evaporated, the residue was mixed with aqua regia (10mL) and diluted to 25 mL with distilled water for determination. During the determination, the concentration of the dissolved solution was firstly measured and the solution was further diluted according to the standard series curve of copper to ensure that the copper to be measured were within the curve range. Finally, the copper leaching was determined as 12 ppm.

Table S8 Intensity of standard series

Entry	Concentration of standard series (μg/L)	Cu/CPS
1	0	147
2	5	4548
3	10	8907
4	20	17525
5	50	44548
6	100	88083
7	200	180765
8	500	447673

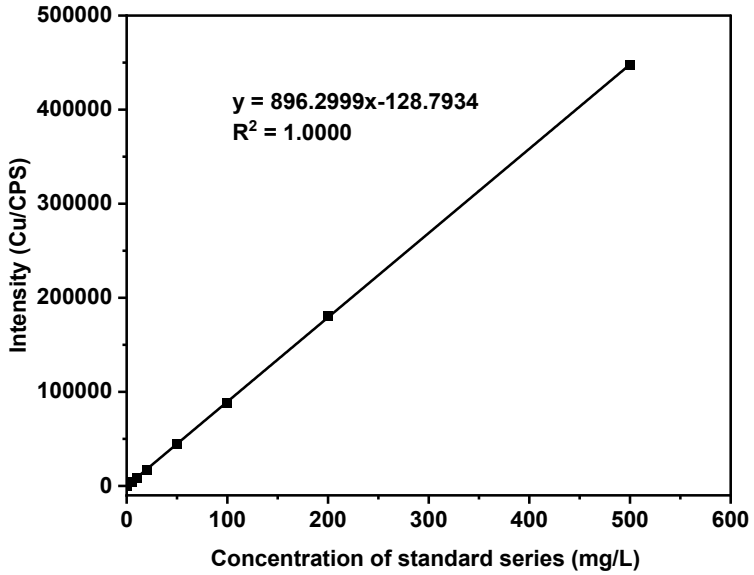
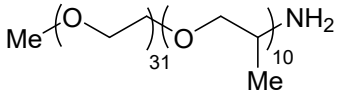
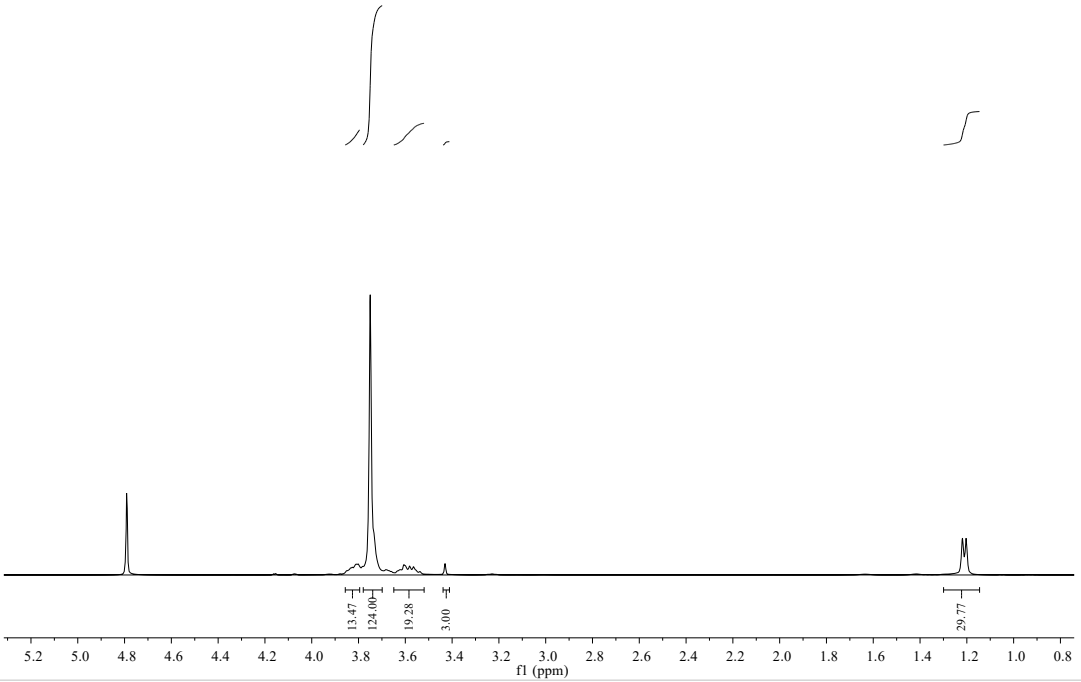
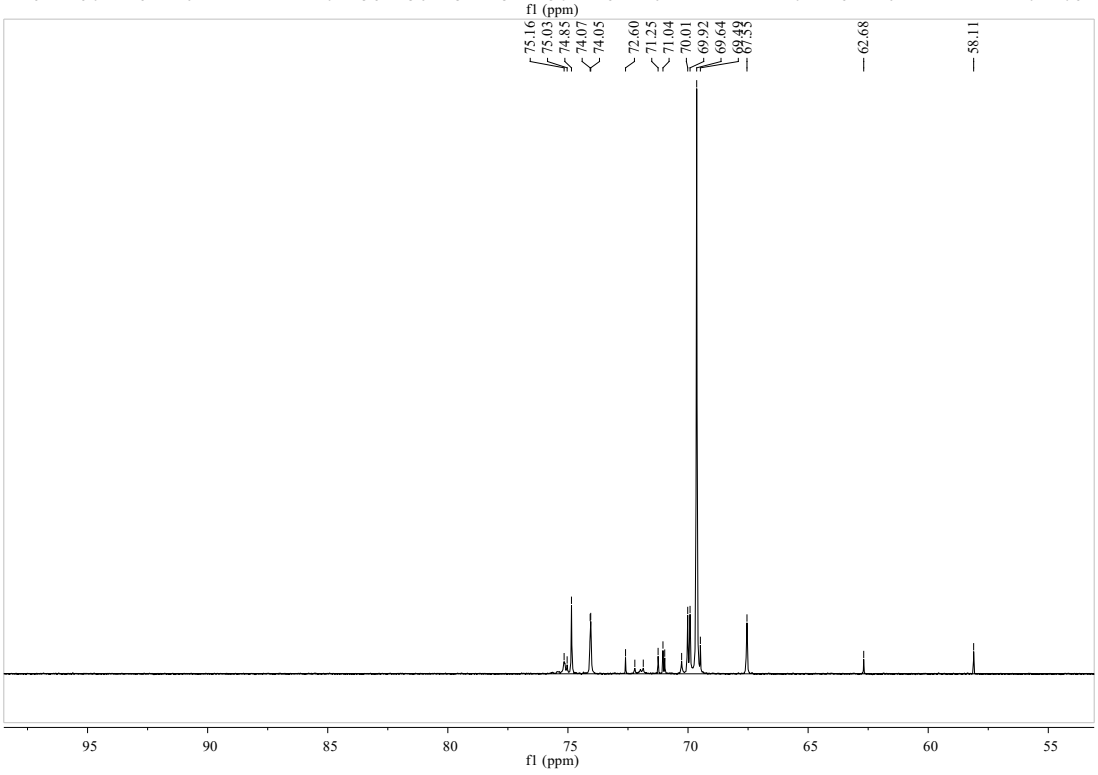


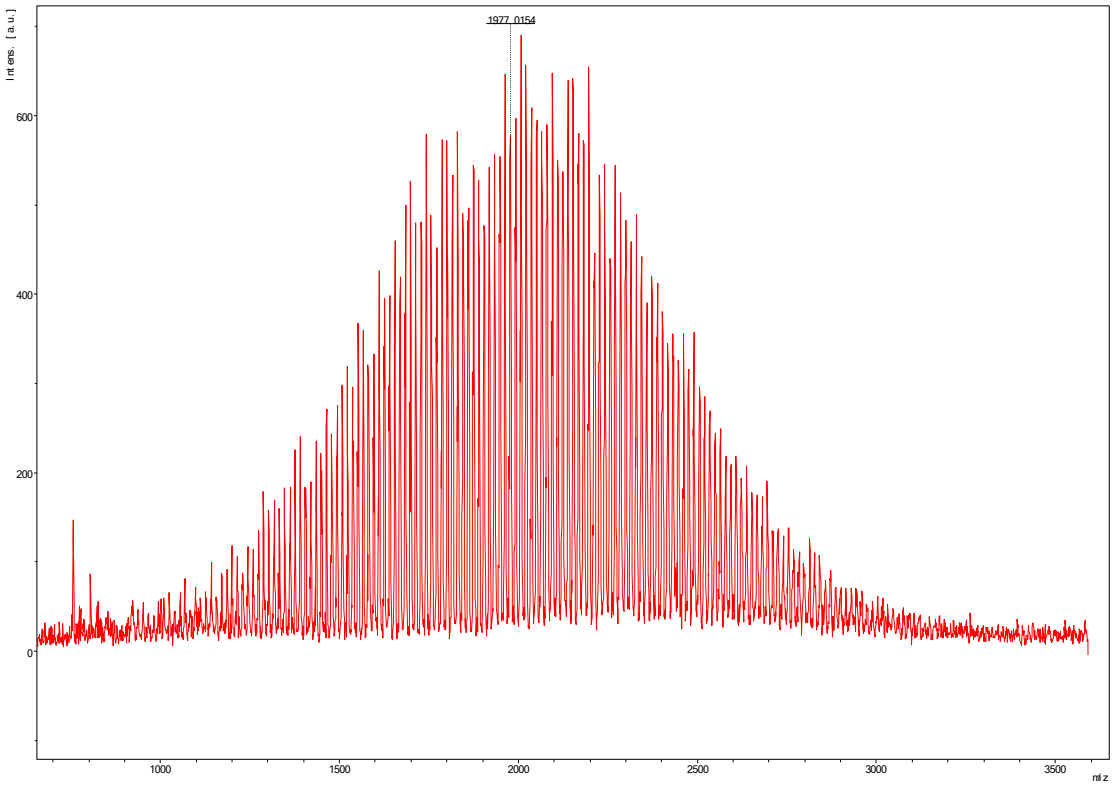
Fig. S8 Standard series curve of copper for ICP-OES

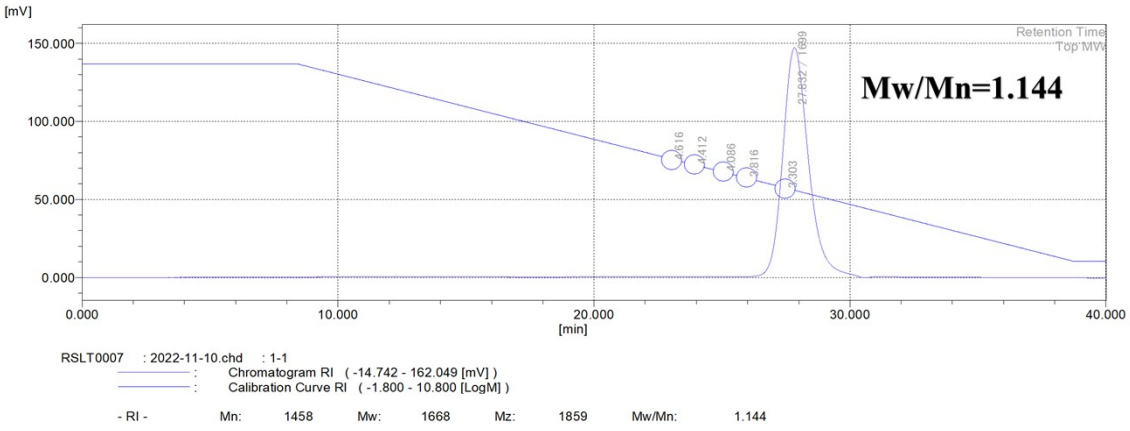
6. Spectra of products











RSLT0007 : 2022-11-10.chd : 1-1

: Chromatogram RI (-14.742 - 162.049 [mV])

: Calibration Curve RI (-1.800 - 10.800 [LogM])

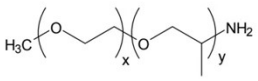
- RI -	Mn:	1458	Mw:	1668	Mz:	1859	Mw/Mn:	1.144

HUNTSMAN
Enriching lives through innovation

Technical Bulletin

JEFFAMINE® M-2070 Polyetheramine

JEFFAMINE M-2070 polyetheramine is a monoamine based on a copolymer backbone. As shown by the representative structure, JEFFAMINE M-2070 polyetheramine is a monofunctional, primary amine with an average molecular weight of about 2,000. The propylene oxide/ethylene oxide (PO/EO) mol ratio is 10/31.



APPLICATIONS
- Formulating emulsifiers, pressure sensitive adhesives, and corrosion inhibitors
- Reactive dispersant

BENEFITS
- Surfactant properties to modify a variety of resin types
- Water soluble

SALES SPECIFICATIONS

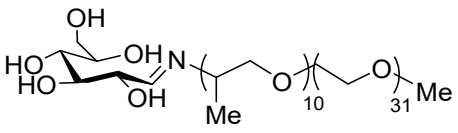
Property	Specifications	Test Method*
Appearance	Colorless to pale yellow liquid with slight haze permitted	ST-30.1
Color, Pt-Co	75 max.	ST-30.12
Conversion, total amine as % of total acetylatables	95 min.	Calculated
Primary amine, % of total amine	95 min.	ST-5.34
Total acetylatables, meq/g	0.48 – 0.52	ST-31.39
Total amine, meq/g	0.45 min	ST-5.35
Water, wt%	0.25 max.	ST-31.53, 6

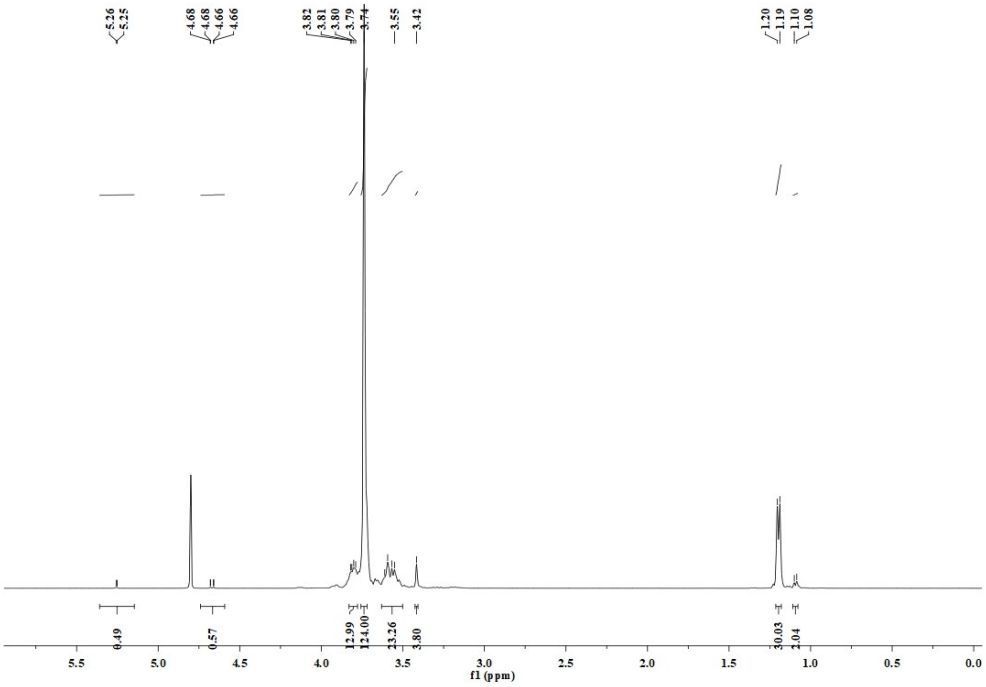
*Methods of Test are available from Huntsman Corporation upon request.

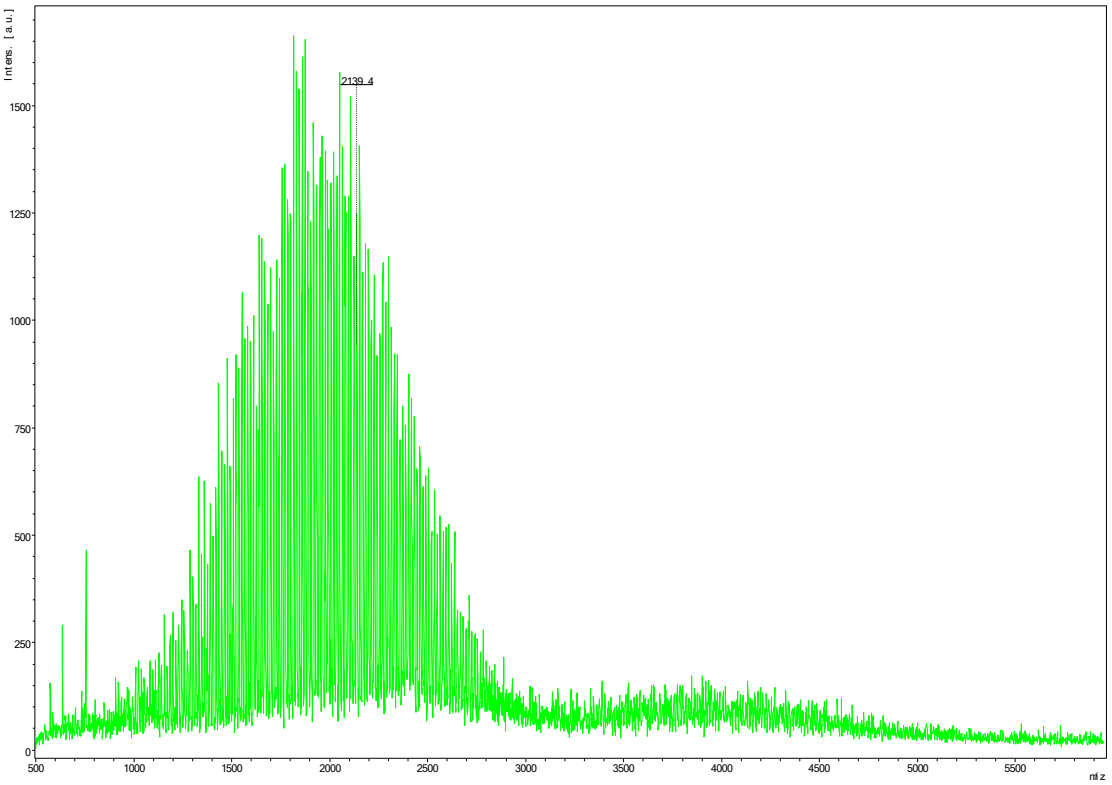
ADDITIONAL INFORMATION

Regulatory Information	
DOT/TDG Classification	Not regulated
HMIS Code	0-1-0
CAS Number	83713-01-3
US, TSCA	Listed
Canadian WHMIS Classification	Not regulated
Canada, DSL	Listed
European Union, EINECS/ELINCS	Polymer Exempt
Australia, AICS	Listed
Japan, METI	Contact Huntsman Regulatory
Korea, ECL	Listed
China, IECSC	Listed

Typical Properties	
AHEW (Amine hydrogen equivalent wt.), g/eq	1040
Viscosity, cSt, 37.8°C (100°F)	186
Density, g/ml (lb/gal), 25°C	1.072 (8.92)
Melting point, °C (°F)	17 (63)
Flash point, PMCC, °C (°F)	243 (469)
pH	11



