Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting information

Radical-chain reaction of Isocyanides with Selenosulfonates and Water: Facile Synthesis of Selenocarbamates Under Metal-free Conditions

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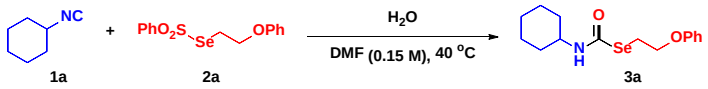
1. General Information

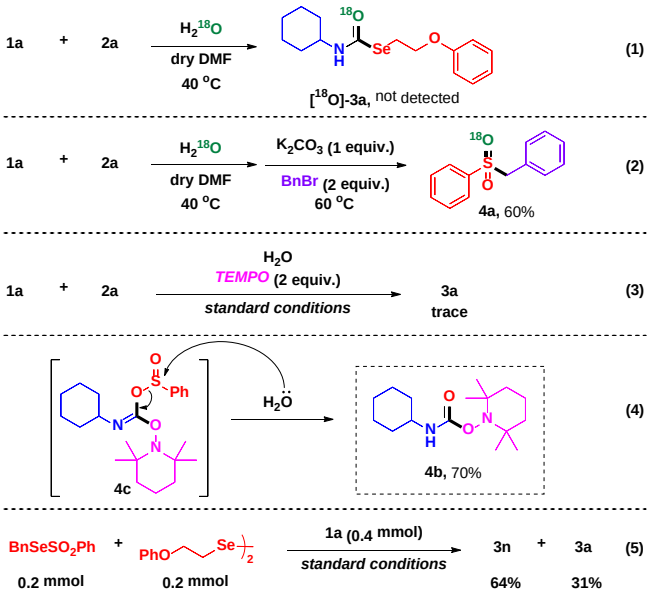
Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were analytical grade and used without further purification. Anhydrous MeCN, DMF, DMA, DMSO and THF (99.9%, Extra Dry with molecular sieves, Water≤50 ppm, in resealable bottle under Ar) was purchased from Adamas-beta®. Alkyl-selenosulfonates were purchased from Suzhou Chukai Pharma Tech Co., Ltd. Analytical thin-layer chromatography (TLC) was performed on silica gel, visualized by I_2 or irradiation with UV light. For column chromatography, 200-300 mesh silica gel was used. Flash chromatography was performed with SepaBean® machine of Santai Technologies. ^{1}H-NMR and ^{13}C-NMR were recorded on a BRUKER 300 MHz or 400 MHz spectrometer in $CDCl_3$. Chemical shifts (δ) were reported referenced to an internal tetramethylsilane standard or the $CDCl_3$ residual peak (δ 7.26) for ^{1}H NMR. Chemical shifts of ^{13}C NMR are reported relative to $CDCl_3$ (δ 77.16). Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), bs (broad singlet), d (doublet), t (triplet), m (multiplet); coupling constants (J) are in Hertz (Hz). Melting points were measured on an Electrothermal digital melting point apparatus and were uncorrected. IR spectra were recorded on a BRUKER VERTEX 70 spectrophotometer and are reported in terms of frequency of absorption (cm^{-1}). HRMS spectra were recorded on a Waters Q-Tof Permier Spectrometer with ESI source. ESR spectra were detected by JES-X320 electron spin resonance instrument.

2. Typical Procedure for the synthesis of 3a



In an oven-dried screw-capped 8-mL vial equipped with a magnetic stir bar, selenosulfonate **2a** (0.3 mmol, 1.0 equiv.) was dissolved in DMF (2 mL). Cyclohexyl isocyanide **1a** (0.60 mmol, 2.0 equiv) and H_2O (3.0 mmol, 10 equiv.) were added subsequently. The system was stirred at 40 °C under air. After 12 h, the crude reaction mixture was cooled to room temperature and diluted with ethyl acetate (50 mL). The organic phase was washed with water (20 mL × 3). The organic layer was dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography (PE/EtOAc = 40:1) to obtain the desired product **3a**.

3. Controlled experiments for Scheme 2



For eq. (1): In an oven-dried screw-capped 8-mL vial equipped with a magnetic stir bar, selenosulfonate **2a** (0.3 mmol, 1.0 equiv.) was dissolved in anhydrous DMF (2 mL). Cyclohexyl isocyanide **1a** (0.60 mmol, 2.0 equiv) and $H_2{}^{18}O$ (3.0 mmol, 10 equiv.) were added subsequently. The system was stirred at 40 °C under air. After 12 h, the crude reaction mixture was cooled to room temperature and diluted with ethyl acetate (5 mL). The crude mixture was analyzed by LC-MS.

For eq. (2): In an oven-dried screw-capped 8-mL vial equipped with a magnetic stir bar, selenosulfonate **2a** (0.2 mmol, 1.0 equiv.) was dissolved in anhydrous DMF (2 mL). Cyclohexyl isocyanide **1a** (0.40 mmol, 2.0 equiv) and $H_2{}^{18}O$ (2.0 mmol, 10 equiv.) were added subsequently. The system was stirred at 40 °C under air. After 12 h, the crude reaction mixture was cooled to room temperature. Then K_2CO_3 (0.2 mmol, 1.0 equiv.) and BnBr (0.40 mmol, 2.0 equiv) were added and the mixture was stirred at 60 °C for another 12 h. After cooling down to room temperature, it was diluted with ethyl acetate (50 mL) and

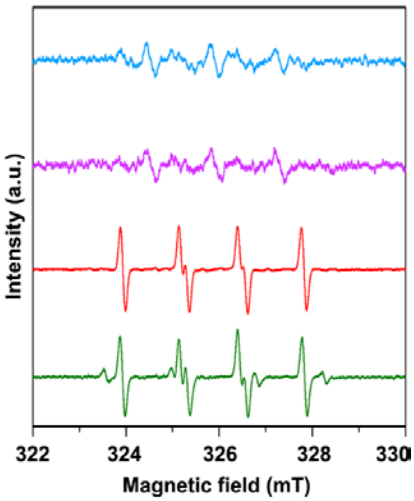
washed with water (20 mL × 3). The organic layer was dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography to obtain the desired product **4a**

For eq. (3) & (4): In an oven-dried screw-capped 8-mL vial equipped with a magnetic stir bar, selenosulfonate **2a** (0.3 mmol, 1.0 equiv.) was dissolved in anhydrous DMF (2 mL). Cyclohexyl isocyanide **1a** (0.60 mmol, 2.0 equiv) and H_2O (3.0 mmol, 10 equiv.) were added subsequently. Radical scavenger TEMPO (0.60 mmol, 2.0 equiv) were added to the above mixture and stirred at 40 °C under air for 12 h. After cooling down to room temperature, it was diluted with ethyl acetate (50 mL) and washed with water (20 mL × 3). The organic layer was dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography to obtain the desired product **4b**.

For eq. (5): In an oven-dried screw-capped 8-mL vial equipped with a magnetic stir bar, *Se*-benzyl benzenesulfonoselenoate (0.20 mmol, 1.0 equiv), 1,2-bis(2-phenoxyethyl)diselane (0.20 mmol, 1.0 equiv.) were dissolved in DMF (2 mL). Cyclohexyl isocyanide **1a** (0.40 mmol, 2.0 equiv) and H_2O (2.0 mmol, 10 equiv.) were added subsequently. The system was stirred at 40 °C under air for 12 h. After cooling down to room temperature, it was diluted with ethyl acetate (50 mL) and washed with water (20 mL × 3). The organic layer was dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography to obtain the corresponding product **3n** and **3a**.

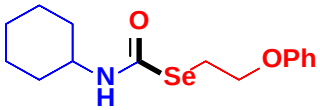
4. EPR experiments

EPR Studies of Interaction between **1a**, **2a** and H_2O. Four dried tubes equipped with a stir bar were respectively loaded with (1) DMPO + **2a** in DMF; (2) DMPO + **2a** + H_2O in DMF; (3) DMPO + **1a** + **2a** in DMF; (4) DMPO + **1a** + **2a** + H_2O in DMF. They were all stirred at 40 °C. After 5 min, the solution samples were taken by four 0.3mm glass capillaries and analyzed by ESR. ESR spectra was recorded at room temperature on ESR spectrometer operated at 9146.941 MHz. Typical spectrometer parameters are shown as follows, Mod freq = 100 kHz, width = 0. 05000 mT, Field center = 326.000 mT, width = +/- 4.000 mT, Sweep time = 30 s.



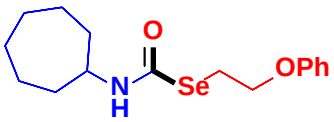
Scheme S1. Room temperature EPR spectra of (blue) DMPO + **2a** in DMF; (purple) DMPO + **2a** + H_2O in DMF; (red) DMPO + **1a** + **2a** in DMF; (green) DMPO + **1a** + **2a** + H_2O in DMF.

5. Spectroscopic Data of Compounds



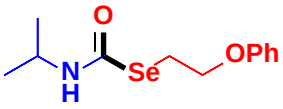
***Se*-(2-phenoxyethyl) cyclohexylcarbamoselenoate (3a)**

White solid. **Mp**: 90.8-91.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (dd, J = 8.6, 7.2 Hz, 2H), 6.93 (dd, J = 11.6, 7.7 Hz, 3H), 5.55 (d, J = 7.8 Hz, 1H), 4.23 (t, J = 6.7 Hz, 2H), 3.78 (dtq, J = 11.4, 7.8, 3.8 Hz, 1H), 3.27 (t, J = 6.7 Hz, 2H), 1.94 (dd, J = 12.3, 4.3 Hz, 2H), 1.70 (dt, J = 13.6, 3.9 Hz, 2H), 1.59 (dq, J = 12.2, 4.0 Hz, 1H), 1.33 (dddd, J = 16.1, 12.6, 9.7, 3.4 Hz, 2H), 1.15 (ttd, J = 11.8, 8.1, 4.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.8, 158.5, 129.5, 121.0, 114.7, 68.0, 51.3, 33.1, 25.4, 25.2, 24.8. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 376.4. **IR (neat)**: ν = 3344, 2928, 2853, 1656, 1500 cm^{-1}; **HRMS** (ESI): calcd. for $C_{15}H_{22}NO_2Se$ $[M+H]^+$: 328.0810, found: 328.0820.



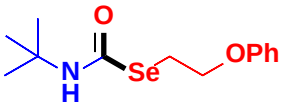
***Se*-(2-phenoxyethyl) cycloheptylcarbamoselenoate (3b)**

White solid. **Mp**: 94.3-95.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (dd, J = 8.6, 7.2 Hz, 2H), 6.93 (dd, J = 11.6, 7.7 Hz, 3H), 5.55 (d, J = 7.8 Hz, 1H), 4.23 (t, J = 6.7 Hz, 2H), 3.78 (dtq, J = 11.4, 7.8, 3.8 Hz, 1H), 3.27 (t, J = 6.7 Hz, 2H), 1.94 (dd, J = 12.3, 4.3 Hz, 2H), 1.70 (dt, J = 13.6, 3.9 Hz, 2H), 1.59 (dq, J = 12.2, 4.0 Hz, 1H), 1.33 (dddd, J = 16.1, 12.6, 9.7, 3.4 Hz, 2H), 1.15 (ttd, J = 11.8, 8.1, 4.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.6, 158.5, 129.6, 121.0, 114.8, 68.1, 53.6, 35.1, 28.1, 25.3, 24.0. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 376.9. **IR (neat)**: ν = 3346, 2925, 2850, 1648, 1498 cm^{-1}; **HRMS** (ESI): calcd. for $C_{16}H_{24}NO_2Se$ $[M+H]^+$: 342.0967, found: 342.0973.



***Se*-(2-phenoxyethyl) isopropylcarbamoselenoate (3c)**

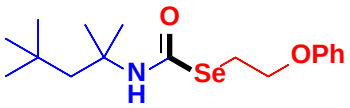
White solid. **Mp**: 81.0-81.9 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.33 – 7.23 (m, 2H), 7.00 – 6.85 (m, 3H), 5.43 (s, 1H), 4.24 (t, J = 6.6 Hz, 2H), 4.08 (s, 1H), 3.27 (t, J = 6.6 Hz, 2H), 1.18 (d, J = 6.6 Hz, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 160.9, 158.5, 129.6, 121.1, 114.8, 68.1, 44.5, 25.2, 22.8. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 377.4. **IR (neat)**: ν = 3345, 2970, 1651, 1499 cm^{-1}; **HRMS** (ESI): calcd. for $C_{12}H_{17}NO_2SeNa$ $[M+Na]^+$: 310.0317, found: 310.0324.



***Se*-(2-phenoxyethyl) tert-butylcarbamoselenoate (3d)**

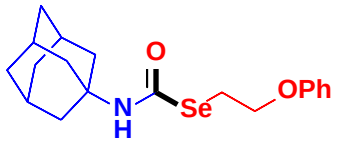
Yellow solid. **Mp**: 68.8-70.0 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 2H), 6.93 (dd, J = 14.4,

7.6 Hz, 3H), 5.34 (s, 1H), 4.22 (t, J = 6.6 Hz, 2H), 3.24 (t, J = 6.6 Hz, 2H), 1.36 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.9, 158.6, 129.5, 121.0, 114.8, 68.1, 54.2, 29.0, 25.5. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 386.4. **IR (neat)**: ν = 3309, 2924, 1657, 1495 cm^{-1}; **HRMS** (ESI): calcd. for $C_{13}H_{19}NO_2SeNa$ $[M+Na]^+$: 324.0473, found: 324.0479.



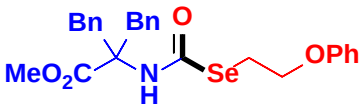
***Se*-(2-phenoxyethyl) (2,4,4-trimethylpentan-2-yl)carbamoselenoate (3e)**

Off-white solid. **Mp**: 42.3-43.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.23 (m, 2H), 6.92 (dd, J = 15.1, 7.5 Hz, 3H), 5.26 (s, 1H), 4.21 (t, J = 6.7 Hz, 2H), 3.23 (t, J = 6.6 Hz, 2H), 1.73 (s, 2H), 1.40 (s, 6H), 1.00 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.7, 158.6, 129.5, 121.0, 114.8, 68.2, 58.0, 51.8, 31.7, 31.5, 29.6, 25.5. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 389.5. **IR (neat)**: ν = 3391, 2929, 1671, 1494 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{27}NO_2Se$ $[M]^+$: 357.1207, found: 357.1208.



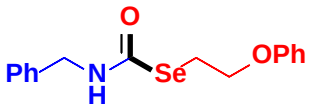
***Se*-(2-phenoxyethyl) ((1s,3s)-adamantan-1-yl)carbamoselenoate (3f)**

White solid. **Mp**: 88.0-88.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (dd, J = 8.6, 7.3 Hz, 2H), 6.99 – 6.85 (m, 3H), 5.18 (s, 1H), 4.22 (t, J = 6.6 Hz, 2H), 3.22 (t, J = 6.6 Hz, 2H), 2.13 – 2.04 (m, 3H), 1.99 (d, J = 2.9 Hz, 6H), 1.66 (t, J = 3.1 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.4, 158.6, 129.5, 121.0, 114.8, 68.1, 55.0, 42.0, 36.3, 29.6, 25.5. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 386.2. **IR (neat)**: ν = 3286, 2903, 2850, 1650 cm^{-1}; **HRMS** (ESI): calcd. for $C_{19}H_{26}NO_2Se$ $[M+H]^+$: 380.1123, found: 380.1106.



methyl 2-benzyl-2-((((2-phenoxyethyl)selanyl)carbonyl)amino)-3-phenylpropanoate (3g)

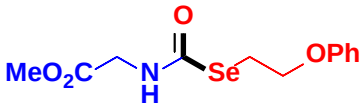
White solid. **Mp**: 92.6-93.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 7.19 (dd, J = 5.2, 1.9 Hz, 6H), 7.10 – 7.03 (m, 4H), 6.98 – 6.88 (m, 3H), 6.21 (s, 1H), 4.26 (t, J = 6.7 Hz, 2H), 3.91 (d, J = 13.6 Hz, 2H), 3.69 (s, 3H), 3.30 (t, J = 6.7 Hz, 2H), 3.22 (d, J = 13.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.8, 161.7, 158.6, 135.7, 129.6, 129.6, 128.4, 127.2, 121.0, 114.7, 69.8, 68.0, 52.6, 41.4, 25.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 401.2. **IR (neat)**: ν = 3272, 1745, 1642, 1200, 670 cm^{-1}; **HRMS** (ESI): calcd. for $C_{26}H_{27}NO_4SeNa$ $[M+Na]^+$: 520.1003, found: 520.0982.



***Se*-(2-phenoxyethyl) benzylcarbamoselenoate (3h)**

Pale yellow solid. **Mp**: 104.7-105.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (dt, J = 23.3, 7.1 Hz, 7H), 6.97 – 6.83 (m, 3H), 6.03 (t, J = 5.8 Hz, 1H), 4.42 (d, J = 5.7 Hz, 2H), 4.21 (t, J = 6.6 Hz, 2H), 3.27 (t, J

= 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.4, 158.4, 137.4, 129.5, 128.8, 127.8, 127.8, 121.0, 114.7, 68.0, 45.8, 25.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 380.7. **IR (neat)**: ν = 3309, 3030, 2924, 2852, 1649, 1213, 693 cm^{-1}; **HRMS** (ESI): calcd. for $C_{16}H_{18}NO_2Se$ $[M+H]^+$: 336.0497, found: 336.0502.

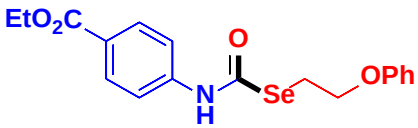


methyl (((2-phenoxyethyl)selanyl)carbonyl)glycinate (3i)

Light brown solid. **Mp**: 87.4-88.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 2H), 6.93 (dd, J = 16.3, 7.8 Hz, 3H), 6.30 (d, J = 5.5 Hz, 1H), 4.23 (t, J = 6.6 Hz, 2H), 4.09 (d, J = 5.2 Hz, 2H), 3.76 (s, 3H), 3.29 (t, J = 6.7 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.8, 163.1, 158.4, 129.6, 121.1, 114.7, 67.8, 52.7, 42.9, 25.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 383.7. **IR (neat)**: ν = 3340, 2946, 1730, 1673, 1201, 750 cm^{-1}; **HRMS** (ESI): calcd. for $C_{12}H_{15}NO_4SeNa$ $[M+Na]^+$: 340.0059, found: 340.0062.

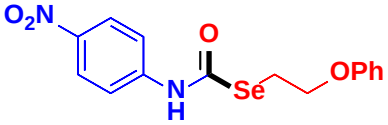
ethyl (((2-phenoxyethyl)selanyl)carbonyl)glycinate (3j)

Off-white solid. **Mp**: 62.3-63.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.23 (m, 2H), 6.97 – 6.88 (m, 3H), 6.33 (s, 1H), 4.22 (q, J = 6.8 Hz, 4H), 4.07 (d, J = 5.1 Hz, 2H), 3.29 (t, J = 6.7 Hz, 2H), 1.28 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.4, 163.0, 158.4, 129.5, 121.1, 114.7, 67.8, 61.9, 43.1, 25.3, 14.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 383.6. **IR (neat)**: ν = 3321, 2936, 1752, 1644, 1175 cm^{-1}; **HRMS** (ESI): calcd. for $C_{13}H_{17}NO_4SeNa$ $[M+Na]^+$: 354.0215, found: 354.0221.



ethyl 4-((((2-phenoxyethyl)selanyl)carbonyl)amino)benzoate (3k)

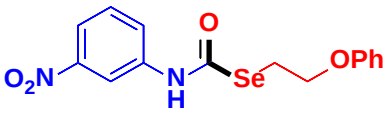
Light brown solid. **Mp**: 105.7-106.3 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.11 (s, 1H), 8.03 – 7.96 (m, 2H), 7.56 – 7.48 (m, 2H), 7.27 (dd, J = 8.7, 7.3 Hz, 2H), 6.98 – 6.88 (m, 3H), 4.36 (q, J = 7.1 Hz, 2H), 4.27 (t, J = 6.5 Hz, 2H), 3.35 (t, J = 6.5 Hz, 2H), 1.38 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 166.4, 161.7, 158.4, 141.9, 131.1, 129.6, 126.1, 121.2, 118.7, 114.8, 67.8, 61.2, 26.1, 14.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 411.3. **IR (neat)**: ν = 3339, 1696, 1592, 1519, 1240, 1108, 746 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{19}NO_4SeNa$ $[M+Na]^+$: 416.0372, found: 416.0377.



