# *Supplementary Information*

**A Fast and Direct Iodide-Catalyzed Oxidative 2-Selenylation of Tryptophan**

Yu-Ting Gao, Shao-Dong Liu, Liang Cheng,* and Li Liu*

*Beijing National Laboratory for Molecular Sciences (BNLMS), CAS Key Laboratory of Molecular Recognition and Function, CAS Research/Education Center for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China and University of Chinese Academy of Sciences, Beijing 100049, China.*

chengl@iccas.ac.cn; lliu@iccas.ac.cn

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Note added after first publication:
This supplementary information file replaces that originally published on 02 March 2021. Some of the NMR assignments in the original version were incorrect but these data have now been corrected in this revised version. Some of the structures included with the NMR spectra were also incorrect, as some COOMe groups were drawn as OMe. These structures have also been corrected. This does not affect any of the results or conclusions of the paper.

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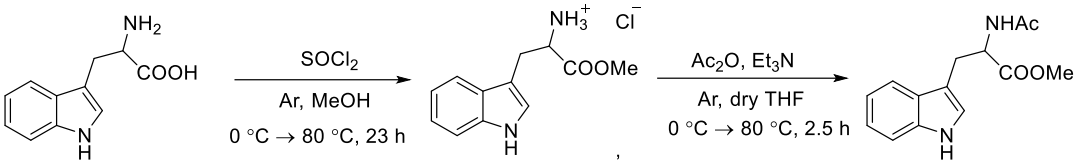
## 1. General Information

Unless otherwise noted, all reagents were obtained from commercially suppliers and were used without further purification. All reactions were carried out under the air atmosphere. Trp-substrates **1** and diselenides **2** were obtained from commercially suppliers or prepared according to the literature procedures.[1-4]

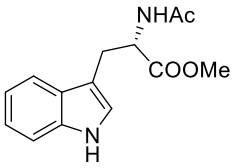
TLC analysis was performed on glass-baked silica plates and visualized with UV light. Column chromatography was performed on silica gel (200-300 mesh) using petroleum ether / ethyl acetate / dichloromethane/methanol. $^{1}H$, $^{13}C$ and $^{19}F$ NMR spectra were obtained on Bruker 300 MHz, 400 MHz or 500 MHz NMR spectrometer in the deuterated solvents indicated. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, h = heptet, m = multiplet. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or (br). Melting points were measured on Beijing Tech X-4 apparats without correction. IR spectra were recorded on a Nicolet 6700 FT-IR spectrometer. HRMS were obtained using electrospray ionization (ESI), nano electrospray ionization (nano ESI), electron ionization (EI) and atmospheric pressure chemical ionization (APCI) mass spectrometers. HPLC analyses were performed on Varian Prostar 210 liquid chromatograph and Agilent 1260 liquid chromatograph. Circular dichroism spectra was JASCO J-815 spectropolarimeter.

## 2. Synthesis of substrates

2.1 Preparation of methyl acetyl-*L*-tryptophanate and methyl acetyl-*DL*-tryptophanate[1]



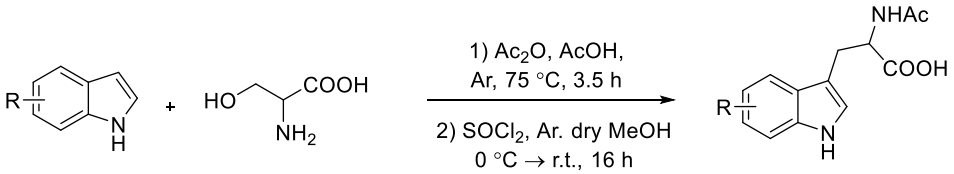

*General procedure*: *L*-Tryptophan or *DL*-Tryptophan (4.9 mmol, 1.0 g) was dispersed in MeOH (9.8 mL) under the argon atmosphere. To the suspension was added thionyl chloride (5.4 mmol, 0.39 mL) dropwise at 0 °C. The mixture was then heated to reflux for 23 hours and then cooled to room temperature. MeOH and excess thionyl chloride were removed in vaccum. The pink solid (methyl *L*-tryptophanate hydrochloride) was obtained and was used for the next step without further purification. The pink solid was dispersed in dry THF (20 mL) under the argon atmosphere and $Et_3N$ (9.8 mmol, 1.4 mL) was added. The mixture was stirred at room temperature for 5 minutes. Acetic anhydride (5.4 mmol, 0.5 mL) was then added dropwise at 0 °C. The resulting solution was heated to reflux for 2.5 hours. After cooling to room temperature, the mixture was diluted with ethyl acetate (50 mL) and the organic layer was washed by 1M HCl (20 mL), saturated $NaHCO_3$ (20 mL) and saturated NaCl (10 mL). Ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: dichloromethane /methanol 50/1) to afford the desired product methyl acetyl-*L*-tryptophanate or methyl acetyl-*DL*-tryptophanate **1a**.




**(*L*)-1a**

**methyl acetyl-*L*-tryptophanate *L*-1a**. White solid, m.p. 55-57 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) δ 10.85 (s, 1H), 8.29 (d, *J* = 7.5 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 2.1 Hz, 1H), 7.09-6.96 (m, 2H), 4.49 (dd, *J* = 13.5, 8.1 Hz, 1H), 3.57 (s, 3H), 3.17-2.97 (m, 2H), 1.81 (s, 3H). $^{13}$C NMR (75 MHz, DMSO-$d_6$) δ 172.5, 169.3, 136.1, 127.0, 123.6, 120.9, 118.4, 117.9, 111.4, 109.5, 53.1, 51.7, 27.1, 22.3. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 2389, 3058, 2951, 2926, 2850, 1738, 1655, 1530, 1458, 1437, 1375, 1216, 1010, 743. HRMS (ESI): calcd for $C_{14}H_{24}O_{16}O_3N_2Na^+$ $[M+Na]^+$: 283.1053, found: 283.1053.

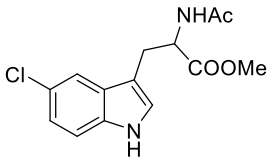
2.2 Preparation of substituted methyl acetyl tryptophanate **1**[2,3]




*General procedure*: The substituted indole (3.3 mmol) and *DL*-serine (6.6 mmol, 693.6 mg) were dissolved in acetic acid (7.7 mL) under the argon atmosphere, acetic anhydride (6.6 mmol, 0.6 mL) was then added dropwise. The mixture was stirred at 75 °C for 3.5 hours. After cooling to room temperature, the solution was adjusted to pH = 11 by addition of 30% aqueous sodium hydroxide carefully in ice bath and extracted with ether (10 mL × 3). The ether phase was washed by 1M NaOH (30 mL). All the aqueous solutions were combined and adjusted to pH = 2 using concentrated hydrochloric acid at 0 °C. The resulting mixture was extracted by EA/MeOH (10/1, 30 mL × 3). The organic was dried over anhydrous sodium sulfate,

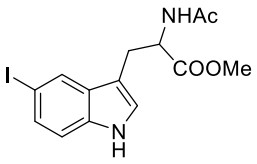
evaporated and got the crude intermediate product.

To the crude intermediate product we got above was added dry MeOH (10 mL) under argon atmosphere, the mixture was stirred at 0 °C for 5 minutes. Then the thionyl chloride (3.6 mmol, 0.7 mL) was added dropwise and the reaction was stirred at 0 °C for another 1.5 hours. After stirring at room temperature overnight, MeOH and excess thionyl chloride were removed in vaccum. The crude product was diluted with ethyl acetate (50 mL) and washed by $H_2O$ (50 mL). Ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3) to afford the desired product substituted methyl acetyl tryptophanate **1b-g**.



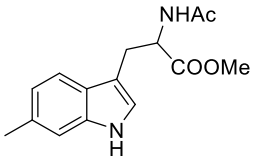

**1b**

**methyl 2-acetamido-3-(5-chloro-1*H*-indol-3-yl)propanoate 1b**. White solid, m.p. 72-73 °C. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.49 (s, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.00 (s, 1H), 6.19 (d, *J* = 7.5 Hz, 1H), 4.95 (dd, *J* = 13.0, 5.0 Hz, 1H), 3.73 (s, 3H), 3.34-3.24 (m, 2H), 2.00 (s, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 172.2, 169.9, 134.5, 128.7, 125.3, 124.3, 122.4, 118.0, 112.4, 109.6, 53.0, 52.4, 27.5, 23.1. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3282, 2951, 1734, 1654, 1528, 1437, 1374, 1215, 893, 729. HRMS (ESI): calcd for $C_{14}H_{15}O_3N_2ClNa^+$ $[M+Na]^+$: 317.0663, found: 317.0669.



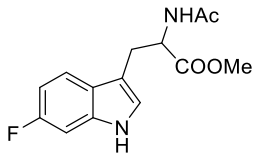

**1c**

**methyl 2-acetamido-3-(5-iodo-1*H*-indol-3-yl)propanoate 1c**. White solid, m.p. 72-73 °C. $^1$H NMR (300 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.84 (s, 1H), 7.42 (d, *J* = 8.7 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 6.93 (d, *J* = 2.1 Hz, 1H), 6.04 (d, *J* = 7.2 Hz, 1H), 4.93 (dd, *J* = 12.9, 8.1 Hz, 1H), 3.72 (s, 3H), 3.34-3.20 (m, 2H), 2.00 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 169.7, 135.1, 130.5, 130.3, 127.7, 123.6, 113.3, 109.6, 83.1, 53.0, 52.5, 27.5, 23.3. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3276, 2951, 2923, 2850, 1737, 1655, 1527, 1455, 1436, 1373, 1213, 879, 795. HRMS (ESI): calcd for $C_{14}H_{15}O_3N_2INa^+$ $[M+Na]^+$: 409.0020, found: 409.0020.



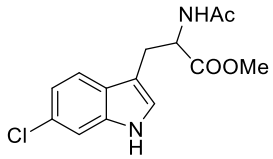

**1d**

**methyl 2-acetamido-3-(6-methyl-1*H*-indol-3-yl)propanoate 1d**. Yellow solid, m.p. 53-54 °C. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.15 (s, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.89 (s, 1H), 6.00 (d, *J* = 6.5 Hz, 1H), 4.94 (dd, *J* = 12.3, 5.3 Hz, 1H), 3.70 (s, 3H), 3.34-3.25 (m, 2H), 2.45 (s, 3H), 1.95 (s, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 172.4, 169.7, 136.6, 132.1, 125.6, 122.0, 121.5, 118.2, 111.2, 109.8, 53.0, 52.3, 27.6, 23.2, 21.6. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3292, 3011, 2951, 2922, 2855, 1740, 1655, 1528, 1437, 1374, 1215, 801. HRMS (ESI): calcd for $C_{15}H_{18}O_3N_2Na^+$ $[M+Na]^+$: 297.1210, found: 297.1211.



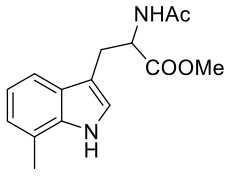

**1e**

**methyl 2-acetamido-3-(6-fluoro-1*H*-indol-3-yl)propanoate 1e**. White solid, m.p. 144-145 °C. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 10.93 (s, 1H), 8.31 (d, *J* = 7.2 Hz, 1H), 7.50-7.44 (m, 1H), 7.14-7.09 (m, 2H), 6.85 (t, *J* = 8.8 Hz, 1H), 4.47 (dd, *J* = 14.0, 7.2 Hz, 1H), 3.57 (s, 3H), 3.13-2.97 (m, 2H), 1.80 (s, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 172.5, 169.3, 158.8 (d, *J* = 187.9 Hz), 135.9 (d, *J* = 10.1 Hz), 124.2 (d, *J* = 2.0 Hz), 123.9, 119.0 (d, *J* = 8.1 Hz), 109.8, 106.9 (d, *J* = 19.2 Hz), 97.4 (d, *J* = 20.2 Hz), 53.1, 51.8, 27.0, 22.3. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -121.0 (s). IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3291, 3067, 2953, 2925, 2850, 1738, 1657, 1629, 1550, 1458, 1438, 1374, 1216, 1140, 952, 804. HRMS (ESI): calcd for $C_{14}H_{15}O_3N_2FNa^+$ [M+Na]$^+$: 301.0959, found: 301.0962.



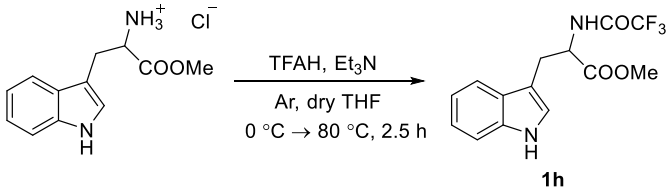

**1f**

**methyl 2-acetamido-3-(6-chloro-1*H*-indol-3-yl)propanoate 1f.** White solid, m.p. 144-145 °C. $^1$H NMR (300 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.35 (d, *J* = 1.5 Hz, 1H), 7.09 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.96 (d, *J* = 2.4 Hz, 1H), 5.98 (d, *J* = 6.9 Hz, 1H), 4.94 (dd, *J* = 13.2, 5.4 Hz, 1H), 3.69 (s, 3H), 3.36-3.23 (m, 2H), 1.97 (s, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 172.3, 169.7, 136.4, 128.2, 126.4, 123.2, 120.5, 119.5, 111.2, 110.4, 53.0, 52.4, 27.6, 23.3. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3282, 2925, 2852, 1737, 1657, 1544, 1456, 1327, 1374, 1215, 907, 805. HRMS (ESI): calcd for $C_{14}H_{15}O_3N_2ClNa^+$ [M+Na]$^+$: 317.0663, found: 317.0668.



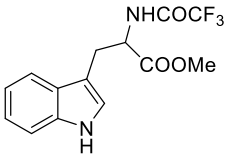

**1g**

**methyl 2-acetamido-3-(7-methyl-1*H*-indol-3-yl)propanoate 1g**. White solid, m.p. 172-173 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 10.82 (s, 1H), 8.28 (d, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.13 (d, *J* = 1.5 Hz, 1H), 6.92-6.86 (m, 2H), 4.48 (dd, *J* = 14.0, 8.0 Hz, 1H), 3.58 (s, 3H), 3.13–2.98 (m, 2H), 2.43 (s, 3H), 1.81 (s, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 172.6, 169.3, 135.6, 126.7, 123.3, 121.5, 120.5, 118.6, 115.6, 109.9, 53.1, 51.7, 27.2, 22.3, 16.7. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3292, 3054, 2924, 2854, 1738, 1657, 1527, 1437, 1374, 1216, 779, 747. HRMS (ESI): calcd for $C_{15}H_{18}O_3N_2Na^+$ [M+Na]$^+$: 297.1210, found: 297.1212.



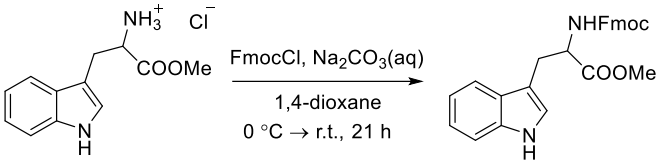

**1h**

*Preparation of **1h***: methyl *L*-tryptophanate hydrochloride (2.0 mmol, 509.4 mg) was dispersed in dry THF (8 mL) under the argon atmosphere and $Et_3N$ (4.0 mmol, 0.6 mL) was added. The mixture was stirred at room temperature for 5 minutes. Trifluoroacetic anhydride (2.2 mmol, 0.3 mL) was then added dropwise at 0 °C. The resulting solution was heated to reflux for 2.5 hours. After cooling to room temperature, the mixture was diluted with ethyl acetate (50 mL) and the organic layer was washed by water (15 mL) and saturated NaCl (10 mL). Ethyl acetate was removed *in vacuum* and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate from 50/1 to 7/1) to afford the desired product methyl (2,2,2-trifluoroacetyl)-*L*-tryptophanate **1h**.



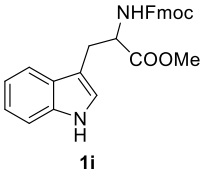
**1h**

**methyl (2,2,2-trifluoroacetyl)-*L*-tryptophanate 1h**. Pale yellow solid, m.p. 109 -111 °C. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 10.89 (s, 1H), 9.92 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.15 (s, 1H), 7.08 (t, *J* = 7.4 Hz, 1H), 6.99 (t, *J* = 7.4 Hz, 1H), 4.59 (dd, *J* = 13.2, 9.2 Hz, 1H), 3.67 (s, 3H), 3.33-3.16 (m, 2H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 170.7, 156.4 (q, *J* = 37.0 Hz), 136.1, 126.9, 123.7, 121.1, 118.5, 117.9, 115.7 (q, *J* = 289.1 Hz), 111.5, 109.1, 53.7, 52.3, 25.9. $^{19}$F NMR (377 MHz, DMSO-$d_6$) δ -74.2 (s). IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3408, 2925, 2851, 1714, 1550, 1458, 1439, 1213, 1175,745. HRMS (ESI): calcd for $C_{14}H_{12}O_3N_2F_2^+$ [M-H]$^+$: 313.0806, found: 313.0800.



**1i**

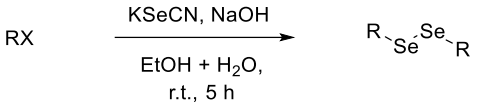
*Preparation of **1i***: methyl *L*-tryptophanate hydrochloride (2.0 mmol, 509.4 mg) was dispersed in 1,4-dioxane (2 mL), $Na_2CO_3$ aqueous solution (10%, 4.0 mL) was then added at 0 °C. After stirring 30 min at 0 °C, FmocCl (1.95 mmol, 504.5 mg in 2 mL of 1,4-dioxane) was added dropwise. The mixture was stirred at 0 °C for another 2 hour and continued overnight at room temperature. After the reaction completed, the mixture was diluted with ethyl acetate (50 mL) and the organic layer was washed by water and saturated NaCl (10 mL). Ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate from 5/1 to 3/1) to afford the desired product methyl (((9*H*-fluoren-9-yl)methoxy)carbonyl)-*L*-tryptophanate **1i**.



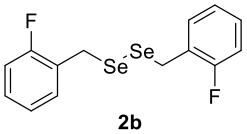
**1i**

**methyl (((9*H*-fluoren-9-yl)methoxy)carbonyl)-*L*-tryptophanate 1i**. Pale yellow solid, m.p. 72 -74 °C. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 10.89 (s, 1H), 7.88 (d, *J* = 7.2 Hz, 3H), 7.67 (t, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.43-7.27 (m, 5H), 7.19 (s, 1H), 7.08 (t, *J* = 7.4 Hz, 1H), 7.00 (t, *J* = 7.4 Hz, 1H), 4.32 (dd, *J* = 13.8, 8.6 Hz, 1H), 4.26-4.19 (m, 3H), 3.62 (s, 3H), 3.22-3.04 (m, 2H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 172.7, 155.9, 143.7, 143.7, 140.7, 136.1, 127.6, 127.1, 125.2, 123.8, 121.0, 120.1, 118.4, 118.0, 111.5, 109.7, 65.7, 55.0, 51.9, 46.6, 26.9. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3414, 3062, 2951, 1710, 1517, 1451, 1340, 1214, 1053, 739. HRMS (ESI): calcd for $C_{27}H_{24}O_4N_2Na^+$ [M+Na]$^+$: 463.1628, found: 463.1625.

2.3 Preparation of substituted diselenides **2**[4]

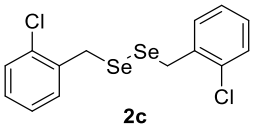



*General procedure*: To the solution of benzyl or alkyl bromide (5 mmol) in ethanol (15 mL) was added KSeCN (6.0 mmol). The solution became cloudy very quickly. The 3.0 M NaOH (4 mL) was added into the mixture after the benzyl or alkyl bromide converted to the intermediates completely (monitored by TLC). The reaction was allowed to stir at room temperature until the intermediates totally converted to the products (monitored by TLC). Most ethanol was removed *in vacuum* and the mixture was diluted with DCM (20 mL) and washed by $H_2O$ (50 mL). The organic layer was dried over anhydrous sodium sulfate, evaporated and purified by silica column chromatography (elute: petroleum ether /dichloromethane) to afford the desired product substituted diselenides **2**.



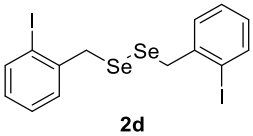

**2b**

**1,2-bis(2-fluorobenzyl)diselane 2b**. Yellow solid, m.p. 58-59 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.25-7.17 (m, 4H), 7.10-7.01 (m, 4H), 3.91 (s, 4H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 160.6 (d, *J* = 248.5 Hz), 131.0 (d, *J* = 4.0 Hz), 128.9 (d, *J* = 9.1 Hz), 126.4 (d, *J* = 14.1 Hz), 123.9 (d, *J* = 3.0 Hz), 115.5 (d, *J* = 21.2 Hz), 25.1 (d, *J* = 2.0 Hz). $^{19}$F NMR (377 MHz, $CDCl_3$) δ -116.9 (s). IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3069, 2921, 1581, 1489, 1457, 1234, 1171, 1079, 1074, 856, 764. HRMS (APCI): calcd for $C_{14}H_{13}F_2Se_2^+$ [M+H]+: 378.9310, found: 378.9307.



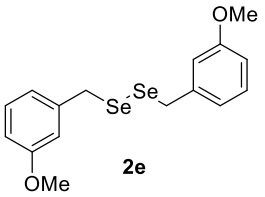

**2c**

**1,2-bis(2-chlorobenzyl)diselane 2c**. Yellow solid, m.p. 102-103 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.40-7.34 (m, 2H ), 7.20-7.19 (m, 6H), 3.99 (s, 4H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 136.7, 133.8, 130.8, 129.7, 128.5, 126.6, 30.5. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3060, 2996, 2923, 1589, 1475, 1442, 1414, 1172, 1050, 1032, 831, 757, 725. HRMS (EI): calcd for $C_{14}H_{12}Cl_2Se_2^+$ $[M]^+$: 409.8641, found: 409.8634.



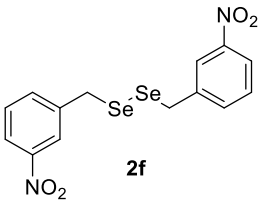

**2d**

**1,2-bis(2-iodobenzyl)diselane 2d.** Yellow solid, m.p. 96-97 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.30-7.27 (m, 2H), 7.21-7.19 (m, 2H), 6.93 (t, *J* = 7.4 Hz, 2H), 3.99 (s, 4H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 141.4, 139.7, 130.0, 128.7, 128.2, 100.5, 38.5. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3356, 2922, 2851, 2372, 2320, 1658, 1632, 1467, 1435, 1362, 1010, 752. HRMS (APCI): calcd for $C_{14}H_{13}I_2Se_2^+$ $[M+H]^+$: 594.7432, found: 594.7428.



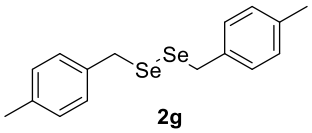

**2e**

**1,2-bis(3-methoxybenzyl)diselane 2e**. Yellow oil. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 7.21 (t, *J* = 7.7 Hz, 2H), 6.84-6.78 (m, 6H), 3.83 (s, 4H), 3.81 (s, 6H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 159.6, 140.5, 129.4, 121.3, 114.5, 112.7, 55.2, 32.7. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 2998, 2936, 2833, 1598, 1584, 1486, 1465, 1452, 1436, 1294, 1264, 1152, 1044, 780, 734, 695. HRMS (APCI): calcd for $C_{16}H_{17}O_2Se_2^+$ $[M+H]^+$: 402.9710, found: 402.9706.



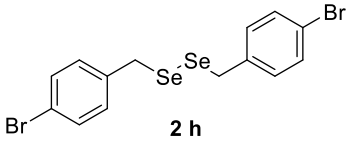

**2f**

**1,2-bis(3-nitrobenzyl)diselane 2f.** Yellow solid, m.p. 108-109 °C. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.10-8.05 (m, 4H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 2H), 4.12 (s, 4H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 147.5, 141.9, 135.5, 129.8, 123.3, 121.8, 29.6. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3083, 2924, 1525, 1353, 1315, 1097, 1075, 807, 738, 684, 673. HRMS (APCI): calcd for $C_{14}H_{13}O_4N_2Se_2^+$ $[M+H]^+$: 432.9200, found: 432.9202.



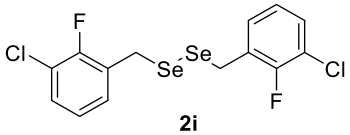

**2g**

**1,2-bis(4-methylbenzyl)diselane 2g**. Yellow solid, m.p. 58-59 °C. $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.12 (s, 8H), 3.85 (s, 4H), 2.33 (s, 6H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 136.8, 135.9, 129.1, 128.9, 32.5, 21.2. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3020, 2919, 2854, 1896, 1152, 1448, 1417, 1171, 814. HRMS (nano ESI): calcd for $C_{16}H_{18}Se_2Na^+$ $[M+Na]^+$: 392.9634, found: 392.9616.




**2 h**

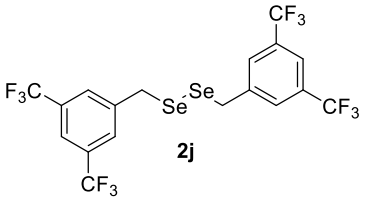
**1,2-bis(4-bromobenzyl)diselane 2h**. Yellow solid, m.p. 105-106 °C. $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.5 Hz, 4H), 7.06 (d, *J* = 8.0 Hz, 4H), 3.79 (s, 4H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 137.9, 131.6, 130.6, 121.0, 31.7. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 2923, 2850, 1900, 1527, 1483, 1399, 1352, 1168, 1070, 1009, 847, 819, 802, 475. HRMS (EI): calcd for $C_{14}H_{12}Br_2Se_2^+$ $[M]^+$: 497.7631, found: 497.7621.




**2i**

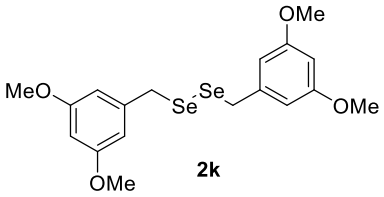
**1,2-bis(3-chloro-2-fluorobenzyl)diselane 2i**. Yellow solid, m.p. 54-55 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.4 Hz, 2H), 7.05-7.00 (m, 4H), 3.92 (s, 4H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 156.1 (d, *J* = 251.5 Hz), 129.6, 129.1 (d, *J* = 3.0 Hz), 128.1 (d, *J* = 15.2 Hz), 124.3 (d, *J* = 4.0 Hz), 121.2 (d, *J* = 18.2 Hz), 24.8 (d, *J* = 2.0 Hz). $^{19}$F NMR (377 MHz, $CDCl_3$) δ -118.7 (s). IR $\nu_{max}$

(KBr, film, $cm^{-1}$): 2921, 2850, 2320, 1468, 1458, 1229, 1189, 1170, 894, 778, 725. HRMS (EI): calcd for $C_{14}H_{12}F_2Cl_2Se_2^+$ $[M]^+$: 445.8453, found: 445.8444.



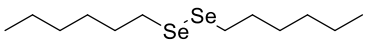
**2j**

**1,2-bis(3,5-bis(trifluoromethyl)benzyl)diselane 2j**. Yellow solid, m.p. 62-63 °C. $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 2H), 7.61 (s, 4H), 3.86 (s, 4H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 141.1, 131.7 (q, *J* = 34.3 Hz), 128.6 (q, *J* = 3.0 Hz), 122.9 (q, *J* = 267.3 Hz), 120.9 (q, *J* = 4.0 Hz), 30.2. $^{19}F$ NMR (377 MHz, $CDCl_3$) δ -63.0 (s). IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3359, 3189, 2923, 2851, 1464, 1374, 1278, 1171, 1132, 923, 896, 857, 729, 704, 683. HRMS (APCI): calcd for $C_{18}H_{19}F_{12}Se_2^+$ $[M+H]^+$: 612.8849, found:612.8842.



**2k**

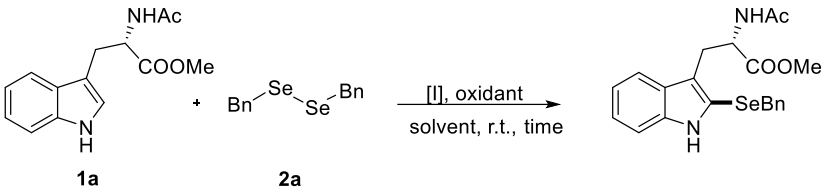
**1,2-bis(3,5-dimethoxybenzyl)diselane 2k**. Yellow solid, m.p. 53-54 °C. $^1H$ NMR (500 MHz, $CDCl_3$) δ 6.40 (s, 4H), 6.36 (s, 2H), 3.83 (s, 4H), 3.79 (s, 12H). $^{13}C$ NMR (126 MHz, $CDCl_3$) δ 160.7, 141.2, 106.9, 99.3, 55.3, 33.0. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 2998, 2937, 2835, 1595, 1462, 1429, 1345, 1322, 1297, 1206, 1156, 1059, 833, 694. HRMS (APCI): calcd for $C_{18}H_{23}O_4Se_2^+$ $[M+H]^+$: 462.9921, found: 462.9919.



**2m**

**1,2-dihexyldiselane 2m.** Yellow oil. $^1H$ NMR (400 MHz, $CDCl_3$) δ 2.91 (t, *J* = 7.4 Hz, 4H), 1.76-1.69 (m, 4H), 1.41-1.26 (m, 12H), 0.89 (t, *J* = 6.6 Hz, 6H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 31.3, 31.0, 30.3, 29.2, 22.6, 14.0. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 2956, 2925, 2854, 1466, 1378, 1227, 1183, 723. HRMS (EI): calcd for $C_{12}H_{26}Se_2^+$ $[M+H]^+$: 330.0359, found: 330.0357.

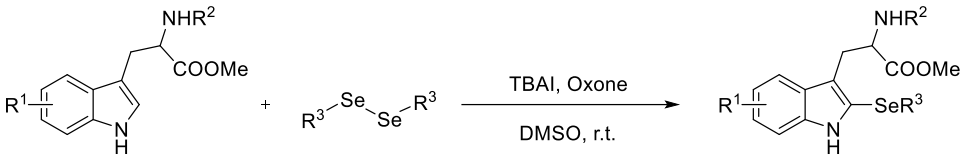
### 3. Optimizaiton of reaction conditions



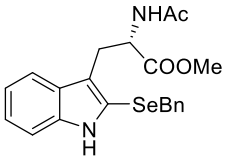

| Entry | [I] (equiv.) | Oxidant (equiv.) | solvent | time | Yield (%) |
|---|---|---|---|---|---|
| 1[b] | TBAI (0.1) | 35% $H_2O_2$ (1.02) | $CH_3CN$ | 24 h | 31 |
| 2[b] | TBAI (0.1) | 35% $H_2O_2$ (1.02) | $H_2O$ | 24 h | N. R. |
| 3[c] | TBAI (0.1) | 35% $H_2O_2$ (1.02) | $H_2O$ + $CH_3CN$ | 24 h | trace |
| 4[b] | TBAI (0.1) | 35% $H_2O_2$ (2.04) | $CH_3CN$ | 19 h | 41 |
| 5[b] | TBAI (1.0) | 35% $H_2O_2$ (1.02) | $CH_3CN$ | 24 h | N. R. |
| 6[b] | TBAI (1.0) | 35% $H_2O_2$ (2.04) | $CH_3CN$ | 24 h | N. R. |
| 7[b] | TBAI (0.1) | 35% $H_2O_2$ (2.04) | DCM | 24 h | 42 |
| 8[b] | TBAI (0.1) | 35% $H_2O_2$ (2.04) | THF | 24 h | 6 |
| 9[b] | TBAI (0.1) | 35% $H_2O_2$ (2.04) | EA | 24 h | 47 |
| 10[b] | TBAI (0.1) | 35% $H_2O_2$ (2.04) | MeOH | 24 h | 21 |
| 11[b] | TBAI (0.1) | 35% $H_2O_2$ (2.04) | DMF | 24 h | N. R. |
| 12[d] | KI (0.1) | Oxone (1.00) | $H_2O$ + $CH_3CN$ | 1 h | 56 |
| 13[d] | KI (0.2)) | Oxone (1.00) | $H_2O$ + $CH_3CN$ | 1 h | 53 |
| 14[d] | KI (0.05) | Oxone (1.00) | $H_2O$ + $CH_3CN$ | 1 h | 49 |
| 15[d] | TBAI (0.05) | Oxone (1.00) | $H_2O$ + $CH_3CN$ | 1 h | 59 |
| 16[d] | NaI (0.05) | Oxone (1.00) | $H_2O$ + $CH_3CN$ | 1 h | 55 |
| 17[d] | KI (0.05) | Oxone (0.75) | $H_2O$ + $CH_3CN$ | 1 h | 54 |
| 18[d] | KI (0.05) | Oxone (0.50) | $H_2O$ + $CH_3CN$ | 1 h | 54 |
| 19[e] | TBAI (0.05) | Oxone (1.00) | $H_2O$ | 1 h | N. D. |
| 20[e] | TBAI (0.05) | Oxone (1.00) | $CH_3CN$ | 1 h | 43 |
| 21[e] | TBAI (0.05) | Oxone (1.00) | DMSO | 20 min | 85 |
| 22[e] | TBAI (0.05) | Oxone (1.00) | DMF | 20 min | 69 |
| 23[e] | TBAI (0.05) | Oxone (1.00) | MeOH | 15 min | 31 |
| 24[e,f] | TBAI (0.05) | Oxone (1.00) | DMSO | 8 min | 94 |
| 25[e,f] | *n*-$Bu_4NI_3$ (0.05) | Oxone (1.00) | DMSO | 10 min | 89 |
| 26[e,f] | TBAI (0.05) | $O_2$ (1 atm) | DMSO | 24 h | N. R. |

[a] Unless noted otherwise, all the reactions were conducted with *L*-methyl acetyl-tryptophanate (0.1 mmol), dibenzyldiselenide (0.1 mmol), catalyst, oxidant in solvent. Isolated yields were given. [b] 0.5 mL solvent. [c] Solvent: 0.25 mL $CH_3CN$ and 0.25 mL $H_2O$. [d] Solvent: 0.5 mL $CH_3CN$ and 0.05 mL $H_2O$. [e] 0.55 mL solvent. [f] Quenched by 1 mL saturated $Na_2S_2O_3$ (aq.) before purification.

**4. General procedure for synthesis of 3, 4 and 5**

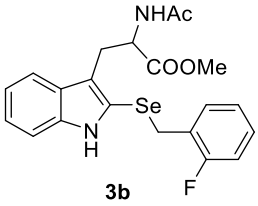



*General procedure*: To the mixture of acetyl tryptophanate (0.1 mmol), diselenide (0.1 mmol) and TBAI (5 mol%) was added DMSO (0.55 mL). And then oxone (0.1 mmol) was added in one portion. The reaction was stirred at room temperature until the acetyl tryptophanate totally disappeared (monitored by TLC). Saturated sodium thiosulfate (1 mL) was added to quench the reaction. The reaction was diluted with ethyl acetate (5 mL) and washed by $H_2O$ (20 mL). Aqueous phase was extracted with ethyl acetate (5 mL × 2). The organic layer was combined, ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3) to afford the desired products **3/4**.



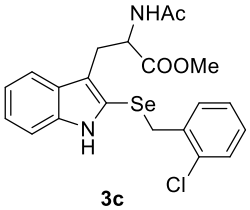

**3a**

**methyl (*S*)-2-acetamido-3-(2-(benzylselanyl)-1*H*-indol-3-yl)propanoate 3a**. Yellow solid, 40.2 mg (from 0.1 mmol), 94% yield, > 99.9% ee, m.p. 55-57 °C. $[\alpha]_D^{28}$ = 20.4 (c 0.25, $CHCl_3$) $^1$H NMR (300 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.22-7.17 (m, 5H), 7.14-7.09 (m, 1H), 7.04-7.01 (m, 2H), 6.00 (d, *J* = 7.6 Hz, 1H), 4.84 (dd, *J* = 13.8, 6.0 Hz, 1H), 3.92 (s, 2H), 3.66 (s, 3H), 3.22-3.06 (m, 2H), 1.91 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 169.7, 138.6, 137.4, 128.7, 128.6, 127.7, 127.1, 123.0, 120.9, 119.8, 118.7, 117.1, 110.7, 52.9, 52.4, 33.5, 27.9, 23.2. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3272, 3059, 2950, 2854, 1738, 1657, 1517, 1494, 1436, 1373, 1340, 1216, 743, 697. HRMS (ESI): calcd for $C_{20}H_{19}O_3N_2Se^+$ $[M-H]^+$: 429.0723, found: 429.0730. The enantiomeric excess was determined by HPLC on the Chiralpak IA column connected in series (*n*-Hexane : isopropanol = 80 :1, flowing rate = 1.0 mL/min, 25 °C, UV detection at λ = 254 nm), $t_R$ = 16.2 min.



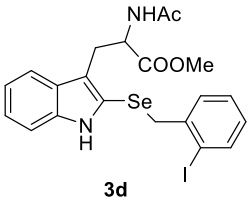

**3b**

**methyl 2-acetamido-3-(2-((2-fluorobenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3b.** Pale yellow solid, 38.5 mg (from 0.1 mmol), 86% yield, m.p. 52-54 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.23 (s, 1H), 7.19-7.16 (m, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 6.97 (t, *J* = 9.2 Hz, 1H), 6.89 (t, *J* = 7.4 Hz, 1H), 6.81 (t, *J* = 7.6 Hz, 1H), 5.99 (d, *J* = 7.6 Hz, 1H), 4.84 (dd, *J* = 12.8, 6.0 Hz, 1H), 3.92 (s, 2H), 3.67 (s, 3H), 3.52 (s, 1H), 3.19-3.03 (m, 2H), 1.90 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 160.45 (d, *J* = 248.5 Hz), 137.4, 130.6 (d, *J* = 4.0 Hz), 129.0 (d, *J* = 8.0 Hz), 127.7, 126.0 (d, *J* = 14.1 Hz), 124.0 (d, *J* = 4.0 Hz), 123.1, 120.6, 119.9, 118.8, 117.5, 115.4 (d, *J* = 21.2 Hz), 110.8, 52.8, 52.4, 27.8, 26.0 (d, *J* = 3.0 Hz), 23.2. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -117.3 (s). IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3271, 3059, 2950, 2922, 2850, 1738, 1657, 1520, 1491, 1437, 1374, 1340, 1233, 1216, 858, 745. HRMS (ESI): calcd for $C_{21}H_{21}O_3N_2FNaSe^+$ $[M+Na]^+$: 471.0594, found: 471.0591.



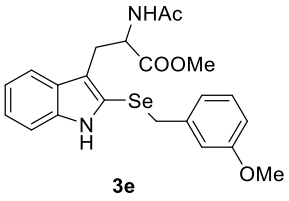

**3c**

**methyl 2-acetamido-3-(2-((2-chlorobenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3c**. Pale yellow solid, 33.6 mg (from 0.1 mmol), 72% yield, m.p. 62-63 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.24 (s, 1H), 7.21-7.09 (m, 3H), 6.98 (t, *J* = 7.2 Hz, 1H), 6.75 (d, *J* = 7.6 Hz, 1H), 5.95 (d, *J* = 6.8 Hz, 1H), 4.83 (dd, *J* = 13.2, 6.0 Hz, 1H), 4.00 (s, 2H), 3.67 (s, 3H), 3.18-3.00 (m, 2H), 1.90 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 137.3, 136.4, 133.7, 130.4, 129.8, 128.6, 127.8, 126.7, 123.2, 120.5, 120.0, 118.9, 117.8, 110.7, 52.8, 52.4, 31.3, 27.9, 23.2. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3264, 3056, 2950, 2921, 2849, 1738, 1658, 1521, 1444, 1374, 1340, 1215, 1052, 1033, 745. HRMS (ESI): calcd for $C_{21}H_{20}O_3N_2ClSe^+$ $[M-H]^+$: 463.0333, found: 463.0329.



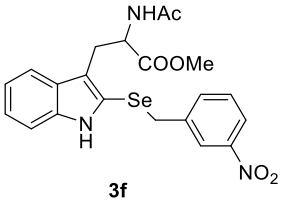

**3d**

**methyl 2-acetamido-3-(2-((2-iodobenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3d**. Pale yellow solid, 49.2 mg (from 0.1 mmol), 89% yield, m.p. 67-69 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.08 (dt, *J* = 22.8, 7.6 Hz, 2H), 6.89 (t, *J* = 7.6 Hz, 1H), 6.75 (d, *J* = 7.6 Hz, 1H), 5.96 (d, *J* = 7.6 Hz, 1H), 4.83 (dd, *J* = 13.2, 6.0 Hz, 1H), 4.02 (s, 2H), 3.68 (s, 3H), 3.17-2.99 (m, 2H), 1.91 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 141.0, 139.8, 137.4, 129.6, 128.8, 128.2, 127.8, 123.2, 120.4, 120.0, 118.9, 117.9, 110.8, 100.3, 52.8, 52.4, 39.4, 27.9, 23.2. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3271, 3055, 2923, 2851, 1737, 1655, 1520, 1436, 1374, 1340, 1215, 1011, 744. HRMS (ESI): calcd for $C_{21}H_{20}O_3N_2ISe^+$ $[M-H]^+$: 554.9689, found: 554.9686.



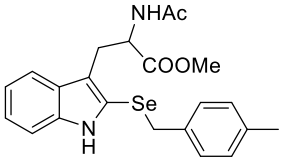

**3e**

**methyl 2-acetamido-3-(2-((3-methoxybenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3e**. Pale yellow solid, 42.6 mg (from 0.1 mmol), 93% yield, m.p. 48-50 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.24-7.22 (m, 1H), 7.19-7.08 (m, 3H), 6.75 (d, *J* = 8.0 Hz, 1H), 6.67 (d, *J* = 7.2 Hz, 1H), 6.47 (s, 1H), 5.97 (d, *J* = 6.8 Hz, 1H), 4.84 (dd, *J* = 12.4, 6.4 Hz, 1H), 3.89 (s, 2H), 3.67 (s, 3H), 3.55 (s, 3H), 3.24-3.11 (m, 2H), 1.91 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 159.5, 140.1, 137.3, 129.5, 127.8, 123.0, 120.1, 120.9, 119.9, 118.7, 117.2, 113.6, 113.3, 110.7, 55.0, 52.9, 52.4, 33.4, 27.9, 23.2. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3268, 3054, 2916, 2849, 1743, 1659, 1599, 1517, 1488, 1437, 1374, 1340, 1265, 1215, 1040, 738, 697. HRMS (ESI): calcd for $C_{22}H_{23}O_4N_2Se^+$ $[M-H]^+$: 459.0829, found: 459.0826.



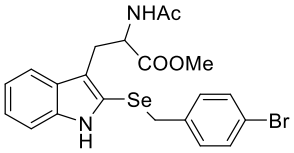

**3f**

**methyl 2-acetamido-3-(2-((3-nitrobenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3f.** Yellow solid, 43.5 mg (from 0.1 mmol), 92% yield, m.p. 64-66 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.04-8.01 (m, 2H), 7.88 (s, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.24 -7.18 (m, 3H), 7.11 (t, *J* = 7.2 Hz, 1H), 5.95 (d, *J* = 7.6 Hz, 1H), 4.84 (dd, *J* = 13.0, 6.2 Hz, 1H), 3.99 (s, 2H), 3.65 (s, 3H), 3.16-3.02 (m, 2H), 1.91 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 169.6, 148.1, 140.8, 137.4, 134.6, 129.3, 127.7, 123.6, 123.5, 122.0, 120.2, 119.5, 118.9, 118.2, 110.8, 52.8, 52.4, 32.1, 28.1, 23.2. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3263, 3059, 2922, 2850, 1737, 1657, 1527, 1436, 1349, 1216, 810, 739, 686. HRMS (ESI): calcd for $C_{21}H_{20}O_5N_3Se^+$ [M-H]$^+$: 474.0574, found: 474.0570.



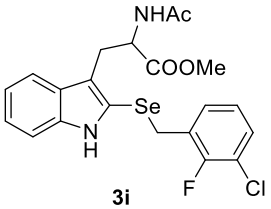

**3g**

**methyl 2-acetamido-3-(2-((4-methylbenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3g**. Pale yellow solid, 35.4 mg (from 0.1 mmol), 80% yield, m.p. 56-57 °C. $^1$H NMR (400 MHz, CDCl3) δ 7.84 (s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.23-7.15 (m, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 7.6 Hz, 2H), 5.97 (d, *J* = 7.2 Hz, 1H), 4.85 (dd, *J* = 13.0, 6.2 Hz, 1H), 3.91 (s, 2H), 3.67 (s, 3H), 3.25-3.12 (m, 2H), 2.32 (s, 3H), 1.91 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 137.3, 137.0, 135.6, 129.2, 128.6, 127.8, 123.0, 121.2, 119.9, 118.8, 117.0, 110.7, 52.9, 52.4, 33.4, 28.0, 23.2, 21.1. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3269, 3051, 2923, 2851, 1737, 1655, 1513, 1437, 1374, 1340, 1216, 817, 742. HRMS (ESI): calcd for $C_{22}H_{23}O_3N_2Se^+$ [M-H]$^+$: 443.0879, found: 443.0878.



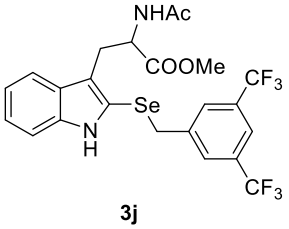

**3h**

**methyl 2-acetamido-3-(2-((4-bromobenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3h**. Pale yellow solid, 45.3 mg (from 0.1 mmol), 89% yield, m.p. 68-69 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 7.6 Hz, 2H), 7.24 (s, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.11 (t, *J* = 7.4 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 2H), 5.96 (d, *J* = 7.6 Hz, 1H), 4.86 (dd, *J* = 13.0, 6.2 Hz, 1H), 3.86 (s, 2H), 3.66 (s, 3H), 3.21-3.07 (m, 2H), 1.91 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 137.8, 137.3, 131.6, 130.3, 127.7, 123.2, 121.0, 120.4, 120.0, 118.8, 117.6, 110.8, 52.8, 52.4, 32.7, 28.0, 23.2. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3270, 3056, 2917, 2849, 1737, 1655, 1521, 1486, 1437, 1374, 1340, 1216, 1011, 744. HRMS (ESI): calcd for $C_{21}H_{20}O_3N_2BrSe^+$ [M-H]$^+$: 506.9828, found: 506.9822.



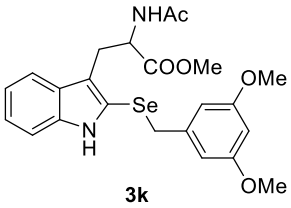

**3i**

**methyl 2-acetamido-3-(2-((3-chloro-2-fluorobenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3i**. Pale yellow solid, 42.4 mg (from 0.1 mmol), 88% yield, m.p. 59-61 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.28 (s, 1H), 7.24-7.18 (m, 2H), 7.10 (t, *J* = 7.2 Hz, 1H), 6.82 (t, *J* = 7.6 Hz, 1H), 6.68 (t, *J* = 7.0 Hz, 1H), 5.95 (d, *J* = 7.2 Hz, 1H), 4.85 (dd, *J* = 12.4, 6.0 Hz, 1H), 3.92 (s, 2H), 3.67 (s, 3H), 3.21-3.04 (m, 2H), 1.90 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 155.9 (d, *J* = 250.5 Hz), 137.4, 129.5, 128.7 (d, *J* = 3.0 Hz), 127.9 (d, *J* = 15.2 Hz), 127.7, 124.3 (d, *J* = 5.1 Hz), 123.3, 121.2 (d, *J* = 17.2 Hz), 120.1, 120.0, 118.9, 117.8, 110.8, 52.8, 52.4, 28.0, 25.9 (d, *J* = 2.0 Hz), 23.2. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -119.0 (s). IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3271, 3056, 2952, 2925, 2848, 1734, 1655, 1516, 1459, 1436, 1373, 1340, 1216, 895, 784, 743, 728. HRMS (ESI): calcd for $C_{21}H_{19}O_3N_2FClSe^+$ [M-H]$^+$: 481.0239, found: 481.0234.



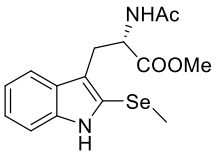

**3j**

**methyl 2-acetamido-3-(2-((3,5-bis(trifluoromethyl)benzyl)selanyl)-1*H*-indol-3-yl)propanoate 3j**. Pale yellow solid, 47.7 mg (from 0.1 mmol), 84% yield, m.p. 54-56 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.66 (s, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.34 (s, 2H), 7.24-7.17 (m, 2H), 7.11 (t, *J* = 7.2 Hz, 1H), 5.95 (d, *J* = 7.6 Hz, 1H), 4.85 (dd, *J* = 13.0, 6.2 Hz, 1H), 3.98 (s, 2H), 3.65 (s, 3H), 3.11-2.95 (m, 2H), 1.89 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 141.4, 137.4, 131.6 (q, *J* = 33.7 Hz), 128.6 (q, *J* = 3.7 Hz), 127.6, 123.6, 123.0 (q, *J* = 274.0 Hz), 120.7 (q, *J* = 3.7 Hz), 120.2, 118.9, 118.8, 118.2, 110.9, 52.9, 52.4, 31.7, 28.0, 23.1. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -63.0 (s). IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3263, 2915, 2850, 1737, 1659, 1521, 1438, 1375, 1278, 1173, 1134, 895, 744, 704, 683. HRMS (ESI): calcd for $C_{23}H_{19}O_3N_2F_6Se^+$ [M-H]$^+$: 565.0471, found: 565.0466.



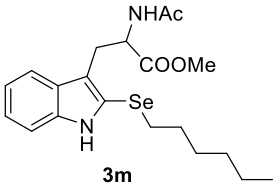

**3k**

**methyl 2-acetamido-3-(2-((3,5-dimethoxybenzyl)selanyl)-1*H*-indol-3-yl)propanoate 3k**. Pale yellow solid, 44.1 mg (from 0.1 mmol), 90% yield, m.p. 55-57 °C. $^1$H NMR (300 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.24-7.07 (m, 3H), 6.30 (s, 1H), 6.13 (d, *J* = 2.1 Hz, 2H), 6.00 (d, *J* = 7.8 Hz, 1H), 4.85 (dd, *J* = 13.6, 5.9 Hz, 1H), 3.84 (s, 2H), 3.67 (s, 3H), 3.55 (s, 6H), 3.28-3.13 (m, 2H), 1.91 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 160.7, 140.9, 137.3, 127.8, 123.1, 120.9, 119.9, 118.7, 117.2, 110.7, 106.3, 99.7, 55.1, 52.9, 52.4, 33.6, 28.0, 23.2. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3271, 3000, 2923, 2849, 1743, 1657, 1595, 1520, 1459, 1430, 1340, 1205, 1152, 1059, 836, 745, 695. HRMS (ESI): calcd for $C_{23}H_{25}O_5N_2Se^+$ [M-H]$^+$: 489.0934, found: 489.0934.