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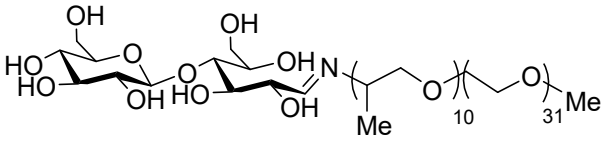
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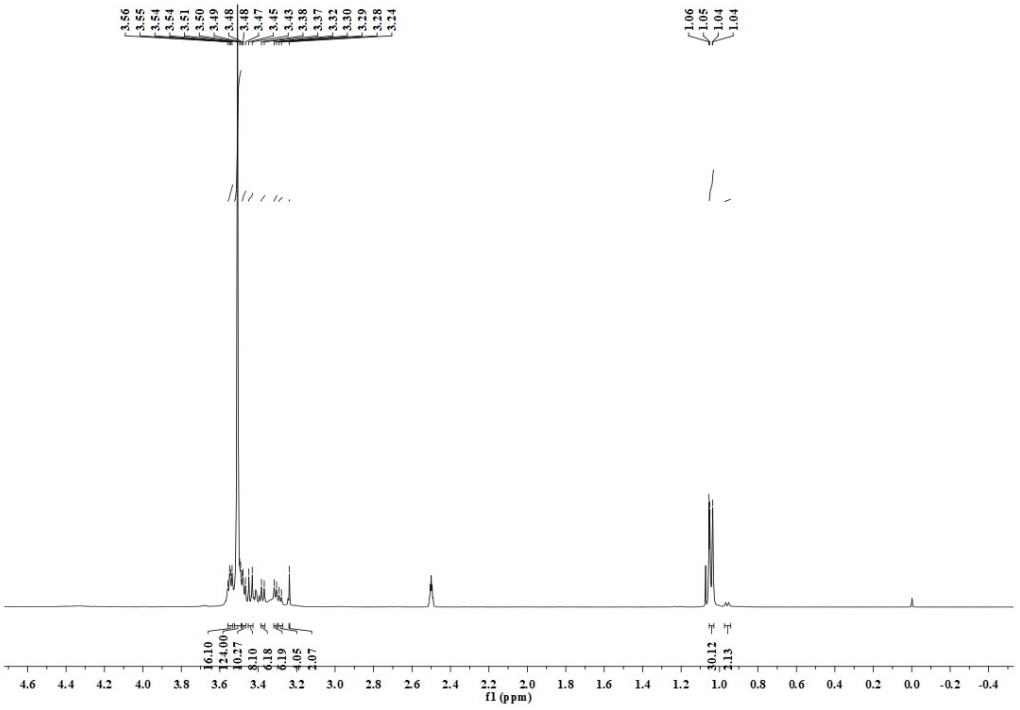
10
O
31
Me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3.37
3.32
3.30
3.29
3.28
3.24
1.06
1.05
1.04
1.04
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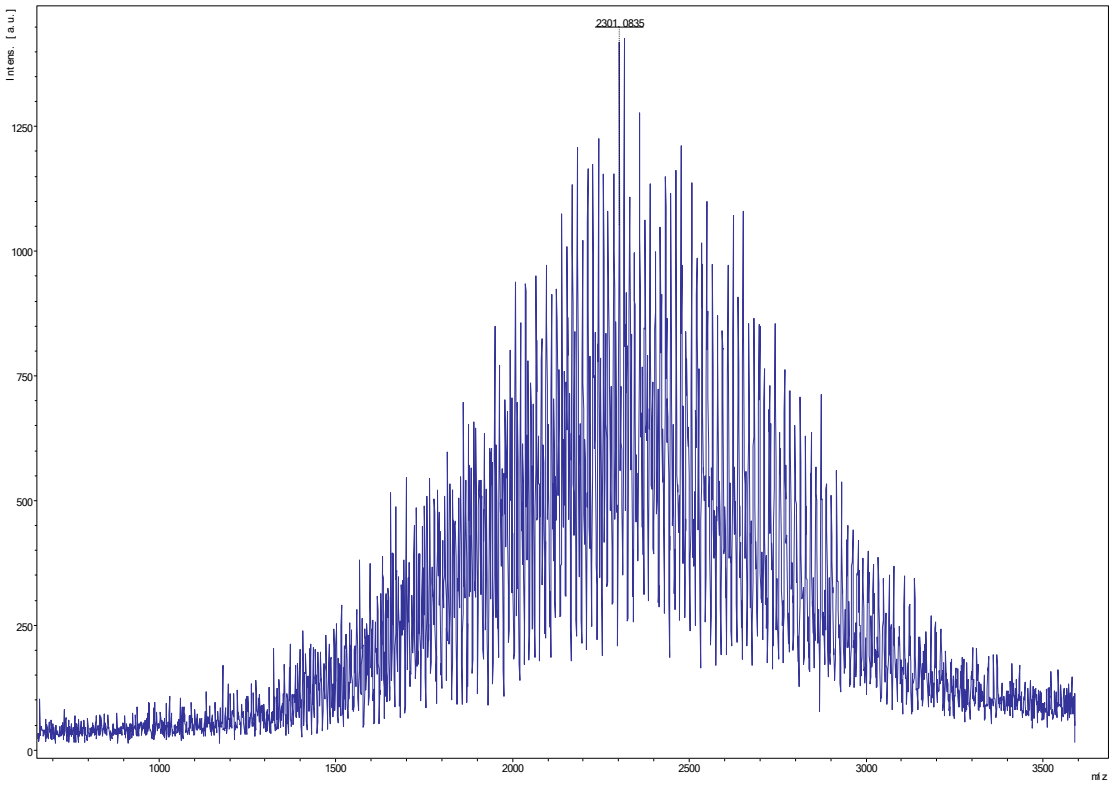
f1 (ppm)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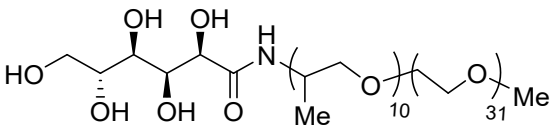
m/z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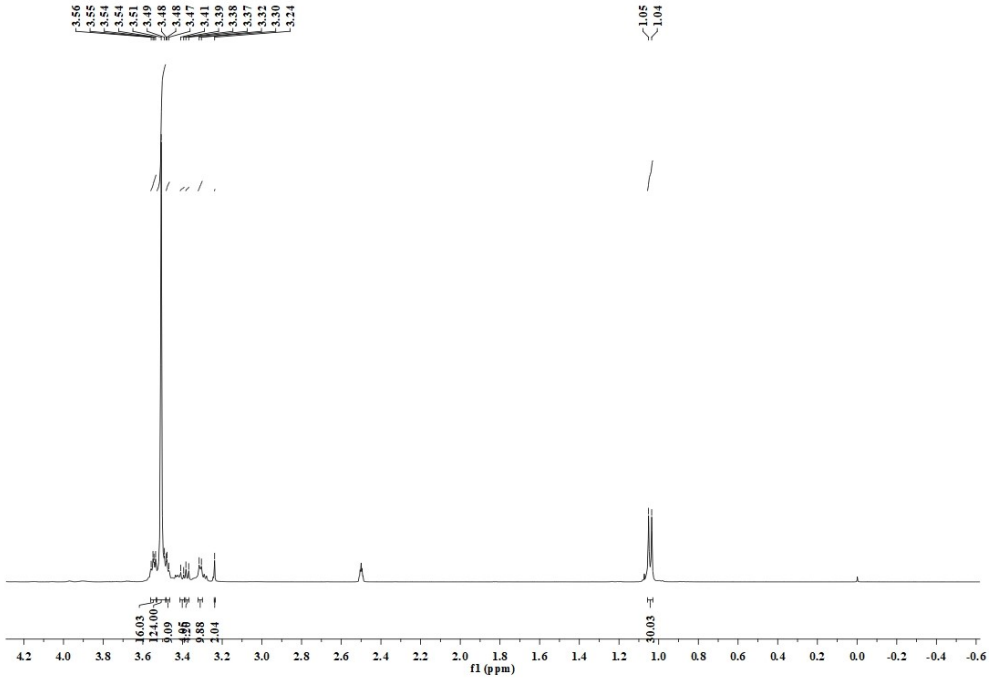
OH
OH
OH
OH
O
H
N
Me
O
10
O
31
Me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3.37
3.32
3.30
3.24
1.05
1.04
16.03
124.00
9.09
9.88
2.04
30.03
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
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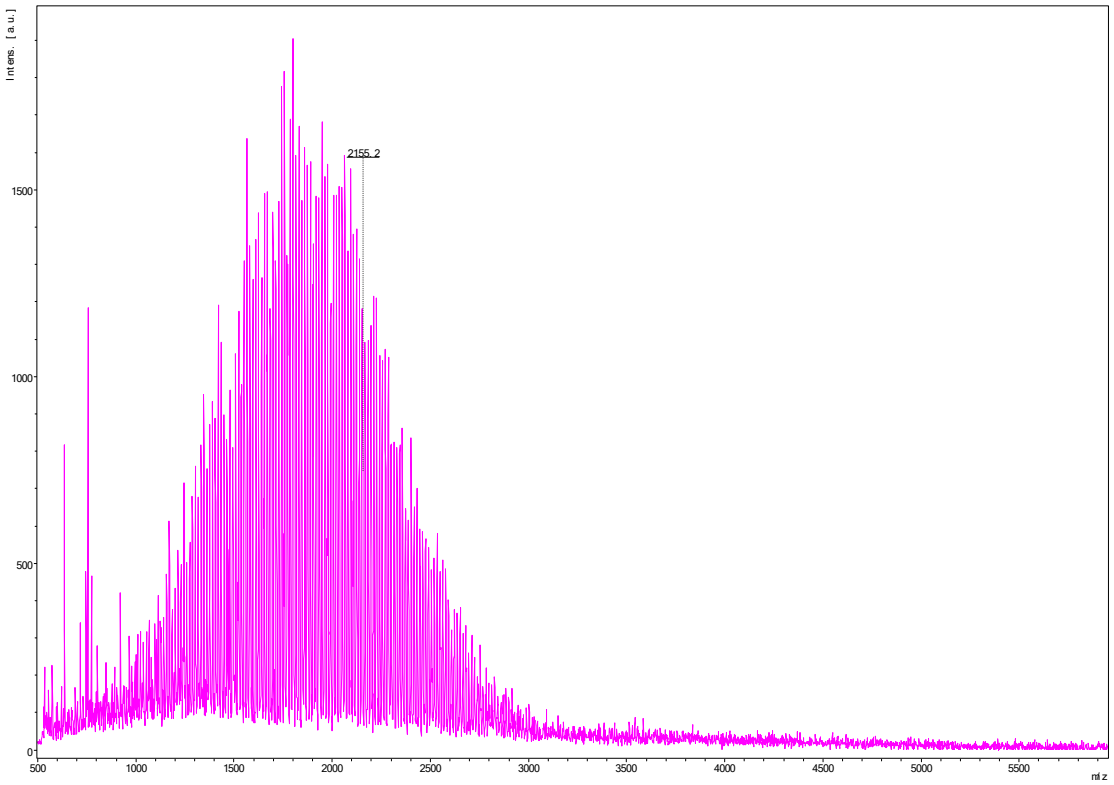
-0.6
f1 (ppm)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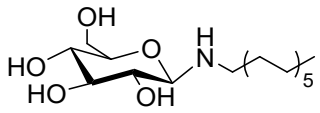
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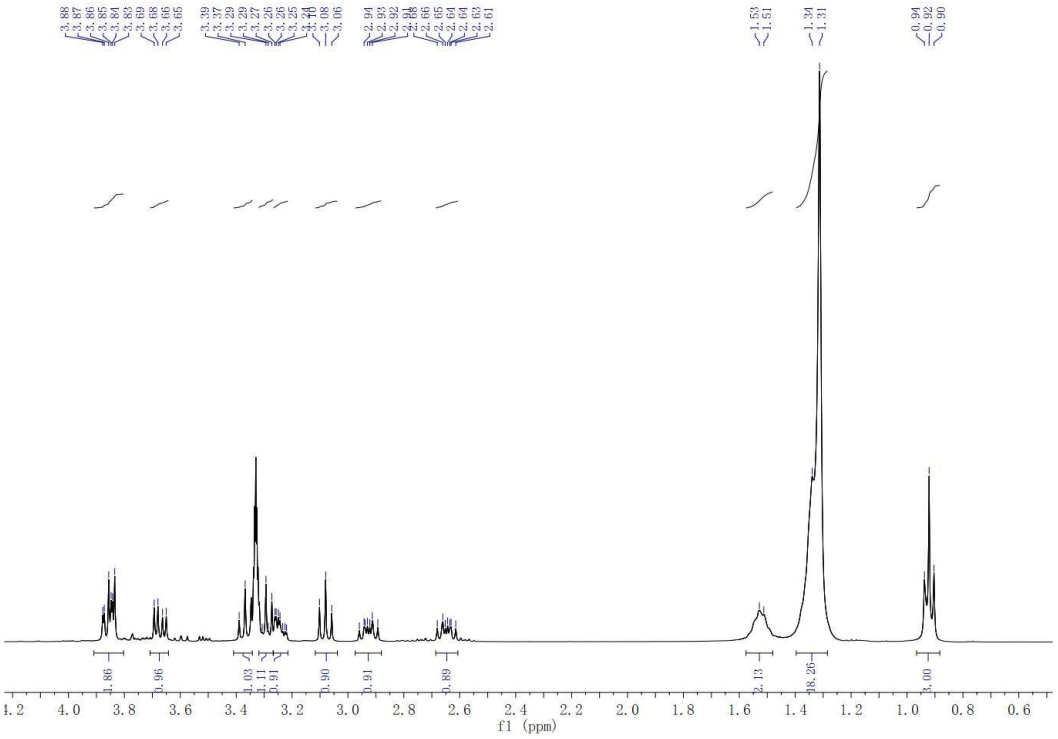
OH
O
H
N
5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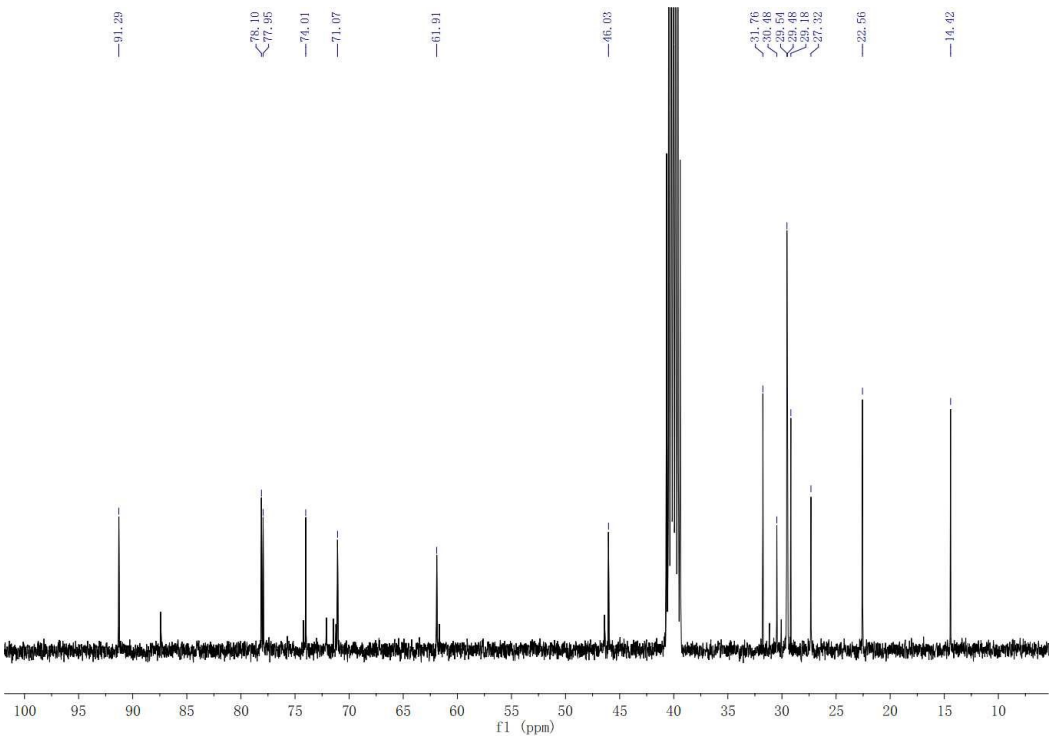
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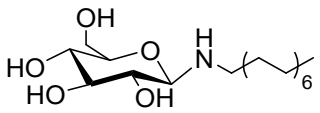
f1 (ppm)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H
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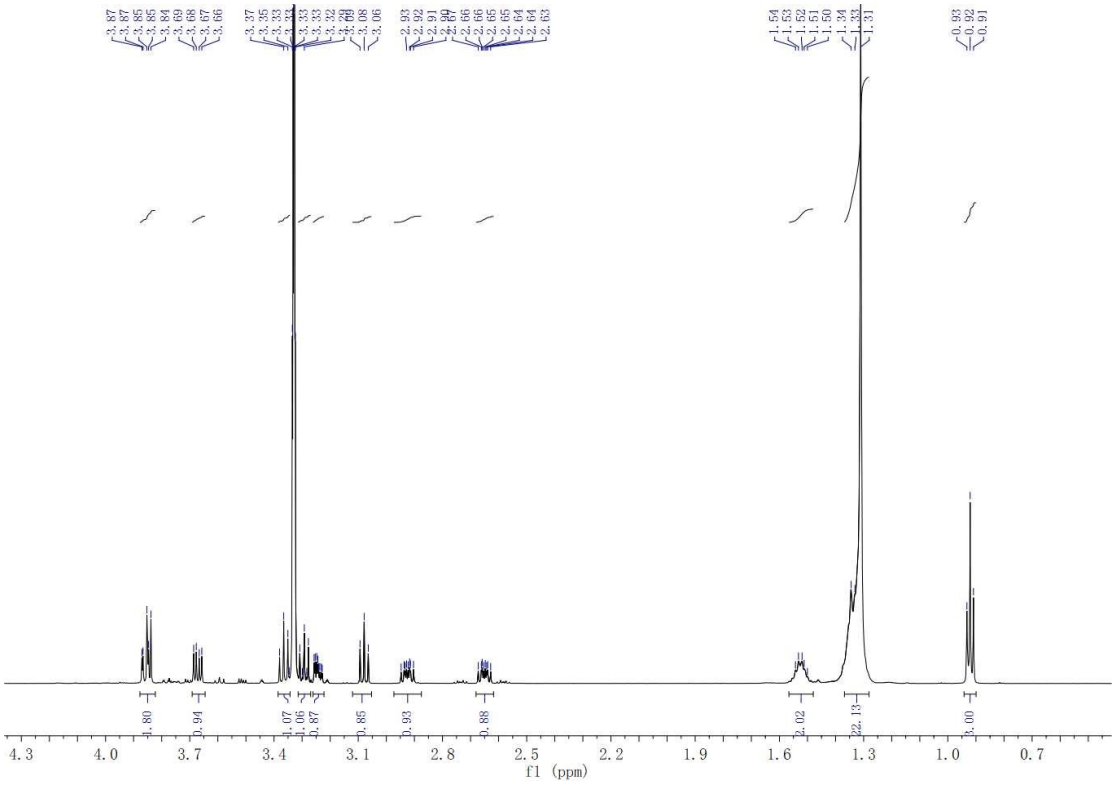
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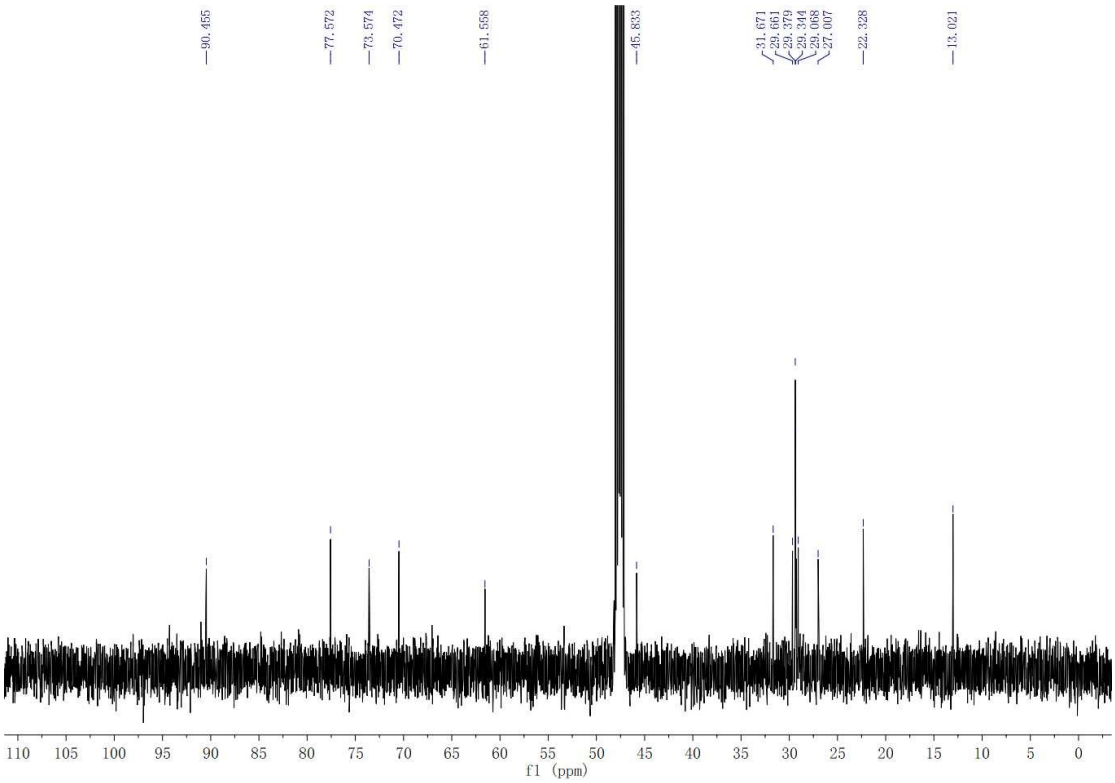
f1 (ppm)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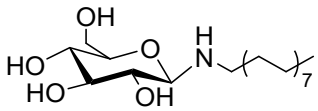
f1 (ppm)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N
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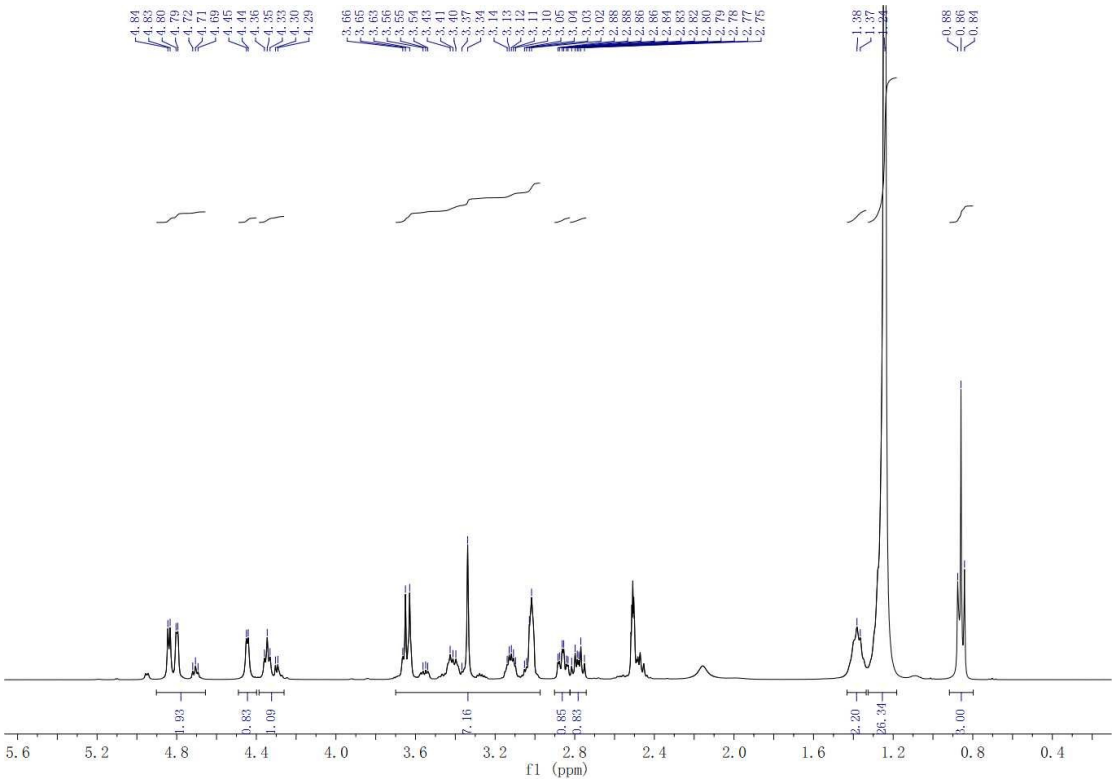
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1.24
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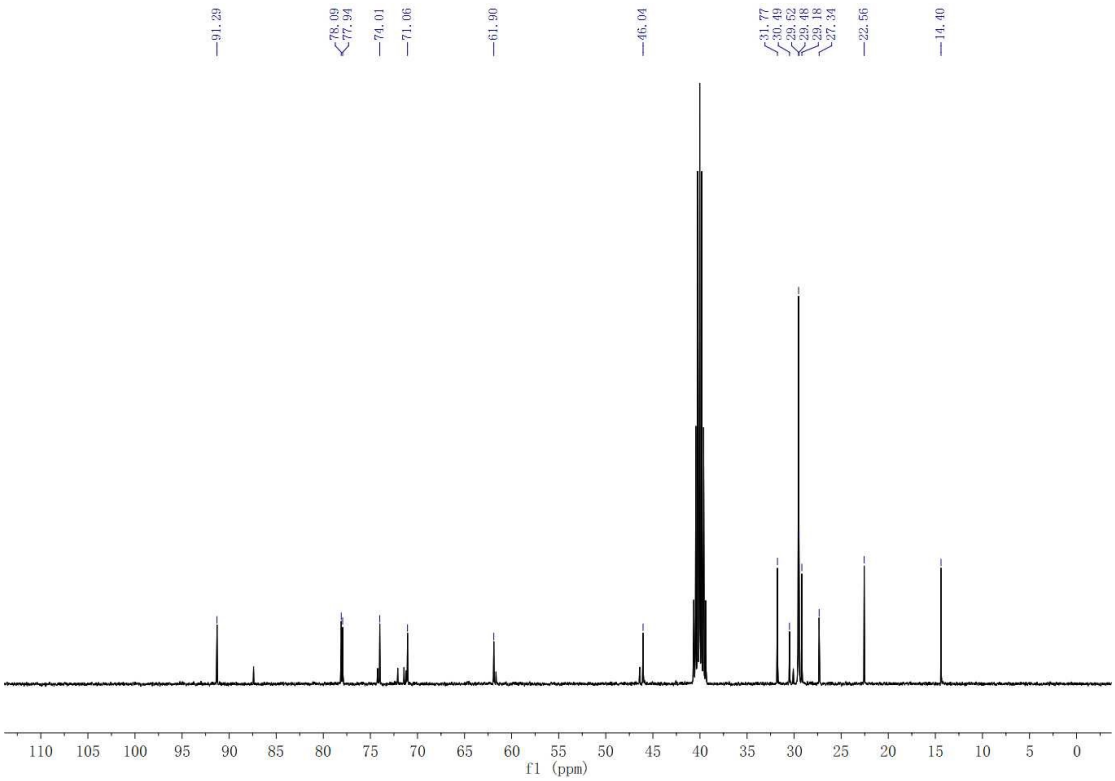
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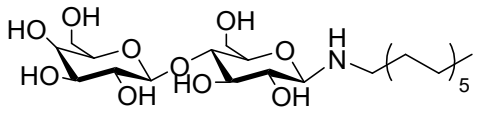
14.40
f1 (ppm)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OH
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OH
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N
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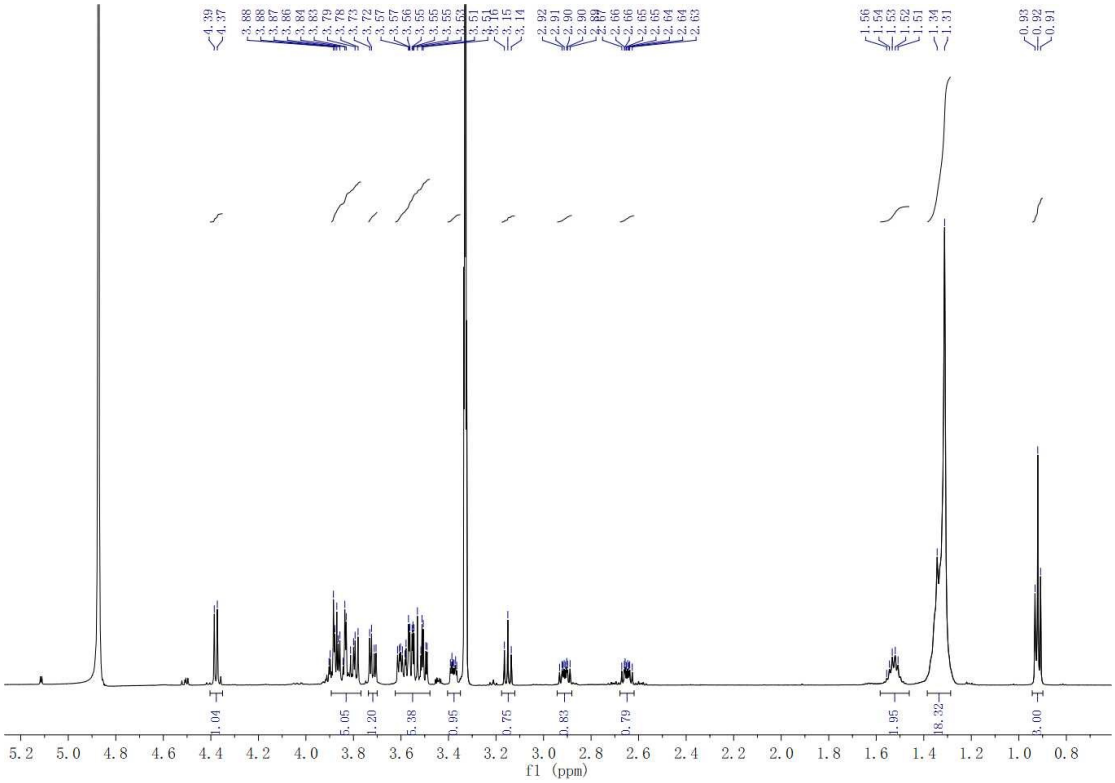
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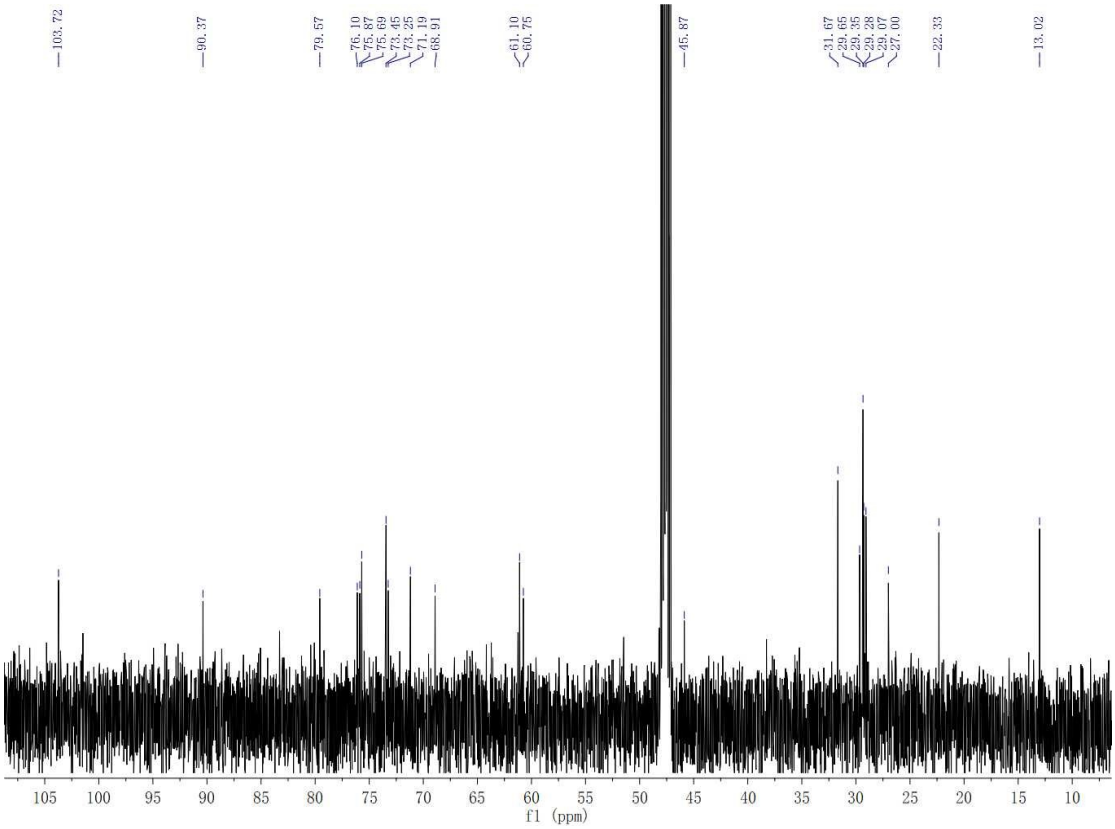
2.64
2.64
2.63
1.56
1.54
1.53
1.52
1.51
1.34
1.31
0.93
0.92
0.91
1.04
5.05
1.20
5.38
0.95
0.75
0.83
0.79
1.95
18.32
3.00
f1 (ppm)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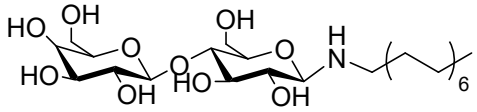
79.57
76.10
75.87
75.69
73.45
73.25
71.19
68.91
61.10
60.75
45.87
31.67
29.65
29.35
29.28
29.07
27.00
22.33
13.02
f1 (ppm)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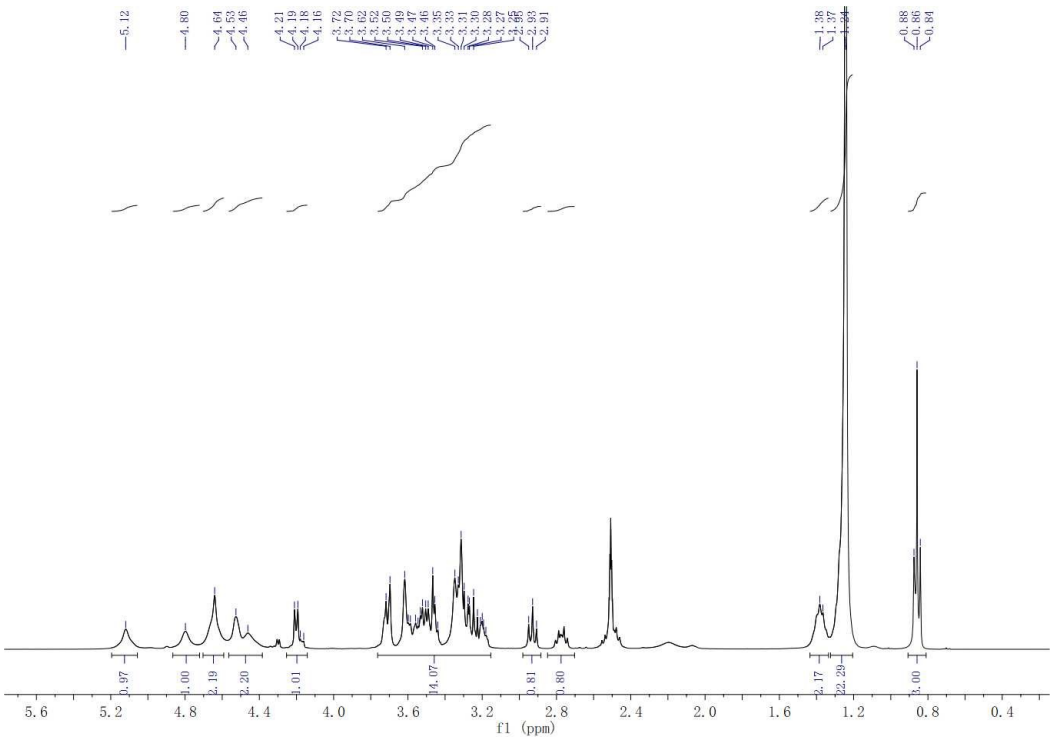
OH
O
HO
OH
O
HO
OH
H
N
6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4.53
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4.21
4.19
4.18
4.16
3.72
3.70
3.62
3.52
3.50
3.49
3.47
3.46
3.35
3.33
3.31
3.30
3.28
3.27
2.93
2.91
1.38
1.37
0.88
0.86
0.84
0.97
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2.20
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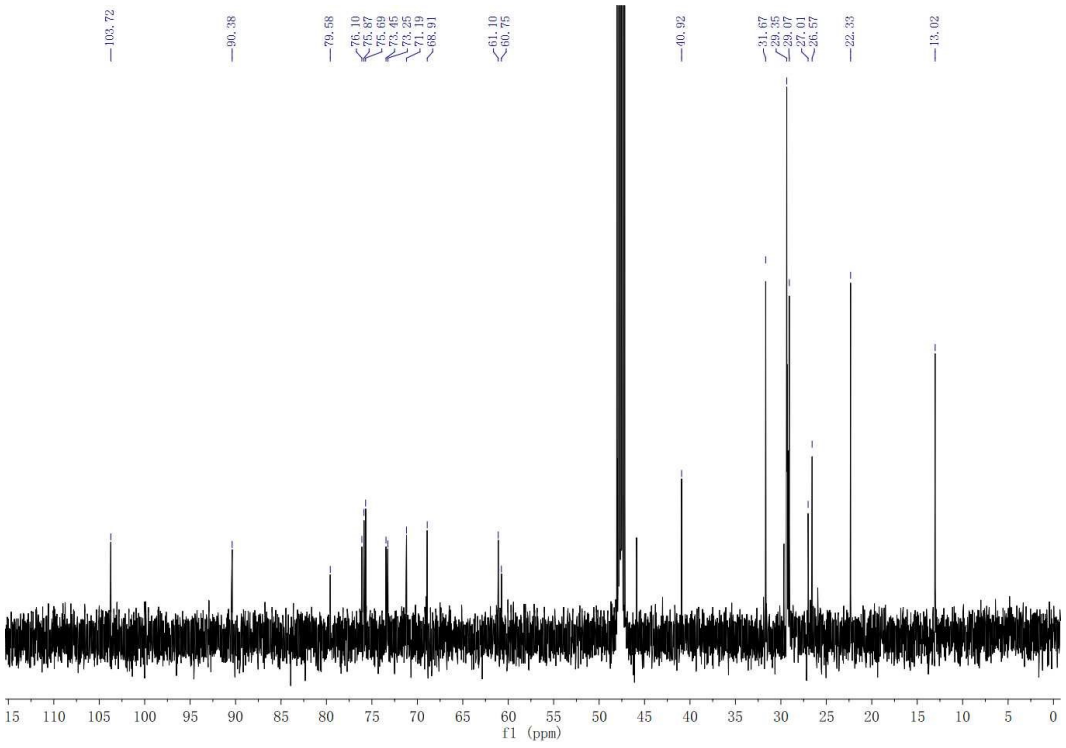
14.07
0.81
0.80
2.17
22.29
3.00
f1 (ppm)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73.25
71.19
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40.92
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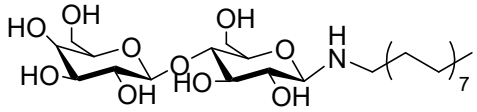
29.35
29.07
27.01
26.57
22.33
13.02
f1 (ppm)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OH
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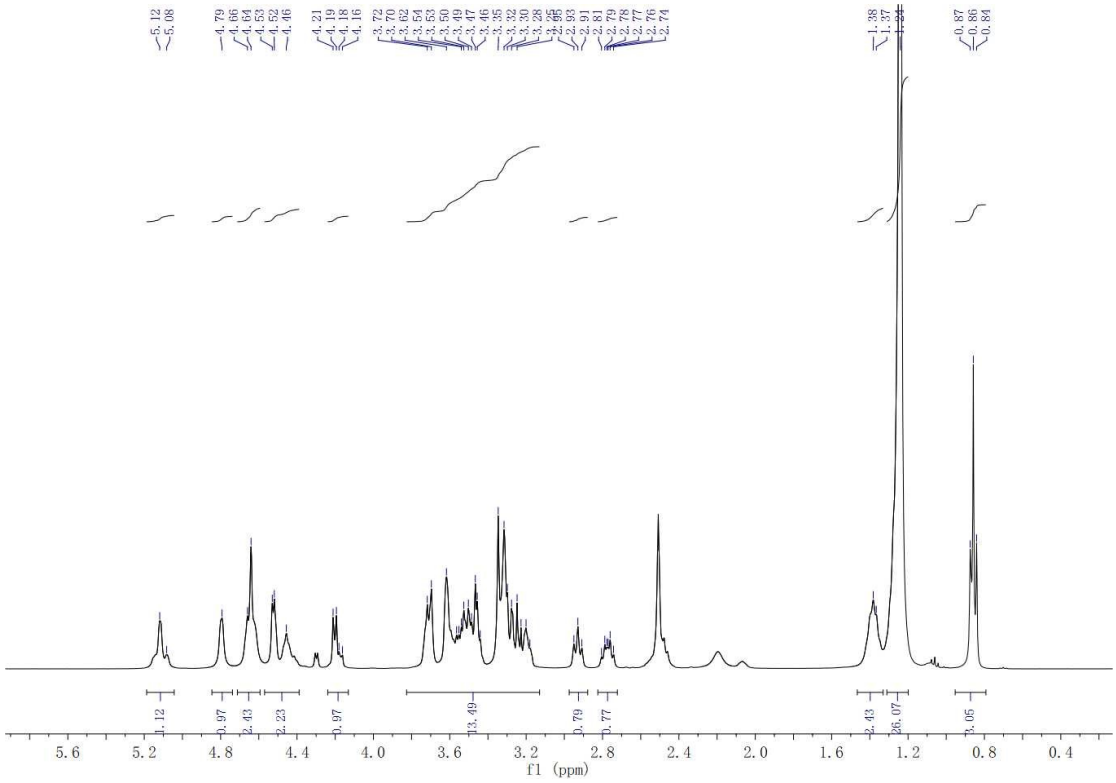
HO
OH
O
OH
HO
O
H
N
7
OH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5.08
4.79
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4.53
4.52
4.46
4.21
4.19
4.18
4.16
3.72
3.70
3.62
3.54
3.53
3.50
3.49
3.47
3.46
3.35
3.32
3.30
3.28
2.93
2.91
2.81
2.79
2.78
2.77
2.76
2.74
1.38
1.37
0.87
0.86
0.84
1.12
0.97
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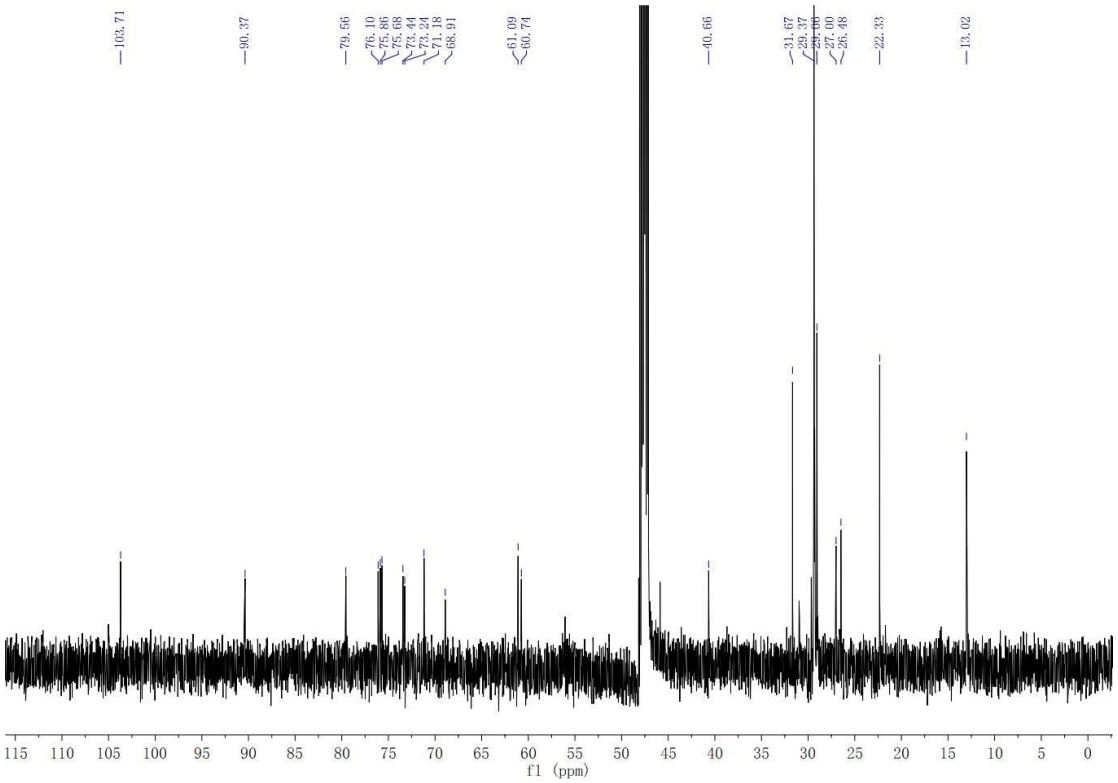
2.23
0.97
13.49
0.79
0.77
2.43
26.07
3.05
f1 (ppm)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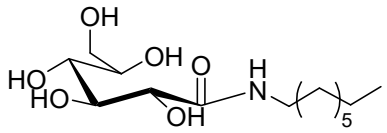
76.10
75.86
75.68
73.44
73.24
71.18
68.91
61.09
60.74
40.66
31.67
29.37
29.06
27.00
26.48
22.33
13.02
115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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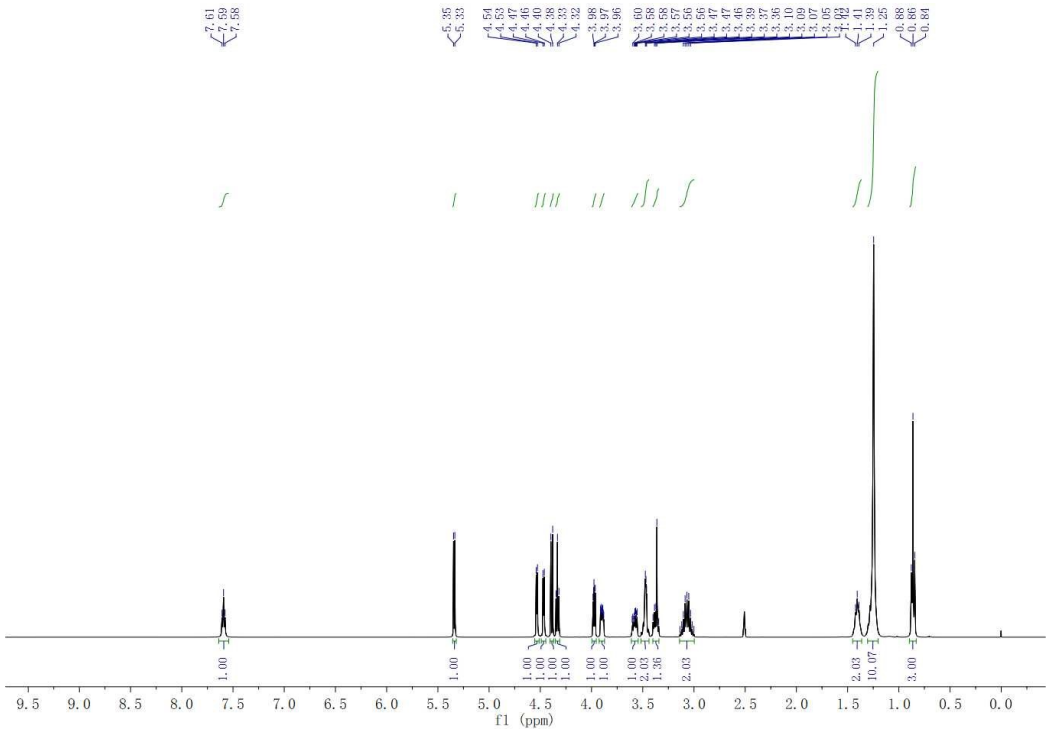
HO
HO
O
H
N
5
OH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7.58
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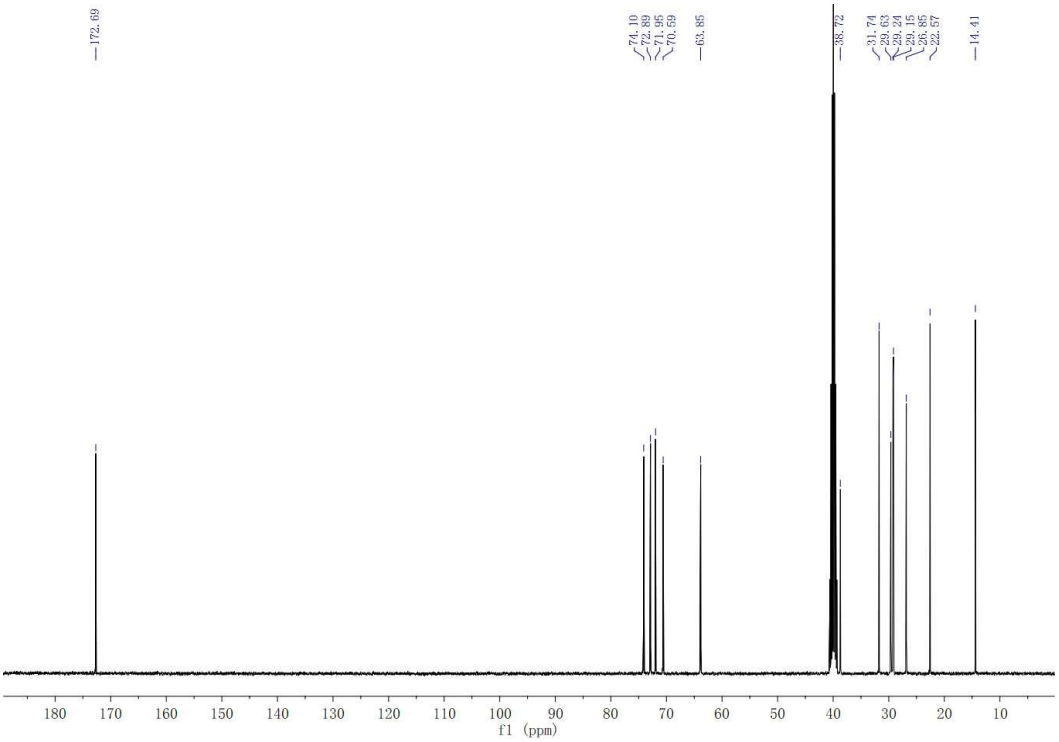
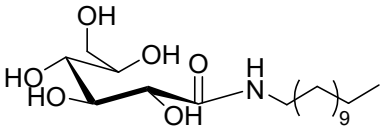
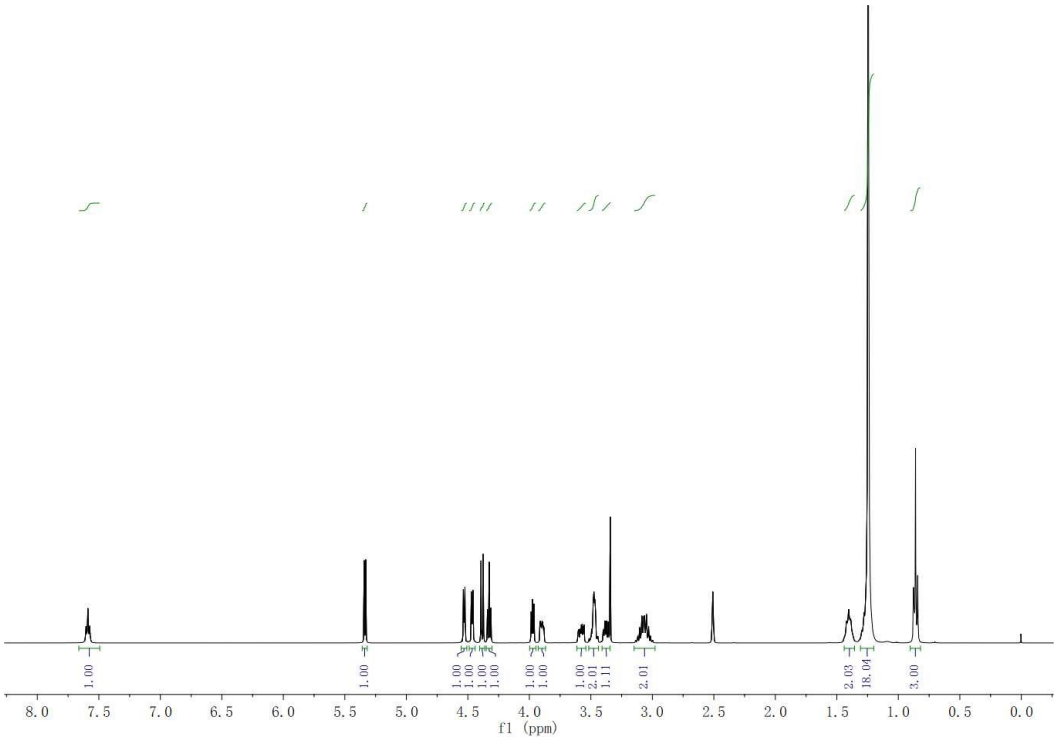
4.53
4.47
4.46
4.40
4.38
4.33
4.32
3.98
3.97
3.96
3.60
3.58
3.58
3.57
3.56
3.56
3.47
3.47
3.46
3.39
3.37
3.36
3.10
3.09
3.07
3.05
1.41
1.39
1.25
0.88
0.86
0.84
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
2.03
1.35
2.03
2.03
10.07
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


172.69
74.10
72.89
71.95
70.59
63.85
38.72
31.74
29.63
29.24
29.15
25.85
22.57
14.41
f1 (ppm)


OH
OH
HO
HO
O
H
N
OH
9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1.00
1.00
1.00
1.00
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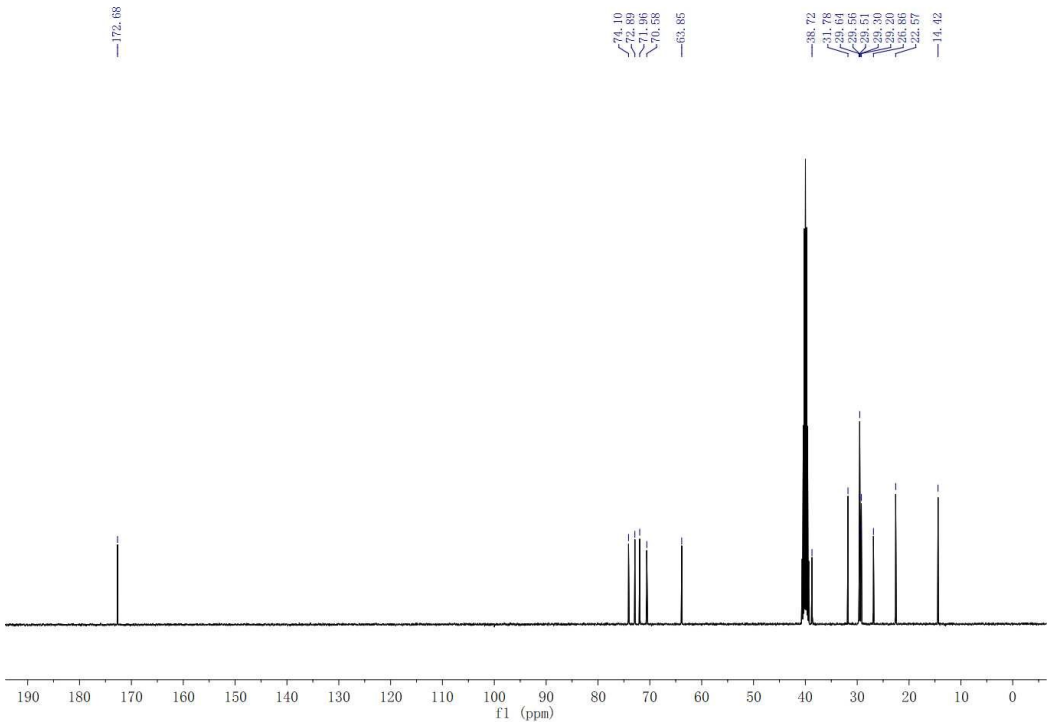
1.00
1.00
2.01
1.11
2.01
2.03
18.04
3.00
f1 (ppm)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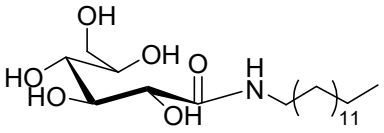
71.96
70.58
63.85
38.72
31.78
29.64
29.56
29.51
29.30
29.20
26.86
22.57
14.42
f1 (ppm)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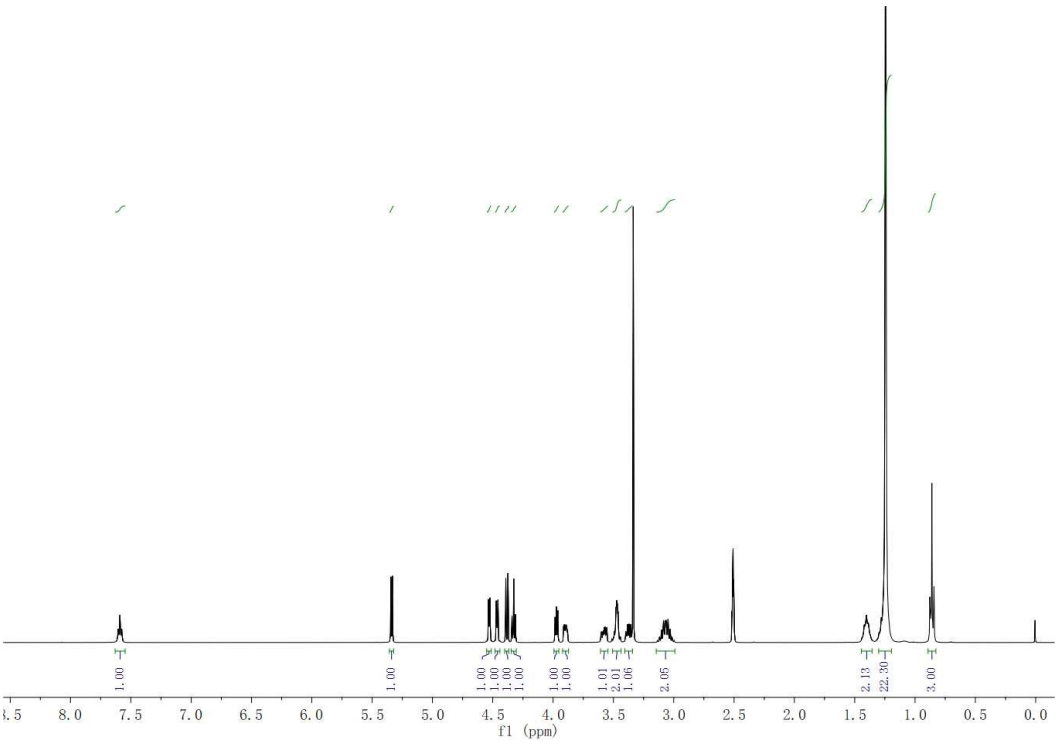
OH
HO
HO
O
H
N
OH
11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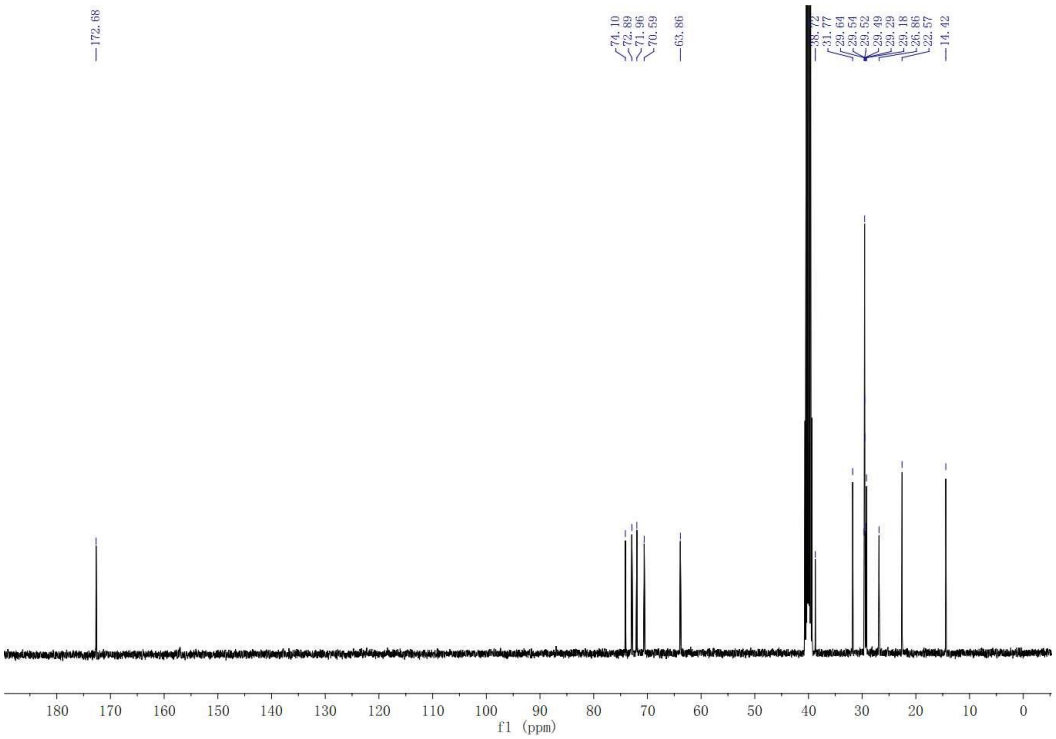
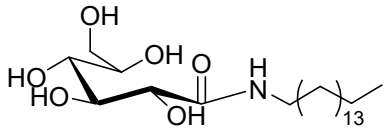
1.00
1.00
1.00
1.00
1.00
1.00
1.01
2.01
1.06
2.05
2.13
22.30
3.00
f1 (ppm)


172.68
74.10
72.89
71.96
70.59
63.86
38.72
31.77
29.64
29.54
29.52
29.49
29.29
29.18
25.86
22.57
14.42
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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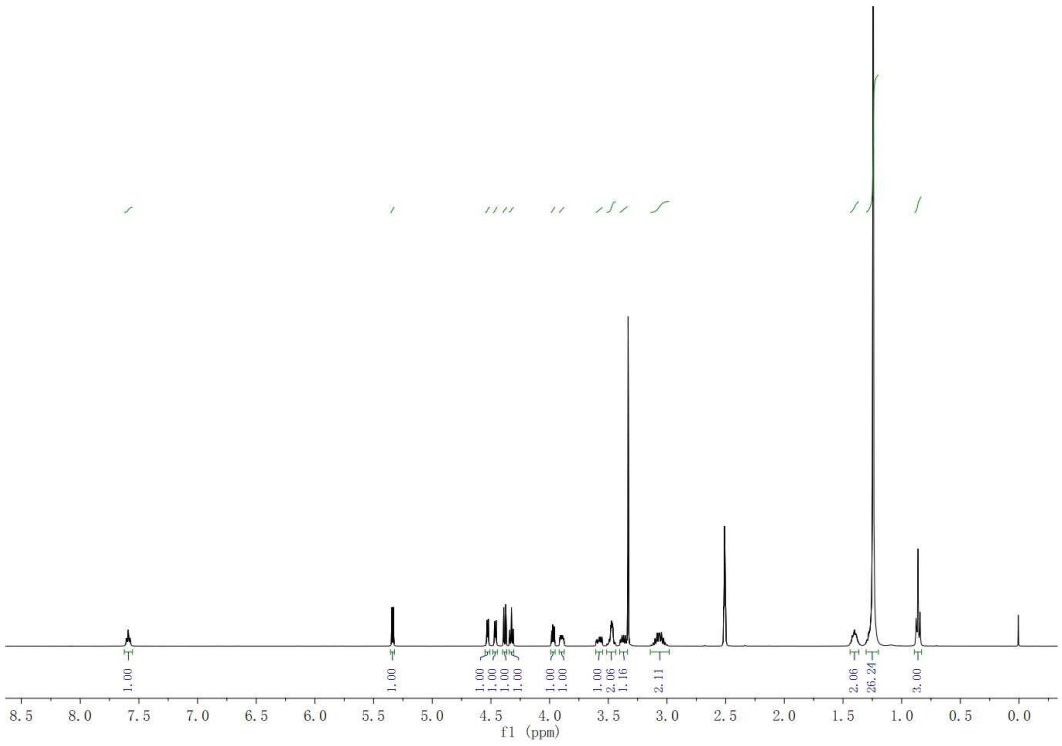
OH
HO
HO
O
H
N
OH
13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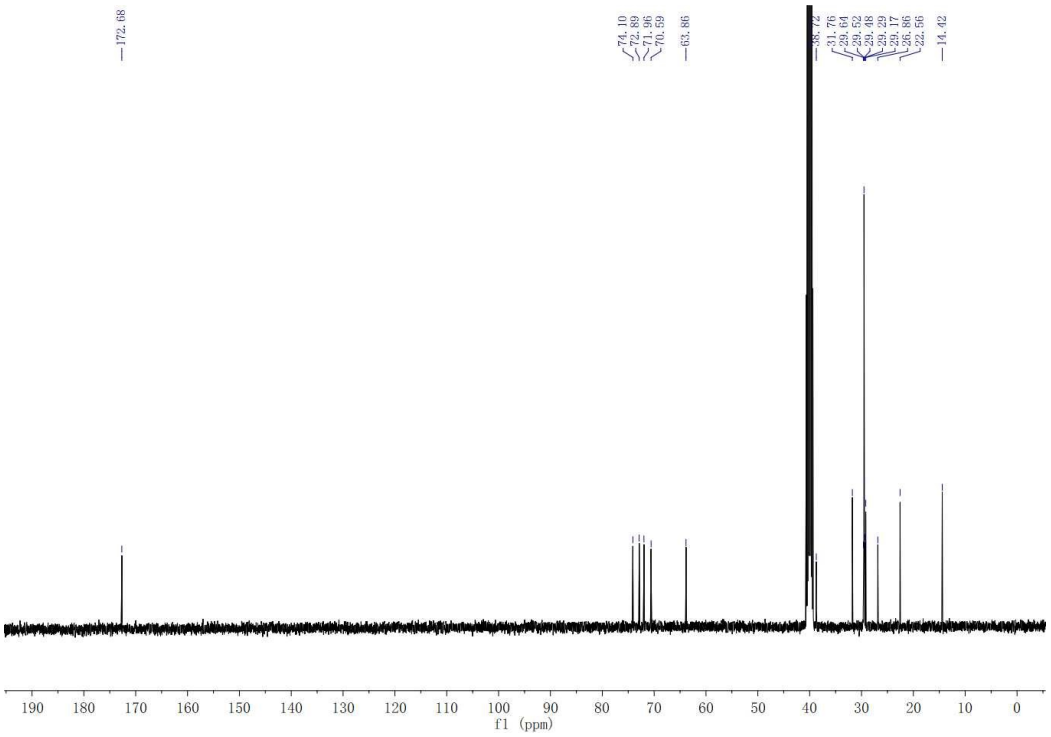
1.00
1.00
1.00
1.00
1.00
2.06
1.16
2.11
2.06
26.24
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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72.89
71.96
70.59
63.86
38.72
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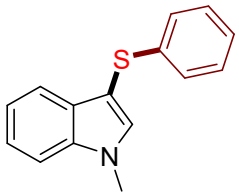
29.64
29.52
29.48
29.29
29.17
25.86
22.56
14.42
f1 (ppm)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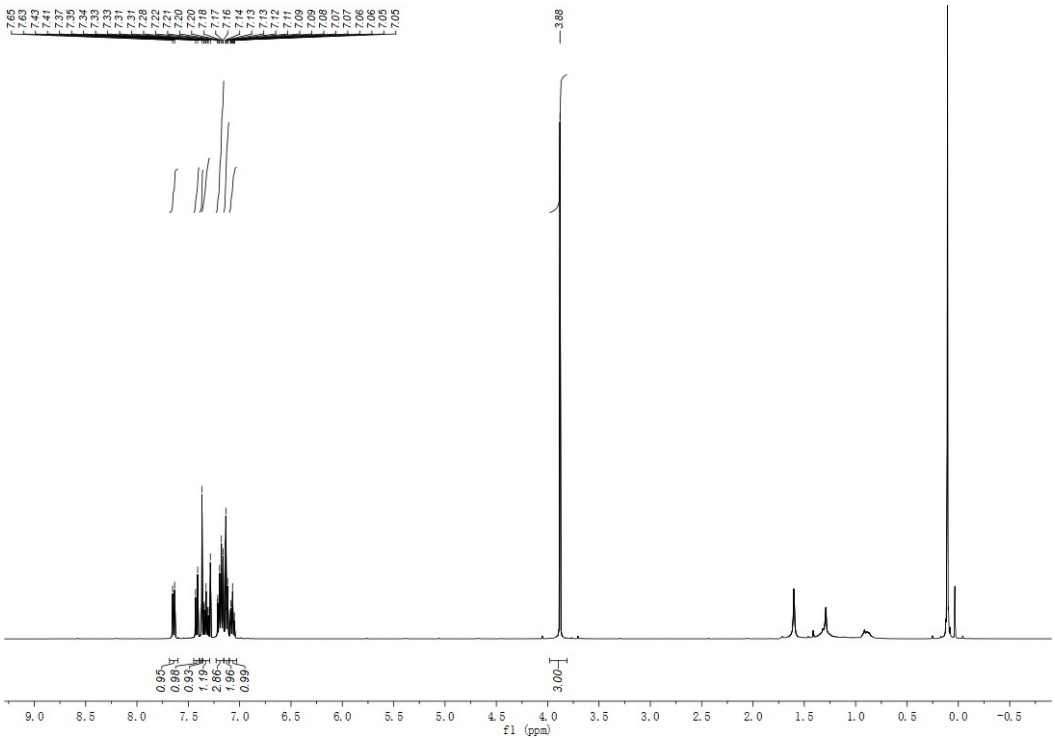
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7.22
7.21
7.20
7.18
7.17
7.16
7.14
7.13
7.12
7.11
7.09
7.08
7.07
7.06
7.05
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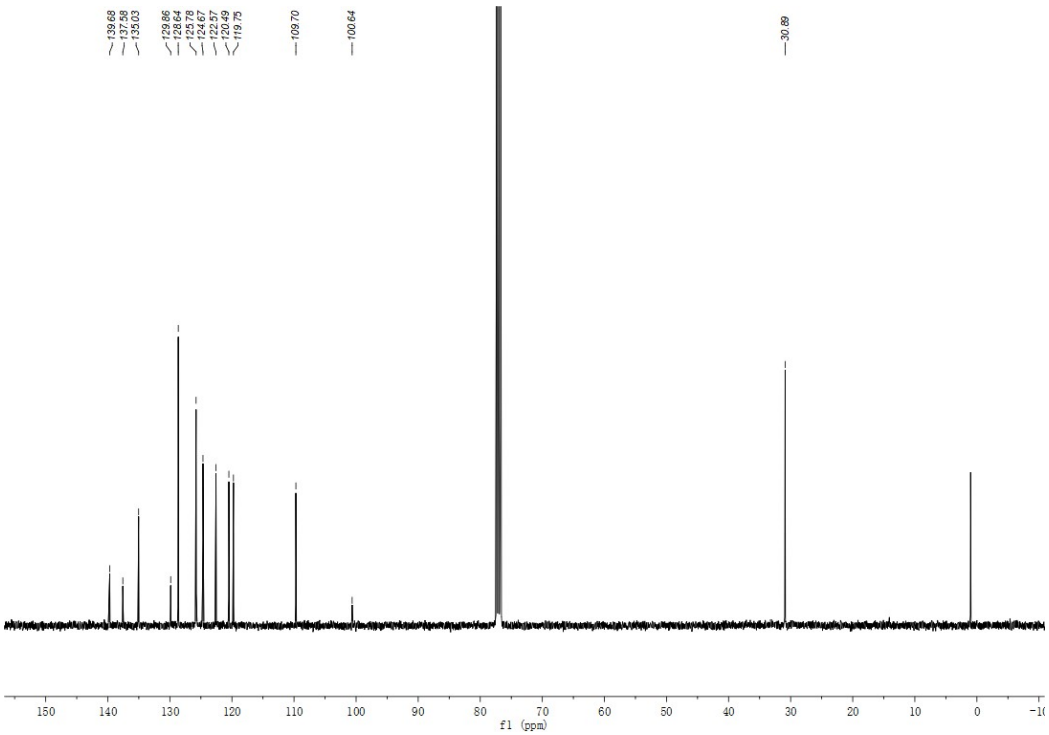
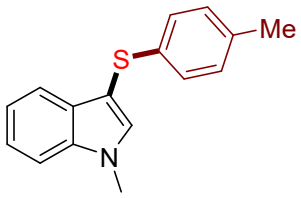
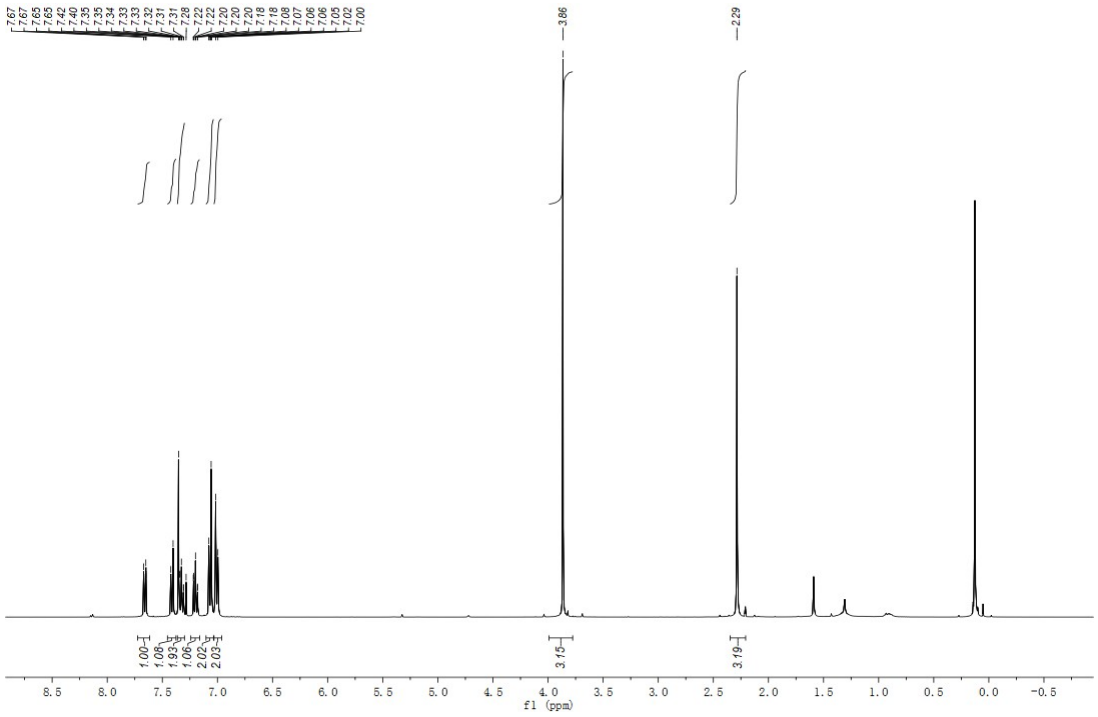
0.95
0.98
0.93
1.19
2.86
1.96
0.99
3.00
f1 (ppm)