***Se*-(2-phenoxyethyl) (4-nitrophenyl)carbamoselenoate (3l)**

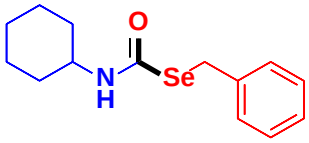
Yellow solid. **Mp**: 112.2-113.8 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.21 (d, J = 8.5 Hz, 2H), 7.81 (s, 1H), 7.61 (d, J = 8.6 Hz, 2H), 7.35 – 7.24 (m, 2H), 6.95 (q, J = 8.4, 8.0 Hz, 3H), 4.40 – 4.23 (m, 2H), 3.62 –

3.25 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 162.2, 158.3, 143.8, 143.2, 129.7, 125.5, 121.5, 118.9, 114.8, 67.7, 26.6. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 419.9. **IR (neat)**: ν = 3339, 2931, 1697, 1487, 1298, 1110, 748 cm^{-1}; **HRMS** (ESI): calcd. for $C_{15}H_{14}N_2O_4SeNa$ $[M+Na]^+$: 389.0011, found: 389.0009.



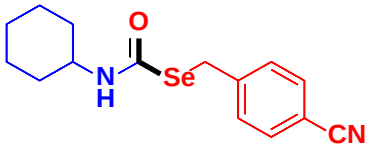
Se-(2-phenoxyethyl) (3-nitrophenyl)carbamoselenoate (3m)

Brown solid. **Mp**: 85.3-86.0 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.34 (t, J = 2.1 Hz, 1H), 7.97 (dd, J = 8.2, 2.1 Hz, 1H), 7.85 – 7.72 (m, 2H), 7.48 (t, J = 8.2 Hz, 1H), 7.29 (t, J = 7.8 Hz, 2H), 6.95 (dd, J = 16.5, 7.8 Hz, 3H), 4.31 (t, J = 6.4 Hz, 2H), 3.40 (t, J = 6.4 Hz, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 162.1, 158.4, 148.7, 138.7, 130.2, 129.7, 125.3, 121.4, 119.3, 114.8, 114.5, 67.8, 26.5. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 412.9. **IR (neat)**: ν = 3339, 2921, 1678, 1525, 1230, 734 cm^{-1}; **HRMS** (ESI): calcd. for $C_{15}H_{15}N_2O_4Se$ $[M+H]^+$: 367.0192, found: 367.0189.



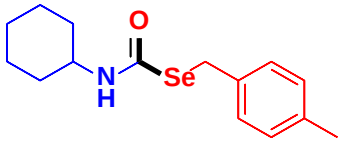
***Se*-benzyl cyclohexylcarbamoselenoate (3n)**

White solid. **Mp**: 81.2-82.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 – 7.23 (m, 4H), 7.18 (t, J = 7.3 Hz, 1H), 5.42 (d, J = 7.6 Hz, 1H), 4.18 (s, 2H), 3.79 (ddt, J = 14.9, 11.1, 6.3 Hz, 1H), 1.93 (dd, J = 12.7, 4.2 Hz, 2H), 1.73 – 1.65 (m, 2H), 1.58 (dt, J = 13.0, 3.9 Hz, 1H), 1.32 (q, J = 12.8, 12.3 Hz, 2H), 1.13 (qd, J = 12.0, 3.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.4, 139.8, 128.9, 128.6, 126.9, 51.3, 33.1, 30.0, 25.4, 24.8. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 477.8. **IR (neat)**: ν = 3302, 2926, 2851, 1643, 1515 cm^{-1}; **HRMS** (ESI): calcd. for $C_{14}H_{20}NOSe$ $[M+H]^+$: 298.0705, found: 298.0733.



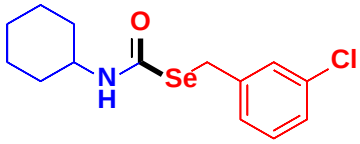
N-(4-nitrophenyl)-3-(p-tolyl)-1,2,4-selenadiazol-5-amine (3o)

White solid. **Mp**: 94.7-95.8 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.64 – 7.54 (m, 2H), 7.53 – 7.36 (m, 2H), 5.37 (d, J = 7.2 Hz, 1H), 4.18 (s, 2H), 3.79 (tq, J = 10.6, 3.8 Hz, 1H), 2.05 – 1.82 (m, 2H), 1.77 – 1.59 (m, 3H), 1.41 – 1.11 (m, 5H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 160.5, 146.1, 132.4, 129.7, 119.0, 110.6, 51.6, 33.1, 29.2, 25.4, 24.8. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 491.8. **IR (neat)**: ν = 3253, 2926, 1646, 1520 cm^{-1}; **HRMS** (ESI): calcd. for $C_{15}H_{19}N_2OSe$ $[M+H]^+$: 323.0657, found: 323.0664.



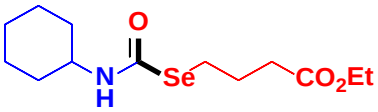
***Se*-(4-methylbenzyl) cyclohexylcarbamoselenoate (3p)**

White solid. **Mp**: 93.7-94.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 – 7.14 (m, 2H), 7.07 (d, J = 7.8 Hz, 2H), 5.35 (s, 1H), 4.16 (s, 2H), 3.78 (dtd, J = 11.3, 7.5, 4.0 Hz, 1H), 2.30 (s, 3H), 1.94 (dd, J = 12.8, 4.0 Hz, 2H), 1.69 (dt, J = 13.5, 3.9 Hz, 2H), 1.59 (dt, J = 13.0, 3.9 Hz, 1H), 1.33 (q, J = 12.1 Hz, 2H), 1.14 (qt, J = 12.5, 3.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.6, 136.7, 136.6, 129.4, 128.8, 51.3, 33.2, 29.8, 25.5, 24.9, 21.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 478.2. **IR (neat)**: ν = 3243, 2928, 1639, 1525 cm^{-1}; **HRMS** (ESI): calcd. for $C_{15}H_{22}NOSe$ $[M+H]^+$: 312.0861, found: 312.0880.



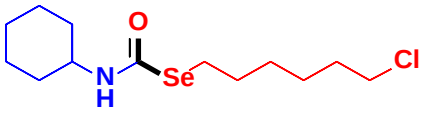
***Se*-(3-chlorobenzyl) cyclohexylcarbamoselenoate (3q)**

White solid. **Mp**: 94.6-96.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (s, 1H), 7.24 – 7.13 (m, 3H), 5.44 (d, J = 7.6 Hz, 1H), 4.12 (s, 2H), 3.79 (dtd, J = 14.8, 7.9, 4.0 Hz, 1H), 1.95 (dd, J = 12.4, 3.3 Hz, 2H), 1.70 (dp, J = 12.0, 4.0 Hz, 2H), 1.60 (dq, J = 12.8, 3.6 Hz, 1H), 1.39 – 1.27 (m, 2H), 1.16 (dddt, J = 16.2, 12.1, 8.5, 3.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.9, 142.1, 134.2, 129.8, 129.0, 127.2, 127.1, 51.4, 33.1, 29.2, 25.4, 24.8. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 482.9. **IR (neat)**: ν = 3255, 2928, 2853, 1638, 1526 cm^{-1}; **HRMS** (ESI): calcd. for $C_{14}H_{19}ClNOSe$ $[M+H]^+$: 332.0315, found: 332.0333.



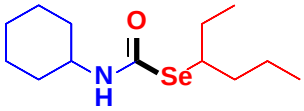
ethyl 4-((cyclohexylcarbamoyl)selanyl)butanoate (3r)

Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.63 (d, J = 7.6 Hz, 1H), 4.13 (q, J = 7.1 Hz, 2H), 3.76 (ddt, J = 13.2, 9.1, 4.2 Hz, 1H), 2.96 (t, J = 7.2 Hz, 2H), 2.42 (t, J = 7.4 Hz, 2H), 2.04 (t, J = 7.3 Hz, 2H), 1.99 – 1.91 (m, 2H), 1.76 – 1.68 (m, 2H), 1.60 (dt, J = 13.1, 3.9 Hz, 1H), 1.40 – 1.30 (m, 2H), 1.26 (t, J = 7.1 Hz, 3H), 1.22 – 1.11 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.1, 161.0, 60.4, 51.1, 34.1, 33.1, 26.5, 25.7, 25.4, 24.8, 14.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 392.4. **IR (neat)**: ν = 3321, 2929, 2854, 1731, 1653, 1508 cm^{-1}; **HRMS** (ESI): calcd. for $C_{13}H_{23}NO_3SeNa$ $[M+Na]^+$: 344.0735, found: 344.0730.



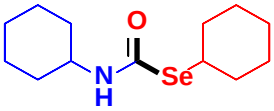
***Se*-(6-chlorohexyl) cyclohexylcarbamoselenoate (3s)**

Light yellow solid. **Mp**: 35.6-36.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.38 (d, J = 7.7 Hz, 1H), 3.77 (dh, J = 14.5, 4.0 Hz, 1H), 3.53 (t, J = 6.7 Hz, 2H), 2.93 (t, J = 7.3 Hz, 2H), 1.95 (dd, J = 12.6, 4.1 Hz, 2H), 1.75 (dp, J = 14.7, 7.0 Hz, 6H), 1.60 (dt, J = 12.9, 3.9 Hz, 1H), 1.49 – 1.29 (m, 6H), 1.17 (dq, J = 16.3, 7.2, 5.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.9, 50.5, 44.5, 32.6, 32.0, 30.5, 28.6, 26.1, 25.9, 24.9, 24.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 395.3. **IR (neat)**: ν = 3331, 2931, 2854, 1654, 1504 cm^{-1}; **HRMS** (ESI): calcd. for $C_{13}H_{25}ClNOSe$ $[M+H]^+$: 326.0784, found: 326.0811.



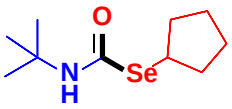
***Se*-(hexan-3-yl) cyclohexylcarbamoselenoate (3t)**

Yellow solid. **Mp**: 41.5-43.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.39 (d, J = 7.3 Hz, 1H), 3.76 (dp, J = 15.2, 5.7, 4.3 Hz, 1H), 3.47 (p, J = 6.8 Hz, 1H), 1.95 (dd, J = 12.2, 4.3 Hz, 2H), 1.84 – 1.54 (m, 8H), 1.53 – 1.28 (m, 5H), 1.21 – 1.10 (m, 3H), 0.99 (t, J = 7.3 Hz, 3H), 0.92 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.2, 50.9, 48.5, 37.9, 33.2, 29.2, 25.5, 24.9, 21.1, 14.0, 12.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 453.0. **IR (neat)**: ν = 3308, 2927, 2853, 1650, 1514 cm^{-1}; **HRMS** (ESI): calcd. for $C_{13}H_{25}NNaOSe$ $[M+Na]^+$: 314.0994, found: 314.0989.



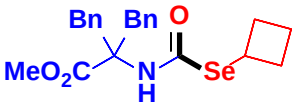
***Se*-cyclohexyl cyclohexylcarbamoselenoate (3u)**

Off-white solid. **Mp**: 111.7-113.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.38 (d, J = 7.6 Hz, 1H), 3.76 (tdt, J = 11.4, 8.1, 4.0 Hz, 1H), 3.58 (tt, J = 9.7, 4.1 Hz, 1H), 2.08 (dt, J = 13.0, 4.6 Hz, 2H), 1.95 (dd, J = 12.5, 4.2 Hz, 2H), 1.66 (dddd, J = 30.0, 13.3, 9.2, 3.8 Hz, 7H), 1.56 (dd, J = 7.1, 3.9 Hz, 1H), 1.46 (ddt, J = 13.9, 6.7, 3.5 Hz, 2H), 1.32 (td, J = 11.8, 10.6, 6.0 Hz, 3H), 1.16 (tdd, J = 12.0, 8.5, 4.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.9, 50.9, 43.8, 34.8, 33.2, 26.9, 25.8, 25.5, 24.9. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 489.7. **IR (neat)**: ν = 3259, 2921, 2849, 1643, 1518, 1446 cm^{-1}; **HRMS** (ESI): calcd. for $C_{13}H_{23}NNaOSe$ $[M+Na]^+$: 312.0837, found: 312.0835.



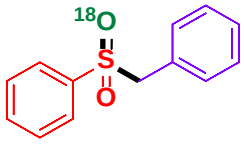
***Se*-cyclopentyl tert-butylcarbamoselenoate (3v)**

Pale yellow solid. **Mp**: 95.3-96.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.18 (s, 1H), 3.75 – 3.63 (m, 1H), 2.20 – 2.10 (m, 2H), 1.75 – 1.66 (m, 4H), 1.63 – 1.55 (m, 2H), 1.36 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.7, 53.9, 42.2, 34.6, 29.1, 24.9. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 494.3. **IR (neat)**: ν = 3293, 2958, 1656, 1518 cm^{-1}; **HRMS** (ESI): calcd. for $C_{10}H_{20}NOSe$ $[M+H]^+$: 250.0705, found: 250.0711.



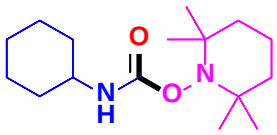
methyl 2-benzyl-2-(((cyclobutylselanyl)carbonyl)amino)-3-phenylpropanoate (3w)

Light yellow solid. **Mp**: 61.9-63.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 (qd, J = 7.7, 6.7, 3.6 Hz, 6H), 7.10 – 7.05 (m, 4H), 6.02 (s, 1H), 4.19 (p, J = 8.3 Hz, 1H), 3.92 (d, J = 13.6 Hz, 2H), 3.73 (s, 3H), 3.21 (d, J = 13.6 Hz, 2H), 2.58 – 2.46 (m, 2H), 2.32 – 2.20 (m, 2H), 2.11 – 1.98 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.0, 163.1, 135.9, 129.7, 128.4, 127.2, 69.6, 52.7, 41.4, 35.6, 31.8, 20.6. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 511.5. **IR (neat)**: ν = 3375, 2936, 2102, 1739, 1681 cm^{-1}; **HRMS** (ESI): calcd. for $C_{13}H_{12}NO_3SeNa$ $[M+Na]^+$: 454.0892, found: 454.0876.



(benzylsulfonyl-^{18}O)benzene (4a)

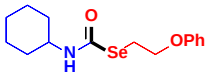
White solid. **Mp**: 140.6-141.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 – 7.52 (m, 3H), 7.44 (t, J = 7.8 Hz, 2H), 7.34 – 7.28 (m, 1H), 7.28 – 7.22 (m, 2H), 7.13 – 7.03 (m, 2H), 4.31 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.9, 133.8, 130.9, 129.0, 128.9, 128.7, 128.7, 128.2, 63.0. **IR (neat)**: ν = 1447, 1244, 793, 757, 687, 542 cm^{-1}; **HRMS** (ESI): calcd. for $C_{13}H_{12}O^{18}OSNa$ $[M+Na]^+$: 257.0493, found: 257.0488.



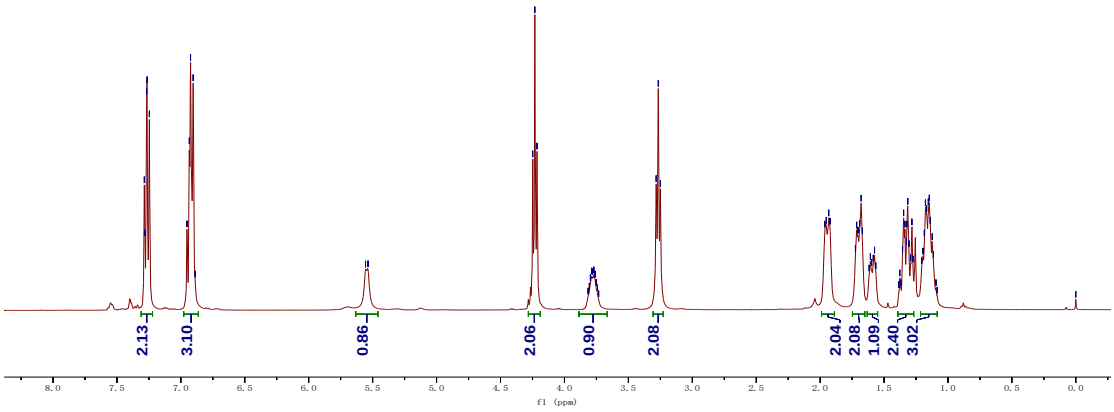
2,2,6,6-tetramethylpiperidin-1-yl cyclohexylcarbamate (4b)

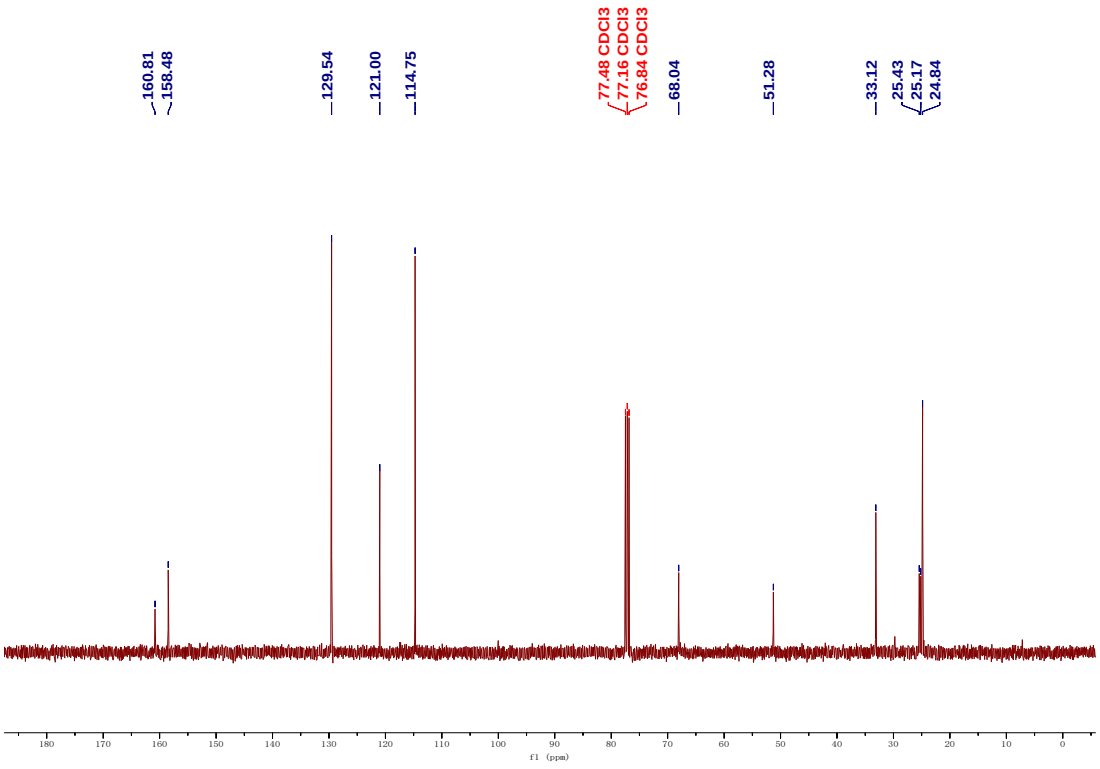
Off-white solid. **Mp**: 105.8-106.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.74 (d, J = 8.1 Hz, 1H), 3.69 – 3.49 (m, 1H), 1.92 (dq, J = 12.6, 3.9 Hz, 2H), 1.62 (tdt, J = 28.9, 13.4, 3.2 Hz, 8H), 1.45 – 1.32 (m, 3H), 1.26 – 1.14 (m, 9H), 1.10 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.8, 60.8, 49.6, 39.9, 33.3, 31.9, 25.6, 24.9, 20.6, 16.8. **IR (neat)**: ν = 3330, 2924, 2853, 1702, 1492 cm^{-1}; **HRMS** (ESI): calcd. for $C_{16}H_{30}N_2O_2Na$ $[M+Na]^+$: 305.2199, found: 305.2204.