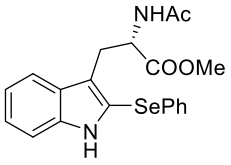

**3l**

**methyl (*S*)-2-acetamido-3-(2-(methylselanyl)-1H-indol-3-yl)propanoate 3l**. Yellow solid, 27.9 mg (from 0.1 mmol), 79% yield, m.p. 52-54 °C. $[\alpha]_D^{28}$ = 45.6 (c 0.25, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 6.10 (d, *J* = 7.4 Hz, 1H), 4.92 (dd, *J* = 13.4, 5.8 Hz, 1H), 3.69 (s, 3H), 3.43-3.31 (m, 2H), 2.23 (s, 3H), 1.94 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 169.7, 137.3, 127.9, 122.8, 121.9, 119.9, 118.5, 115.5, 110.7, 53.0, 52.4, 28.2, 23.2, 9.7. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3271, 3056, 2928, 2852, 1737, 1657, 1525, 1436, 1374, 1340, 1265, 1216, 1010, 802, 743. HRMS (ESI): calcd for $C_{15}H_{17}O_3N_2Se^+$ [M-H]$^+$: 353.0410, found: 353.0417.



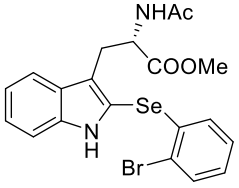

**3m**

**methyl 2-acetamido-3-(2-(hexylselanyl)-1*H*-indol-3-yl)propanoate 3m**. Orange oil, 34.0 mg (from 0.1 mmol), 80% yield. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 6.11 (d, *J* = 7.4 Hz, 1H), 4.91 (dd, *J* = 12.2, 5.4 Hz, 1H), 3.69 (s, 3H), 3.41-3.33 (m, 2H), 2.75 (t, *J* = 7.4 Hz, 2H), 1.94 (s, 3H), 1.63-1.56 (m, 2H), 1.37-1.20 (m, 6H), 0.85 (t, *J* = 6.4 Hz, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 169.7, 137.3, 127.8, 122.8, 121.2, 119.8, 118.5, 116.2, 110.7, 53.0, 52.4, 31.2, 30.6, 30.0, 29.3, 28.2, 23.2, 22.5, 14.0. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3271, 3057, 2955, 2926, 2854, 1737, 1657, 1521. 1436, 1374, 1340, 1261, 1216, 1011 799, 743. HRMS (ESI): calcd for $C_{20}H_{28}O_3N_2NaSe^+$ [M+Na]$^+$: 447.1157, found: 447.1164.




**3n**

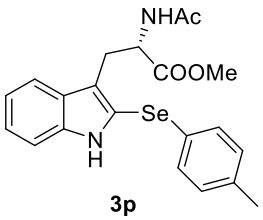
**methyl (*S*)-2-acetamido-3-(2-(phenylselanyl)-1*H*-indol-3-yl)propanoate 3n**. Pale yellow solid, 31.5 mg (from 0.1 mmol), 76% yield, m.p. 65-66 °C. $[\alpha]_D^{28}$ = 38.8 (c 0.25, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.24-7.20 (m, 6H), 7.14 (t, *J* = 7.6 Hz, 1H), 5.99 (d, *J* = 7.6 Hz, 1H), 4.91 (dd, *J* = 13.4, 5.8 Hz, 1H), 3.68 (s, 3H), 3.46-3.33 (m, 2H), 1.78 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.8, 137.7, 131.4, 129.6, 129.6, 127.8, 126.9, 123.4, 120.1, 119.8, 119.0, 117.6, 111.0, 52.9, 52.4, 28.2, 23.0. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3261, 3056, 2924, 2853, 1734, 1657, 1517, 1477, 1438, 1374, 1340, 1218, 1021, 799, 737, 689. HRMS (ESI): calcd for $C_{20}H_{19}O_3N_2Se^+$ [M-H]$^+$: 415.0566, found: 415.0577.




**3o**

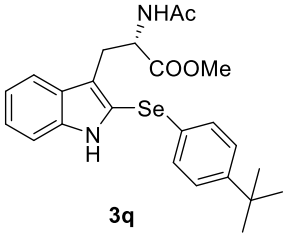
**methyl (*S*)-2-acetamido-3-(2-((2-bromophenyl)selanyl)-1*H*-indol-3-yl)propanoate 3o**. Yellow solid, 15.7 mg (from 0.1

mmol), 32% yield, m.p. 80-81 °C. $[\alpha]_D^{28}$ = 37.6 (c 0.125, $CHCl_3$). $^1H$ NMR (400 MHz, $CDCl_3$) δ, 8.41 (s, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.49-7.47 (m, 1H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.27-7.25 (m, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.06-7.00 (m, 2H), 6.59-6.56 (m, 1H), 5.99 (d, *J* = 7.6 Hz, 1H), 4.92 (dd, *J* = 13.4, 5.8 Hz, 1H), 3.68 (s, 3H), 3.46-3.30 (m, 2H), 1.77 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 172.2, 169.8, 138.0, 135.4, 132.8, 129.0, 128.3, 127.9, 127.6, 123.9, 121.8, 120.3, 119.4, 119.3, 119.0, 111.2, 52.9, 52.5, 28.2, 23.0. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3261, 3055, 2950, 2923, 2850, 1737, 1657, 1521, 1441, 1374, 1341, 1218, 1010, 744. HRMS (ESI): calcd for $C_{20}H_{18}O_3N_2BrSe^+$ $[M-H]^+$: 492.9672, found: 492.9681.



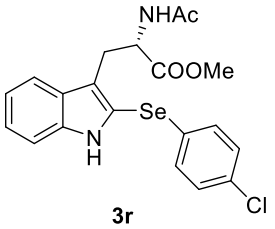
**3p**

**methyl (*S*)-2-acetamido-3-(2-(*p*-tolylselanyl)-1*H*-indol-3-yl)propanoate 3p**. Pale yellow solid, 26.6 mg (from 0.1 mmol), 62% yield, m.p. 65-66 °C. $[\alpha]_D^{28}$ = 42.9 (c 0.245, $CHCl_3$). $^1H$ NMR (400 MHz, CDCl3) δ 8.21 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.18-7.11 (m, 3H), 7.04 (d, *J* = 8.0 Hz, 2H), 5.99 (d, *J* = 7.6 Hz, 1H), 4.91 (dd, *J* = 13.2, 6.0 Hz, 1H), 3.69 (s, 3H), 3.45-3.33 (m, 2H), 2.28 (s, 3H), 1.80 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 172.3, 169.8, 137.6, 137.1, 130.4, 130.3, 127.9, 127.2, 123.2, 120.6, 120.1, 118.9, 116.9, 110.9, 52.9, 52.5, 28.2, 23.0, 21.0. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3271, 3056, 2950, 2925, 2855, 1743, 1657, 1517, 1489, 1436, 1374, 1340, 1216, 1014, 802, 744. HRMS (ESI): calcd for $C_{20}H_{21}O_3N_2Se^+$ $[M-H]^+$: 429.0723, found: 429.0733.



**3q**

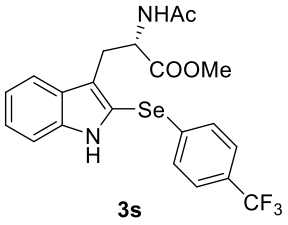
**methyl (*S*)-2-acetamido-3-(2-((4-(*tert*-butyl)phenyl)selanyl)-1*H*-indol-3-yl)propanoate 3q**. Pale yellow solid, 36.9 mg (from 0.1 mmol), 78% yield, m.p. 80-82 °C. $[\alpha]_D^{28}$ = 29.0 (c 0.255, $CHCl_3$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.24-7.23 (m, 2H), 7.21-7.12 (m, 4H), 5.98 (d, *J* = 7.6 Hz, 1H), 4.91 (dd, *J* = 13.2, 6.0 Hz, 1H), 3.70 (s, 3H), 3.47-3.34 (m, 2H), 1.76 (s, 3H), 1.26 (s, 9H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 172.3, 169.8, 150.4, 137.7, 129.7, 127.8, 127.5, 126.7, 123.3, 120.3, 120.1, 118.9, 117.2, 110.9, 53.0, 52.5, 34.5, 31.2, 28.2, 23.0. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3271, 3054, 2960, 2865, 1738, 1659, 1517, 1498, 1436, 1374, 1341, 1217, 1113, 1010, 820, 743, 542. HRMS (ESI): calcd for $C_{24}H_{27}O_3N_2Se^+$ $[M-H]^+$: 471.1192, found: 471.1202.



**3r**

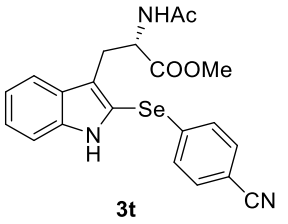
**methyl (*S*)-2-acetamido-3-(2-((4-chlorophenyl)selanyl)-1*H*-indol-3-yl)propanoate 3r.** Pale yellow solid, 32.9 mg (from 0.1 mmol), 73% yield, m.p. 72-74 °C. $[\alpha]_D^{28}$ = 41.2 (c 0.255, $CHCl_3$). $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.19-7.10 (m, 5H), 5.99 (d, *J* = 8.0 Hz, 1H), 4.92 (dd, *J* = 13.4, 5.8 Hz, 1H),

3.67 (s, 3H), 3.45-3.31 (m, 2H), 1.84 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.7, 137.7, 133.1, 130.9, 129.7, 129.6, 127.8, 123.6, 120.3, 119.4, 119.1, 117.9, 111.1, 52.9, 52.5, 28.3, 23.1. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3271, 3056, 2951, 2926, 2854, 2738, 1651, 1517, 1473, 1436, 1374, 1340, 1218, 1088, 1009, 812, 744. HRMS (ESI): calcd for $C_{20}H_{18}O_3N_2ClSe^+$ $[M-H]^+$: 449.0177, found: 449.0186.



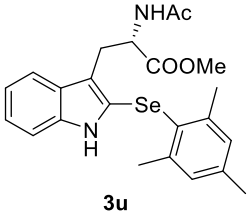
**3s**

**methyl (*S*)-2-acetamido-3-(2-((4-(trifluoromethyl)phenyl)selanyl)-1*H*-indol-3-yl)propanoate 3s**. Yellow solid, 32.1 mg (from 0.1 mmol), 66% yield, m.p. 77-79 °C. $[\alpha]_D^{28}$ = 45.6 (c 1.01, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.27-7.25 (m, 1H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.00 (d, *J* = 7.6 Hz, 1H), 4.92 (dd, *J* = 13.6, 6.0 Hz, 1H), 3.66 (s, 3H), 3.45-3.31 (m, 2H), 1.81 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 169.7, 137.9, 137.2, 128.8 (q, *J* = 33.3 Hz), 127.7, 126.2 (q, *J* = 3.7 Hz), 123.9 (q, *J* = 273.2 Hz), 123.8, 122.5, 120.3, 119.2, 118.7, 118.2, 111.2, 52.9, 52.5, 28.4, 23.0. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -62.7 (s). IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3258, 2921, 1737, 1659, 1601, 1522, 1438, 1325, 1165, 1123, 1074, 1012, 827, 745. HRMS (ESI): calcd for $C_{21}H_{18}O_3N_2F_3Se^+$ $[M-H]^+$: 483.0440, found: 483.0450.



**3t**

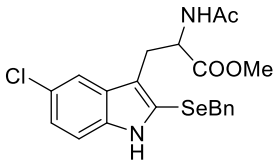
**methyl (*S*)-2-acetamido-3-(2-((4-cyanophenyl)selanyl)-1*H*-indol-3-yl)propanoate 3t.** Pale yellow solid, 39.1 mg (from 0.1 mmol), 89% yield, m.p. 87-88 °C. $[\alpha]_D^{29}$ = 48.4 (c 0.25, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.28-7.27 (m, 1H), 7.18 (t, *J* = 8.2 Hz, 3H), 6.00 (d, *J* = 8.0 Hz, 1H), 4.91 (dd, *J* = 13.8, 5.8 Hz, 1H), 3.65 (s, 3H), 3.43-3.29 (m, 2H), 1.84 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.1, 169.6, 139.8, 137.9, 132.7, 128.7, 127.7, 124.1, 120.5, 119.3, 119.2, 118.5, 117.4, 111.3, 109.9, 52.9, 52.5, 28.4, 23.1. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3356, 3059, 2951, 2922, 2851, 2226, 1740, 1657, 1586, 1523, 1483, 1437, 1374, 1341, 1218, 1014, 821, 746, 544. HRMS (ESI): calcd for $C_{21}H_{18}O_3N_3Se^-$ $[M-H]^-$: 440.0519, found: 440.0526.



**3u**

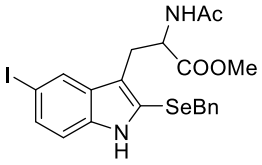
**methyl (*S*)-2-acetamido-3-(2-(mesitylselanyl)-1*H*-indol-3-yl)propanoate 3u.** Pale yellow solid, 7.4 mg (from 0.1 mmol), 16% yield, m.p. 74-76 °C. $[\alpha]_D^{29}$ = 38.2(c 0.11, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.15-7.13 (m, 1H), 7.07-7.06 (m, 2H), 6.97 (s, 2H), 6.03 (d, *J* = 7.2 Hz, 1H), 4.97 (dd, *J* = 12.8, 5.2 Hz, 1H), 3.73 (s, 3H), 3.37-3.36 (m, 2H), 2.42 (s, 6H), 2.30 (s, 3H), 1.99 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 142.9, 139.4, 137.7, 129.3, 128.5,

125.3, 123.2, 121.8, 119.8, 117.8, 111.9, 110.3, 52.7, 52.5, 28.4, 24.2, 23.3, 20.9. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3271, 2951, 2923, 2852, 1737, 1661, 1517, 1436, 1374, 1340, 1261, 1217, 1021, 851, 801, 742. HRMS (ESI): calcd for $C_{23}H_{25}O_3N_2Se^+$ $[M-H]^+$: 457.1036, found: 457.1045.



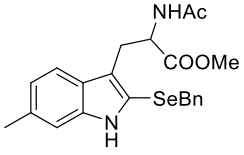

**4a**

**methyl 2-acetamido-3-(2-(benzylselanyl)-5-chloro-1*H*-indol-3-yl)propanoate 4a**. Yellow solid, 28.3 mg (from 0.1 mmol), 61% yield, m.p. 61-63 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.44 (s, 1H), 7.19-7.16 (m, 3H), 7.09 (s, 2H), 7.00-6.98 (m, 2H), 6.00 (d, *J* = 7.6 Hz, 1H), 4.84 (dd, *J* = 13.2, 5.6 Hz, 1H), 3.92 (s, 2H), 3.69 (s, 3H), 3.14-3.01 (m, 2H), 1.94 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 169.6, 138.4, 135.6, 128.7, 128.6, 127.2, 125.6, 123.3, 122.5, 118.2, 116.9, 111.7, 52.7, 52.5, 33.5, 27.9, 23.2. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3262, 3061, 3028, 2926, 1851, 1737, 1657, 1520, 1437, 1374, 1263, 1215, 800, 737, 697. HRMS (ESI): calcd for $C_{21}H_{21}O_3N_2ClNaSe^+$ $[M+Na]^+$: 487.0298, found: 487.0297.



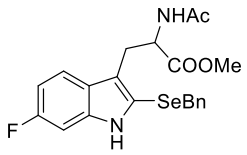

**4b**

**methyl 2-acetamido-3-(2-(benzylselanyl)-5-iodo-1*H*-indol-3-yl)propanoate 4b**. Yellow solid, 43.1 mg (from 0.1 mmol), 78% yield, m.p. 70-72 °C. $^1$H NMR (300 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.80 (s, 1H), 7.39 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.20-7.15 (m, 3H), 7.01-6.94 (m, 3H), 5.97 (d, *J* = 8.1 Hz, 1H), 4.84 (dd, *J* = 13.5, 5.4 Hz, 1H), 3.92 (s, 2H), 3.71 (s, 3H), 3.16-3.01 (m, 2H), 1.96 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.1, 169.6, 138.5, 136.3, 131.2, 130.2, 128.7, 128.6, 127.8, 127.3, 122.1, 116.5, 112.6, 83.3, 52.7, 52.5, 33.5, 27.8, 23.3. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3262, 3059, 3028, 2923, 2851, 1734, 1657, 1517, 1436, 1374, 1213, 797, 759, 696. HRMS (ESI): calcd for $C_{21}H_{21}O_3N_2INaSe^+$ $[M+Na]^+$: 578.9654, found: 578.9659.



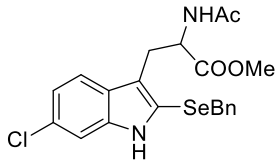

**4c**

**methyl 2-acetamido-3-(2-(benzylselanyl)-6-methyl-1*H*-indol-3-yl)propanoate 4c**. Yellow solid, 32.7 mg (from 0.1 mmol), 74% yield, m.p. 52-54 °C. $^1$H NMR (300 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.21-7.19 (m, 3H), 7.03-7.01 (m, 3H), 6.93 (d, *J* = 8.1 Hz, 1H), 5.95 (d, *J* = 7.5 Hz, 1H), 4.82 (dd, *J* = 13.5, 6.0 Hz, 1H), 3.90 (s, 2H), 3.67 (s, 3H), 3.18-3.03 (m, 2H), 2.44 (s, 3H), 1.91 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 169.6, 138.8, 137.8, 133.0, 128.7, 128.5, 127.1, 125.7, 121.7, 119.9, 118.5, 117.2, 110.6, 52.8, 52.4, 33.6, 27.9, 23.2, 21.7. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3271, 3061, 3028, 2917, 2849, 1739, 1657, 1520, 1437, 1373, 1340, 2161, 1216, 1029, 802, 760, 736, 697. HRMS (ESI): calcd for $C_{22}H_{24}O_3N_2NaSe^+$ $[M+Na]^+$: 467.0844, found: 467.0847.



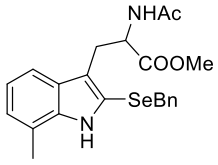

**4d**

**methyl 2-acetamido-3-(2-(benzylselanyl)-6-fluoro-1*H*-indol-3-yl)propanoate 4d**. Yellow solid, 40.8 mg (from 0.1 mmol), 91% yield, m.p. 52-54 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.43-7.40 (m, 1H), 7.22-7.15 (m, 3H), 7.00 (d, *J* = 6.0 Hz, 2H), 6.88-6.84 (m, 2H), 6.02 (d, *J* = 7.6 Hz, 1H), 4.83 (dd, *J* = 13.2, 6.0 Hz, 1H), 3.90 (s, 2H), 3.66 (s, 3H), 3.15-3.03 (m, 2H), 1.92 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.7, 160.4 (d, *J* = 16.6 Hz), 138.5, 137.2(d, *J* = 12.4 Hz), 128.7, 128.5, 127.2, 124.3, 120.8 (d, *J* = 4.0 Hz), 119.6 (d, *J* = 11.1 Hz), 117.5, 108.7 (d, *J* = 24.2 Hz), 97.0 (d, *J* = 26.3 Hz), 52.8, 52.4, 33.5, 28.0, 23.2. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -119.5 (s). IR $\nu_{max}$ (KBr, film, cm$^{-1}$):3268, 3061, 3028, 2918, 2849, 1739, 1657, 1525, 1439, 1346, 1291, 1216, 1120, 958, 836, 803, 760, 697. HRMS (ESI): calcd for $C_{21}H_{21}O_3N_2FNaSe^+$ [M+Na]$^+$: 471.0594, found: 471.0597.



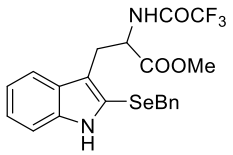

**4e**

**methyl 2-acetamido-3-(2-(benzylselanyl)-6-chloro-1*H*-indol-3-yl)propanoate 4e**. Yellow solid, 36.3 mg (from 0.1 mmol), 78% yield, m.p. 62-64 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.22-7.16 (m, 4H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.99 (d, *J* = 6.4 Hz, 2H), 6.00 (d, *J* = 7.6 Hz, 1H), 4.83 (dd, *J* = 13.2, 6.0 Hz, 1H), 3.91 (s, 2H), 3.66 (s, 3H), 3.15-3.02 (m, 2H), 1.92 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.6, 138.5, 137.5, 129.0, 128.7, 128.5, 127.2, 126.3, 121.6, 120.6, 119.6, 117.4, 110.6, 52.8, 52.5, 33.5, 27.9, 23.2. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3261, 3062, 3029, 2951, 2849, 1737, 1657, 1520, 1437, 1374, 1336, 1217, 1063, 917, 803, 759, 737, 697. HRMS (ESI): calcd for $C_{21}H_{21}O_3N_2ClNaSe^+$ [M+Na]$^+$: 487.0298, found: 487.0297.



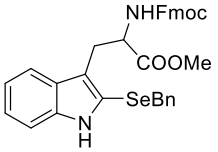

**4f**

**methyl 2-acetamido-3-(2-(benzylselanyl)-7-methyl-1*H*-indol-3-yl)propanoate 4f**. Yellow solid, 38.0 mg (from 0.1 mmol), 86% yield, m.p. 60-62 °C. $^1$H NMR (300 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.35 (d, *J* = 7.8 Hz, 1H), 7.23-7.19 (m, 3H), 7.09-6.94 (m, 4H), 5.97 (d, *J* = 7.8 Hz, 1H), 4.86 (dd, *J* = 13.8, 5.7 Hz, 1H), 3.93 (s, 2H), 3.68 (s, 3H), 3.26-3.10 (m, 2H), 2.31 (s, 3H), 1.91 (s, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 172.3, 169.6, 139.0, 136.9, 128.9, 128.6, 127.3, 127.2, 123.4, 120.4, 120.1, 119.9, 117.5, 116.5, 52.9, 52.4, 33.5, 28.1, 23.3, 16.3. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3271, 3026, 3027, 2920, 2849, 1737, 1657, 1517, 1453, 1374, 1218, 1029, 759, 748, 670. HRMS (ESI): calcd for $C_{22}H_{24}O_3N_2NaSe^+$ [M+Na]$^+$: 467.0844, found: 467.0847.



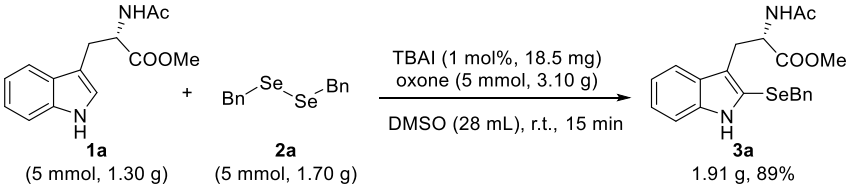

**4g**

**methyl 3-(2-(benzylselanyl)-1*H*-indol-3-yl)-2-(2,2,2-trifluoroacetamido)propanoate 4g**. Yellow solid, 45.3 mg (from 0.1 mmol), 94% yield, m.p. 129-131 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.25-7.18 (m, 5H), 7.12 (t, *J* = 7.4 Hz, 1H), 7.02-7.00 (m, 2H), 6.86 (d, *J* = 7.6 Hz, 1H), 4.80 (dd, *J* = 13.4, 6.2 Hz, 1H), 3.92 (s, 2H), 3.69 (s, 3H), 3.22-3.10 (m, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.6, 156.7 (q, *J* = 37.8 Hz), 138.6, 137.3, 128.7, 128.5, 127.4, 127.2, 123.3, 120.9, 120.1, 118.4, 116.3, 115.5 (q, *J* = 37.8 Hz), 110.8, 53.2, 52.8, 33.5, 27.5. $^{19}$F NMR (377 MHz, $CDCl_3$) δ -75.8 (s). IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3366, 3059, 2925, 2854, 1714, 1545, 1441, 1340, 1212, 1173, 745, 697. HRMS (ESI): calcd for $C_{21}H_{18}O_3N_2F_3Se^+$ $[M-H]^+$: 483.0429, found: 483.0436.

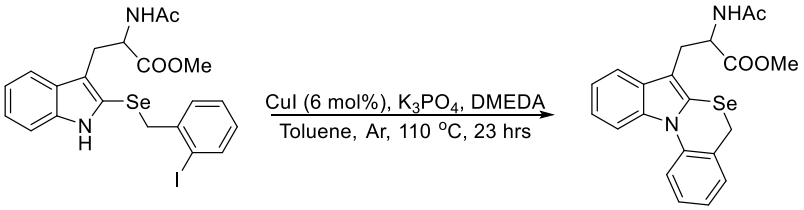



**4h**

**methyl 2-((((9*H*-fluoren-9-yl)methoxy)carbonyl)amino)-3-(2-(benzylselanyl)-1*H*-indol-3-yl)propanoate 4h**. White solid, 47 mg (from 0.1 mmol), 77% yield, m.p. 70-72 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.74 (d, *J* = 7.6 Hz, 2H), 7.57-7.50 (m, 3H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.29-7.25 (m, 2H), 7.23-7.16 (m, 5H), 7.11 (t, *J* = 7.2 Hz, 1H), 7.04-7.03 (m, 2H), 5.38 (d, *J* = 8.0 Hz, 1H), 4.66 (dd, *J* = 14.0, 6.4 Hz, 1H), 4.33 (d, *J* = 6.8 Hz, 2H), 4.17 (t, *J* = 7.0 Hz, 1H), 3.91 (s, 2H), 3.69 (s, 3H), 3.26-3.12 (m, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 155.6, 143.9, 143.8, 141.2, 138.8, 137.3, 128.7, 128.5, 127.6, 127.1, 127.0, 125.1, 123.1, 121.0, 119.9, 119.9, 118.8, 117.2, 110.7, 67.0, 54.6, 52.4, 47.1, 33.5, 28.3. IR $\nu_{max}$ (KBr, film, cm$^{-1}$): 3353, 3060, 2921, 2850, 1706, 1517, 1448, 1340, 1214, 1057, 759, 740, 697. HRMS (ESI): calcd for $C_{34}H_{31}O_4N_2Se^+$ $[M+H]^+$: 611.1444, found: 611.1436.

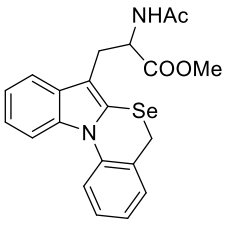



*Gram-Scale preparation*: To the mixture of *L*-acetyl tryptophanate ***L*-1a** (5 mmol, 1.3 g), dibenzyldiselenide (5 mmol, 1.7 g), TBAI (1 mol%, 18.5 mg) was added DMSO (27.5 mL). And then oxone (5 mmol, 3.1 g) was added in one portion. The mixture was stirred at room temperature for 15 min. Saturated sodium thiosulfate (30 mL) was added to quench the reaction. The reaction was diluted with ethyl acetate (50 mL) and washed by $H_2O$ (200 mL). Aqueous phase was extracted with ethyl acetate (50 mL × 4). The organic layer was combined, ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3) to afford the desired product **3a** in the yield of 89%.




To the mixture of methyl 2-acetamido-3-(2-((2-iodobenzyl)selanyl)-1*H*-indol-3-yl)propanoate **3d** (0.050 mmol, 27.76 mg), CuI (0.003 mmol, 0.57 mg), $K_3PO_4$ (0.075 mmol, 15.92 mg) was added toluene (0.5 mL) under argon atmosphere. *N*,*N*'-diethylethylenediamine (0.005 mmol, 0.52 μL) was then added. The mixture was heated to reflux for 23 hours. After

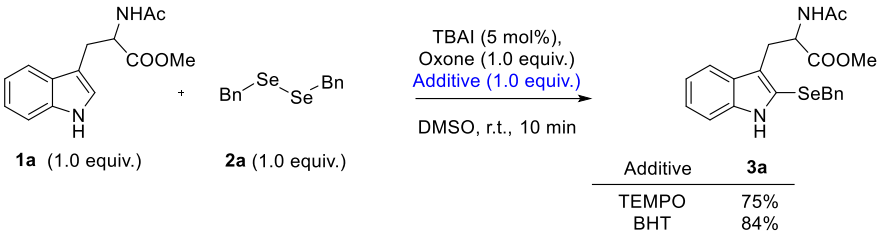
cooling to room temperature, the mixture was filtered through silica gel, the filter cake was washed with ethyl acetate (30 mL) and the filtrate was concentrated *in vacuum*. The crude was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3) to afford desired compound **5** as a white solid.




**5**

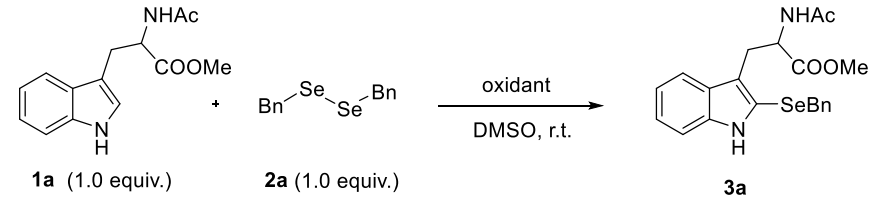
**methyl 2-acetamido-3-(5*H*-benzo[4,5][1,3]selenazino[3,2-*a*]indol-7-yl)propanoate 5**. White solid, 19.2 mg (from 0.05 mmol), 90% yield, m.p. 92-93 $^{o}$C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.85-7.84 (m, 2H), 7.50-7.38 (m, 3H), 7.24-7.17 (m, 3H), 6.06 (d, *J* = 7.6 Hz, 1H), 5.06-5.02 (m, 1H), 3.84-3.74 (m, 2H), 3.70 (s, 3H), 3.44-3.27 (m, 2H), 1.99 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.0, 169.6, 137.3, 136.3, 130.0, 129.8, 128.2, 127.9, 127.0, 124.7, 122.2, 121.3, 121.2, 117.9, 112.0, 111.5, 52.7, 52.6, 29.2, 23.9, 23.4. IR $\nu_{max}$ (KBr, film, $cm^{-1}$): 3357, 3194, 2922, 2850, 1943, 1659, 1632, 1490, 1448, 1369, 1212, 744. HRMS (ESI): calcd for $C_{21}H_{20}O_3N_2NaSe^+$ $[M+Na]^+$: 451.0531, found: 451.0537.

## 5. Control experiments




| Additive | 3a |
|---|---|
| TEMPO | 75% |
| BHT | 84% |

To the mixture of acetyl tryptophanate **1a** (0.1 mmol, 26.0 mg), diselenide (0.1 mmol, 34.0 mg), TBAI (5 mol%, 1.85 mg) and additive (TEMPO or BHT, 0.1 mmol) was added DMSO (0.55 mL). And then oxone (0.1 mmol, 61.5 mg) was added in one portion. The reaction was stirred at room temperature until the acetyl tryptophanate **1a** totally disappeared (monitored by TLC). Saturated sodium thiosulfate (1 mL) was added to quench the reaction. The reaction was diluted with ethyl acetate (5 mL) and washed by $H_2O$ (20 mL). The organic layer was combined, ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3) to afford the desired product **3a**.




| | | |
|---|---|---|
| $I_2$ (1.0 equiv.), 24 h : | 61% | (1) |
| $I_2$ (1.0 equiv.) + *n*-$Bu_4OH$ (2.0 equiv.), 24 h : | 0% | (2) |
| $TBAI_3$ (1.0 equiv.), 24 h: | 0% | (3) |
| $NaIO_3$ (1.0 equiv.), 24 h : | 0% | (4) |
| $NaIO_4$ (1.0 equiv.), 24 h : | 0% | (5) |
| $I_2$ (1.0 equiv.) + $KHSO_4$ (2.0 equiv.), 24 h : | 76% | (6) |
| $TBAI_3$ (1.0 equiv.) + $KHSO_4$ (2.0 equiv.), 24 h : | 45% | (7) |

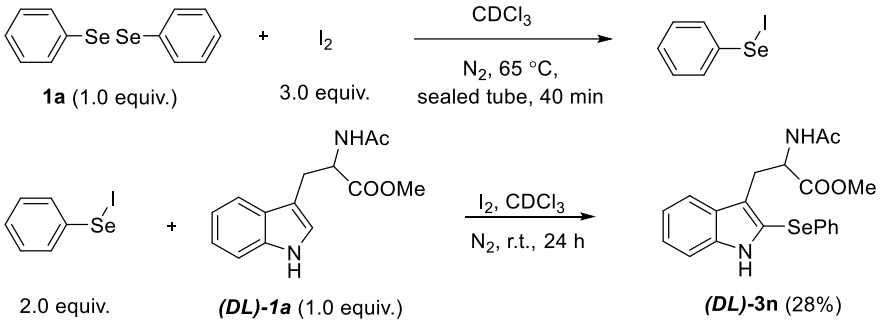
*Entries (1), (3), (4) and (5)*: To solution of acetyl tryptophanate **1a** (0.1 mmol, 26.0 mg) and diselenide (0.1 mmol, 34.0 mg) in DMSO (0.55 mL) was added iodine (0.1 mmol, 25.4 mg) or tetrabutylammonium triiodide (0.1 mmol, 62.3 mg) or sodium iodate (0.1 mmol, 19.8 mg) or sodium periodate (0.1 mmol, 21.4 mg) in one portion. The mixture was stirred at room temperature and monitored by TLC. Saturated sodium thiosulfate (1 mL) was added to quench the reaction. The reaction was diluted with ethyl acetate (5 mL) and washed by $H_2O$ (20 mL). Aqueous phase was extracted with ethyl acetate (5 mL × 2). The organic layer was combined, ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3). (26.2 mg, yield 61% for entry 1, no reaction for entry3, 4, 5)

*Entry (2)*: Iodine (0.1 mmol, 25.4 mg) and 25% aqueous tetrabutylammoniumhydroxide (0.2 mmol, 205 μL) were mixed in DMSO (0.55 mL), and the mixture was stirred at room temperature for 10 minutes. Acetyl tryptophanate **1a** (0.1 mmol, 26.0 mg), diselenide (0.1 mmol, 34.0 mg) was added to the mixture in sequence. The mixture was stirred at room temperature and monitored by TLC. After stirring for 24 hours, saturated sodium thiosulfate (1 mL) was added to quench the reaction.(,

yield 85%)

*Entry (6)*: To solution of acetyl tryptophanate **1a** (0.1 mmol, 26.0 mg), diselenide (0.1 mmol, 34.0 mg) and $KHSO_4$ (0.2 mmol, 27.2 mg) in DMSO (0.55 mL) was added iodine (0.1 mmol, 25.4 mg) in one portion. The mixture was stirred at room temperature and monitored by TLC. After stirring for 24 hours at room temperature, saturated sodium thiosulfate (1 mL) was added to quench the reaction. The reaction was diluted with ethyl acetate (5 mL) and washed by $H_2O$ (20 mL). Aqueous phase was extracted with ethyl acetate (5 mL × 2). The organic layer was combined, ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3) to afford the desired product **3a** (36.5 mg, yield 85%).

*Entry (7)*: To solution of acetyl tryptophanate **1a** (0.1 mmol, 26.0 mg), diselenide (0.1 mmol, 34.0 mg) and $KHSO_4$ (0.2 mmol, 27.2 mg) in DMSO (0.55 mL) was added tetrabutylammonium triiodide (0.1 mmol, 62.3 mg) in one portion. The mixture was stirred at room temperature and monitored by TLC. After stirring for 24 hours at room temperature, saturated sodium thiosulfate (1 mL) was added to quench the reaction. The reaction was diluted with ethyl acetate (5 mL) and washed by $H_2O$ (20 mL). Aqueous phase was extracted with ethyl acetate (5 mL × 2). The organic layer was combined, ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3) to afford the desired product **3a** (19.5 mg, yield 45%).




The PhSeI[5] synthesised herein are sensitive to moisture, therefore the reaction techniques were employed throughout, with all additions being performed in an $N_2$ filled glove box. Under the $N_2$ atmosphere, $I_2$ (0.75 mmol, 190.5 mg) was dissolved in $CDCl_3$ (5 mL), and then diphenyldiselenide was added. The mixture was sealed tube and stirred at 65 °C for 40 minutes. The dark purple solution containing PhSeI (0.1 M in $CDCl_3$) was obtained. NMR spectra of the resulting solution under $N_2$ atmosphere also proved the formation of PhSeI ($^1$H NMR (300 MHz, CDCl3) δ 7.73-7.70 (m, 2H), 7.34–7.26 (m, 3H). $^{13}$C NMR (101 MHz, CDCl3) δ 134.1, 129.4, 129.3.). Under the $N_2$ atmosphere, ***(DL)-1a*** (0.1 mmol, 26.0 mg) in the reaction tube was added PhSeI (0.1 M in $CDCl_3$, 2 mL). The mixture was stirred at room temperature for 24 h. Saturated sodium thiosulfate (1 mL) was added to quench the reaction. The reaction was diluted with ethyl acetate (5 mL) and washed by $H_2O$ (20 mL). Aqueous phase was extracted with ethyl acetate (5 mL × 2). The organic layer was combined, ethyl acetate was removed by rotary evaporator and the crude product was purified by silica column chromatography (elute: petroleum ether / ethyl acetate 1/3) to afford the products ***(DL)*-3n** with the yield of 28%.

**6. X-ray crystallographic date**

X-ray crystallography of compound **3j** (CCDC 2058699)

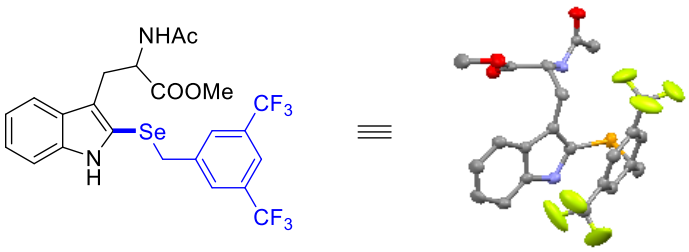



Table 1 Crystal data and structure refinement for A.

| | |
|---|---|
| Identification code | A |
| Empirical formula | $C_{23}H_{20}F_6N_2O_3Se$ |
| Formula weight | 565.37 |
| Temperature/K | 169.99(11) |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 9.17100(10) |
| b/Å | 10.0901(3) |
| c/Å | 13.7727(3) |
| α/° | 109.3780(10) |
| β/° | 91.5750(10) |
| γ/° | 100.5370(10) |
| Volume/Å$^3$ | 1176.65(5) |
| Z | 2 |
| ρcalcg/cm$^3$ | 1.596 |
| μ/mm$^{-1}$ | 2.860 |
| F(000) | 568.0 |
| Crystal size/mm3 | 0.11 × 0.08 × 0.05 |
| Radiation | Cu Kα (λ = 1.54178) |
| 2Θ range for data collection/° | 6.834 to 150.786 |
| Index ranges | -11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -17 ≤ l ≤ 17 |
| Reflections collected | 16758 |
| Independent reflections | 4667 [Rint = 0.0262, Rsigma = 0.0261] |
| Data/restraints/parameters | 4667/0/318 |
| Goodness-of-fit on F2 | 1.109 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0642, wR2 = 0.1983 |
| Final R indexes [all data] | R1 = 0.0648, wR2 = 0.1986 |
| Largest diff. peak/hole / e Å$^{-3}$ | 1.70/-0.72 |

Table 2 Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å2×103) for A. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| Se1 | 2904.5(6) | 6652.2(6) | 8098.8(4) | 34.1(2) |
| F1 | 3743(6) | 4133(6) | 3724(5) | 90.0(17) |
| F2 | 4251(6) | 2670(8) | 4380(4) | 95.5(19) |
| F3 | 2597(5) | 1979(7) | 3101(4) | 97(2) |
| F4 | -1869(8) | 1364(7) | 6202(4) | 120(3) |
| F5 | -1736(6) | 285(5) | 4681(4) | 93.1(19) |
| F6 | -2892(6) | 1927(8) | 5093(10) | 172(5) |
| O1 | 5509(4) | 3098(4) | 9575(3) | 38.3(9) |
| O2 | 5345(5) | 1352(4) | 8044(3) | 40.8(9) |
| O3 | 8318(4) | 5515(4) | 8214(3) | 40.0(9) |
| N1 | 921(5) | 4583(4) | 8675(3) | 29.6(9) |
| N2 | 5982(5) | 5177(4) | 8657(3) | 30.4(9) |
| C00V | 3112(7) | 3002(8) | 3980(5) | 46.0(14) |
| C1 | 2204(6) | 4838(5) | 8216(4) | 29.1(10) |
| C2 | 2775(5) | 3600(5) | 7851(4) | 26.9(10) |
| C3 | 1741(5) | 2517(5) | 8097(4) | 25.7(9) |
| C4 | 1644(6) | 1043(5) | 7898(4) | 31.8(11) |
| C5 | 467(6) | 303(6) | 8234(5) | 39.7(13) |
| C6 | -635(6) | 986(6) | 8752(5) | 41.4(13) |
| C7 | -598(6) | 2422(6) | 8930(4) | 35.1(11) |
| C8 | 601(5) | 3169(5) | 8600(4) | 27.8(10) |
| C9 | 4140(6) | 3390(6) | 7299(4) | 32.3(11) |
| C10 | 5585(5) | 3683(5) | 8004(4) | 28.8(10) |
| C11 | 5483(5) | 2719(5) | 8656(4) | 30.5(11) |
| C12 | 5203(8) | 317(7) | 8564(6) | 53.3(17) |
| C13 | 7300(5) | 6001(5) | 8681(4) | 27.1(10) |
| C14 | 7474(6) | 7565(6) | 9280(5) | 37.1(12) |
| C15 | 1355(6) | 6480(6) | 6996(4) | 35.7(12) |
| C16 | 1124(6) | 5038(6) | 6168(4) | 30.5(10) |
| C17 | 2160(6) | 4703(6) | 5455(4) | 33.9(11) |
| C18 | 1953(6) | 3353(6) | 4712(4) | 33.2(11) |
| C19 | 694(6) | 2303(6) | 4658(4) | 35.1(11) |
| C20 | -332(6) | 2652(6) | 5361(4) | 33.6(11) |
| C21 | -125(6) | 4013(6) | 6121(4) | 32.0(11) |
| C22 | -1713(7) | 1575(7) | 5332(5) | 43.5(13) |

Table 3 Anisotropic Displacement Parameters (Å2×103) for A. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+...].

| Atom | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Se1 | 37.1(3) | 24.4(3) | 38.9(3) | 12.6(2) | -5.2(2) | -0.7(2) |
| F1 | 89(4) | 92(4) | 97(4) | 41(3) | 60(3) | 14(3) |
| F2 | 62(3) | 165(6) | 83(3) | 49(4) | 22(3) | 69(4) |
| F3 | 58(3) | 125(5) | 52(3) | -32(3) | 23(2) | -6(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| F4 | 140(6) | 120(5) | 60(3) | 29(3) | 18(3) | -69(4) |
| F5 | 88(4) | 61(3) | 88(4) | -10(3) | 27(3) | -25(3) |
| F6 | 31(3) | 120(5) | 408(15) | 165(8) | -22(5) | -12(3) |
| O1 | 38(2) | 40(2) | 38(2) | 12.7(17) | 5.4(16) | 12.2(17) |
| O2 | 43(2) | 24.2(18) | 53(2) | 8.8(17) | 13.0(18) | 8.8(16) |
| O3 | 27.1(19) | 41(2) | 49(2) | 10.3(18) | 10.7(16) | 8.4(16) |
| N1 | 28(2) | 27(2) | 33(2) | 6.9(17) | 1.8(17) | 9.6(17) |
| N2 | 25(2) | 24(2) | 38(2) | 4.2(17) | 10.2(17) | 4.6(16) |
| C00V | 36(3) | 62(4) | 36(3) | 12(3) | 5(2) | 10(3) |
| C1 | 31(3) | 24(2) | 30(2) | 7.3(19) | -2.1(19) | 4.3(19) |
| C2 | 27(2) | 25(2) | 25(2) | 5.1(18) | -2.0(18) | 1.9(19) |
| C3 | 24(2) | 24(2) | 25(2) | 5.6(18) | -2.7(18) | 1.7(18) |
| C4 | 26(2) | 24(2) | 38(3) | 3(2) | 1(2) | 2.3(19) |
| C5 | 35(3) | 22(2) | 57(4) | 10(2) | 3(3) | 0(2) |
| C6 | 28(3) | 34(3) | 60(4) | 18(3) | 8(2) | -5(2) |
| C7 | 24(2) | 36(3) | 45(3) | 14(2) | 5(2) | 5(2) |
| C8 | 23(2) | 27(2) | 31(2) | 8(2) | -2.5(18) | 3.9(19) |
| C9 | 36(3) | 30(3) | 27(2) | 7(2) | 8(2) | 3(2) |
| C10 | 25(2) | 23(2) | 35(3) | 5(2) | 10.4(19) | 3.0(18) |
| C11 | 19(2) | 28(2) | 45(3) | 10(2) | 8(2) | 7.5(18) |
| C12 | 45(4) | 32(3) | 90(5) | 28(3) | 16(3) | 12(3) |
| C13 | 24(2) | 28(2) | 31(2) | 13(2) | 0.8(19) | 5.9(19) |
| C14 | 29(3) | 27(3) | 54(3) | 14(2) | 3(2) | 2(2) |
| C15 | 40(3) | 30(3) | 38(3) | 13(2) | -3(2) | 9(2) |
| C16 | 32(3) | 35(3) | 29(2) | 14(2) | -2(2) | 10(2) |
| C17 | 29(3) | 42(3) | 33(3) | 18(2) | -1(2) | 4(2) |
| C18 | 30(3) | 44(3) | 29(2) | 13(2) | 2(2) | 11(2) |
| C19 | 37(3) | 37(3) | 31(3) | 10(2) | 1(2) | 9(2) |
| C20 | 36(3) | 36(3) | 30(3) | 14(2) | 0(2) | 7(2) |
| C21 | 32(3) | 36(3) | 31(3) | 14(2) | 3(2) | 10(2) |
| C22 | 43(3) | 41(3) | 43(3) | 13(3) | 5(3) | 2(3) |

Table 4 Bond Lengths for A.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Se1 | C1 | 1.887(5) | C2 | C9 | 1.494(7) |
| Se1 | C15 | 1.993(5) | C3 | C4 | 1.406(7) |
| F1 | C00V | 1.341(9) | C3 | C8 | 1.412(7) |
| F2 | C00V | 1.314(8) | C4 | C5 | 1.378(8) |
| F3 | C00V | 1.310(8) | C5 | C6 | 1.405(8) |
| F4 | C22 | 1.293(8) | C6 | C7 | 1.381(8) |
| F5 | C22 | 1.309(8) | C7 | C8 | 1.391(7) |
| F6 | C22 | 1.265(9) | C9 | C10 | 1.543(7) |
| O1 | C11 | 1.192(7) | C10 | C11 | 1.521(7) |
| O2 | C11 | 1.337(6) | C13 | C14 | 1.495(7) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O2 | C12 | 1.440(8) | C15 | C16 | 1.496(7) | | |
| O3 | C13 | 1.231(6) | C16 | C17 | 1.389(8) | | |
| N1 | C1 | 1.374(7) | C16 | C21 | 1.379(8) | | |
| N1 | C8 | 1.371(7) | C17 | C18 | 1.382(8) | | |
| N2 | C10 | 1.447(6) | C18 | C19 | 1.399(8) | | |
| N2 | C13 | 1.329(7) | C19 | C20 | 1.376(8) | | |
| C00V | C18 | 1.494(8) | C20 | C21 | 1.399(8) | | |
| C1 | C2 | 1.388(7) | C20 | C22 | 1.500(8) | | |
| C2 | C3 | 1.446(7) | | | | | |

Table 5 Bond Angles for A.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C1 | Se1 | C15 | 96.8(2) | N2 | C10 | C11 | 110.4(4) |
| C11 | O2 | C12 | 115.6(5) | C11 | C10 | C9 | 112.4(4) |
| C8 | N1 | C1 | 109.1(4) | O1 | C11 | O2 | 124.0(5) |
| C13 | N2 | C10 | 122.7(4) | O1 | C11 | C10 | 126.1(5) |
| F1 | C00V | C18 | 112.0(6) | O2 | C11 | C10 | 109.8(5) |
| F2 | C00V | F1 | 103.1(6) | O3 | C13 | N2 | 122.1(5) |
| F2 | C00V | C18 | 113.1(5) | O3 | C13 | C14 | 121.3(5) |
| F3 | C00V | F1 | 105.4(6) | N2 | C13 | C14 | 116.5(4) |
| F3 | C00V | F2 | 108.6(6) | C16 | C15 | Se1 | 110.6(3) |
| F3 | C00V | C18 | 113.8(5) | C17 | C16 | C15 | 121.1(5) |
| N1 | C1 | Se1 | 120.6(4) | C21 | C16 | C15 | 119.5(5) |
| N1 | C1 | C2 | 110.4(4) | C21 | C16 | C17 | 119.4(5) |
| C2 | C1 | Se1 | 129.0(4) | C18 | C17 | C16 | 120.5(5) |
| C1 | C2 | C3 | 105.2(4) | C17 | C18 | C00V | 119.4(5) |
| C1 | C2 | C9 | 128.3(5) | C17 | C18 | C19 | 120.7(5) |
| C3 | C2 | C9 | 126.5(4) | C19 | C18 | C00V | 119.8(5) |
| C4 | C3 | C2 | 133.6(5) | C20 | C19 | C18 | 118.3(5) |
| C4 | C3 | C8 | 118.7(5) | C19 | C20 | C21 | 121.3(5) |
| C8 | C3 | C2 | 107.6(4) | C19 | C20 | C22 | 120.6(5) |
| C5 | C4 | C3 | 118.6(5) | C21 | C20 | C22 | 118.1(5) |
| C4 | C5 | C6 | 121.4(5) | C16 | C21 | C20 | 119.8(5) |
| C7 | C6 | C5 | 121.4(5) | F4 | C22 | F5 | 102.9(6) |
| C6 | C7 | C8 | 117.0(5) | F4 | C22 | C20 | 113.0(5) |
| N1 | C8 | C3 | 107.7(4) | F5 | C22 | C20 | 114.0(5) |
| N1 | C8 | C7 | 129.5(5) | F6 | C22 | F4 | 107.1(8) |
| C7 | C8 | C3 | 122.8(5) | F6 | C22 | F5 | 106.2(7) |
| C2 | C9 | C10 | 115.1(4) | F6 | C22 | C20 | 112.9(6) |
| N2 | C10 | C9 | 111.0(4) | | | | |

Table 6 Hydrogen Bonds for A.

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| N1 | H1 | O31 | 0.86 | 2.26 | 2.850(6) | 125.3 |

1-1+X,+Y,+Z

Table 7 Torsion Angles for A.