139.68
137.88
135.03
129.86
128.64
125.78
124.67
122.57
120.49
119.75
109.70
100.64
30.89
f1 (ppm)


S
Me
N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7.31
7.28
7.22
7.20
7.20
7.20
7.18
7.18
7.08
7.07
7.06
7.06
7.05
7.02
7.00
3.86
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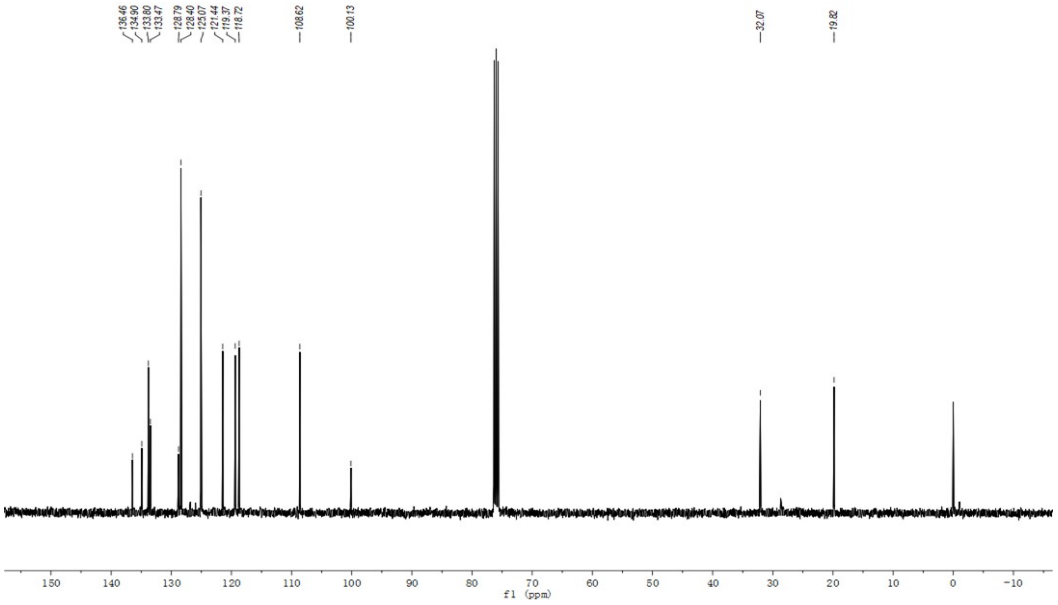
1.00
1.08
1.93
1.06
2.02
2.03
3.15
3.19
f1 (ppm)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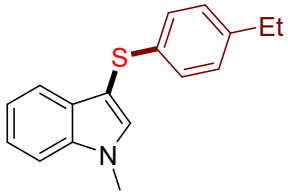
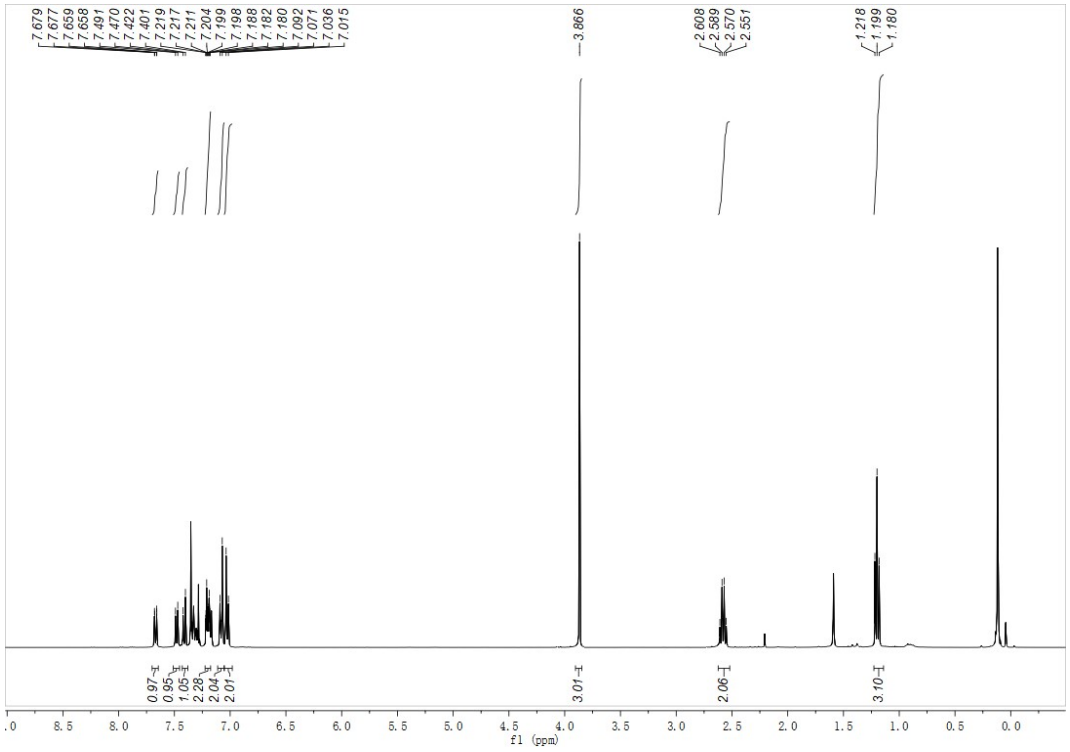
133.80
133.47
128.79
128.40
125.07
121.44
119.37
110.72
108.62
100.13
32.07
19.82
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Et
S
N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7.401
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7.217
7.211
7.204
7.199
7.198
7.188
7.182
7.180
7.092
7.071
7.036
7.015
3.866
2.608
2.589
2.570
2.551
1.218
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1.180
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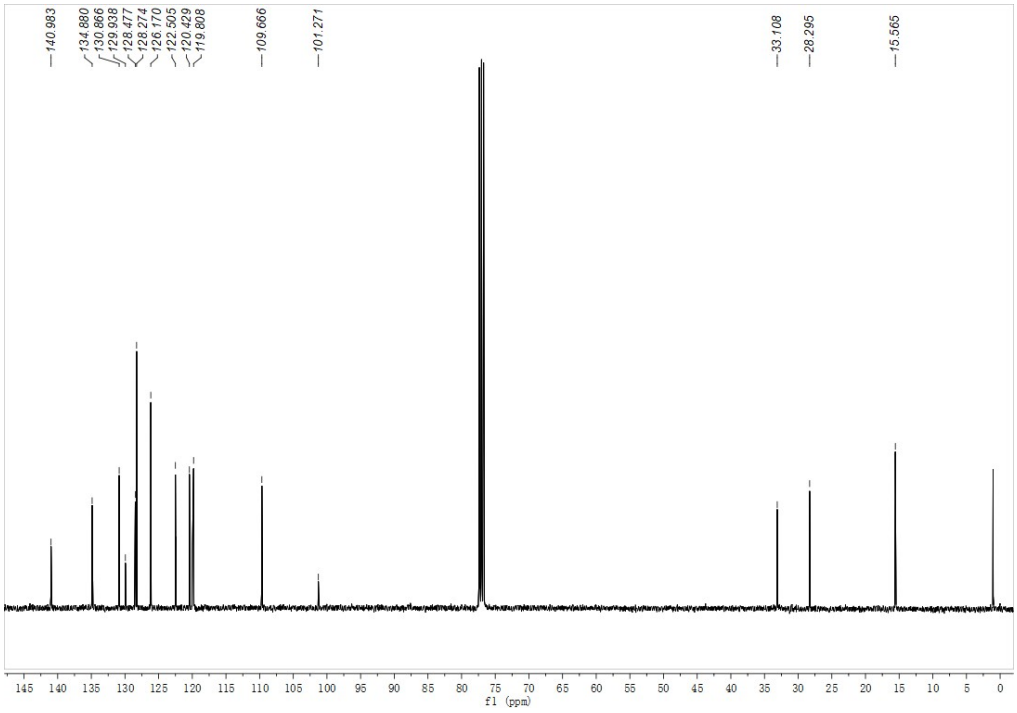
0.95
1.05
2.28
2.04
2.01
3.01
2.06
3.10
f1 (ppm)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101.271
33.108
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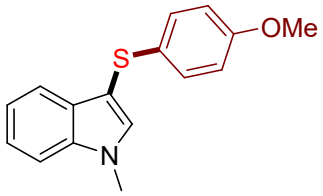
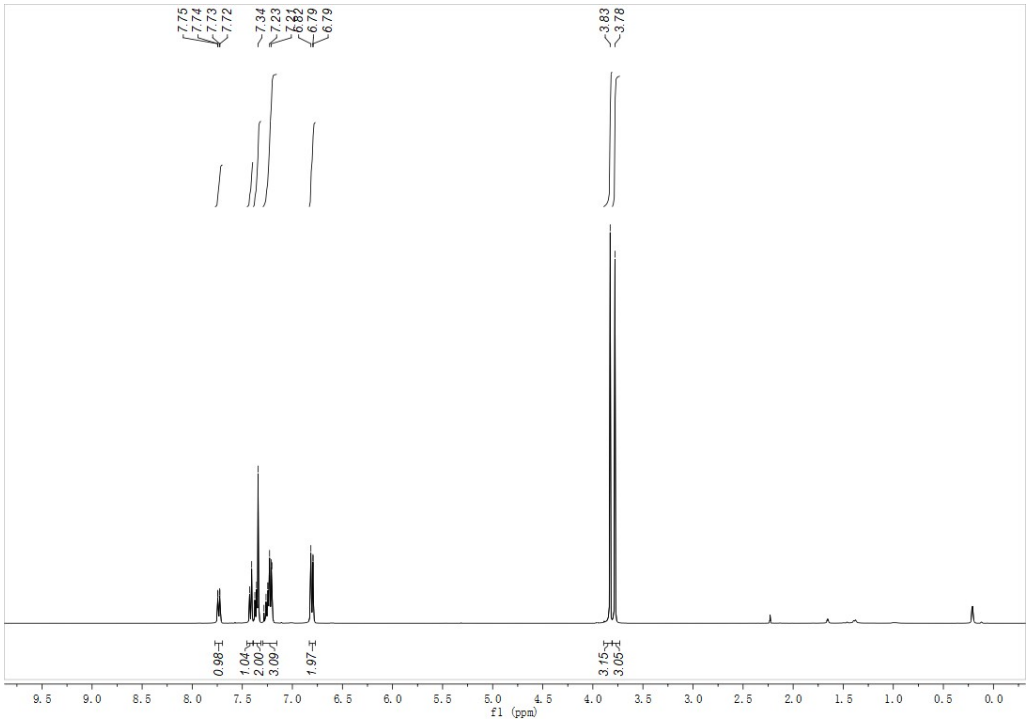
15.565
f1 (ppm)


OMe
S
N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7.72
7.34
7.23
6.82
6.79
6.79
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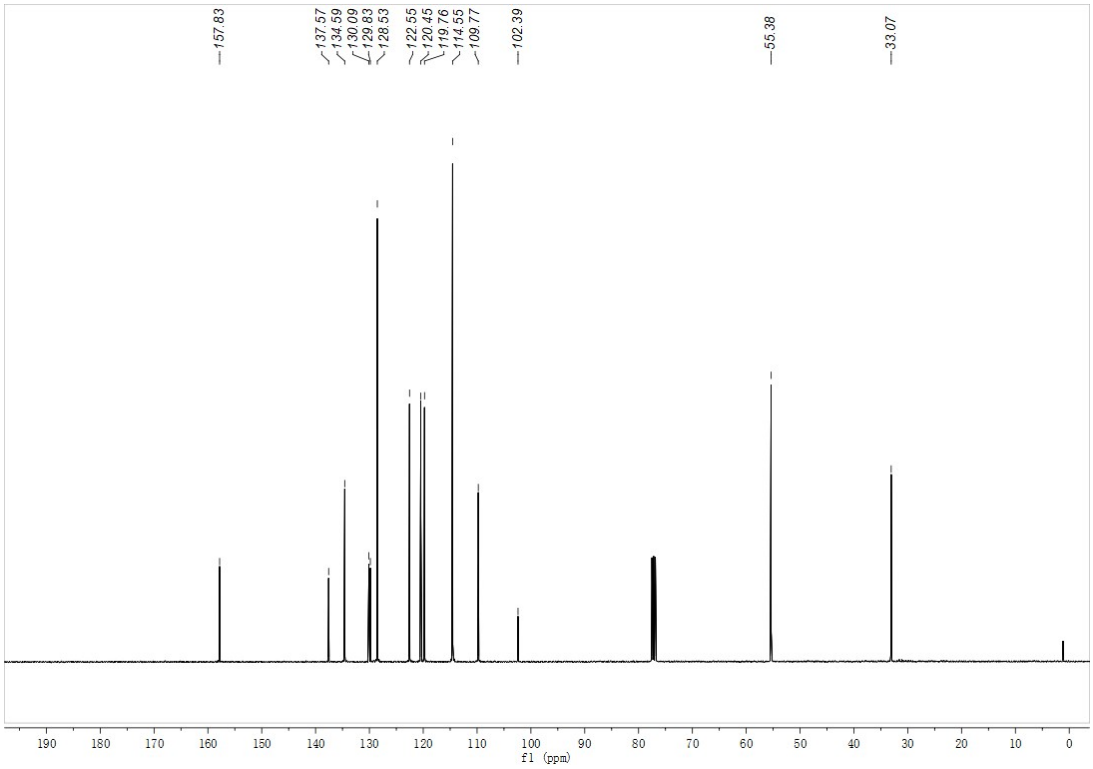
3.78
0.98
1.04
2.00
3.09
1.97
3.15
3.08
f1 (ppm)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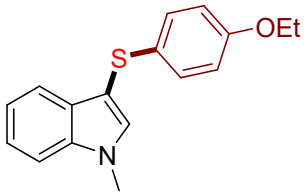
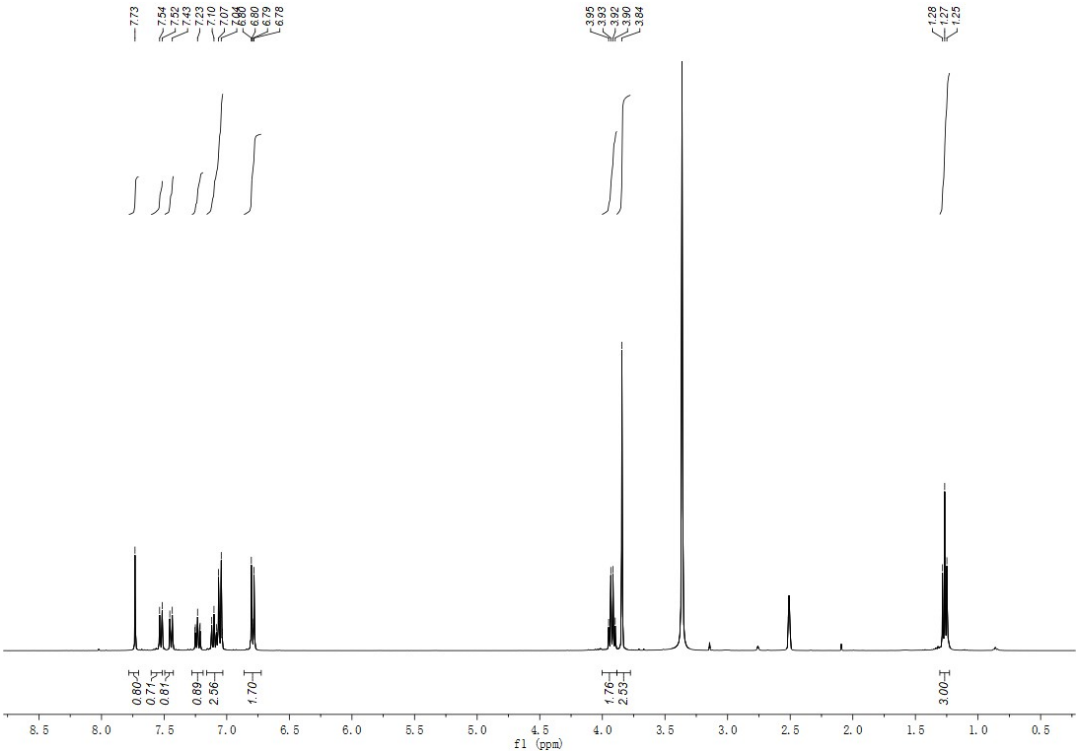
102.39
55.38
33.07
f1 (ppm)


OEt
S
N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6.79
6.78
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3.92
3.90
3.84
1.28
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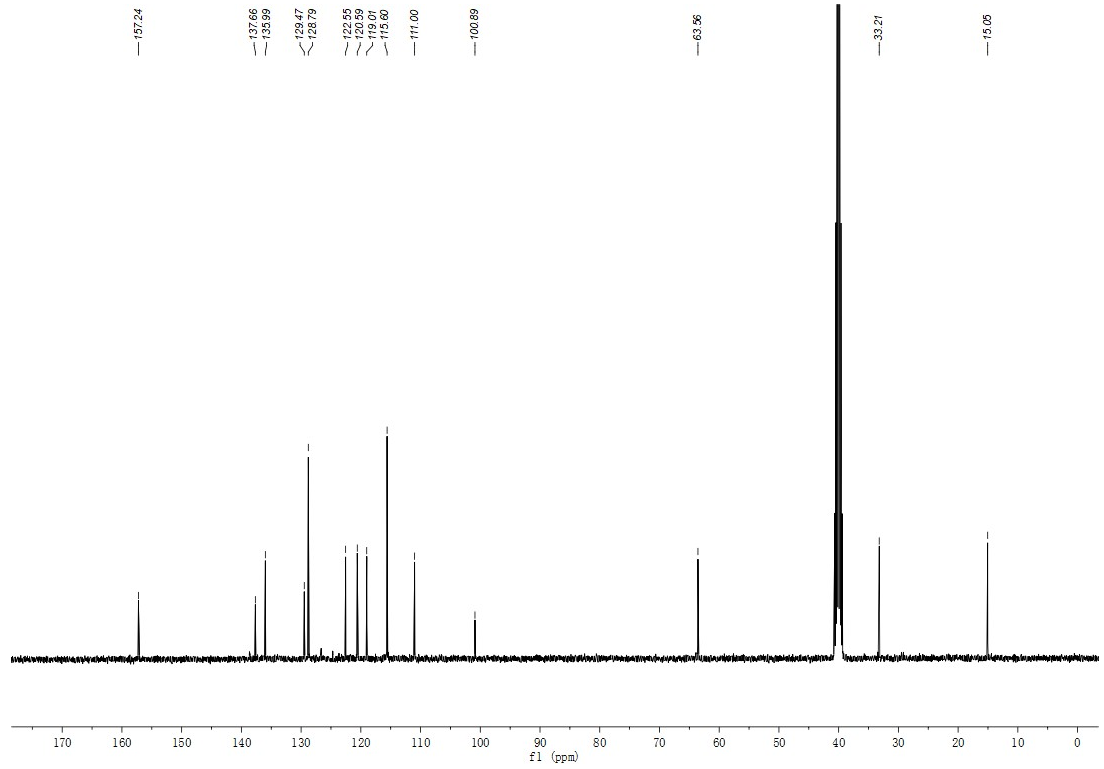
0.89
2.56
1.70
1.76
2.53
3.00
f1 (ppm)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111.00
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63.56
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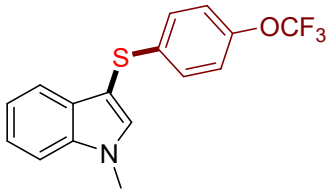
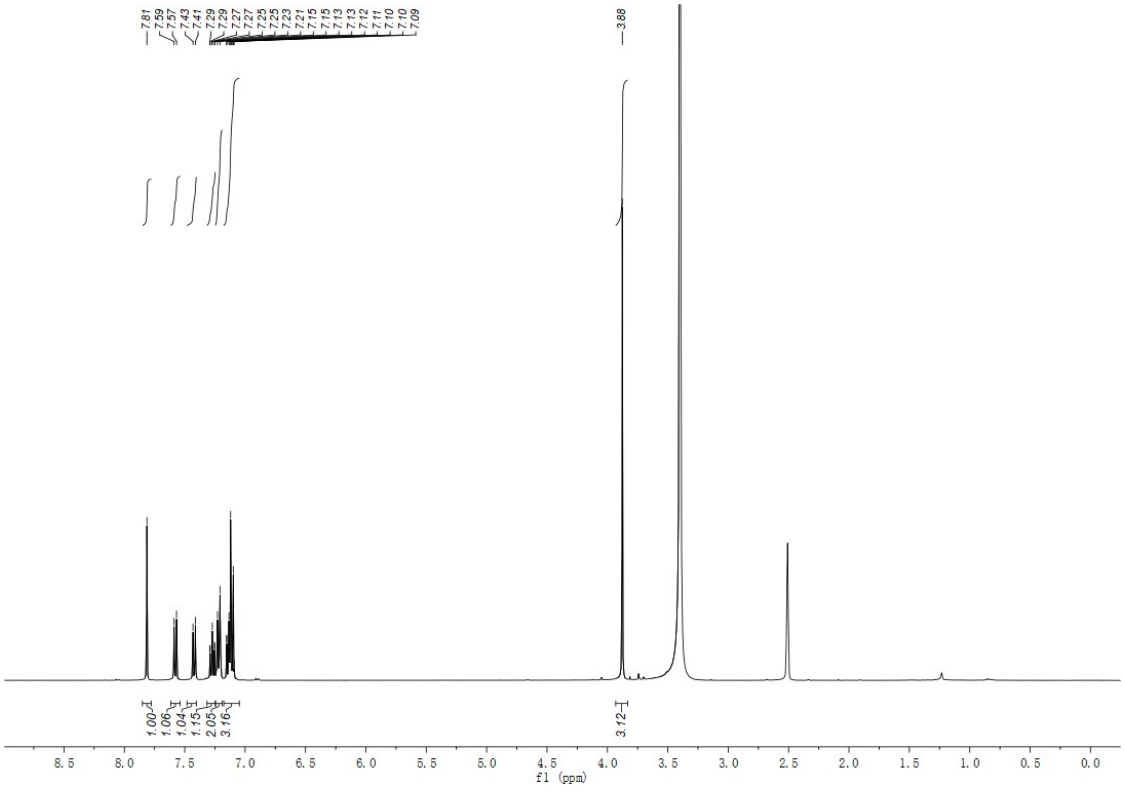
15.05
f1 (ppm)


S
OCF3
N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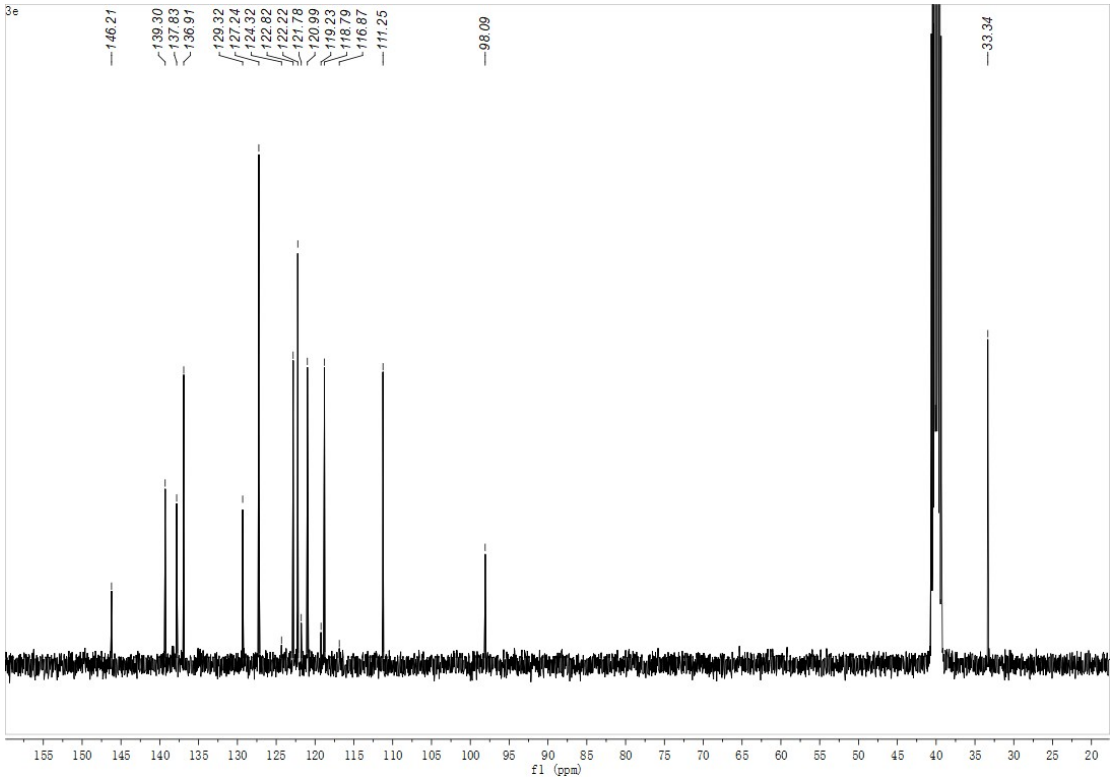
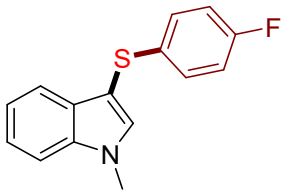
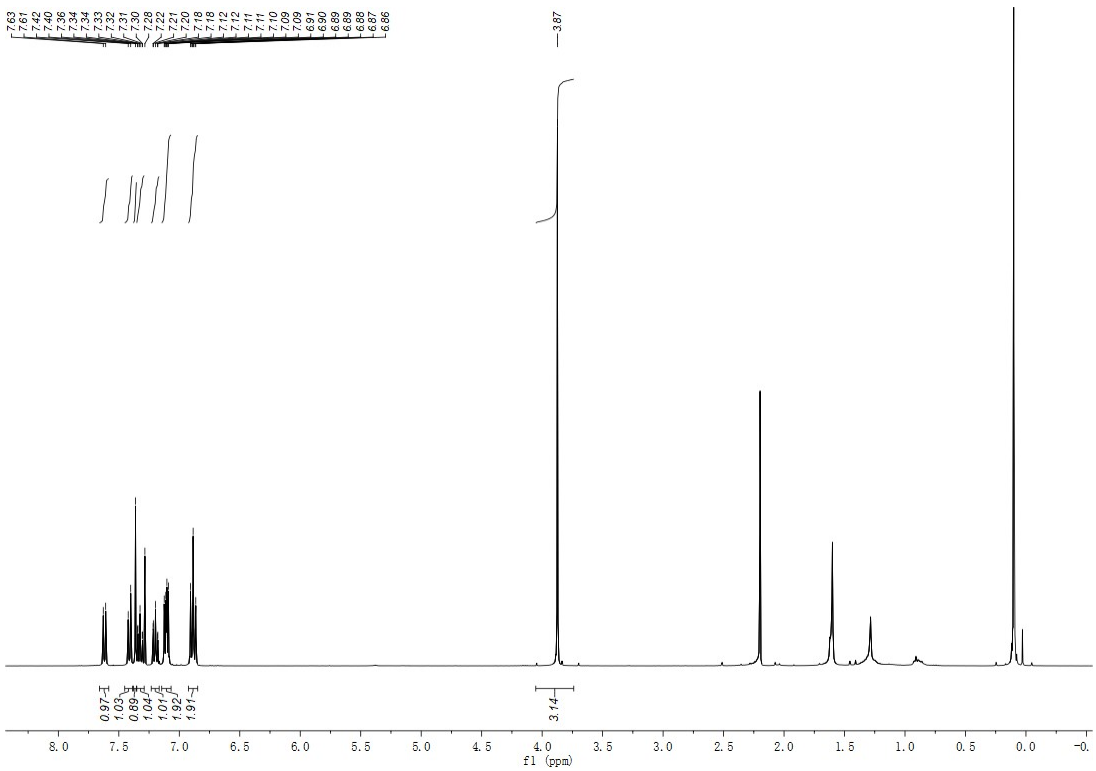
7.10
7.09
3.88
1.00
1.06
1.04
1.15
2.05
3.16
3.12
f1 (ppm)


3e
146.21
139.30
137.83
136.91
129.32
127.24
124.32
122.82
122.22
121.78
120.99
119.23
118.79
116.87
111.25
98.09
33.34
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)


S
F
N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7.33
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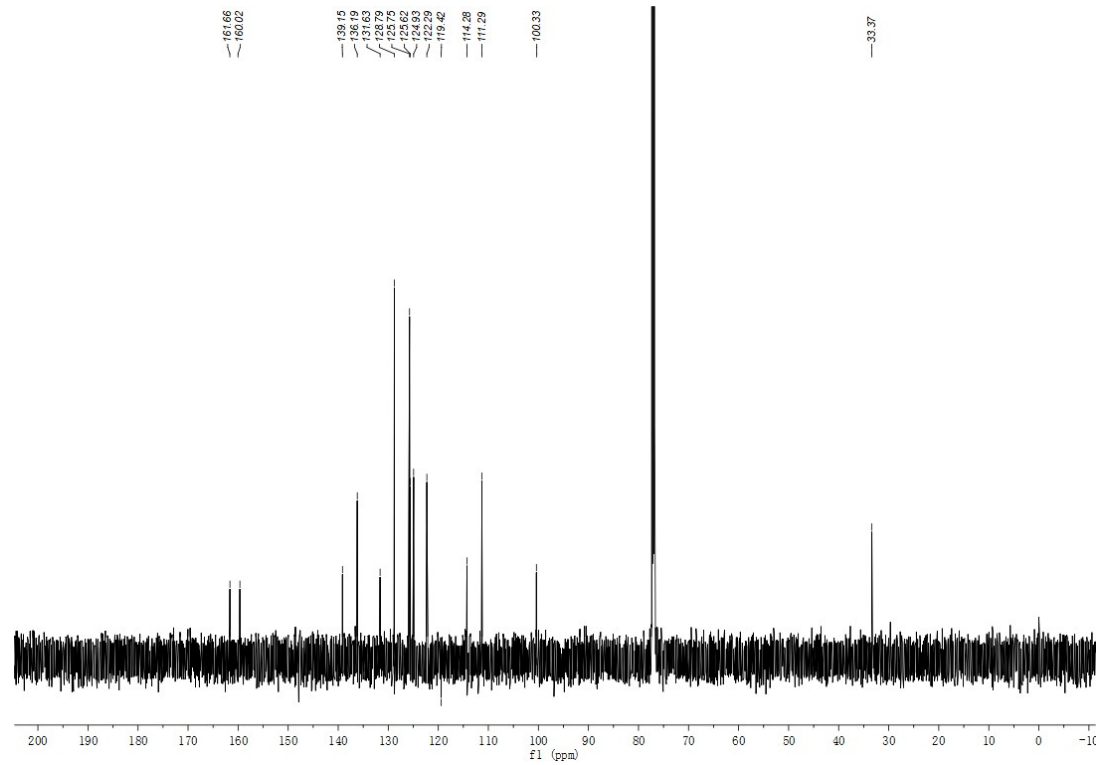
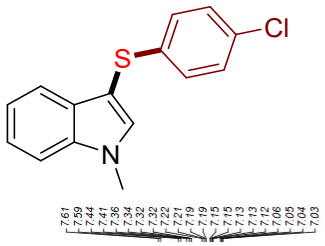
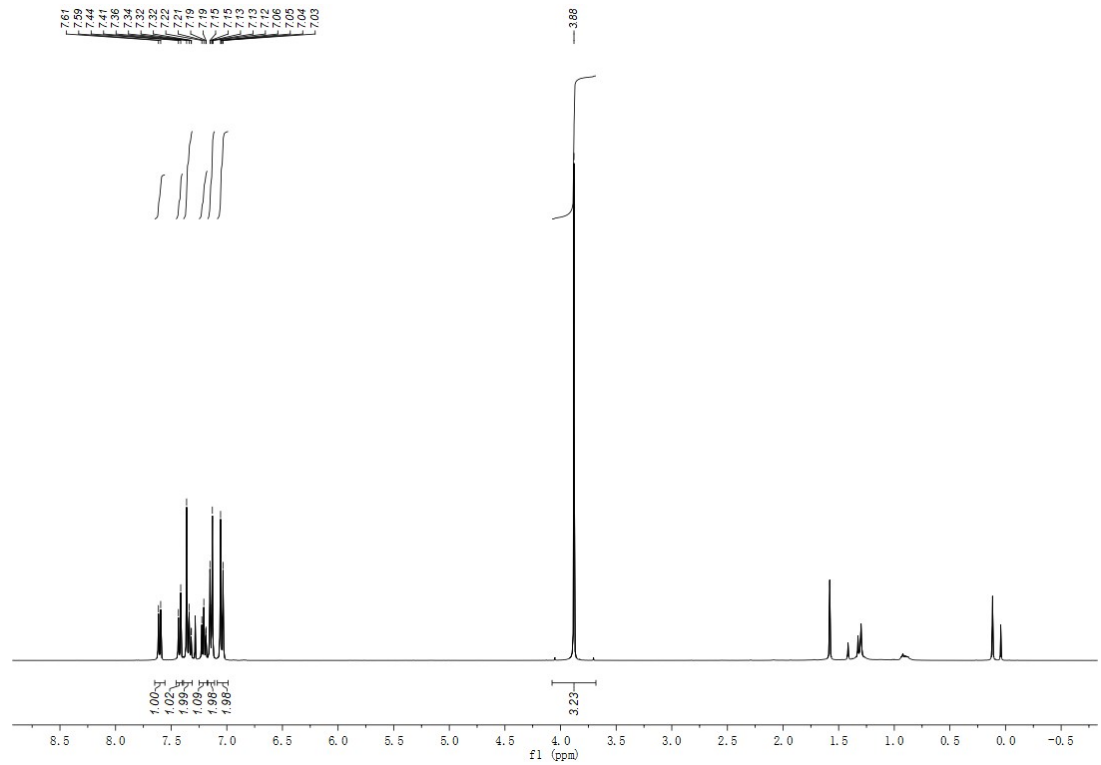
7.31
7.30
7.28
7.22
7.21
7.20
7.18
7.18
7.12
7.12
7.11
7.11
7.10
7.09
7.09
6.91
6.90
6.89
6.89
6.88
6.87
6.86
3.87
0.97
1.03
0.89
1.04
1.01
1.92
1.91
3.14
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


161.66
160.02
139.15
136.19
131.63
128.79
125.75
125.62
124.93
122.29
119.42
114.28
111.29
100.33
33.37
f1 (ppm)


S
Cl
N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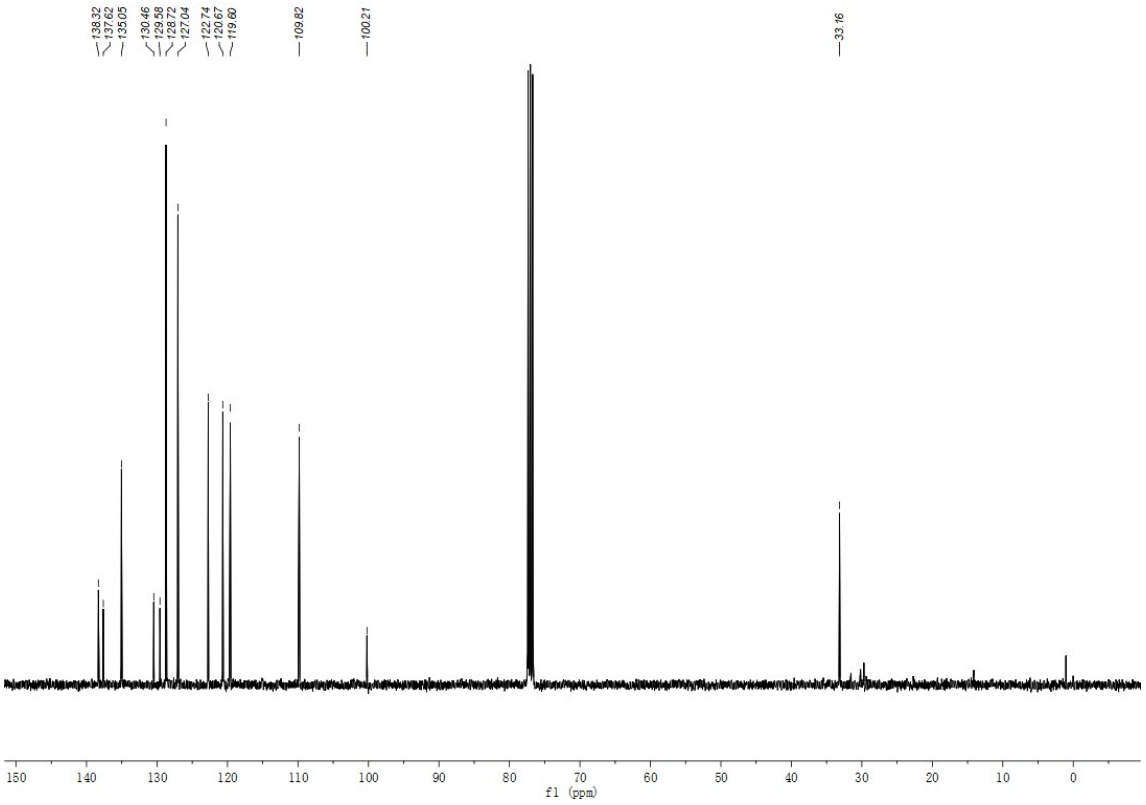
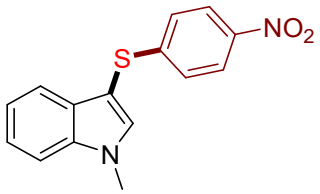
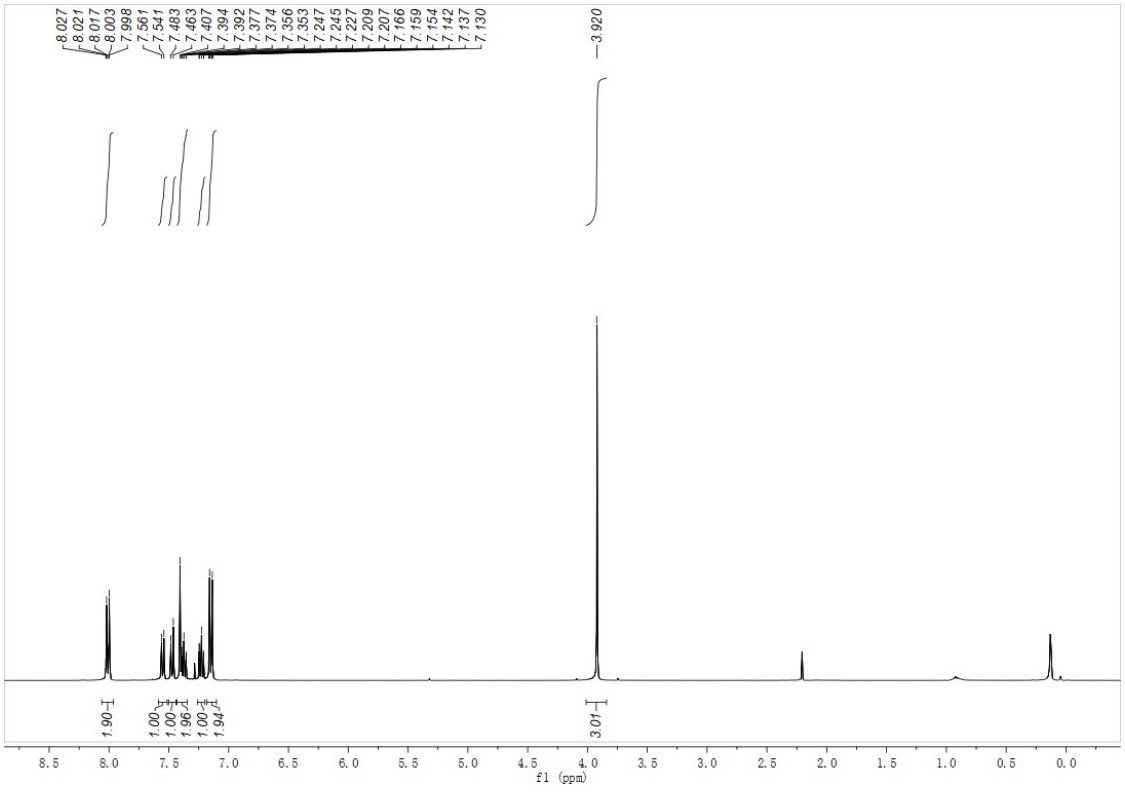
7.34
7.32
7.22
7.21
7.19
7.15
7.13
7.12
7.06
7.05
7.04
7.03
3.88
1.00
1.02
1.99
1.09
1.98
1.98
3.23
f1 (ppm)