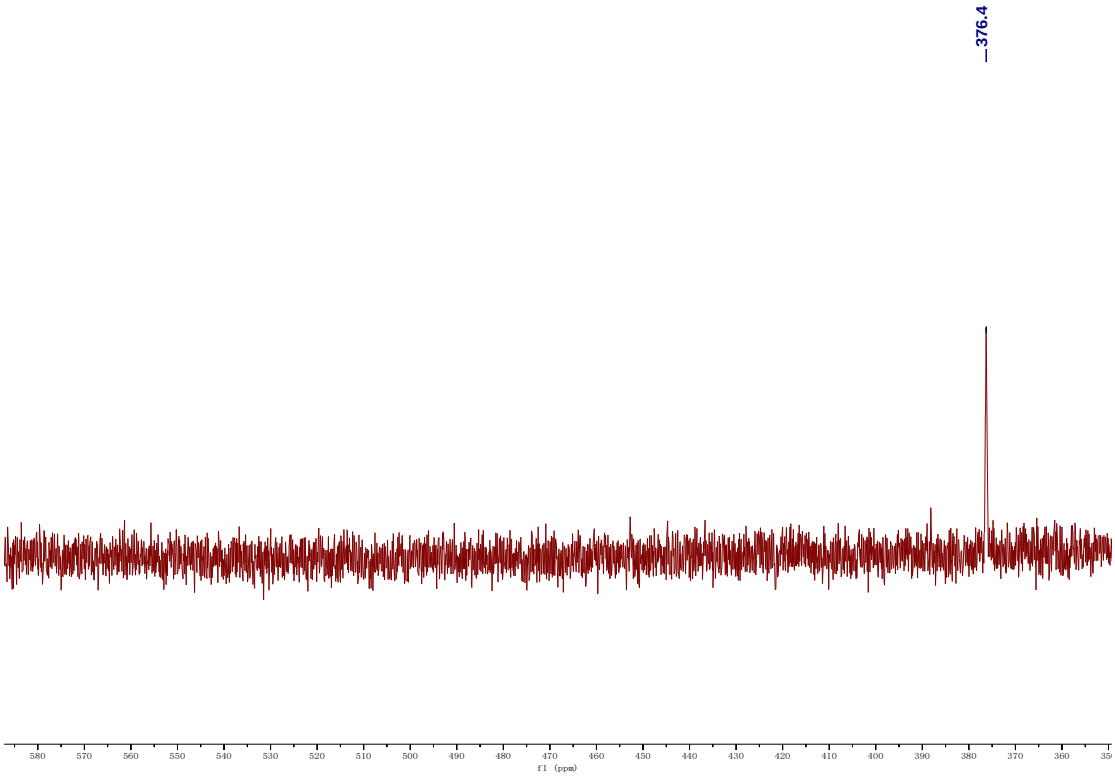
6. Copies of ^{1}H, ^{13}C and ^{77}Se NMR Spectra for Compounds

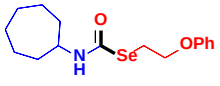


3a

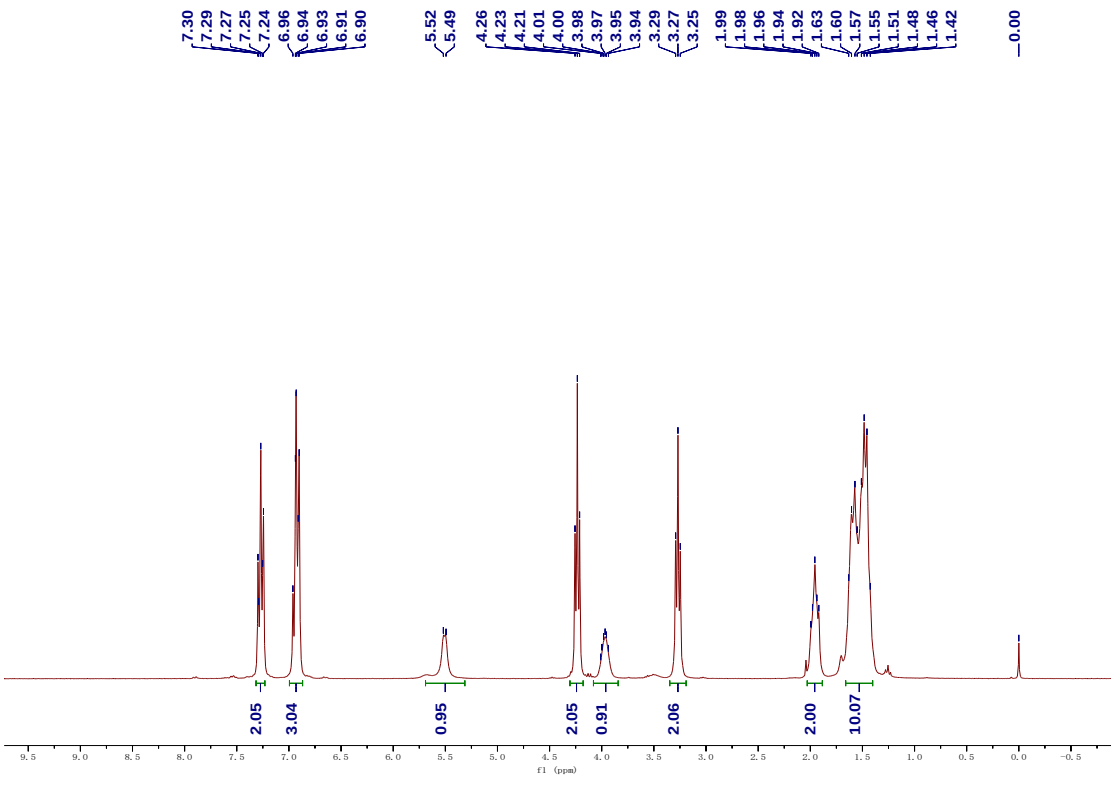


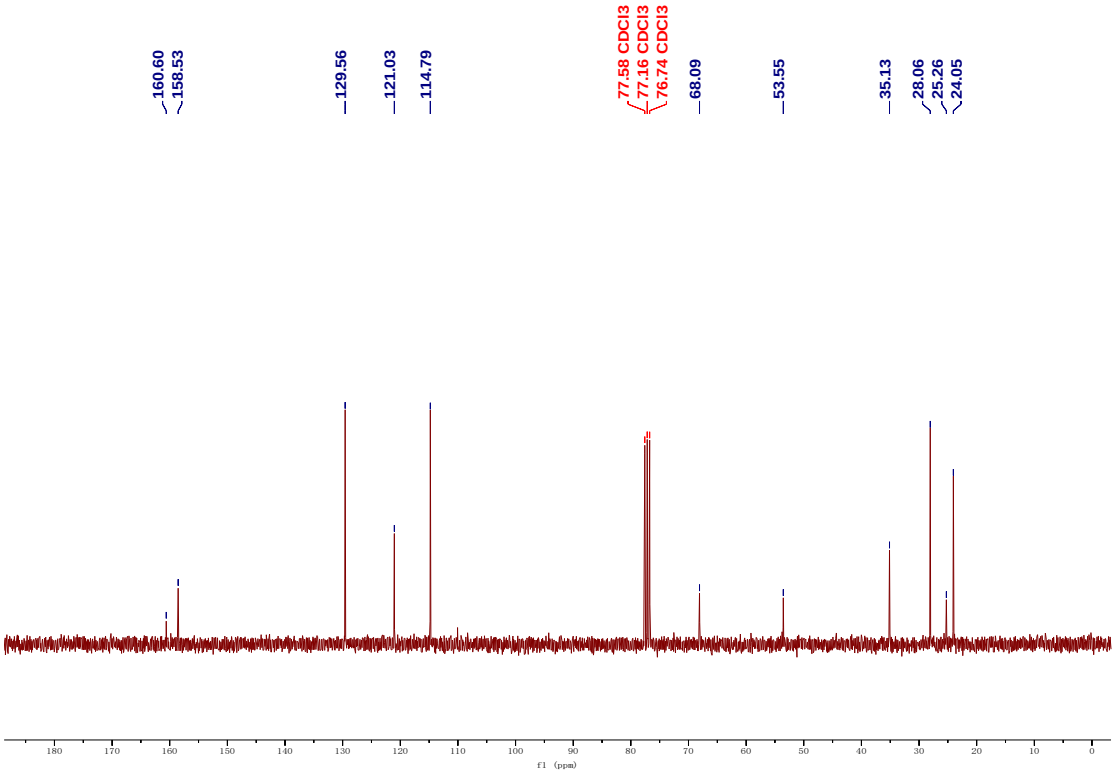


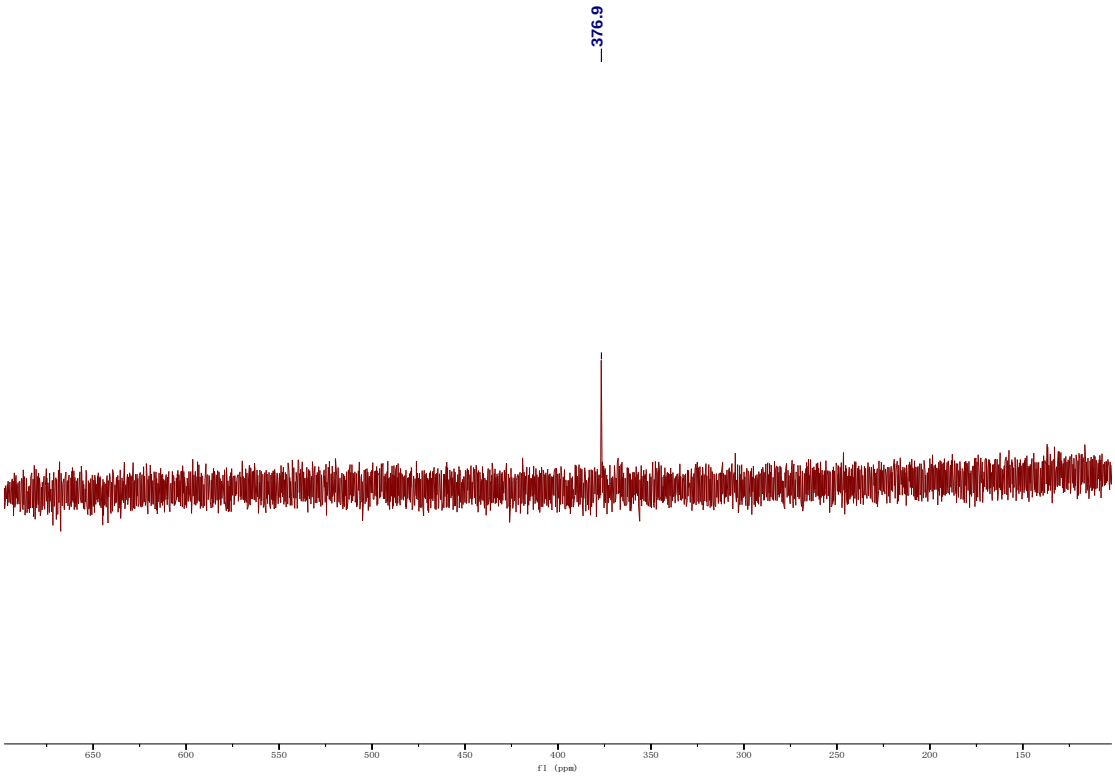

376.4
580 570 560 550 540 530 520 510 500 490 480 470 460 450 440 430 420 410 400 390 380 370 360
f1 (ppm)

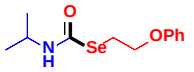

O
N
H
Se
OPh

3b


7.30 7.29 7.27 7.25 7.24 6.96 6.94 6.93 6.91 6.90
5.52 5.49
4.26 4.23 4.21 4.01 4.00 3.98 3.97 3.95 3.94
3.29 3.27 3.25
1.99 1.98 1.96 1.94 1.92 1.63 1.60 1.57 1.55 1.51 1.48 1.46 1.42
0.00
2.05 3.04 0.95 2.05 0.91 2.06 2.00 10.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


160.60
158.53
129.56
121.03
114.79
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
68.09
53.55
35.13
28.06
25.26
24.05
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


376.9
650 600 550 500 450 400 350 300 250 200 150
f1 (ppm)


O
N
H
Se
OPh

3c


7.30
7.29
7.27
7.25
7.25
6.96
6.96
6.94
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6.93
6.92
6.91
6.90
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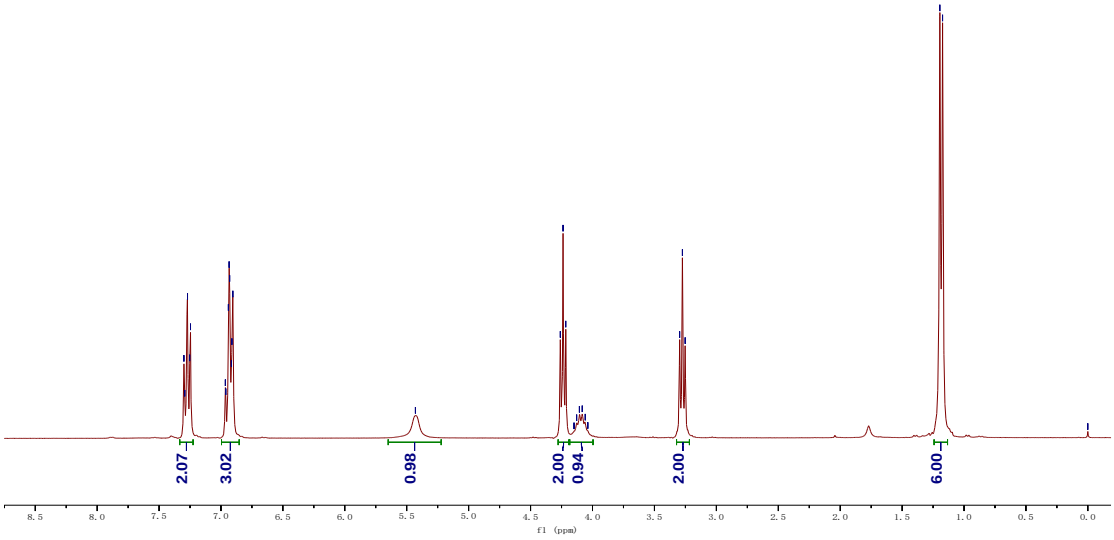
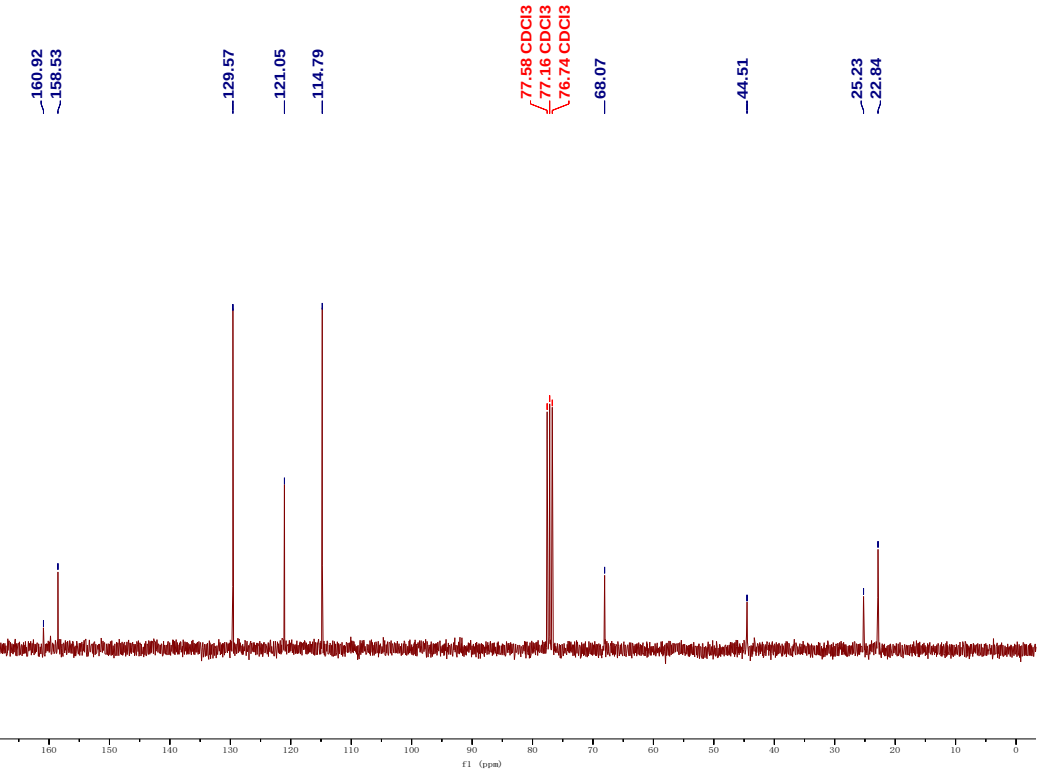
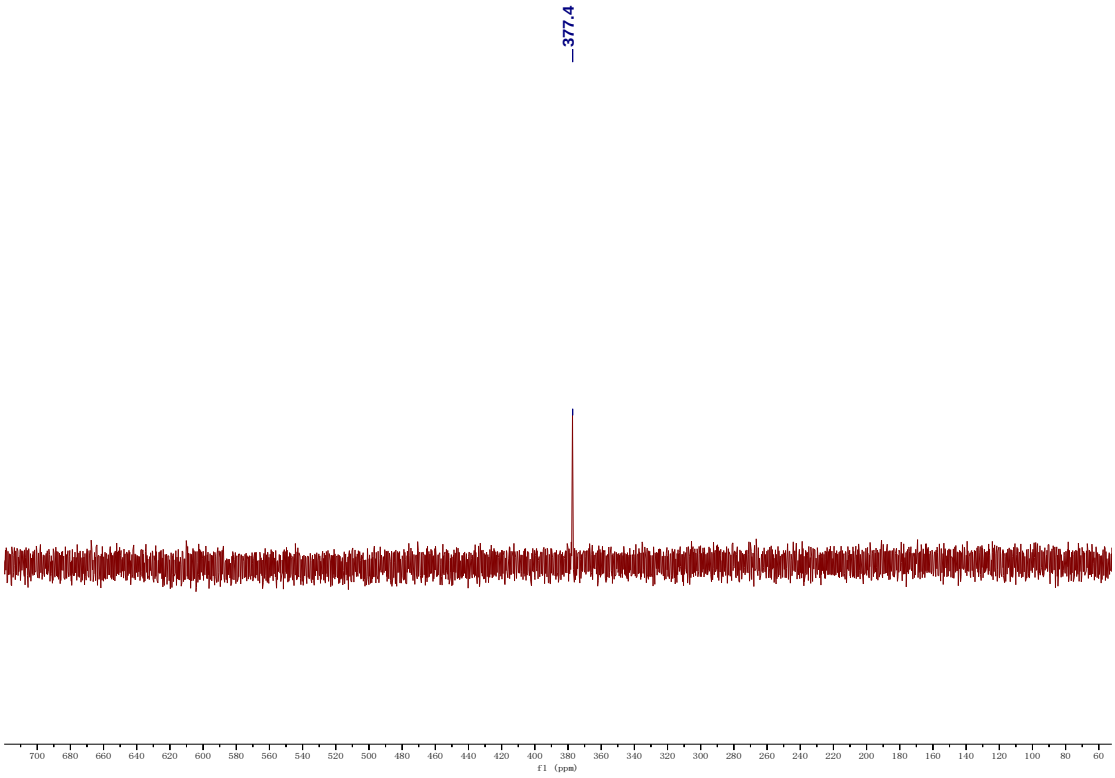
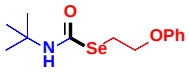
4.15
4.13
4.11
4.08
4.06
4.04
3.30
3.27
3.25
1.20
1.17
0.00