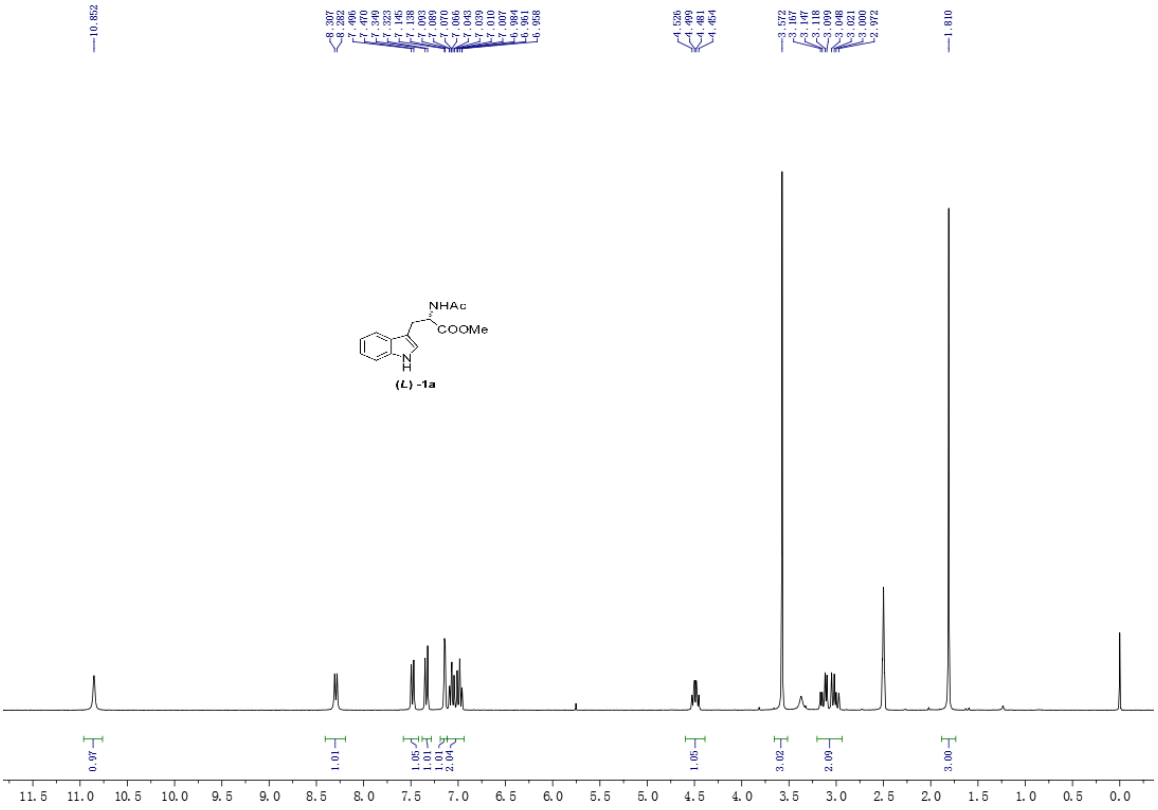
| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| Se1 | C1 | C2 | C3 | -176.2(4) | C8 | N1 | C1 | Se1 | 175.9(3) |
| Se1 | C1 | C2 | C9 | 2.5(8) | C8 | N1 | C1 | C2 | -1.5(6) |
| Se1 | C15 | C16 | C17 | -74.6(5) | C8 | C3 | C4 | C5 | -2.2(8) |
| Se1 | C15 | C16 | C21 | 104.1(5) | C9 | C2 | C3 | C4 | -2.0(9) |
| F1 | C00V | | C18 | C17 -35.5(8) | | C9 | C2 | C3 | C8 -178.8(5) |
| F1 | C00V | | C18 | C19 146.3(6) | | C9 | C10 | C11 | O1 -114.6(6) |
| F2 | C00V | | C18 | C17 80.5(8) | | C9 | C10 | C11 | O2 65.0(5) |
| F2 | C00V | | C18 | C19 -97.7(7) | | C10 | N2 | C13 | O3 -6.2(8) |
| F3 | C00V | | C18 | C17 -154.9(6) | | C10 | N2 | C13 | C14 171.9(5) |
| F3 | C00V | | C18 | C19 26.9(9) | | C12 | O2 | C11 | O1 0.9(7) |
| N1 | C1 | C2 | C3 | 1.0(5) | C12 | O2 | C11 | C10 | -178.7(4) |
| N1 | C1 | C2 | C9 | 179.6(5) | C13 | N2 | C10 | C9 | -124.5(5) |
| N2 | C10 | C11 | O1 | 9.9(7) | C13 | N2 | C10 | C11 | 110.1(5) |
| N2 | C10 | C11 | O2 | -170.5(4) | C15 | Se1 | C1 | N1 | -72.6(4) |
| C00V | | C18 | C19 | C20 178.4(5) | | C15 | Se1 | C1 | C2 104.2(5) |
| C1 | N1 | C8 | C3 | 1.4(5) | C15 | C16 | C17 | C18 | 178.1(5) |
| C1 | N1 | C8 | C7 | -178.3(5) | C15 | C16 | C21 | C20 | -178.6(5) |
| C1 | C2 | C3 | C4 | 176.7(5) | C16 | C17 | C18 | C00V | -177.7(5) |
| C1 | C2 | C3 | C8 | -0.1(5) | C16 | C17 | C18 | C19 | 0.5(8) |
| C1 | C2 | C9 | C10 | 90.2(6) | C17 | C16 | C21 | C20 | 0.2(7) |
| C2 | C3 | C4 | C5 | -178.8(5) | C17 | C18 | C19 | C20 | 0.2(8) |
| C2 | C3 | C8 | N1 | -0.7(5) | C18 | C19 | C20 | C21 | -0.7(8) |
| C2 | C3 | C8 | C7 | 178.9(5) | C18 | C19 | C20 | C22 | 179.2(5) |
| C2 | C9 | C10 | N2 | -64.6(6) | C19 | C20 | C21 | C16 | 0.5(8) |
| C2 | C9 | C10 | C11 | 59.7(6) | C19 | C20 | C22 | F4 | 124.7(7) |
| C3 | C2 | C9 | C10 | -91.4(6) | C19 | C20 | C22 | F5 | 7.7(9) |
| C3 | C4 | C5 | C6 | 1.0(9) | C19 | C20 | C22 | F6 | -113.6(9) |
| C4 | C3 | C8 | N1 | -178.1(4) | C21 | C16 | C17 | C18 | -0.7(8) |
| C4 | C3 | C8 | C7 | 1.5(8) | C21 | C20 | C22 | F4 | -55.4(8) |
| C4 | C5 | C6 | C7 | 1.1(10) | C21 | C20 | C22 | F5 | -172.4(6) |
| C5 | C6 | C7 | C8 | -1.8(9) | C21 | C20 | C22 | F6 | 66.2(9) |
| C6 | C7 | C8 | N1 | -179.9(5) | C22 | C20 | C21 | C16 | -179.4(5) |
| C6 | C7 | C8 | C3 | 0.5(8) | | | | | |

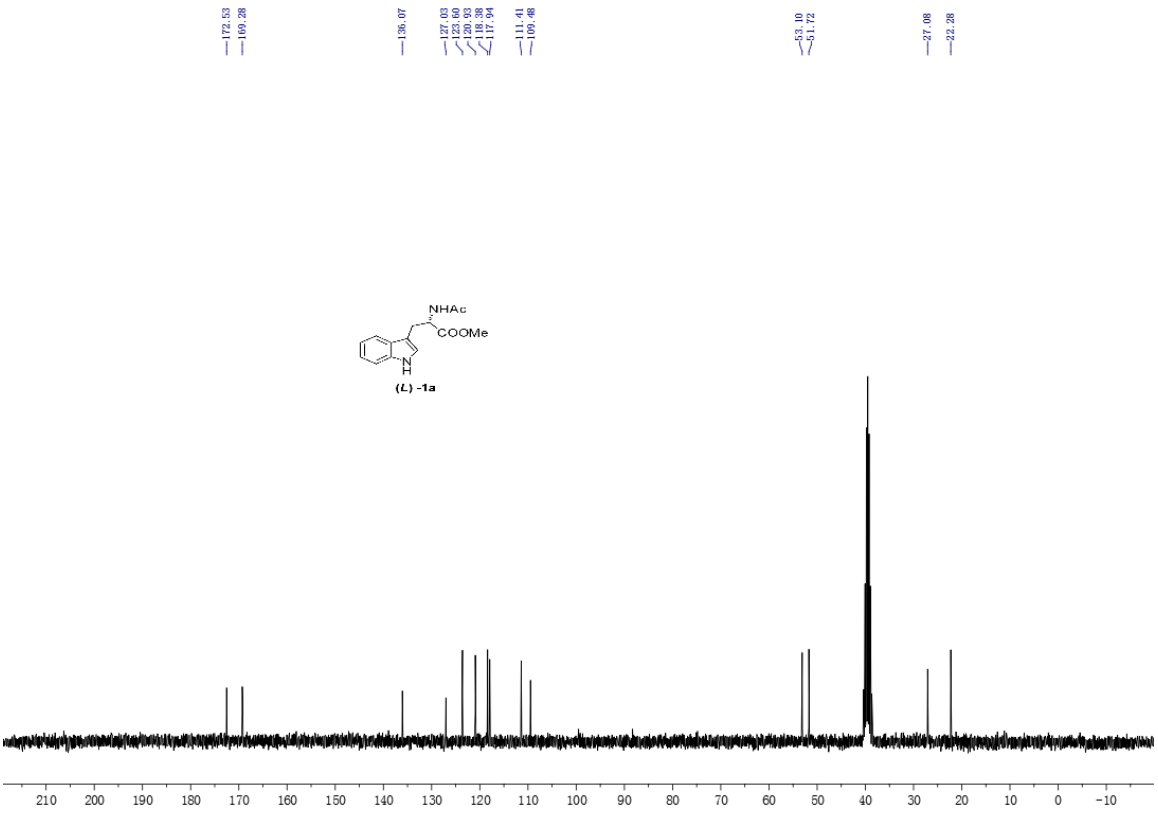
Table 8 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for A.

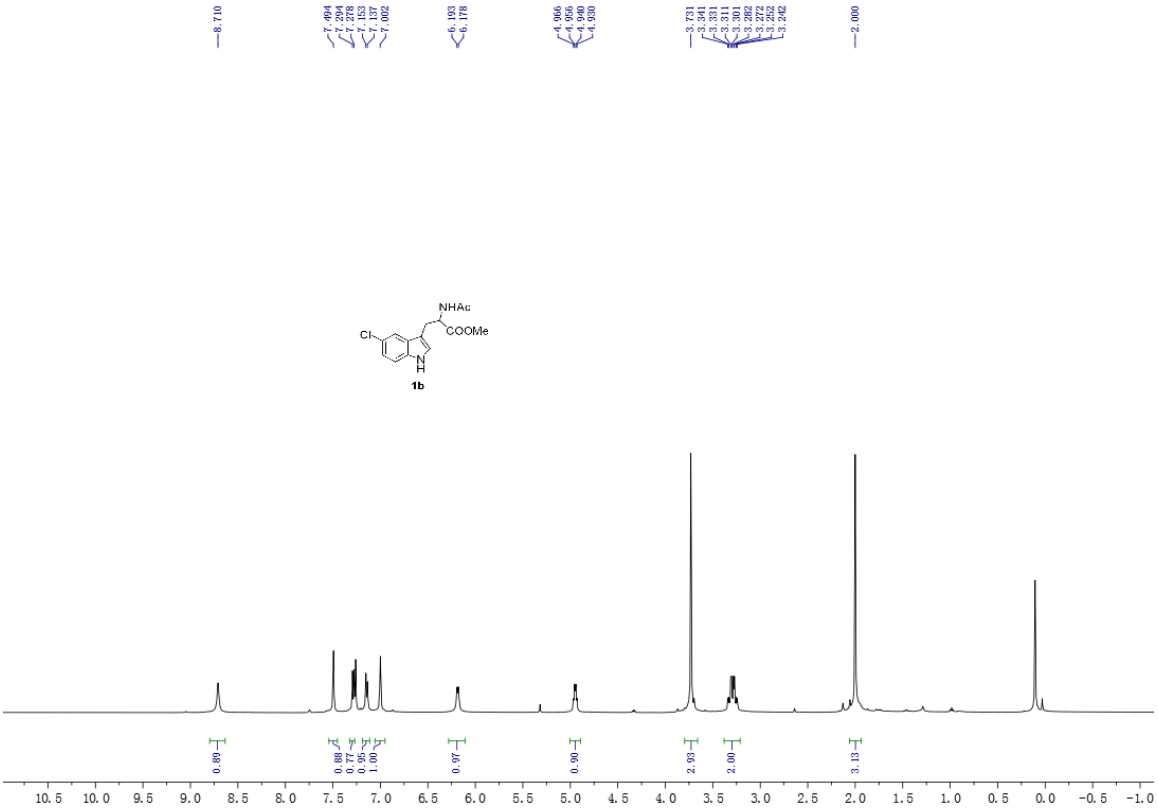
| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| H1 | 401.24 | 5210.98 | 8963.43 | 36 |
| H2 | 5337.9 | 5546.63 | 9044.66 | 37 |
| H4 | 2359.86 | 576.25 | 7547.14 | 38 |
| H5 | 401.04 | -669.85 | 8116.14 | 48 |

| | | | | |
|---|---|---|---|---|
| H6 | -1406.36 | 459.56 | 8979.14 | 50 |
| H7 | -1341.61 | 2869.17 | 9255.18 | 42 |
| H9A | 4284.23 | 4018.01 | 6892.74 | 39 |
| H9B | 3972.49 | 2410.16 | 6822.53 | 39 |
| H10 | 6388.3 | 3478 | 7556.91 | 35 |
| H12A | 5415.73 | -565.25 | 8110.49 | 80 |
| H12B | 4205.37 | 145.26 | 8755.34 | 80 |
| H12C | 5892.8 | 679.61 | 9174.04 | 80 |
| H14A | 8499.8 | 7965.68 | 9538.54 | 56 |
| H14B | 6868.91 | 7691.31 | 9848.2 | 56 |
| H14C | 7166.53 | 8043.96 | 8836.36 | 56 |
| H15A | 424.85 | 6617.18 | 7295.07 | 43 |
| H15B | 1661.93 | 7221.69 | 6698.17 | 43 |
| H17 | 2998.44 | 5392.71 | 5478.23 | 41 |
| H19 | 554.3 | 1393.06 | 4160.1 | 42 |
| H21 | -827.36 | 4227.13 | 6593.14 | 38 |

## 7. NMR spectra

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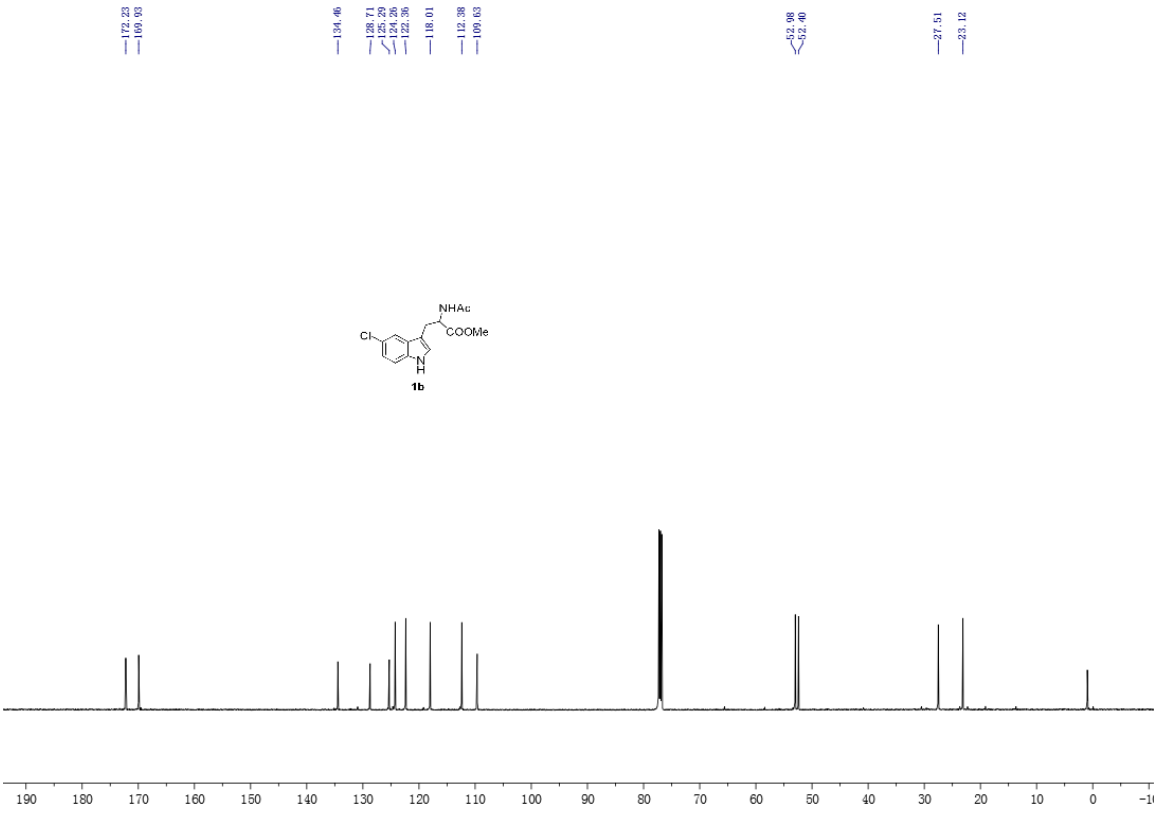
3.731
3.341
3.331
3.311
3.301
3.282
3.272
3.252
3.242
2.000
NHAc
COOMe
Cl
N
H
1b
0.89
0.88
0.77
0.95
1.00
0.97
0.90
2.93
2.00
3.13
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0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124.26
122.36
118.01
112.38
109.63
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27.51
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COOMe
Cl
N
H
1b
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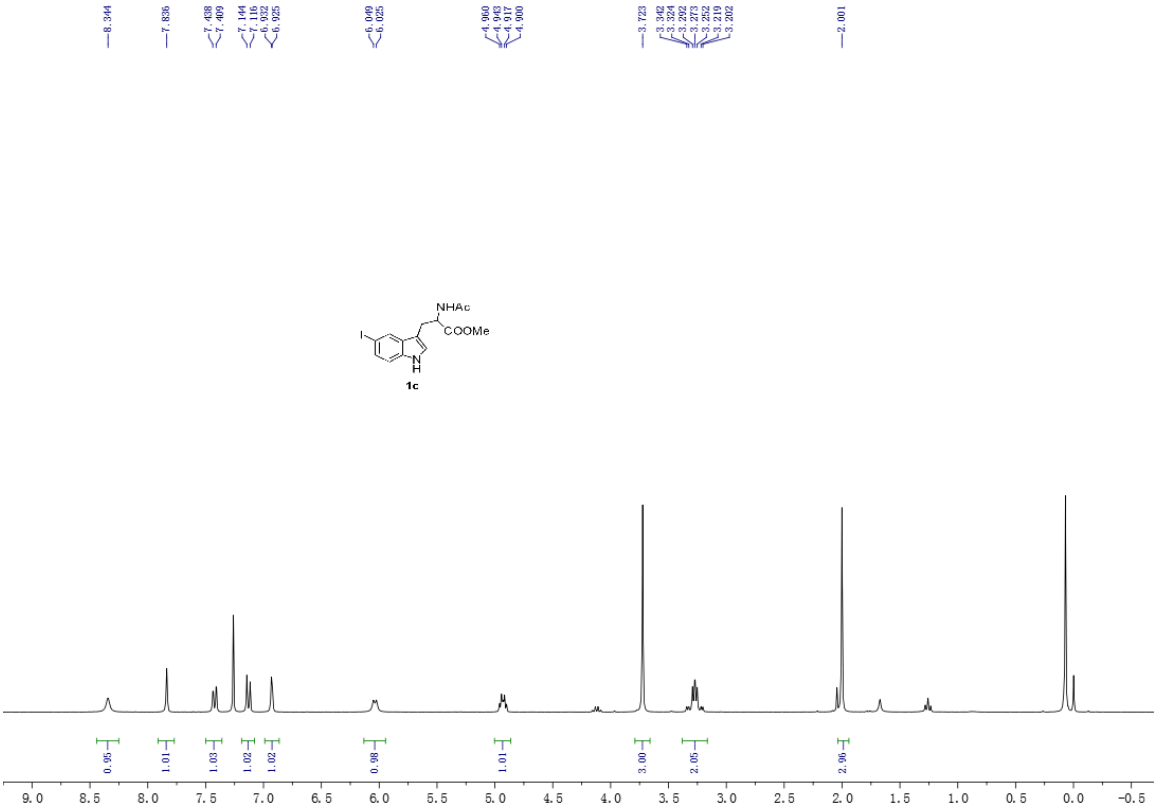
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I
N
H
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1.01
1.03
1.02
1.02
0.98
1.01
3.00
2.05
2.96
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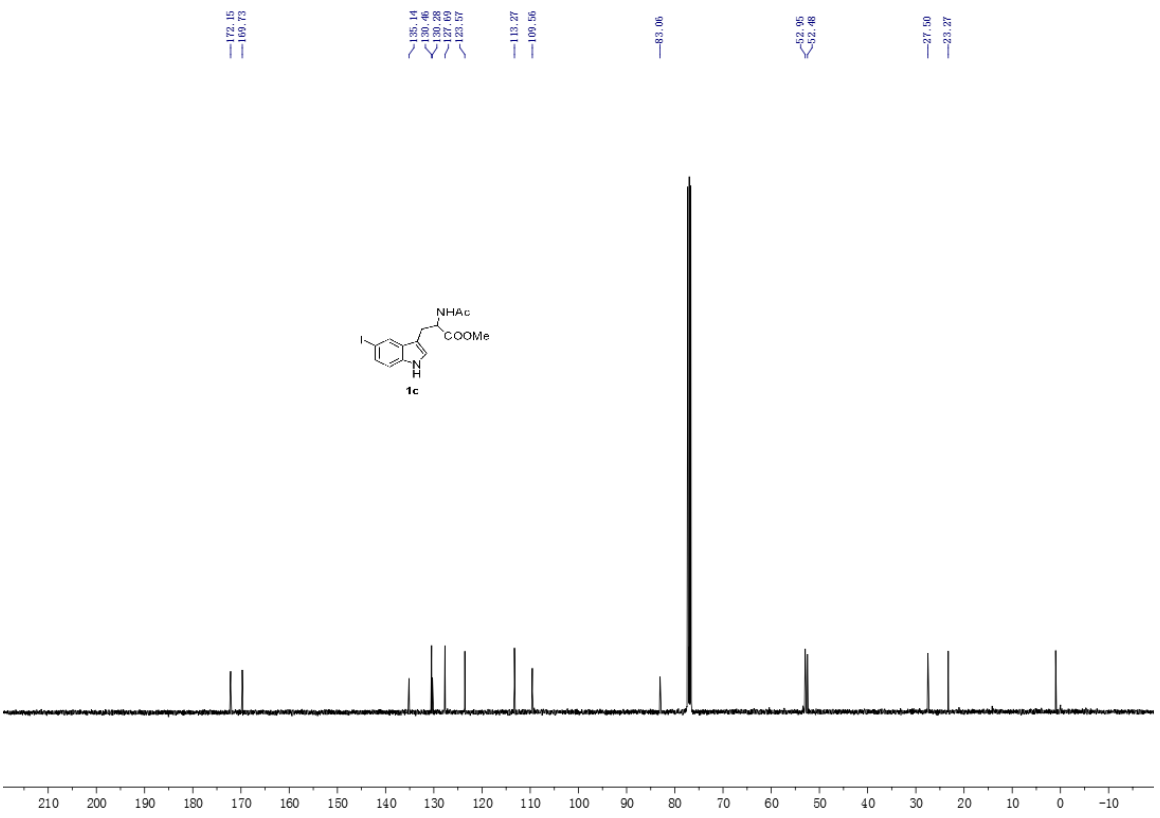
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123.57
113.27
109.56
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COOMe
I
N
H
1c
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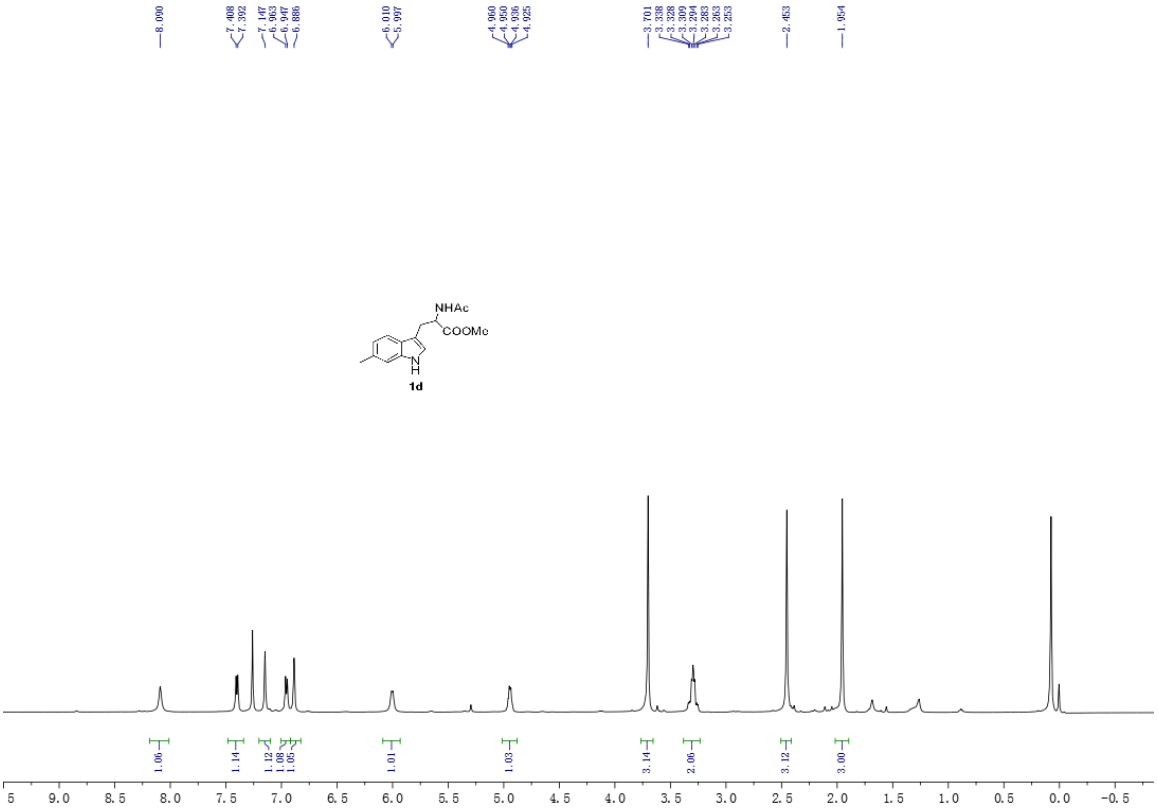
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3.338
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3.309
3.294
3.283
3.263
3.253
2.453
1.954
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COOMe
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1.01
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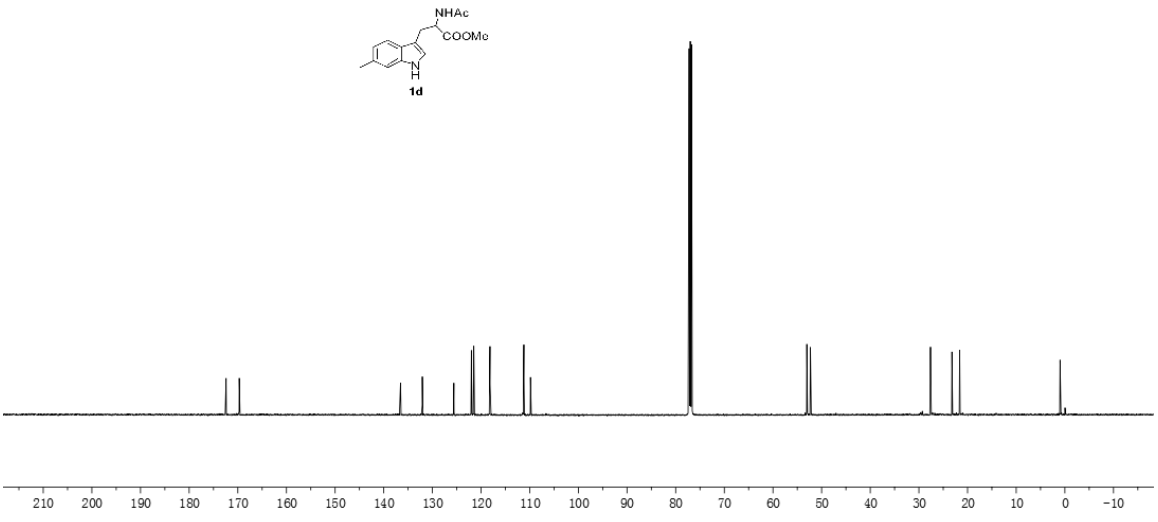
2.06
3.12
3.00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23.22
21.62
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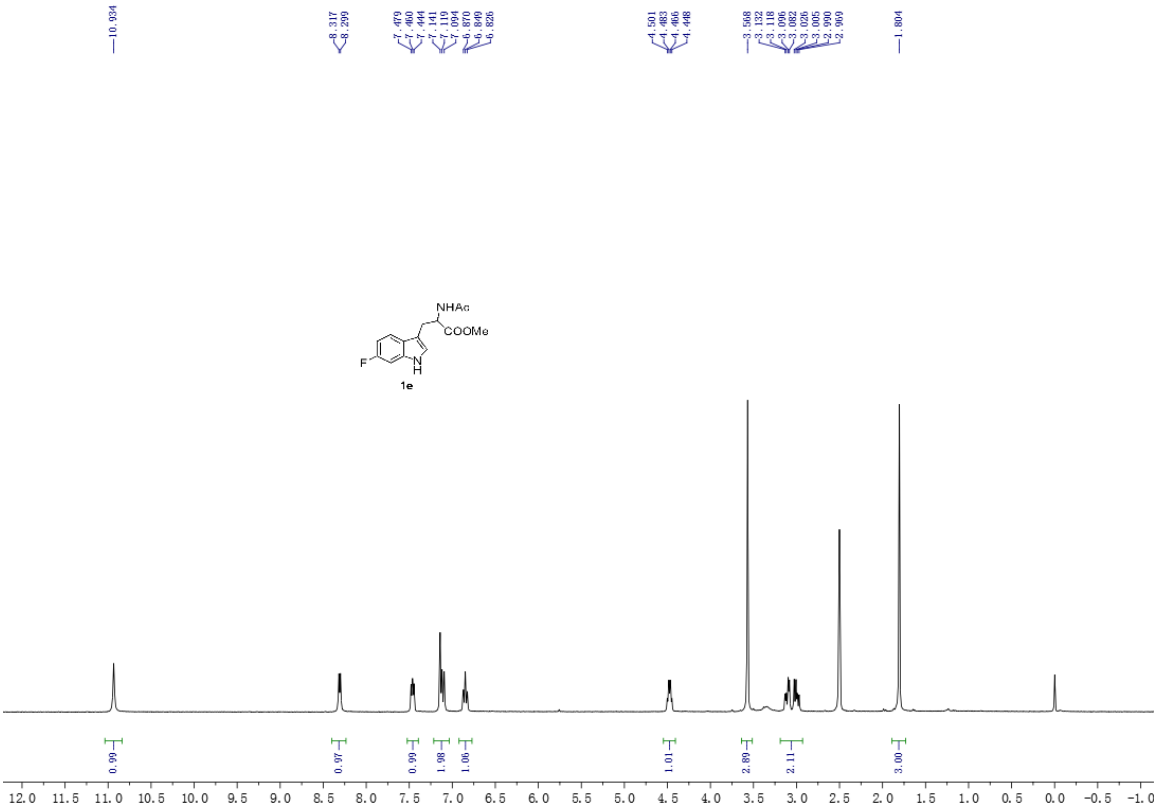
COOMe
1d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H
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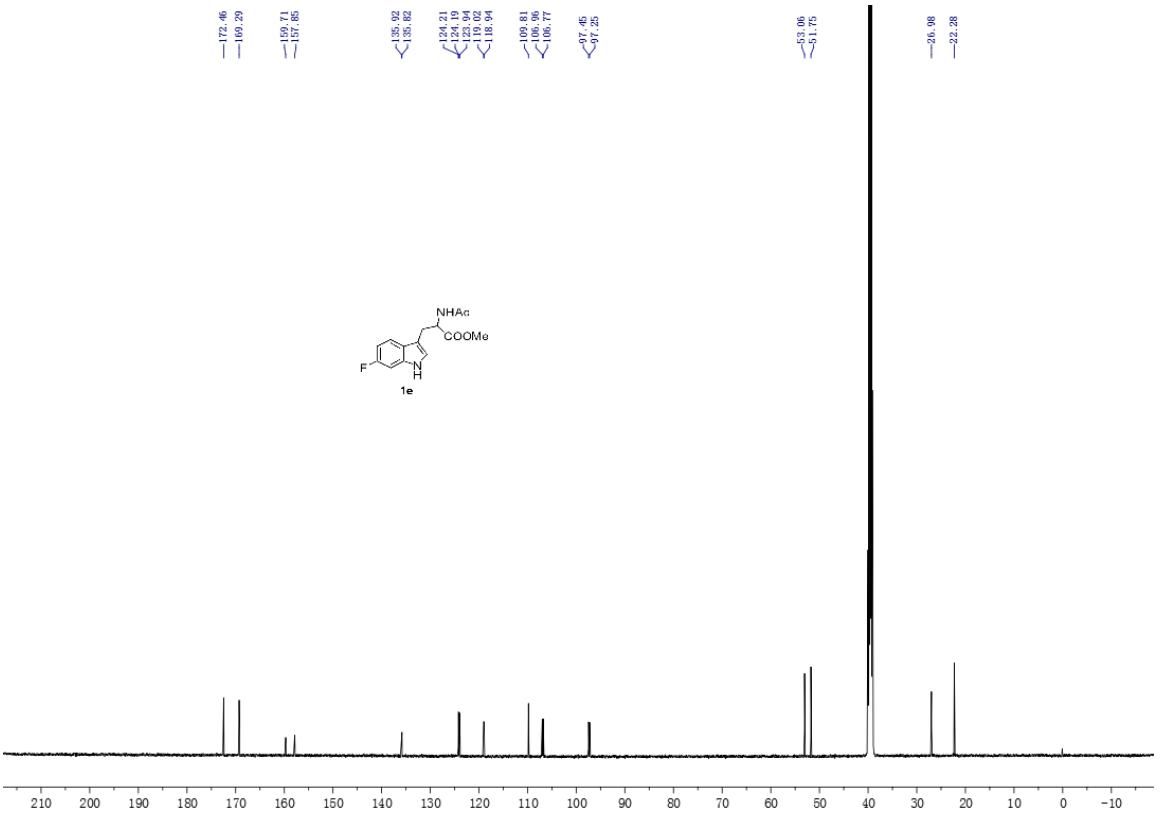
1.98
1.06
1.01
2.89
2.11
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0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53.06
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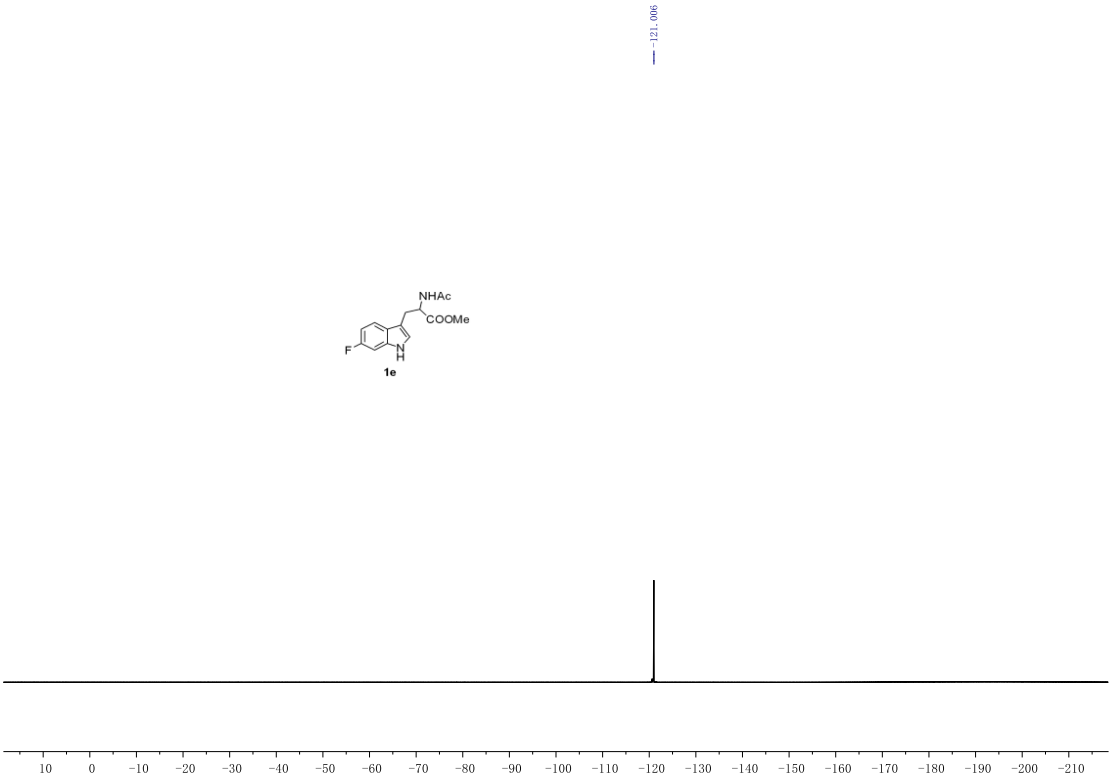
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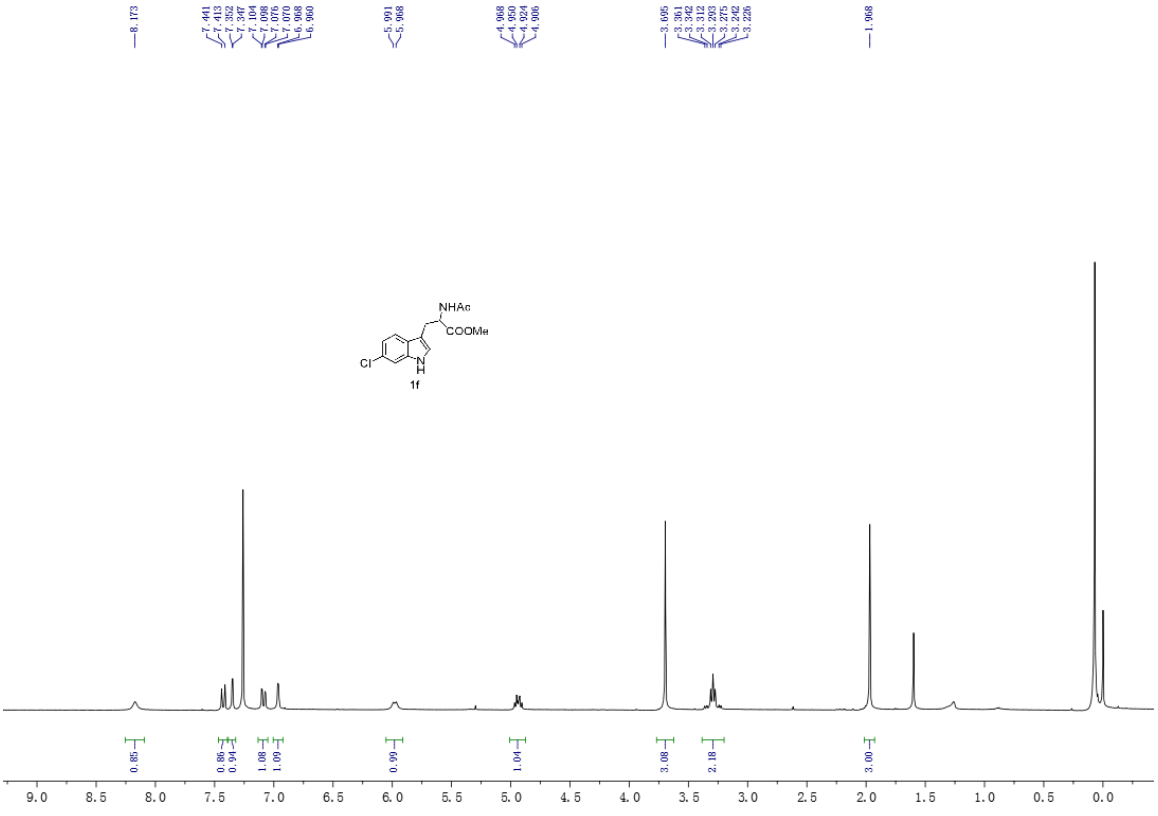
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COOMe
Cl
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0.94
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1.09
0.99
1.04
3.08
2.18
3.00
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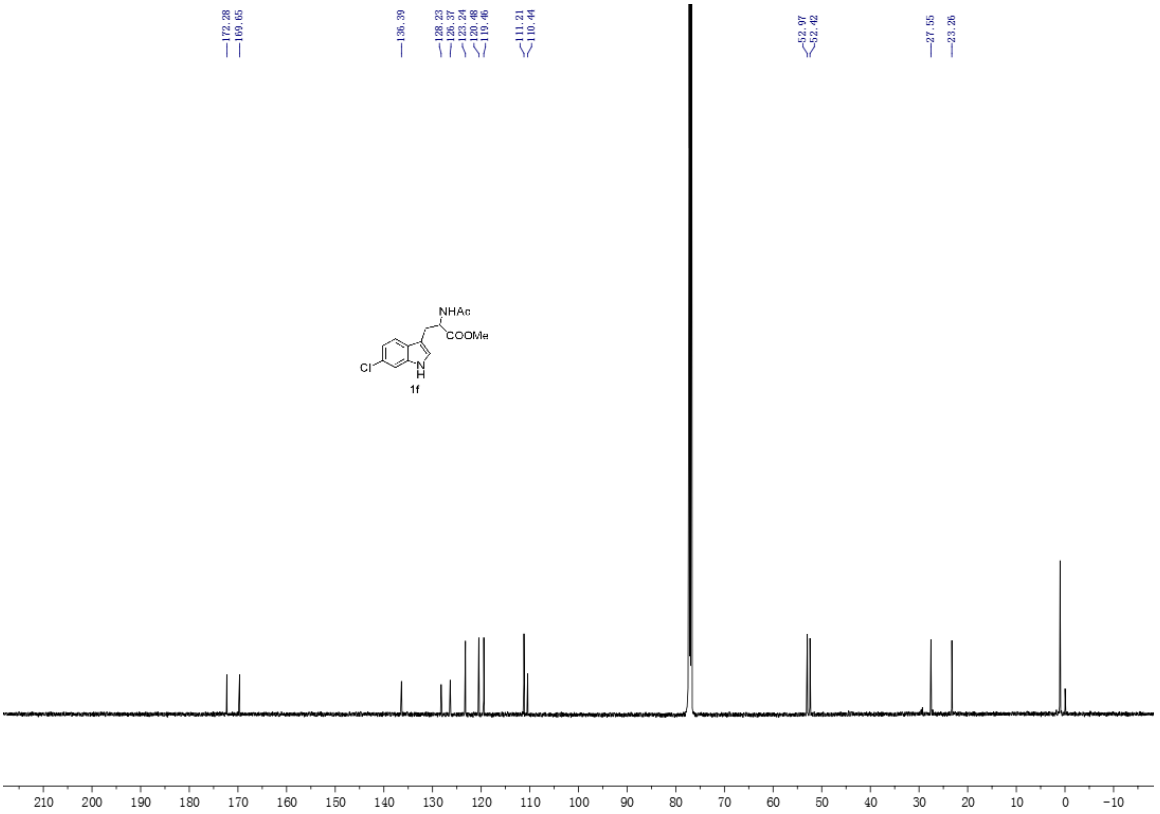
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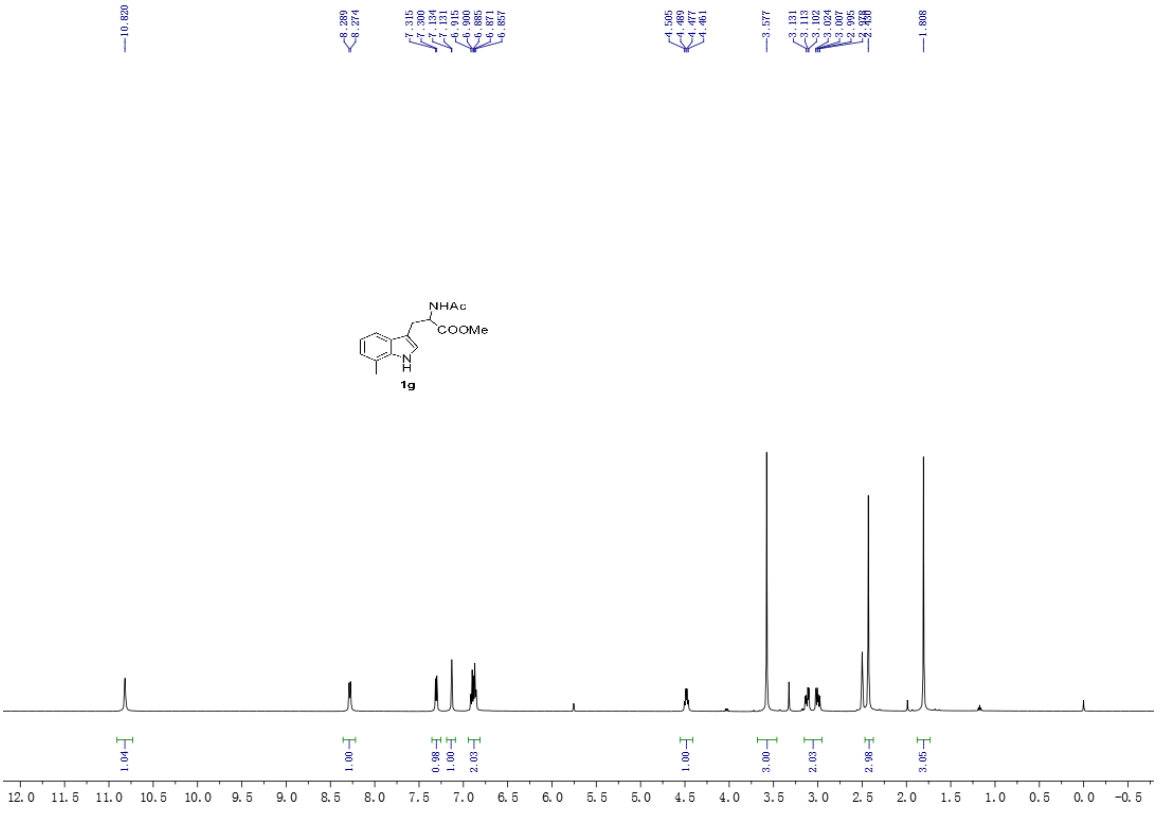
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COOMe
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H
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0.98
1.00
2.03
1.00
3.00
2.03
2.98
3.05
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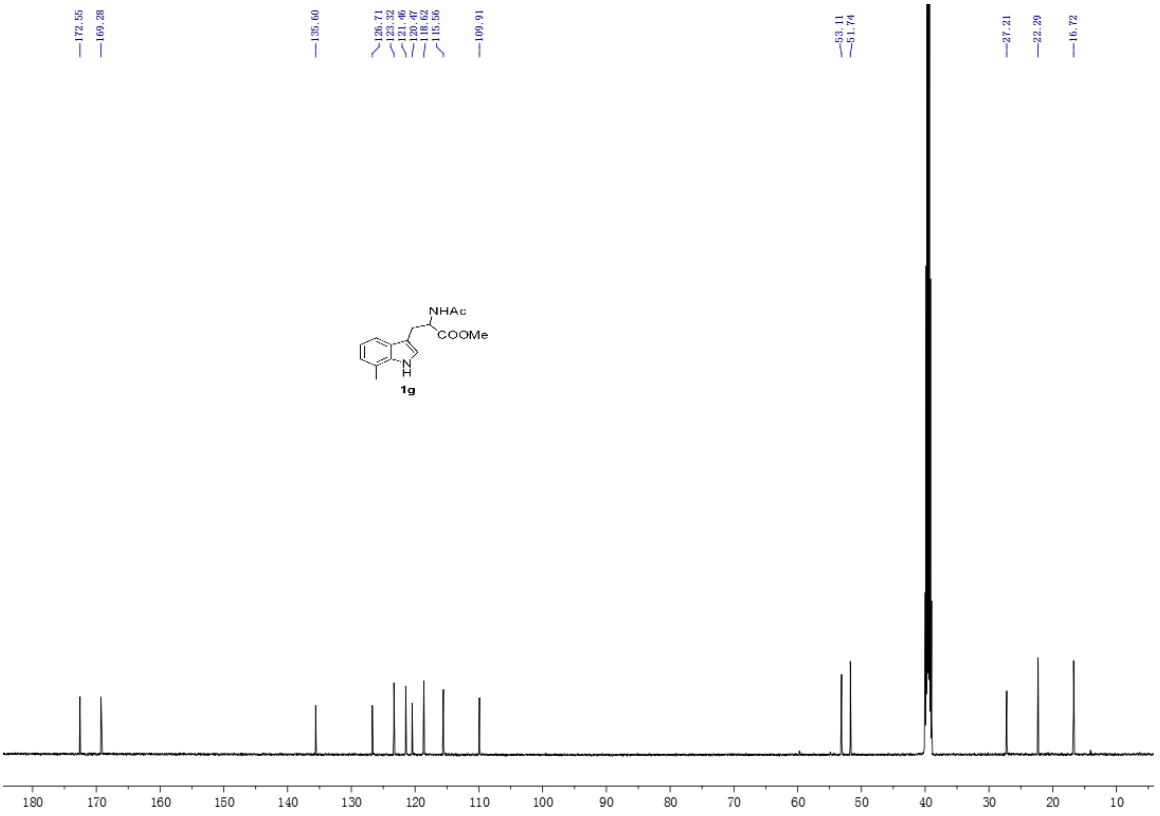
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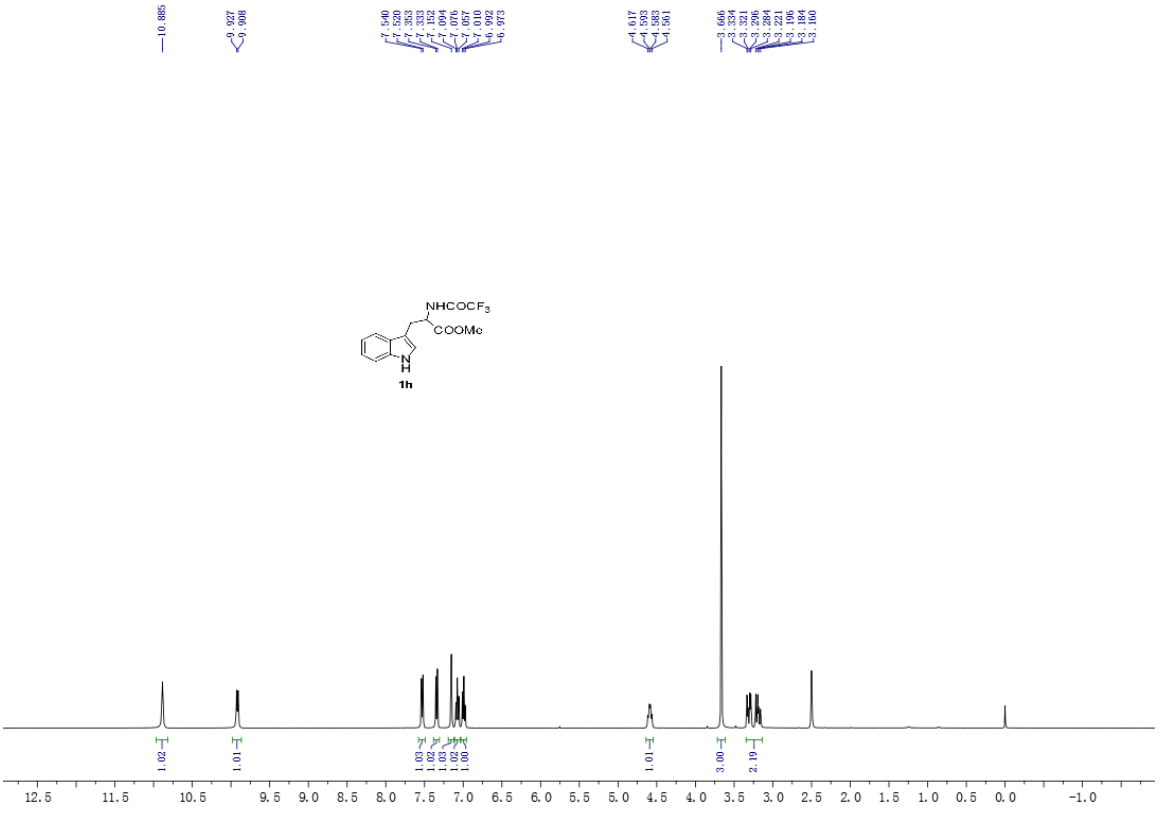
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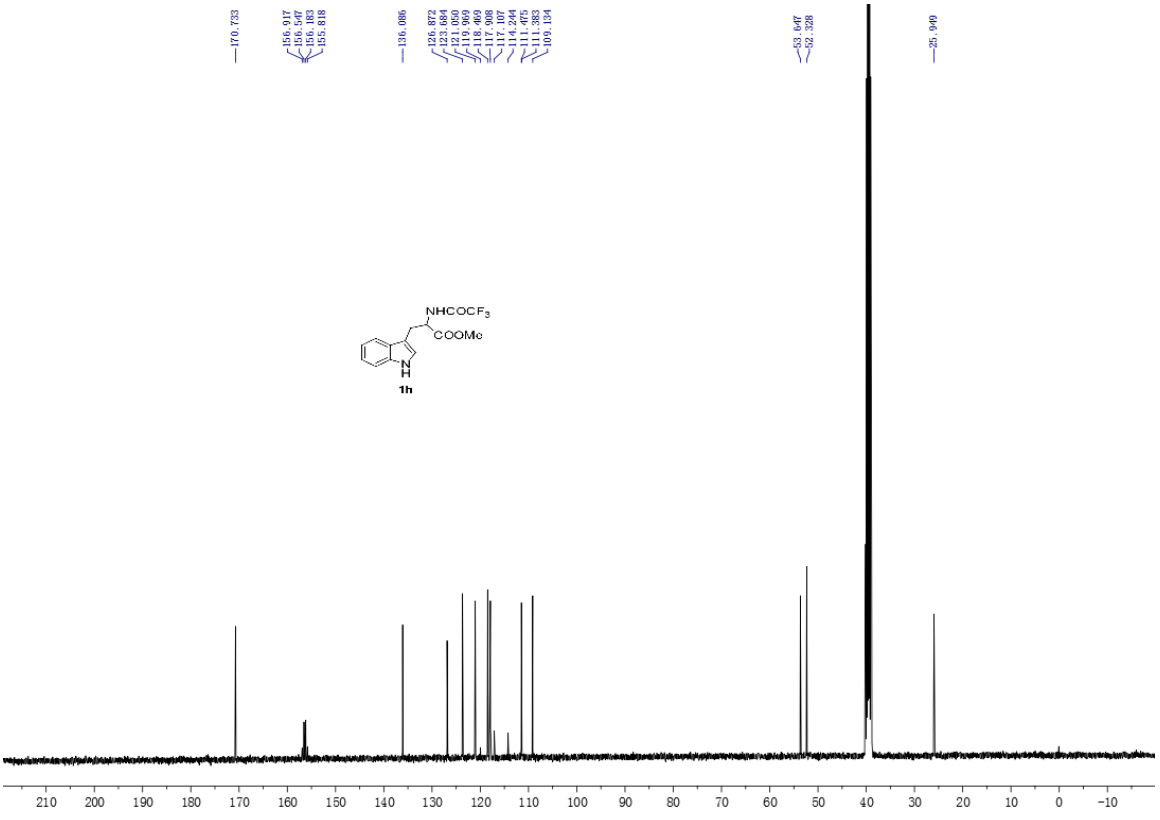
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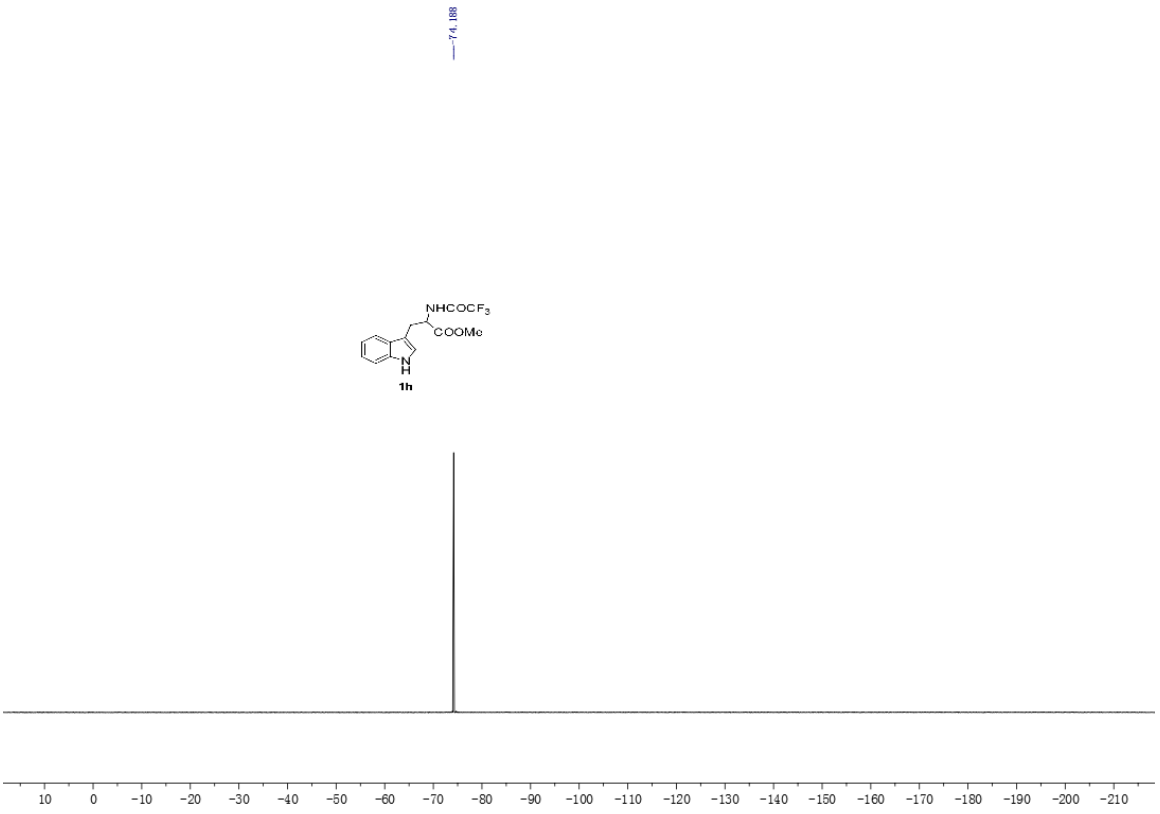
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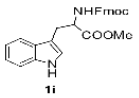
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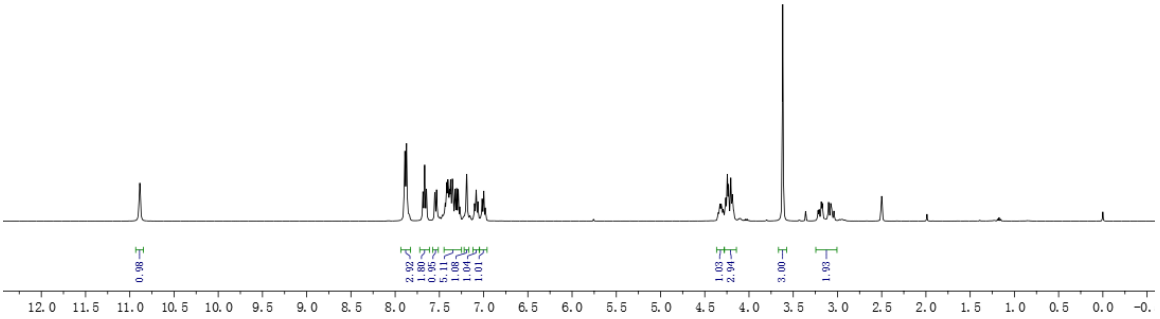
N