138.32
137.62
135.05
130.46
129.58
128.72
127.04
122.74
120.67
119.60
109.82
100.21
33.16
f1 (ppm)


NO2
S
N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8.021
8.017
8.003
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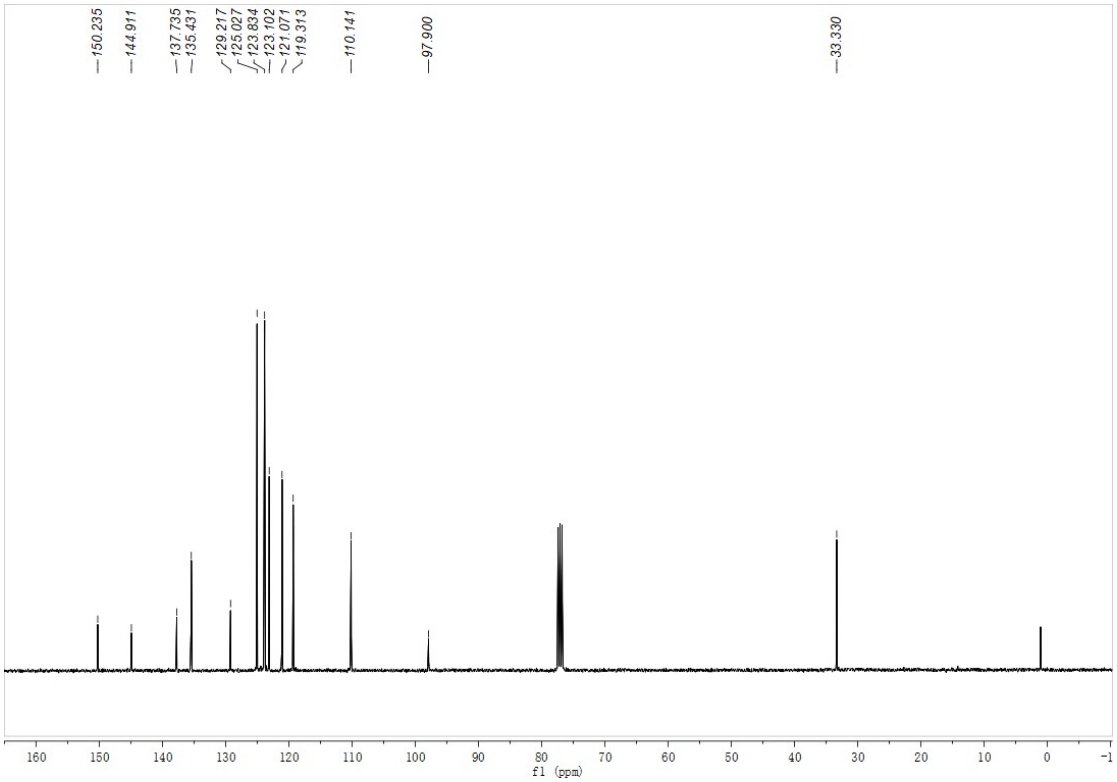
7.561
7.541
7.483
7.463
7.407
7.394
7.392
7.377
7.374
7.356
7.353
7.247
7.245
7.227
7.209
7.207
7.166
7.159
7.154
7.142
7.137
7.130
3.920
1.90
1.00
1.00
1.96
1.00
1.94
3.01
f1 (ppm)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137.735
135.431
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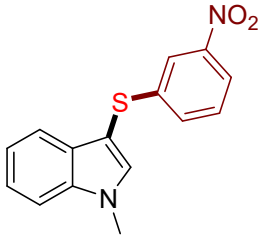
125.027
123.834
123.102
121.071
119.313
110.141
97.900
33.330
f1 (ppm)


NO2
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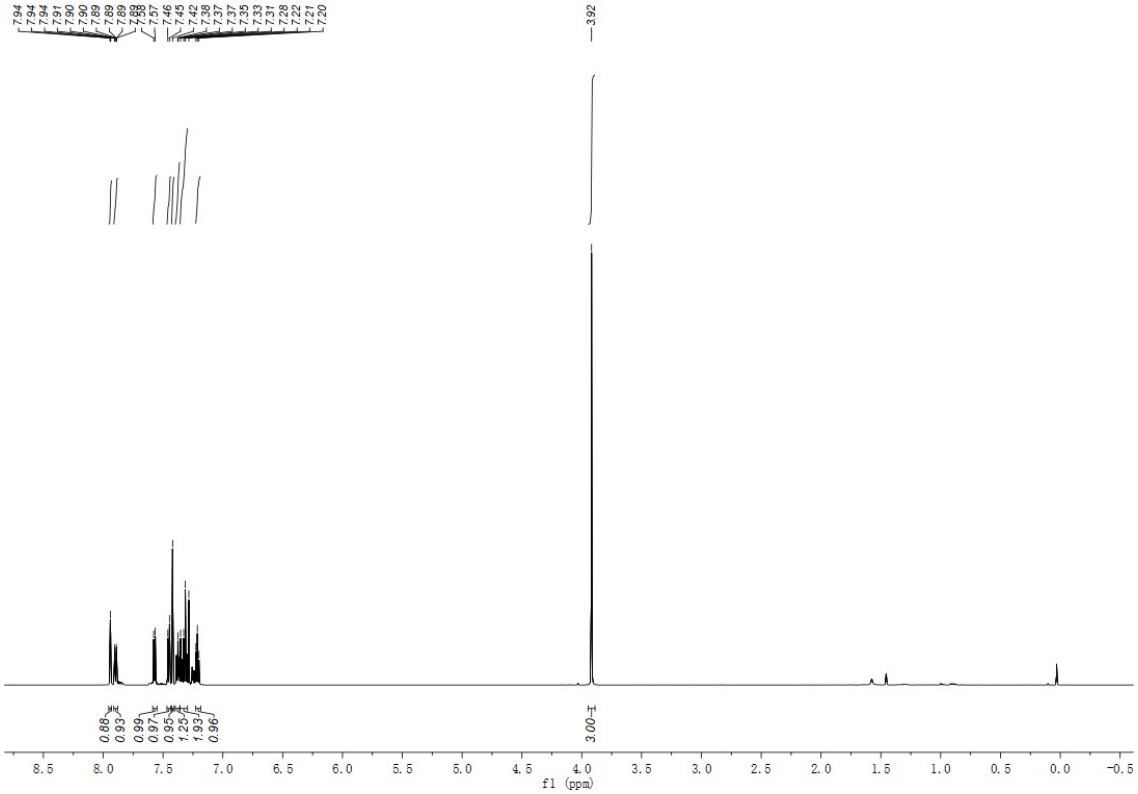
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7.94
7.94
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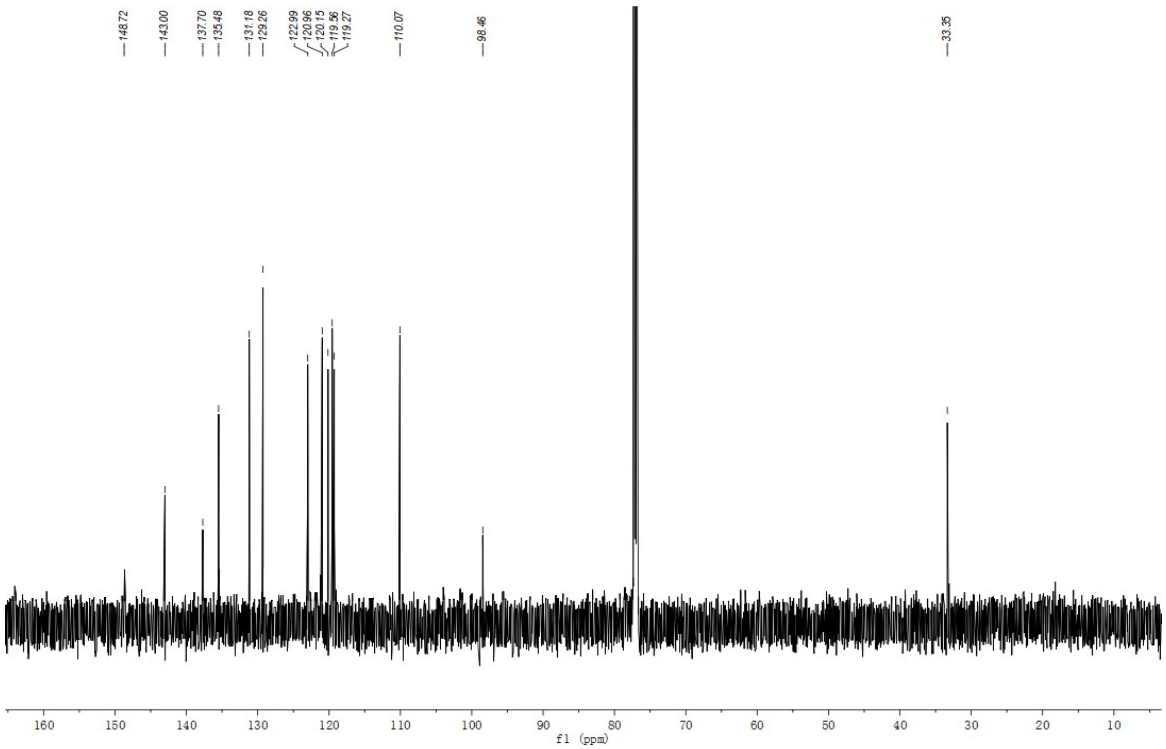
7.90
7.90
7.89
7.89
7.89
7.88
7.88
7.57
7.46
7.45
7.42
7.38
7.37
7.37
7.35
7.33
7.31
7.28
7.22
7.21
7.20
3.92
0.88
0.93
0.99
0.97
0.95
1.25
1.93
0.96
3.00
f1 (ppm)


148.72
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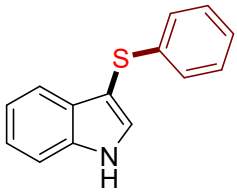
135.48
131.18
129.26
122.99
120.96
120.15
119.56
119.27
110.07
98.46
33.35
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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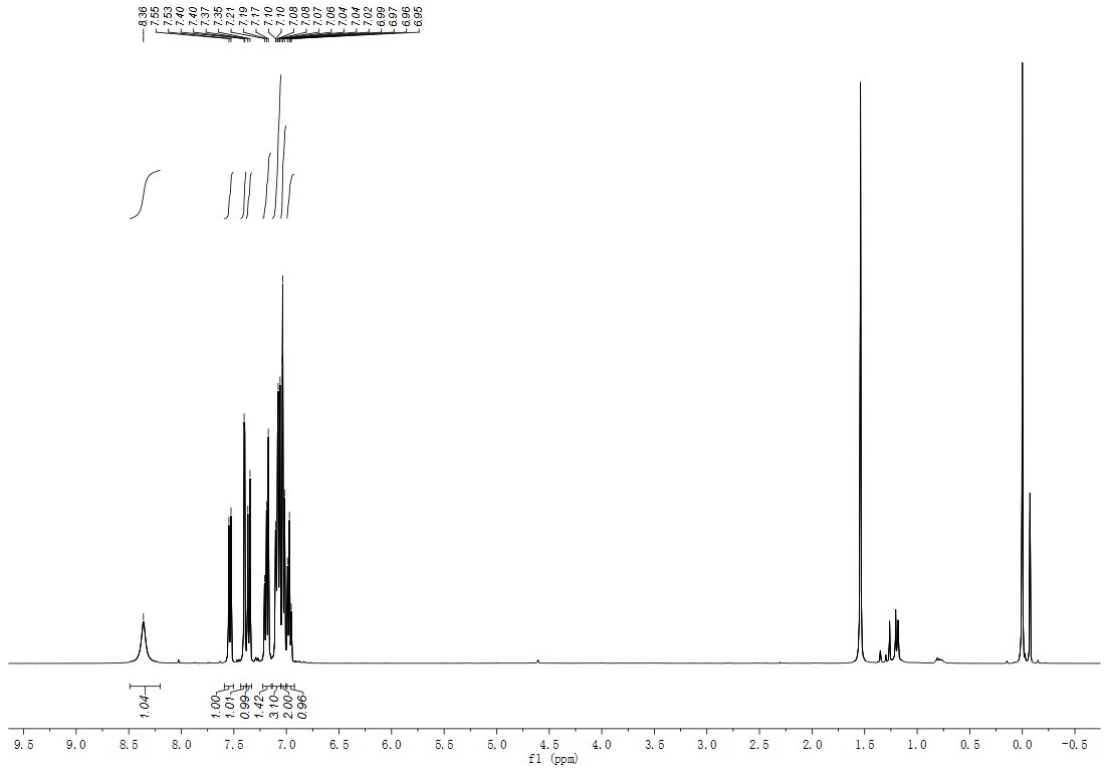
N
H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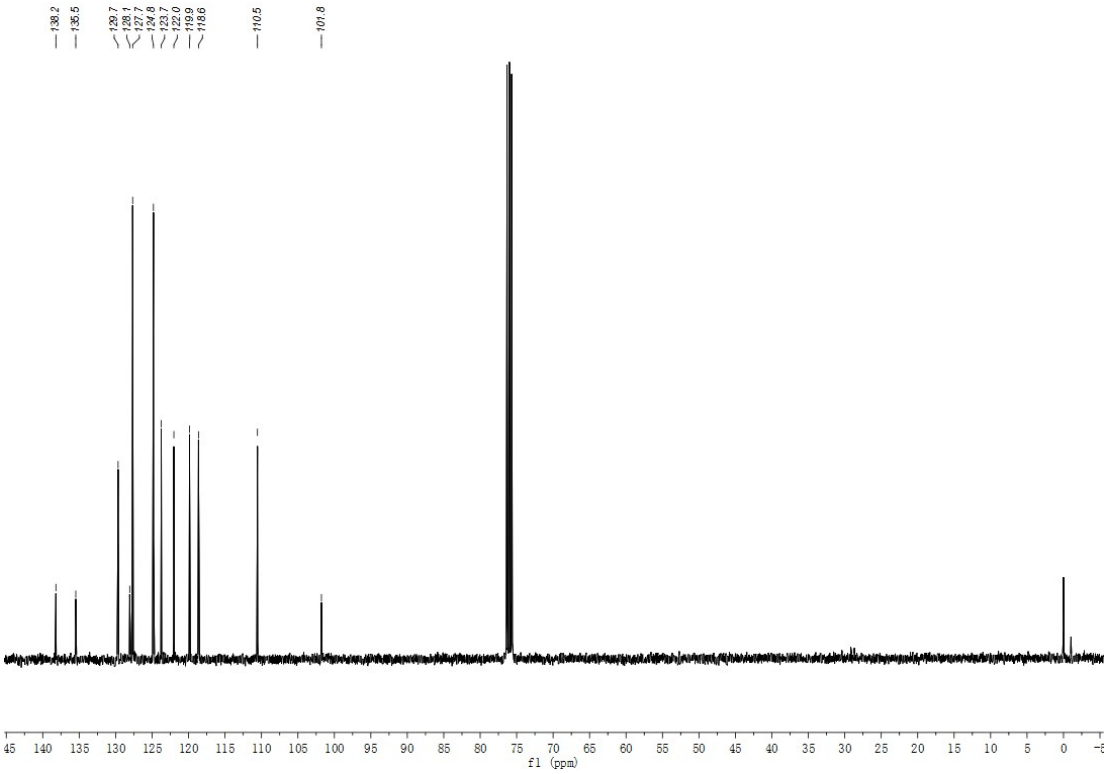
7.35
7.21
7.19
7.17
7.10
7.10
7.08
7.08
7.07
7.06
7.04
7.04
7.02
6.99
6.97
6.96
6.95
1.04
1.00
1.01
0.99
1.42
3.10
2.00
0.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


138.2
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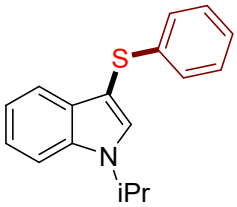
129.1
127.7
124.8
123.7
122.0
119.9
118.6
110.5
101.8
f1 (ppm)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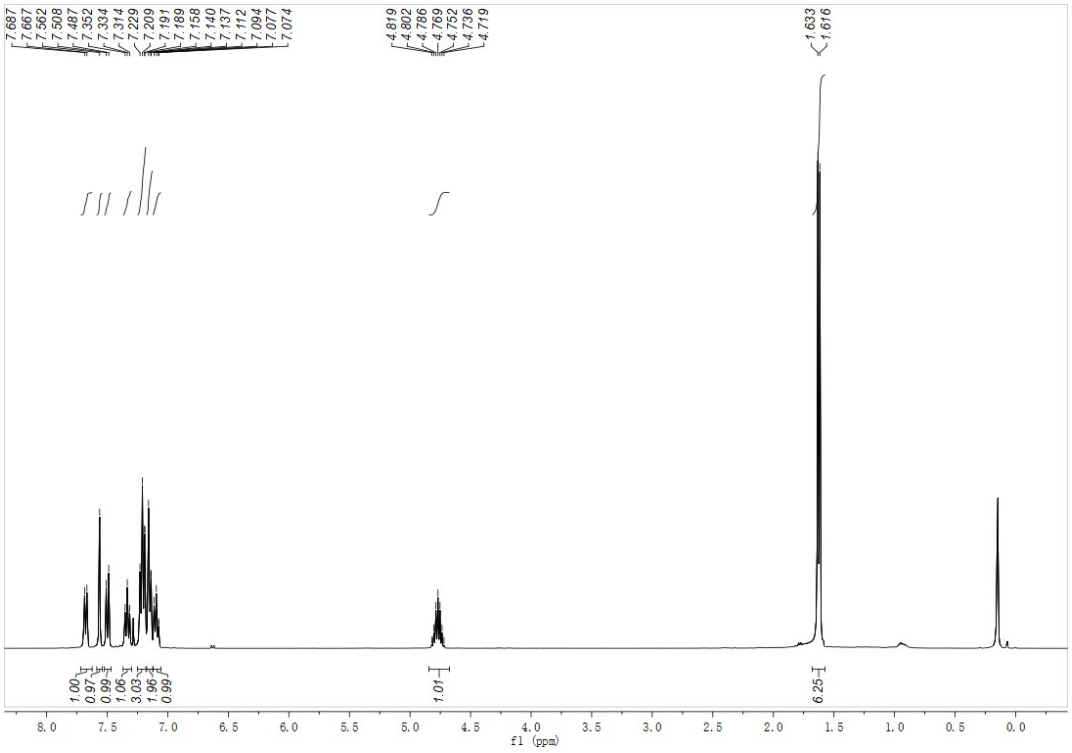
iPr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7.314
7.229
7.209
7.191
7.189
7.158
7.140
7.137
7.112
7.094
7.077
7.074
4.819
4.802
4.786
4.769
4.752
4.736
4.719
1.633
1.616
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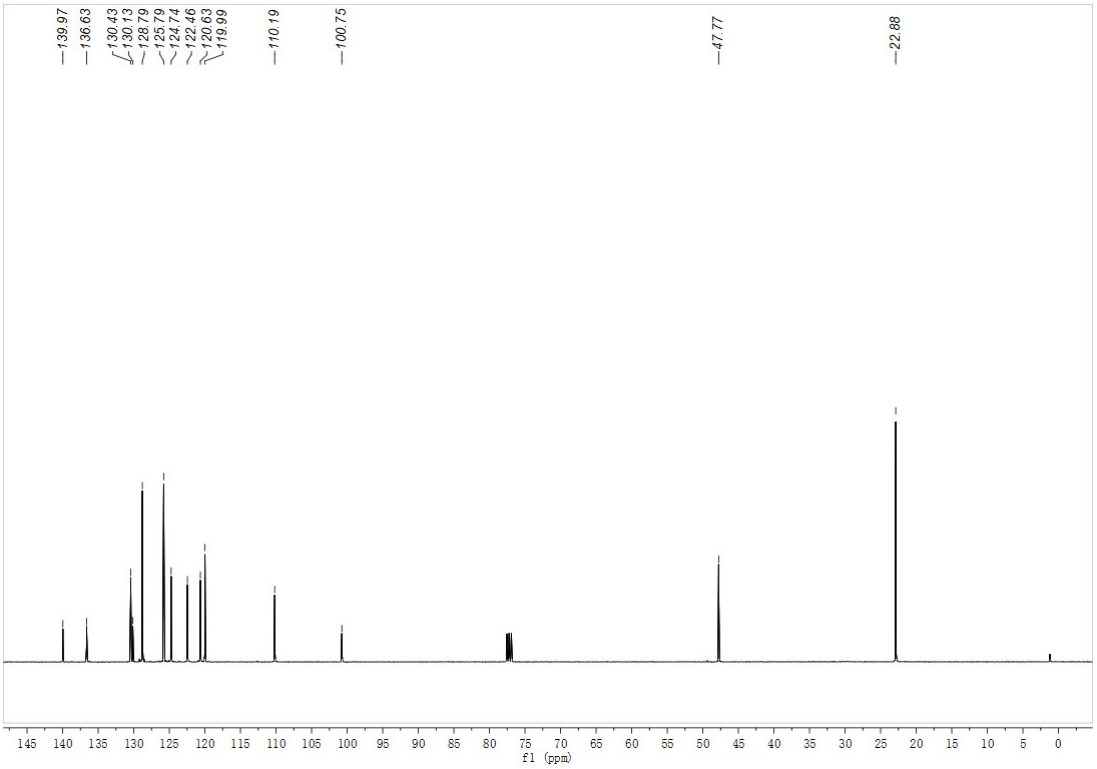
0.97
0.99
1.06
3.03
1.96
0.99
1.01
6.25
f1 (ppm)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128.79
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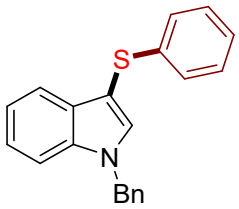
124.74
122.46
120.63
119.99
110.19
100.75
47.77
22.88
f1 (ppm)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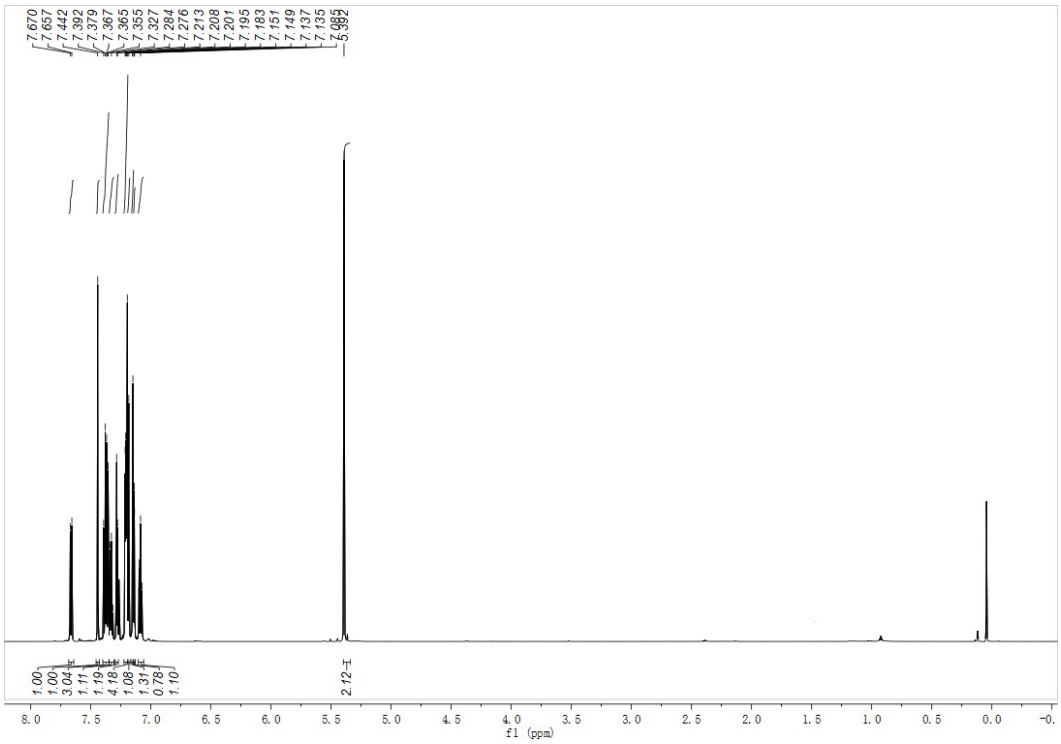
Bn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7.208
7.201
7.195
7.183
7.151
7.149
7.137
7.135
7.085
5.392
1.00
1.00
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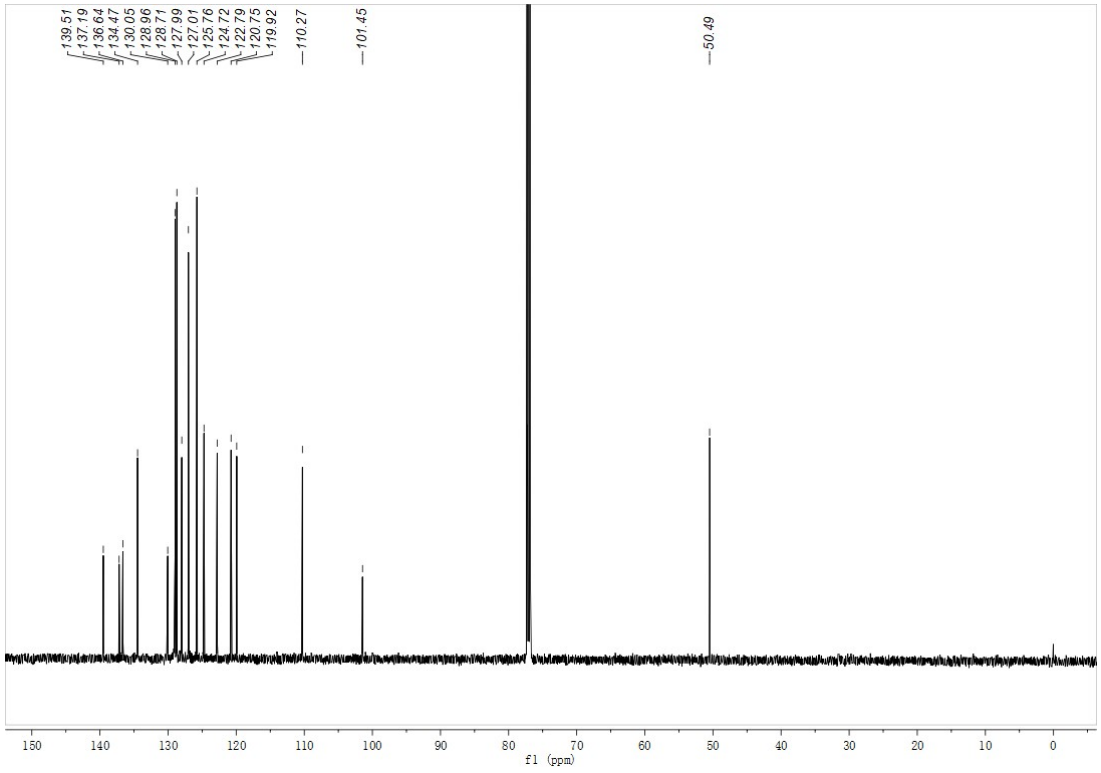
1.11
1.19
4.18
1.08
1.31
0.78
1.10
2.12
f1 (ppm)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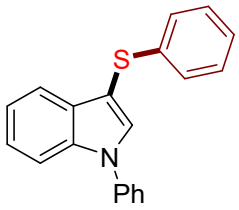
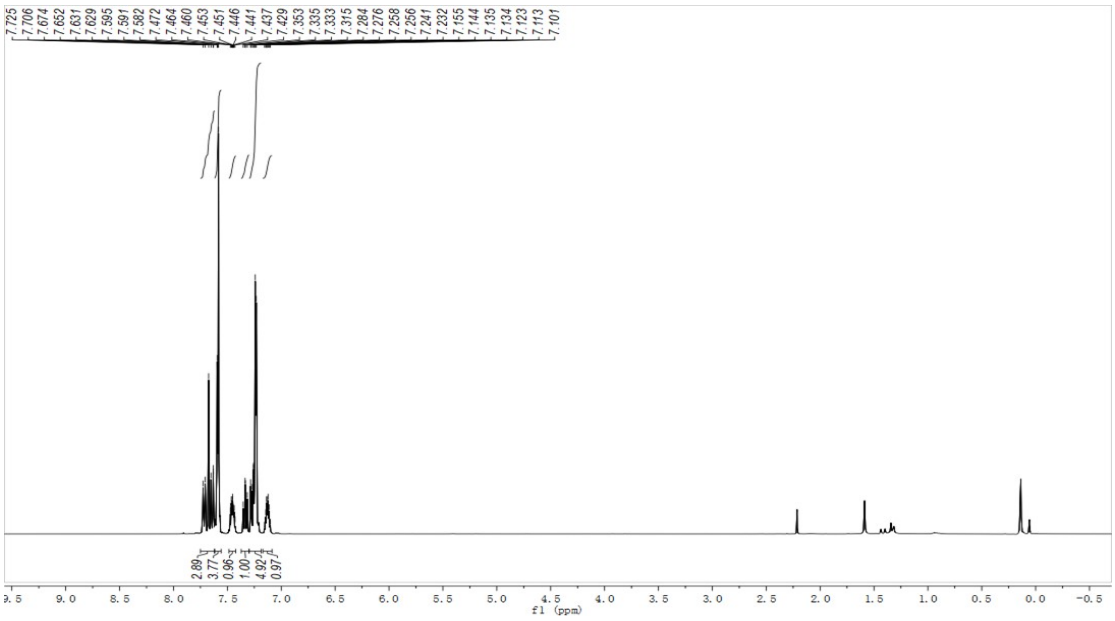
134.47
130.05
128.96
128.71
127.99
127.01
125.76
124.72
122.79
120.75
119.92
110.27
101.45
50.49
f1 (ppm)


S
N
Ph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7.629
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7.591
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7.460
7.453
7.451
7.446
7.441
7.437
7.429
7.353
7.335
7.333
7.315
7.284
7.276
7.258
7.256
7.241
7.232
7.155
7.144
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7.134
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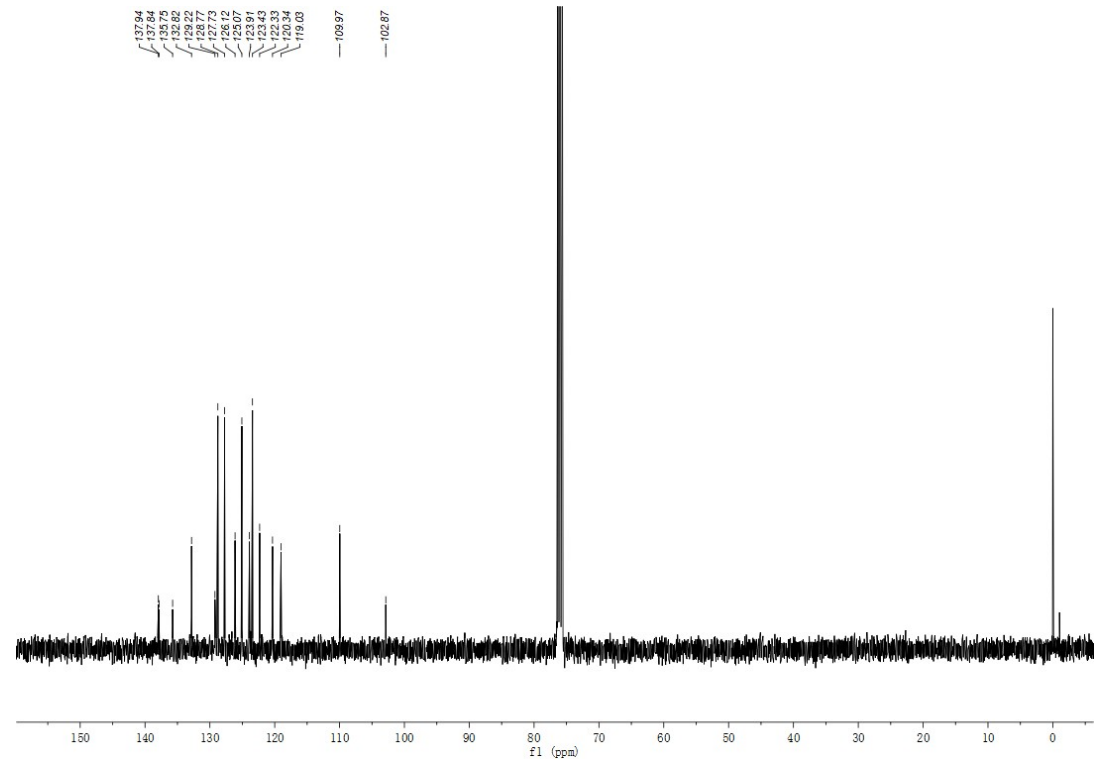
7.113
7.101
2.89
3.77
0.96
1.00
4.92
0.97
f1 (ppm)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126.12
125.97
123.91
123.43
122.33
120.34
119.03
109.97
102.87
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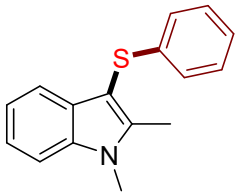
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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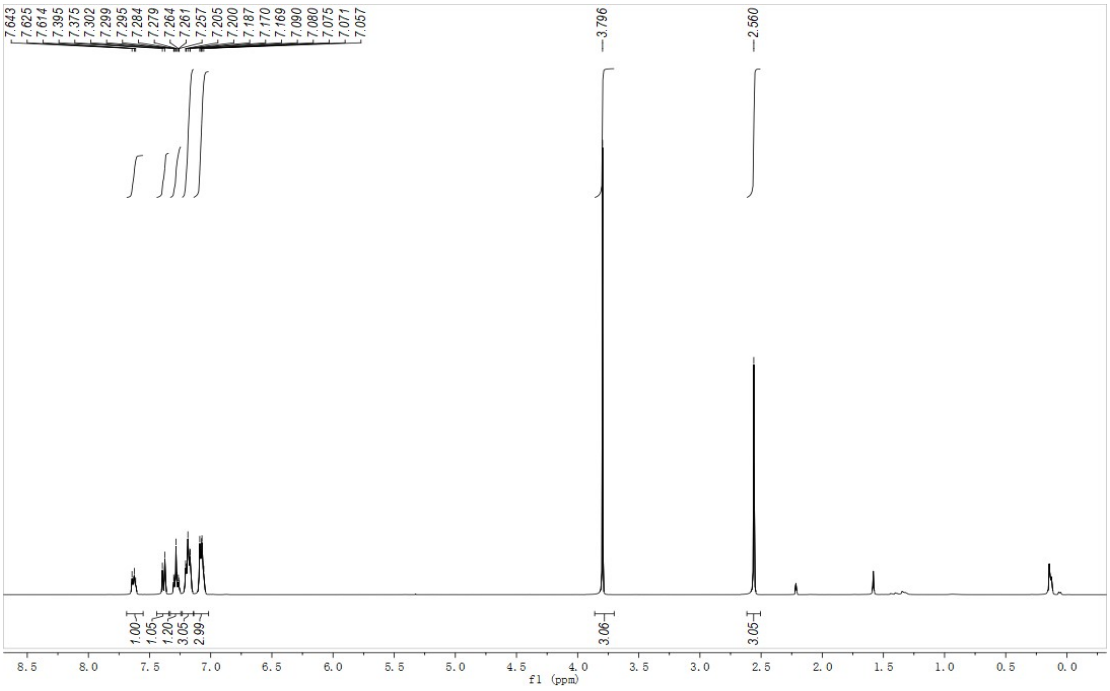
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7.205
7.200
7.187
7.170
7.169
7.090
7.080
7.075
7.071
7.057
3.796
2.560
1.00
1.05
1.20
3.05
2.99
3.06
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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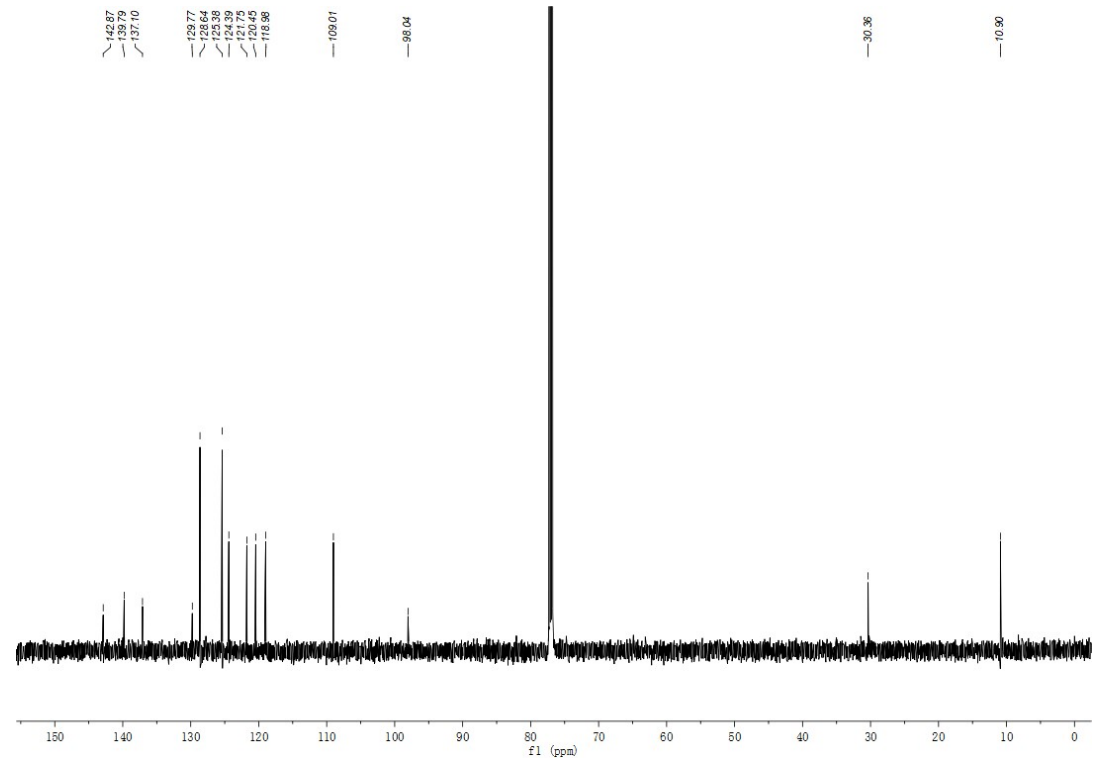
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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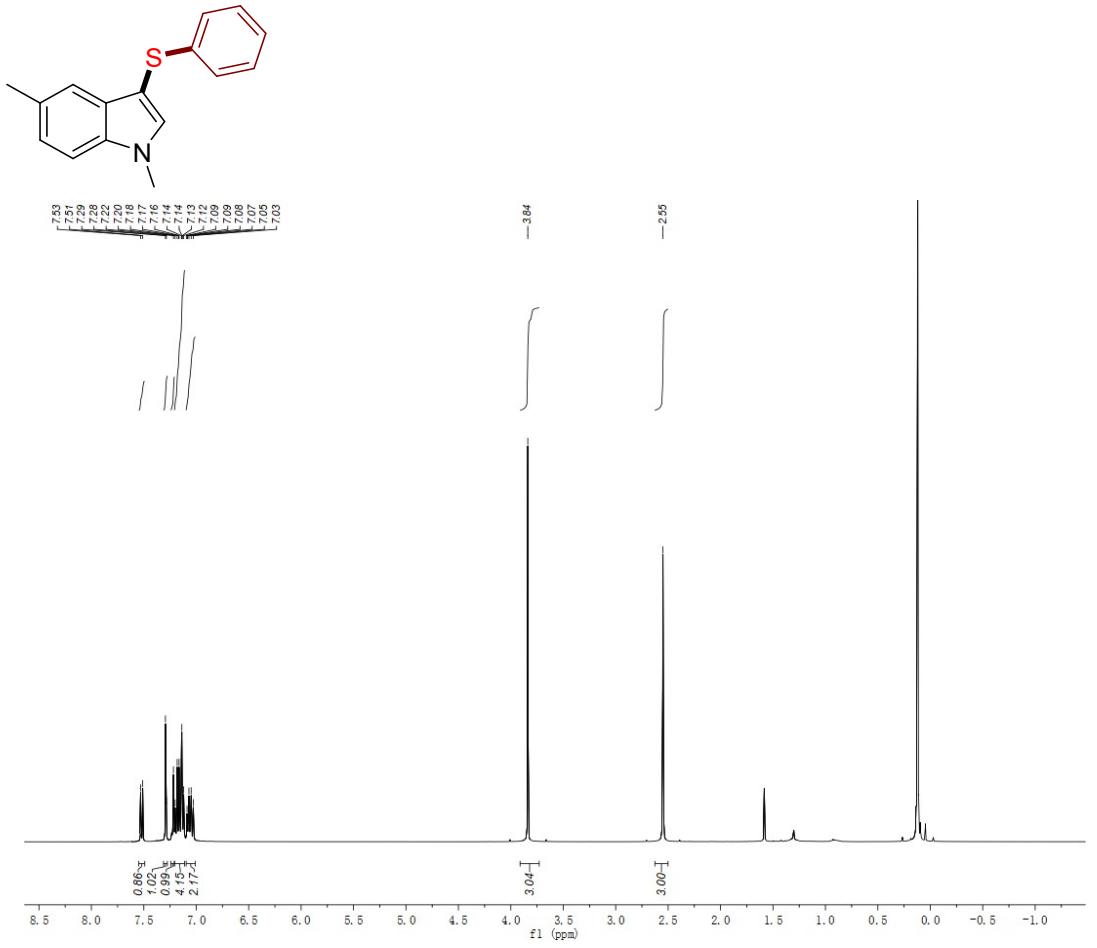
98.04
30.36
10.90
f1 (ppm)


S
N
7.53
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7.18
7.17
7.16
7.14
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7.13
7.12
7.09
7.09
7.08
7.08
7.07
7.07
7.05
7.03
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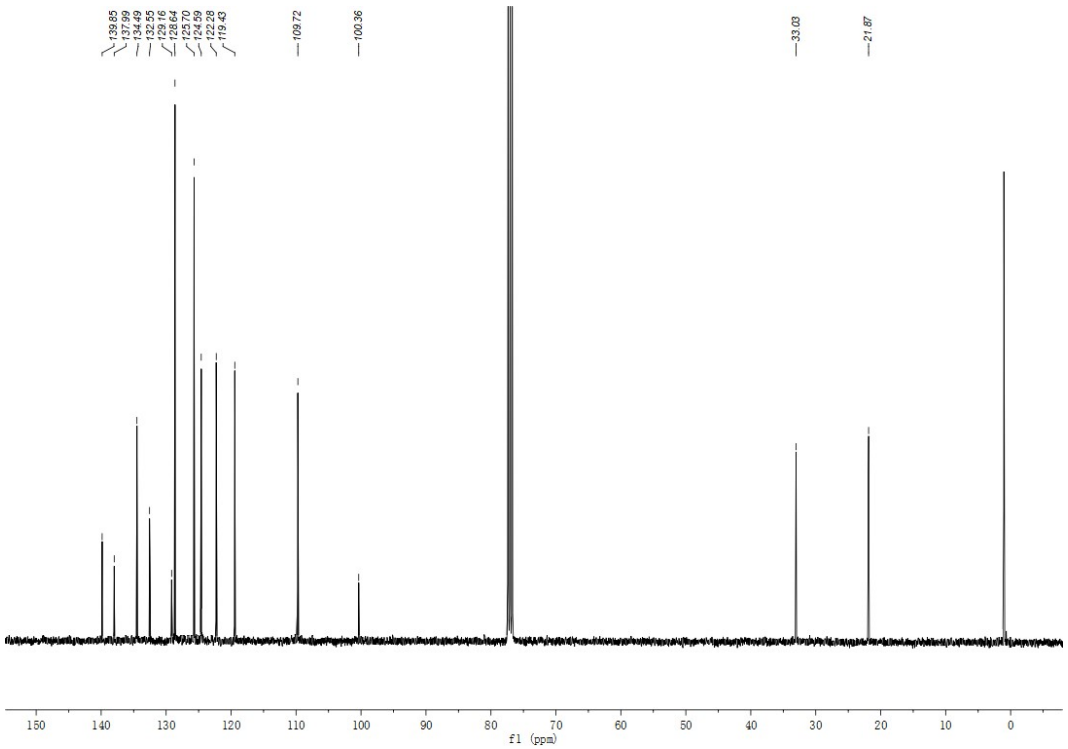
1.02
0.99
4.15
2.17
3.04
3.00
f1 (ppm)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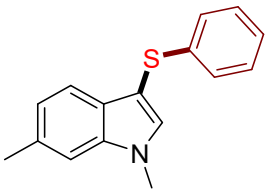
100.36
33.03
21.87
f1 (ppm)