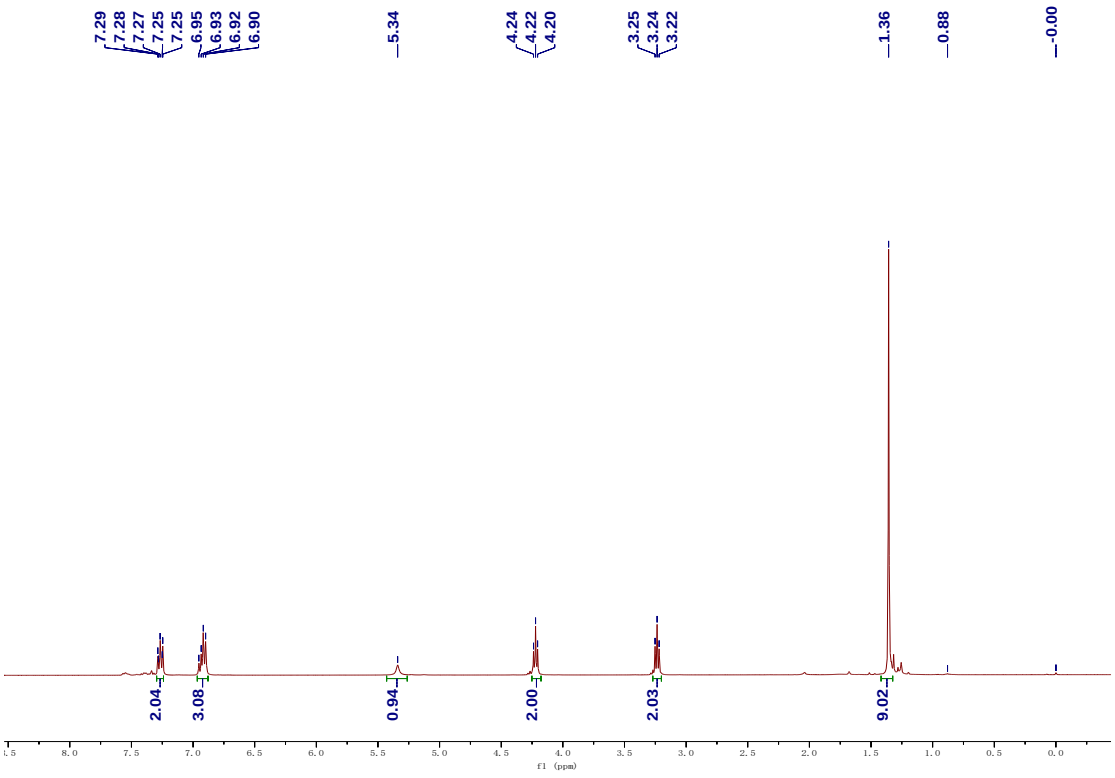

2.07
3.02
0.98
2.00
0.94
2.00
6.00
f1 (ppm)

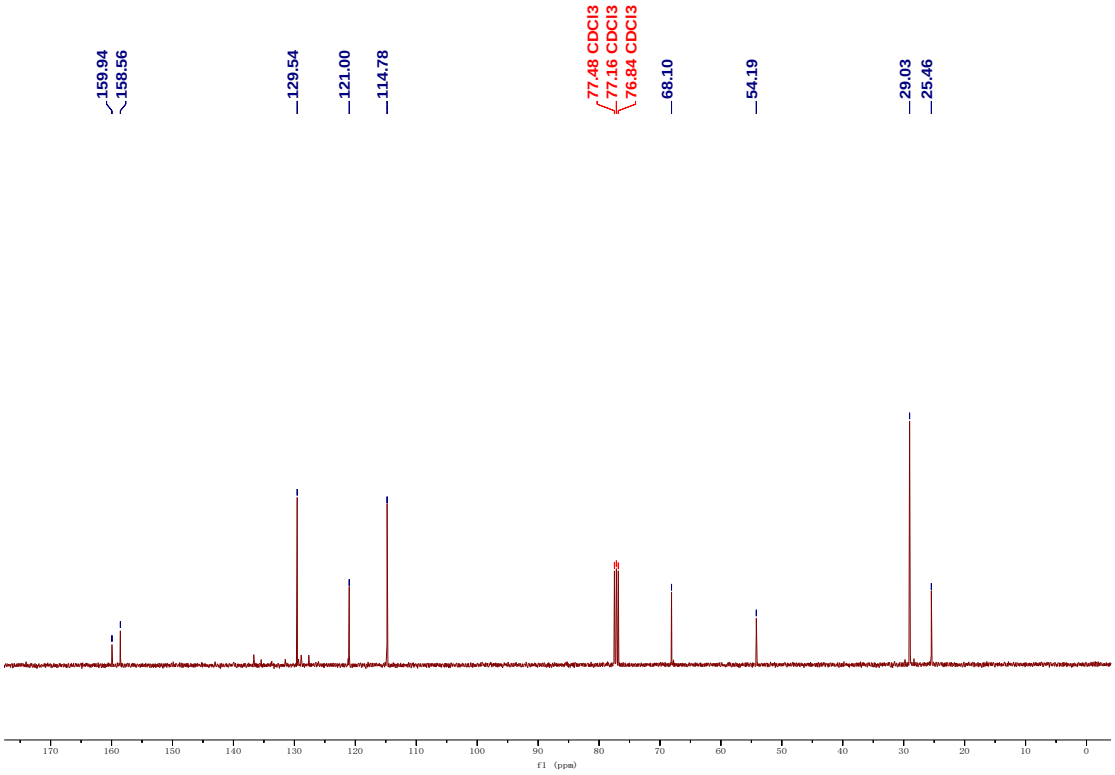

160.92
158.53
129.57
121.05
114.79
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
68.07
44.51
25.23
22.84
f1 (ppm)

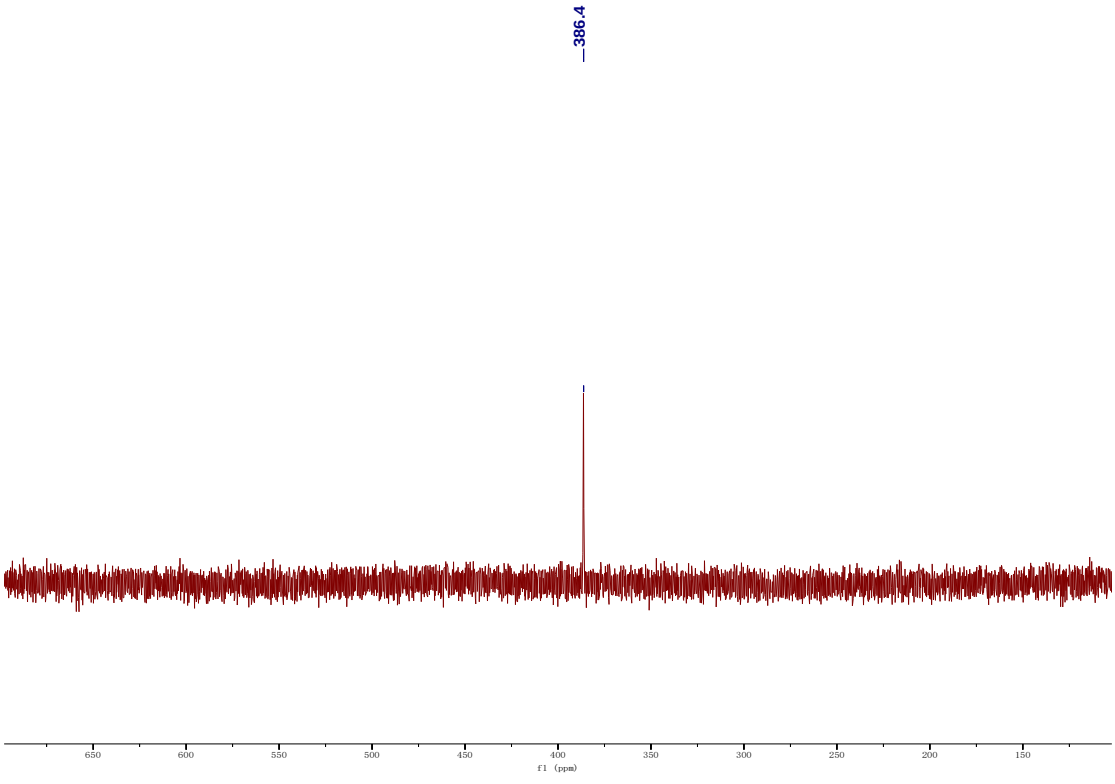

377.4
700 680 660 640 620 600 580 560 540 520 500 480 460 440 420 400 380 360 340 320 300 280 260 240 220 200 180 160 140 120 100 80 60
f1 (ppm)

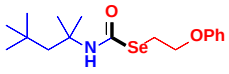

O
N
H
Se
OPh

3d


7.29
7.28
7.27
7.25
7.25
6.95
6.93
6.92
6.90
5.34
4.24
4.22
4.20
3.25
3.24
3.22
1.36
0.88
0.00
2.04
3.08
0.94
2.00
2.03
9.02
f1 (ppm)

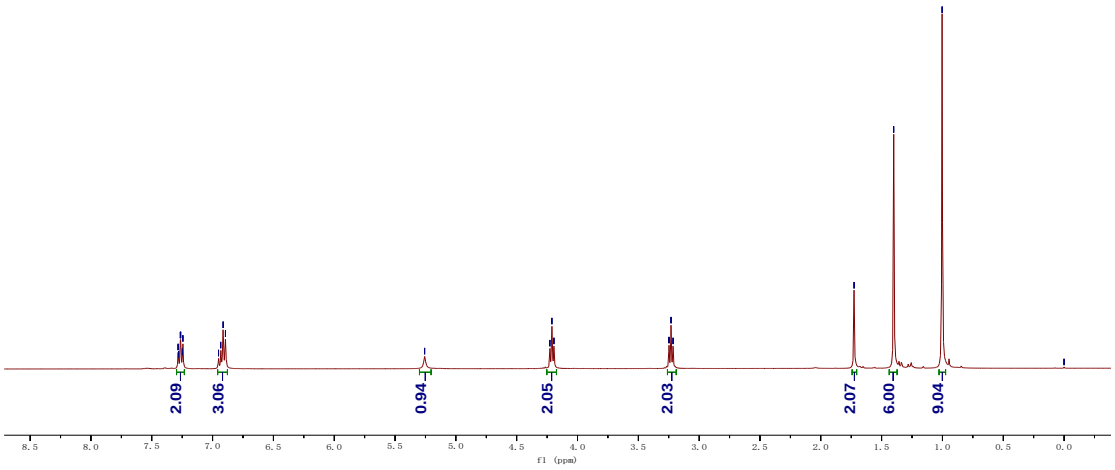

159.94
158.56
129.54
121.00
114.78
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
68.10
54.19
29.03
25.46
f1 (ppm)


386.4
f1 (ppm)

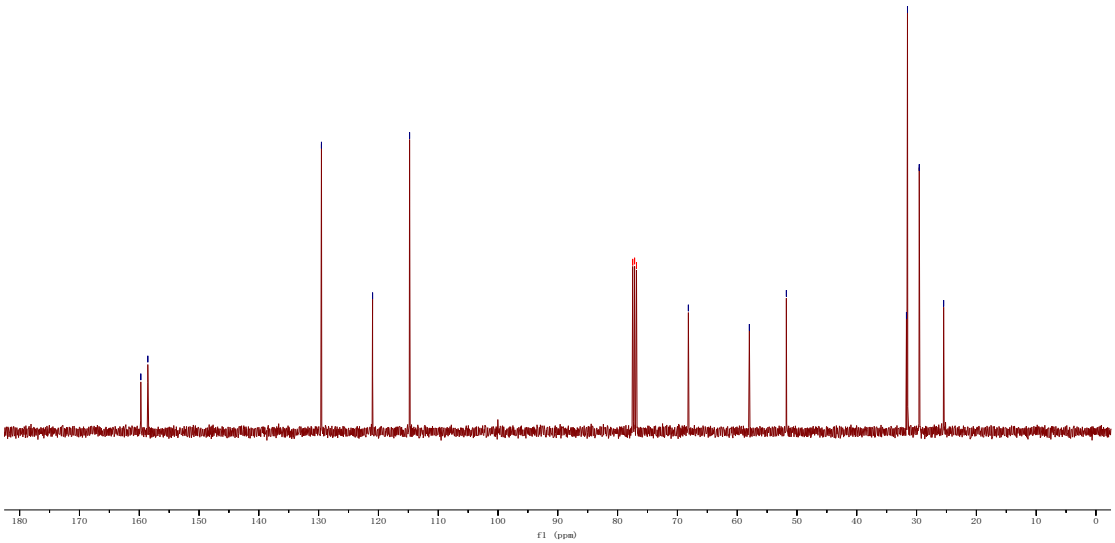

O
N
H
Se
OPh

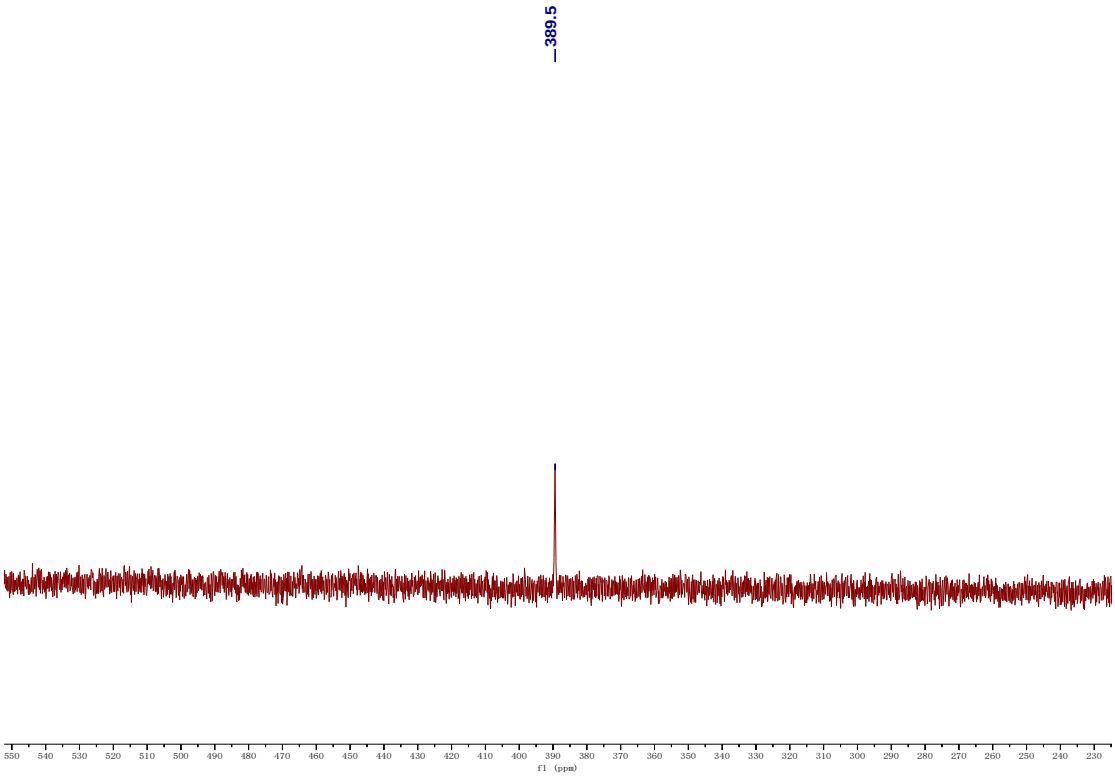
3e

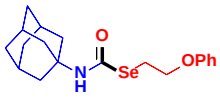

7.28
7.28
7.27
7.26
7.25
7.24
6.95
6.93
6.91
6.89
5.26
4.23
4.21
4.19
3.25
3.23
3.21
1.73
1.40
1.00
0.00


2.09
3.06
0.94
2.05
2.03
2.07
6.00
9.04
f1 (ppm)


159.74
158.57
129.53
120.98
114.79
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
68.16
57.96
51.78
31.69
31.52
29.55
25.47

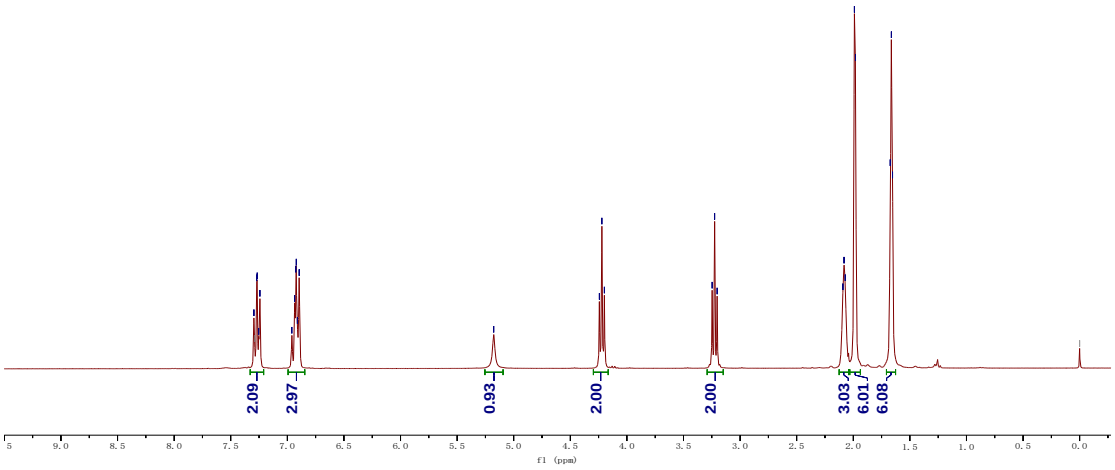

f1 (ppm)

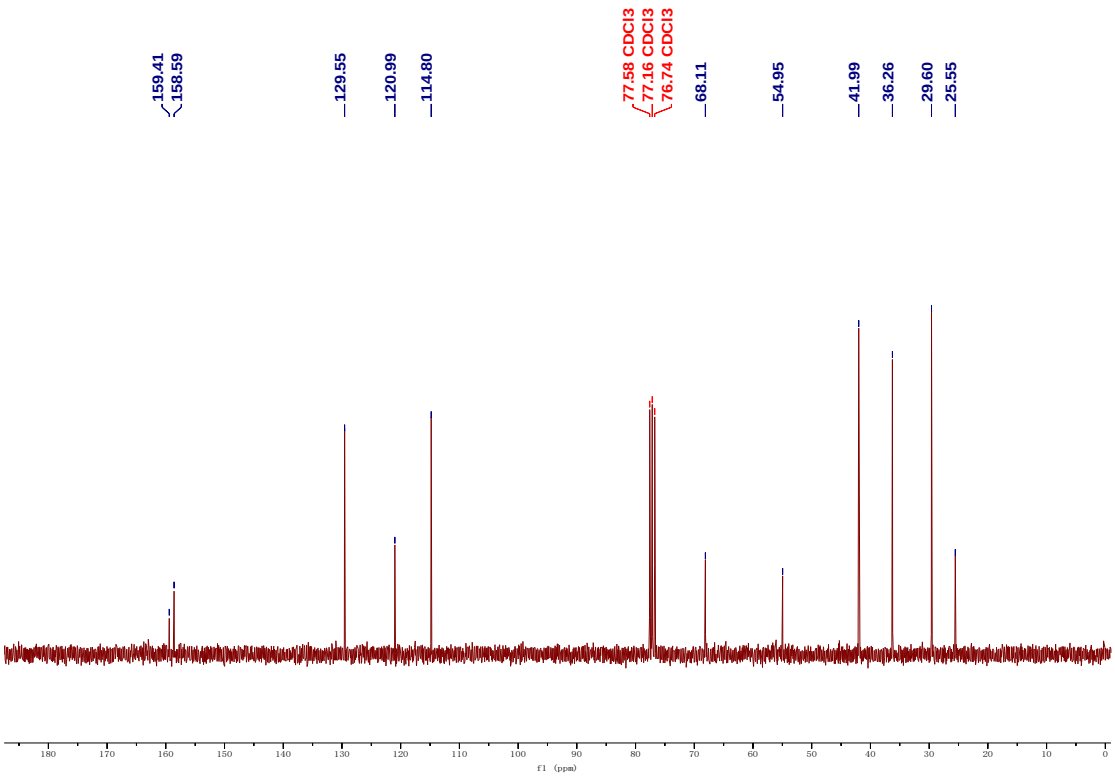

389.5
550 540 530 520 510 500 490 480 470 460 450 440 430 420 410 400 390 380 370 360 350 340 330 320 310 300 290 280 270 260 250 240 230
f1 (ppm)