1i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1.01
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2.94
3.00
1.93
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.


172.71
155.92
143.74
143.71
140.68
136.12
127.60
127.05
125.22
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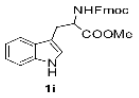
NHFmoc
COOMe
H
N

1i


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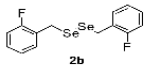
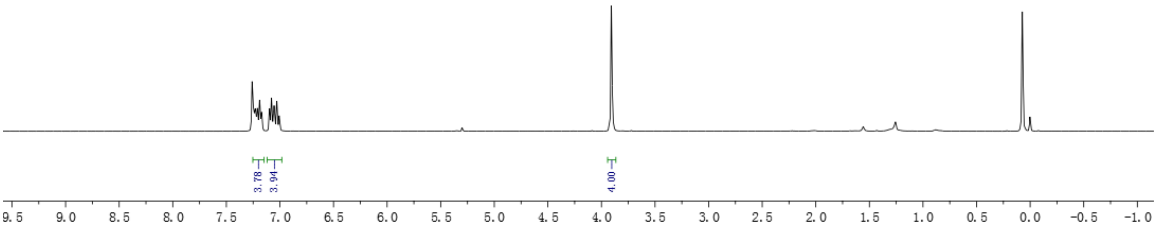
3.907


F
Se
Se
F

2b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7.5
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5.0
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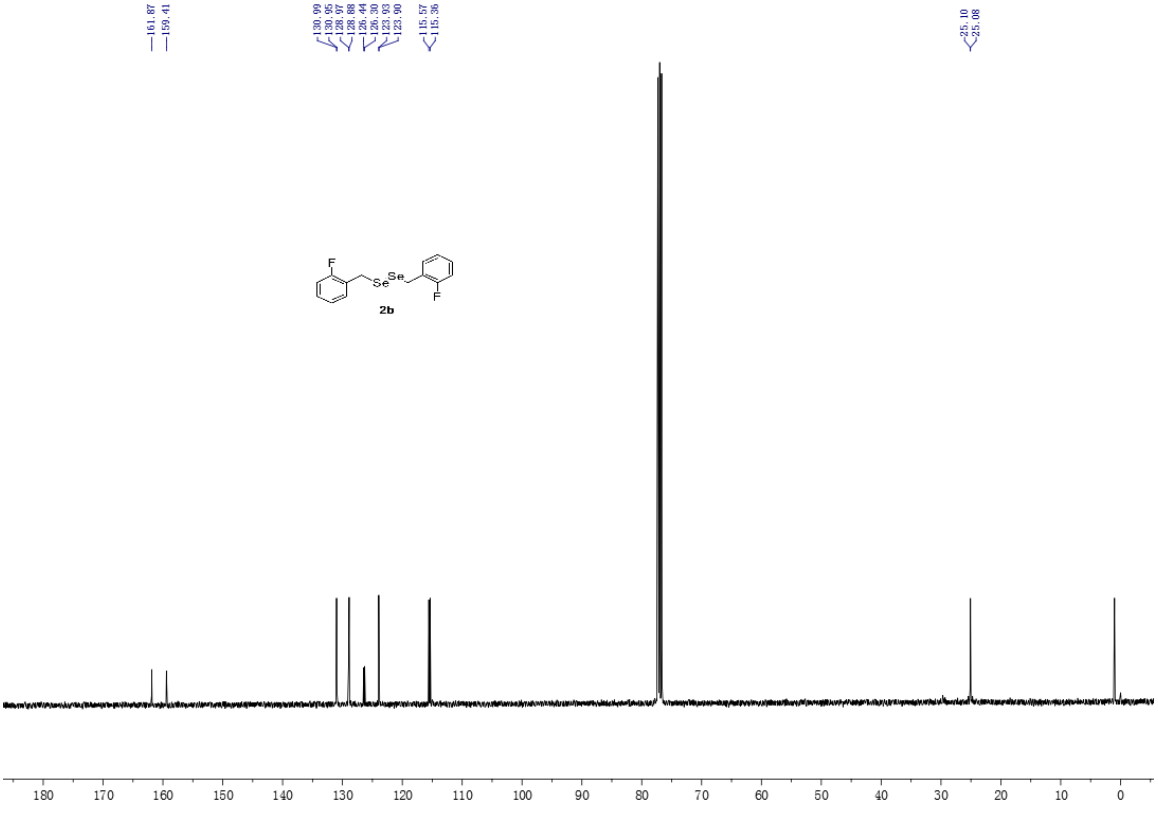
-1.0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126.44
126.30
123.93
123.90
115.57
115.36
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25.08
180
170
160
150
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100
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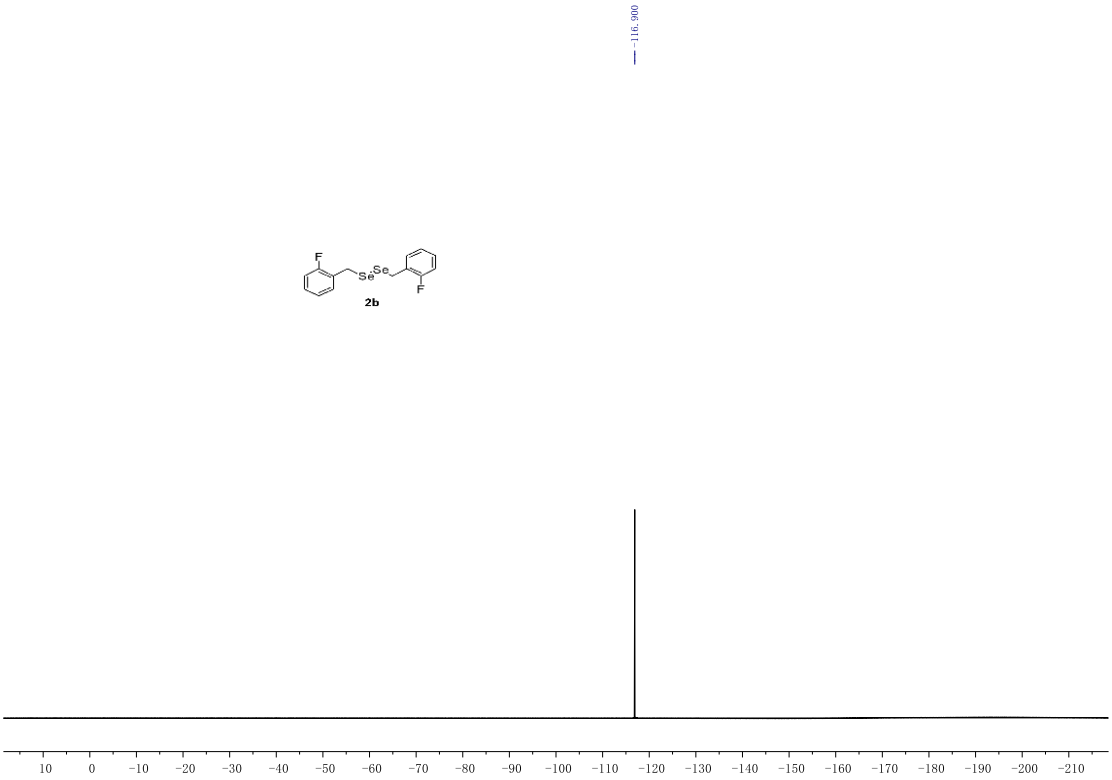
20
10
0