S
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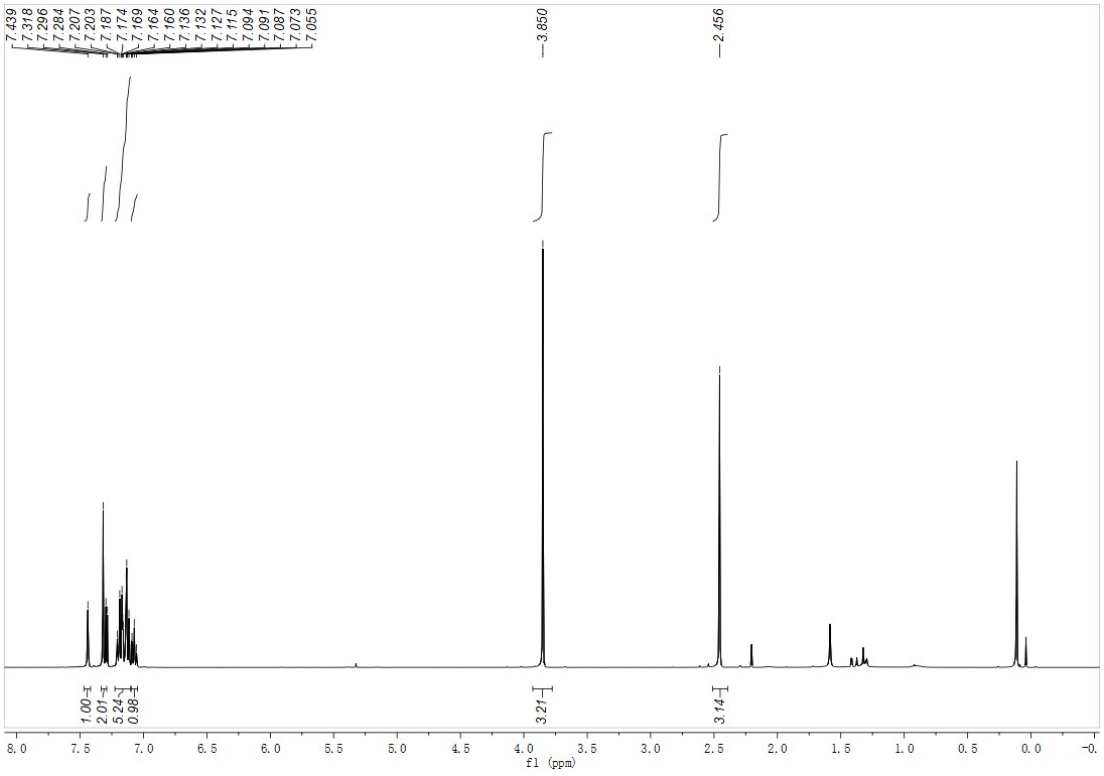
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7.164
7.160
7.136
7.132
7.127
7.115
7.094
7.091
7.087
7.073
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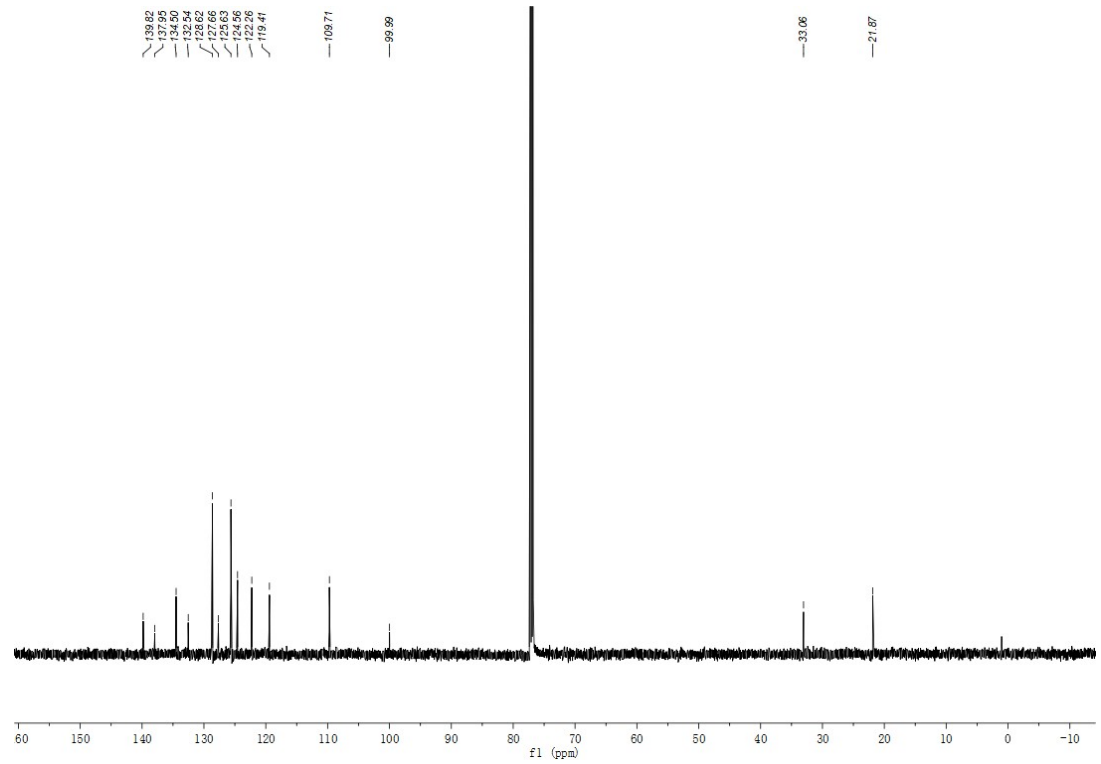
3.21
3.14
f1 (ppm)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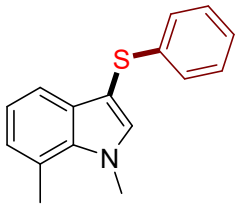
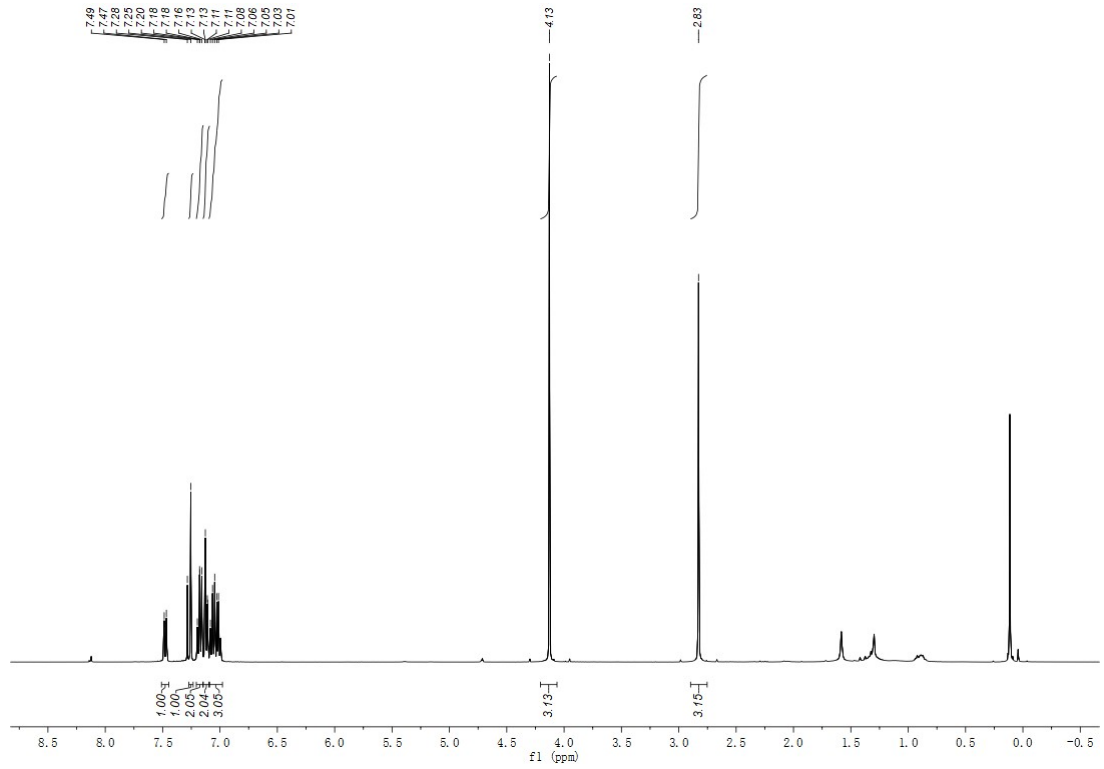
21.87
f1 (ppm)


S
N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7.13
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7.11
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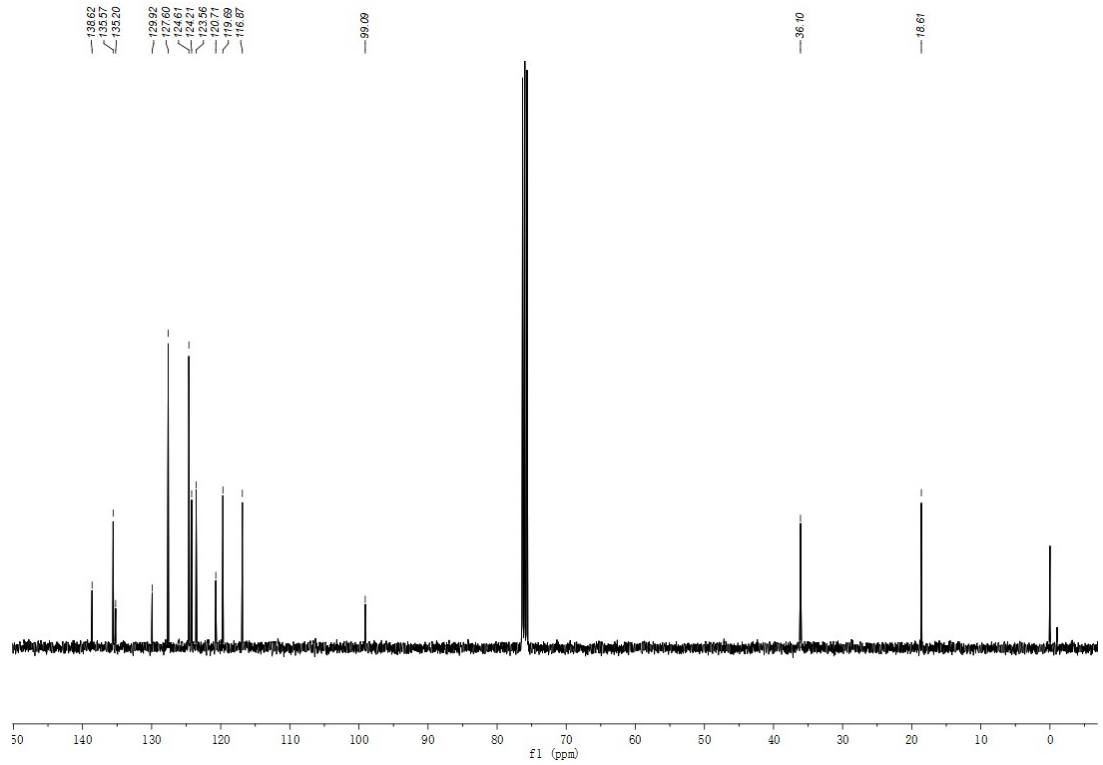
7.06
7.05
7.03
7.01
4.13
2.83
1.00
1.00
2.05
2.04
3.05
3.13
3.15
f1 (ppm)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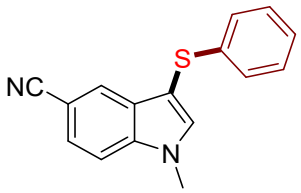
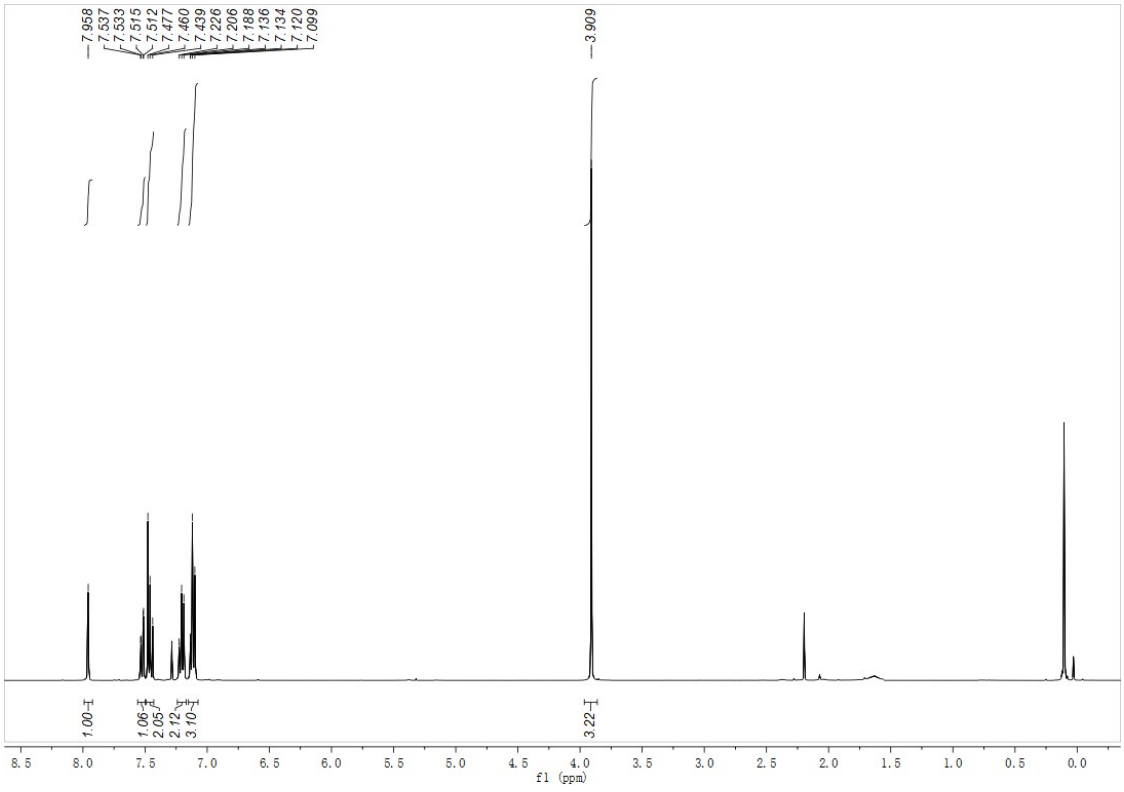
124.21
123.56
120.71
119.69
116.87
99.09
36.10
18.61
f1 (ppm)


S
NC
N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7.439
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7.206
7.188
7.136
7.134
7.120
7.099
3.909
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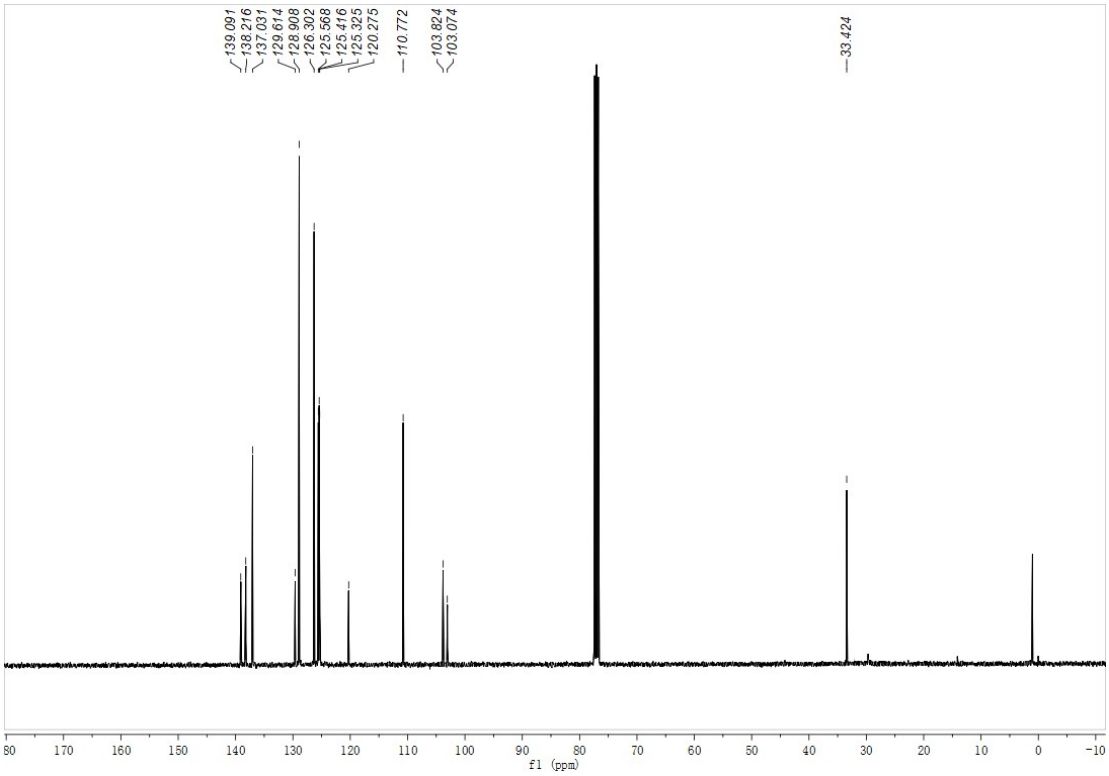
1.06
2.05
2.12
3.10
3.22
f1 (ppm)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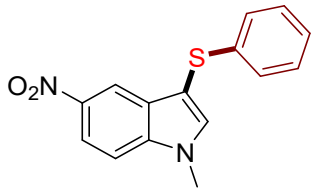
125.416
125.325
120.275
110.772
103.824
103.074
33.424
f1 (ppm)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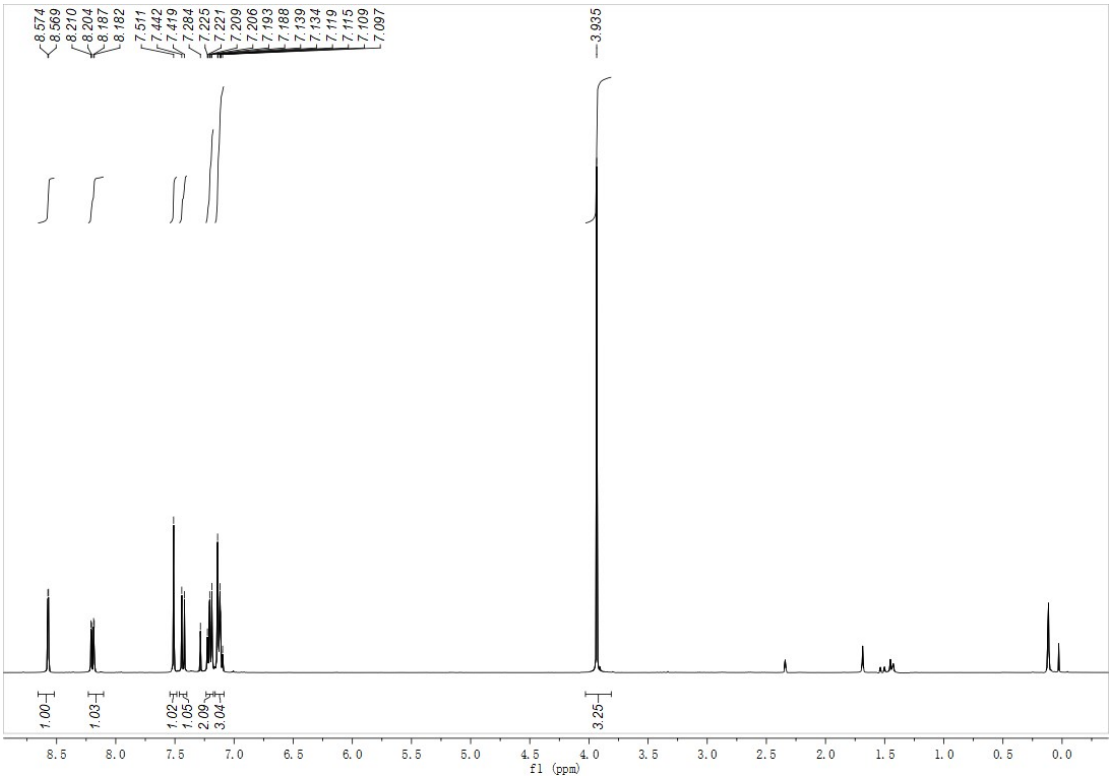
O2N
N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7.442
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7.284
7.225
7.221
7.209
7.206
7.193
7.188
7.139
7.134
7.119
7.115
7.109
7.097
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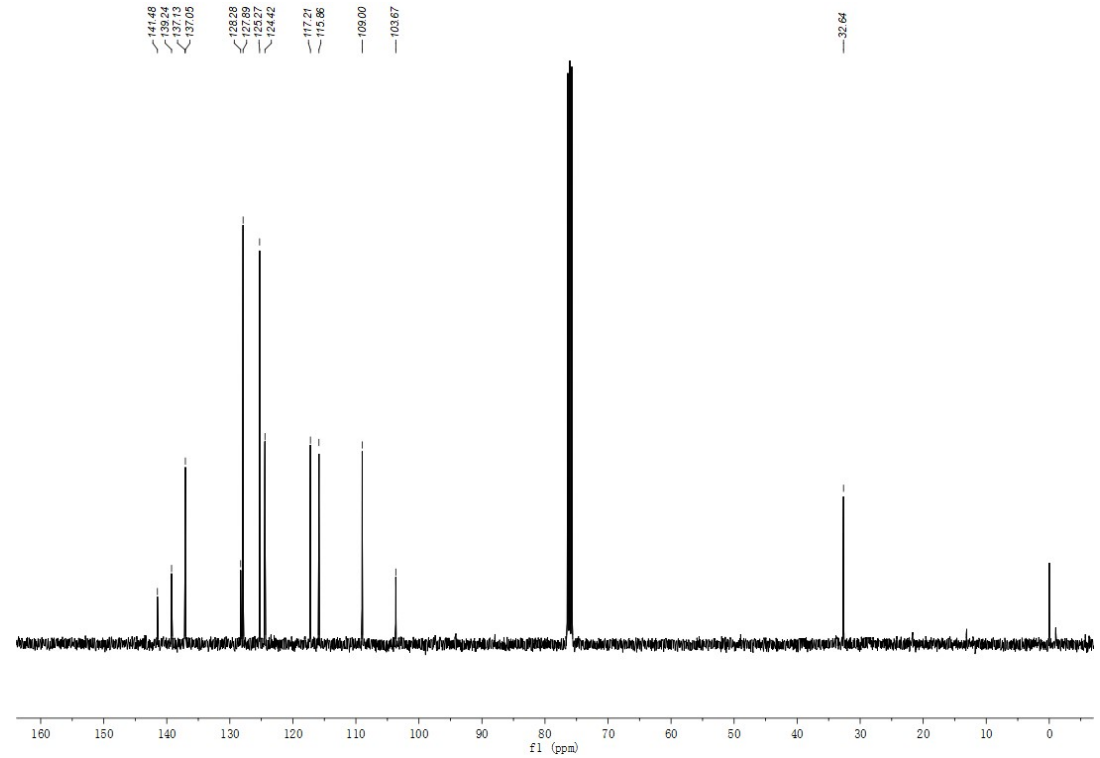
1.03
1.02
1.05
2.09
3.04
3.25
f1 (ppm)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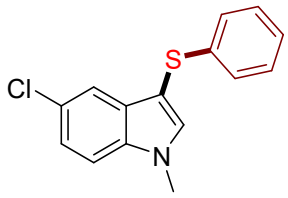
124.42
117.21
115.86
109.00
103.67
32.64
f1 (ppm)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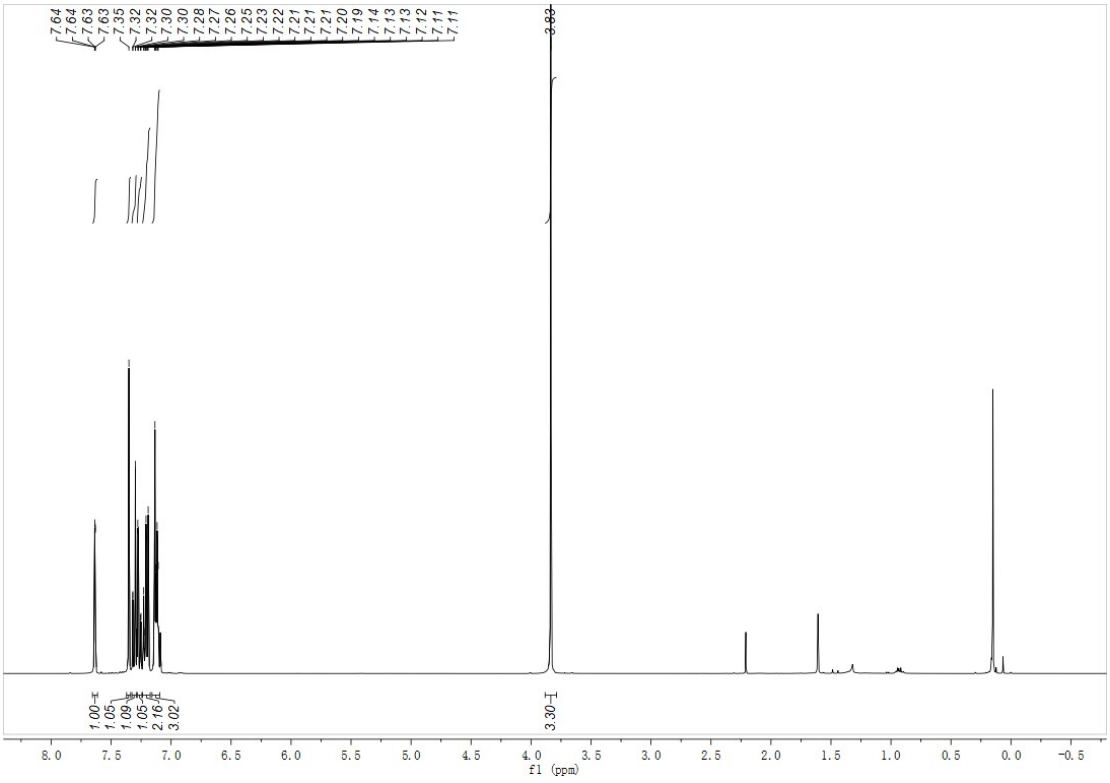
Cl
N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7.25
7.23
7.22
7.21
7.21
7.21
7.20
7.19
7.14
7.13
7.13
7.12
7.11
7.11
3.83
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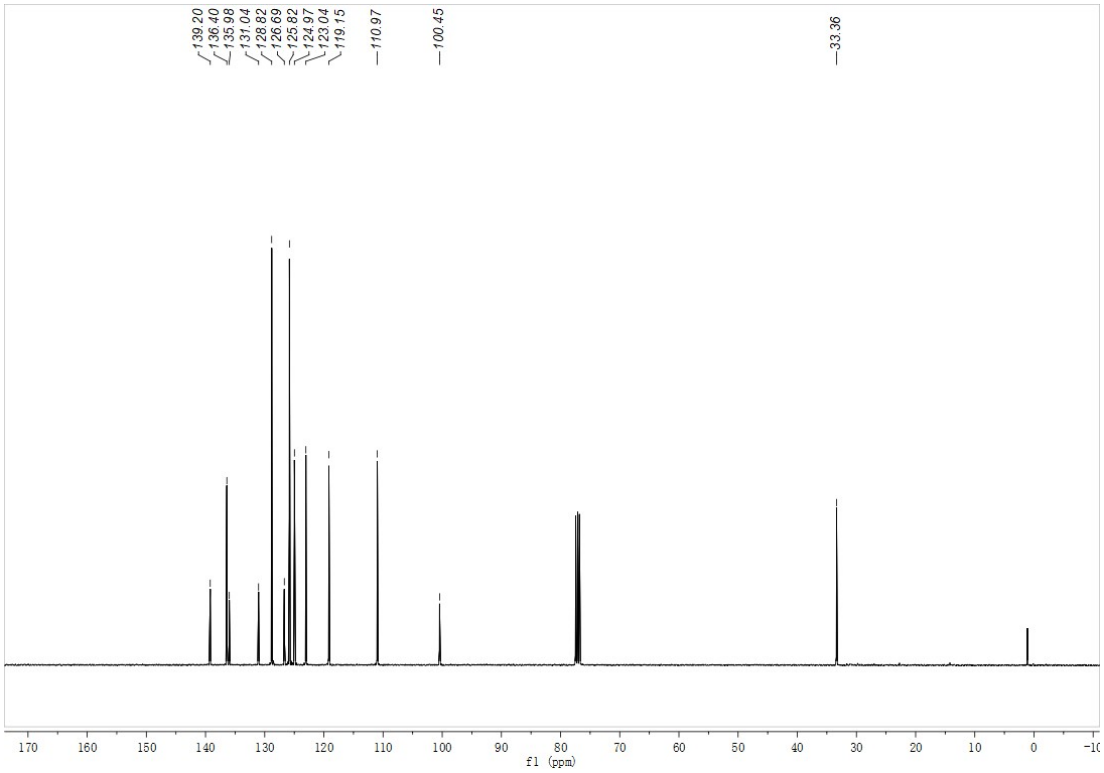
1.05
1.09
1.05
2.16
3.02
3.30
f1 (ppm)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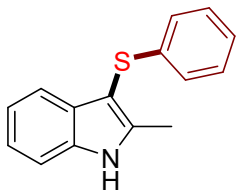
f1 (ppm)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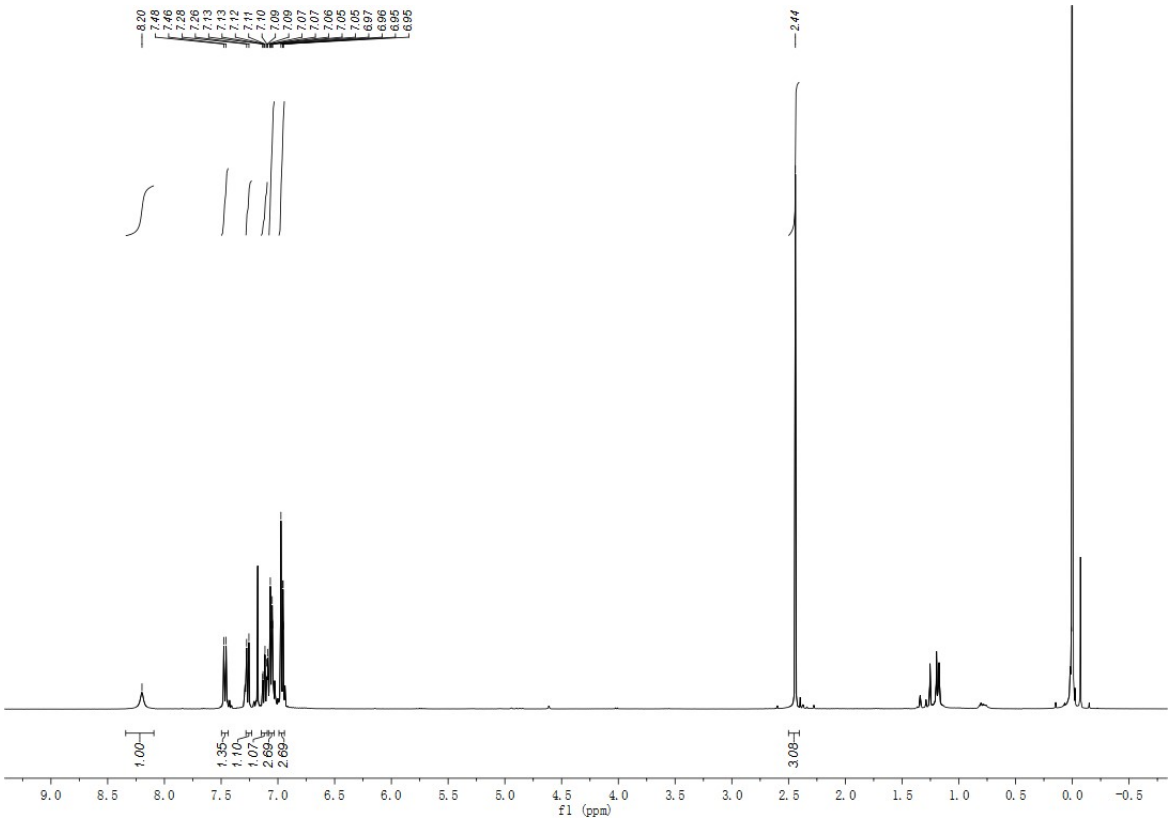
H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7.12
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7.09
7.09
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7.05
7.05
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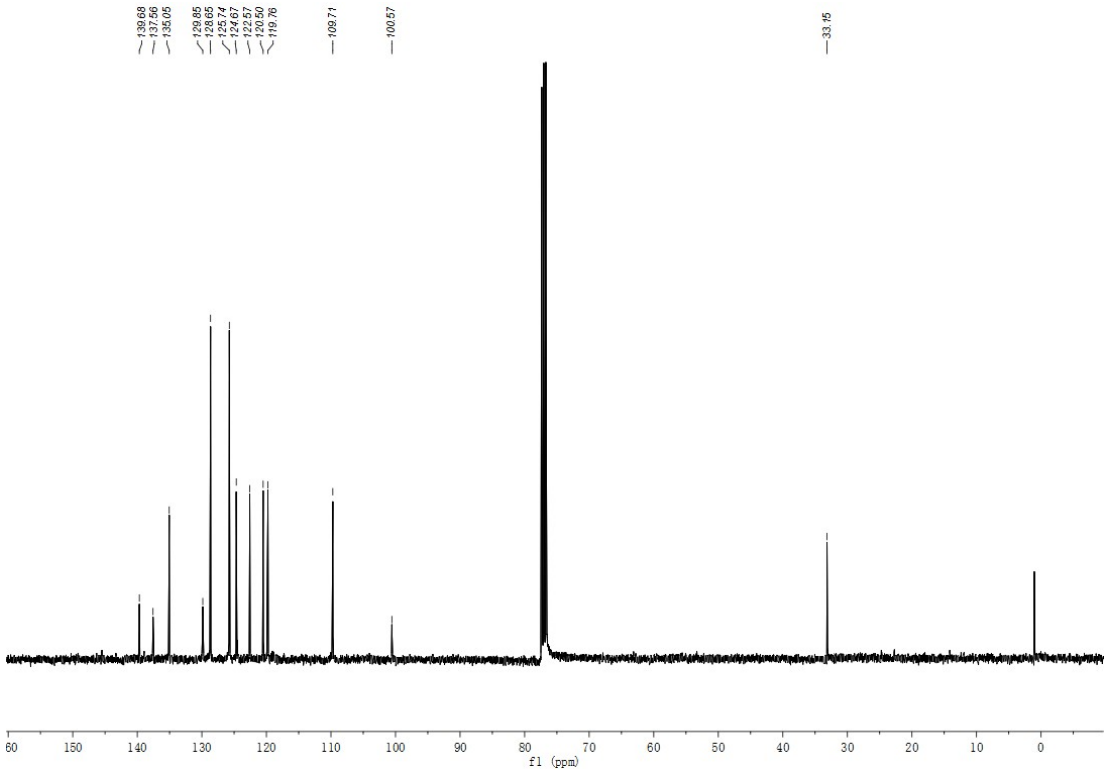
1.07
2.69
2.69
3.08
f1 (ppm)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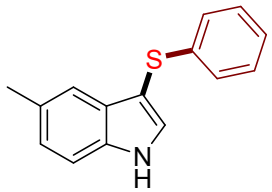
119.76
109.71
100.57
33.15
f1 (ppm)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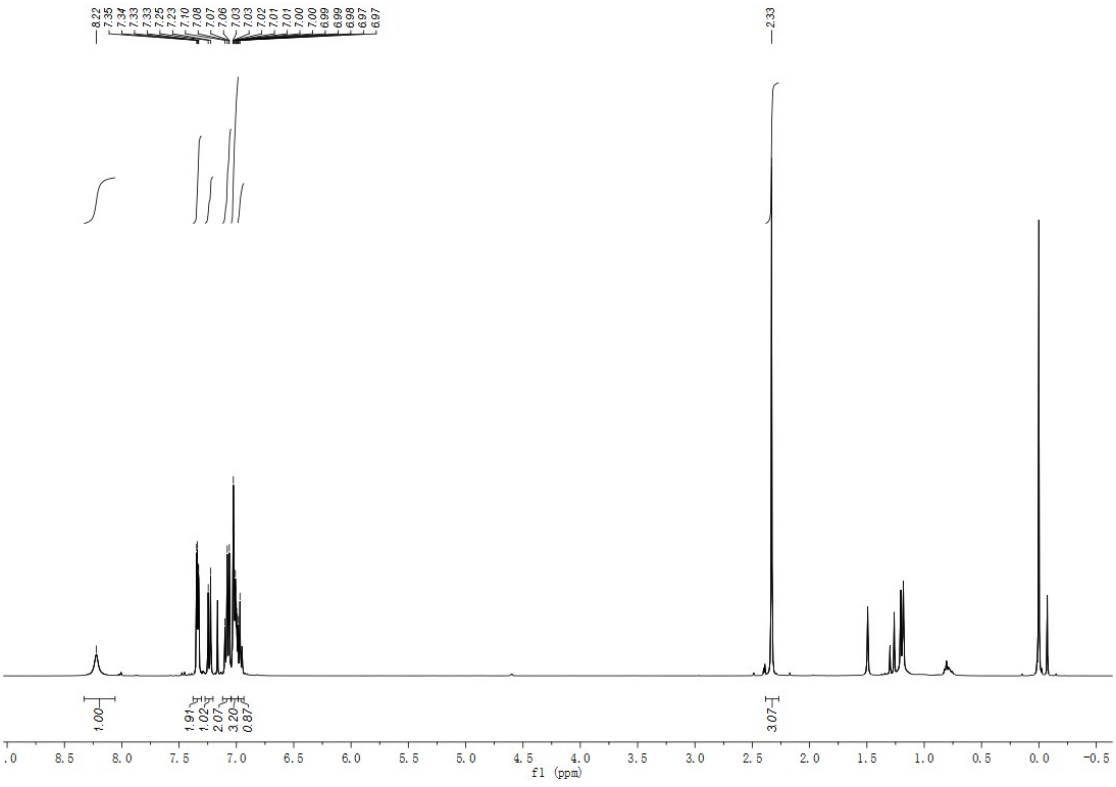
N
H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7.23
7.10
7.08
7.07
7.06
7.03
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7.01
7.00
7.00
6.99
6.99
6.98
6.97
6.97
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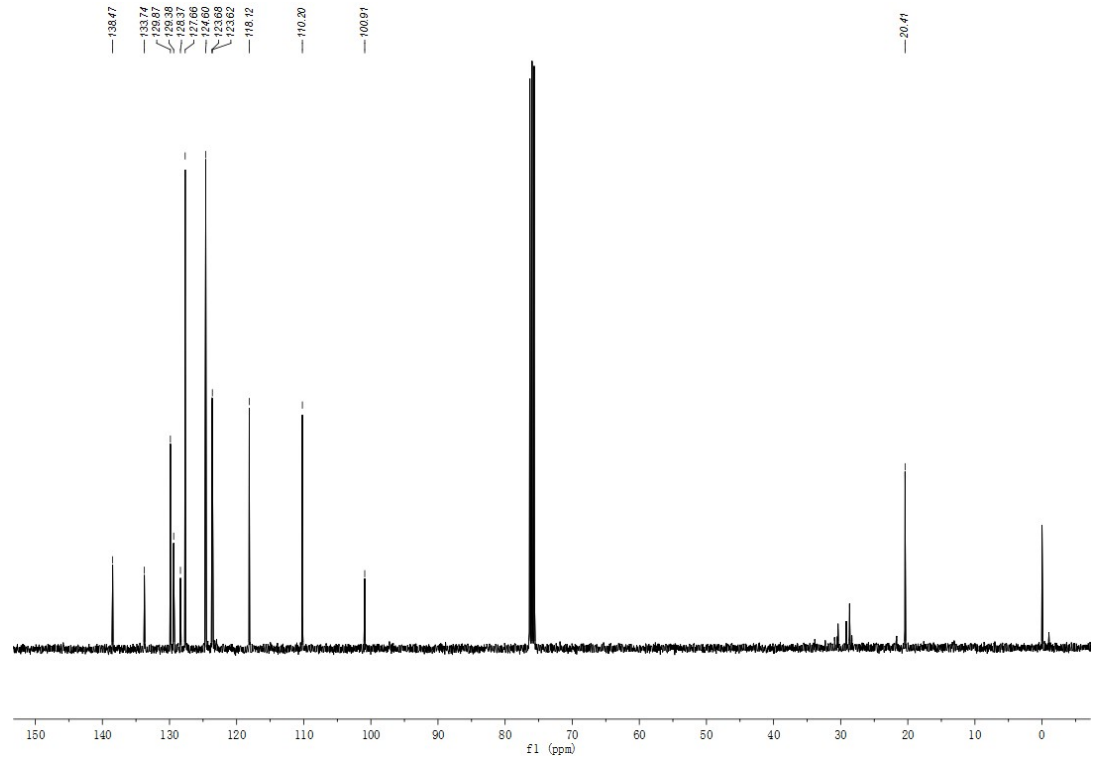
1.00
1.91
1.02
2.07
3.20
0.87
3.07
f1 (ppm)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123.68
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100.91
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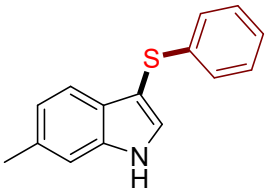
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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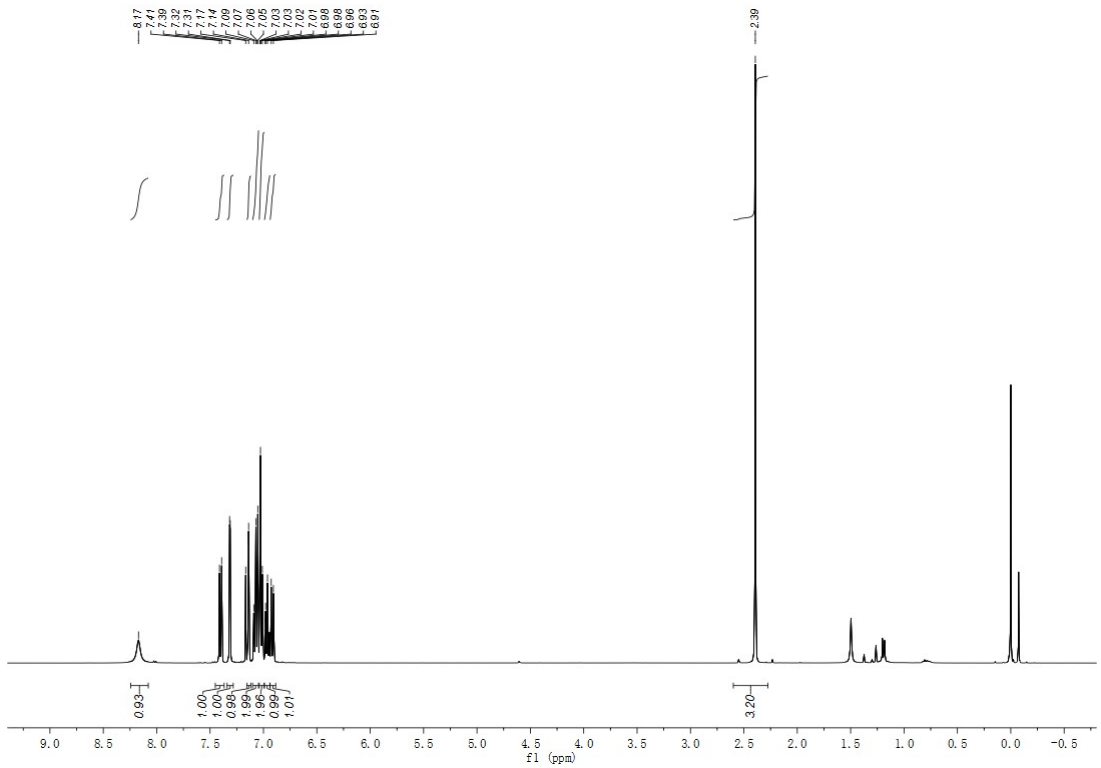
N
H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7.17
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7.09
7.07
7.06
7.05
7.03
7.03
7.02
7.01
6.98
6.98
6.96
6.93
6.91
2.39
0.93
1.00
1.00
0.98
1.99
1.96
0.99
1.01
3.20
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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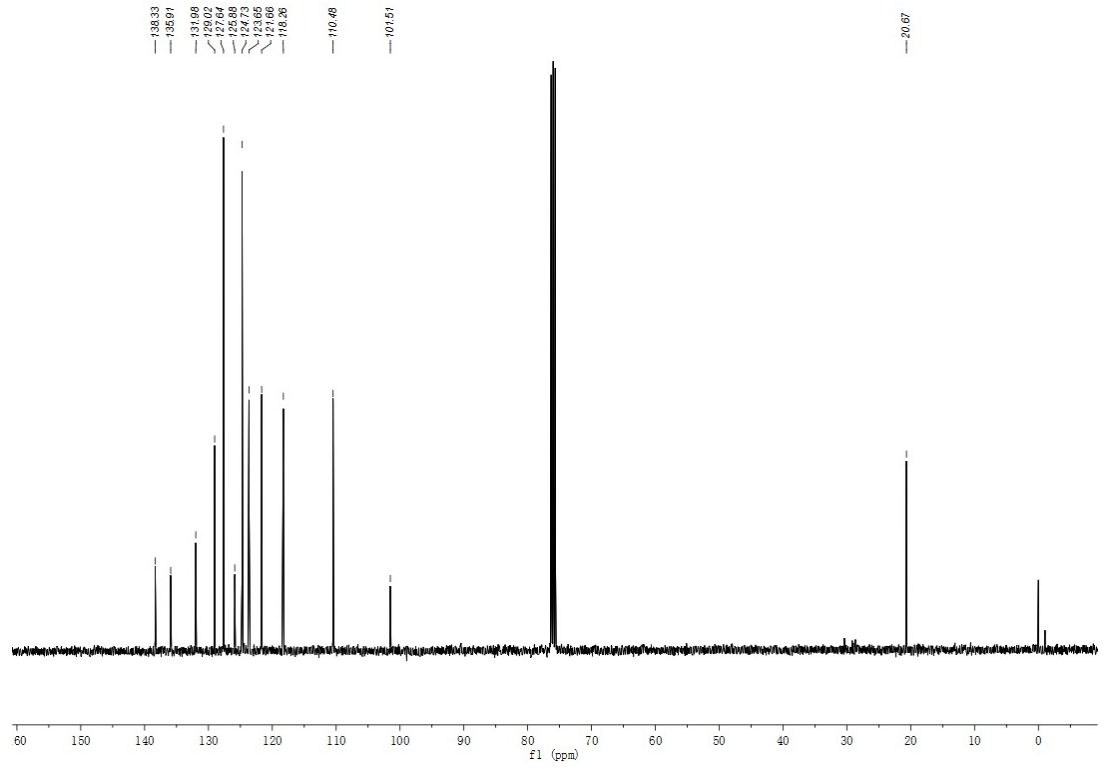
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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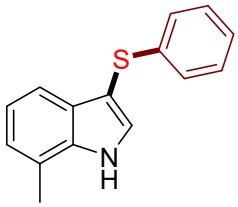
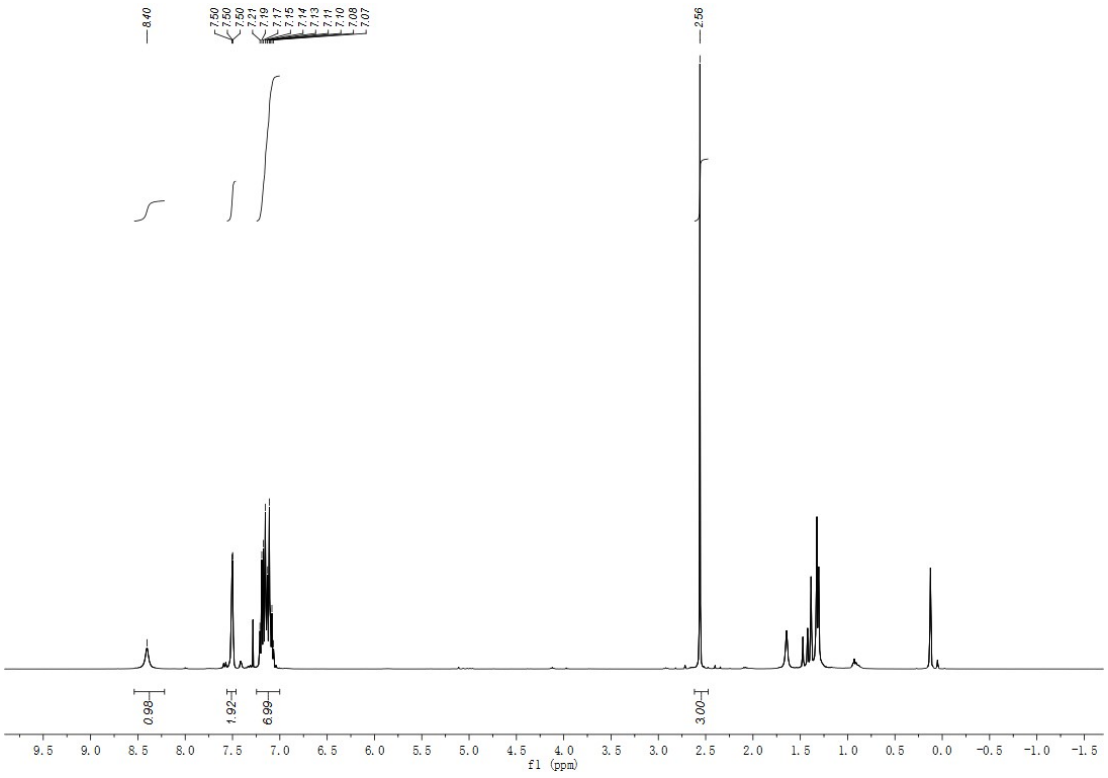
123.65
121.66
118.26
110.48
101.51
20.67
f1 (ppm)