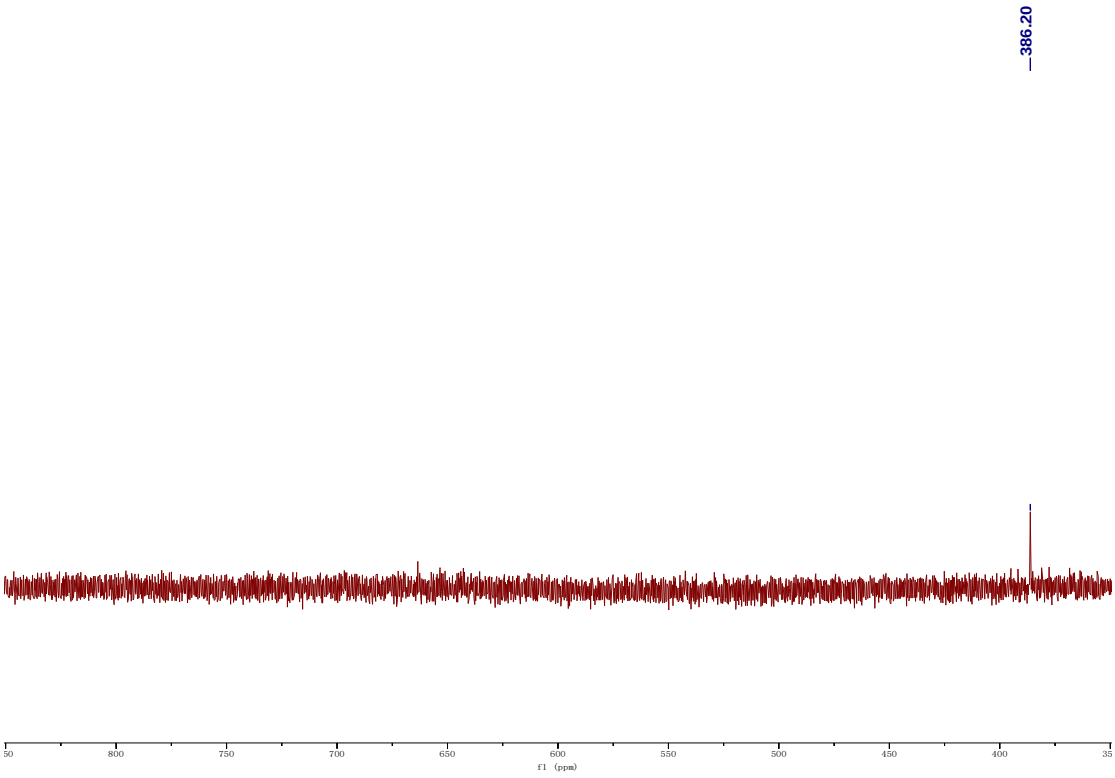

O
N
H
Se
OPh

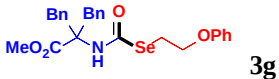
3f


7.30
7.29
7.27
7.27
7.25
7.24
6.96
6.94
6.93
6.92
6.91
6.90
5.18
4.24
4.22
4.20
3.25
3.23
3.20
2.09
2.08
2.07
1.99
1.98
1.67
1.66
1.65
0.00


2.09
2.97
0.93
2.00
2.00
3.03
6.01
6.08
f1 (ppm)


159.41
158.59
129.55
120.99
114.80
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
68.11
54.95
41.99
36.26
29.60
25.55
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


386.20
50 800 750 700 650 600 550 500 450 400 35
f1 (ppm)


Bn
Bn
O
MeO2C
N
H
Se
OPh

3g


7.30
7.28
7.28
7.26
7.25
7.22
7.20
7.20
7.19
7.18
7.17
7.17
7.08
7.07
7.07
7.06
7.05
6.97
6.97
6.95
6.94
6.94
6.93
6.92
6.91
6.91
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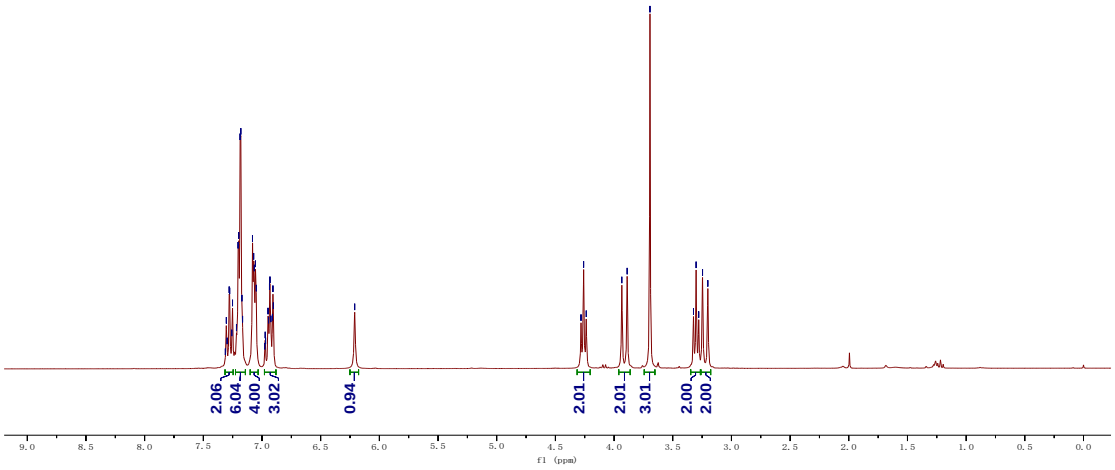
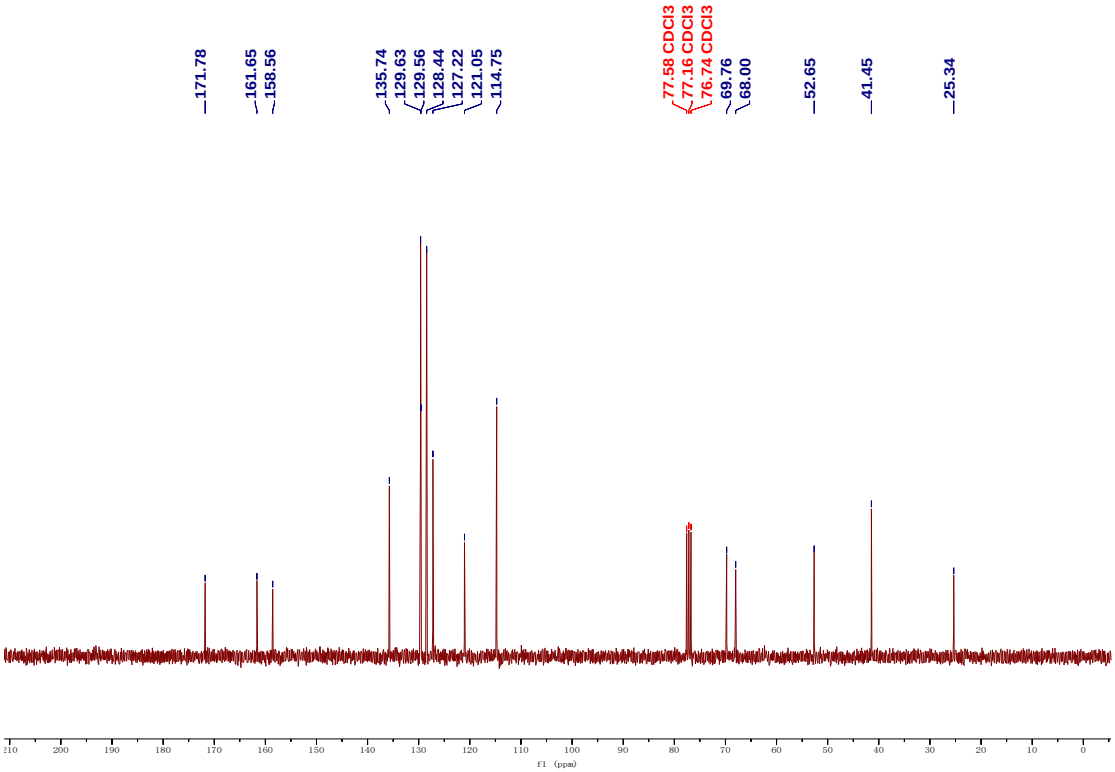
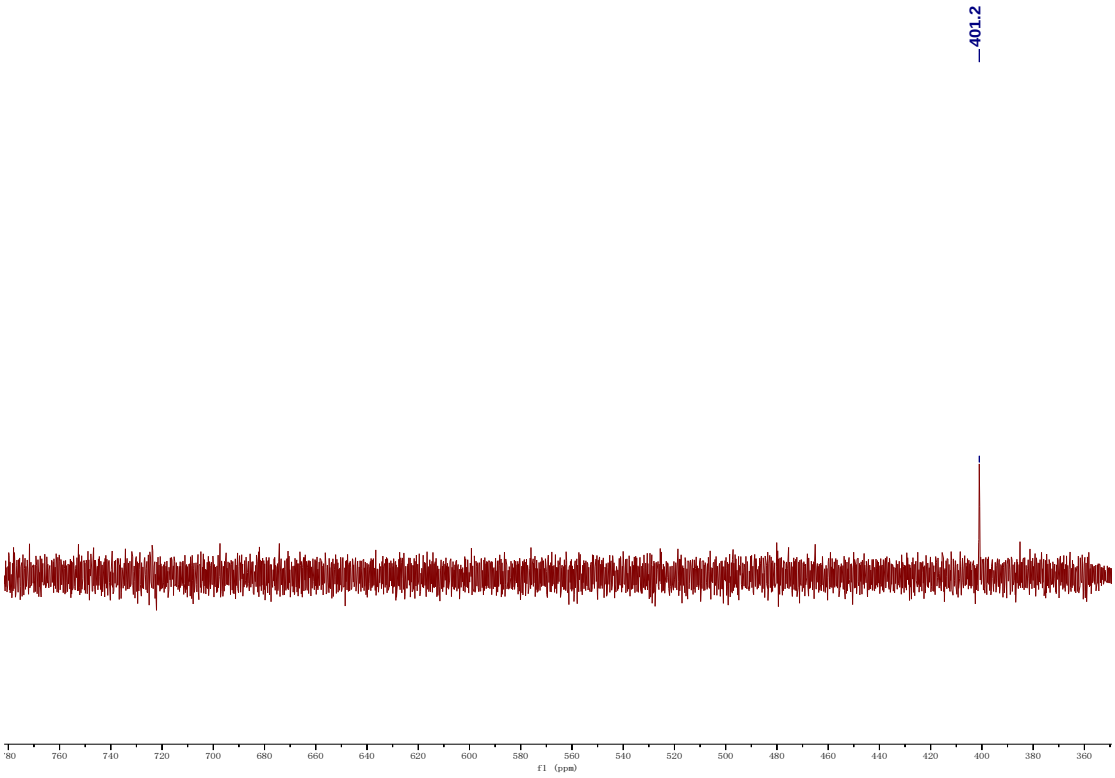
3.89
3.32
3.30
3.28
3.25
3.20

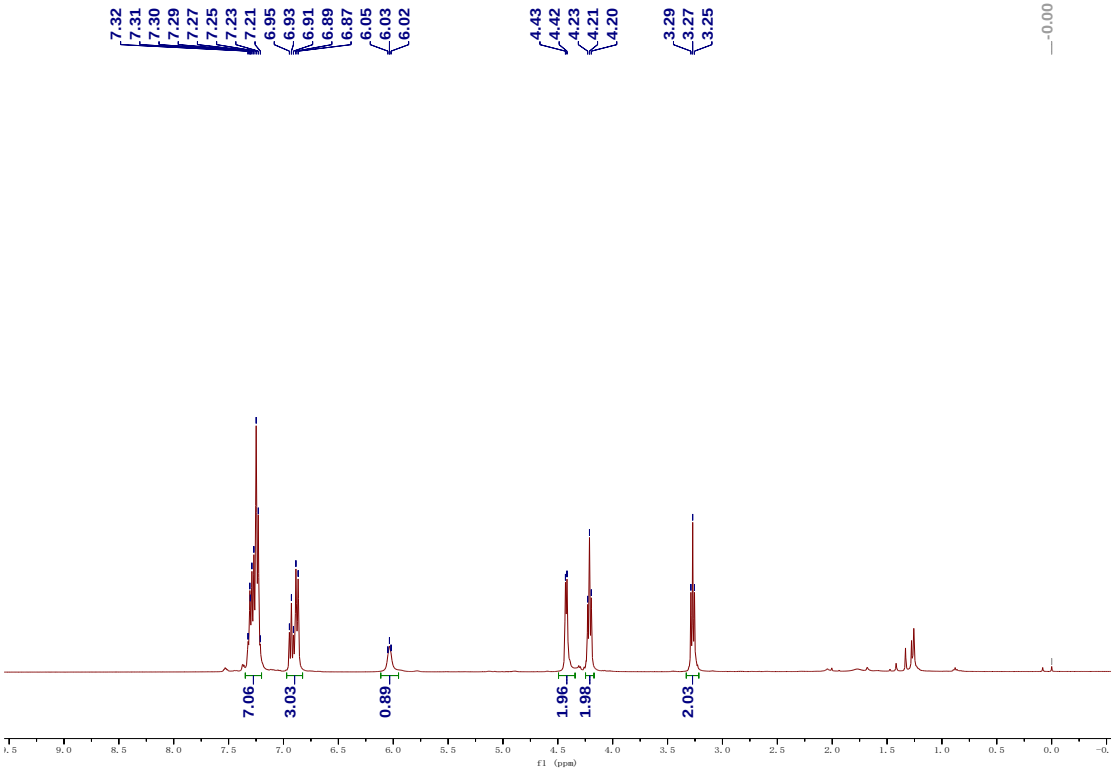

2.06
6.04
4.00
3.02
0.94
2.01
2.01
3.01
2.00
2.00
f1 (ppm)

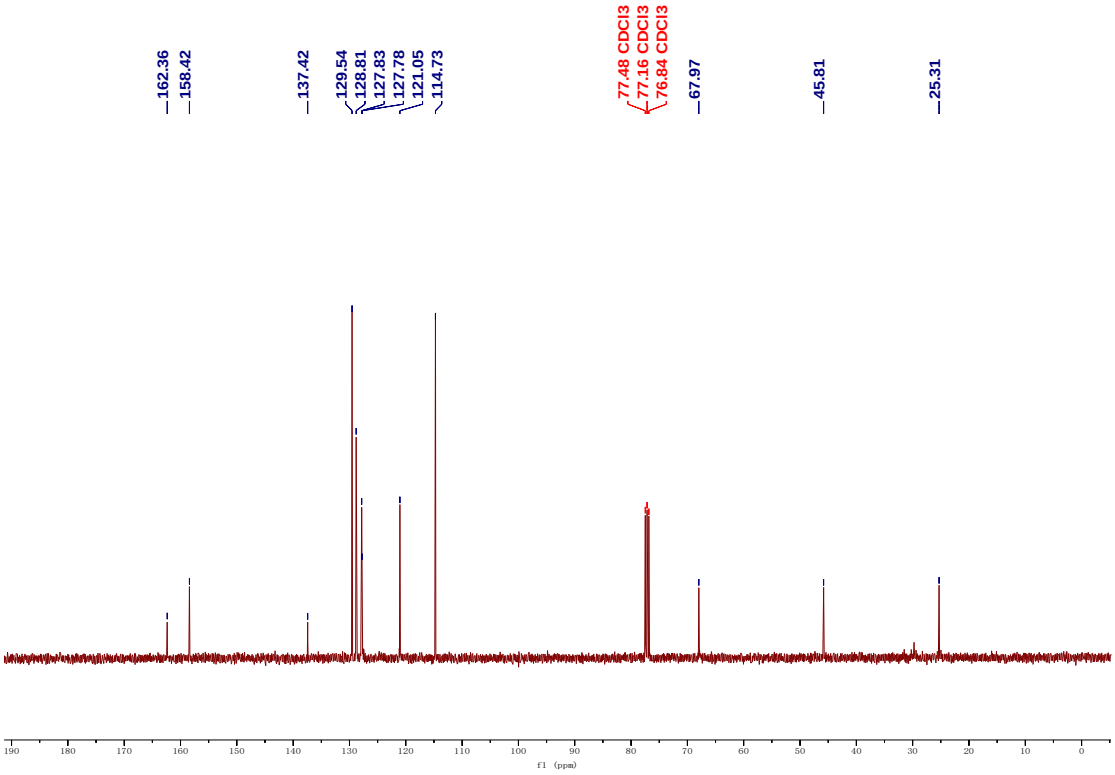

171.78
161.65
158.56
135.74
129.63
129.56
128.44
127.22
121.05
114.75
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
69.76
68.00
52.65
41.45
25.34
f1 (ppm)

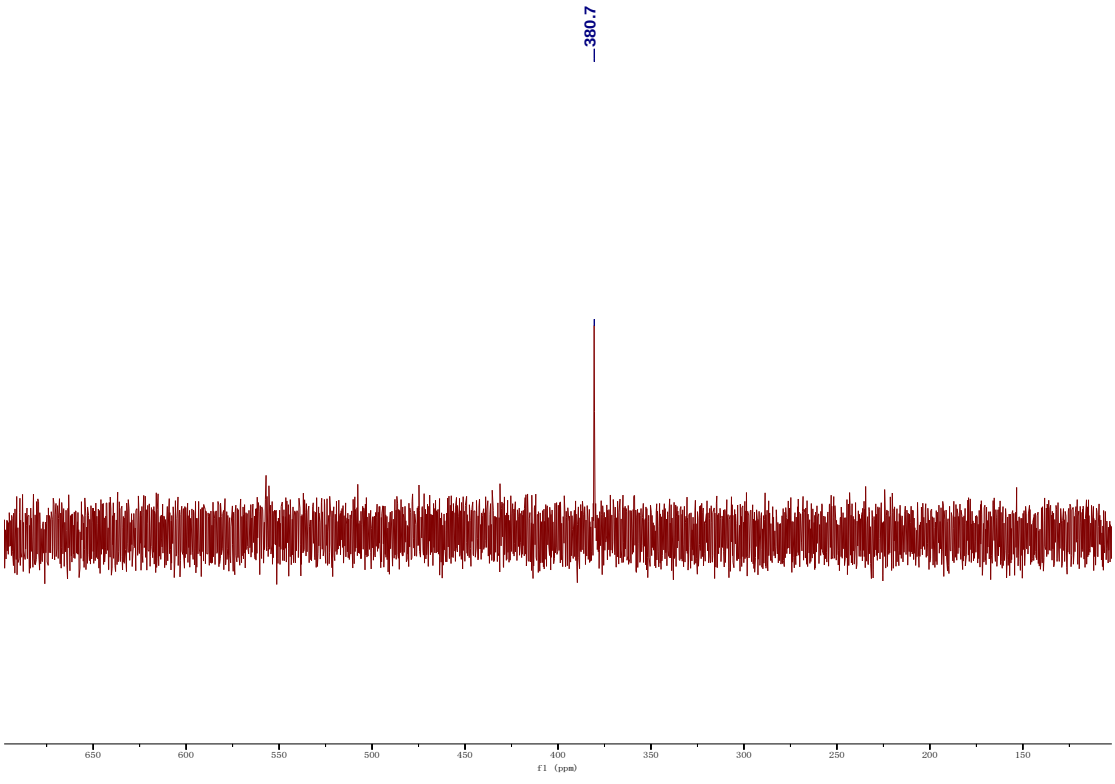

401.2
f1 (ppm)