F
Se
Se
F

2b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Se
Se
F
2b
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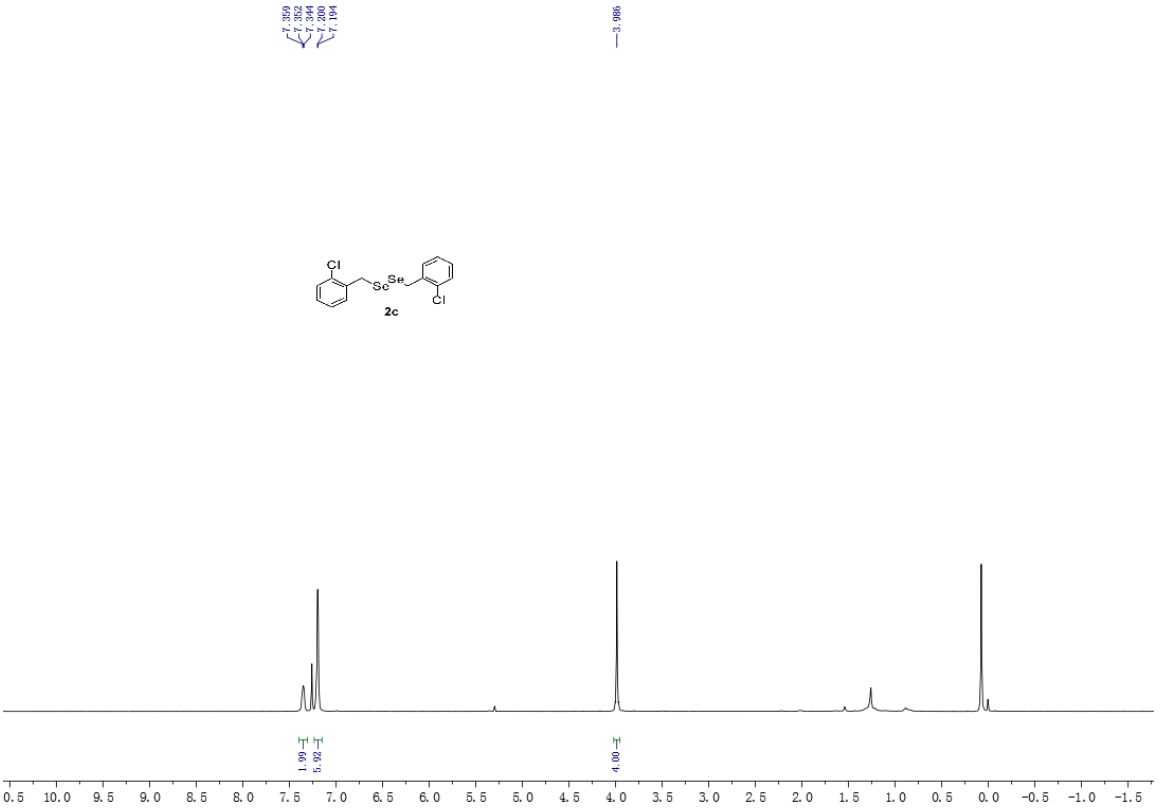
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Se
Se
Cl
2c
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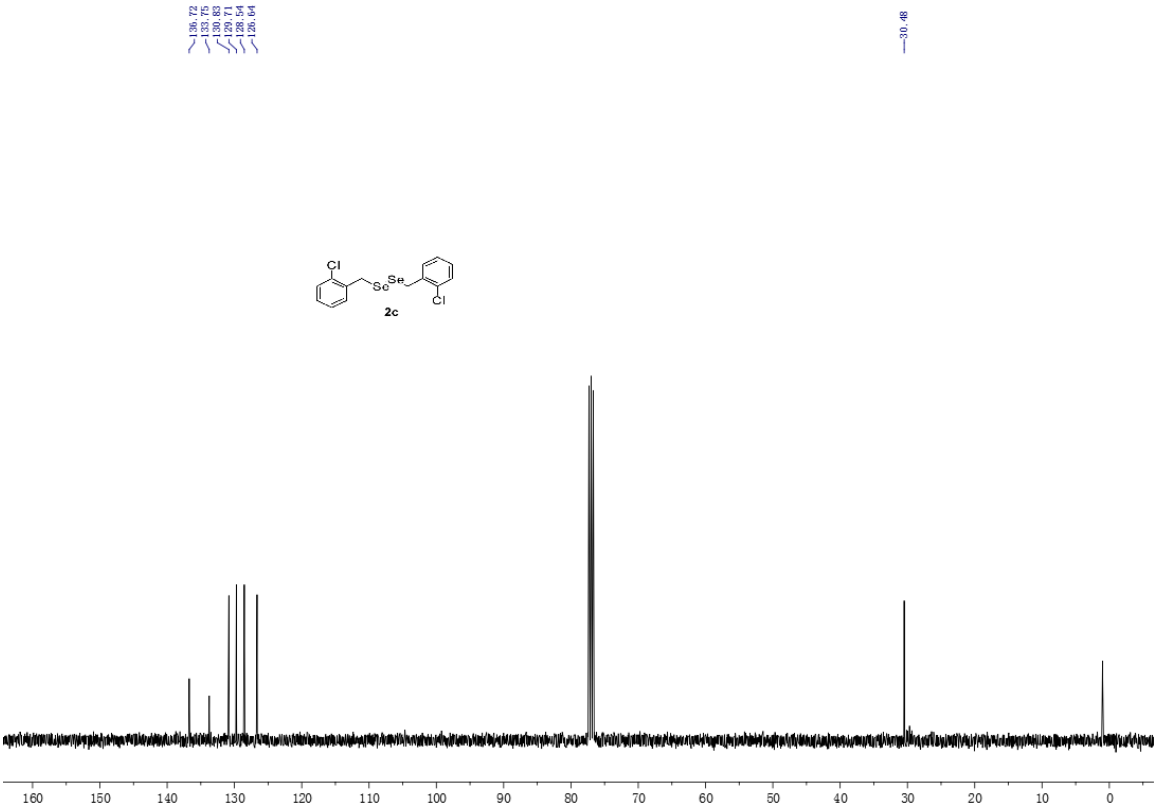
5.92
4.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5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126.64
30.48
Cl
Se
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2c
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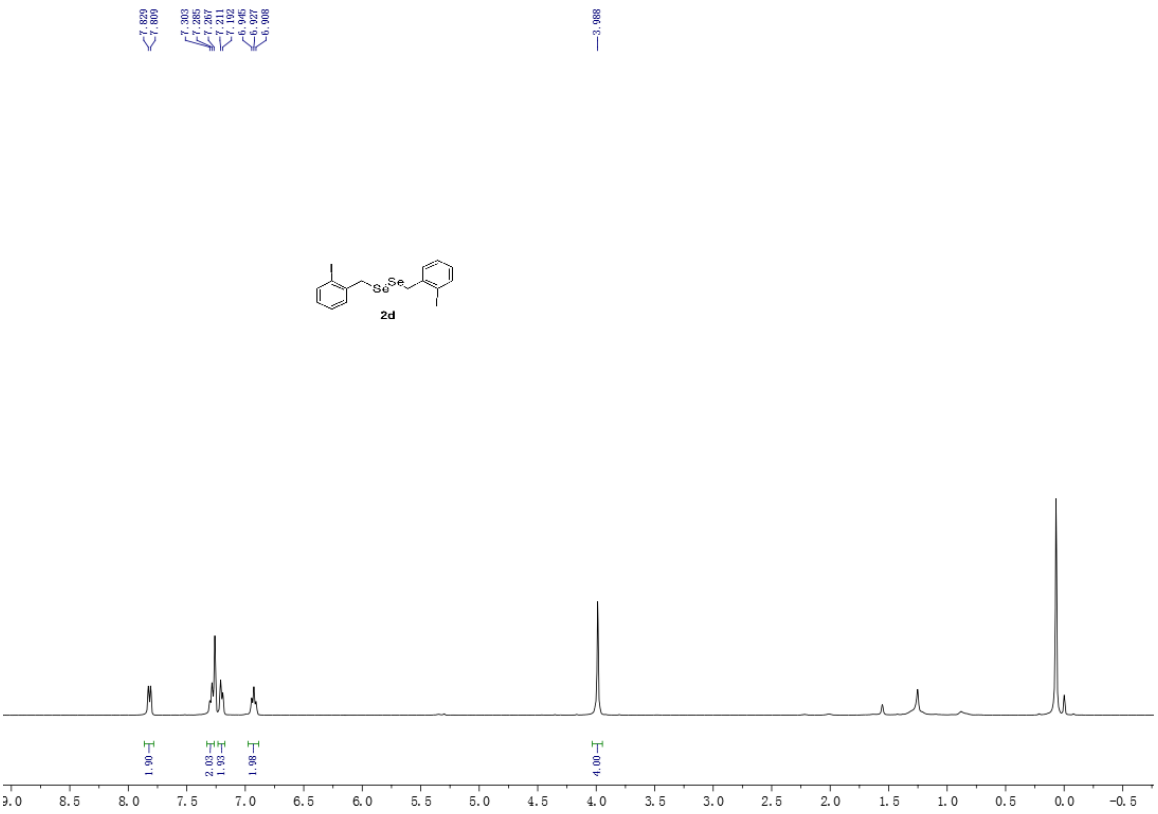
10
0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7.211
7.192
6.946
6.927
6.908
3.988
Se
Se
2d
1.90
2.03
1.93
1.98
4.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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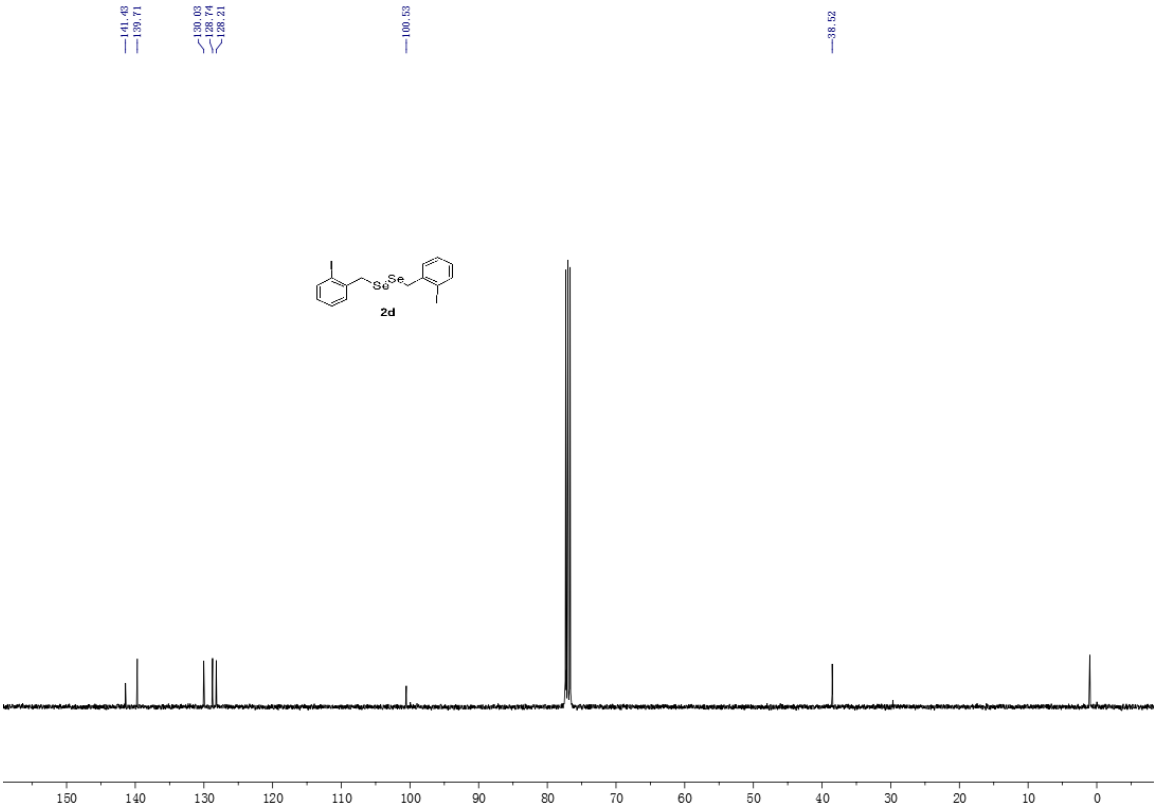
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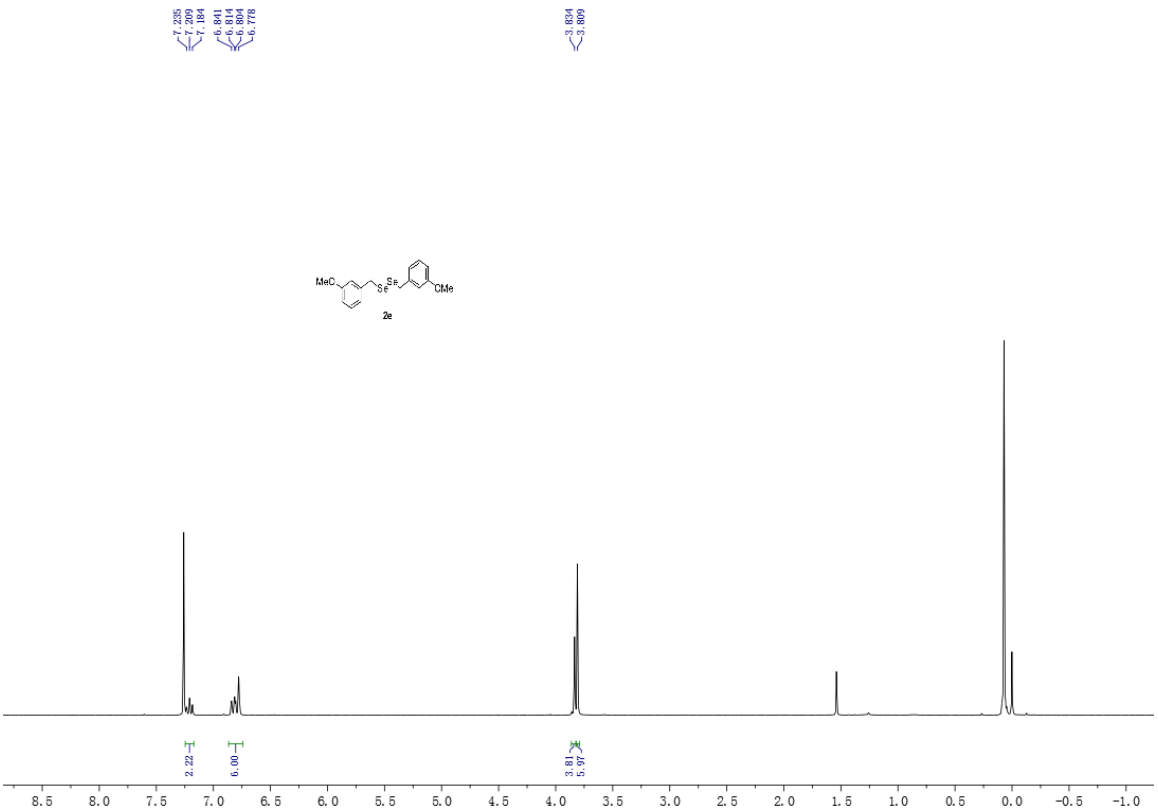
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6.809
6.778
3.834
3.809
MeO
OMe
2e
2.22
6.00
3.81
5.97
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
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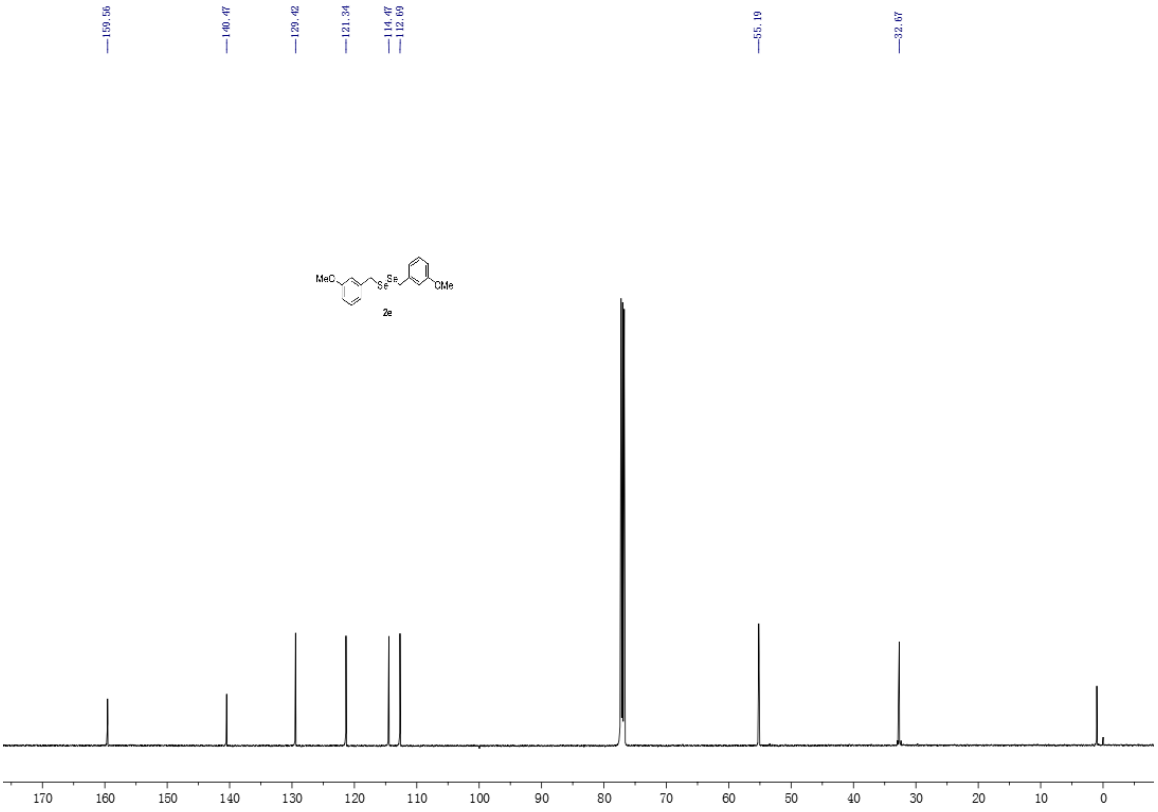
-0.5
-1.0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129.42
121.34
114.47
112.69
55.19
32.67
MeO
Se
Se
OMe
2e
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150
140
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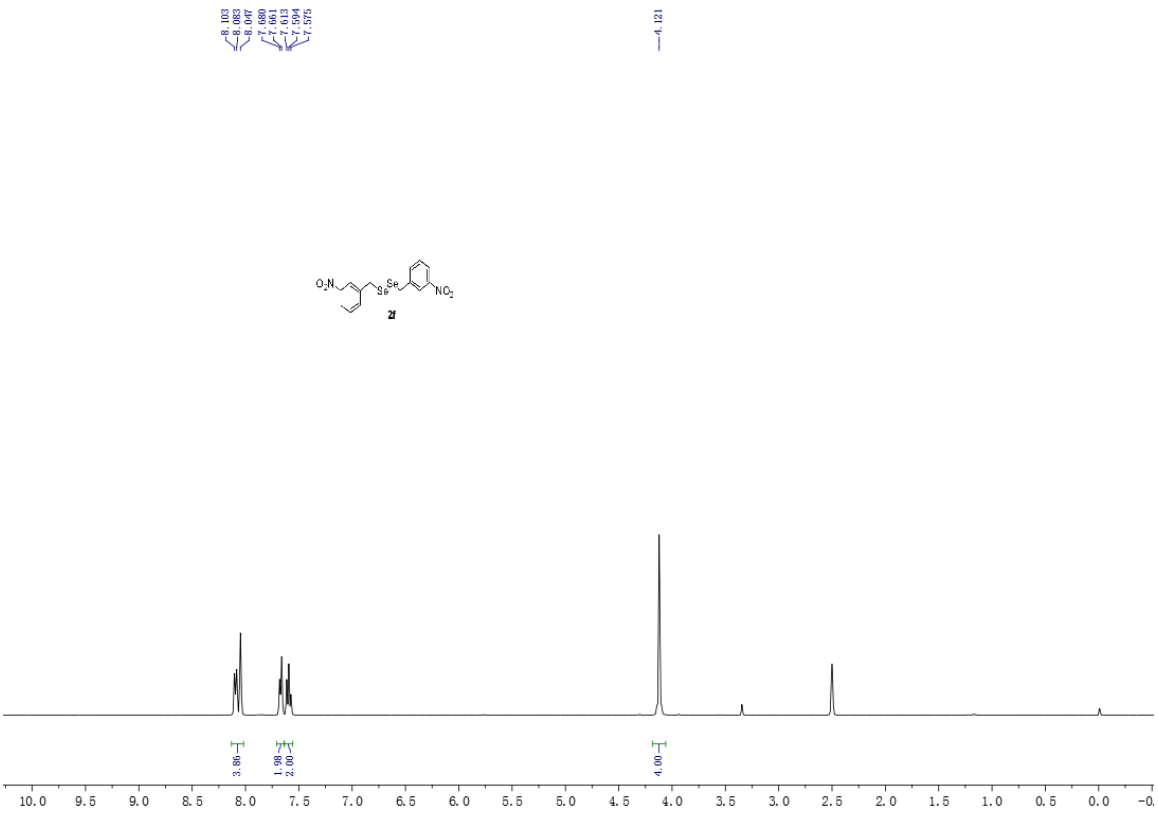
10
0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8.083
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7.613
7.594
7.575
4.121
O2N
Se
Se
NO2
2f
3.86
1.98
2.00
4.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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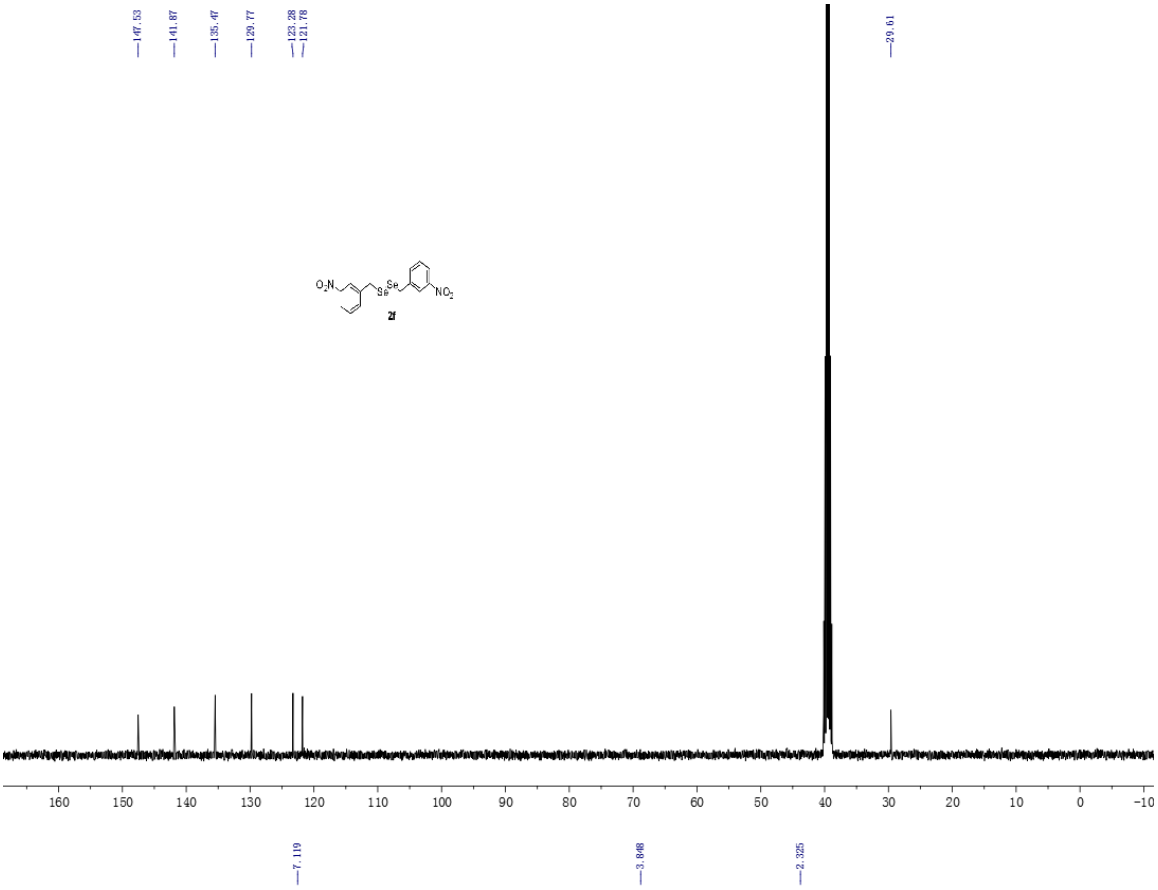
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135.47
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123.28
121.78
29.61
2f
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140
130
120
110
100
90
80
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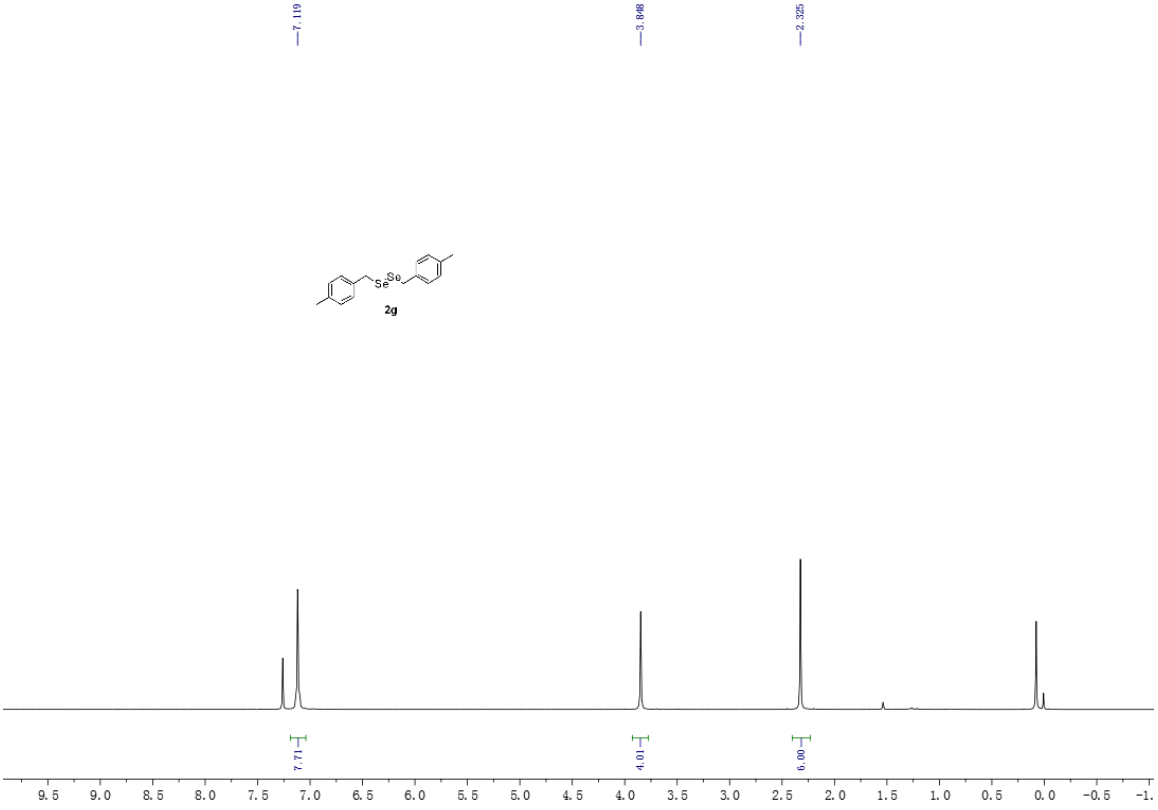
60
50
40
30
20
10
0
-10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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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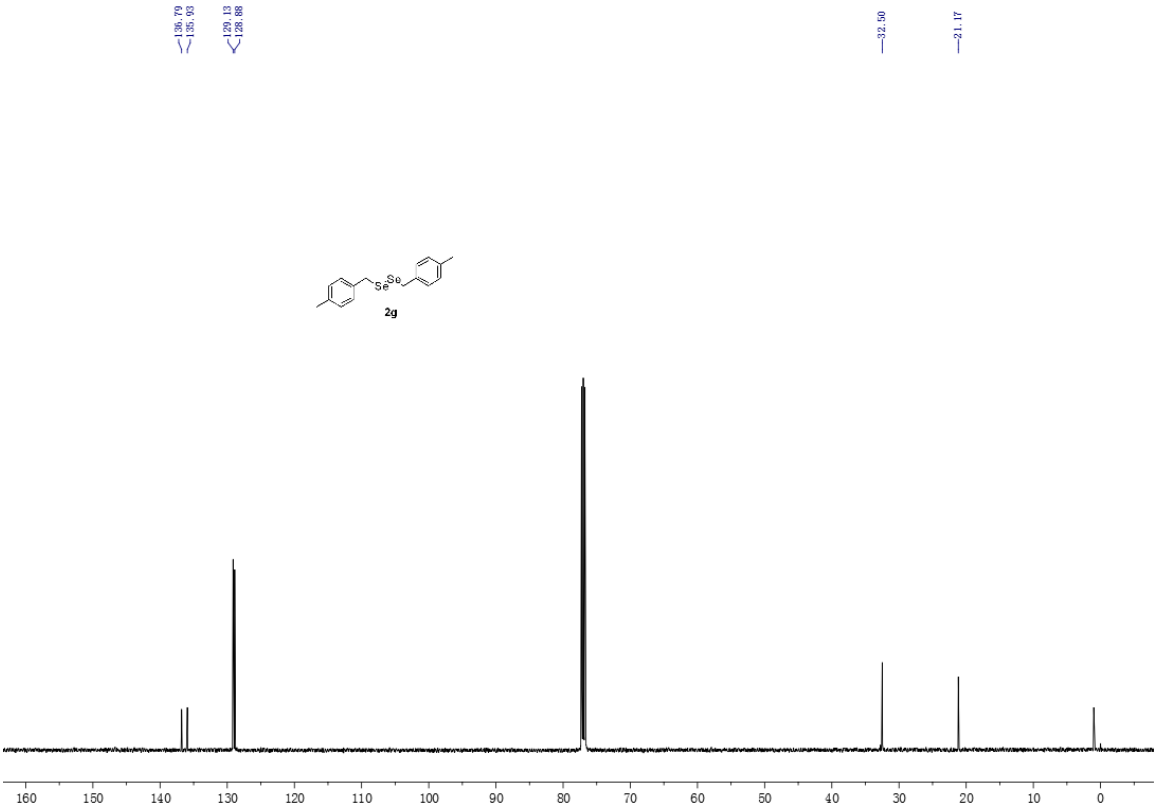
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135.93
129.13
128.88
32.50
21.17
2g
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150
140
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120
110
100
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70
60
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30
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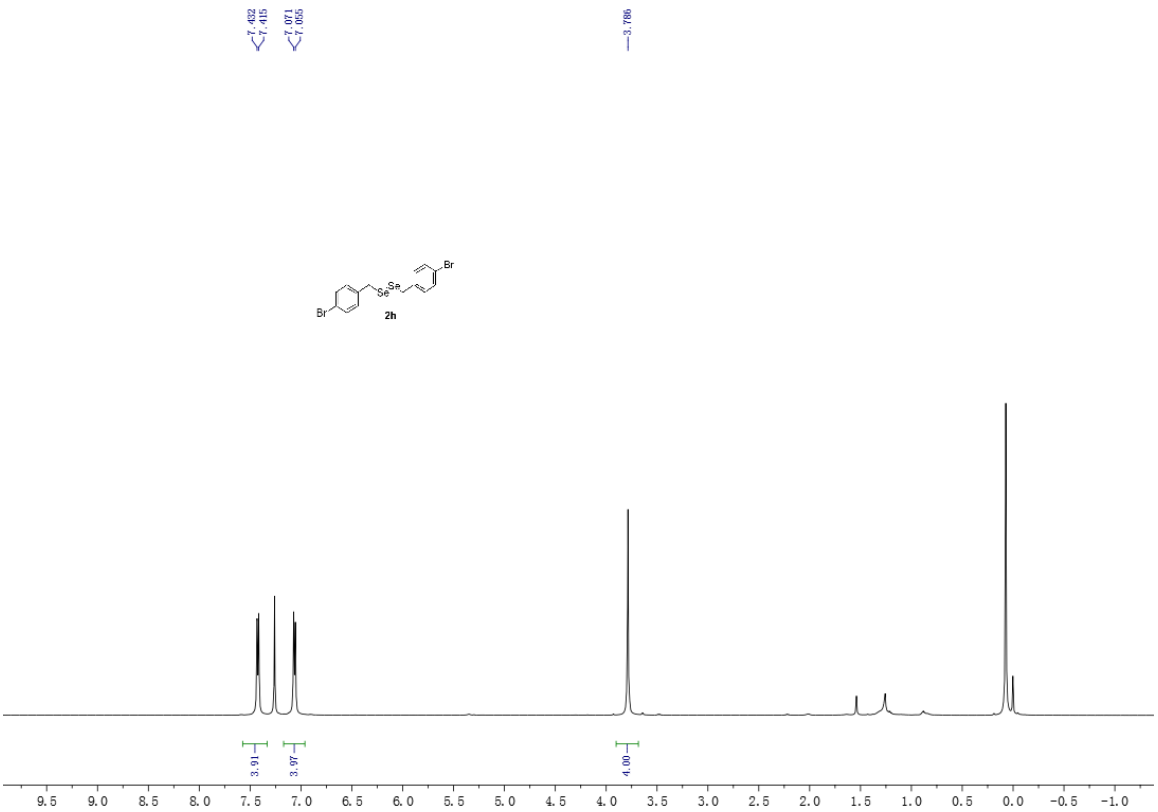
10
0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7.071
7.055
3.786
Br
Br
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3.91
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4.00
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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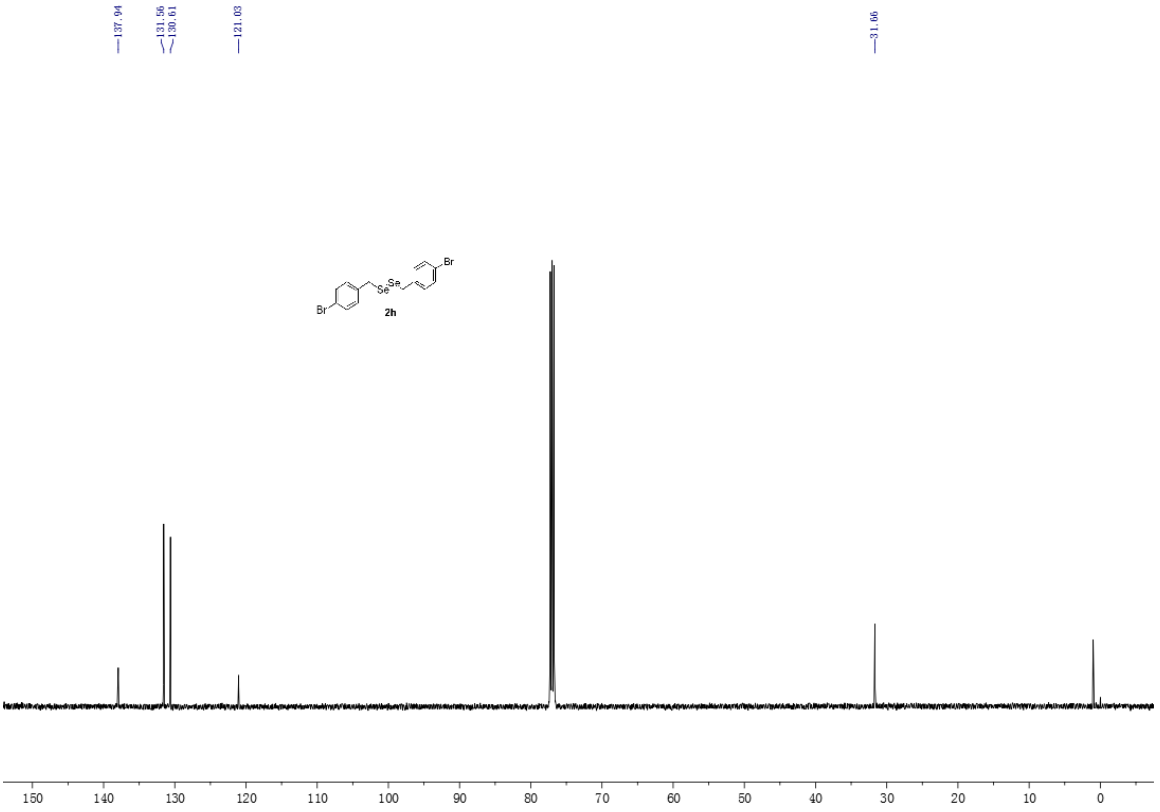
-1.0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131.56
130.61
121.03
31.66
Br
Se
Se
Br
2h
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140
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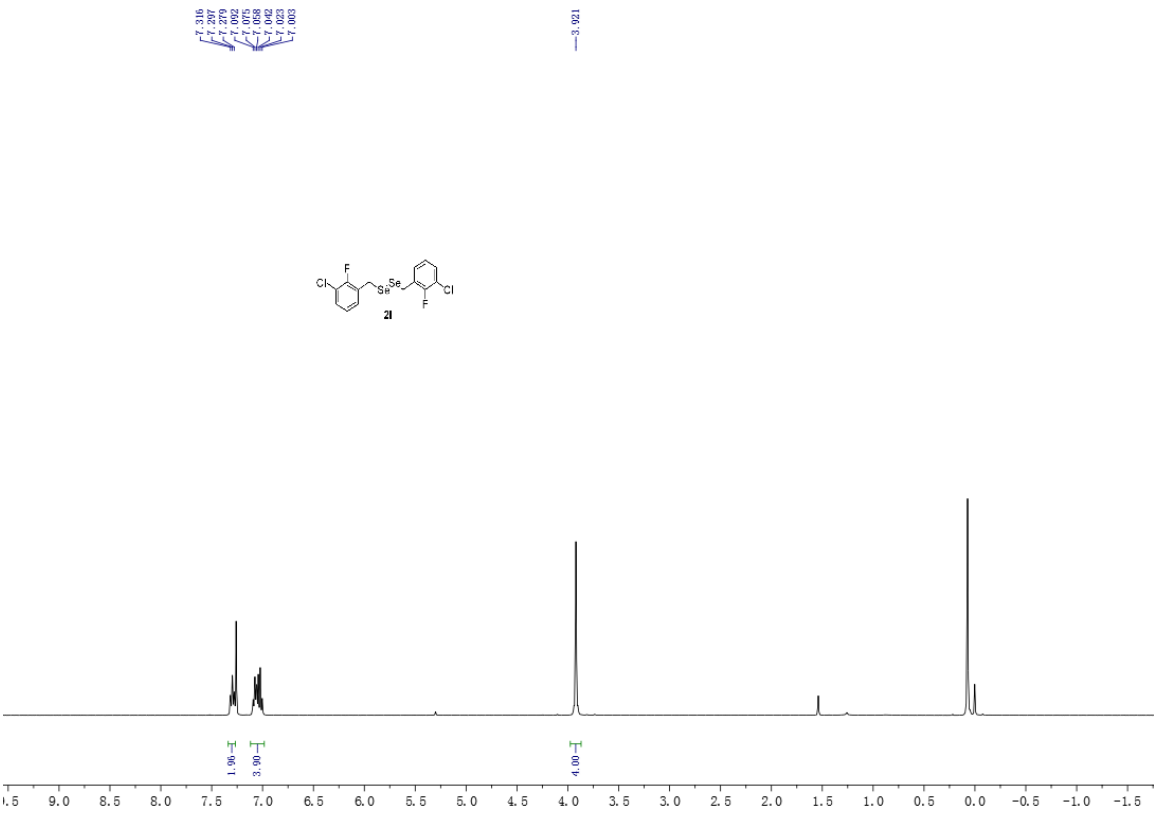
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7.075
7.058
7.042
7.023
7.003
3.921
F
Cl
Se
Se
Cl
F
2l
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3.90
4.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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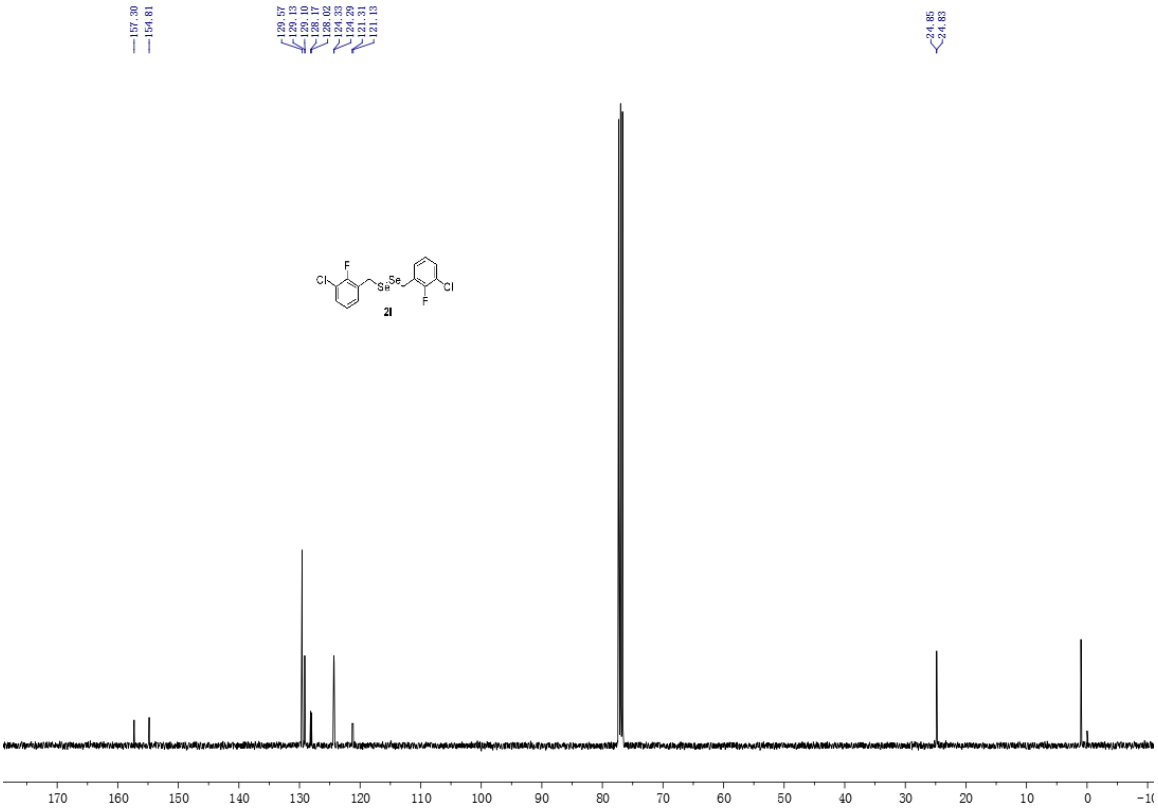
-1.0
-1.5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128.02
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121.31
121.13
24.85
24.63
Cl
F
Se
Se
F
Cl
2l
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130
120
110
100
90
80
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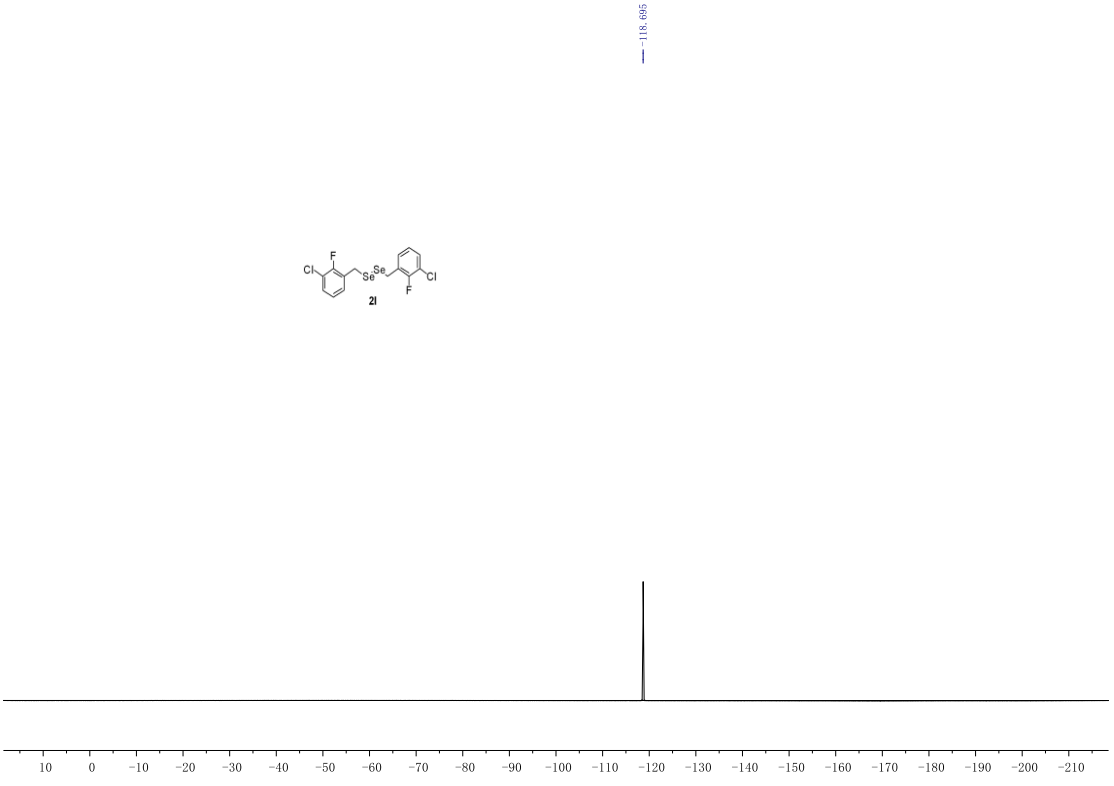
60
50
40
30
20
10
0
-10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Cl
F
Se
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F
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2l
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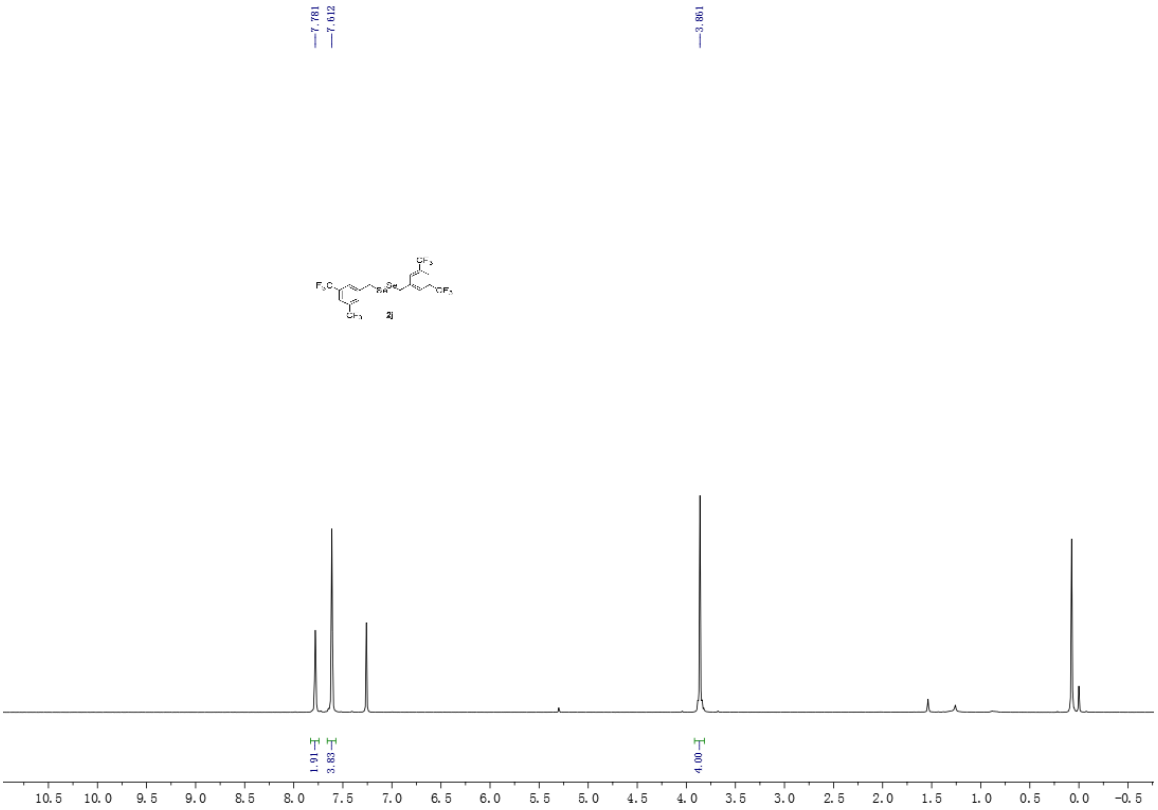
-190
-200
-210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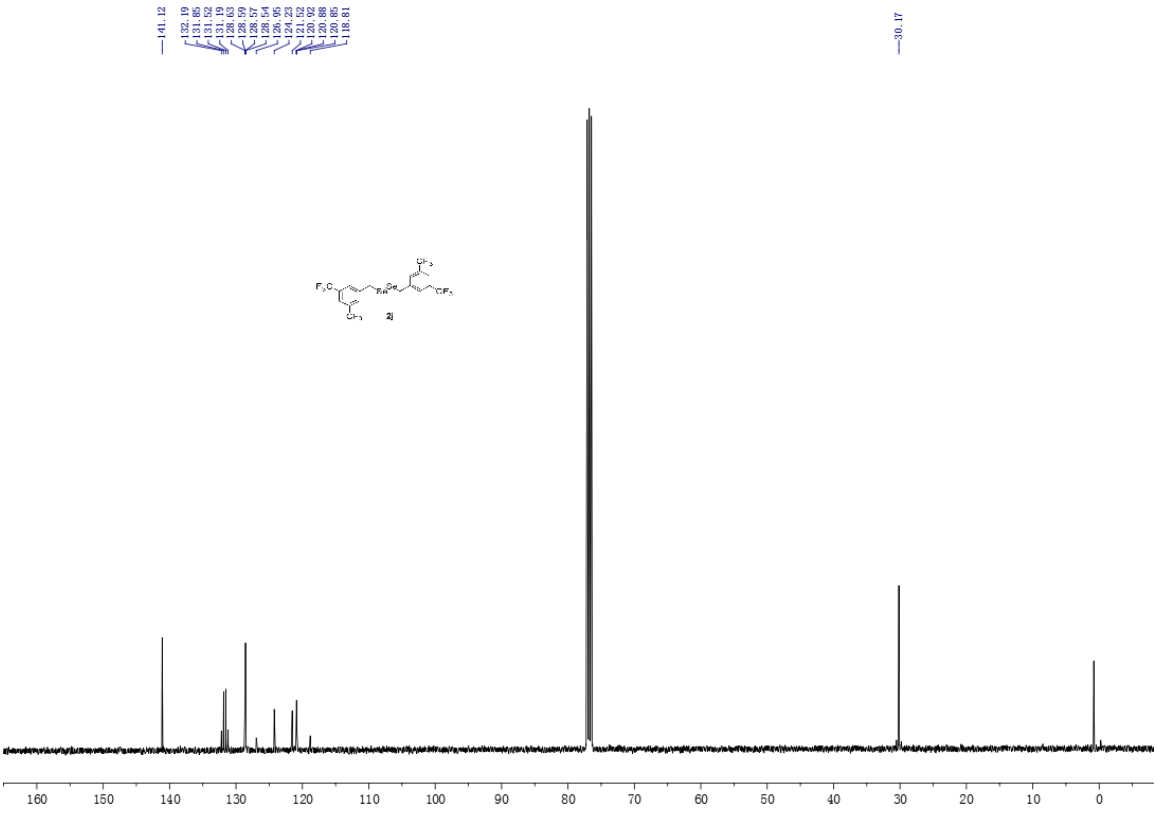
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118.81
30.17
2j
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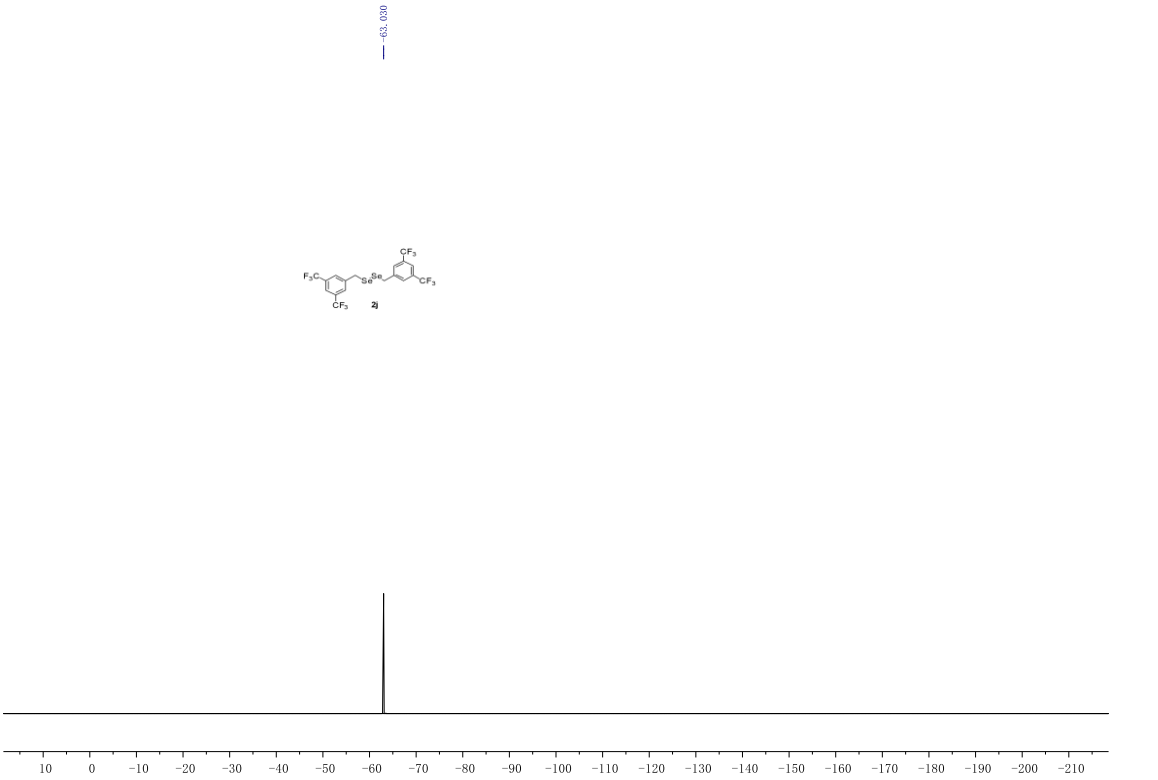
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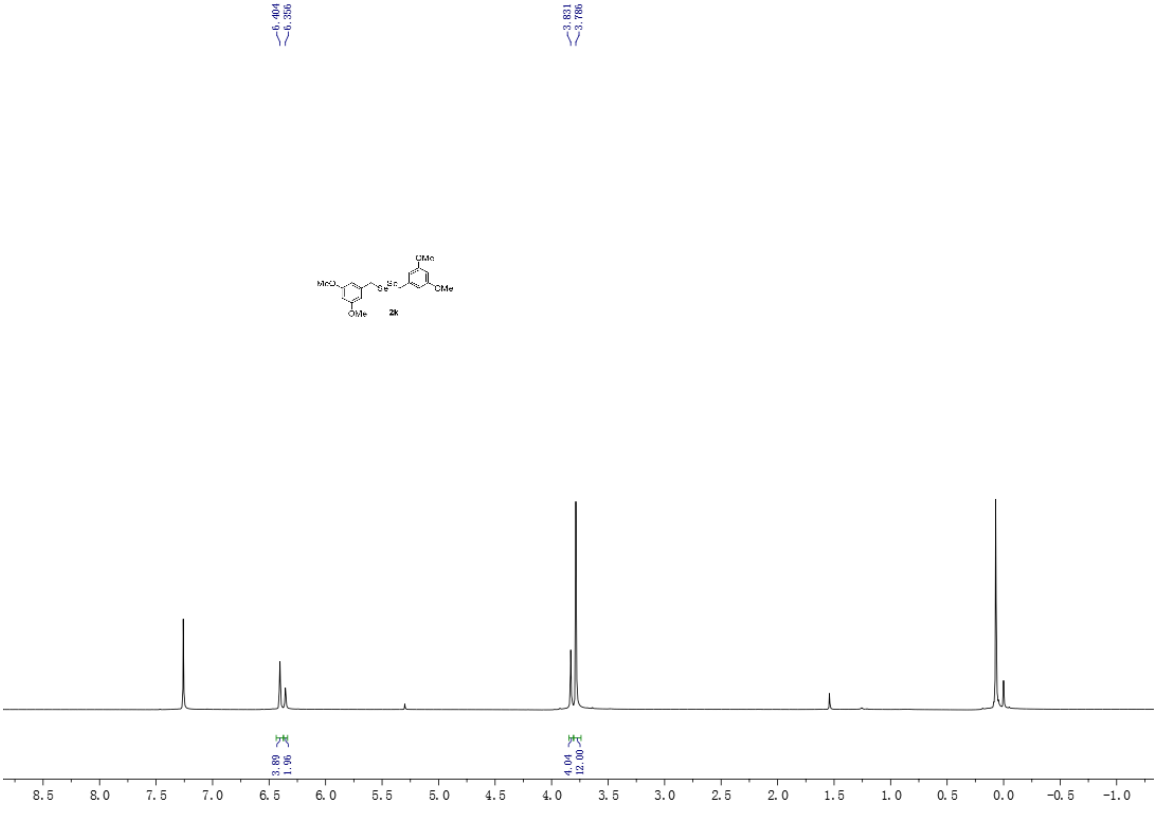
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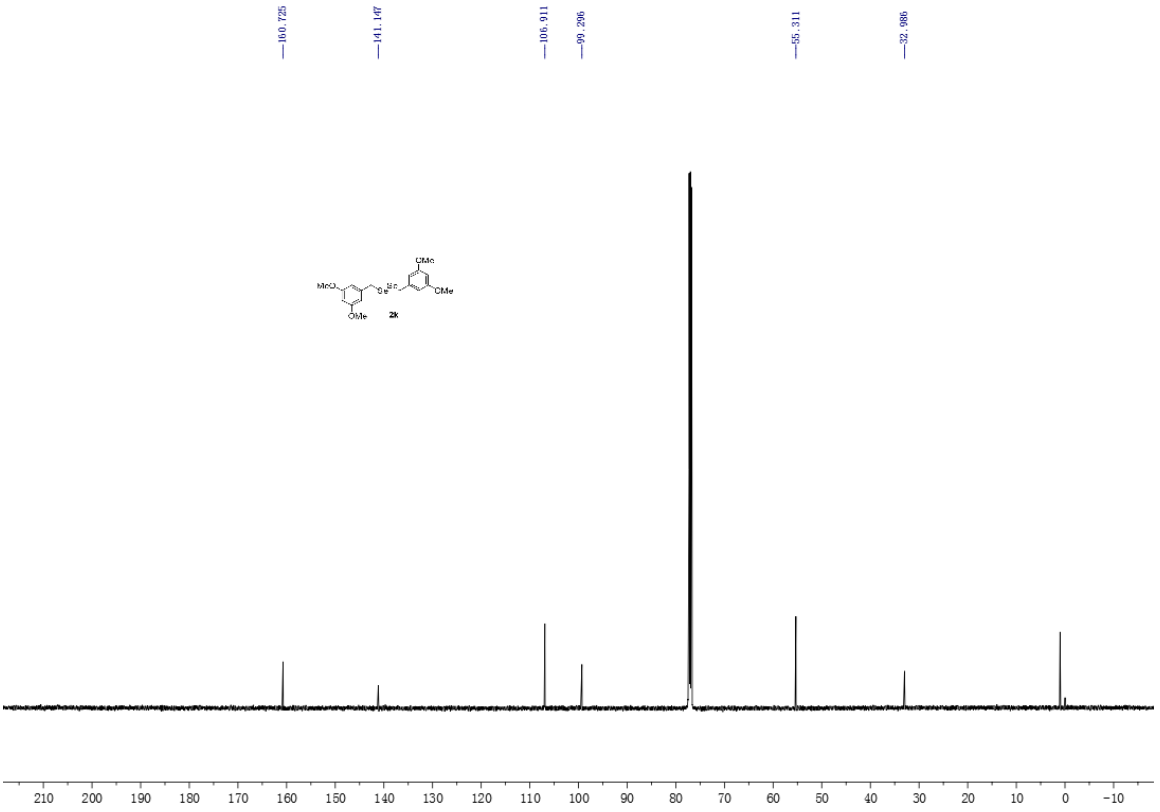
6.356
3.831
3.786
2k
3.89
1.96
4.04
12.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0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32.986
2k
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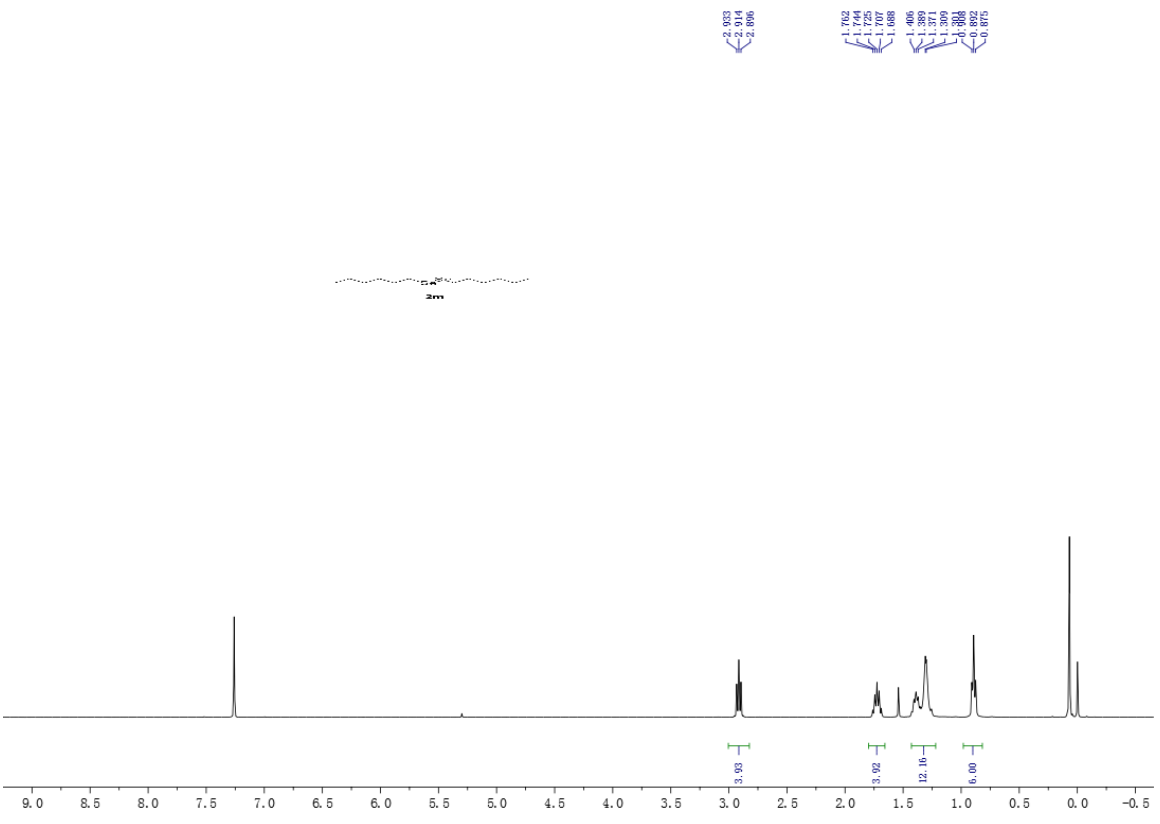
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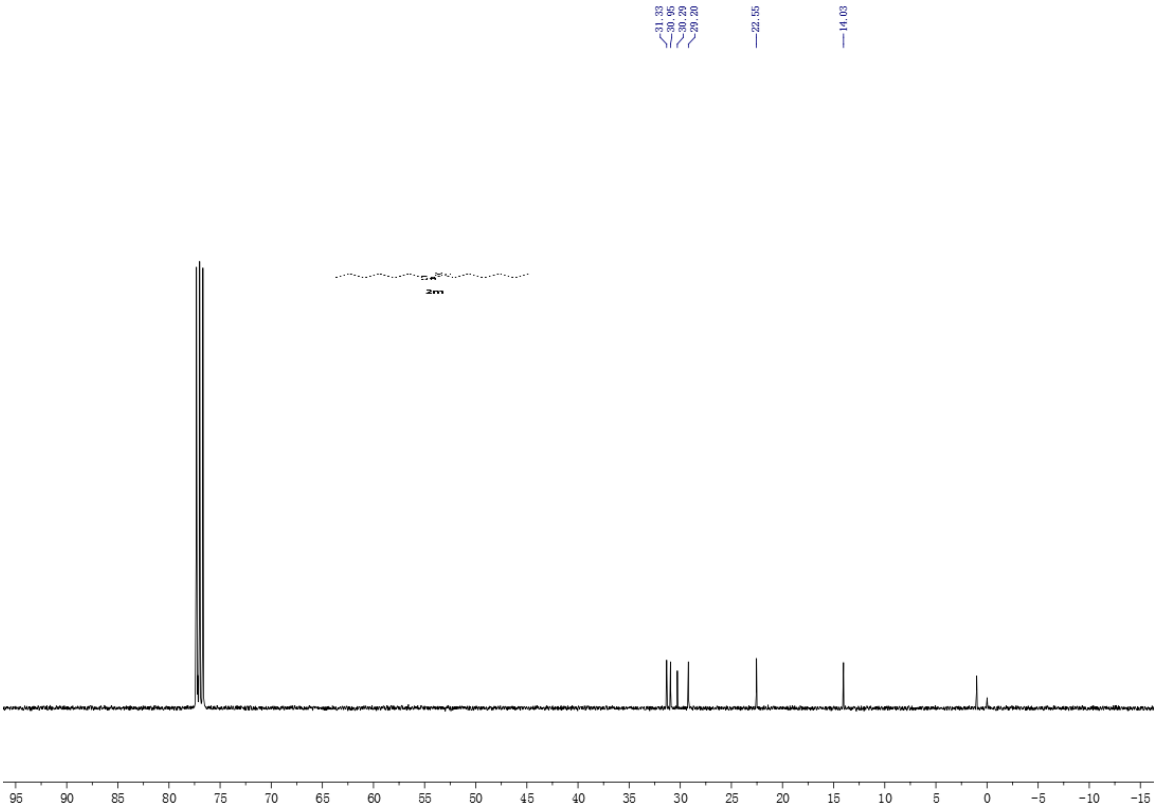
1.406
1.389
1.371
1.309
0.908
0.892
0.875
3m
3.93
3.92
12.16
6.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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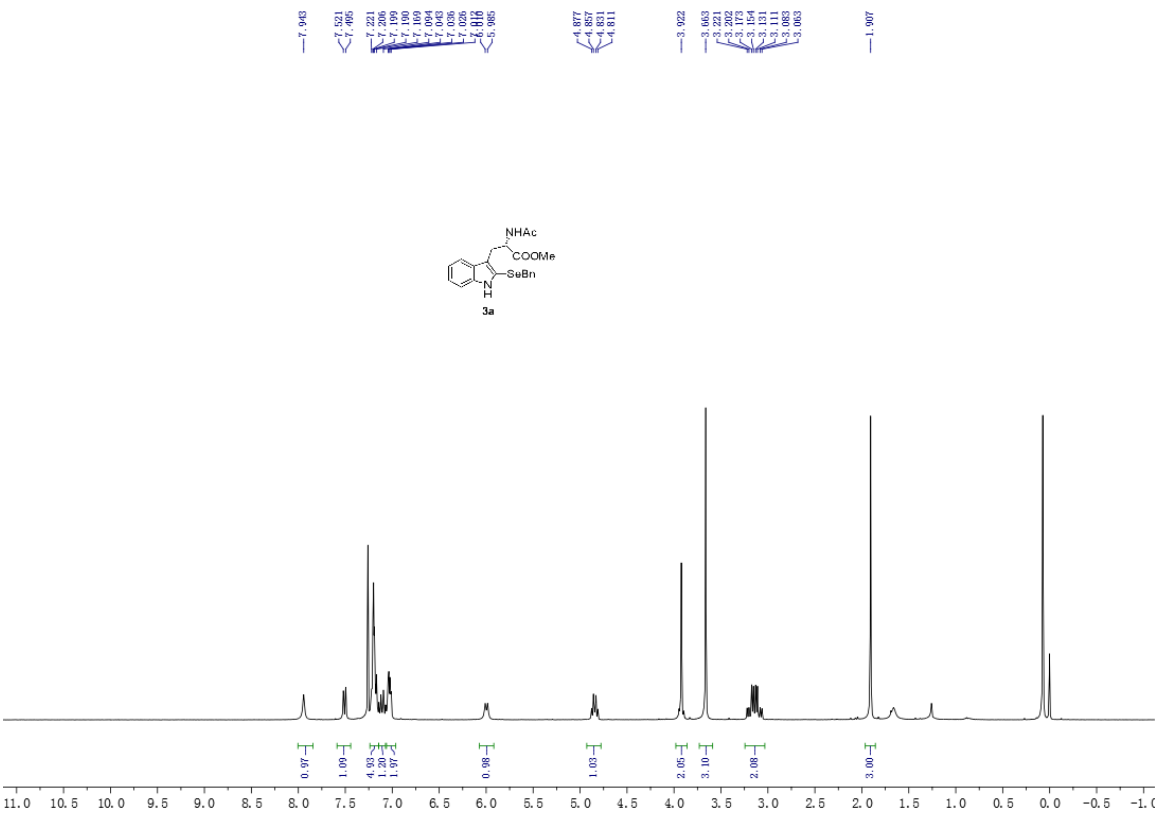
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6.016
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3.111
3.083
3.063
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NHAc
COOMe
SeBn
N
H
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4.93
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1.97
0.98
1.03
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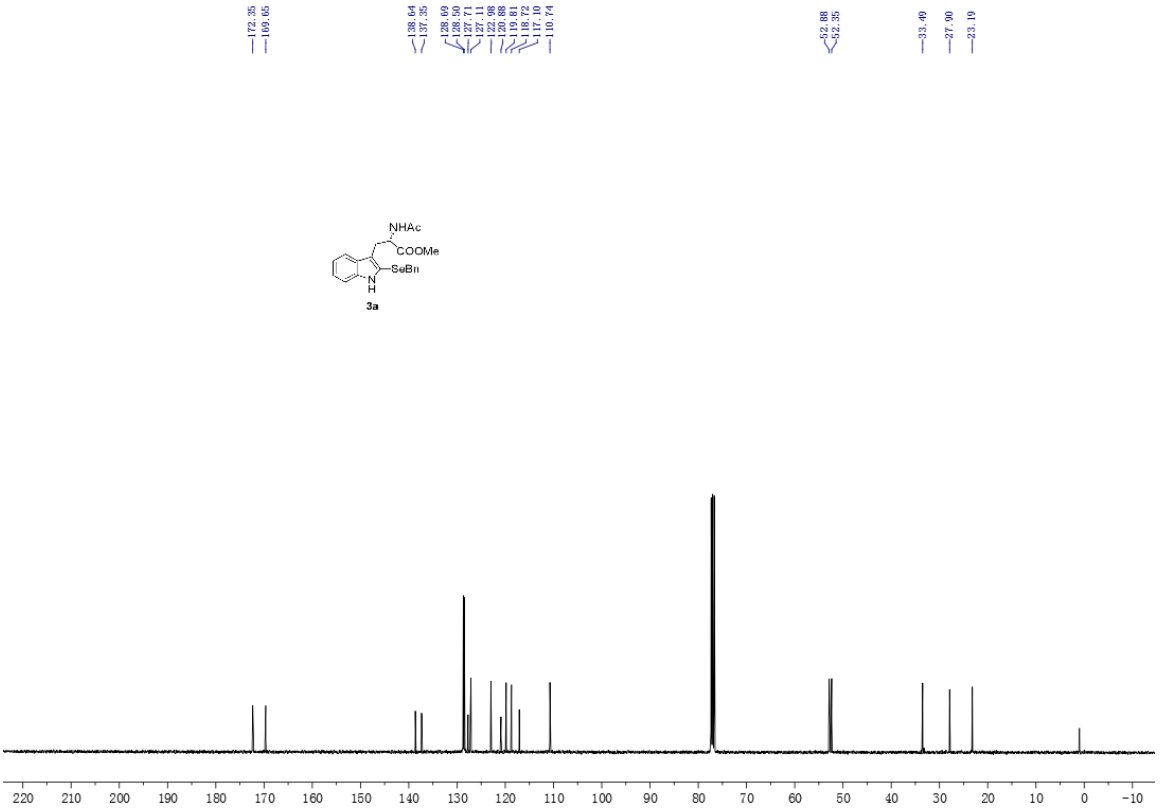
3.10
2.08
3.00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117.19
110.74
52.88
52.35
33.49
27.90
23.19
NHAc
COOMe
SeBn
N
H
3a
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200
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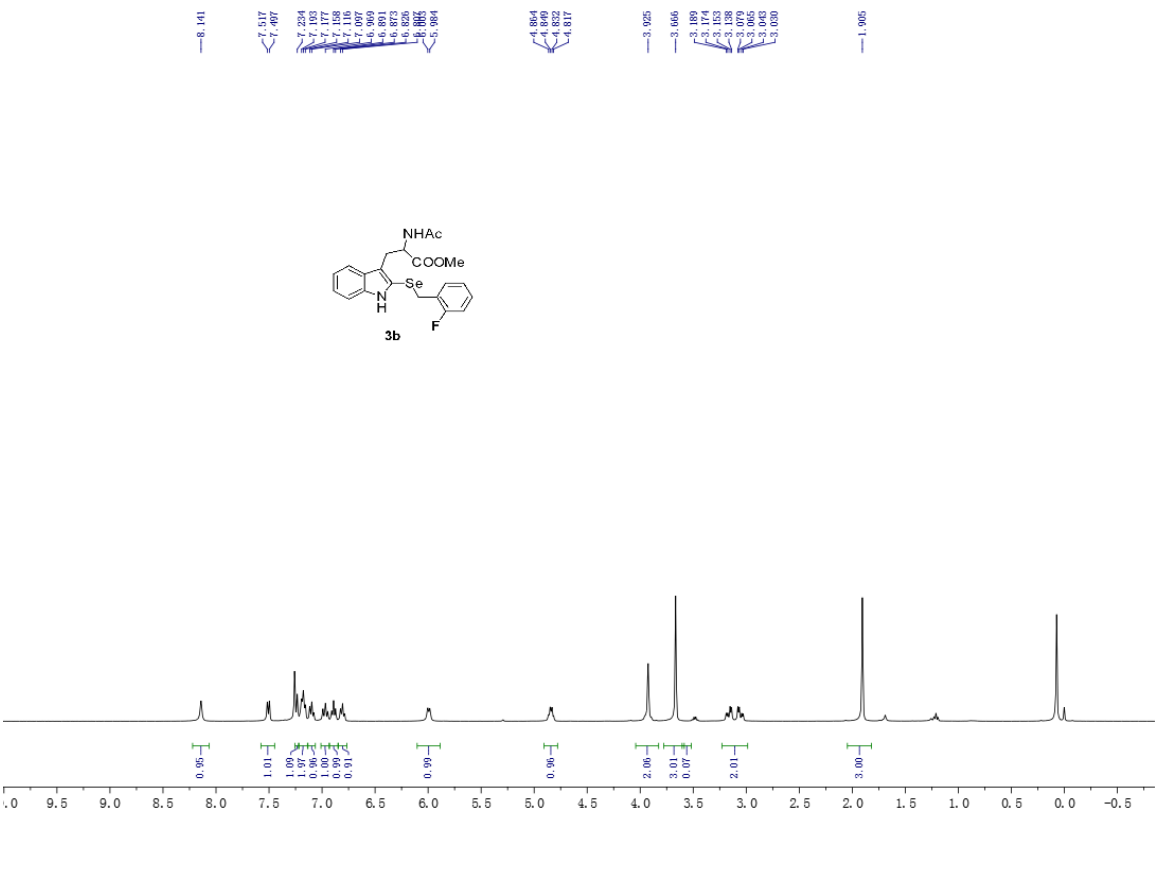
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3.138
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COOMe
Se
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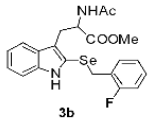
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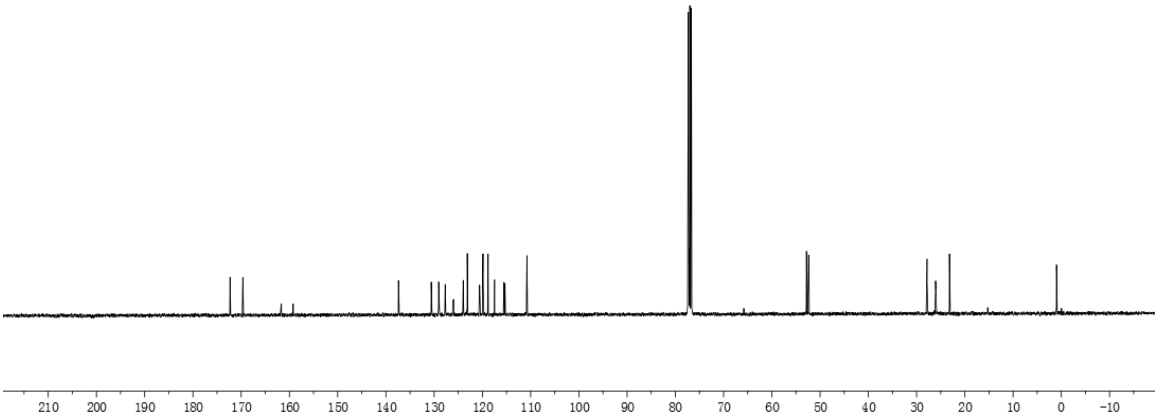
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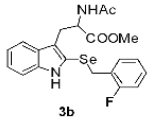
0
-10