S
N
H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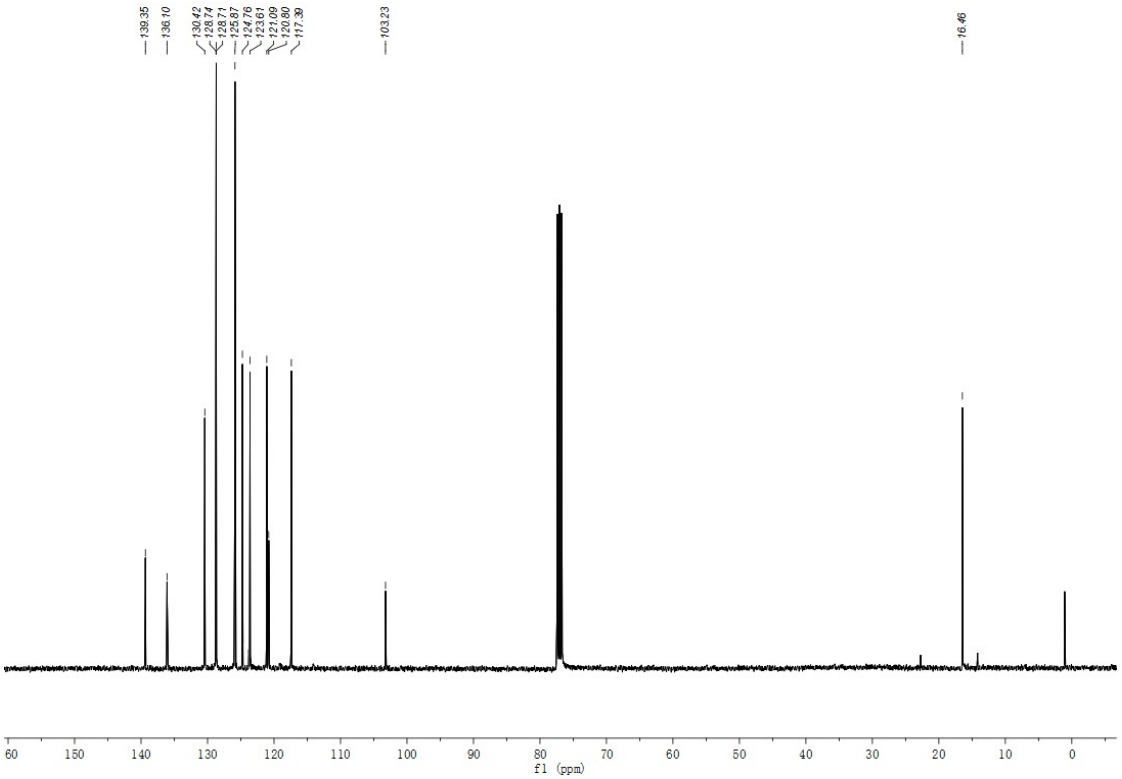
7.10
7.08
7.07
2.56
0.98
1.92
6.99
3.00
f1 (ppm)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121.09
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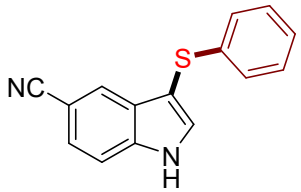
117.39
103.23
16.46
f1 (ppm)


S
NC
N
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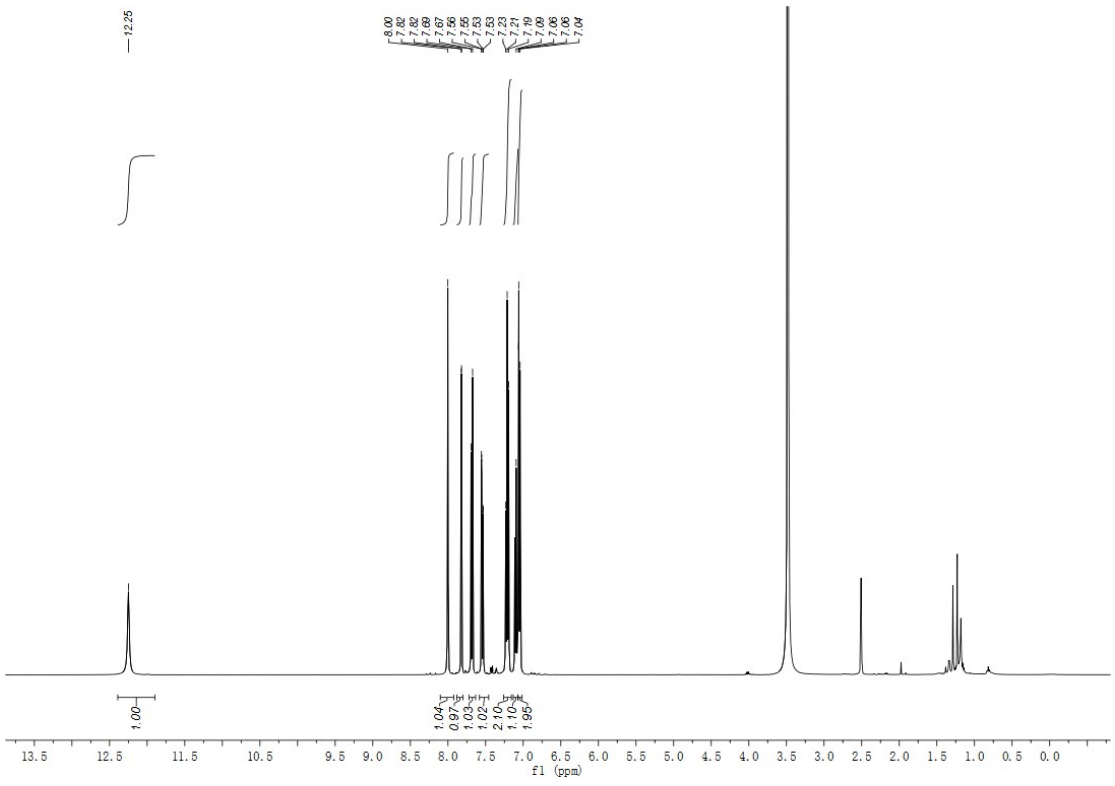
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7.53
7.23
7.21
7.19
7.09
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7.06
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1.03
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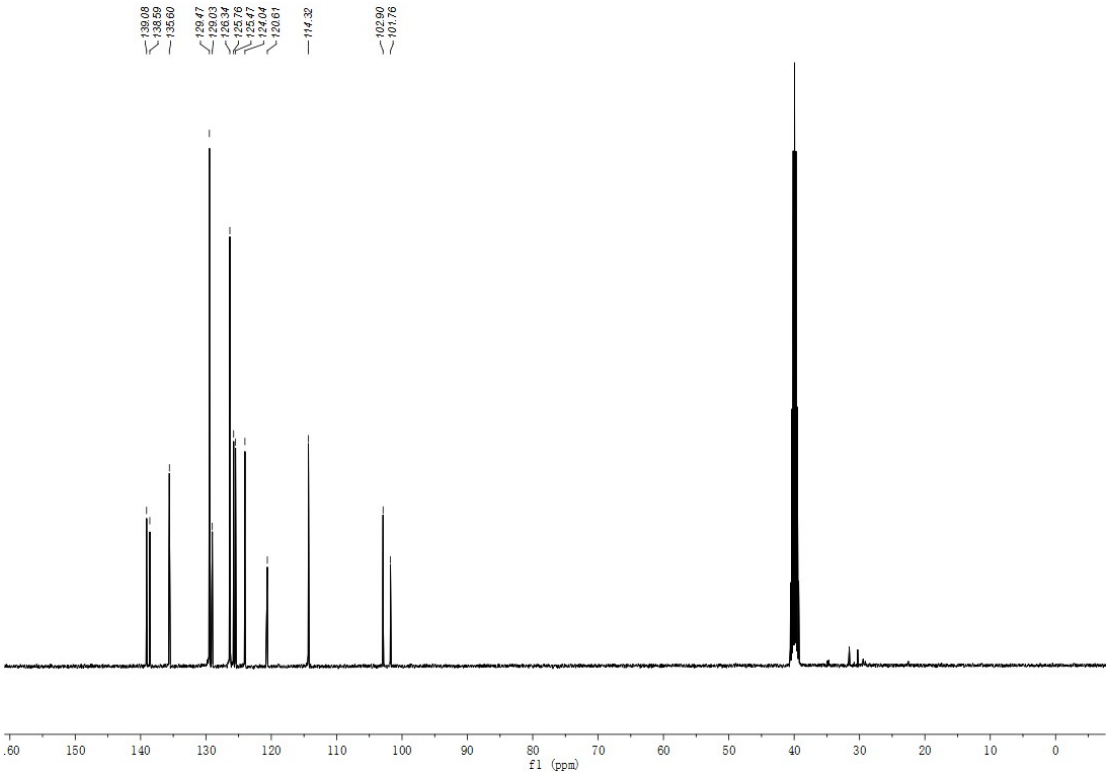
2.10
1.10
1.95
f1 (ppm)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125.47
124.04
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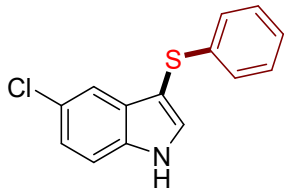
114.32
102.90
101.76
f1 (ppm)


Cl
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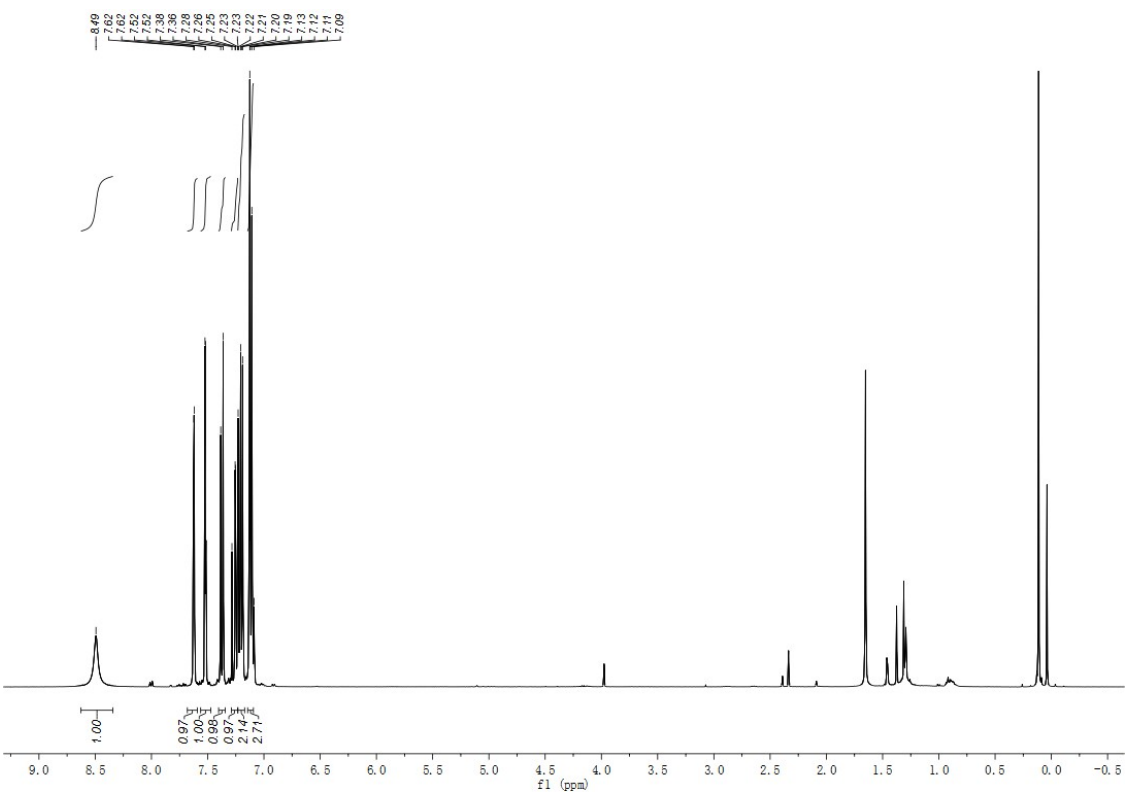
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7.21
7.20
7.19
7.13
7.12
7.11
7.09
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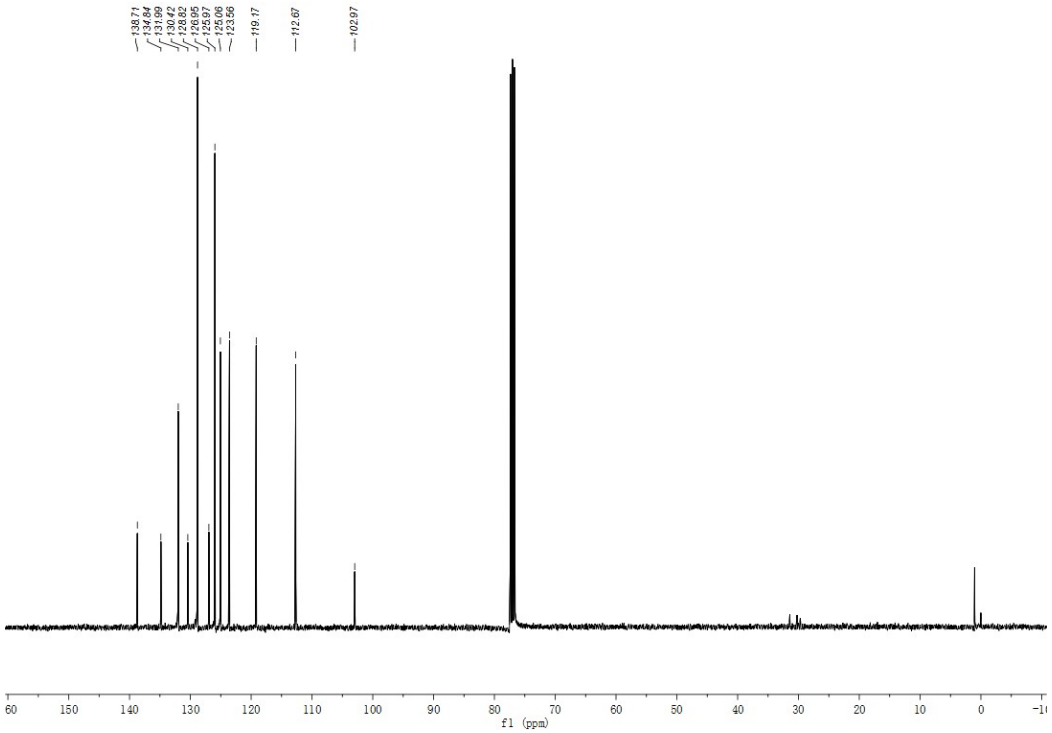
0.97
1.00
0.98
0.97
2.14
2.71
f1 (ppm)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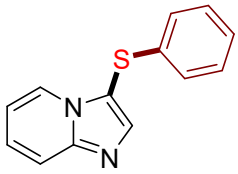
125.06
123.56
119.17
112.67
102.97
f1 (ppm)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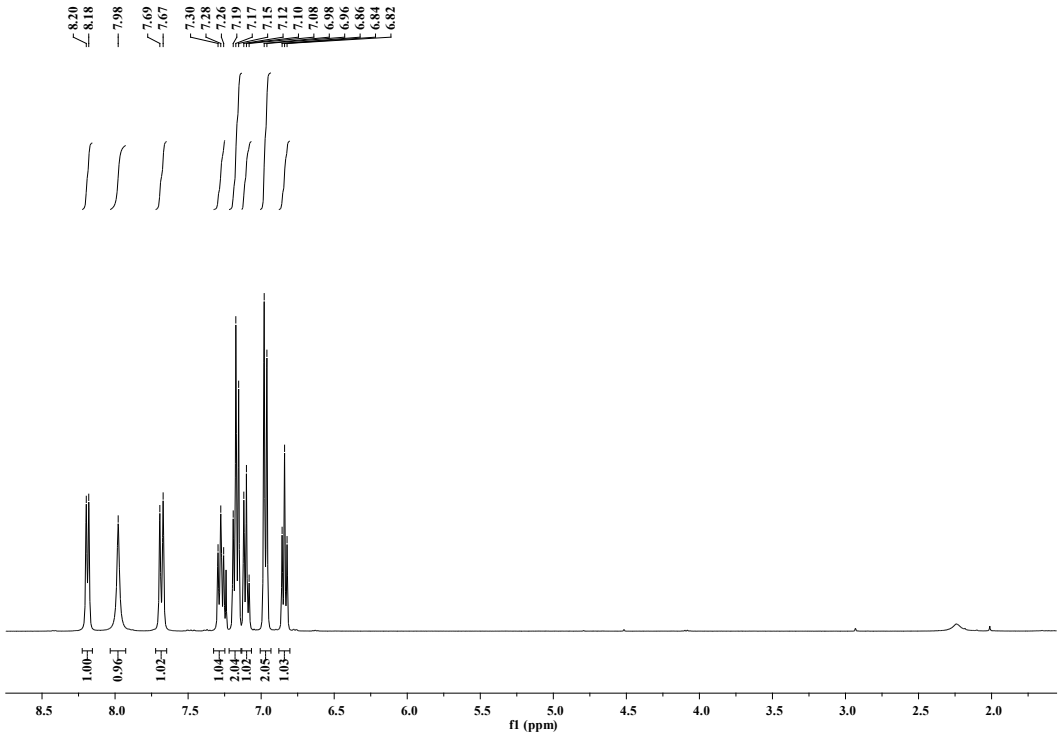
N
N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7.19
7.17
7.15
7.12
7.10
7.08
6.98
6.96
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1.00
0.96
1.02
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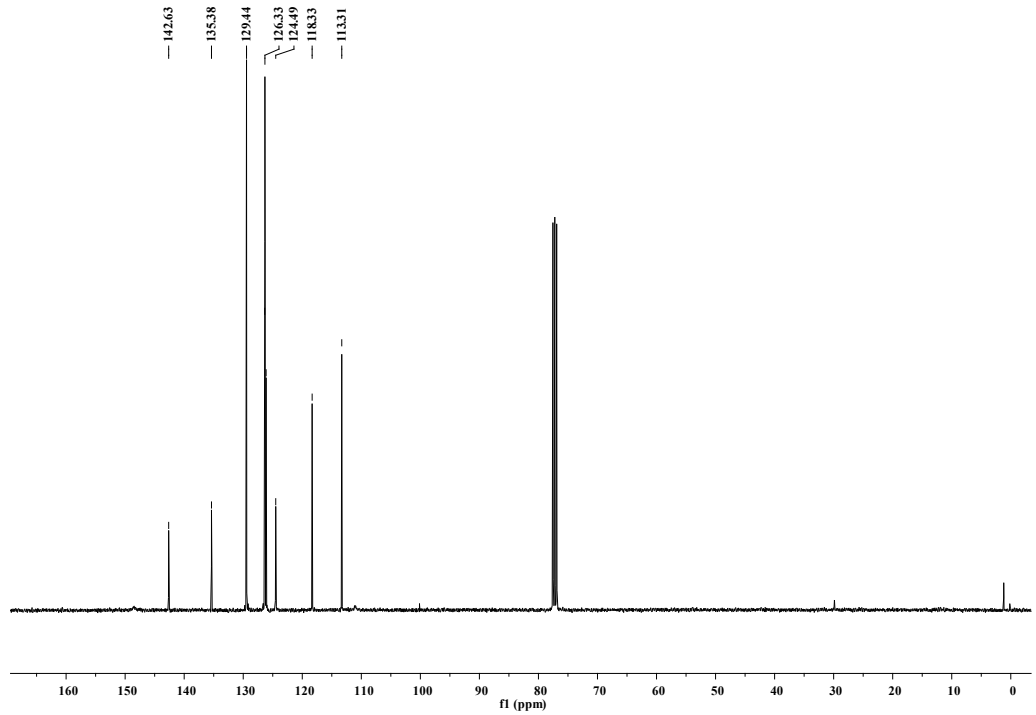
2.04
1.02
2.05
1.03
f1 (ppm)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10
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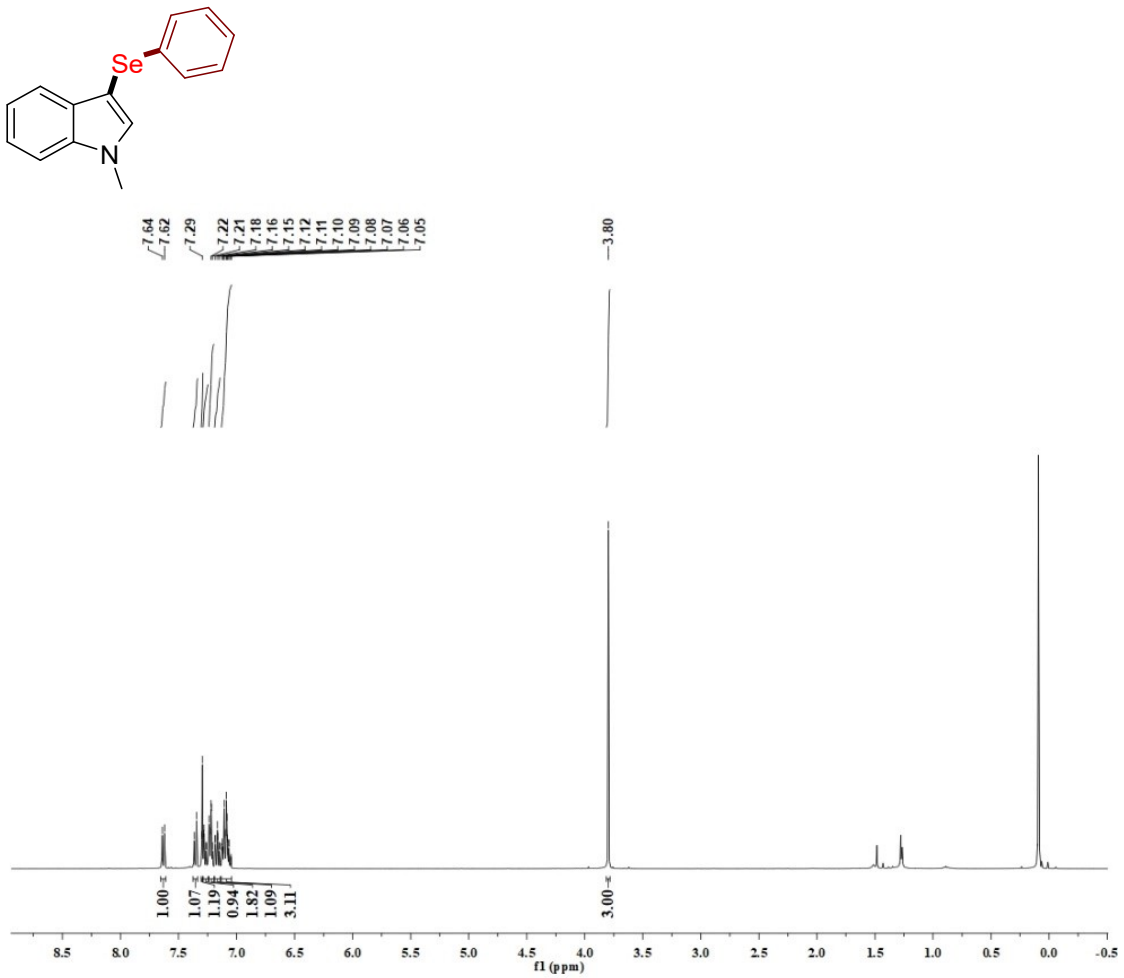
f1 (ppm)


Se
N
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7.12
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7.10
7.09
7.08
7.07
7.06
7.05
3.80
1.00
1.07
1.19
0.94
1.82
1.09
3.11
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
2.5
2.0
1.5
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0.5
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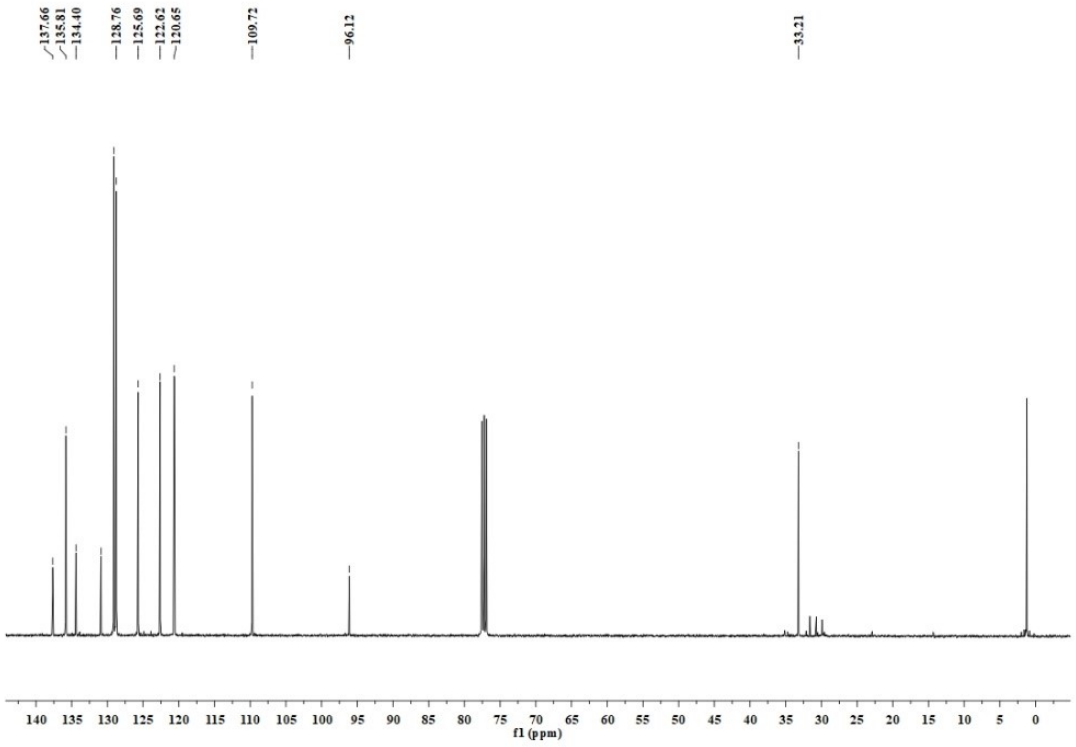
-0.5
f1 (ppm)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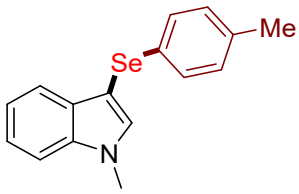
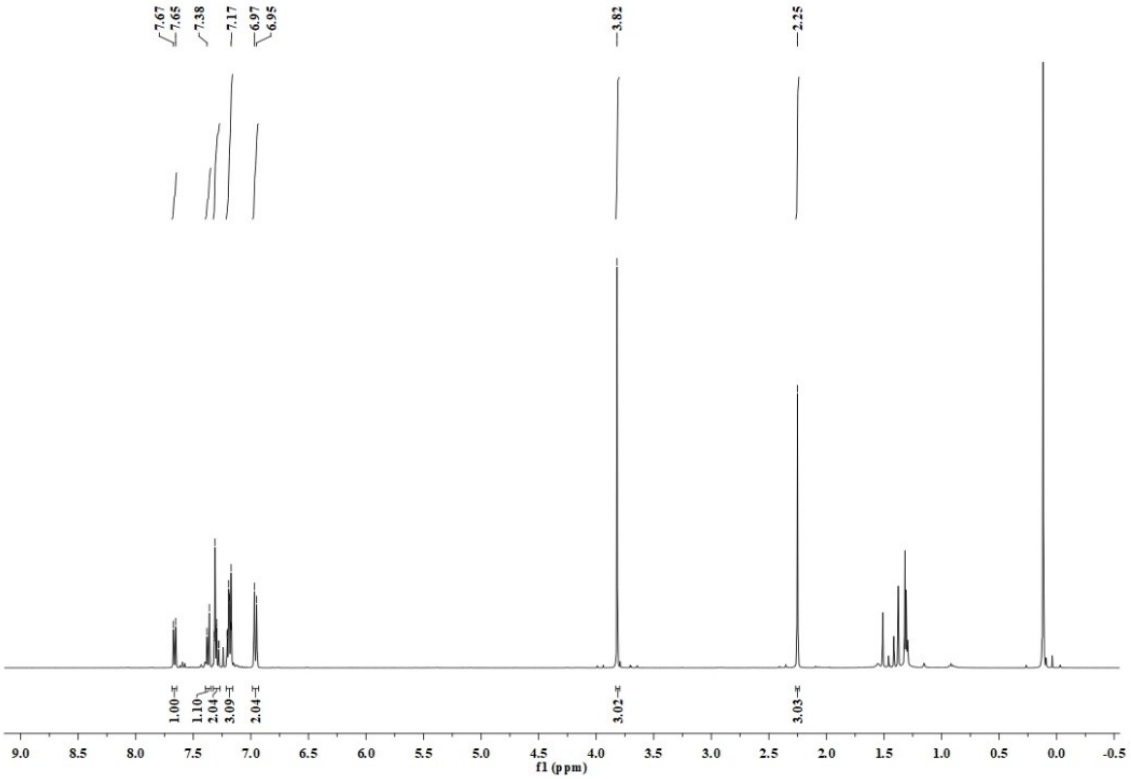
96.12
33.21
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Me
Se
N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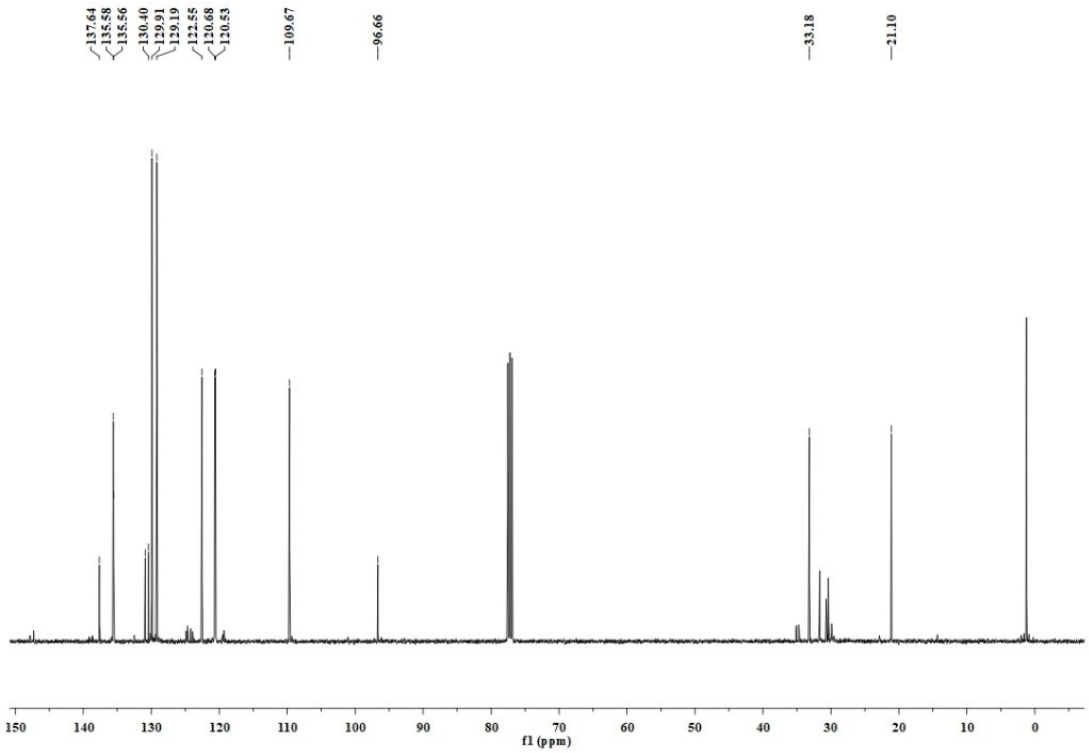
7.17
6.97
6.95
3.82
2.25
1.00
1.10
2.04
3.09
2.04
3.02
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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120.53
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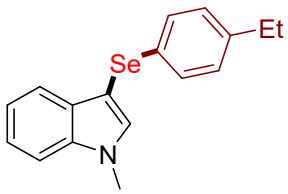
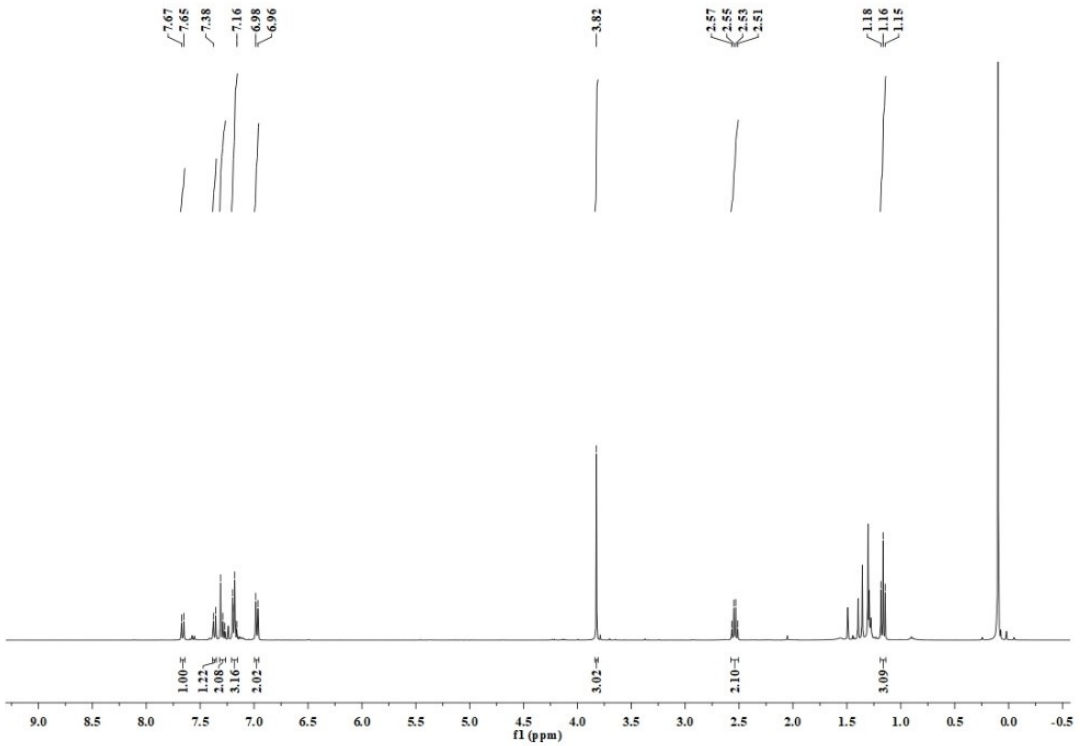
96.66
33.18
21.10
f1 (ppm)


Et
Se
N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6.96
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2.51
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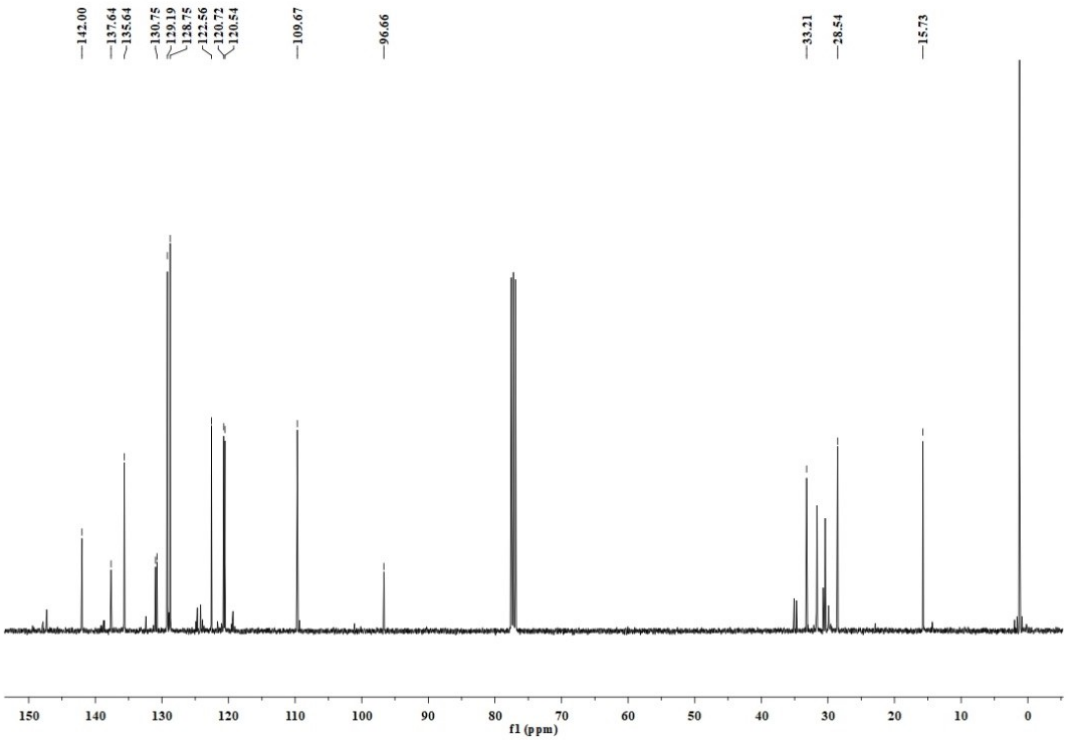
1.15
1.00
1.22
2.08
3.16
2.02
3.02
2.10
3.09
f1 (ppm)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135.64
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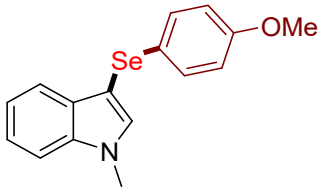
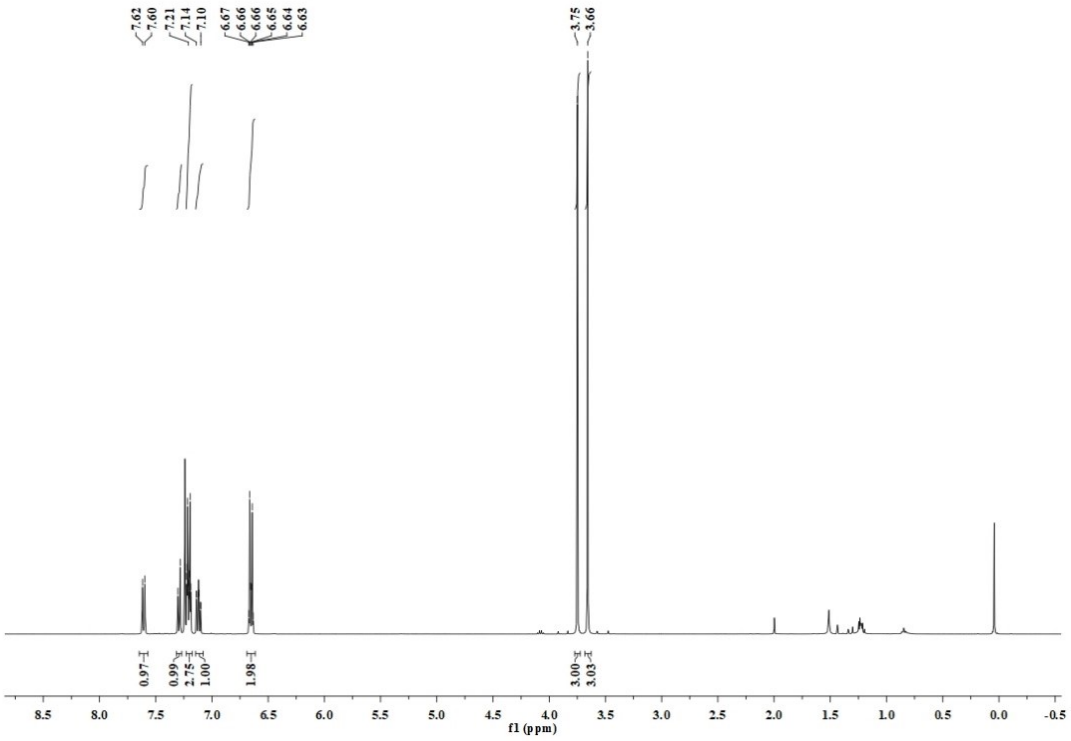
122.56
120.72
120.54
109.67
96.66
33.21
28.54
15.73
f1 (ppm)