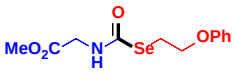

O
Ph
N
H
Se
OPh

3h

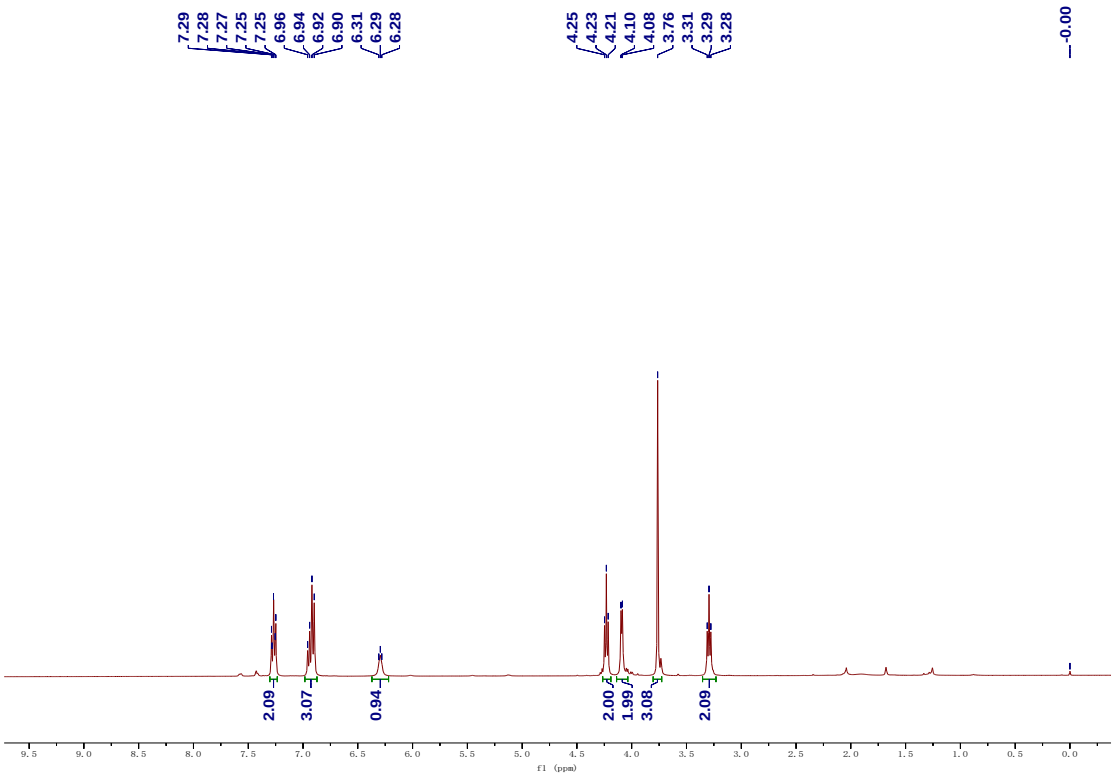

7.32
7.31
7.30
7.29
7.27
7.25
7.23
7.21
6.95
6.93
6.91
6.89
6.87
6.05
6.03
6.02
4.43
4.42
4.23
4.21
4.20
3.29
3.27
3.25
0.00
7.06
3.03
0.89
1.96
1.98
2.03
f1 (ppm)

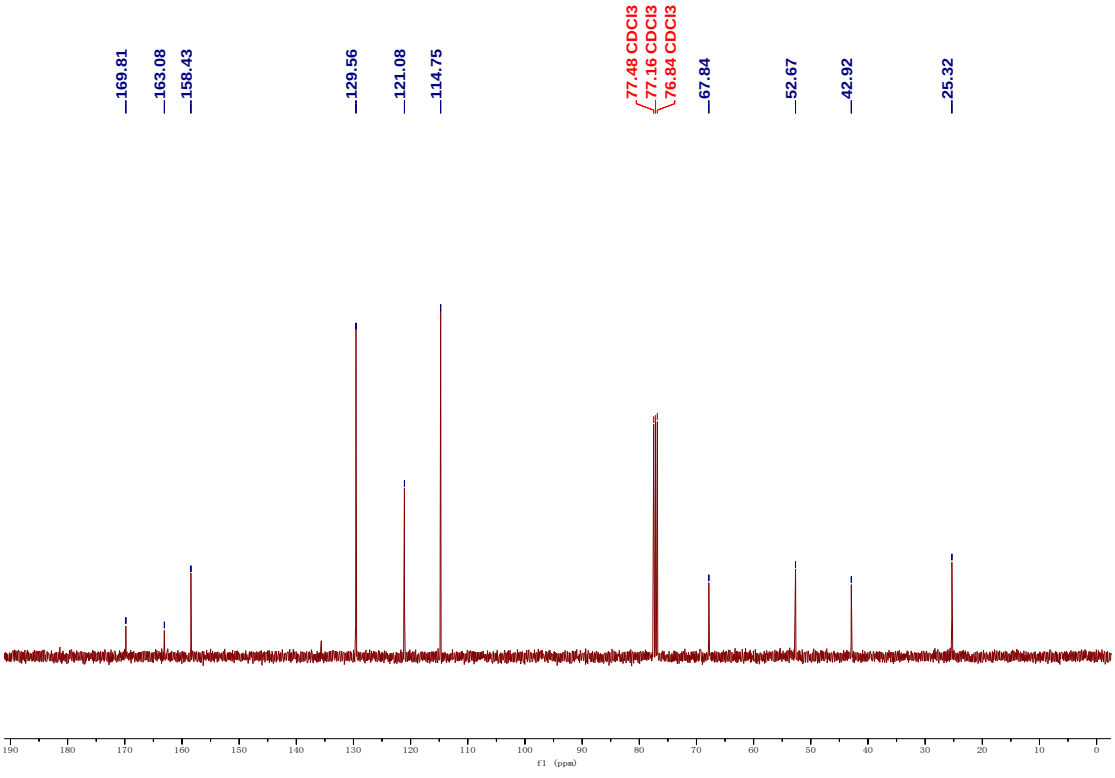

162.36
158.42
137.42
129.54
128.81
127.83
127.78
121.05
114.73
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
67.97
45.81
25.31
f1 (ppm)

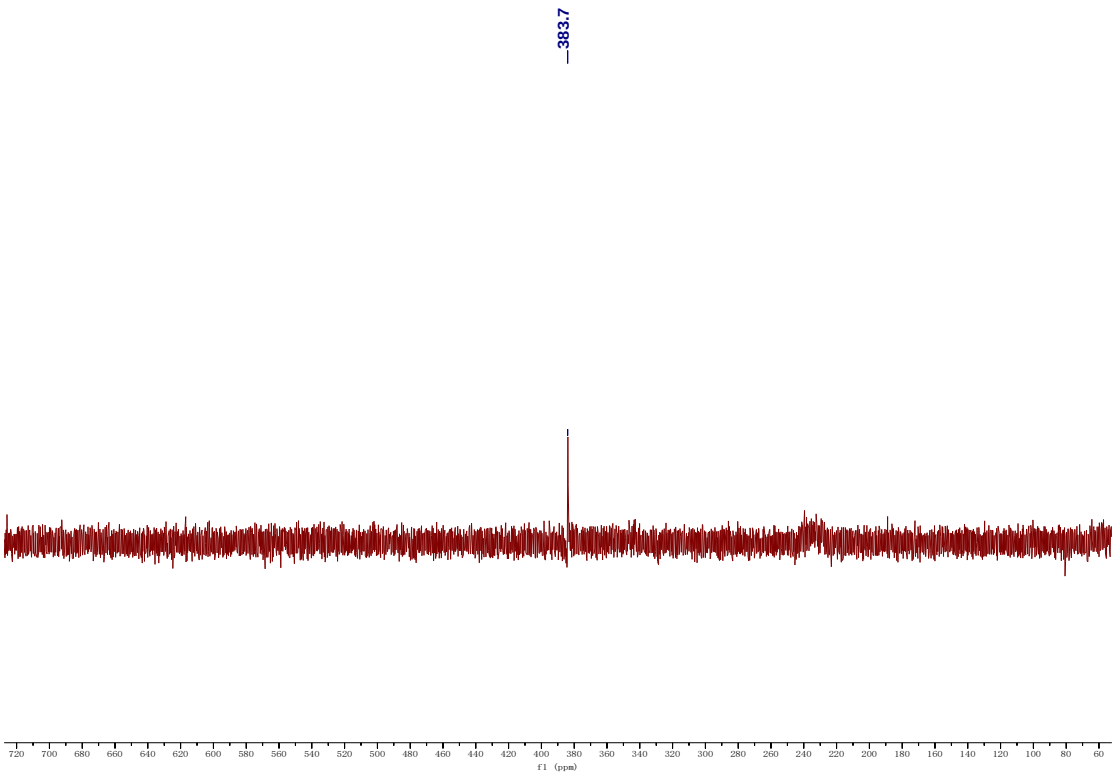

380.7
f1 (ppm)

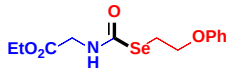

O
MeO2C
N
H
Se
OPh

3i

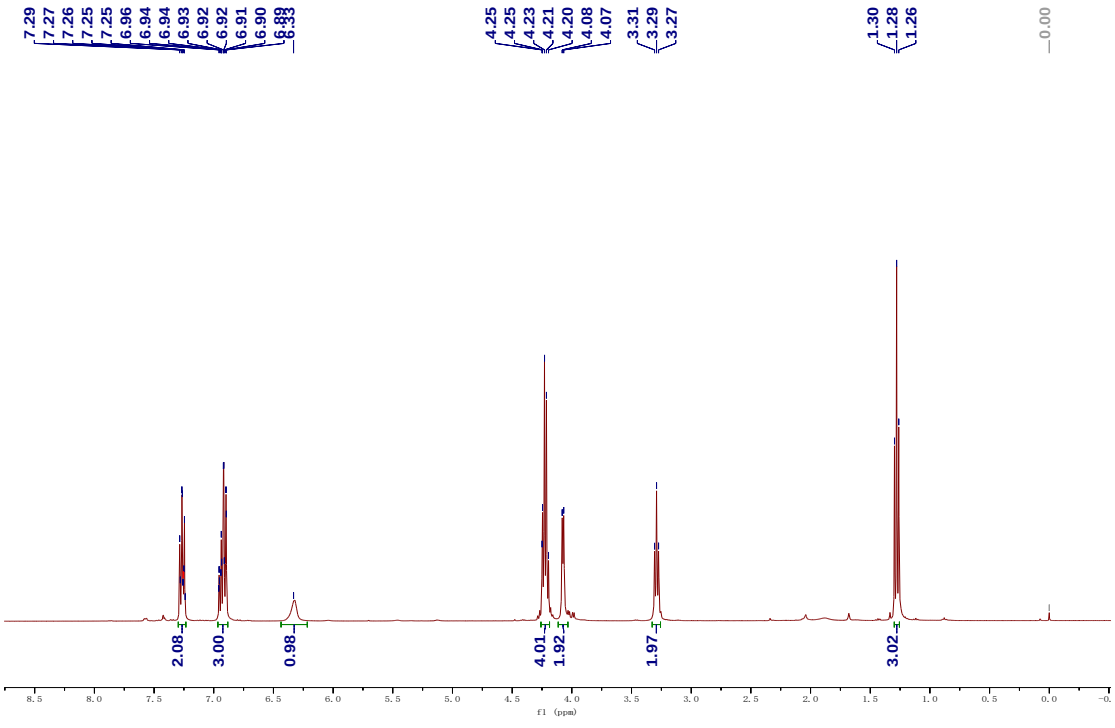

7.29
7.28
7.27
7.25
7.25
6.96
6.94
6.92
6.90
6.31
6.29
6.28
4.25
4.23
4.21
4.10
4.08
3.76
3.31
3.29
3.28
0.00
2.09
3.07
0.94
2.00
1.99
3.08
2.09
f1 (ppm)

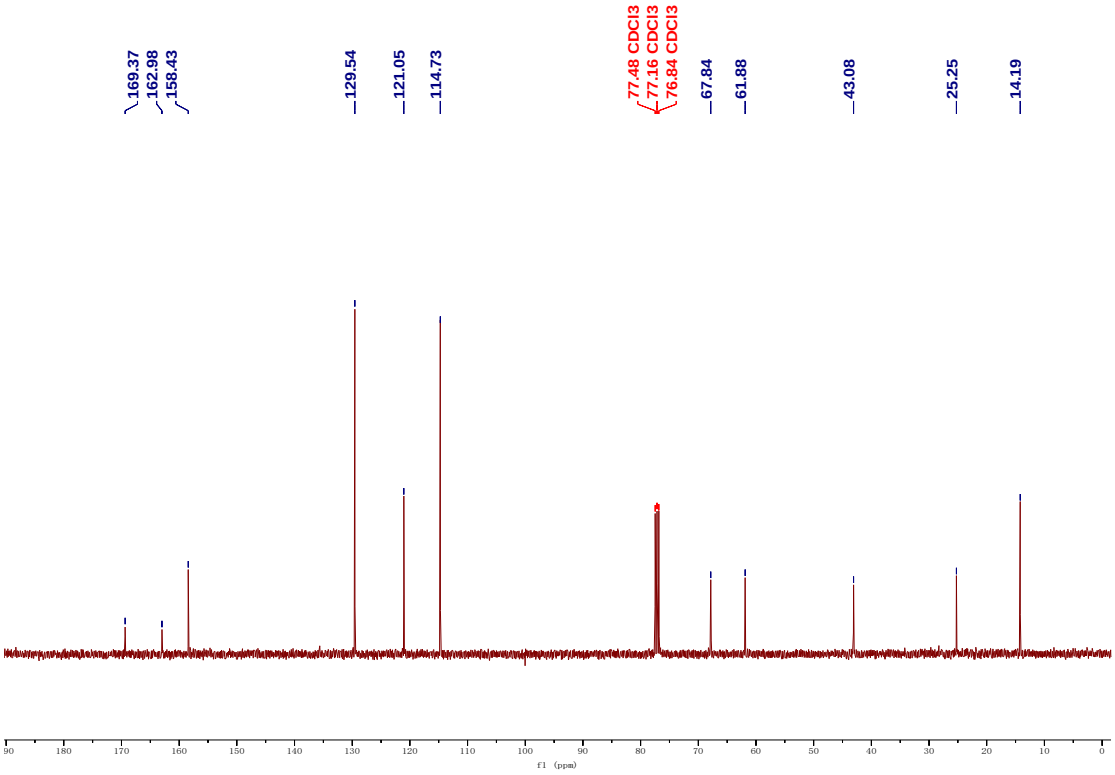

169.81
163.08
158.43
129.56
121.08
114.75
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
67.84
52.67
42.92
25.32
f1 (ppm)

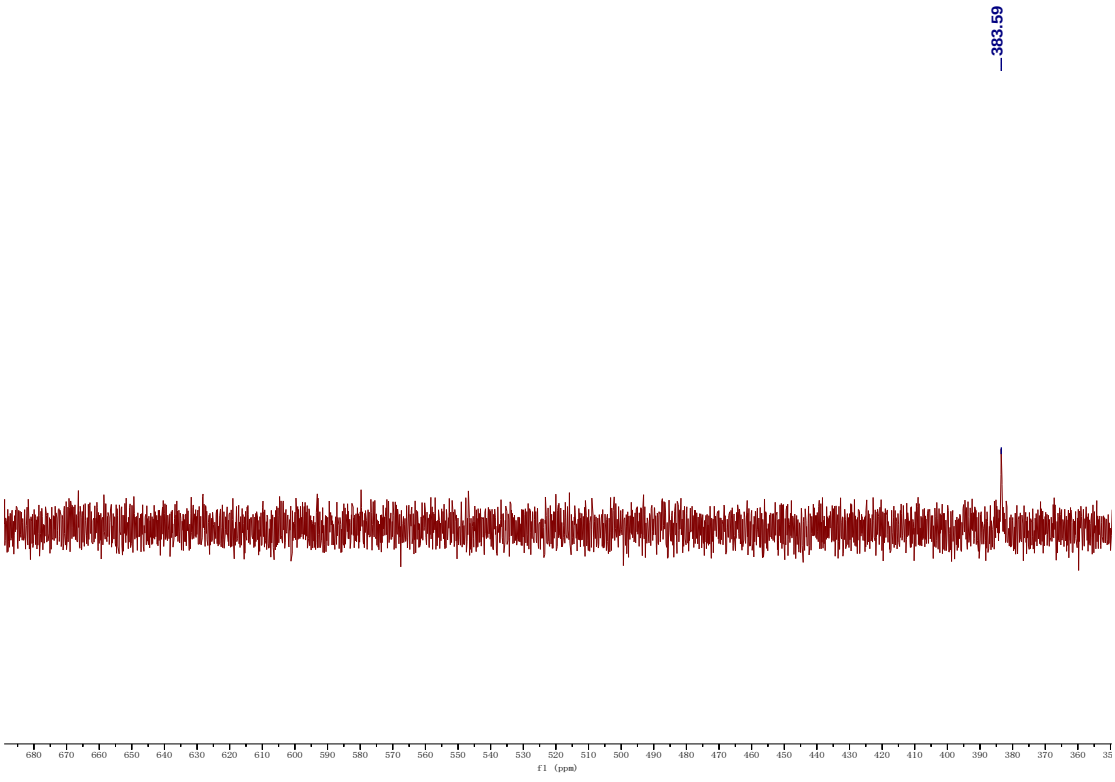

383.7
720 700 680 660 640 620 600 580 560 540 520 500 480 460 440 420 400 380 360 340 320 300 280 260 240 220 200 180 160 140 120 100 80 60
f1 (ppm)

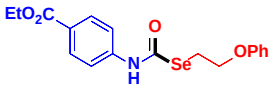

O
EtO2C
N
H
Se
OPh

3j

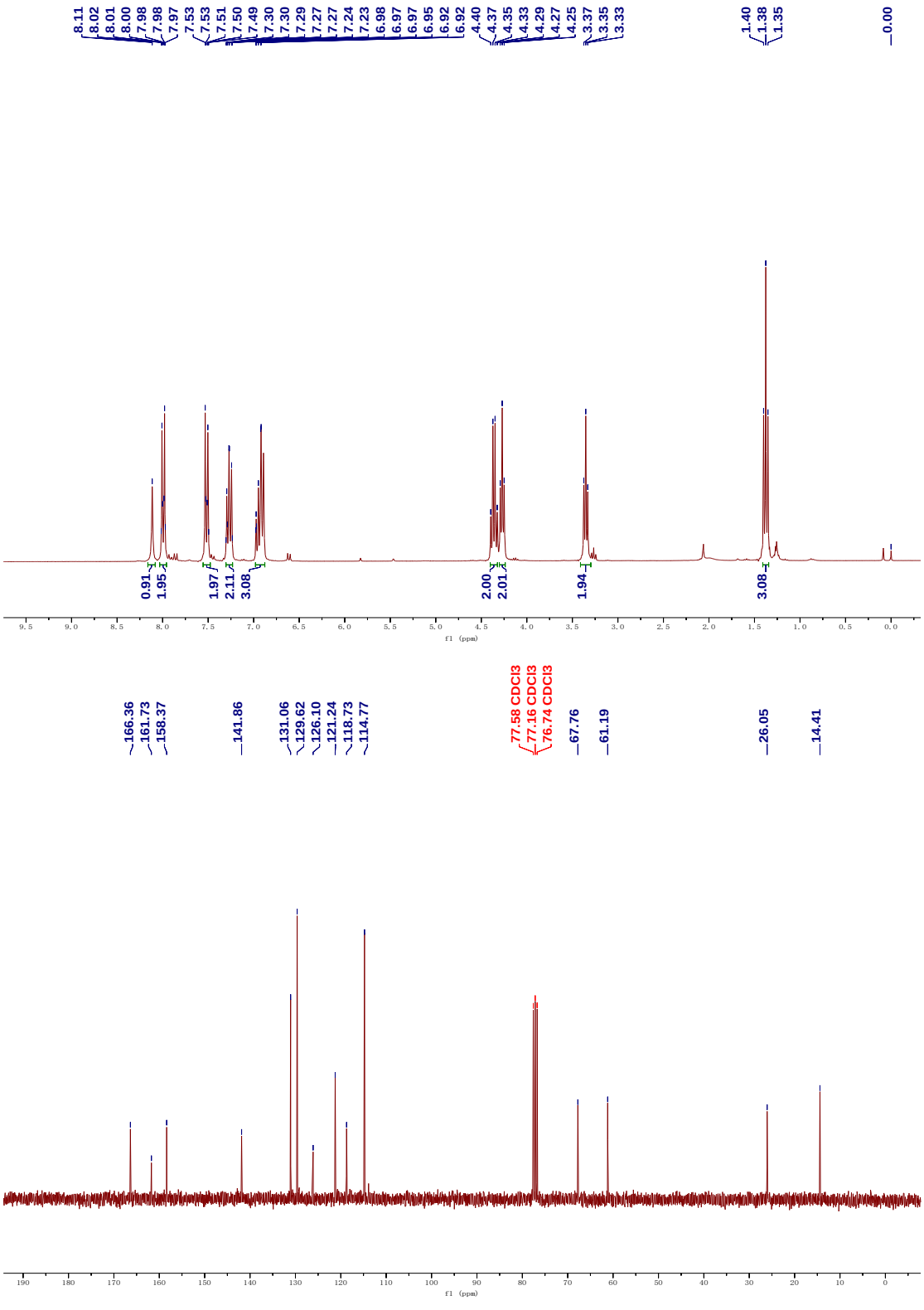

7.29
7.27
7.26
7.25
7.25
6.96
6.94
6.93
6.92
6.92
6.91
6.90
6.89
6.88
4.25
4.25
4.23
4.21
4.20
4.08
4.07
3.31
3.29
3.27
1.30
1.28
1.26
0.00
2.08
3.00
0.98
4.01
1.92
1.97
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