117.254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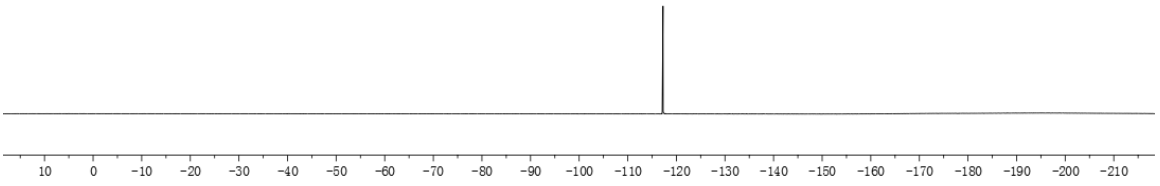
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-200
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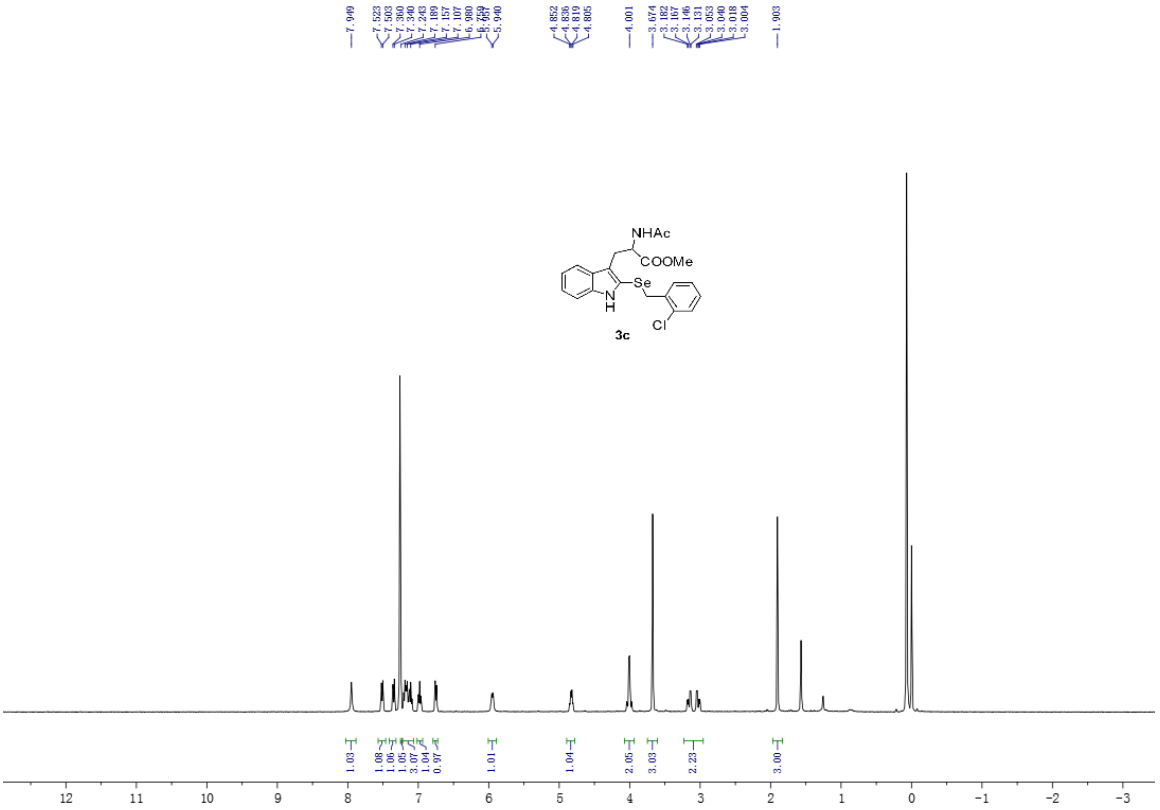
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3.018
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H
Cl
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1.06
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0.97
1.01
1.04
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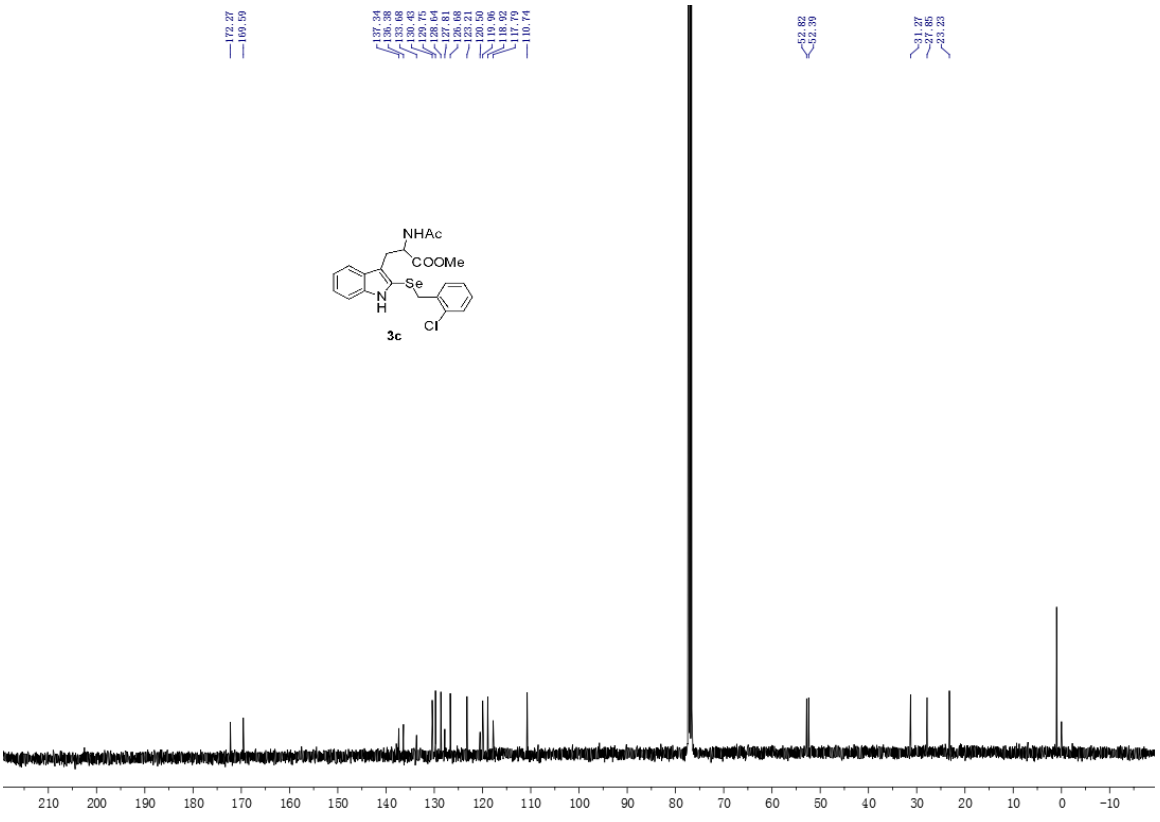
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118.92
117.79
110.74
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52.39
31.27
27.95
23.23
NHAc
COOMe
Se
N
H
Cl
3c
210
200
190
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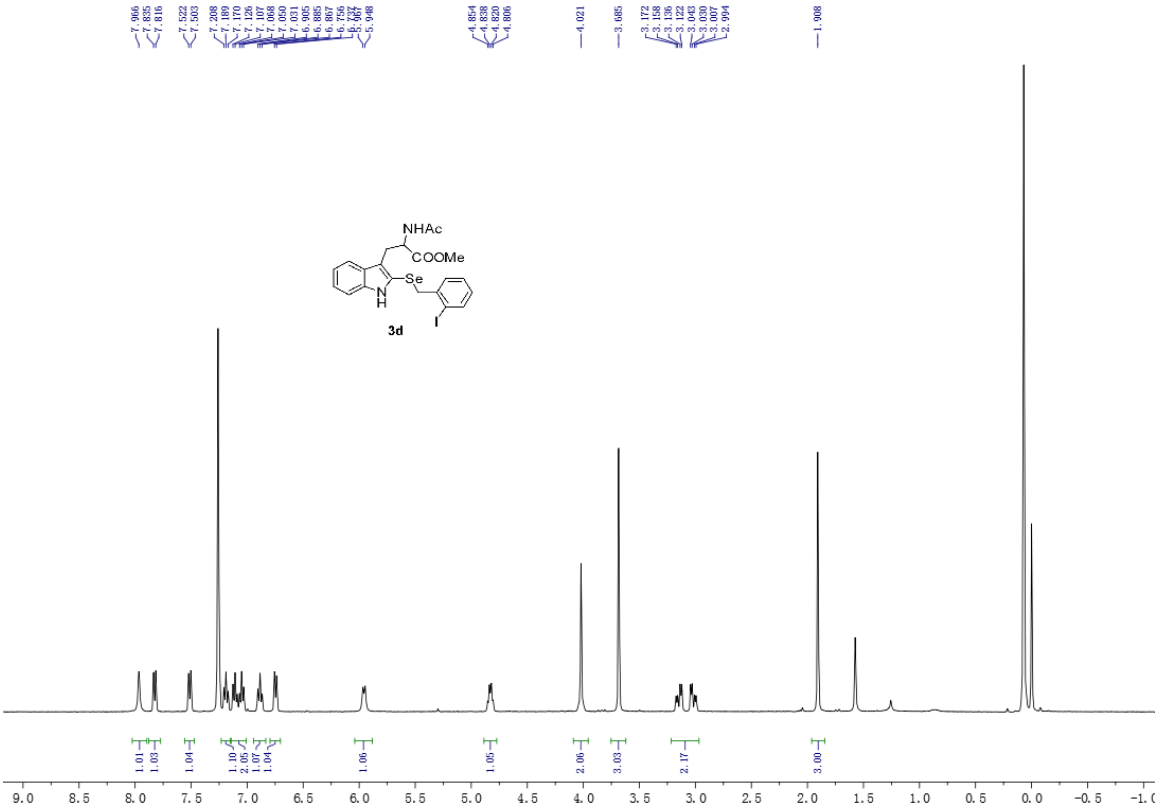
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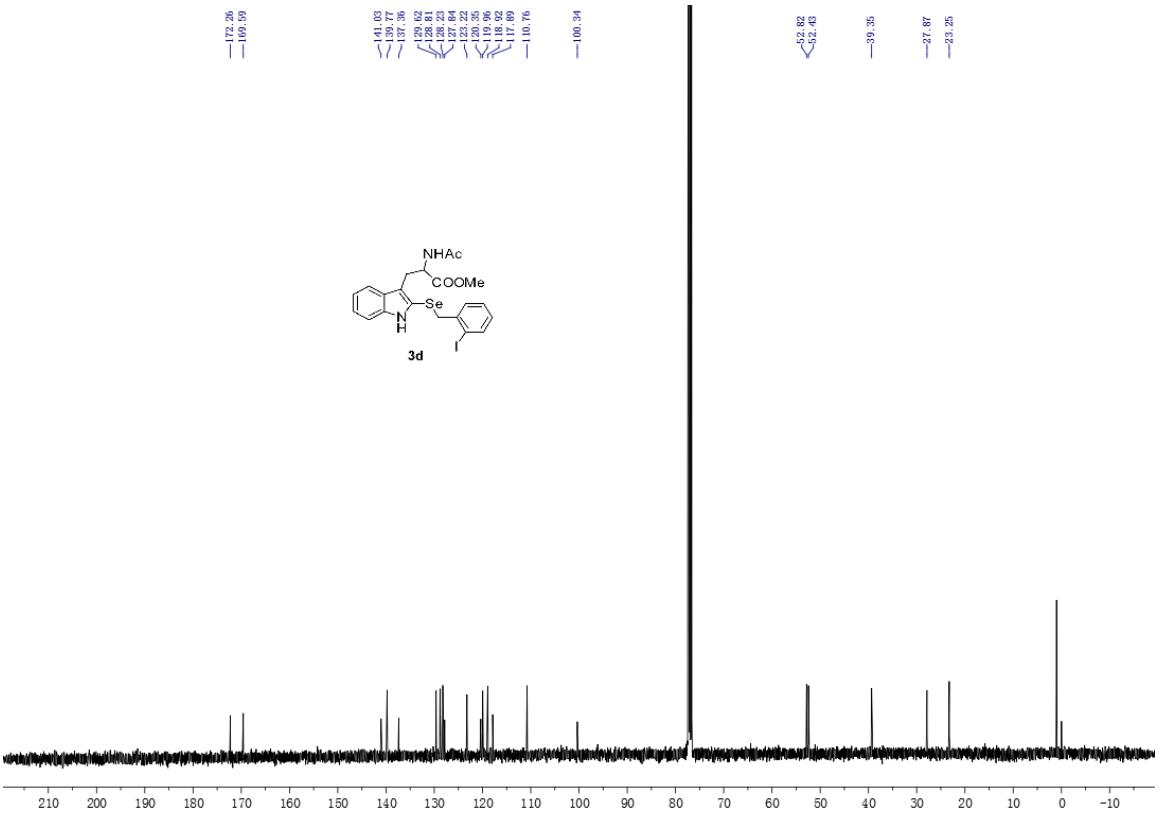
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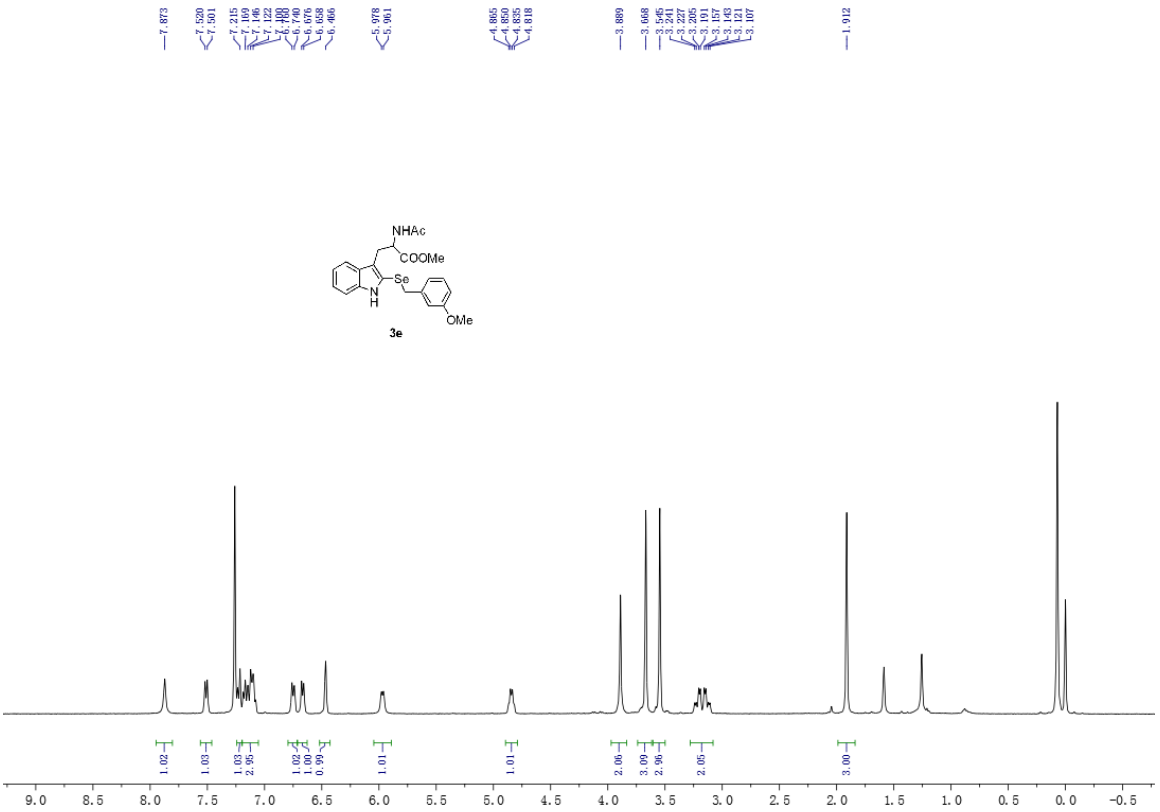
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3.107
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Se
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H
OMe
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2.06
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2.05
3.00
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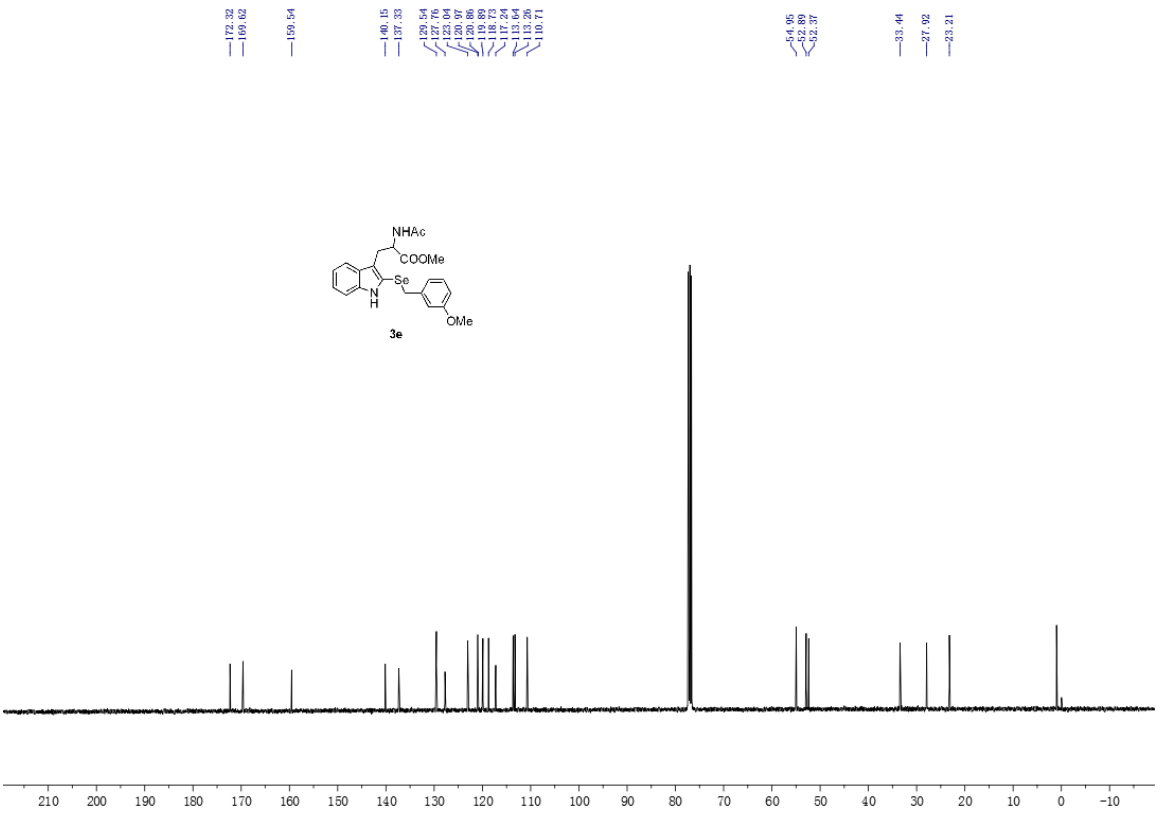
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113.26
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52.37
33.44
27.92
23.21
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COOMe
Se
N
H
OMe
3e
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7.195
7.175
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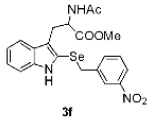
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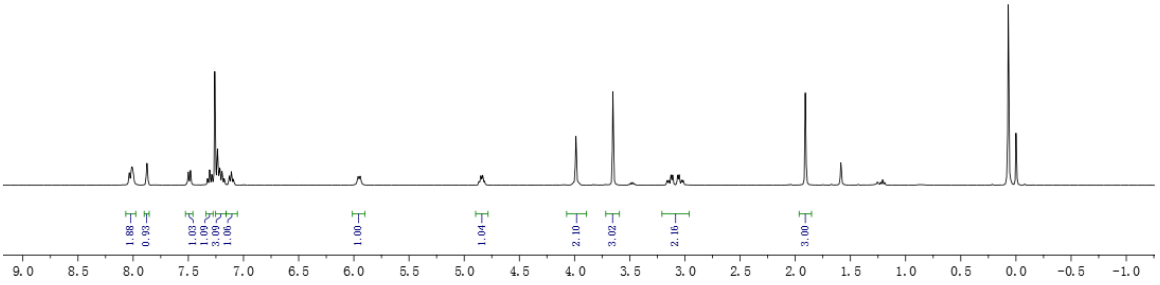
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6.0
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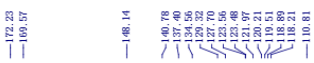
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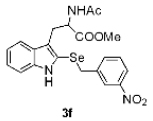
23.22


NHAc
COOMe
Se
N
H
NO2

3f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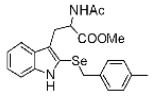
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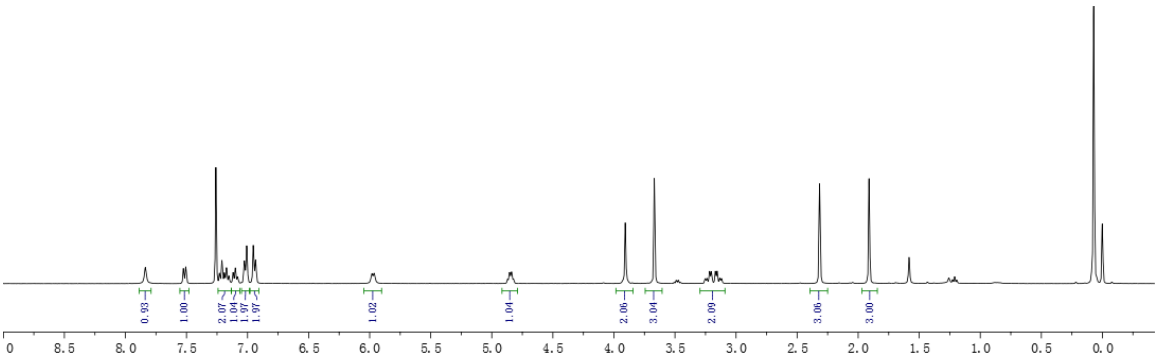
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0.0


172.34
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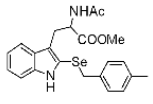
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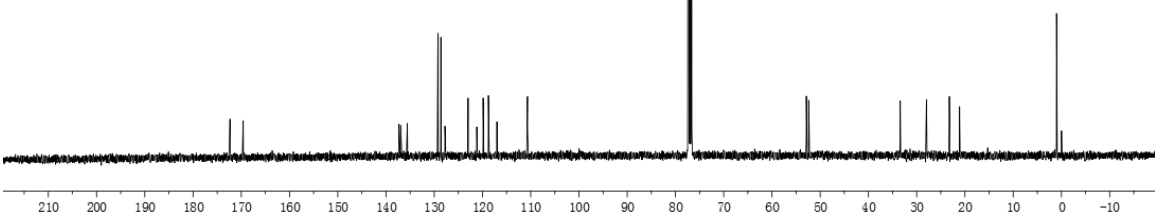
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0
-10


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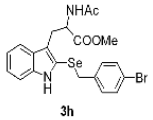
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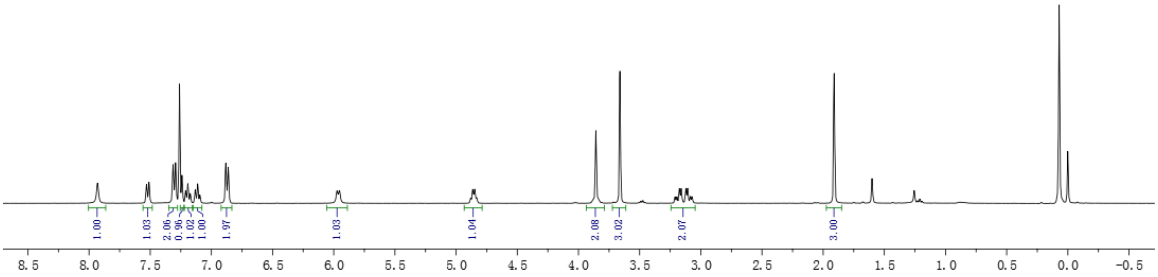
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2.0
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1.0
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0.0
-0.5


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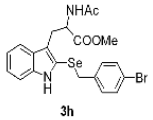
23.23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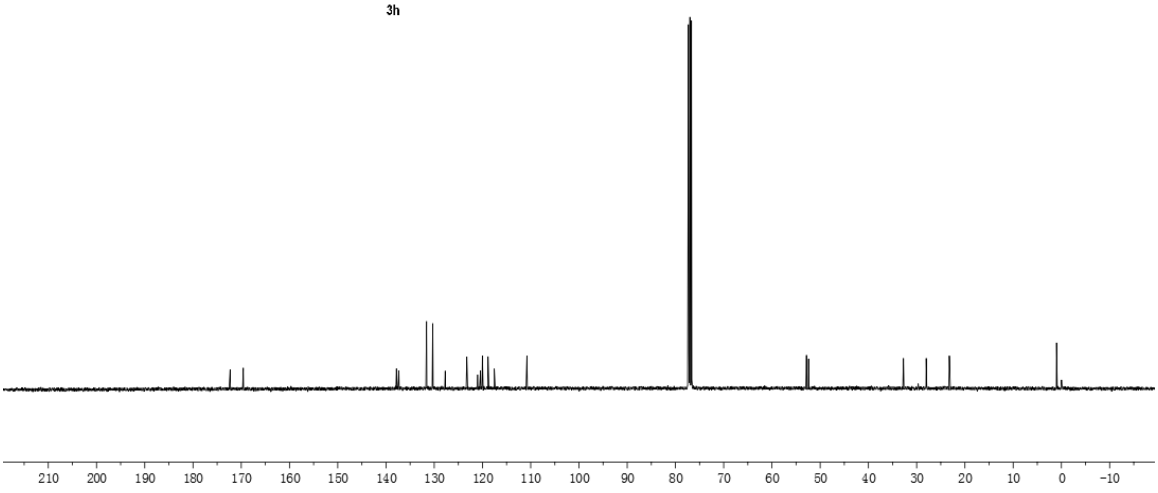
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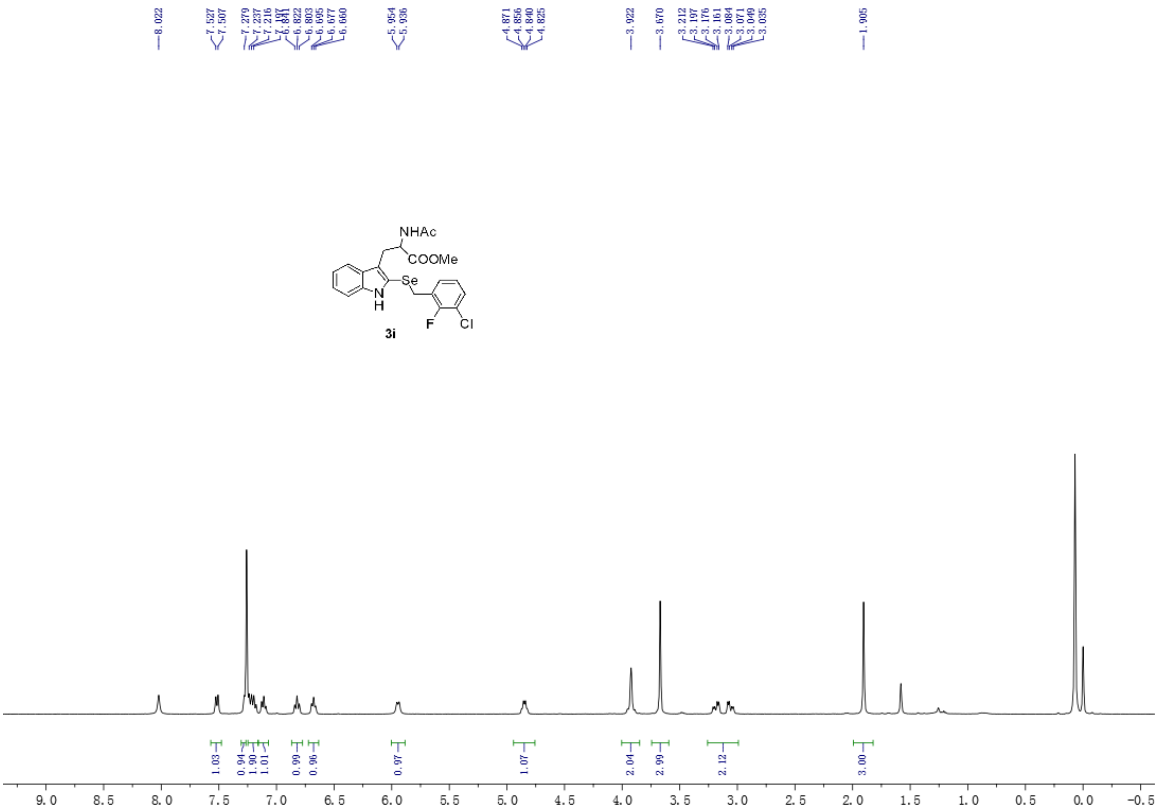
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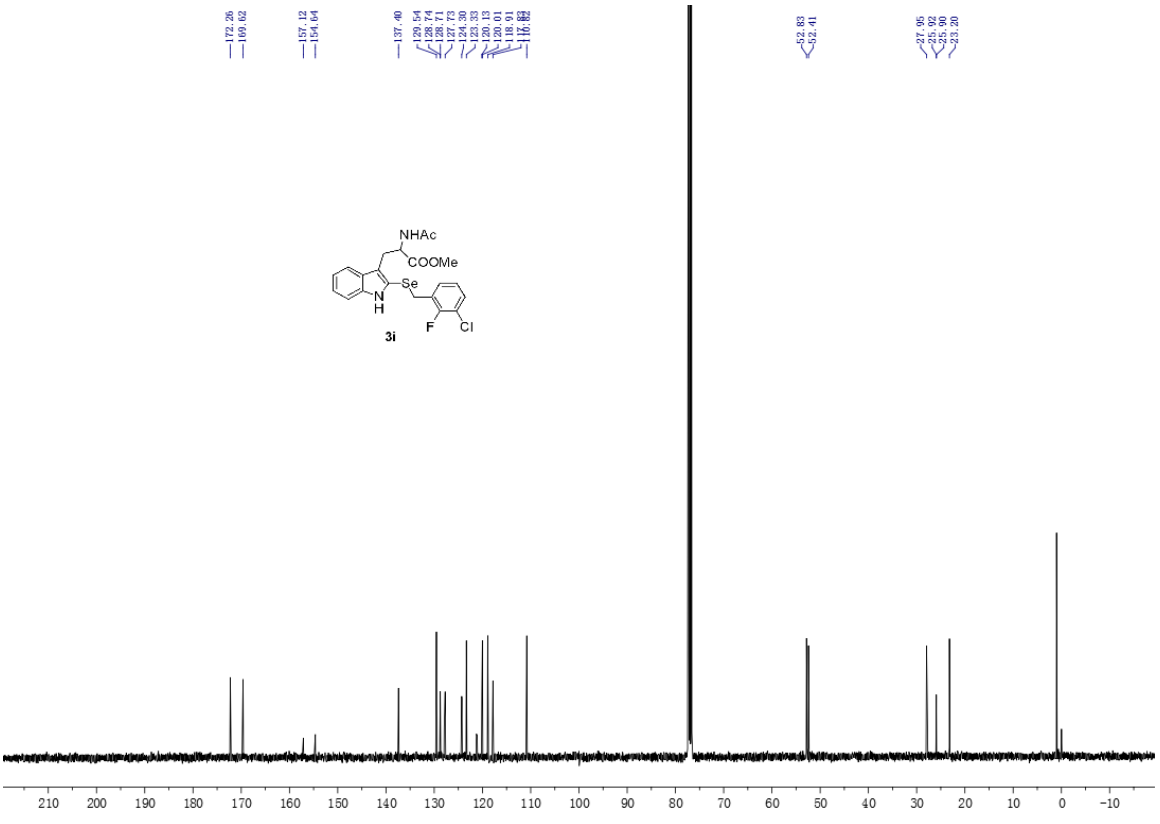
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Cl
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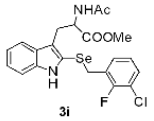
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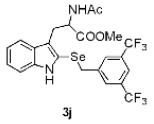
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Se
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CF3

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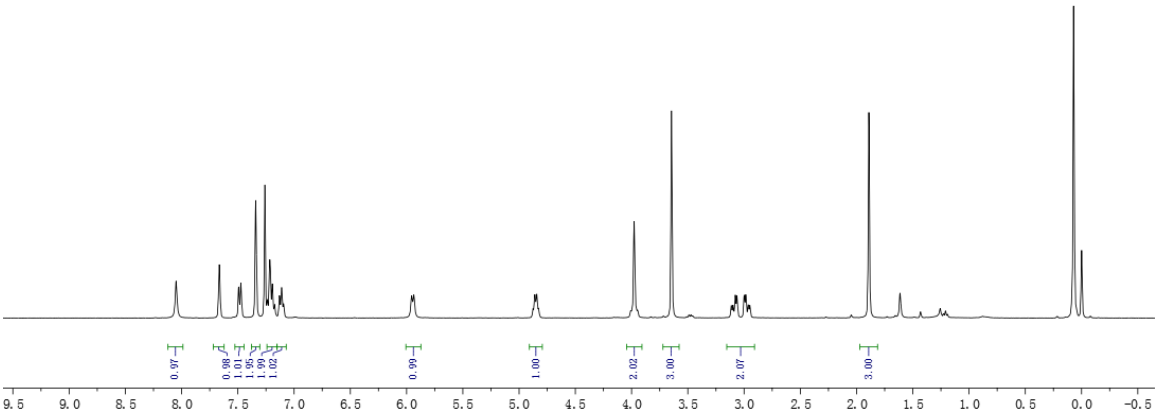
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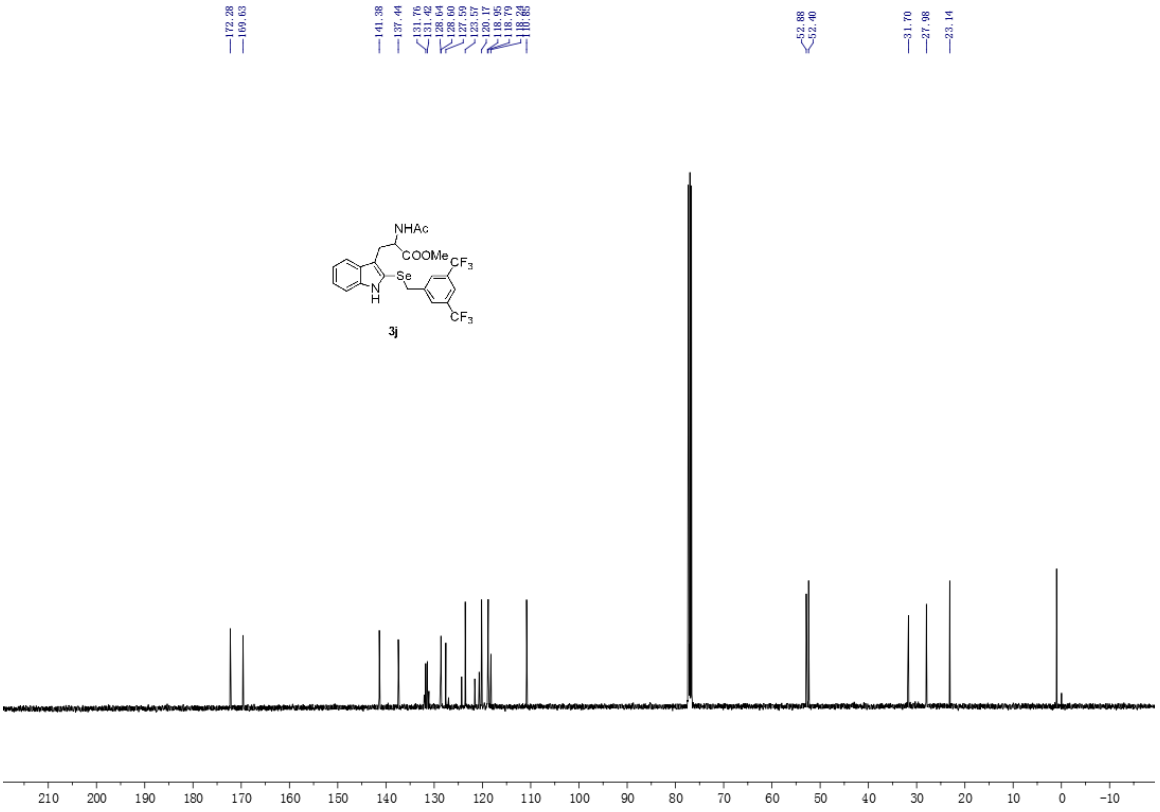
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CF3
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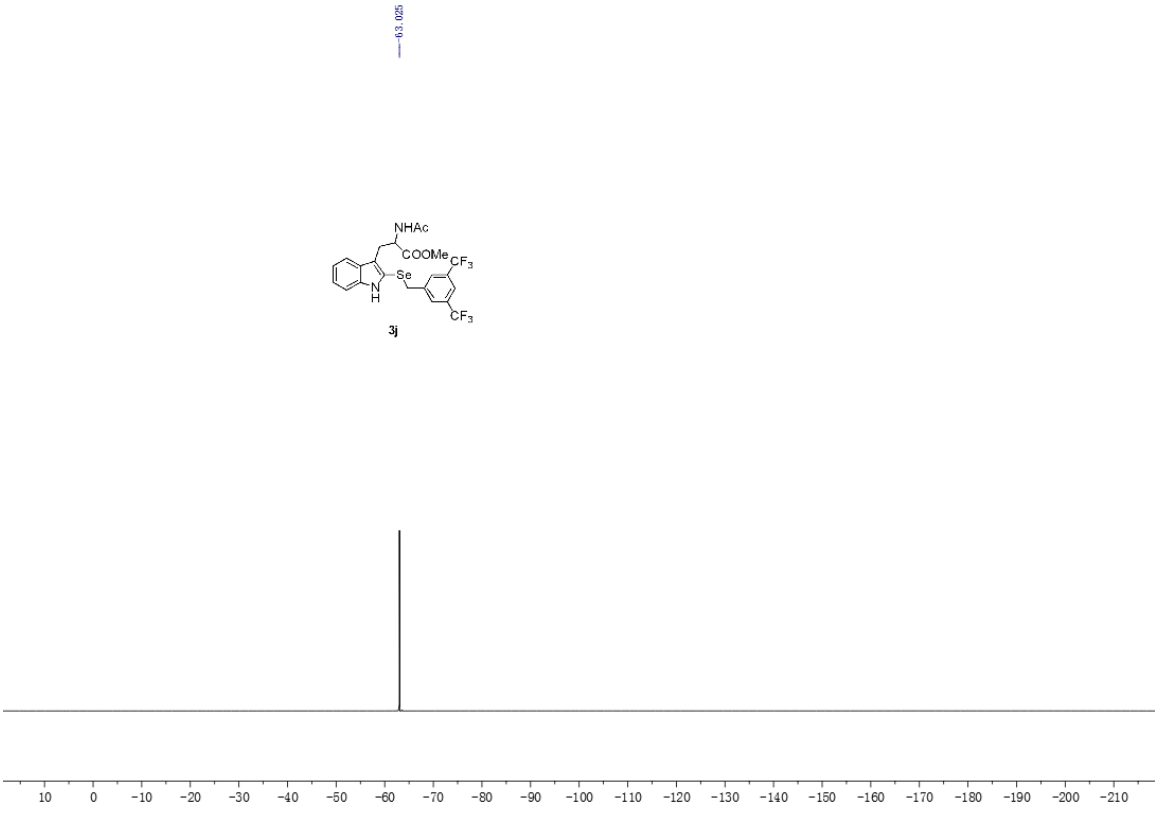
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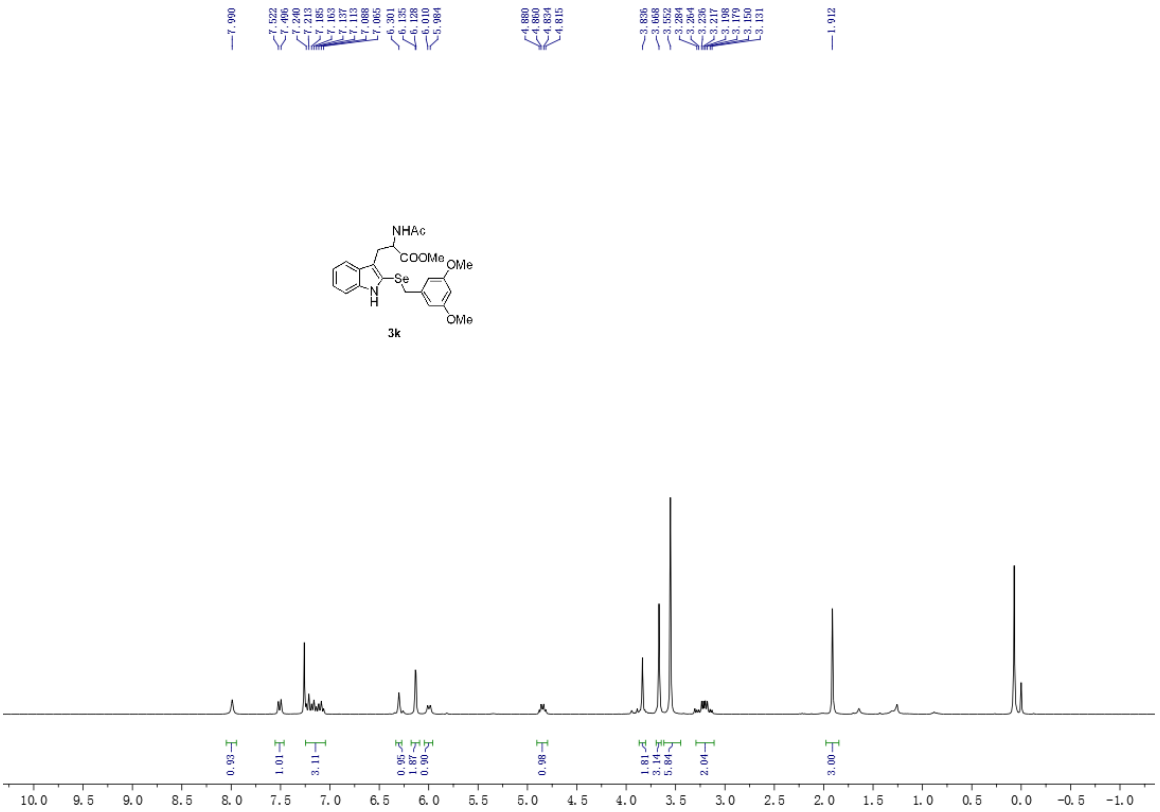
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COOMe
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3.00
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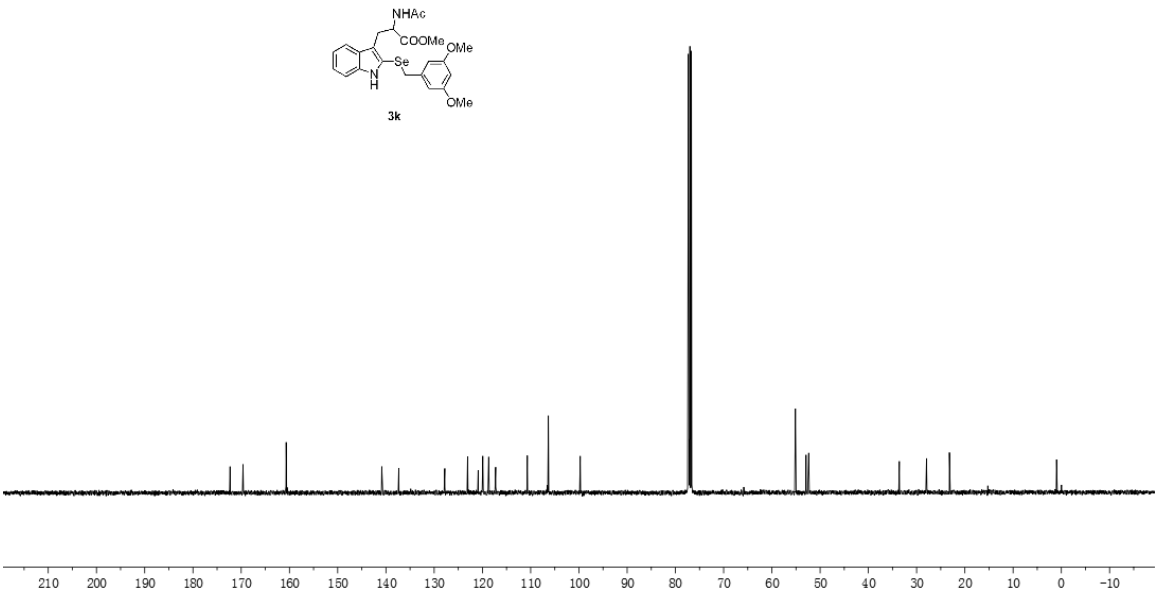
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COOMe
OMe
Se
N
H
OMe
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


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7.170
7.151
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6.113
6.094
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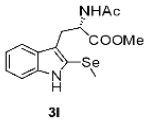
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H

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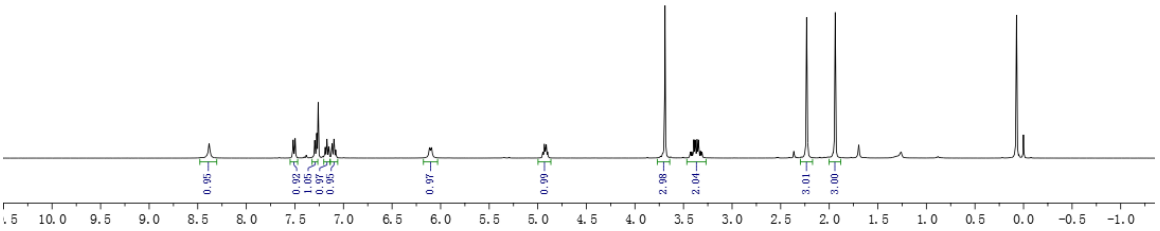
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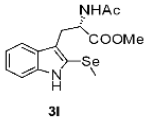
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Se
N
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3l