OMe
Se
N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7.14
7.10
6.67
6.66
6.66
6.65
6.64
6.63
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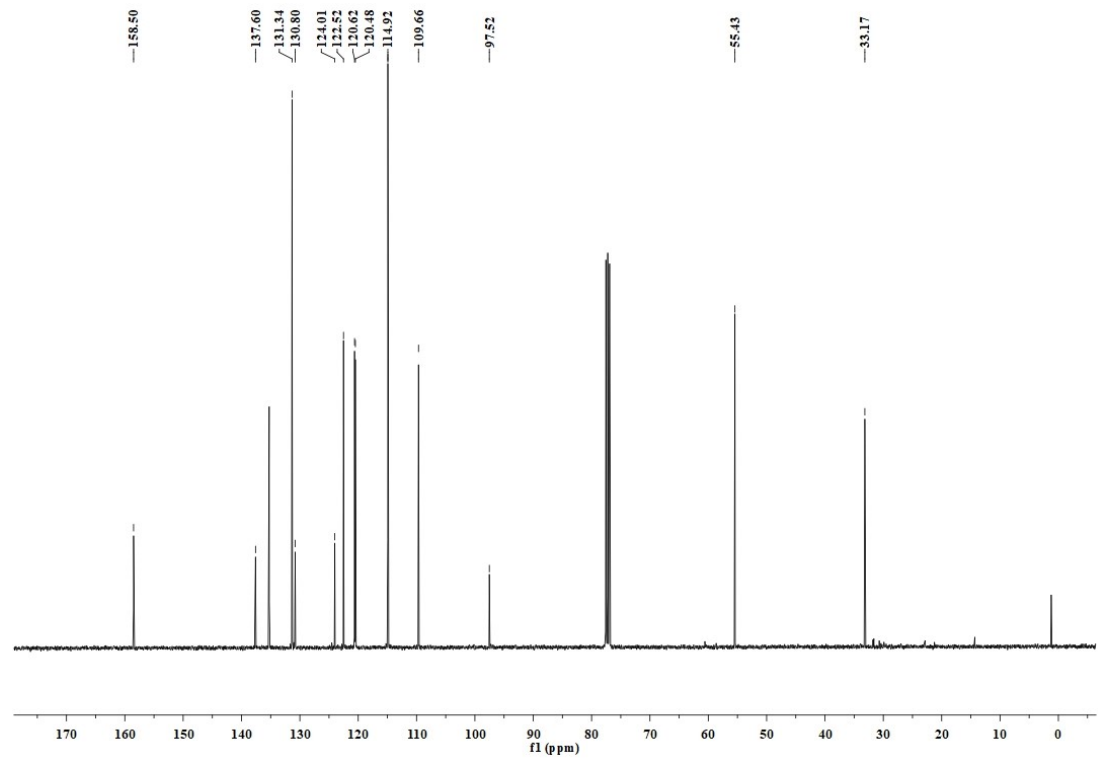
3.66
0.97
0.99
2.75
1.00
1.98
3.00
3.03
f1 (ppm)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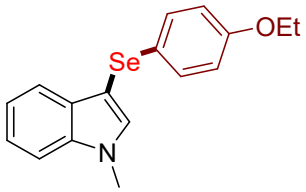
122.52
120.62
120.48
114.92
109.66
97.52
55.43
33.17
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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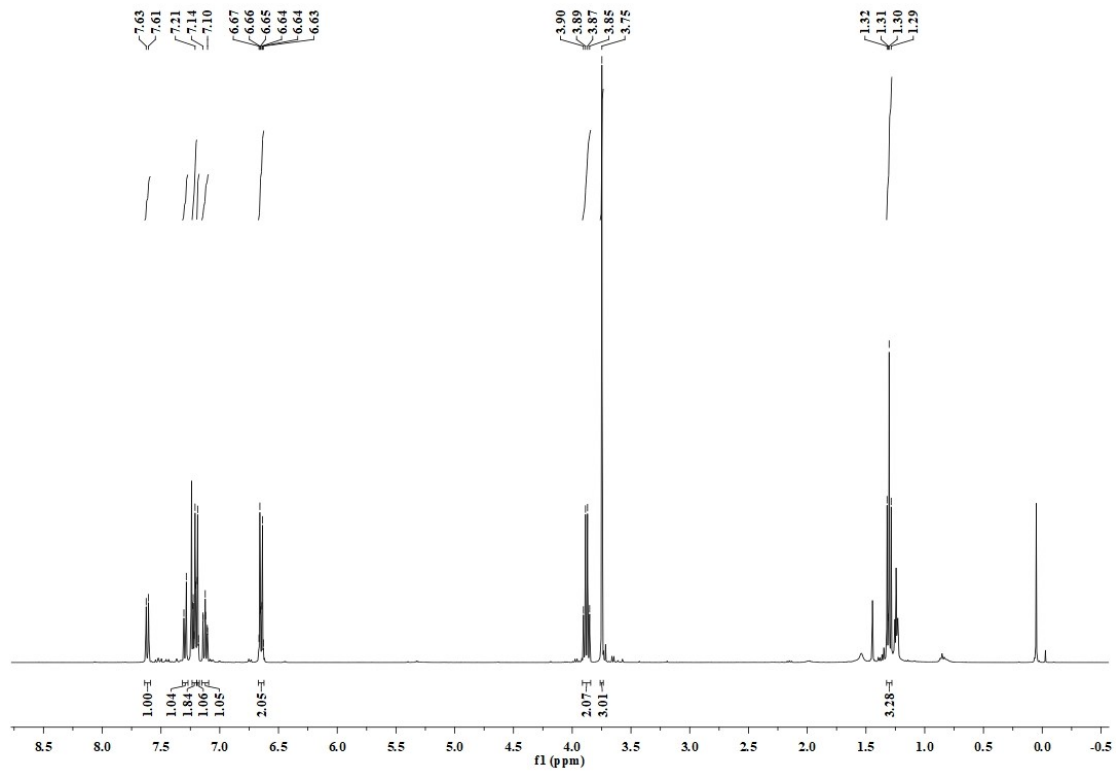
Se
N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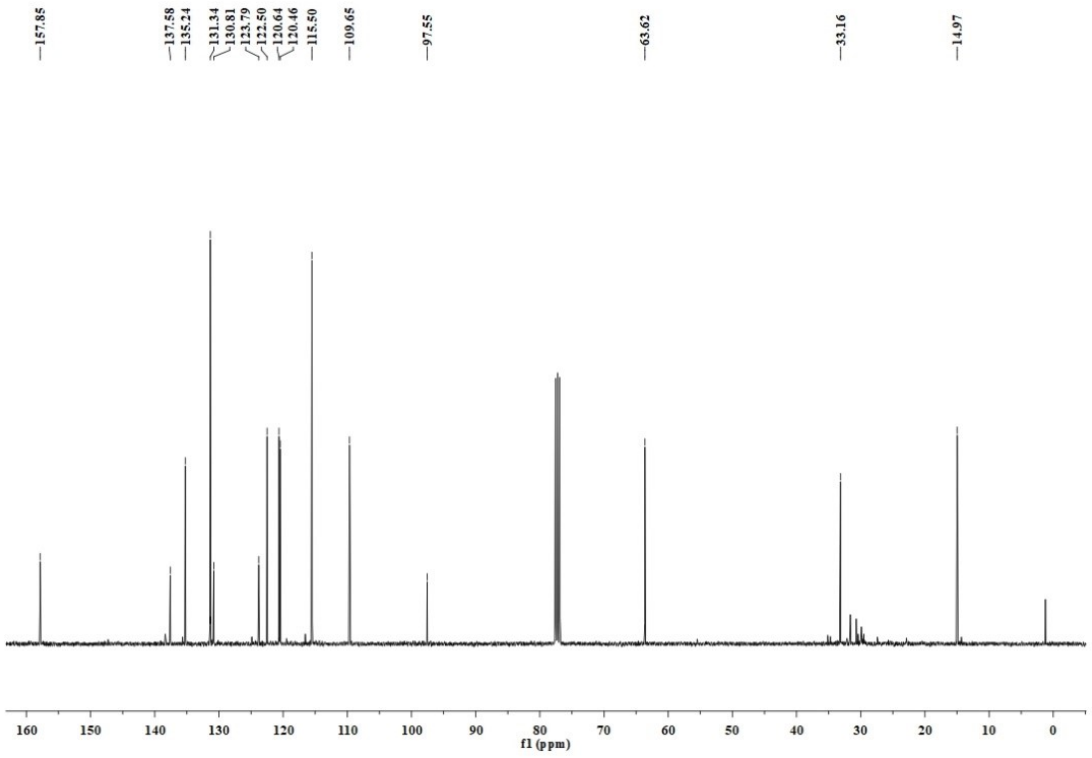
3.90
3.89
3.87
3.85
3.75
1.32
1.31
1.30
1.29
1.00
1.04
1.84
1.06
1.05
2.05
2.07
3.01
3.28
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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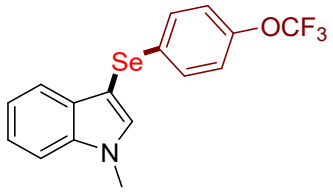
123.79
122.50
120.64
120.46
115.50
109.65
97.55
63.62
33.16
14.97
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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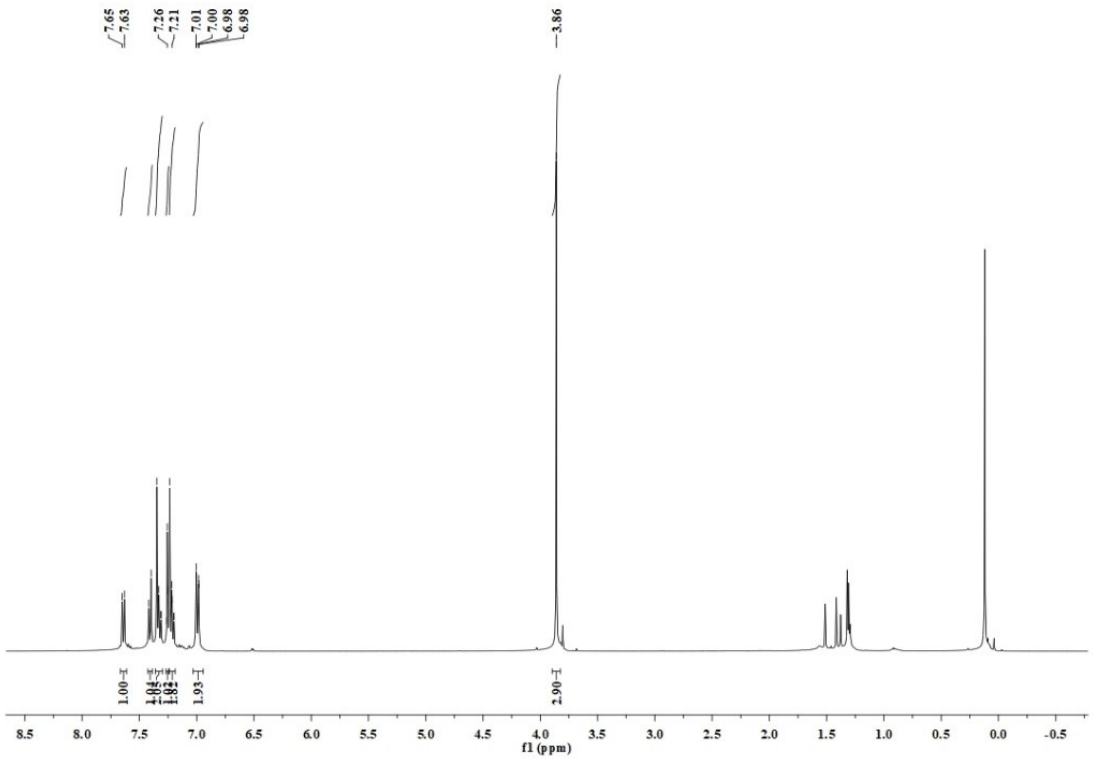
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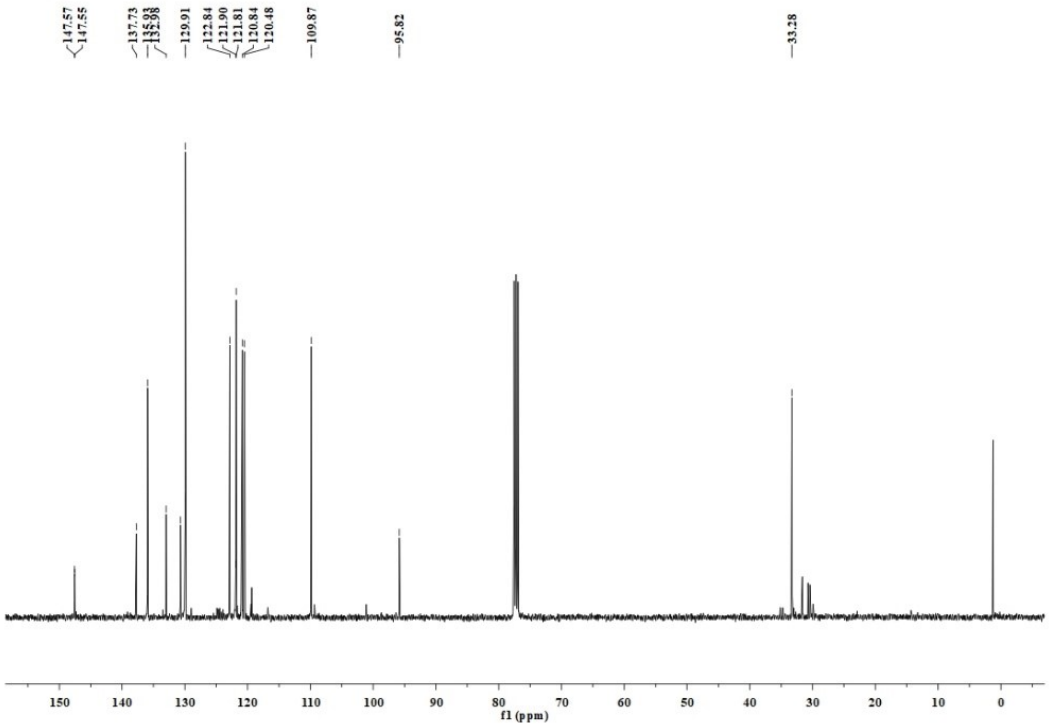
7.00
6.98
6.98
3.86
1.00
1.04
1.02
1.93
2.90
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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147.55
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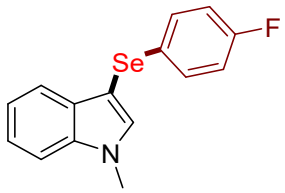
132.98
129.91
122.84
121.90
121.81
120.84
120.48
109.87
95.82
33.28
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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F
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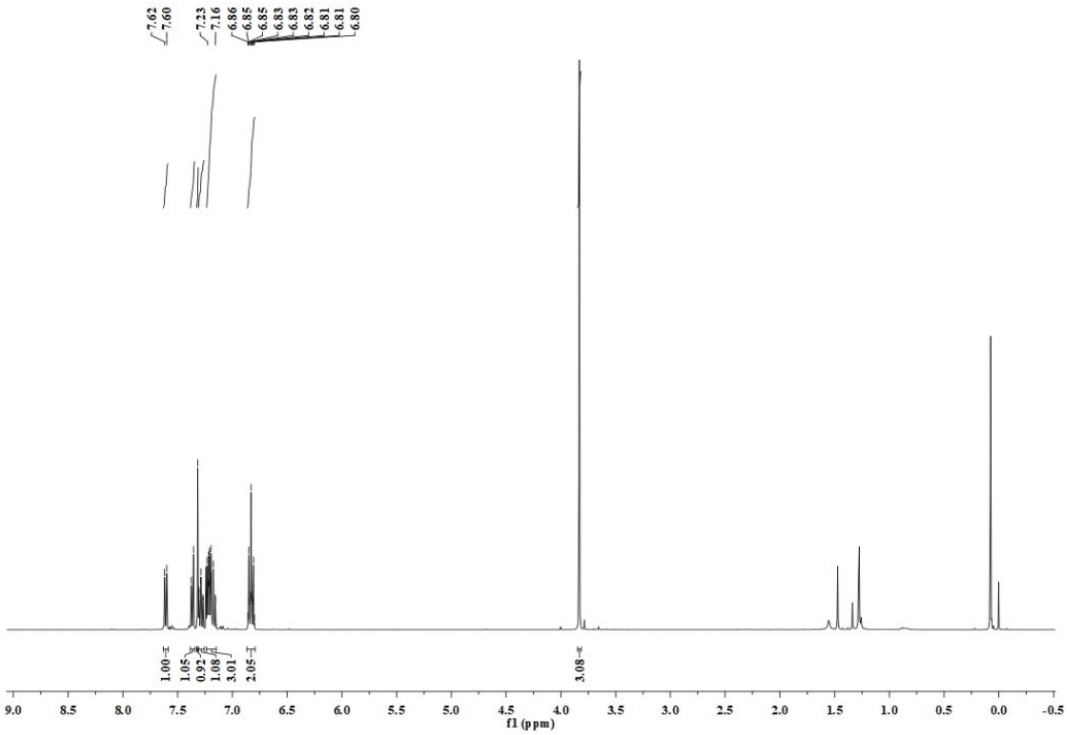
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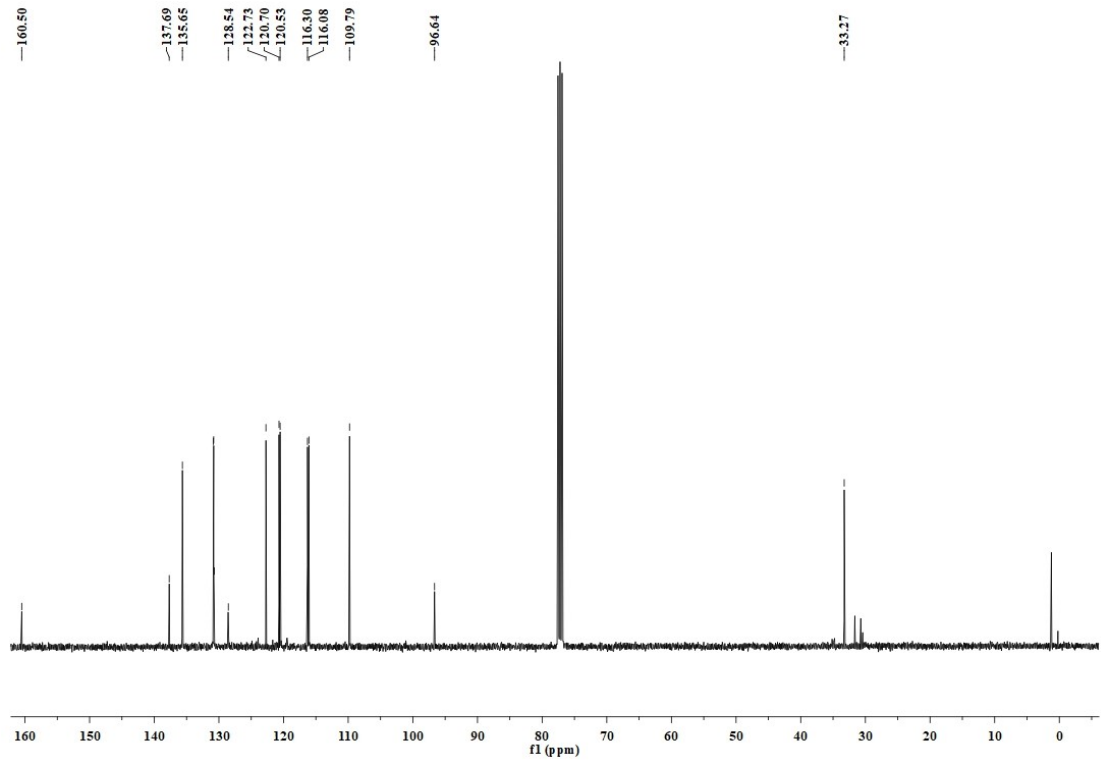
6.86
6.85
6.85
6.83
6.83
6.82
6.81
6.81
6.80
1.00
1.05
0.92
1.08
3.01
2.05
3.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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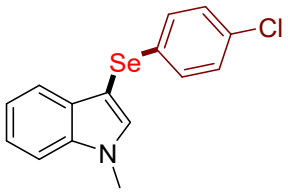
120.70
120.53
116.30
116.08
109.79
96.64
33.27
f1 (ppm)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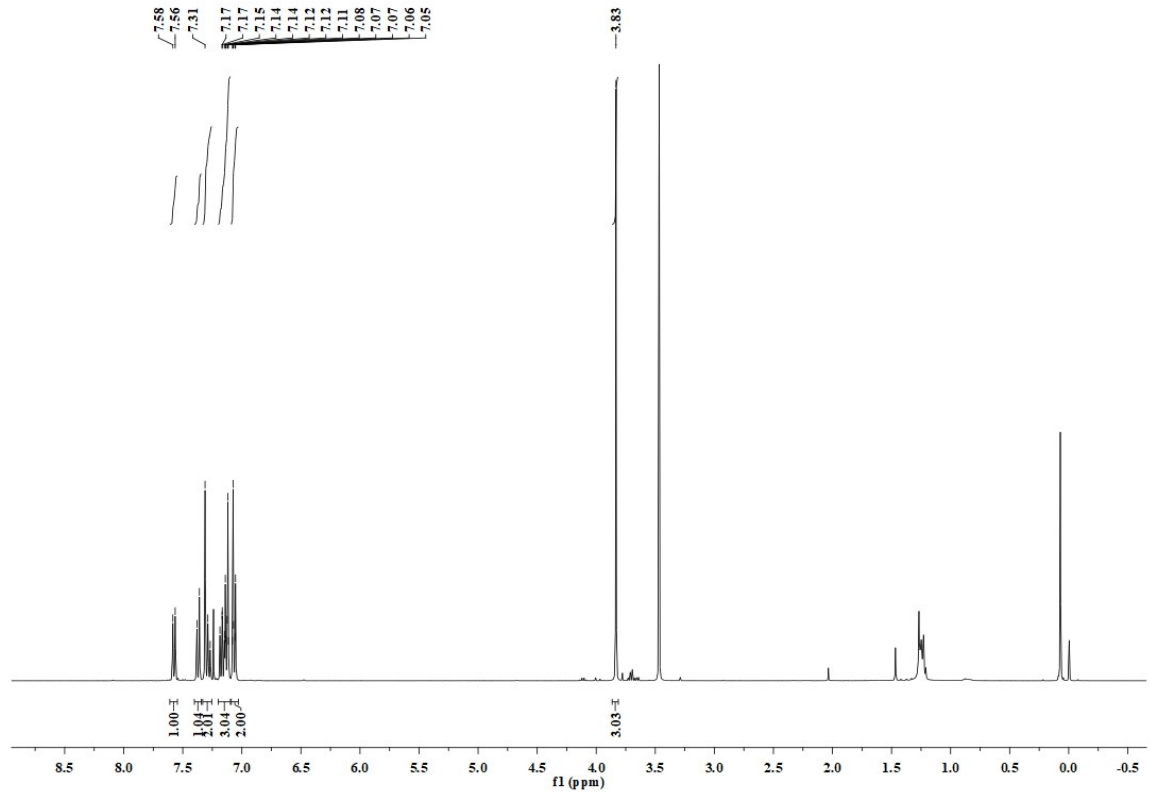
Se
N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7.14
7.14
7.12
7.12
7.11
7.08
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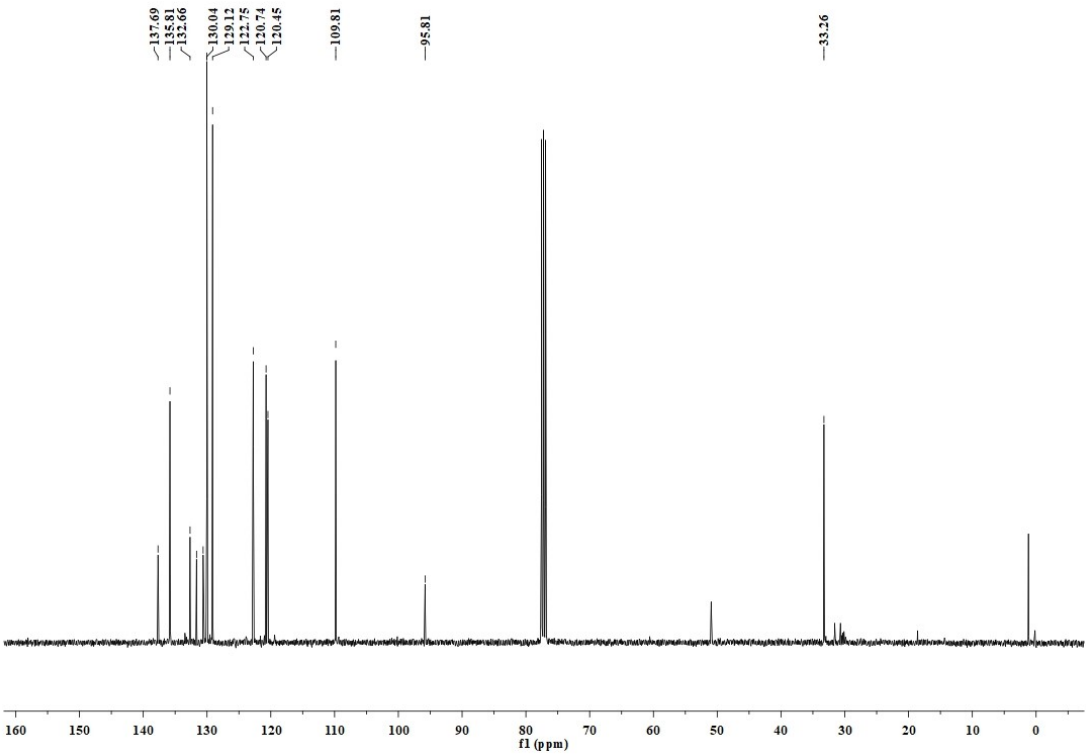
1.01
3.04
2.00
3.03
f1 (ppm)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95.81
33.26
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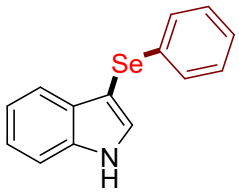
f1 (ppm)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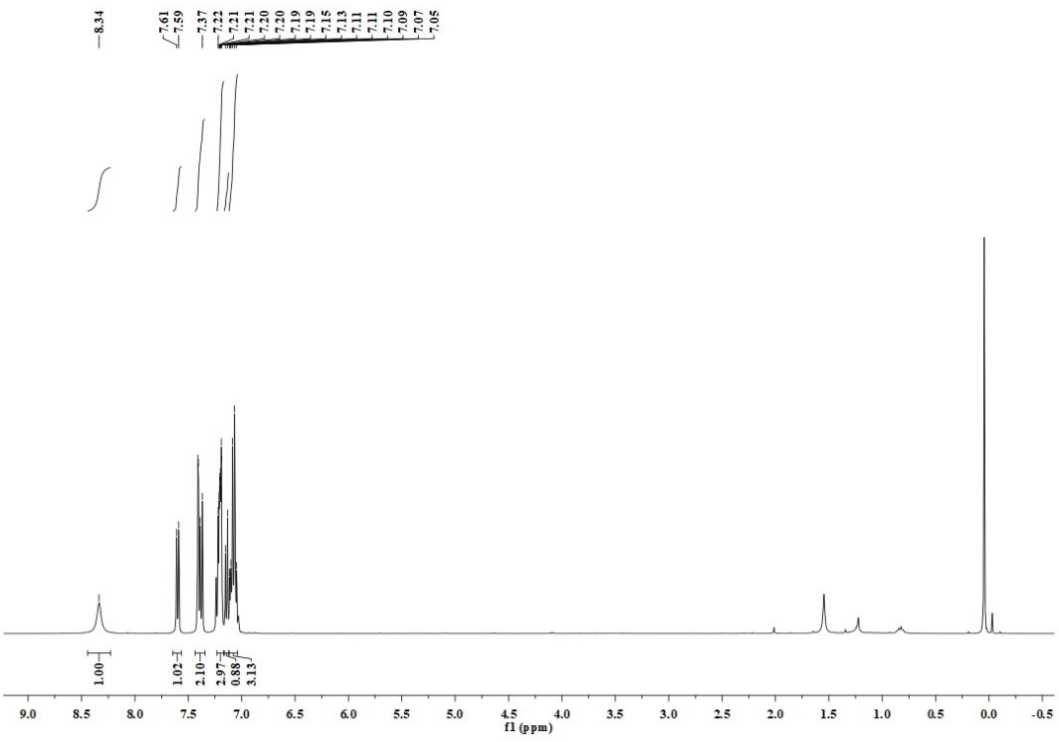
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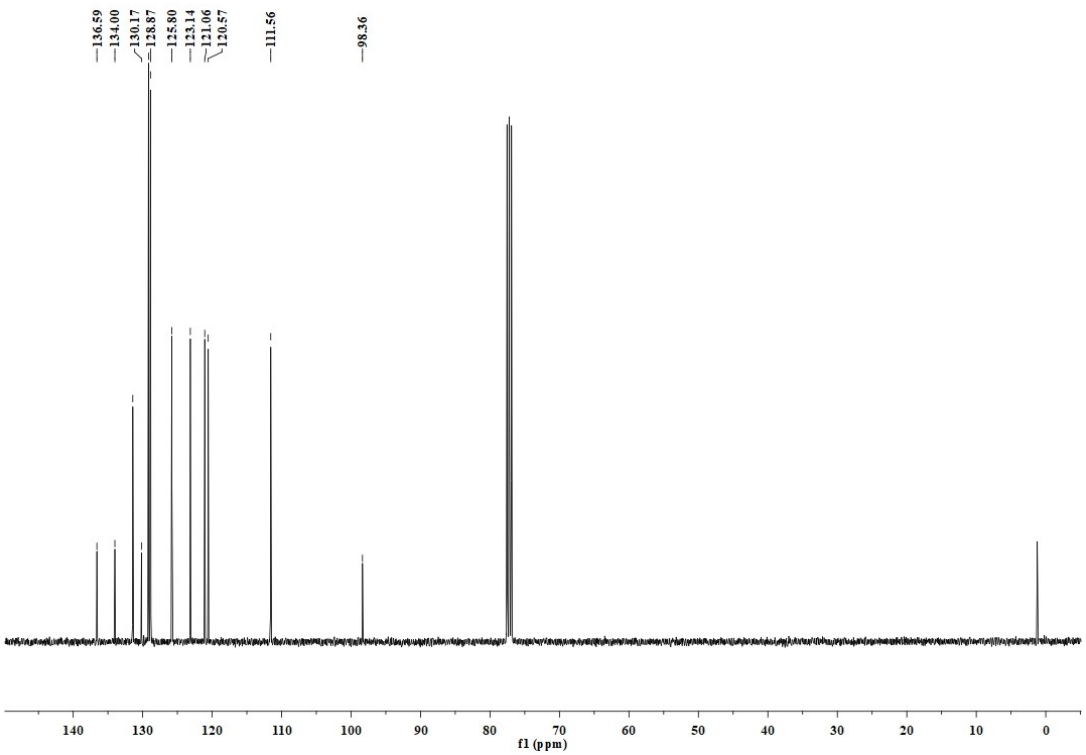
7.19
7.19
7.15
7.13
7.11
7.11
7.10
7.09
7.07
7.05
1.00
1.02
2.10
2.97
0.88
3.13
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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110
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90
80
70
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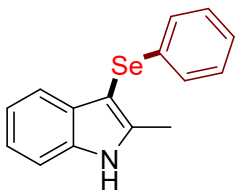
50
40
30
20
10
0
f1 (ppm)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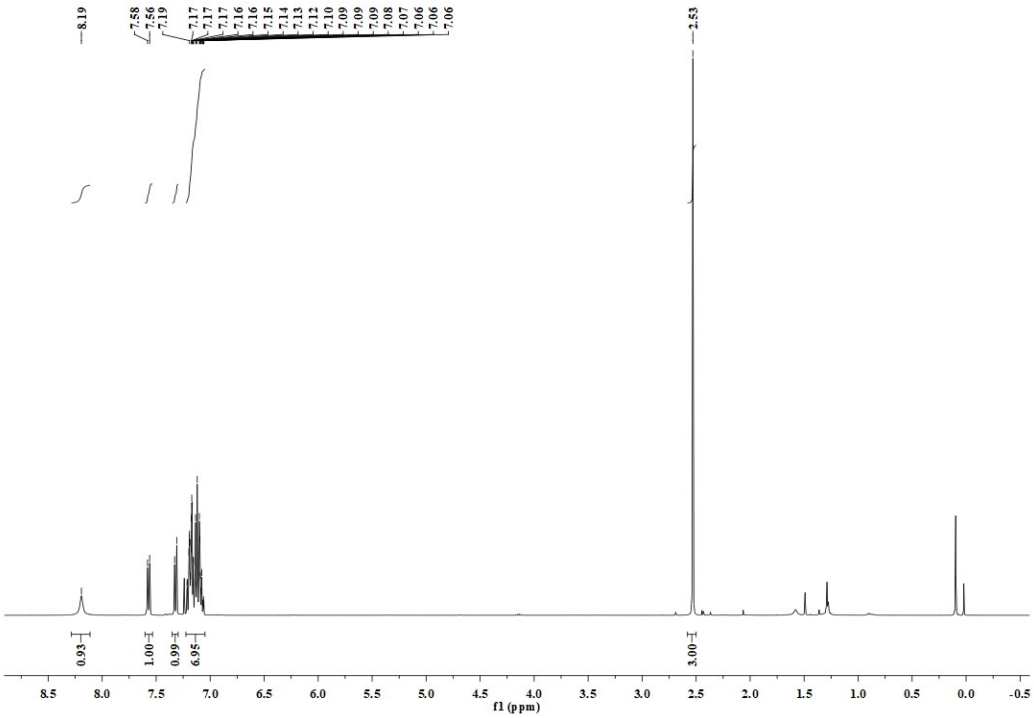
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7.13
7.12
7.10
7.09
7.09
7.09
7.08
7.07
7.06
7.06
7.06
2.53
0.93
1.00
0.99
6.95
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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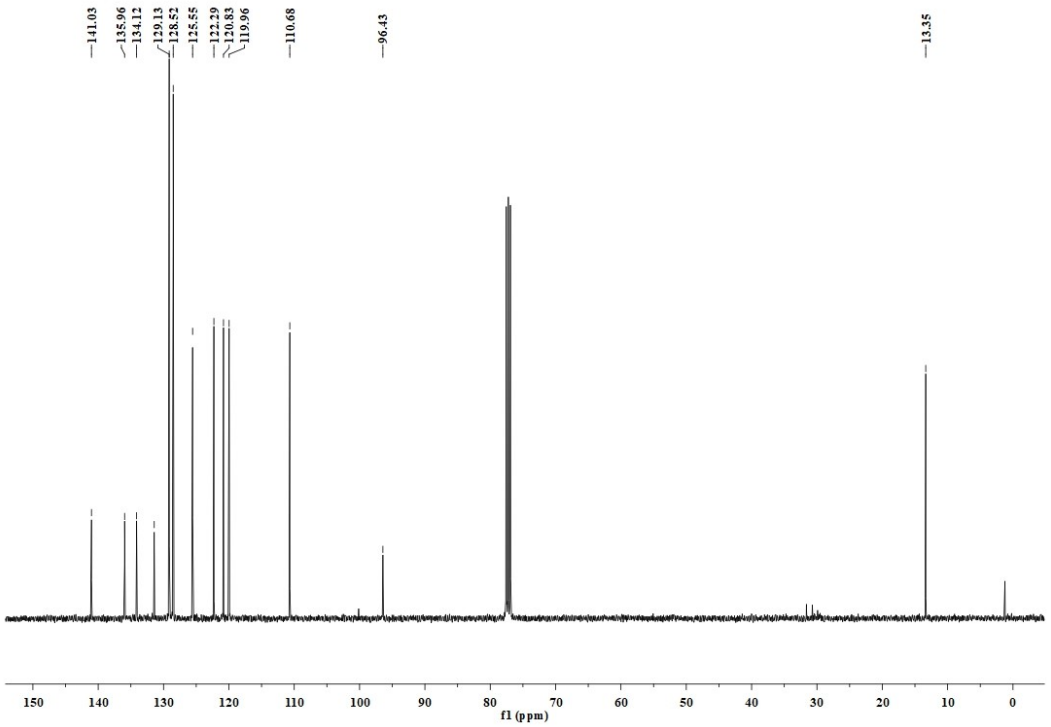
0.5
0.0
-0.5
f1 (ppm)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119.96
110.68
96.43
13.35
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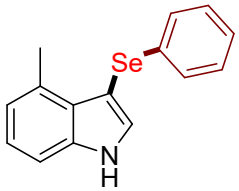
f1 (ppm)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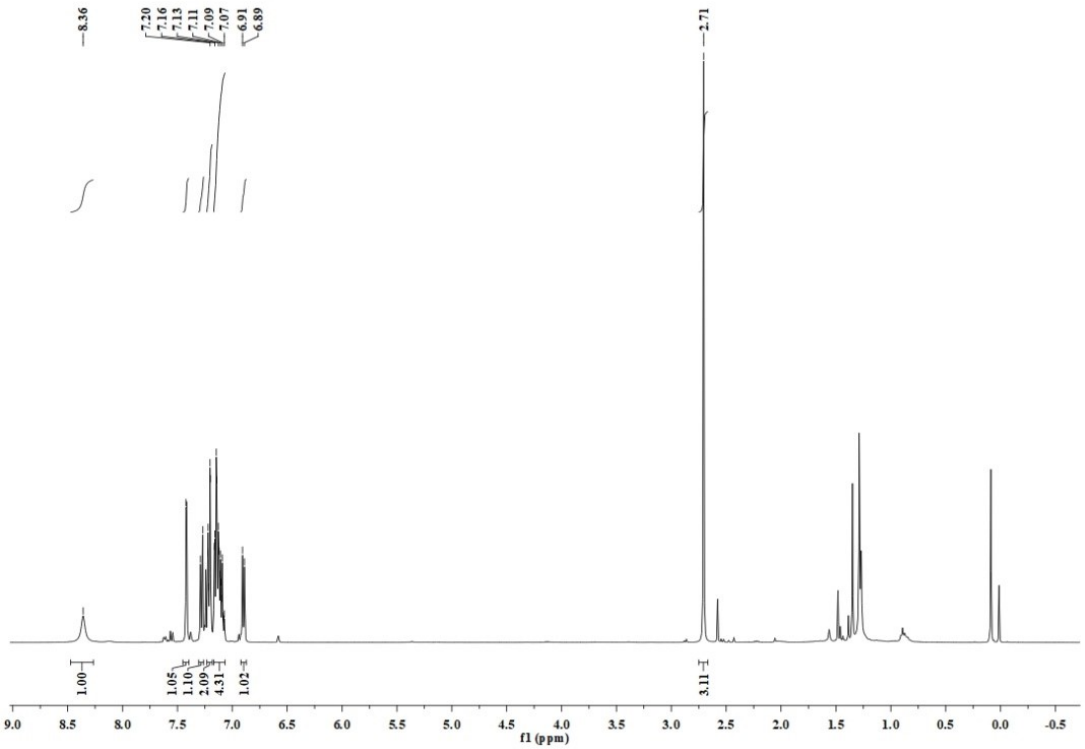
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7.07
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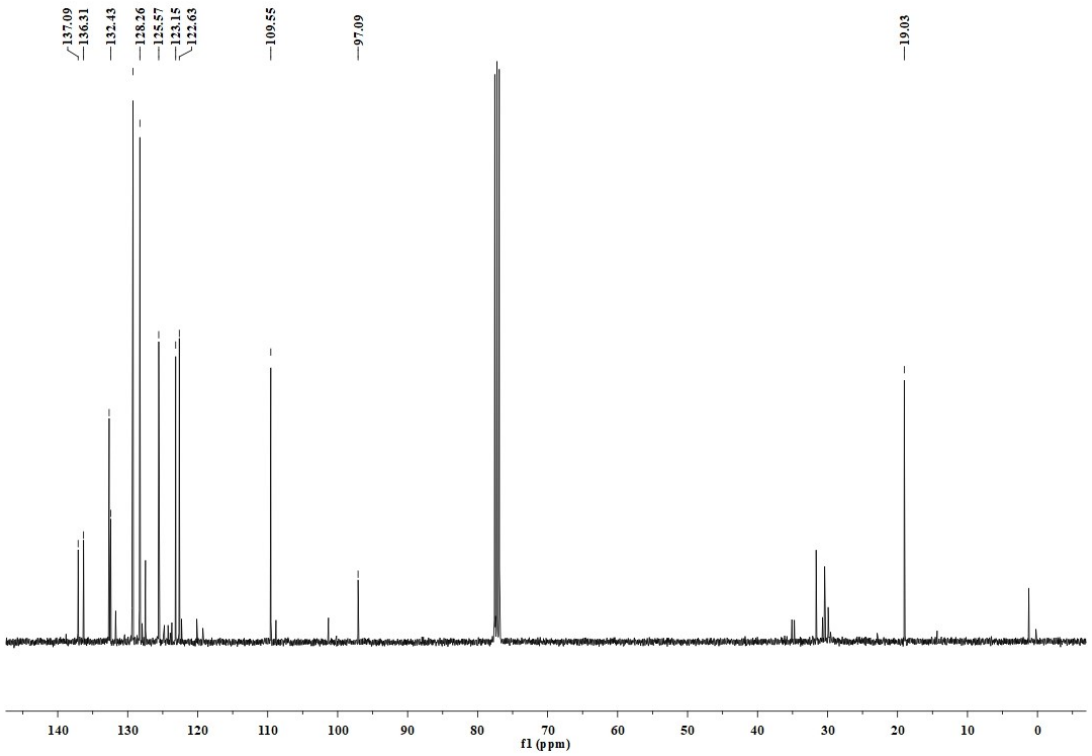
2.71
1.00
1.05
1.10
2.09
4.31
1.02
3.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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50
40
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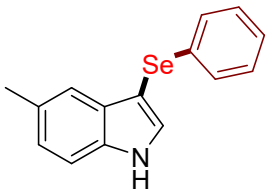
10
0
f1 (ppm)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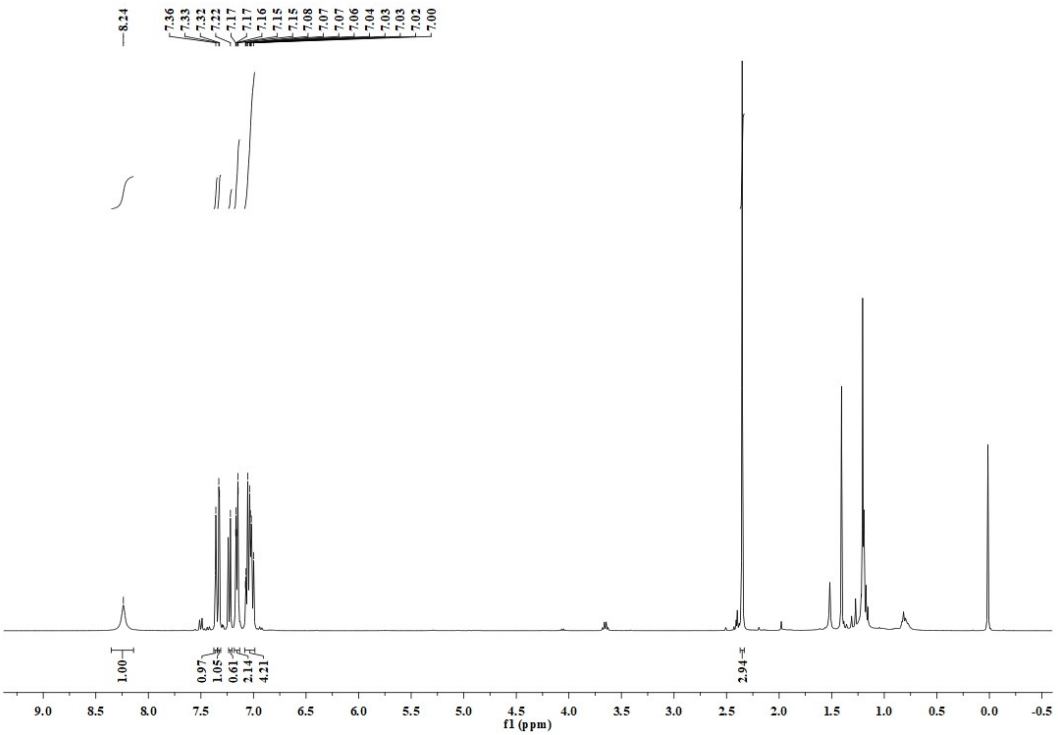
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7.07
7.06
7.04
7.03
7.03
7.02
7.00
1.00
0.97
1.05
0.61
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4.21
2.94
9.0
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8.0
7.5
7.0
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6.0
5.5
5.0
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2.0
1.5
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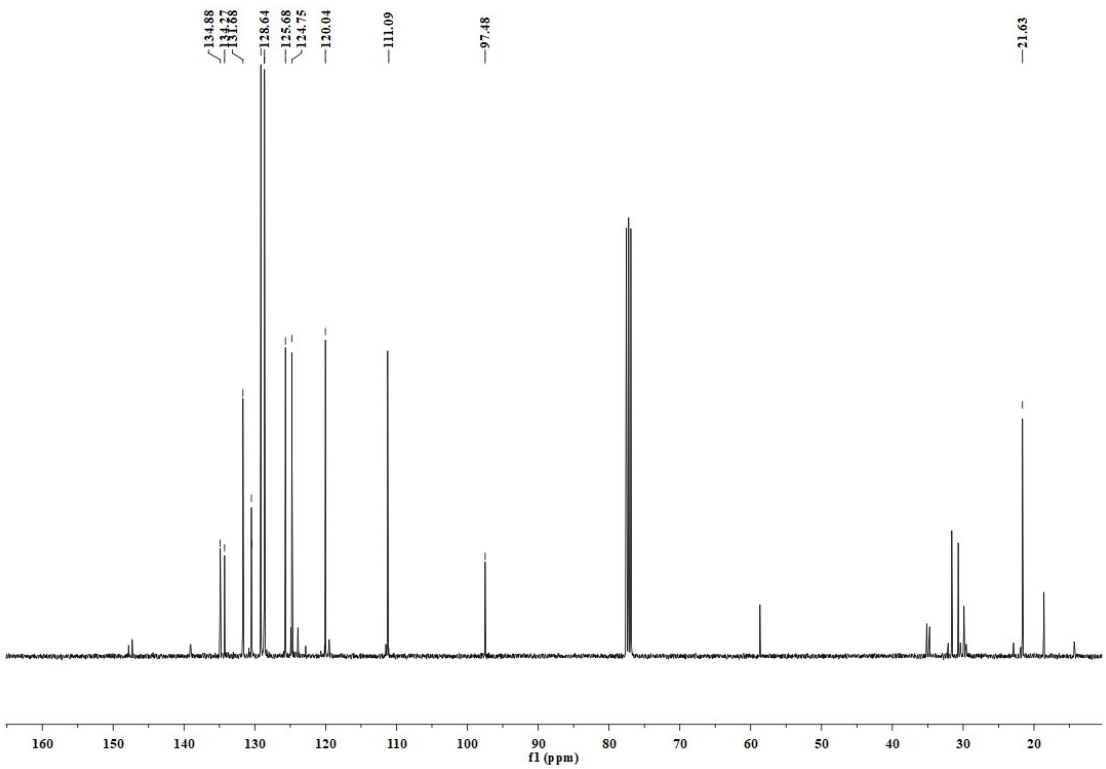
0.5
0.0
-0.5
f1 (ppm)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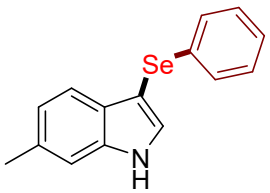
30
20
f1 (ppm)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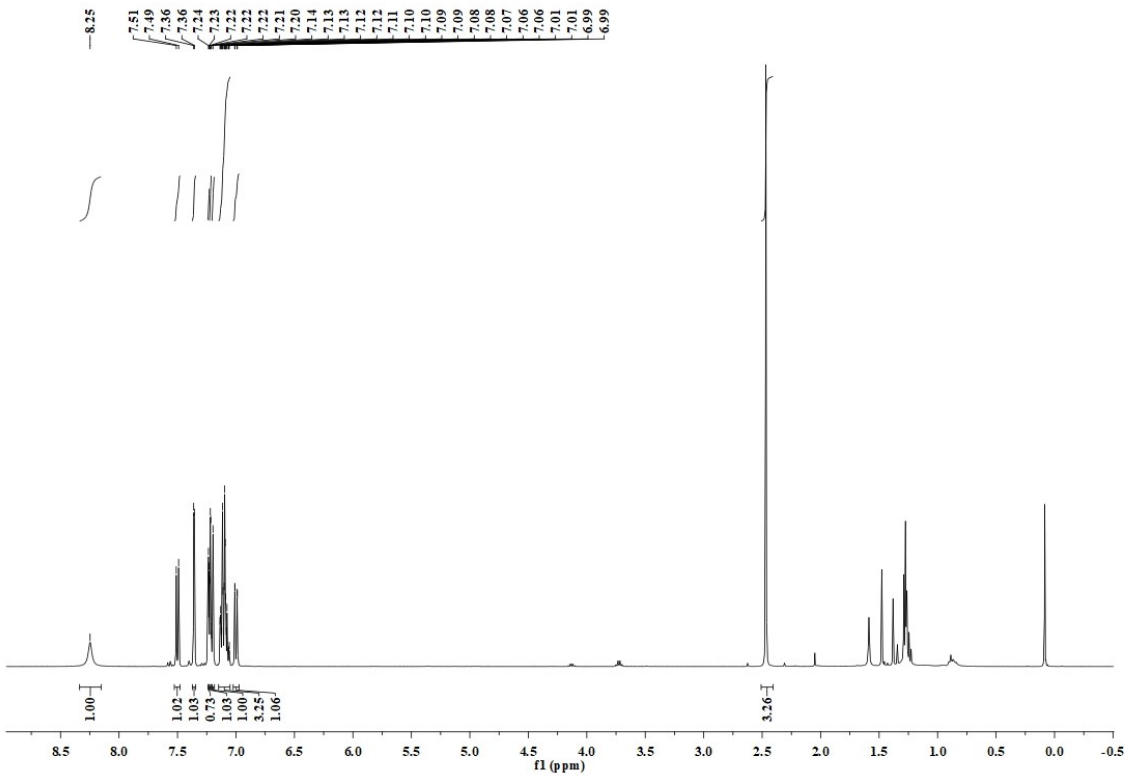
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7.08
7.08
7.07
7.06
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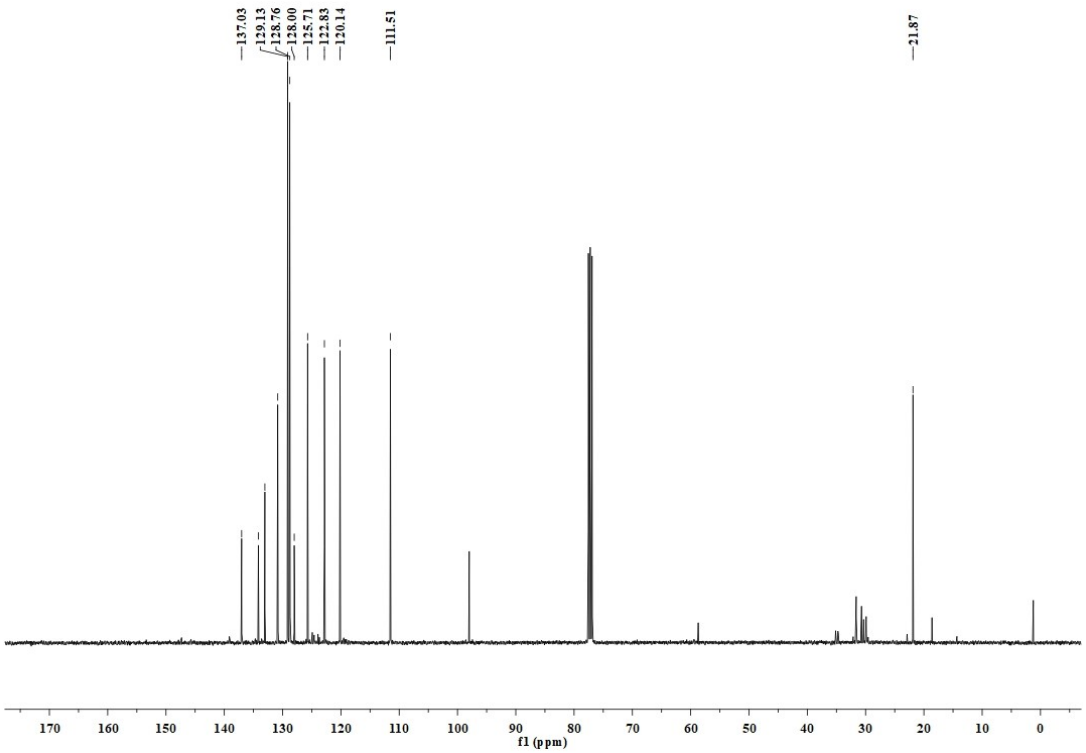
f1 (ppm)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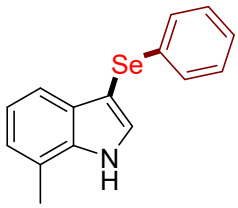
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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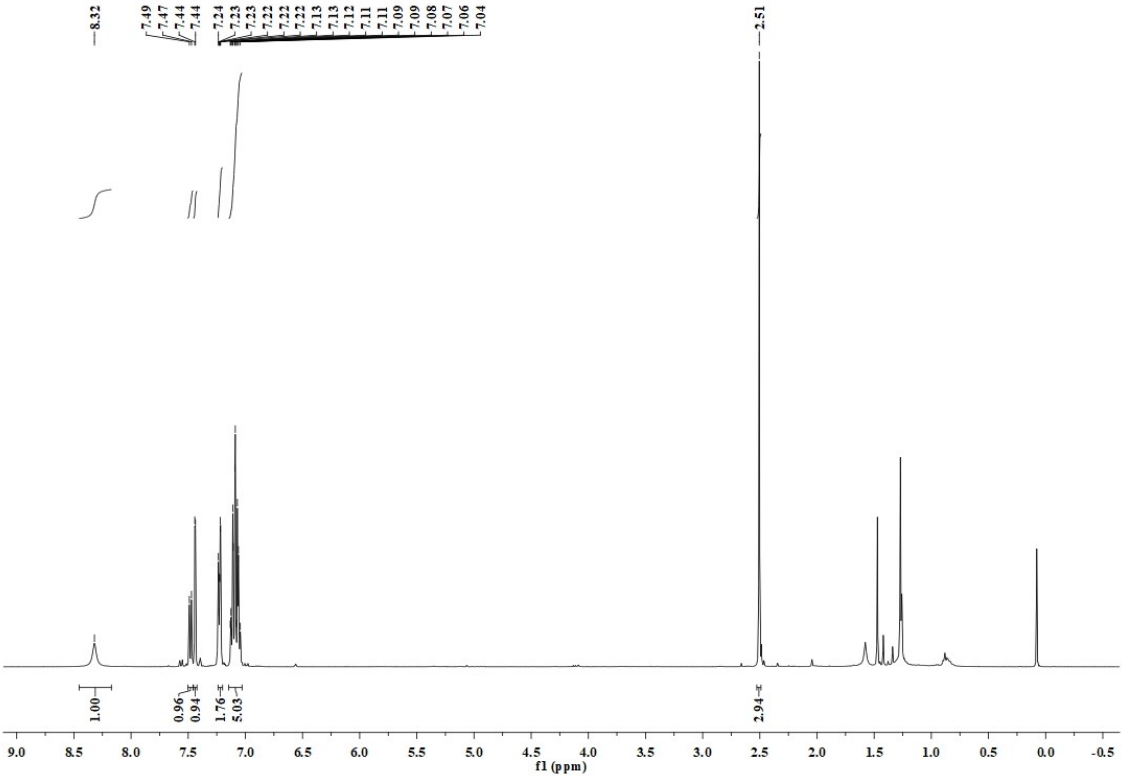
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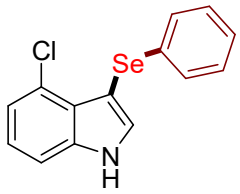
7.11
7.11
7.09
7.09
7.08
7.07
7.06
7.04
2.51
1.00
0.96
0.94
1.76
5.03
2.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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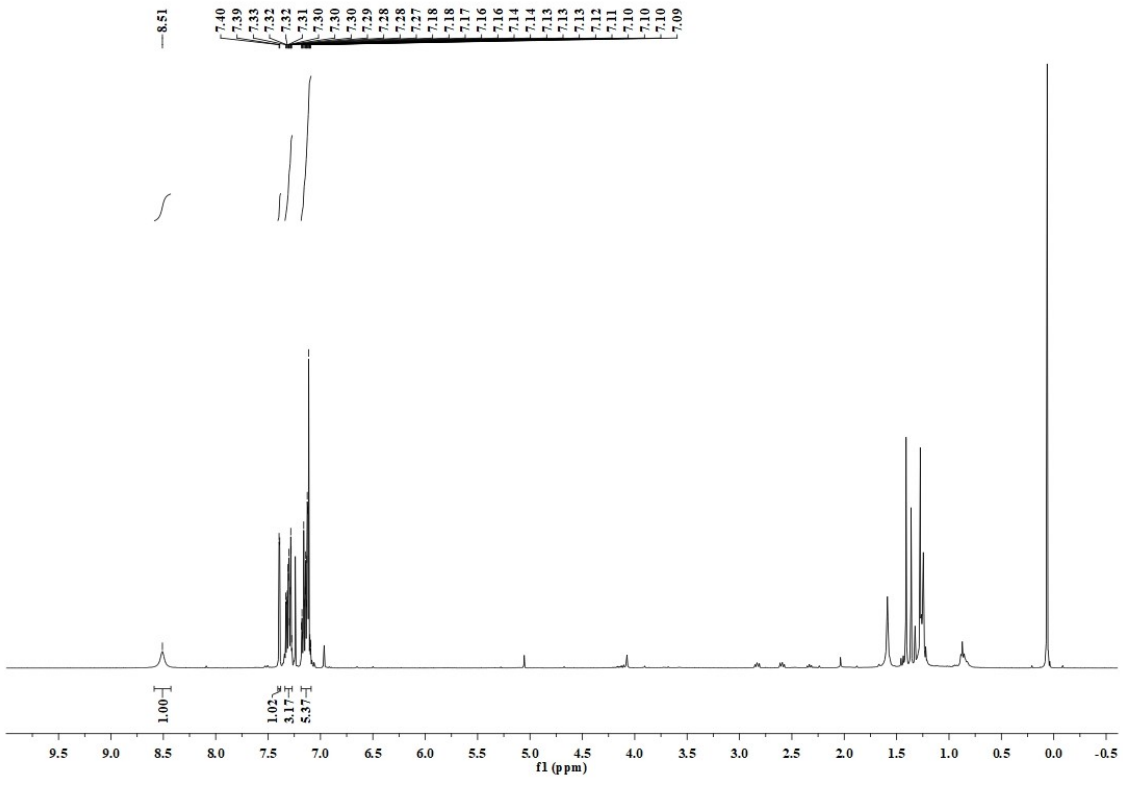
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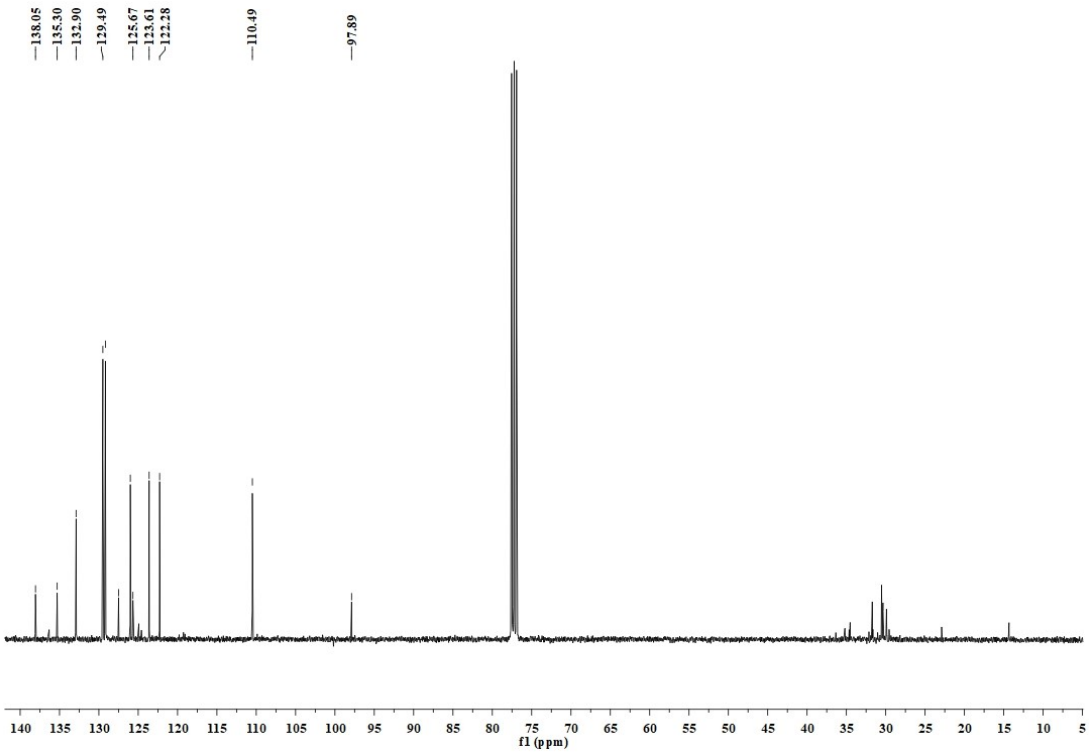
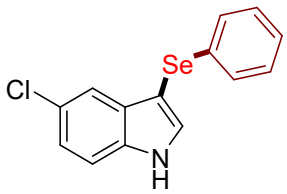
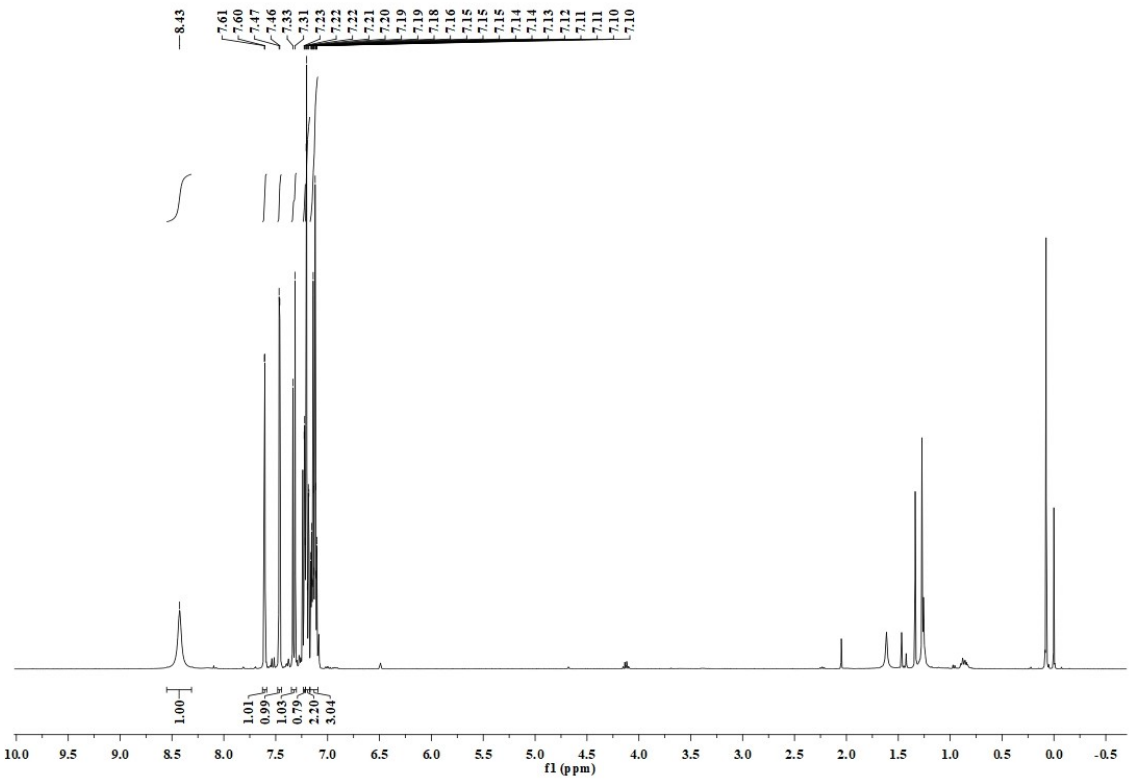
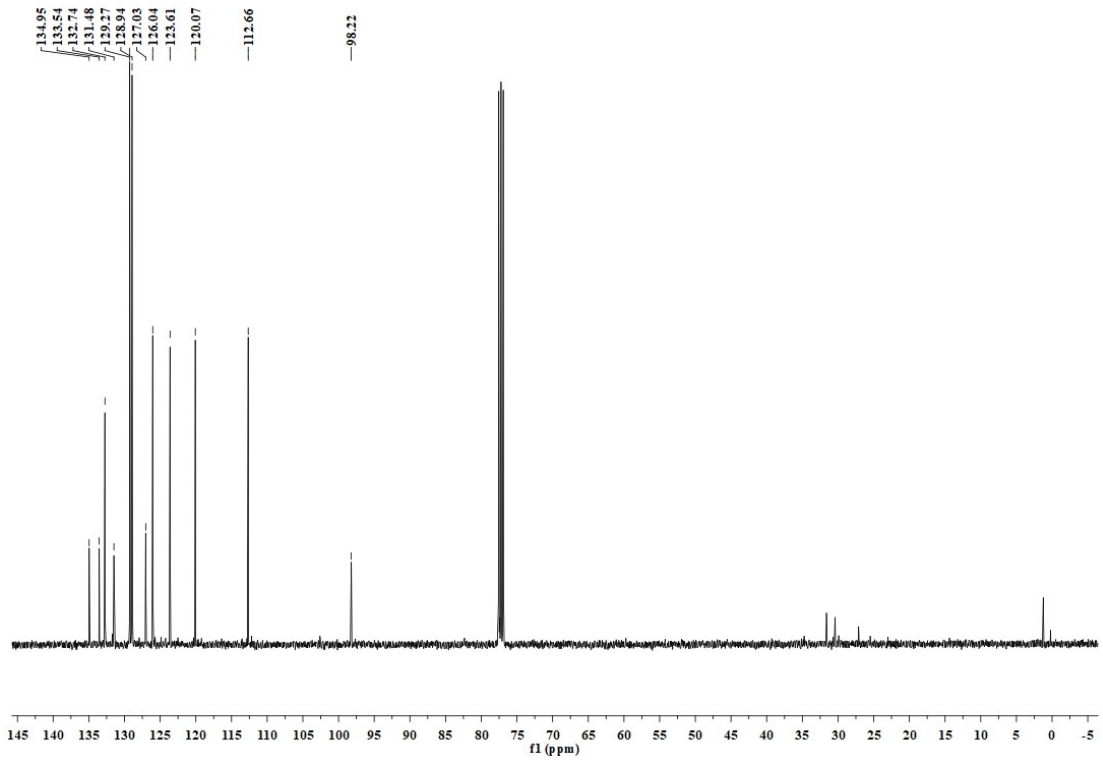
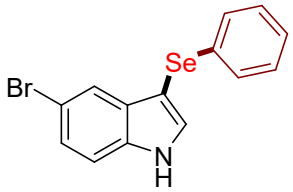
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