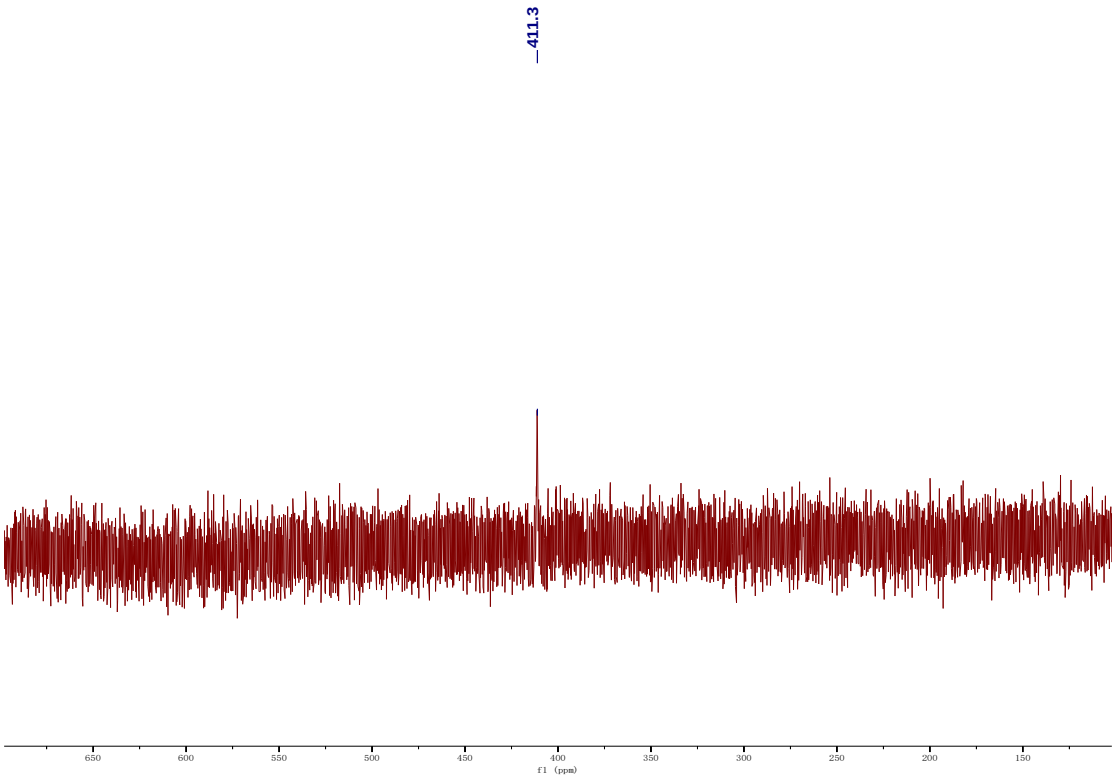

169.37
162.98
158.43
129.54
121.05
114.73
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
67.84
61.88
43.08
25.25
14.19
f1 (ppm)

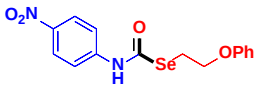

383.59
f1 (ppm)


EtO2C
O
N
H
Se
OPh

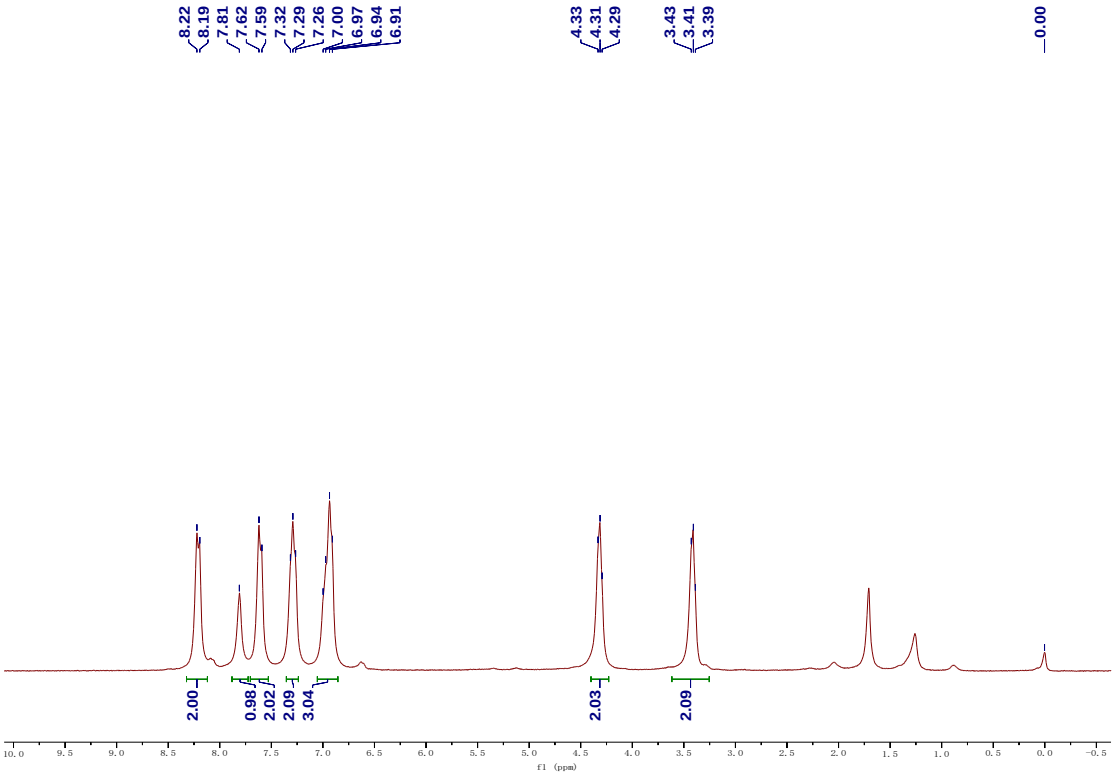
3k

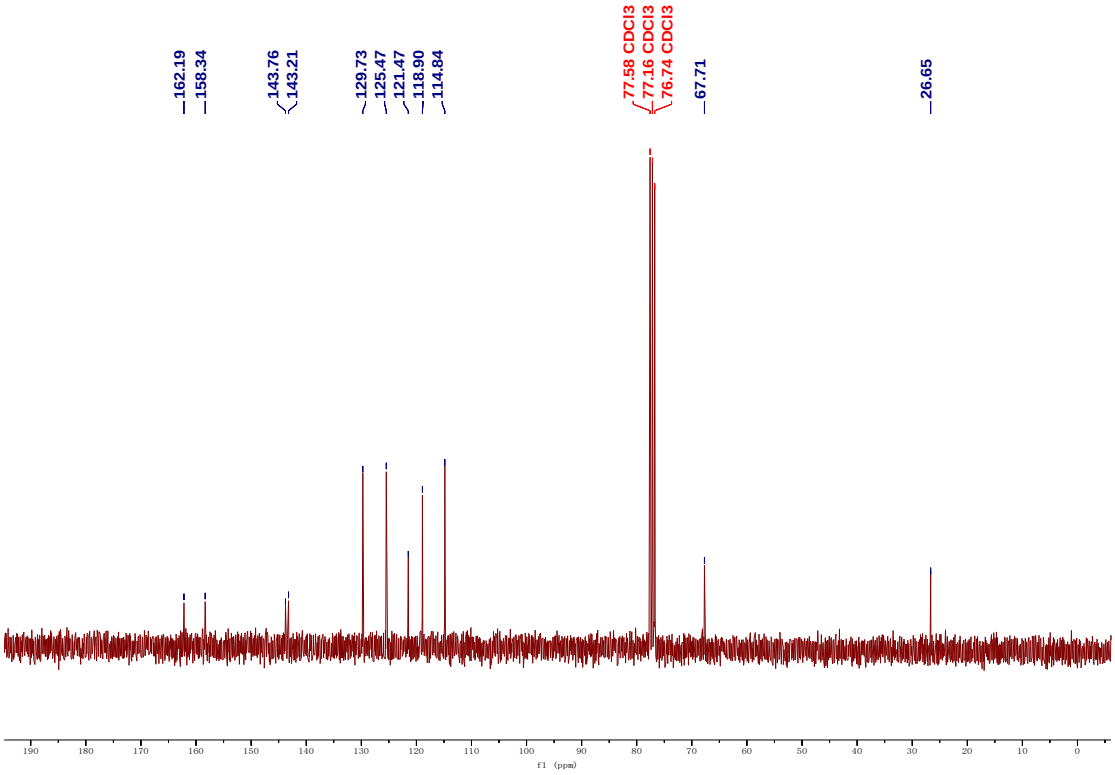

8.11
8.02
8.01
8.00
7.98
7.98
7.97
7.53
7.53
7.51
7.50
7.49
7.30
7.30
7.29
7.27
7.27
7.24
7.23
6.98
6.97
6.97
6.95
6.92
6.92
4.40
4.37
4.35
4.33
4.29
4.27
4.25
3.37
3.35
3.33
1.40
1.38
1.35
0.00
0.91
1.95
1.97
2.11
3.08
2.00
2.01
1.94
3.08
f1 (ppm)
166.36
161.73
158.37
141.86
131.06
129.62
126.10
121.24
118.73
114.77
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
67.76
61.19
26.05
14.41
f1 (ppm)

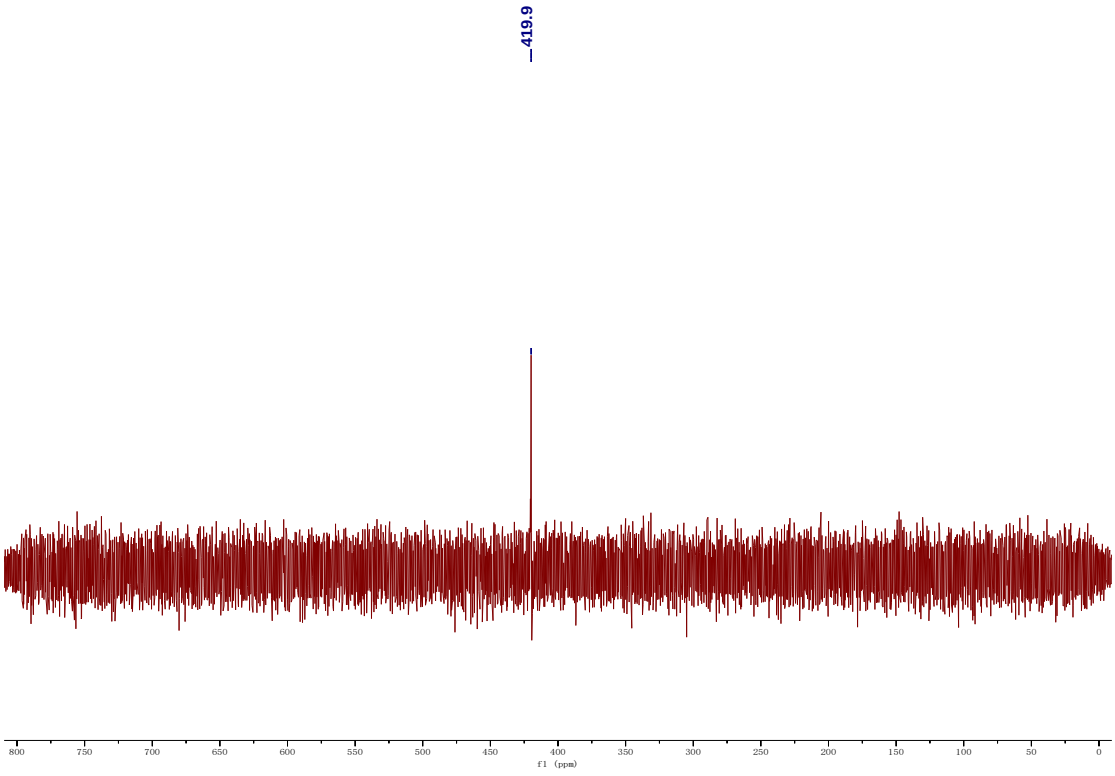

411.3
650
600
550
500
450
400
350
300
250
200
150
f1 (ppm)

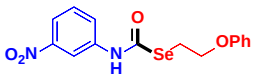

O2N
O
N
H
Se
OPh

3l

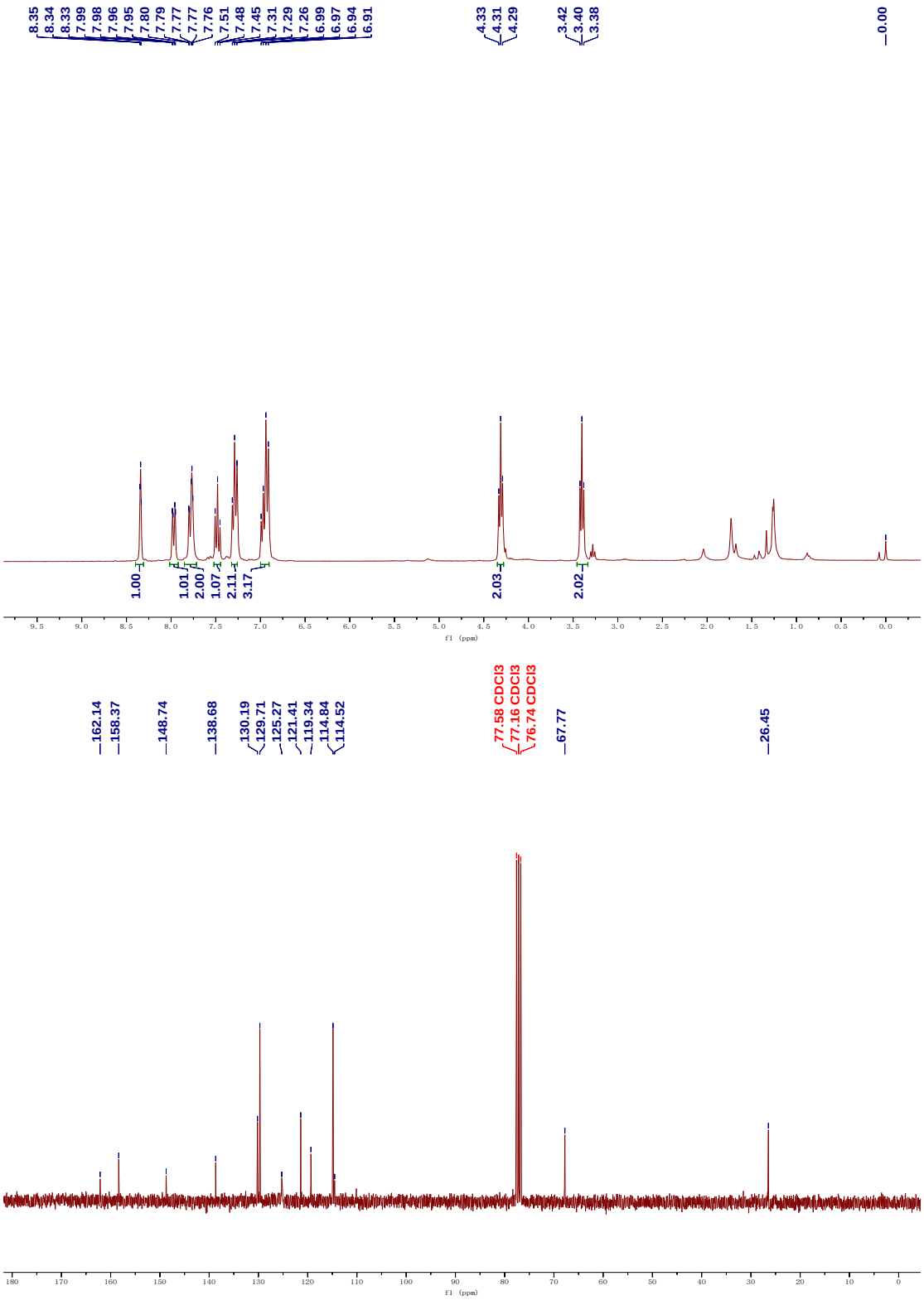

8.22
8.19
7.81
7.62
7.59
7.32
7.29
7.26
7.00
6.97
6.94
6.91
4.33
4.31
4.29
3.43
3.41
3.39
0.00
2.00
0.98
2.02
2.09
3.04
2.03
2.09
f1 (ppm)

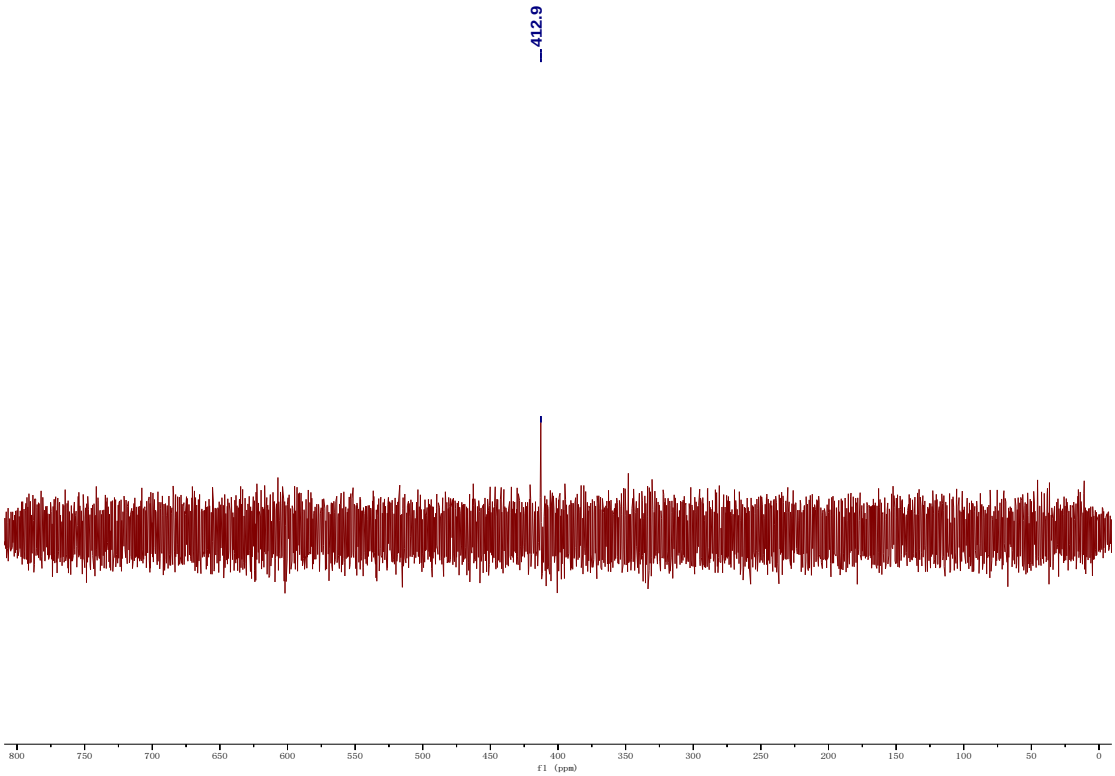

162.19
158.34
143.76
143.21
129.73
125.47
121.47
118.90
114.84
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
67.71
26.65
f1 (ppm)

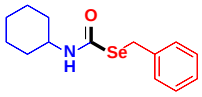

419.9
f1 (ppm)