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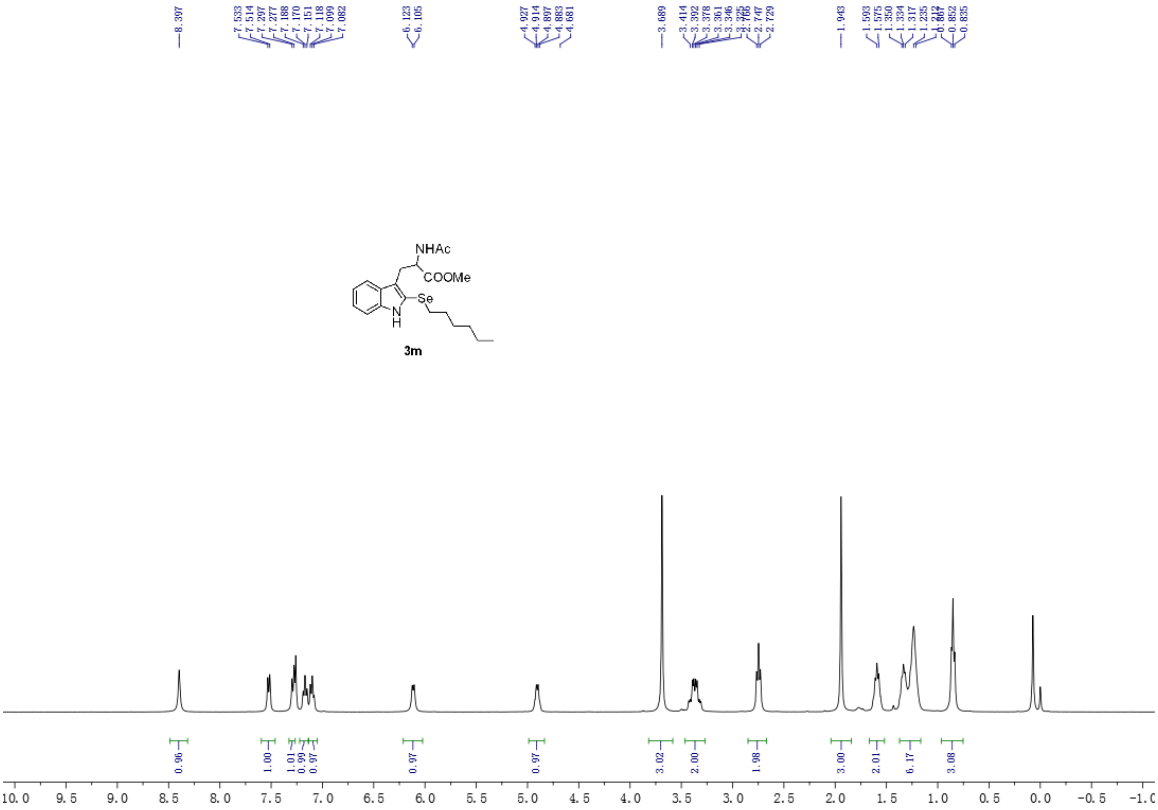
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COOMe
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N
H
3m
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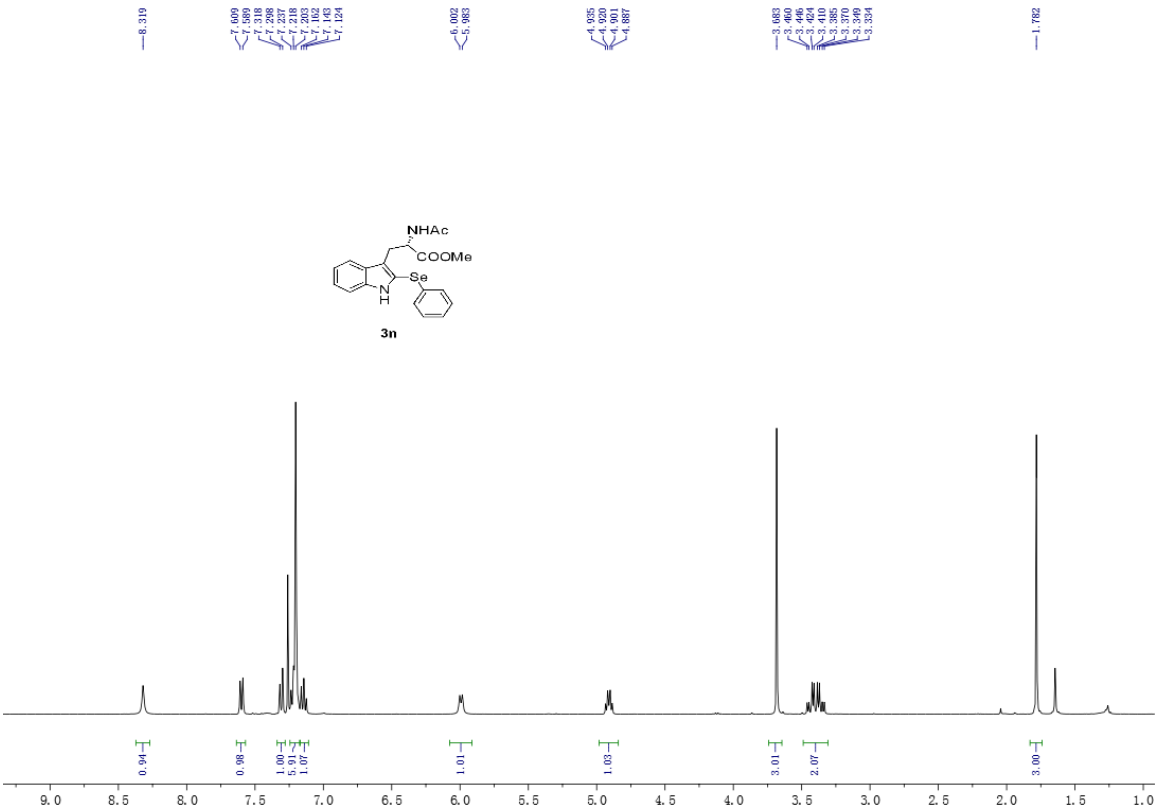
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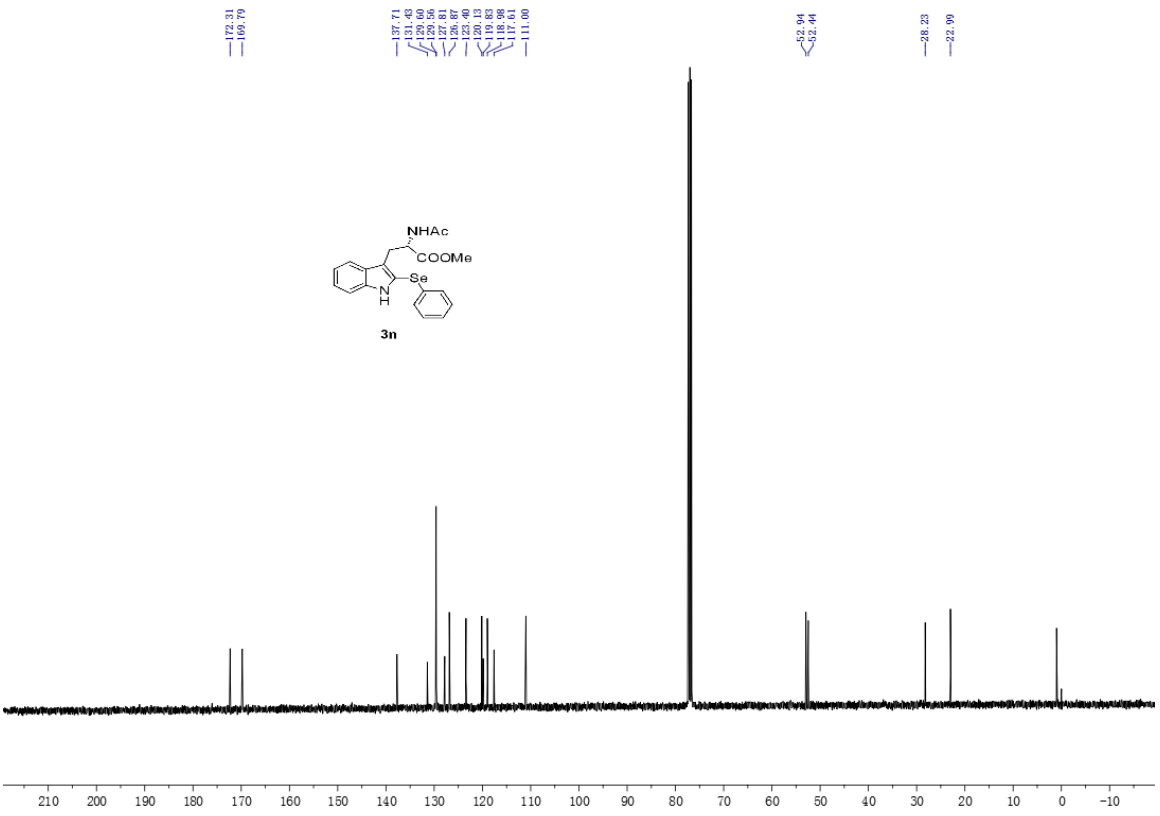
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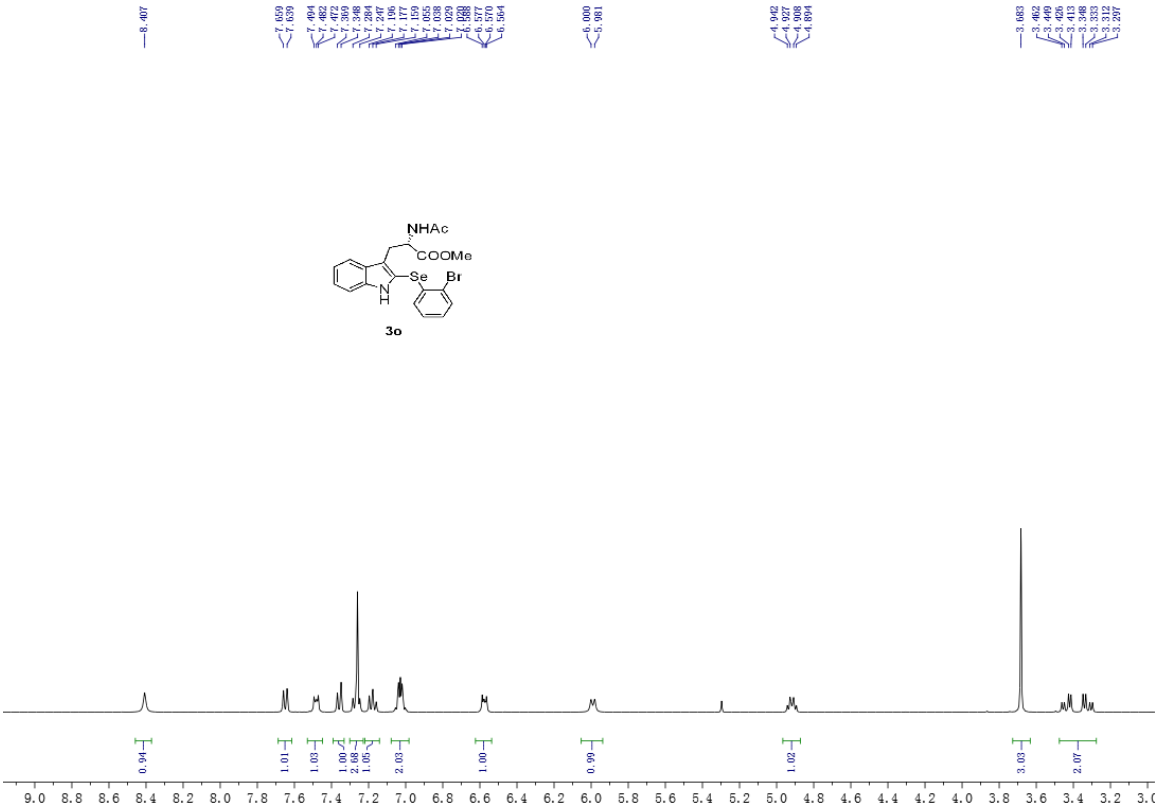
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Br
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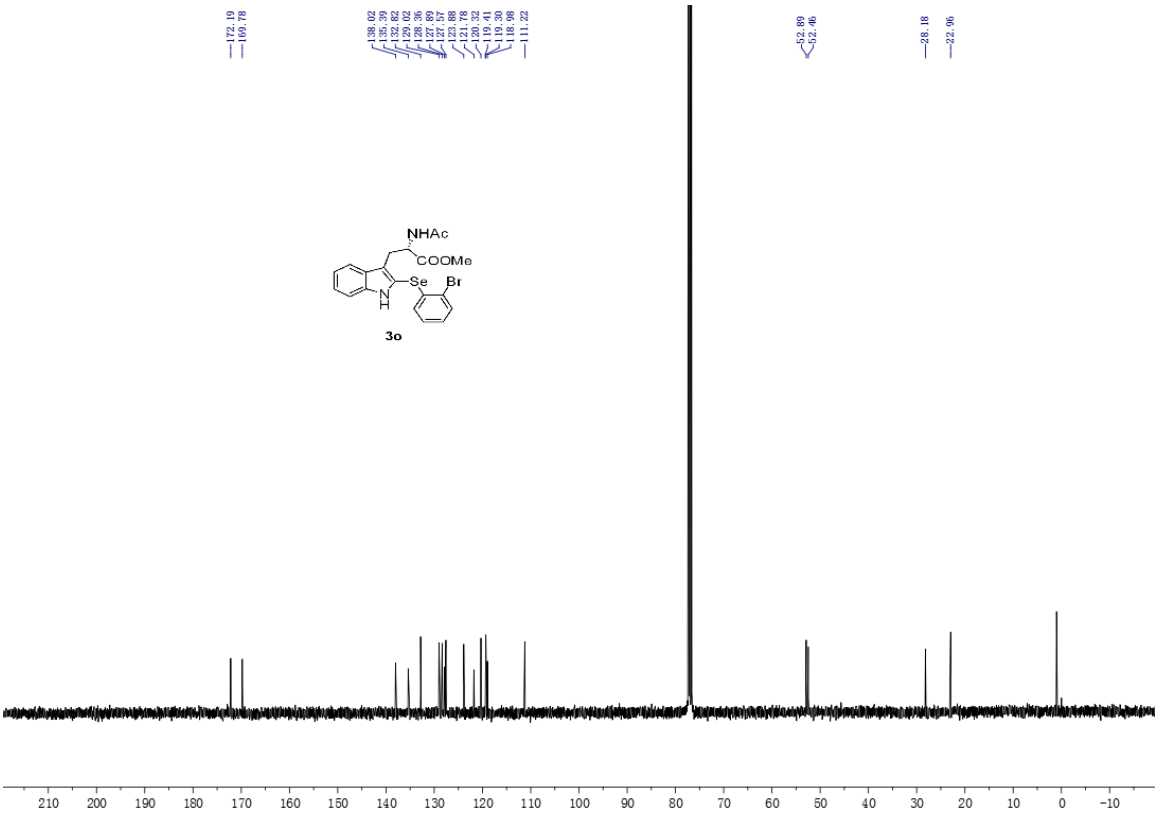
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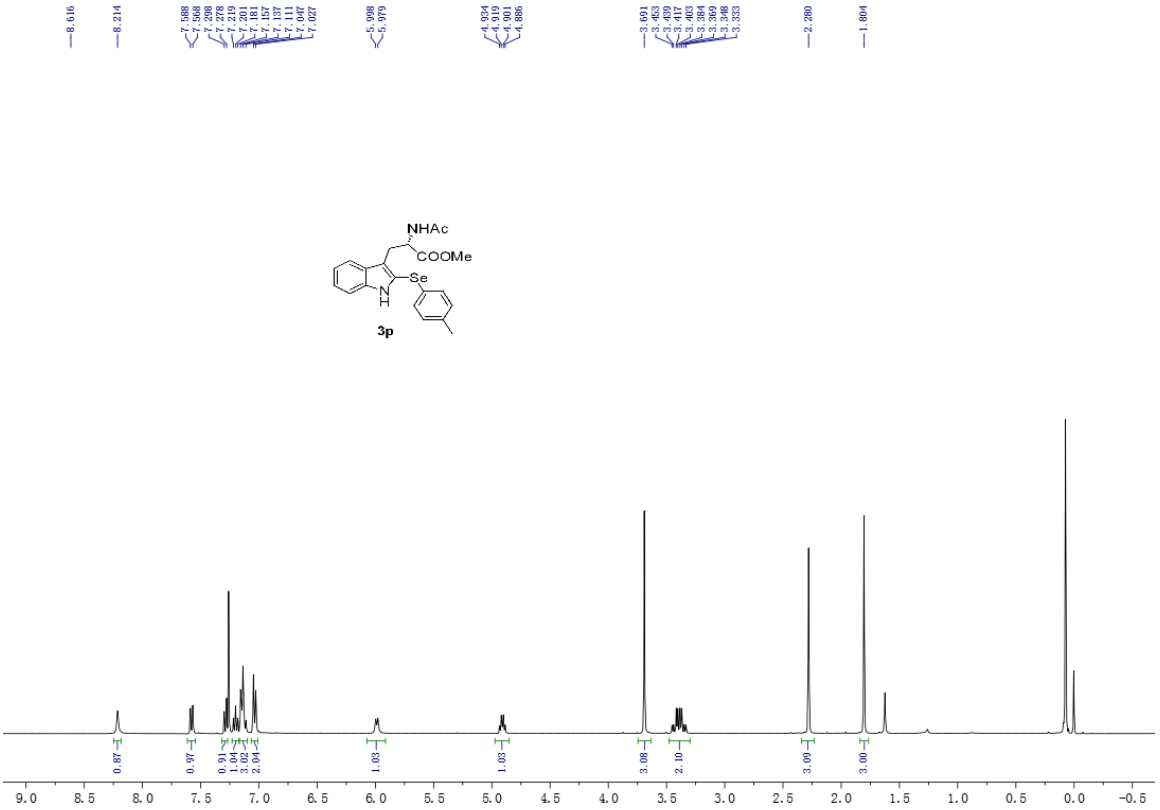
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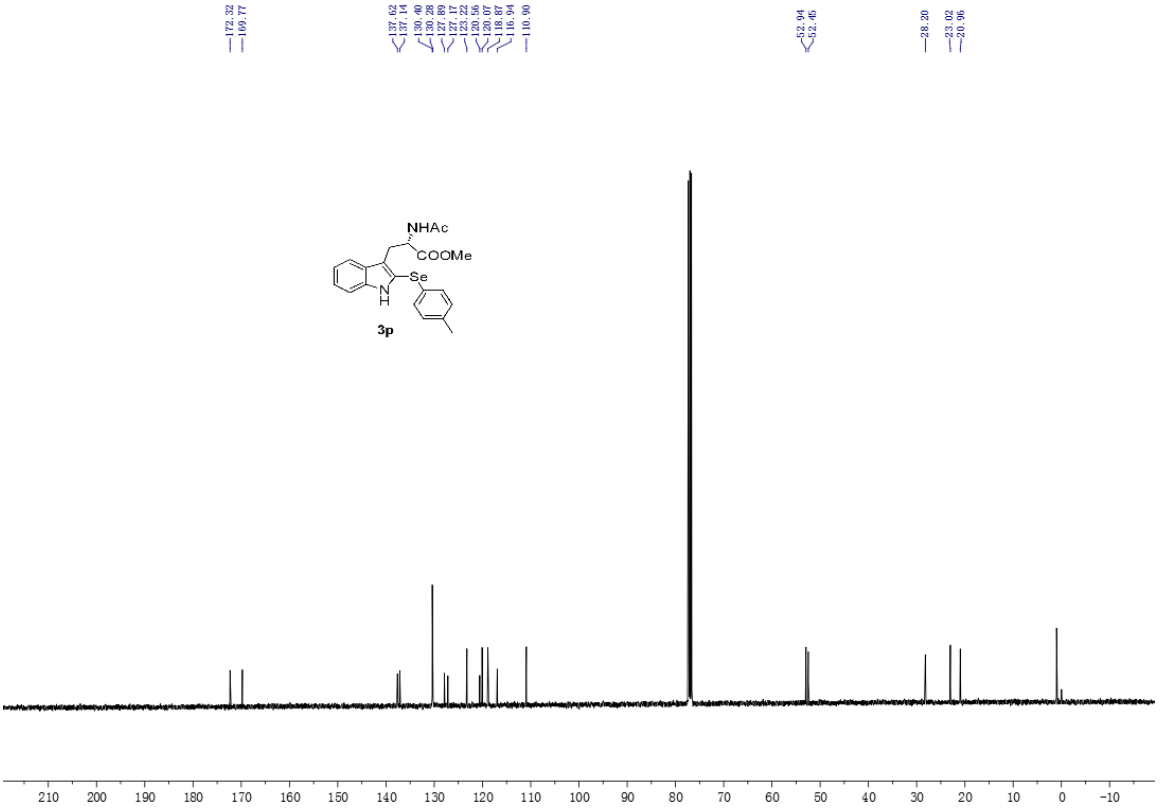
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COOMe
Se
H
3p
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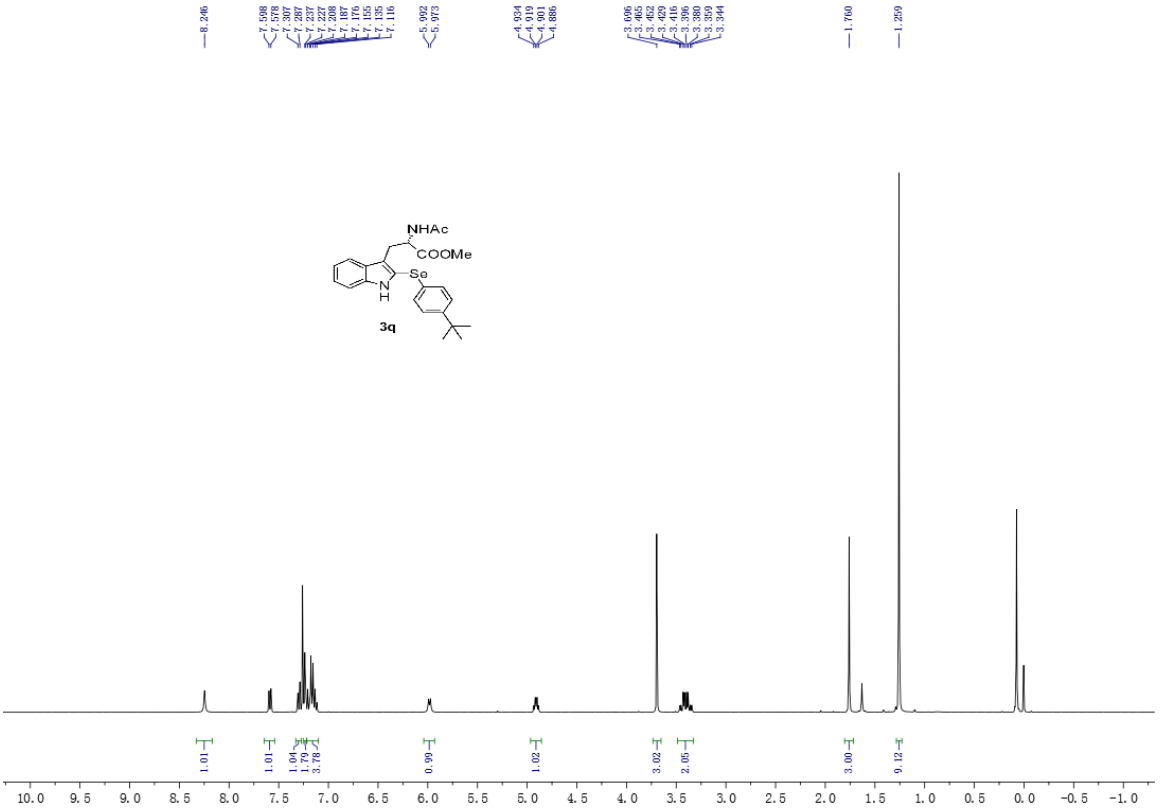
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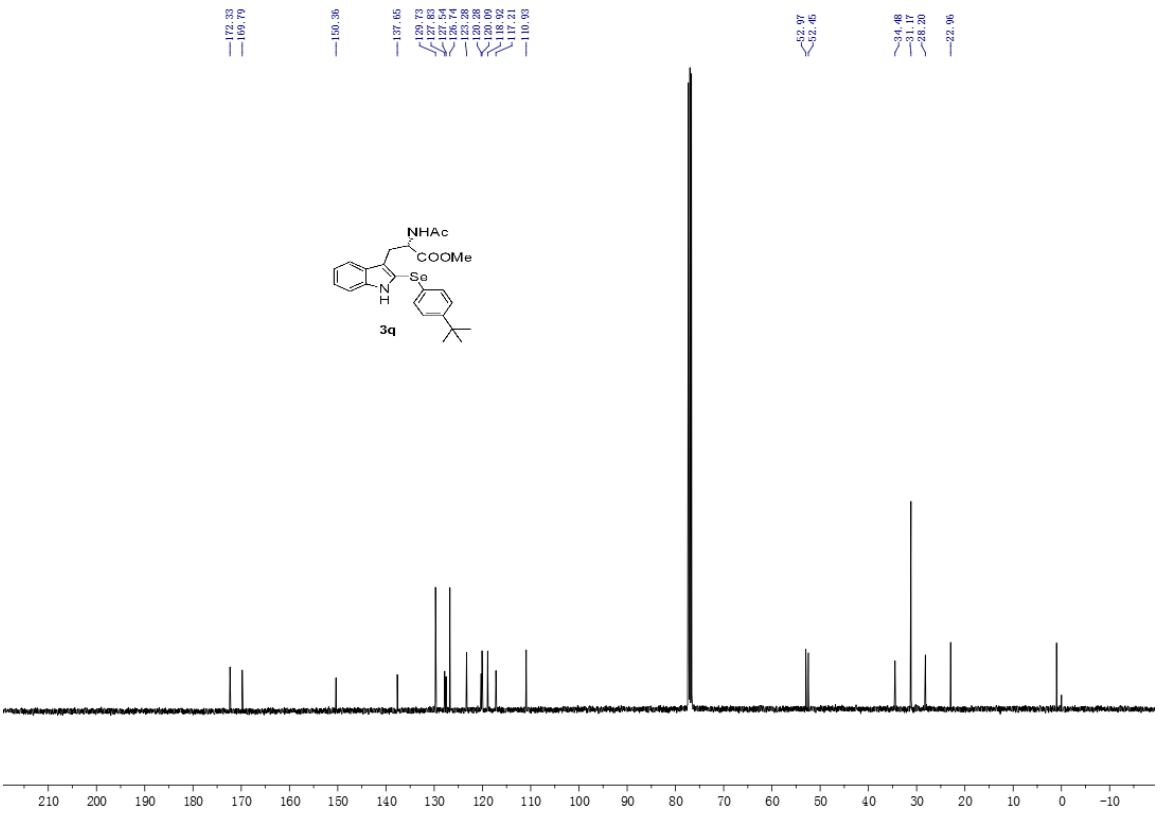
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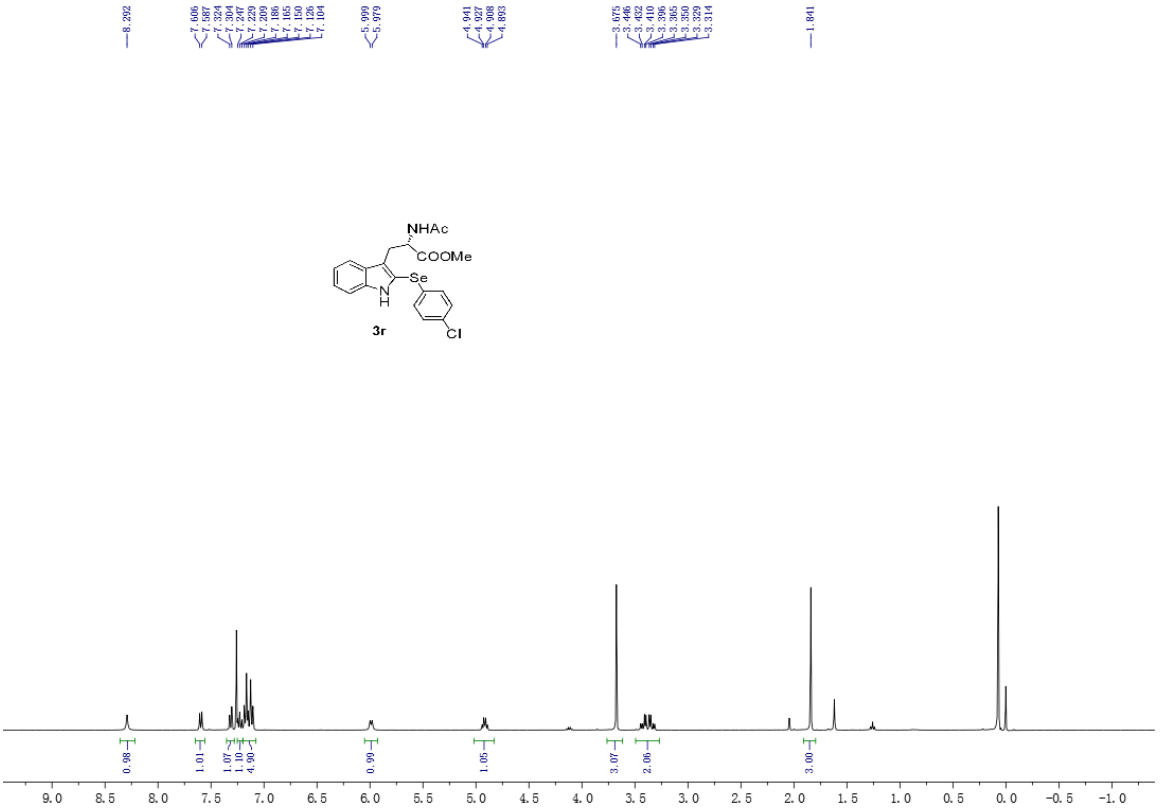
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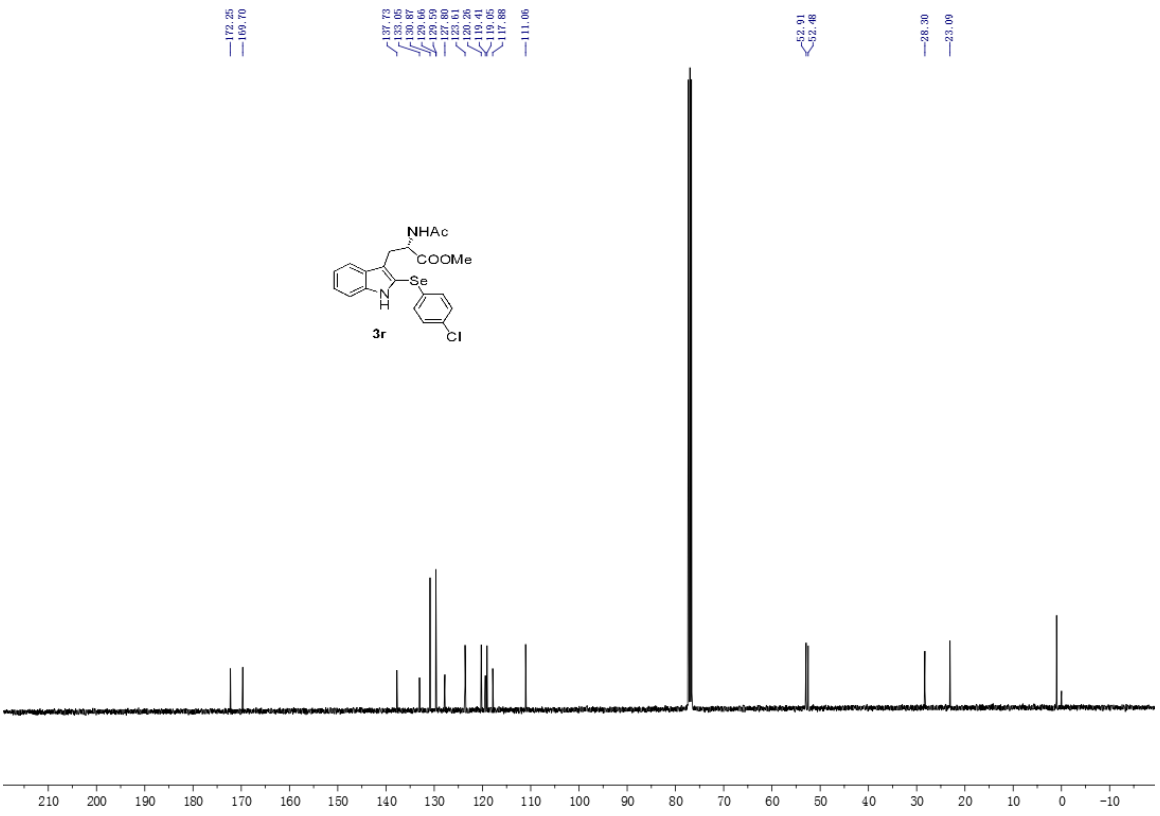
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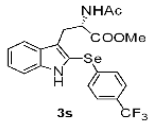
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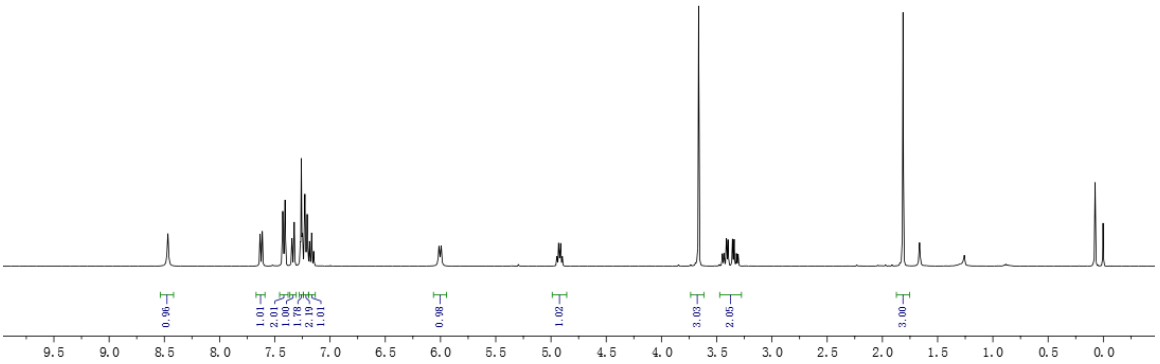
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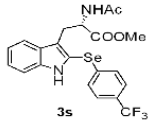
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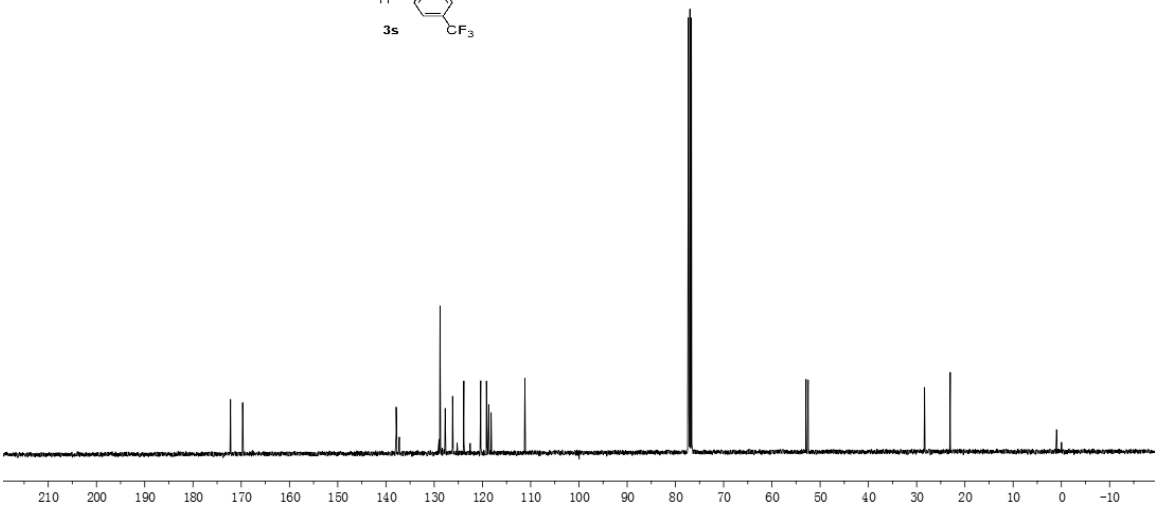
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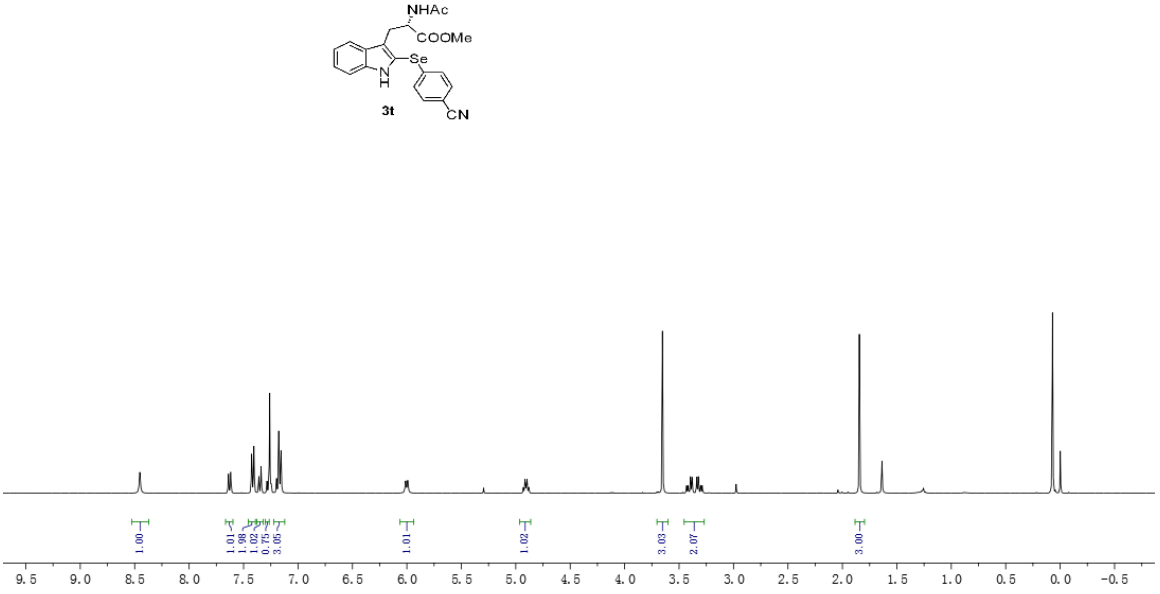
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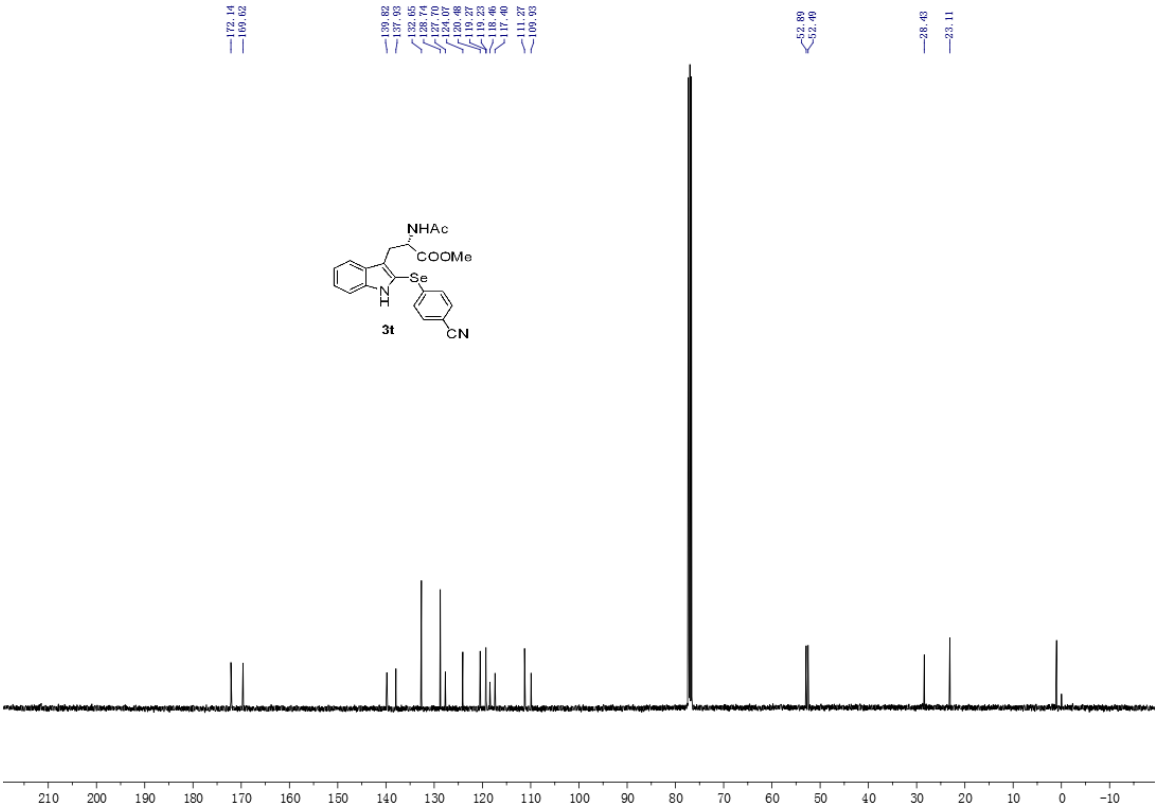
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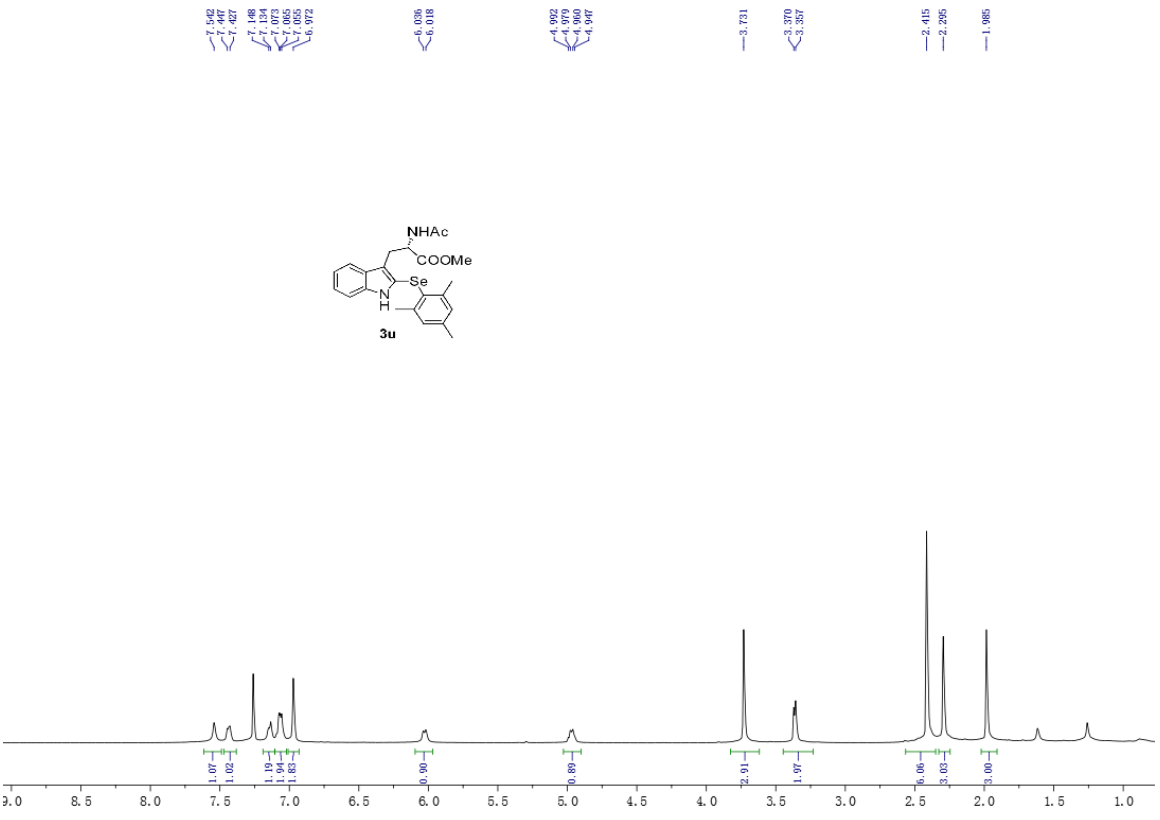
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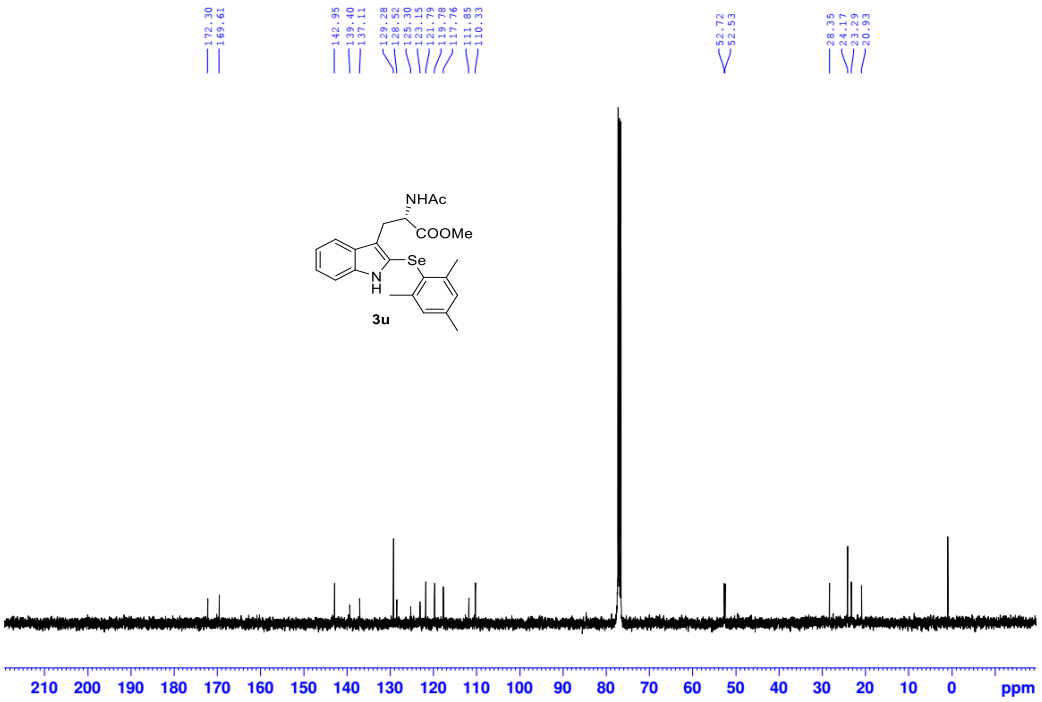
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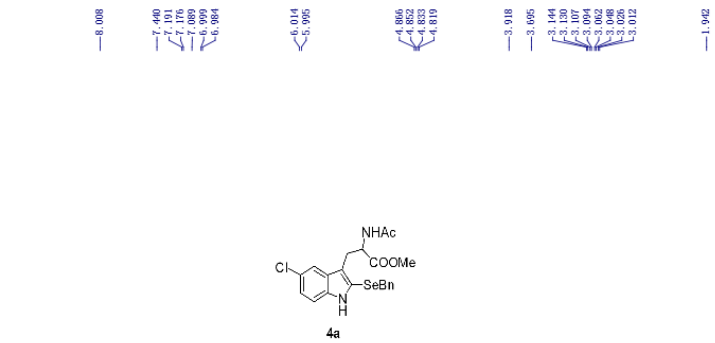
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3.918
3.695
3.144
3.130
3.107
3.094
3.062
3.048
3.026
3.012
1.942
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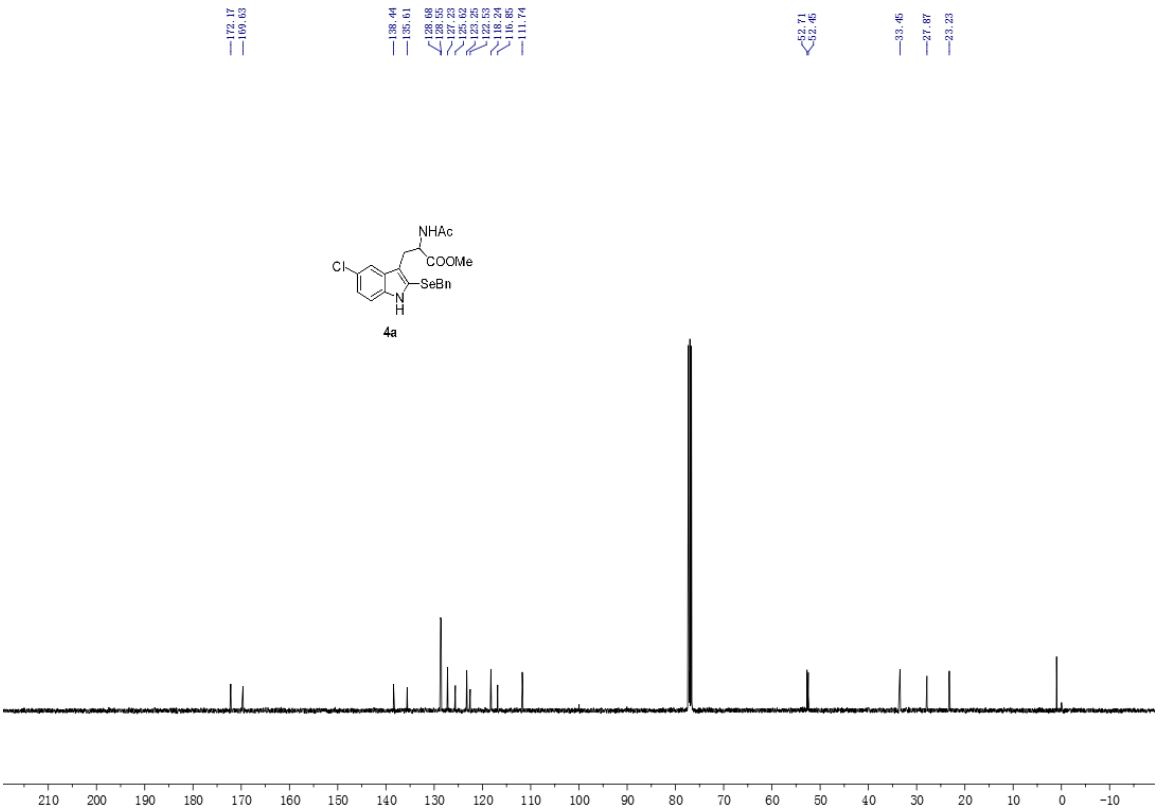
COOMe
Cl
SeBn
N
H
4a
0.89
0.97
2.99
1.95
1.98
0.97
0.99
2.08
3.06
2.04
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5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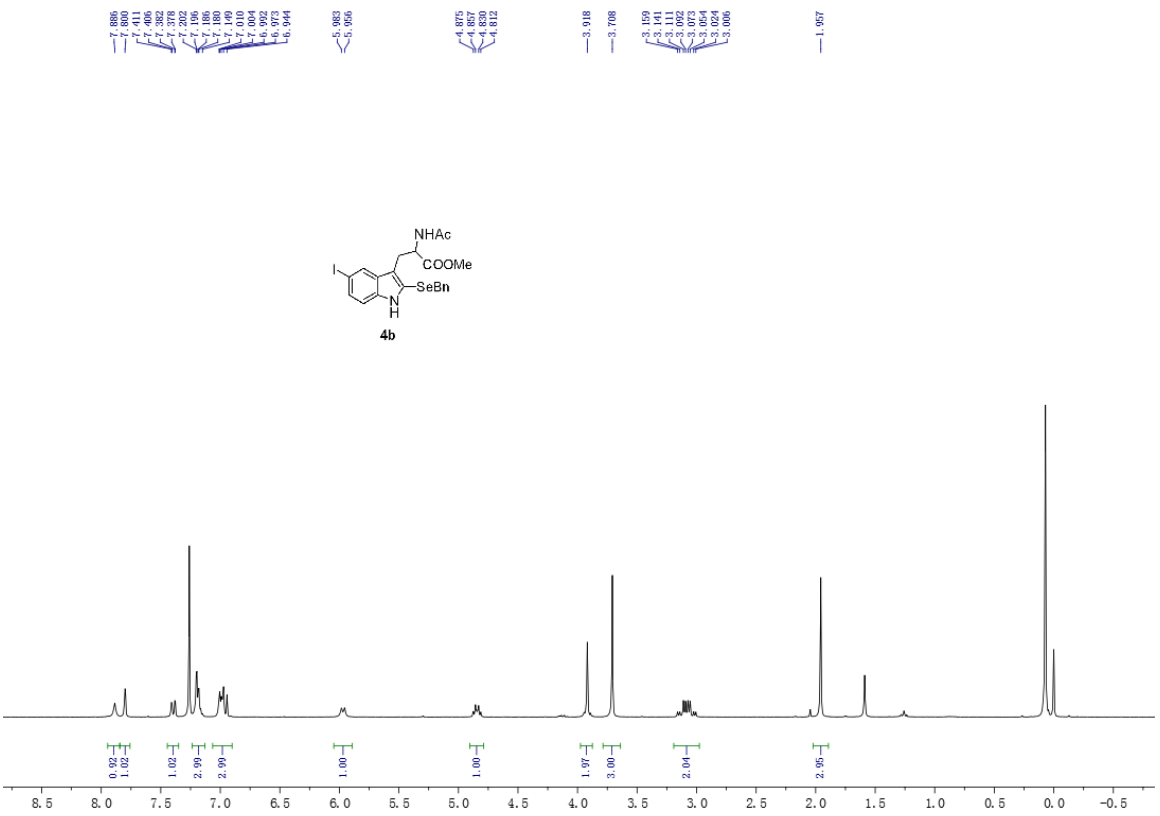
128.23
125.62
123.25
122.53
118.24
116.85
111.74
52.71
52.45
33.45
27.87
23.23
NHAc
COOMe
Cl
SeBn
N
H
4a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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7.378
7.202
7.196
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7.180
7.169
7.010
7.004
6.992
6.973
6.944
5.983
5.956
4.875
4.857
4.830
4.812
3.918
3.708
3.159
3.141
3.111
3.092
3.073
3.054
3.024
3.006
1.957
NHAc
COOMe
I
SeBn
N
H
4b
0.92
1.02
1.02
2.99
2.99
1.00
1.00
1.97
3.00
2.04
2.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
2.0
1.5
1.0
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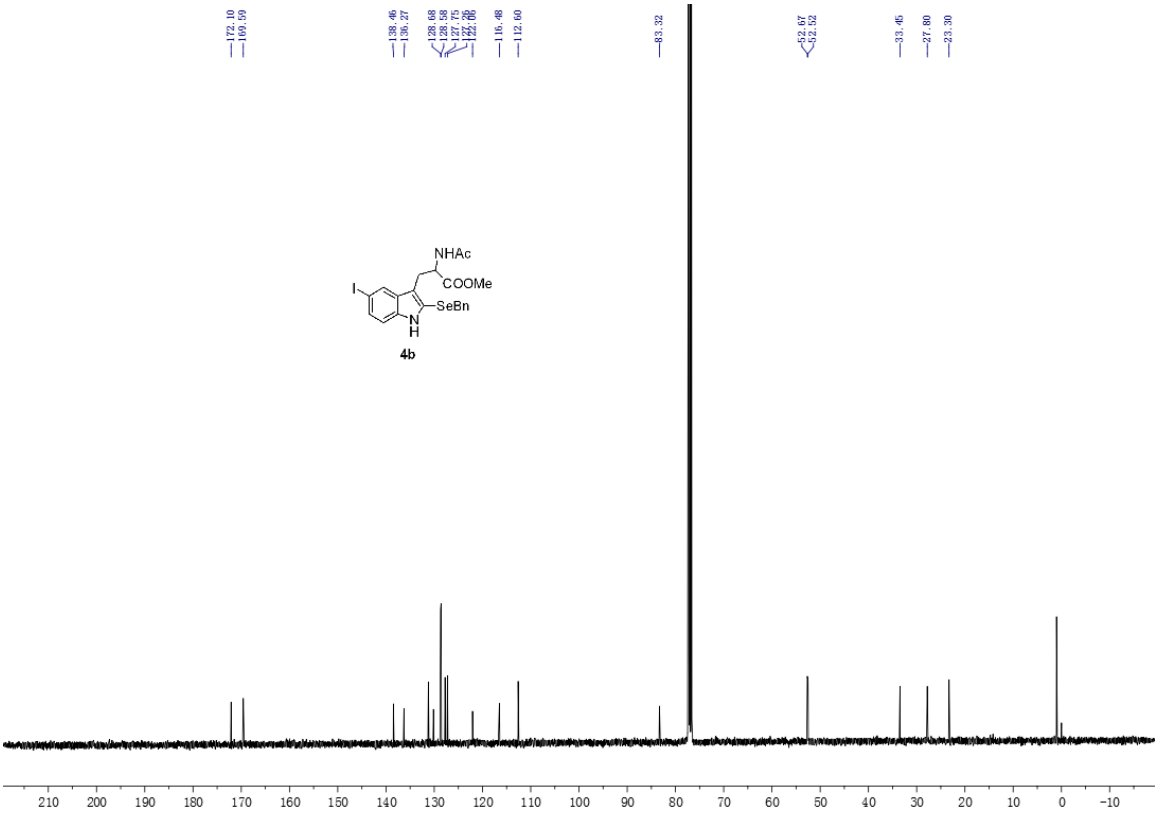
0.0
-0.5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127.75
127.28
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112.60
83.32
52.67
52.52
33.45
27.80
23.30
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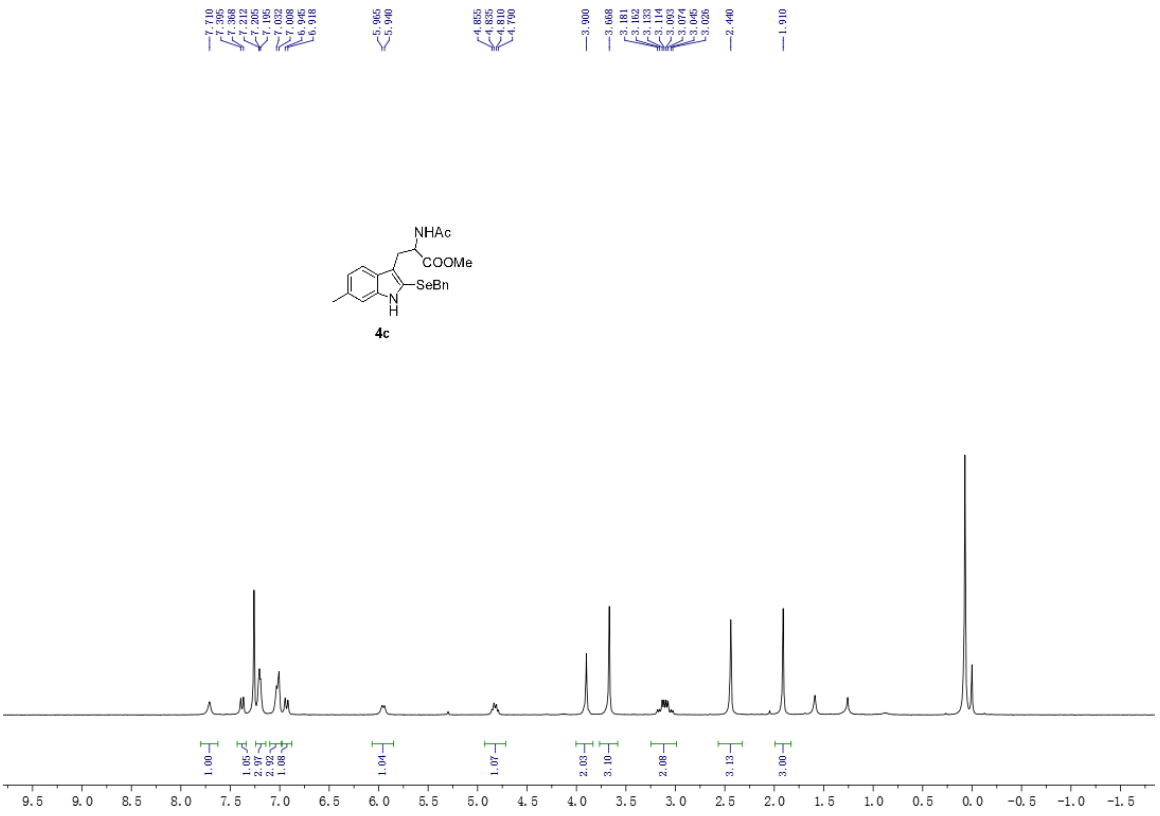
COOMe
SeBn
I
N
H
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.305
7.195
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7.008
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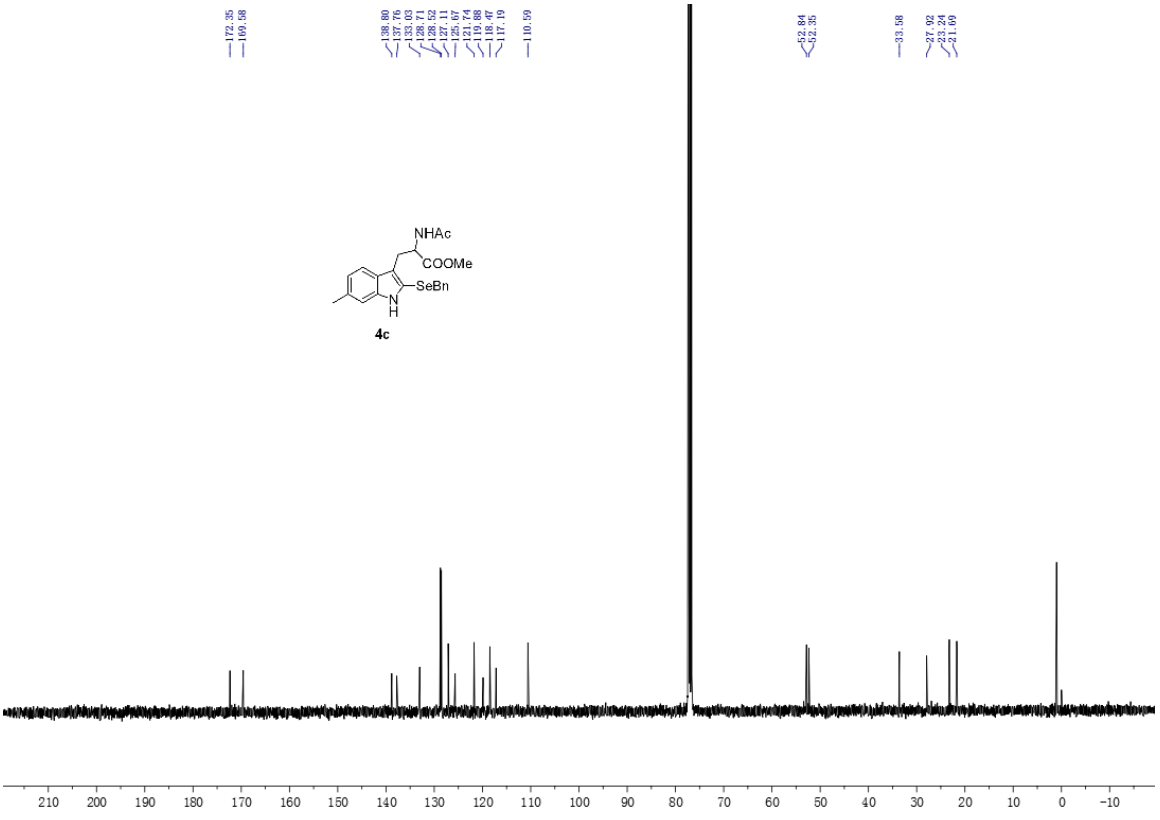
6.918
5.965
5.940
4.855
4.835
4.810
4.790
3.900
3.668
3.181
3.162
3.135
3.114
3.093
3.074
3.045
3.026
2.440
1.910
NHAc
COOMe
SeBn
N
H
4c
1.00
1.05
2.97
2.92
1.08
1.04
1.07
2.03
3.10
2.08
3.13
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5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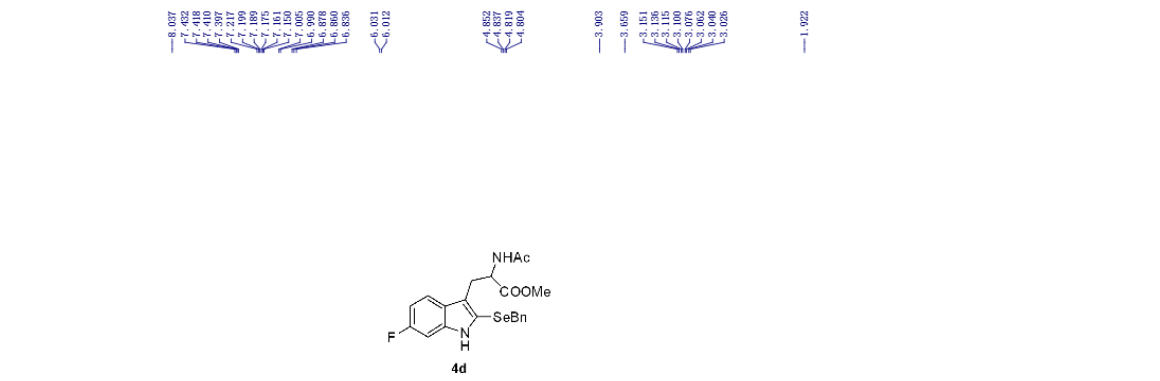
121.74
119.88
118.47
117.19
110.59
52.84
52.35
33.58
27.92
23.24
21.69
NHAc
COOMe
SeBn
N
H
4c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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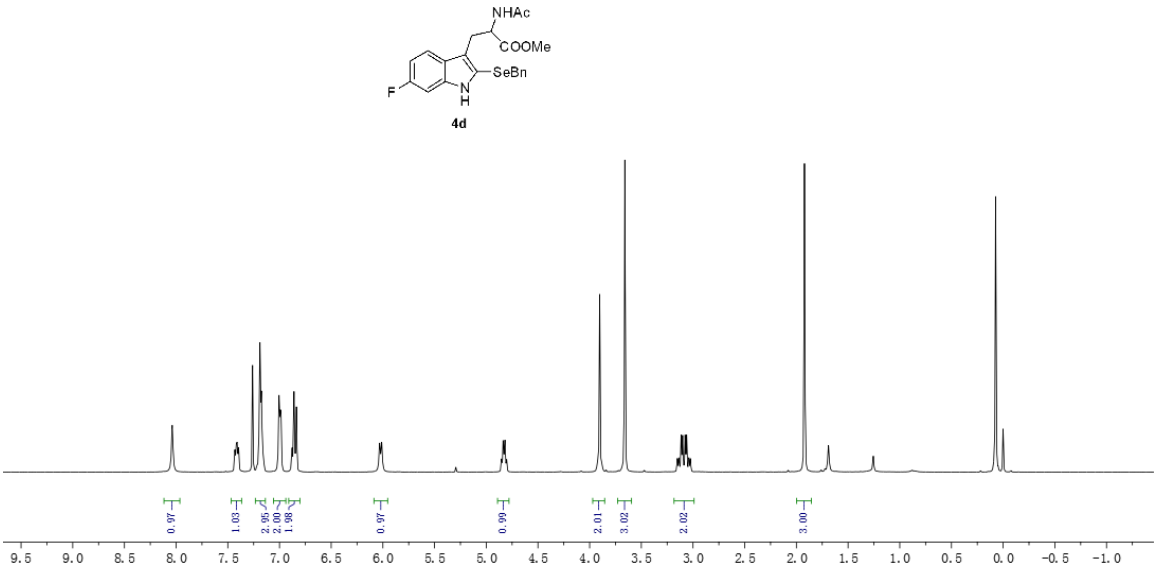
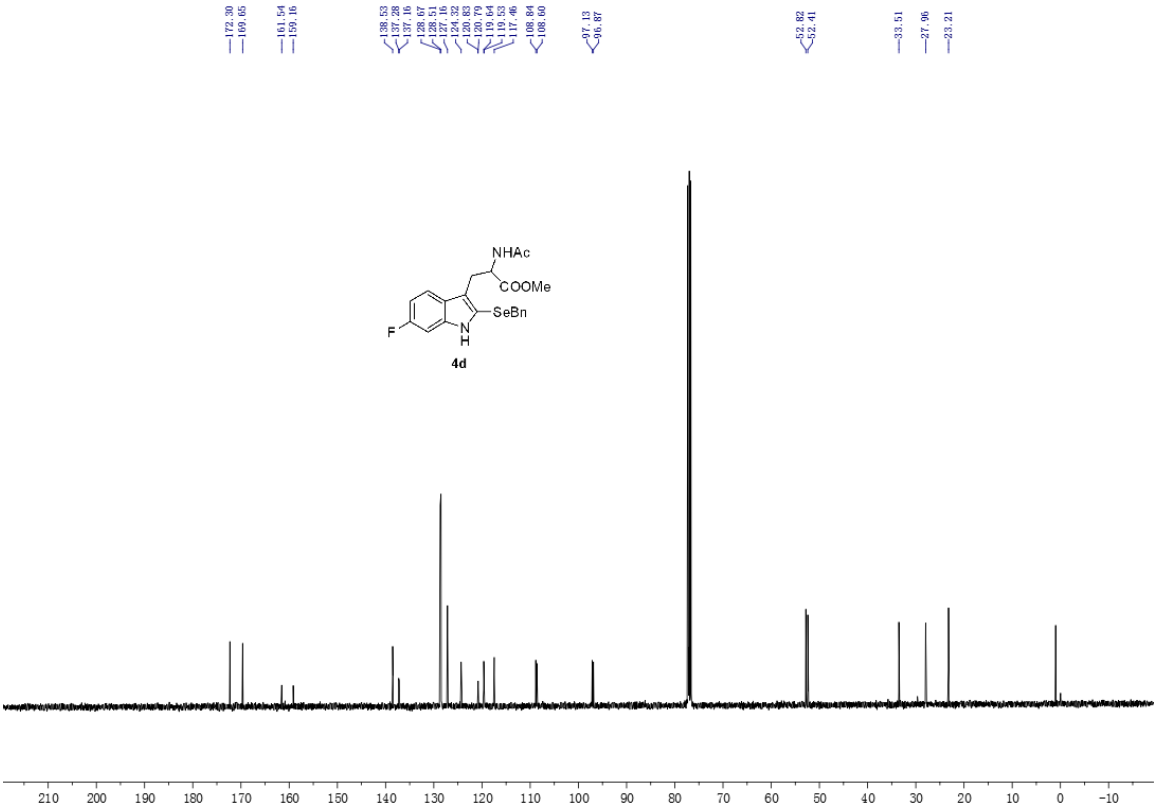
7.418
7.410
7.397
7.217
7.199
7.189
7.175
7.161
7.150
7.095
6.999
6.878
6.860
6.836
6.031
6.012
4.852
4.837
4.819
4.804
3.903
3.659
3.151
3.136
3.115
3.100
3.076
3.062
3.040
3.026
1.922