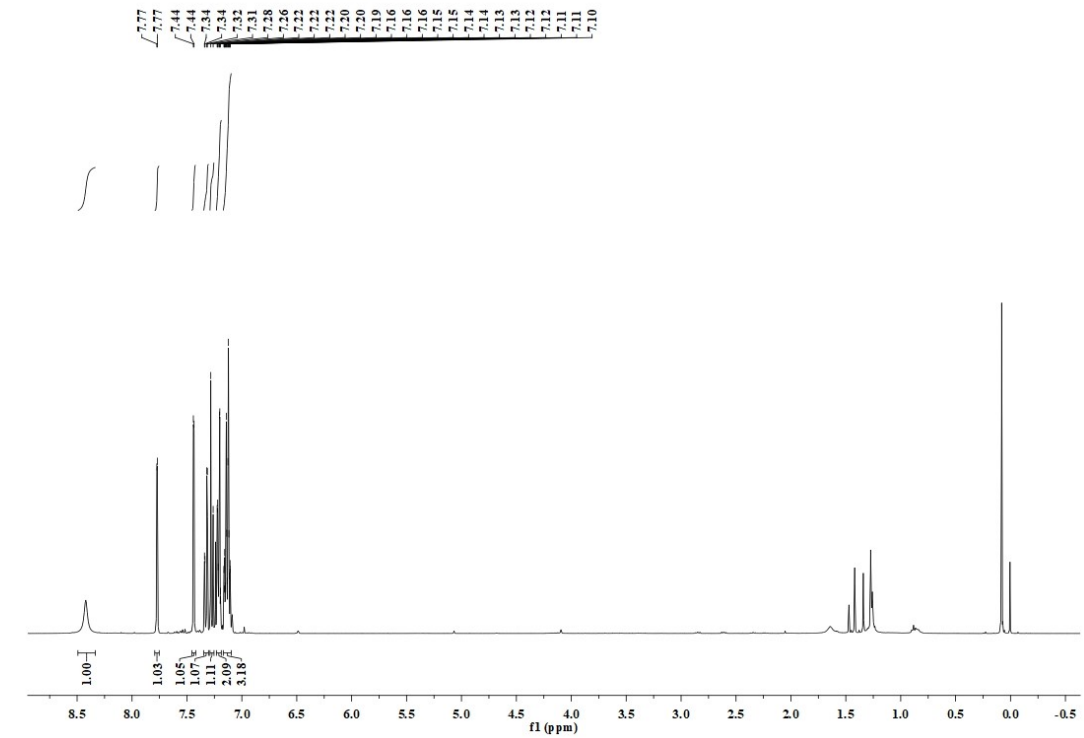

138.05
135.30
132.90
129.49
125.67
123.61
122.28
110.49
97.89
f1 (ppm)

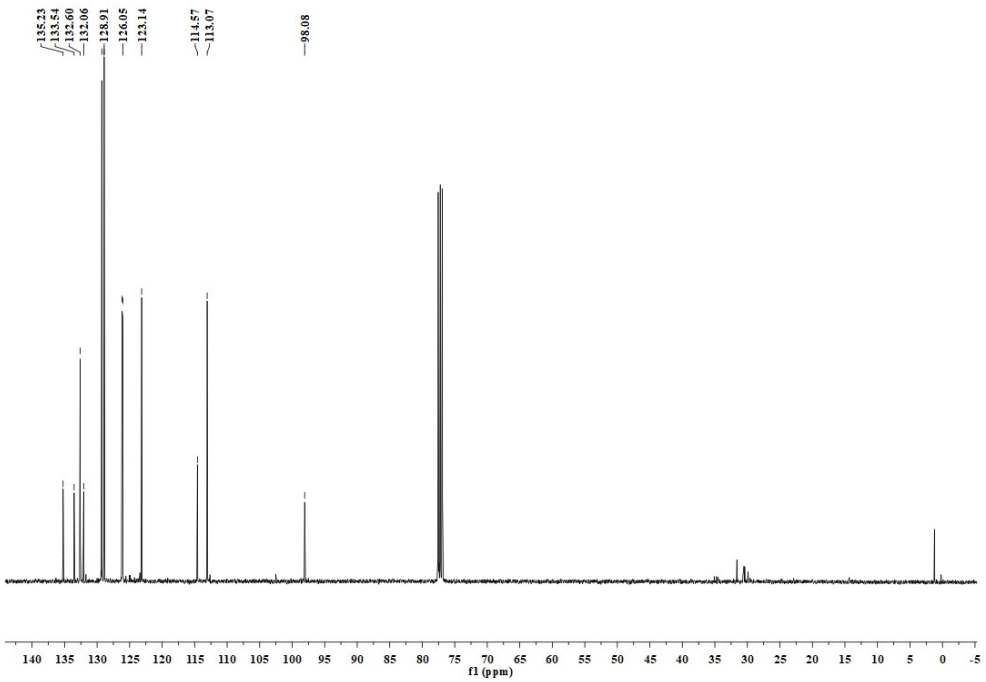

Se
Cl
N
H

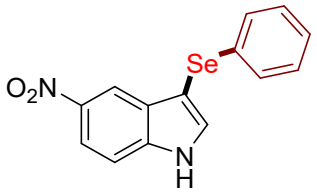

8.43
7.61
7.60
7.47
7.46
7.33
7.31
7.23
7.22
7.22
7.21
7.20
7.19
7.19
7.18
7.16
7.15
7.15
7.15
7.14
7.14
7.13
7.12
7.11
7.11
7.10
7.10
1.00
1.01
0.99
1.03
0.79
2.20
3.04
f1 (ppm)

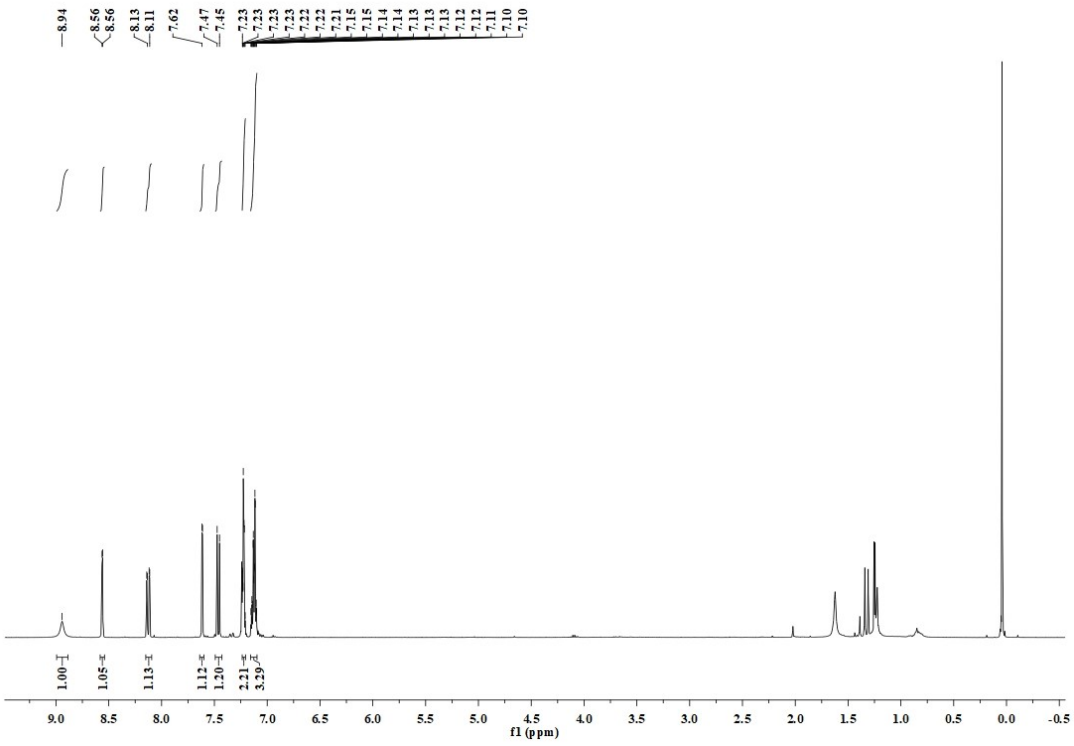

134.95
133.54
132.74
131.48
129.27
128.94
127.03
126.04
123.61
120.07
112.66
98.22
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5
f1 (ppm)

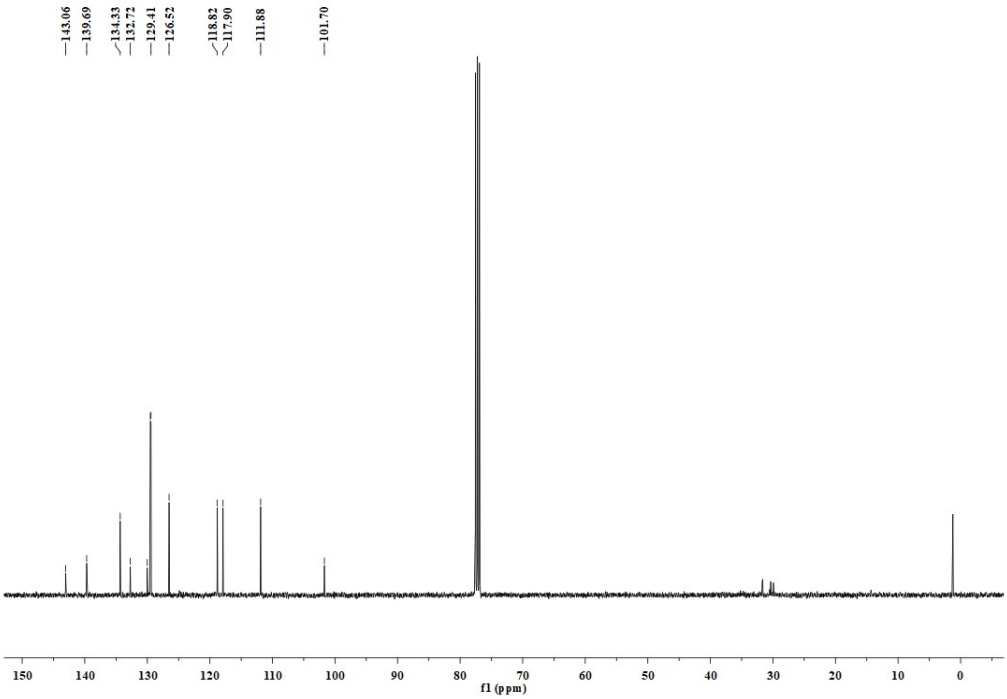

Br
Se
N
H

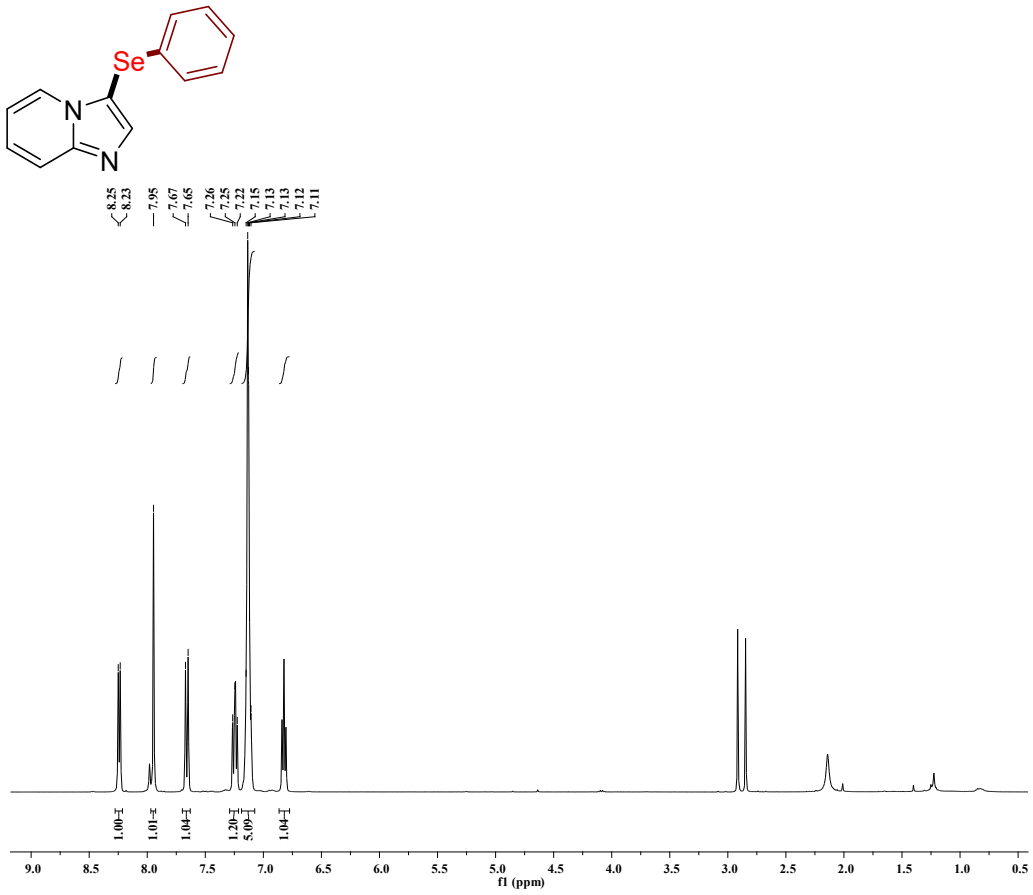

7.77
7.77
7.44
7.34
7.34
7.32
7.31
7.28
7.26
7.22
7.22
7.22
7.20
7.20
7.19
7.16
7.16
7.16
7.15
7.15
7.14
7.14
7.13
7.13
7.12
7.12
7.11
7.11
7.10
1.00
1.03
1.05
1.07
1.11
2.09
3.18
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

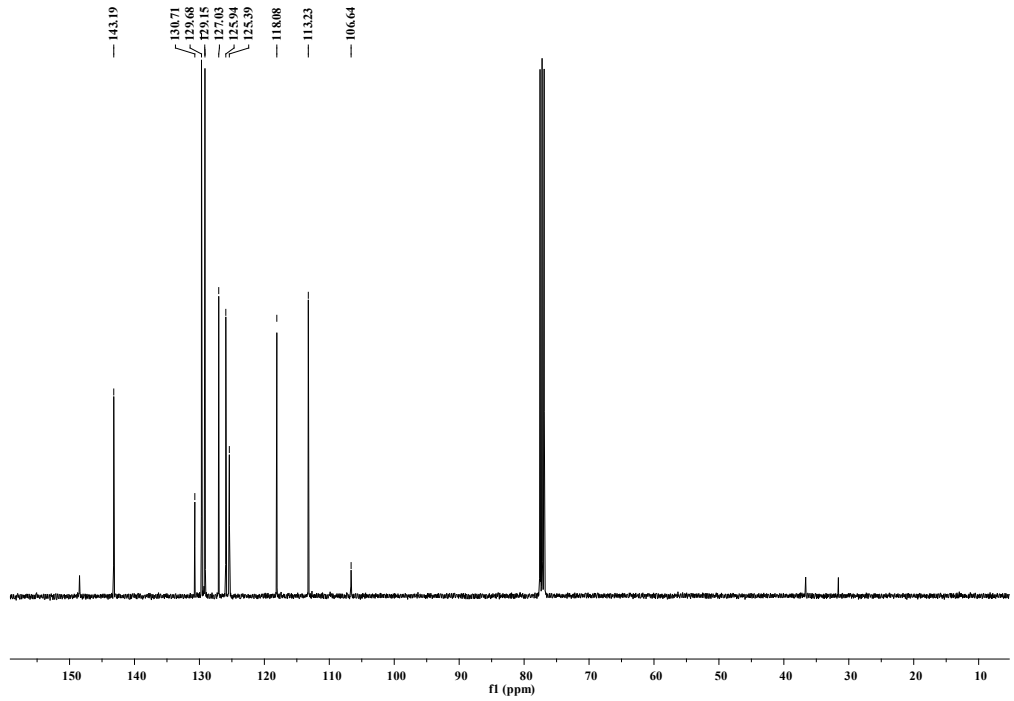

135.23
133.54
132.60
132.06
128.91
126.05
123.14
114.57
113.07
98.08
f1 (ppm)

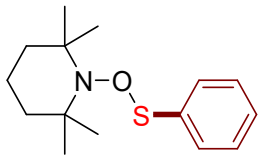

Se
O2N
N
H

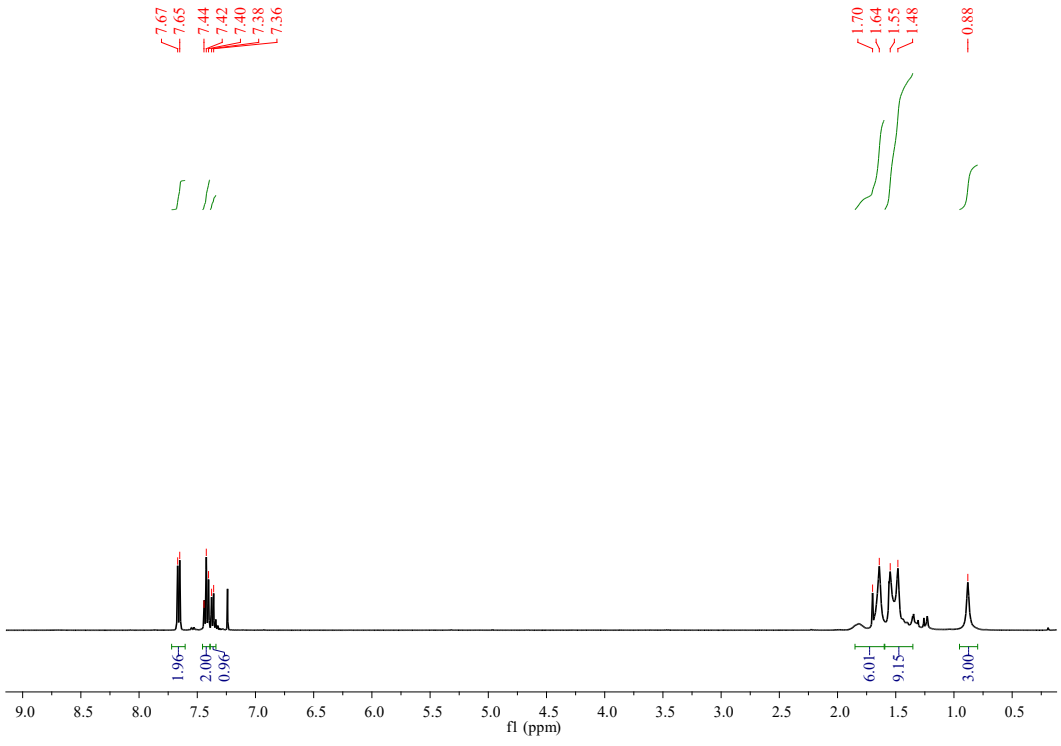

8.94
8.56
8.56
8.13
8.11
7.62
7.47
7.45
1.00
1.05
1.13
1.12
1.20
2.21
3.29
f1 (ppm)

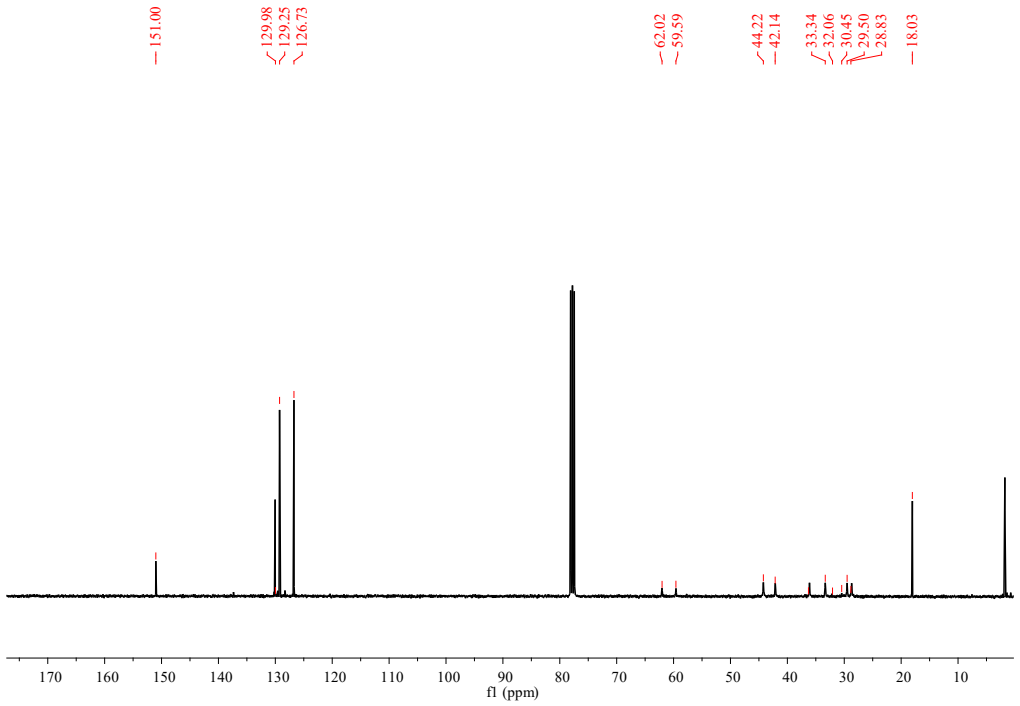

143.06
139.69
134.33
132.72
129.41
126.52
118.82
117.90
111.88
101.70
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Se
N
N
8.25
8.23
7.95
7.67
7.65
7.26
7.25
7.22
7.15
7.13
7.13
7.12
7.11
1.00
1.01
1.04
1.20
5.09
1.04
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
f1 (ppm)


143.19
130.71
129.68
129.15
127.03
125.94
125.39
118.08
113.23
106.64
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


N
O
S


7.67
7.65
7.44
7.42
7.40
7.38
7.36
1.70
1.64
1.55
1.48
0.88
1.96
2.00
0.96
6.01
9.15
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
f1 (ppm)



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