NHAc
COOMe
SeBn
F
N
H
4d
0.97
1.03
2.95
2.00
1.98
0.97
0.99
2.01
3.02
2.02
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 -0.5 -1.0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137.28
137.16
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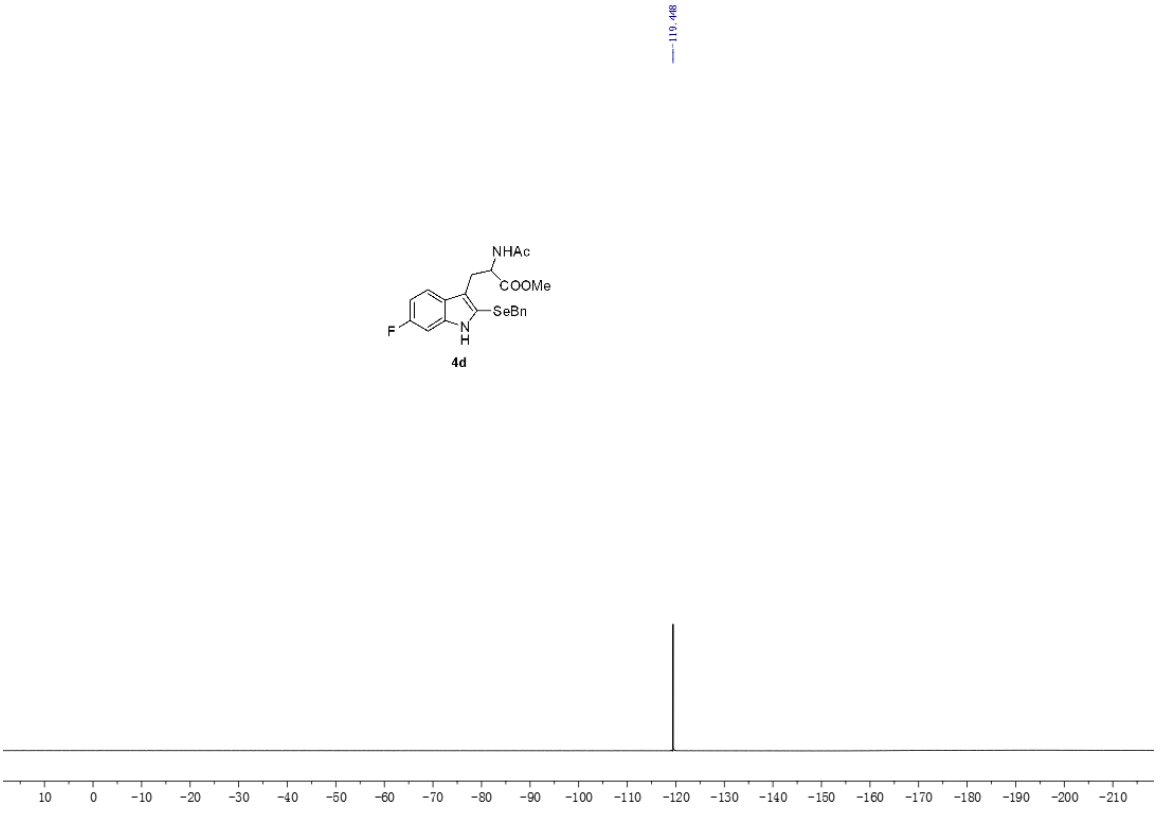
128.51
127.16
124.32
120.83
120.79
119.64
119.53
117.46
108.84
108.60
97.13
96.87
52.82
52.41
33.51
27.96
23.21
NHAc
COOMe
SeBn
F
N
H
4d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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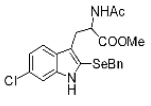
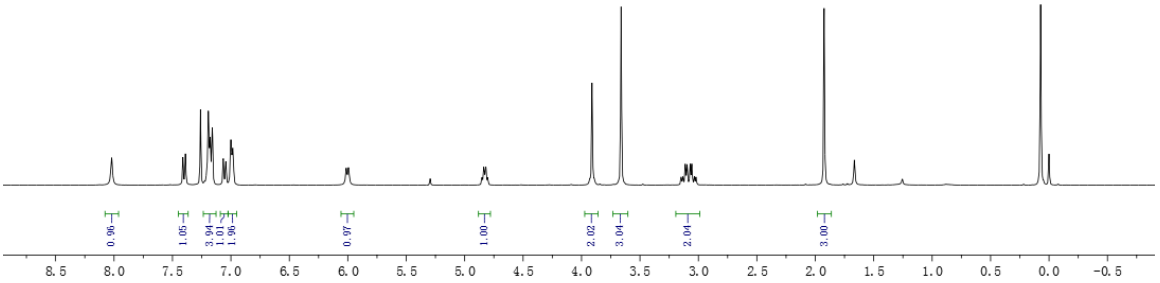
COOMe
SeBn
F
N
H
4d
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210


8.021
7.411
7.390
7.223
7.209
7.193
7.178
7.160
7.065
7.044
7.000
6.984
6.013
5.994
4.852
4.837
4.819
4.804
3.910
3.662
3.148
3.133
3.112
3.097
3.071
3.056
3.035
3.021
1.924


NHAc
COOMe
SeBn
Cl
N
H

4e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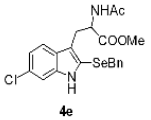
1.96
0.97
1.00
2.02
3.04
2.04
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


172.25
169.64
138.48
137.53
128.96
128.67
128.54
127.22
126.26
121.61
120.59
119.58
117.39
110.61
52.78
52.45
33.47
27.92
23.23


NHAc
COOMe
SeBn
Cl
N
H

4e


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


7.593
7.367
7.341
7.228
7.221
7.211
7.206
7.193
7.086
7.080
7.068
7.055
7.043
7.019
6.993
5.988
5.959
4.891
4.872
4.845
4.826
3.930
3.677
3.261
3.242
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3.194
3.170
3.151
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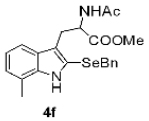
3.103
2.305
1.912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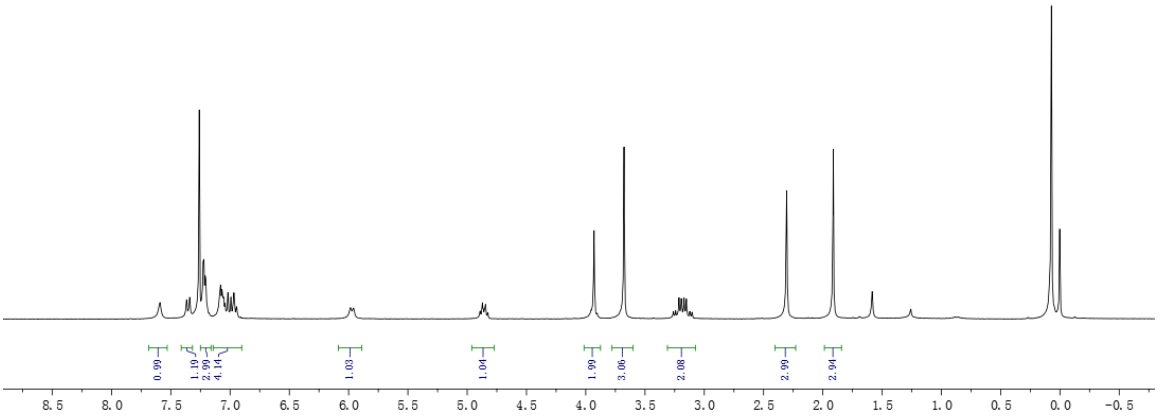
COOMe
SeBn
H
N

4f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4.14
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1.04
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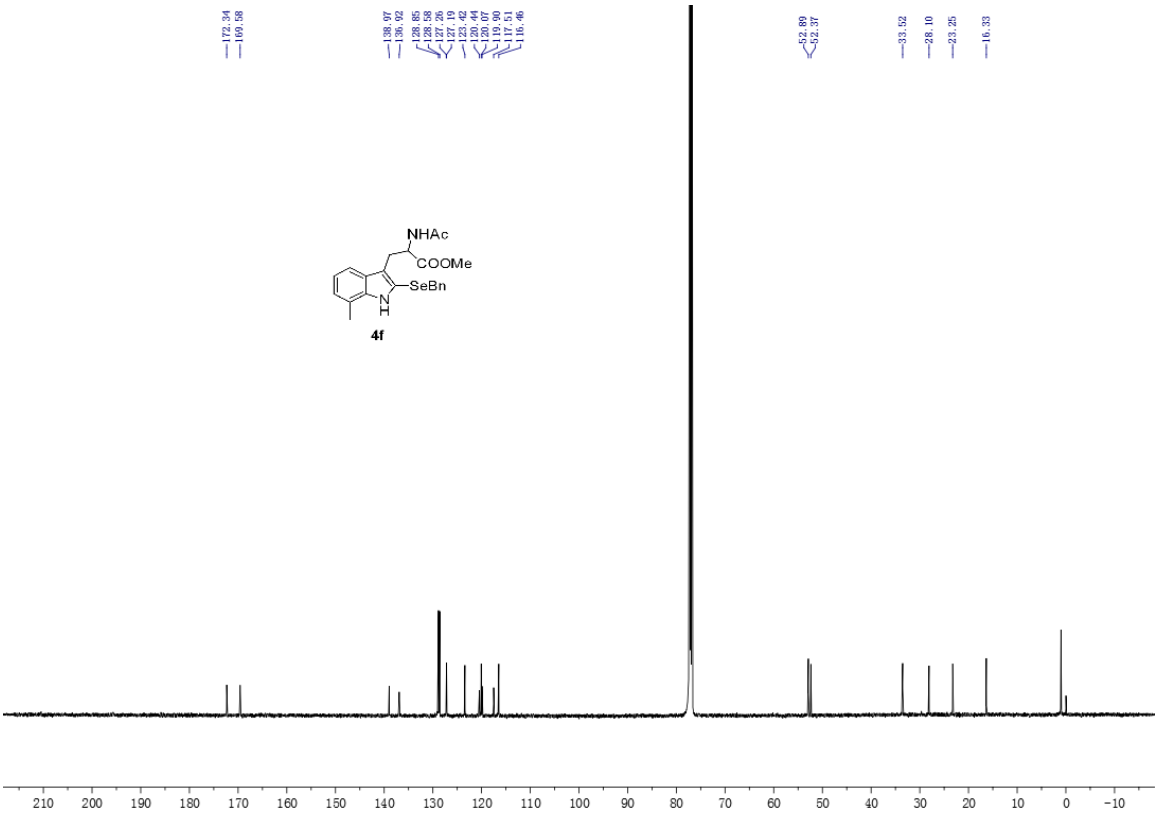
3.06
2.08
2.99
2.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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128.58
127.35
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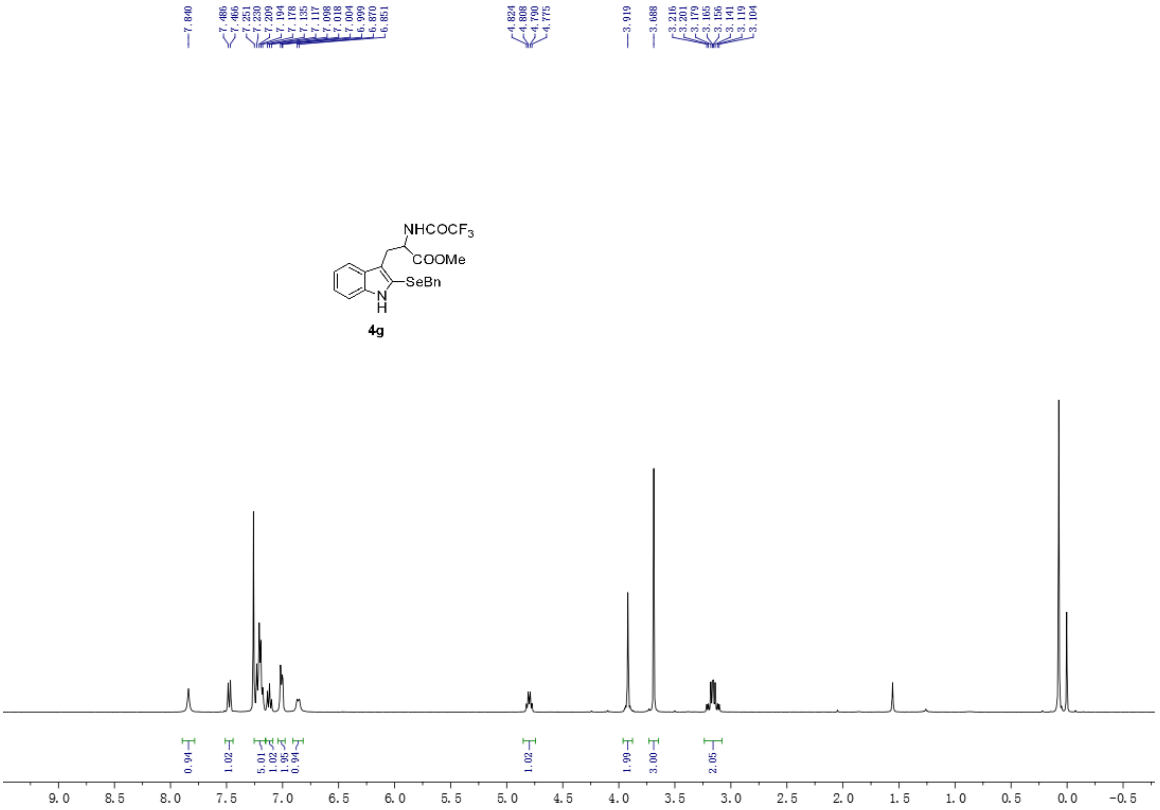
123.42
120.44
120.07
119.90
117.51
116.46
52.89
52.37
33.52
28.10
23.25
16.33
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


NHAc
COOMe
SeBn
H
N

4f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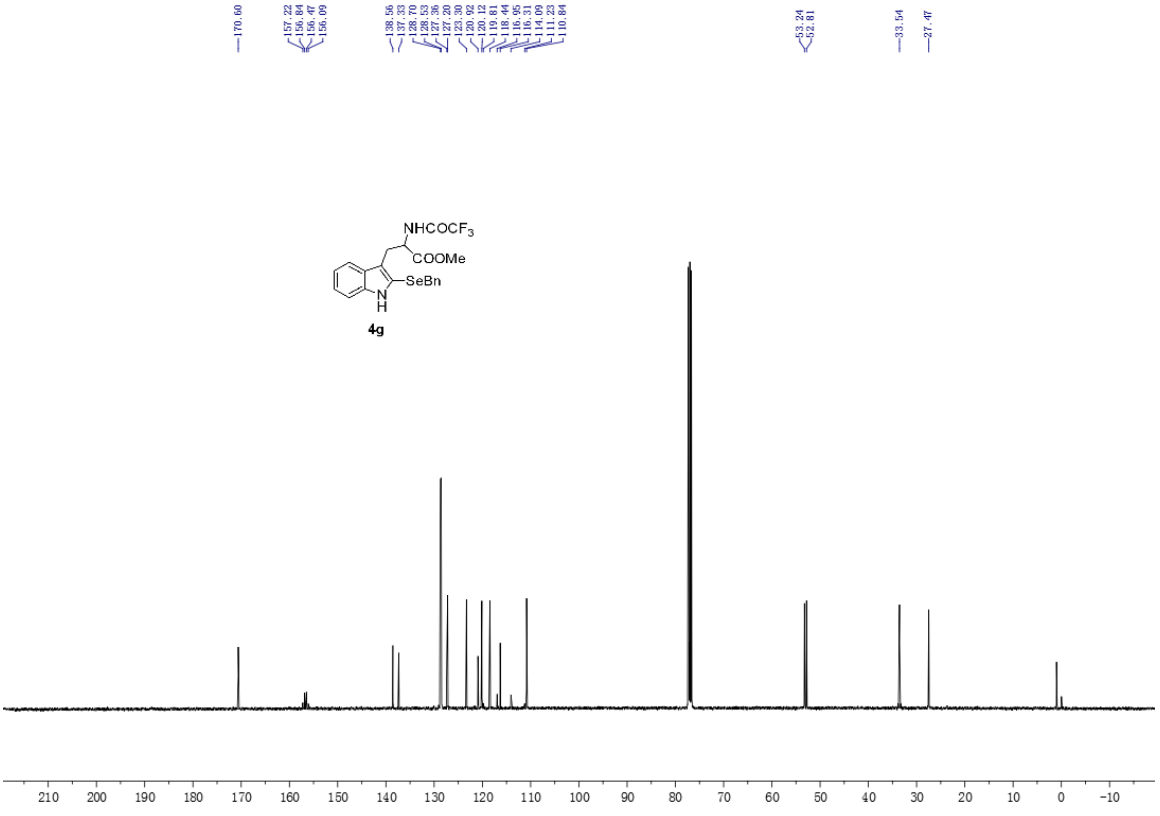
7.230
7.209
7.194
7.178
7.135
7.117
7.098
7.018
7.004
6.999
6.870
6.851
4.824
4.808
4.790
4.775
3.919
3.688
3.216
3.201
3.179
3.165
3.156
3.141
3.119
3.104
NHCOCF3
COOMe
SeBn
N
H
4g
0.94
1.02
5.01
1.02
1.05
0.94
1.02
1.99
3.00
2.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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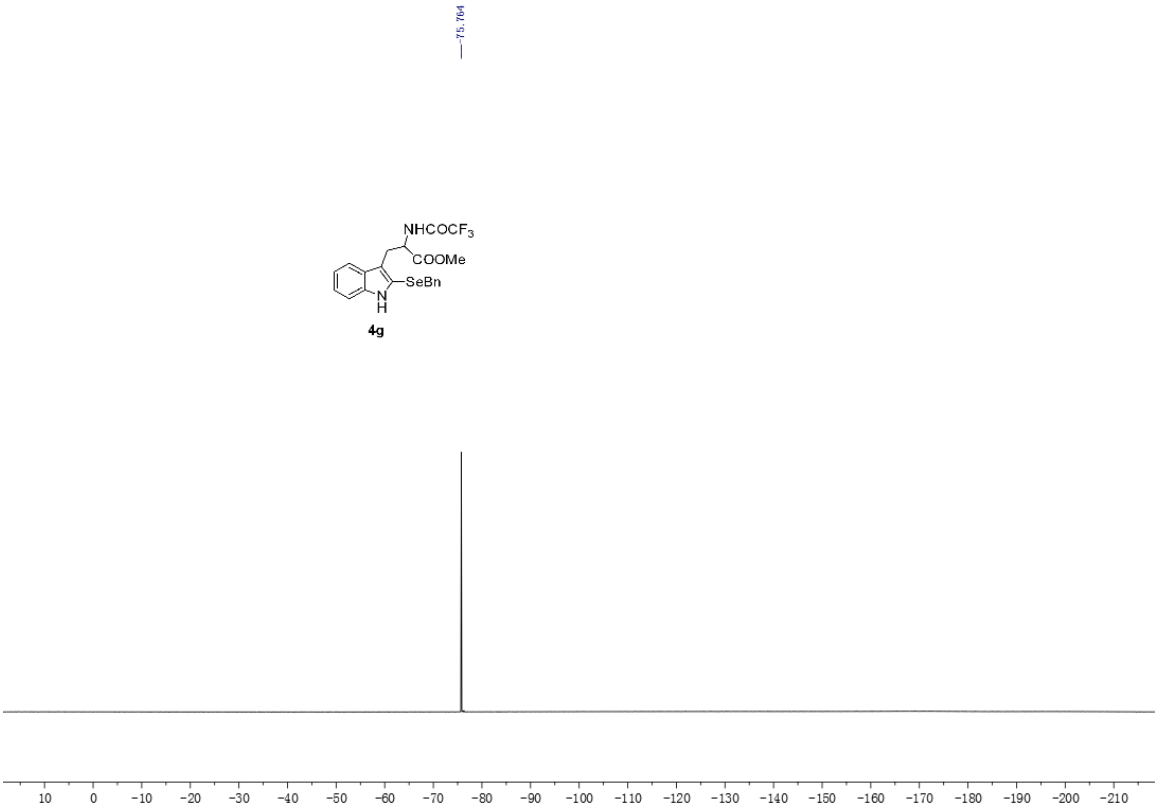
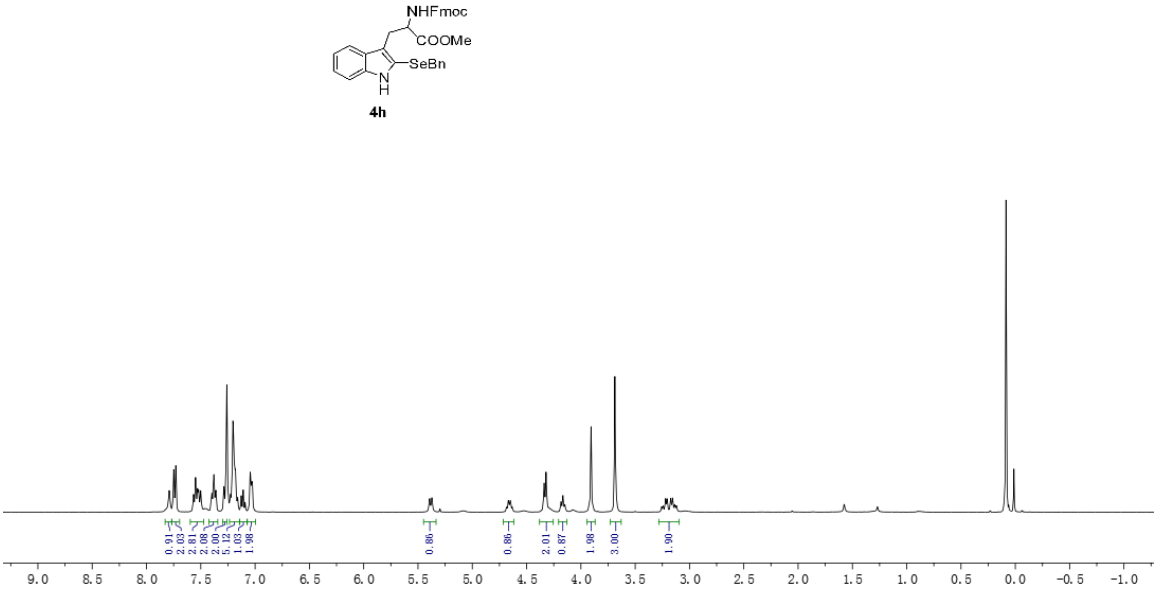
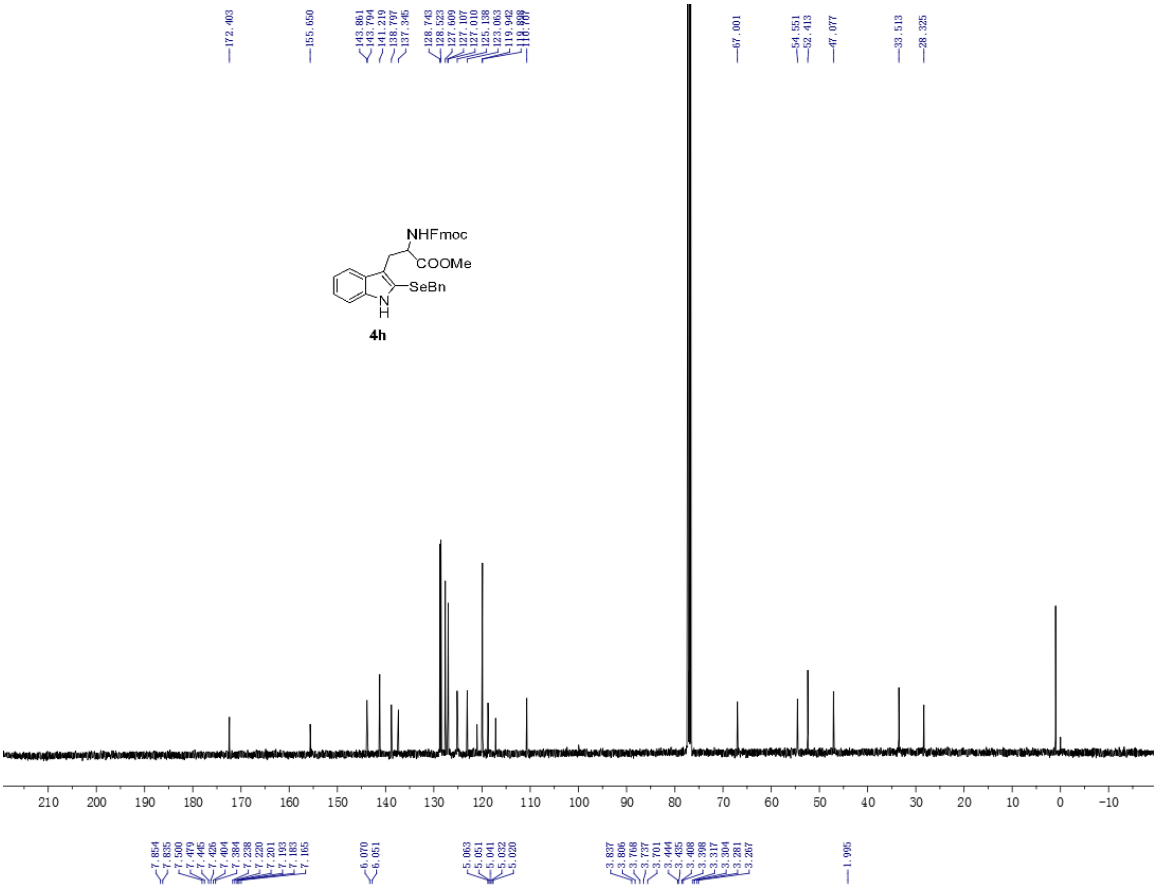
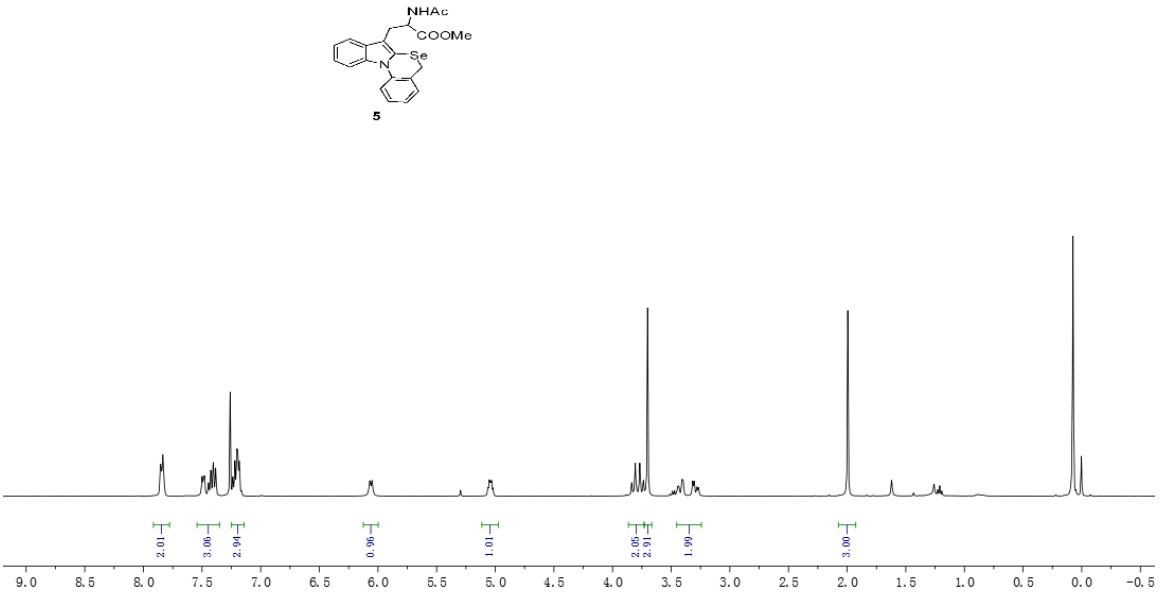
157.22
156.84
156.47
156.09
138.56
137.33
128.70
128.53
127.36
127.20
123.30
120.92
120.12
119.81
118.44
116.95
116.31
114.09
111.23
110.84
53.24
52.81
33.54
27.47
NHCOCF3
COOMe
SeBn
N
H
4g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


-75.764
NHCOCF3
COOMe
SeBn
N
H
4g
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210


7.790 7.779 7.739 7.566 7.548 7.530 7.520 7.511 7.398 7.379 7.361 7.286 7.250 7.236 7.204 7.188 7.181 7.160 7.138 7.109 7.092 7.044 7.030 7.025
5.393 5.373
4.684 4.668 4.649 4.635
4.338 4.321 4.183 4.166
3.687
3.256 3.242 3.220 3.206 3.173 3.156 3.137 3.121


NHFmoc
COOMe
SeBn
N
H
4h
0.91 2.03 2.81 2.08 2.00 2.12 1.03 1.98
0.86
0.86
2.01 0.87
1.98
3.00
1.90
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 -1.0


NHFmoc
COOMe
SeBn
4h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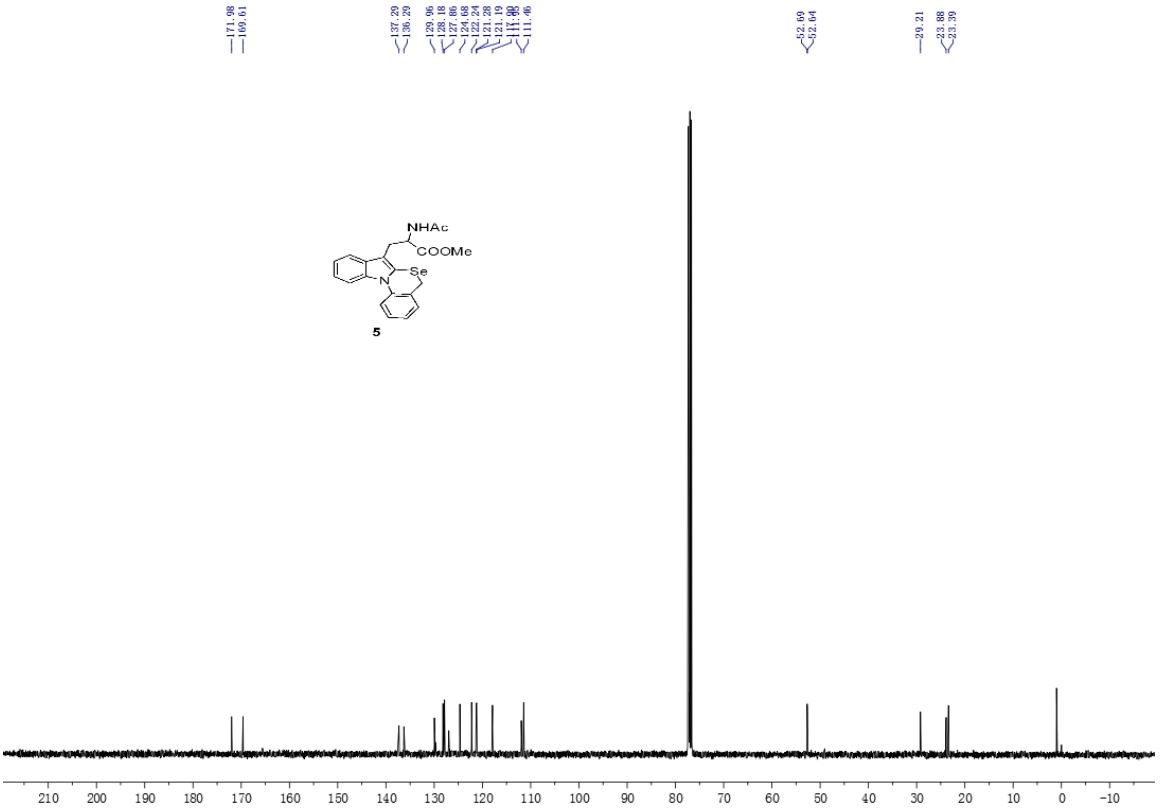
COOMe
Se
5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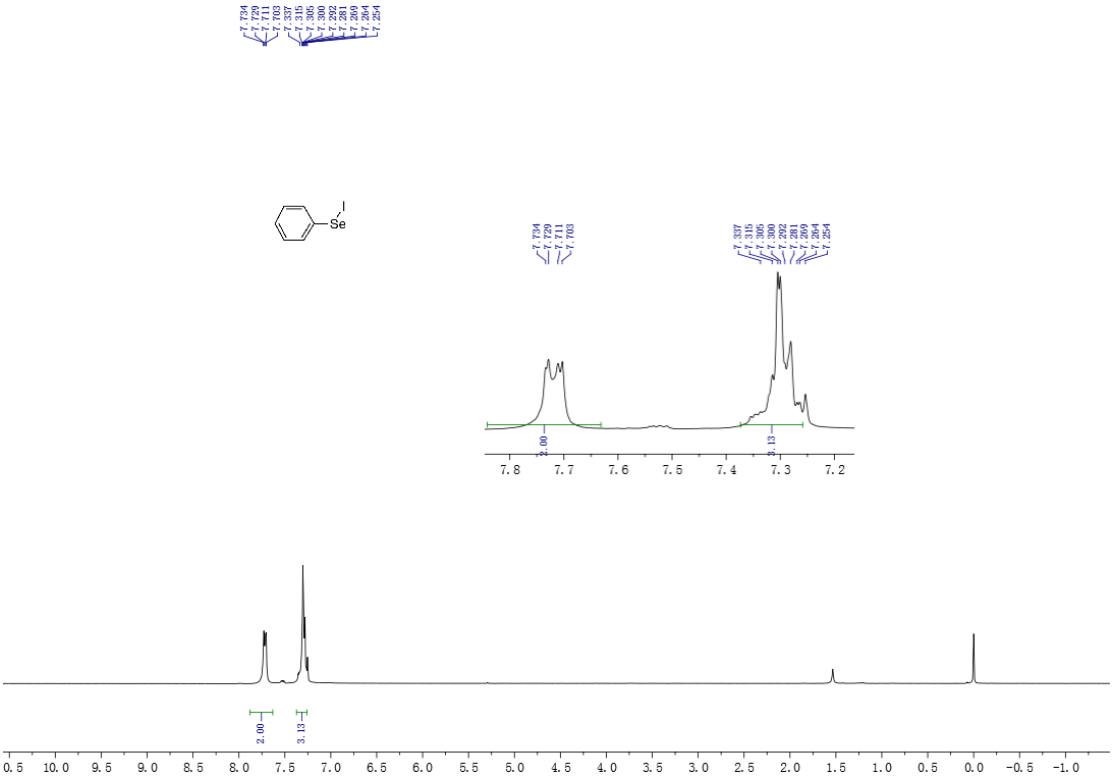
137.29
136.29
129.96
128.18
127.86
124.68
122.24
121.28
121.19
111.80
111.46
52.69
52.64
29.21
23.88
23.39
NHAc
COOMe
Se
N
5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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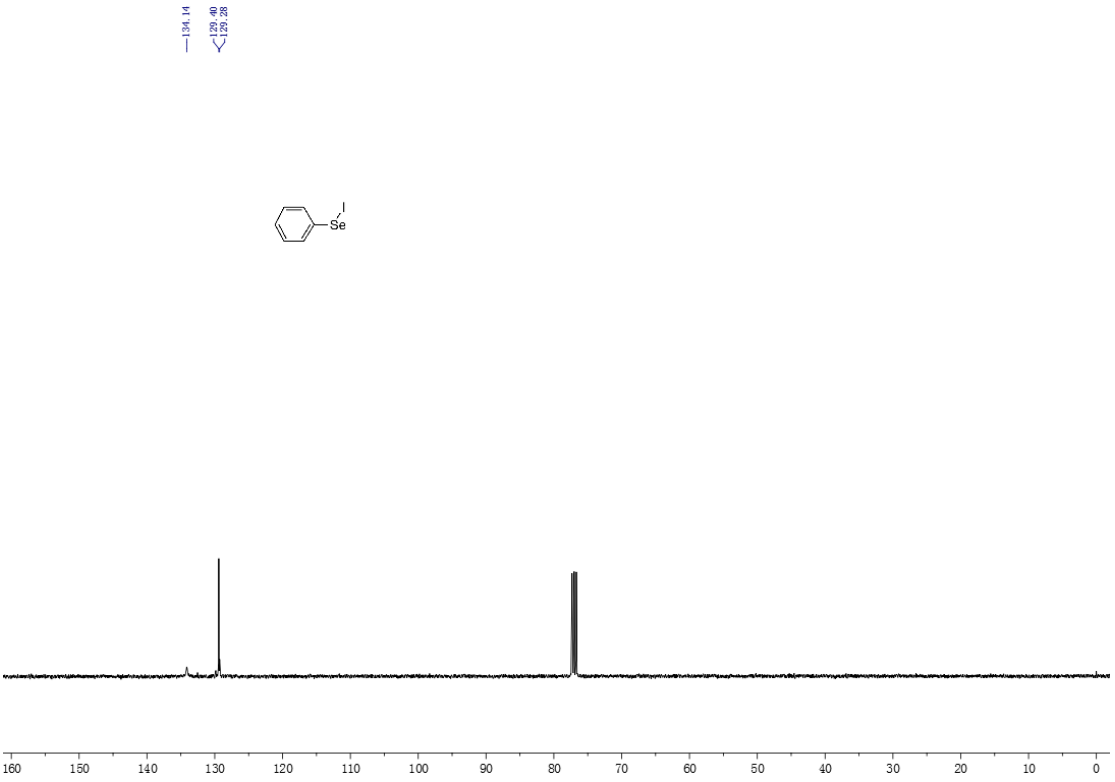
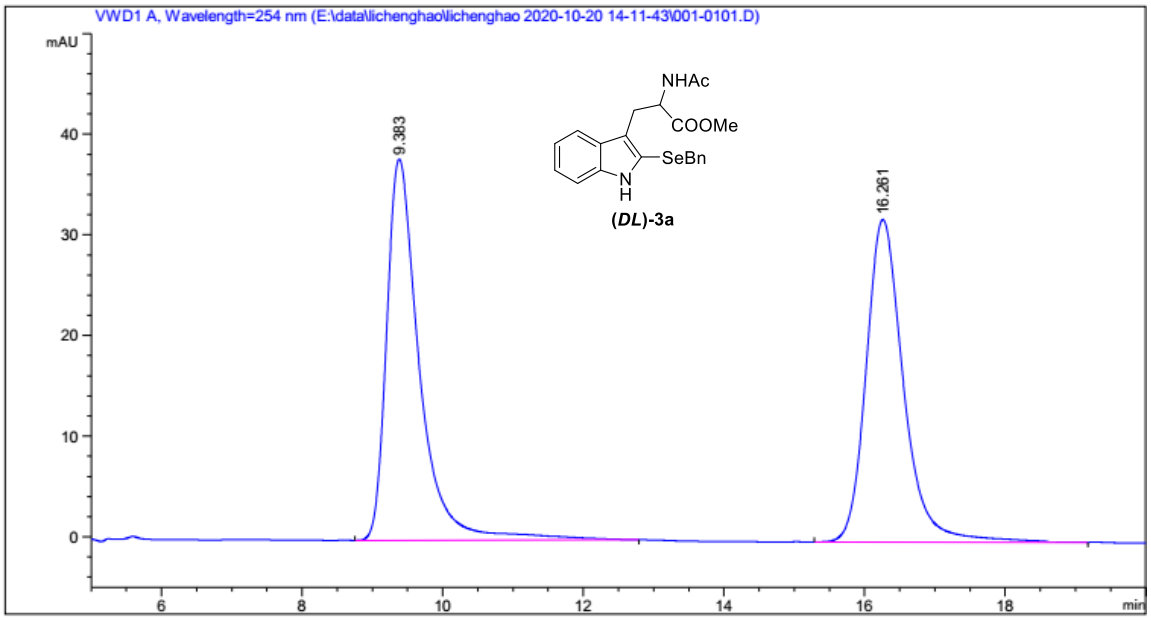
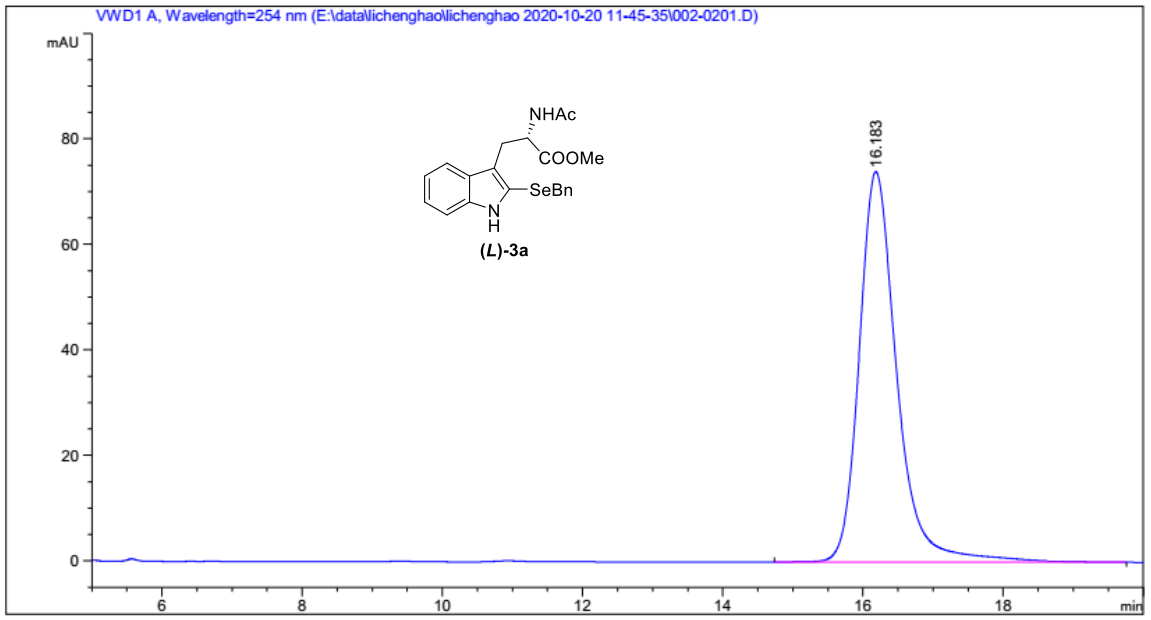
7.337
7.315
7.305
7.300
7.292
7.281
7.269
7.264
7.254
Se
I
2.00
3.13
7.8 7.7 7.6 7.5 7.4 7.3 7.2
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0


134.14
129.40
129.28
Se
I
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

## 8. HPLC spectra



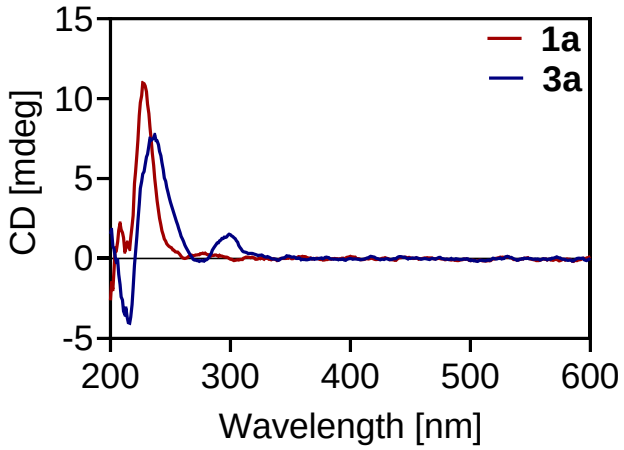

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [mAU*s] | 峰高 [mAU] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 9.383 | BB | 0.4825 | 1232.21887 | 37.87691 | 50.9513 |
| 2 | 16.261 | BB | 0.5590 | 1186.20630 | 32.03588 | 49.0487 |
| 总量： | | | | 2418.42517 | 69.91279 | |

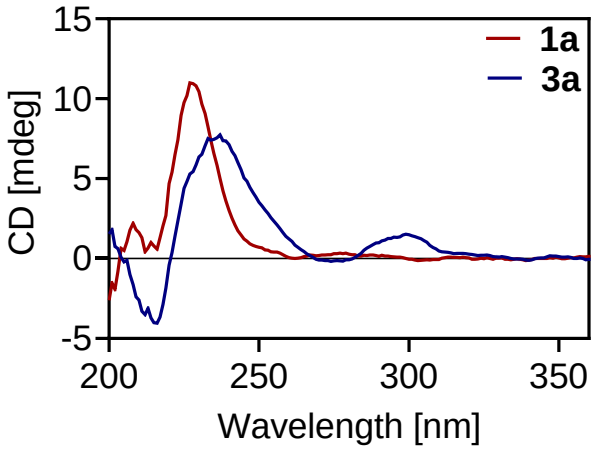



| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [mAU*s] | 峰高 [mAU] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 16.183 | BB | 0.5650 | 2766.55493 | 74.02369 | 100.0000 |

**9. CD Spectra**

CD spectra were recorded on a Jasco J810 instrument using a cell of 1cm path length. Spectral accumulation parameters included the scanning rate at 1000 nm/min with a 1-nm bandwidth, over the wavelength range of 200-600 nm. Each spectrum was obtained from an average of 5 scans. The CD spectra were measured with **1a** (*ca.* $5\times10^{-5}$ M) and **3a** (*ca.* $4\times10^{-5}$ M) in $CH_3CN$ at 25 °C. The CD spectra were corrected for solvent contributions.



**10. References**

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