O
O2N
N
H
Se
OPh

3m

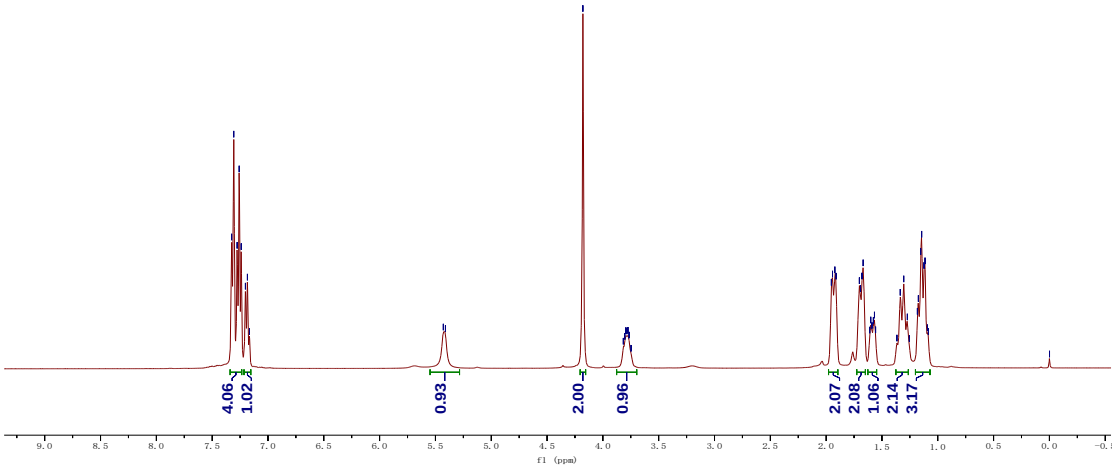

8.35
8.34
8.33
7.99
7.98
7.96
7.95
7.80
7.79
7.77
7.77
7.76
7.51
7.48
7.45
7.31
7.29
7.26
6.99
6.97
6.94
6.91
4.33
4.31
4.29
3.42
3.40
3.38
0.00
1.00
1.01
2.00
1.07
2.11
3.17
2.03
2.02
f1 (ppm)
162.14
158.37
148.74
138.68
130.19
129.71
125.27
121.41
119.34
114.84
114.52
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
67.77
26.45
f1 (ppm)

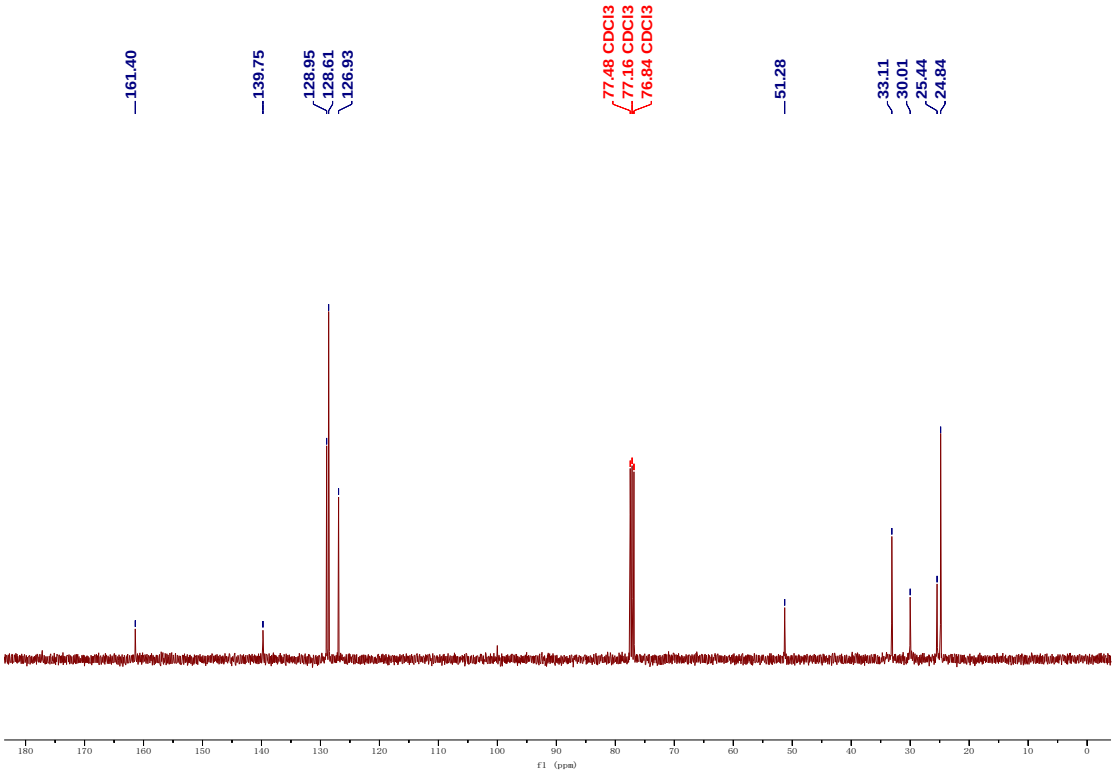

412.9
800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0
f1 (ppm)

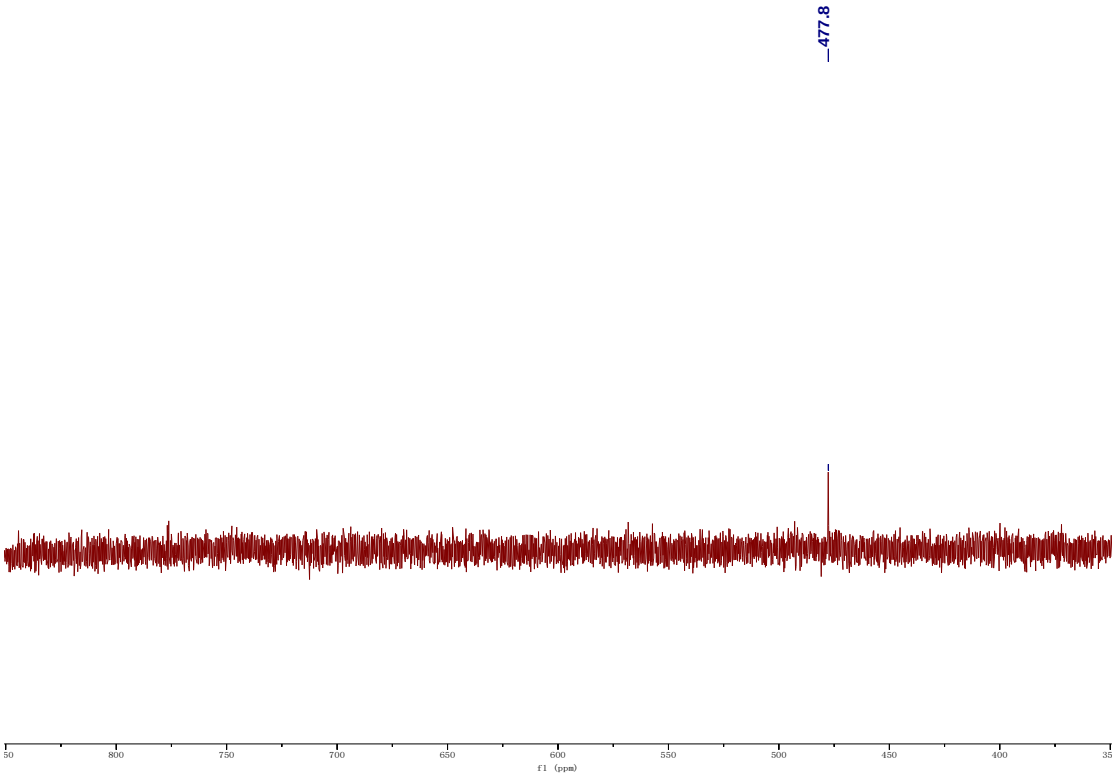

O
N
H
Se

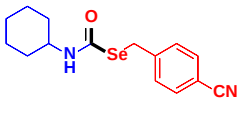
3n


7.33 7.31 7.28 7.26 7.24 7.20 7.18 7.17
5.43 5.41 4.18 3.82 3.80 3.79 3.78 3.78 3.77 3.75 1.95 1.94 1.92 1.91 1.70 1.69 1.68 1.67 1.61 1.60 1.59 1.58 1.57 1.56 1.37 1.34 1.30 1.27 1.25 1.18 1.17 1.15 1.14 1.12 1.11 1.09 1.08 -0.00

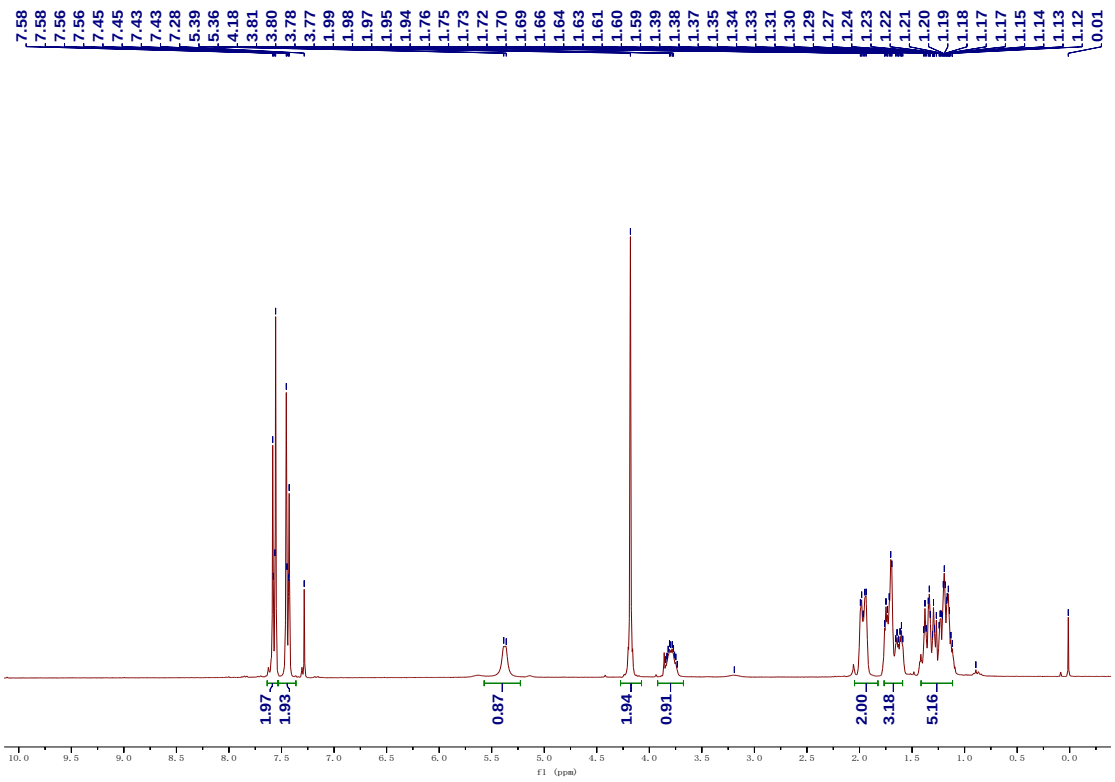

4.06 1.02 0.93 2.00 0.96 2.07 2.08 1.06 2.14 3.17
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

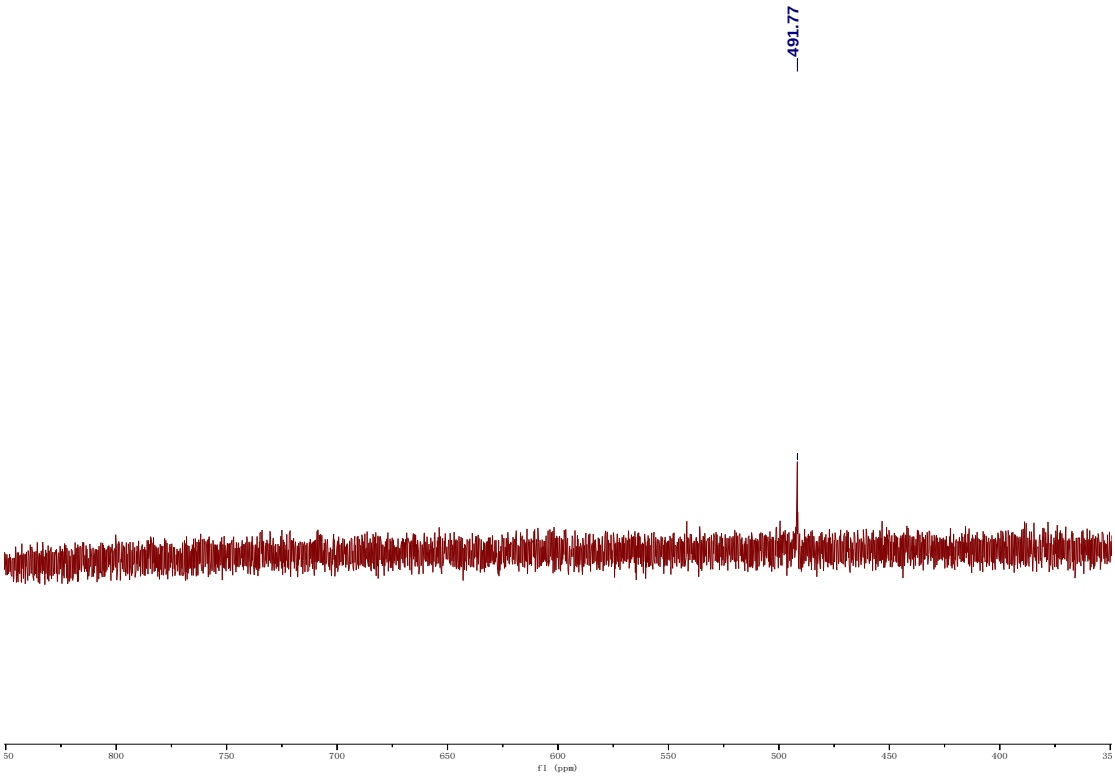

161.40
139.75
128.95
128.61
126.93
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
51.28
33.11
30.01
25.44
24.84
f1 (ppm)

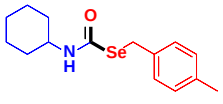

477.8
f1 (ppm)


O
N
H
Se
CN

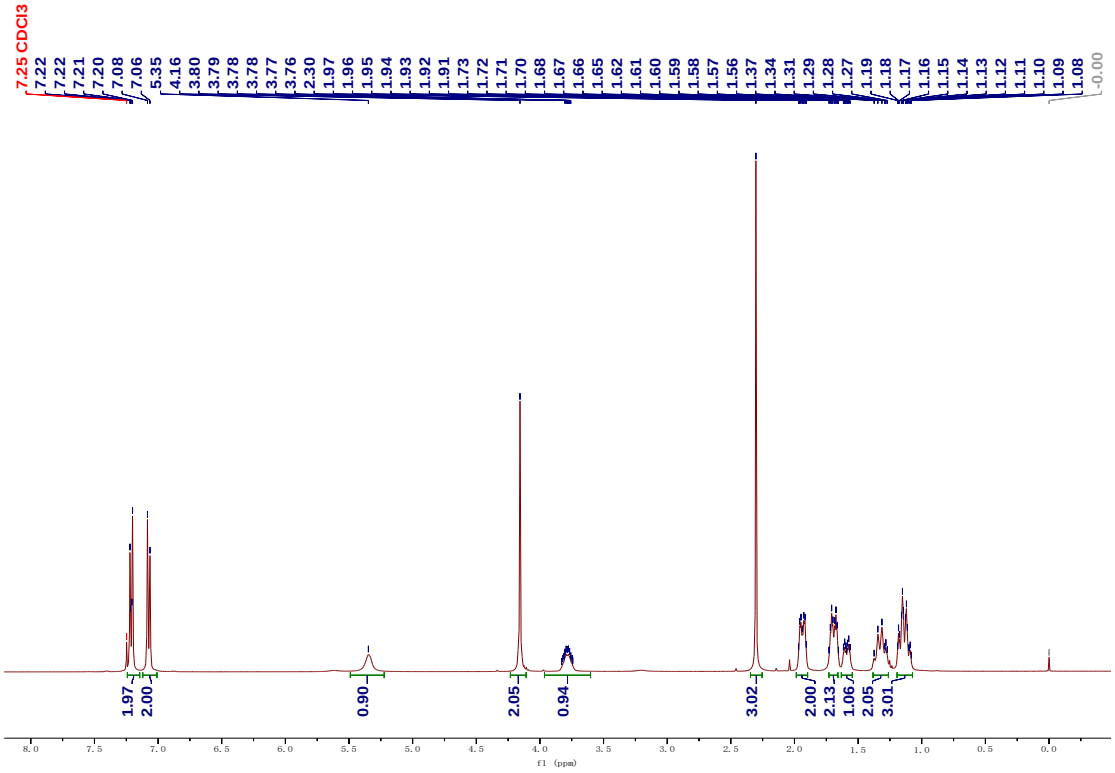
3o

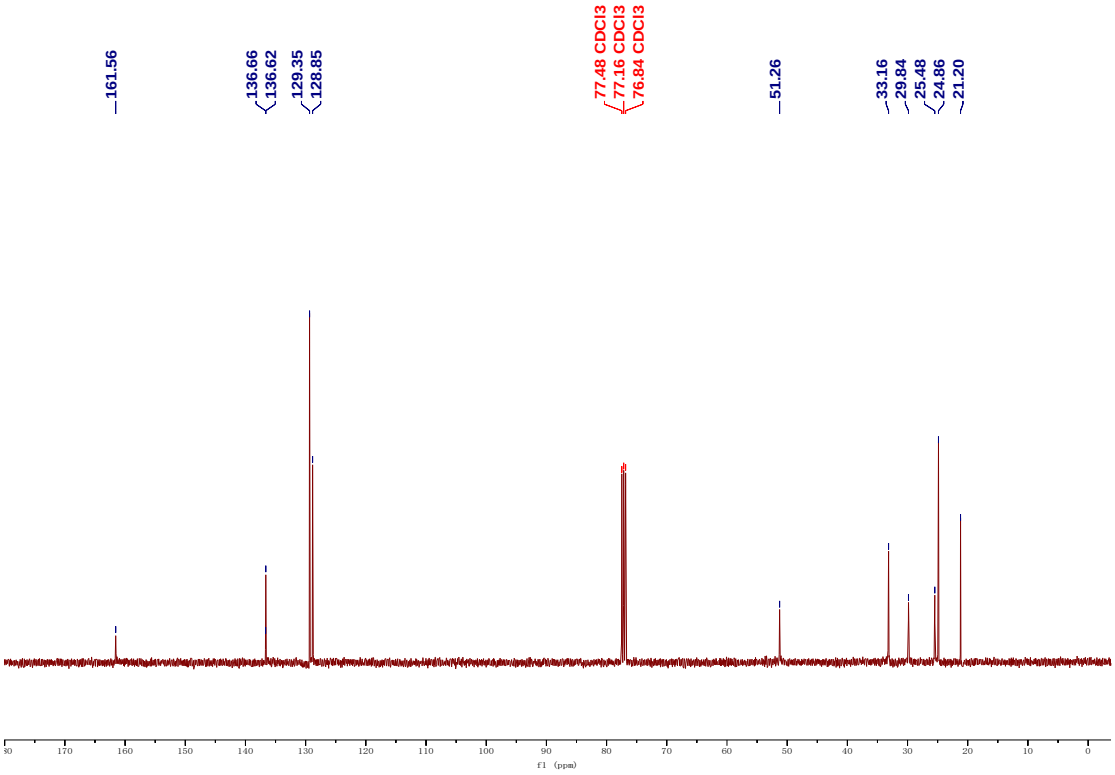

7.58
7.58
7.56
7.56
7.45
7.45
7.43
7.43
7.28
5.39
5.36
4.18
3.81
3.80
3.78
3.77
1.99
1.98
1.97
1.95
1.94
1.76
1.75
1.73
1.72
1.70
1.69
1.66
1.64
1.63
1.61
1.60
1.59
1.39
1.38
1.37
1.35
1.34
1.33
1.31
1.30
1.29
1.27
1.24
1.23
1.22
1.21
1.20
1.19
1.18
1.17
1.17
1.15
1.14
1.13
1.12
0.01
1.97
1.93
0.87
1.94
0.91
2.00
3.18
5.16
f1 (ppm)
160.46
146.08
132.43
129.75
118.98
110.61
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
51.63
33.14
29.24
25.43
24.84
f1 (ppm)

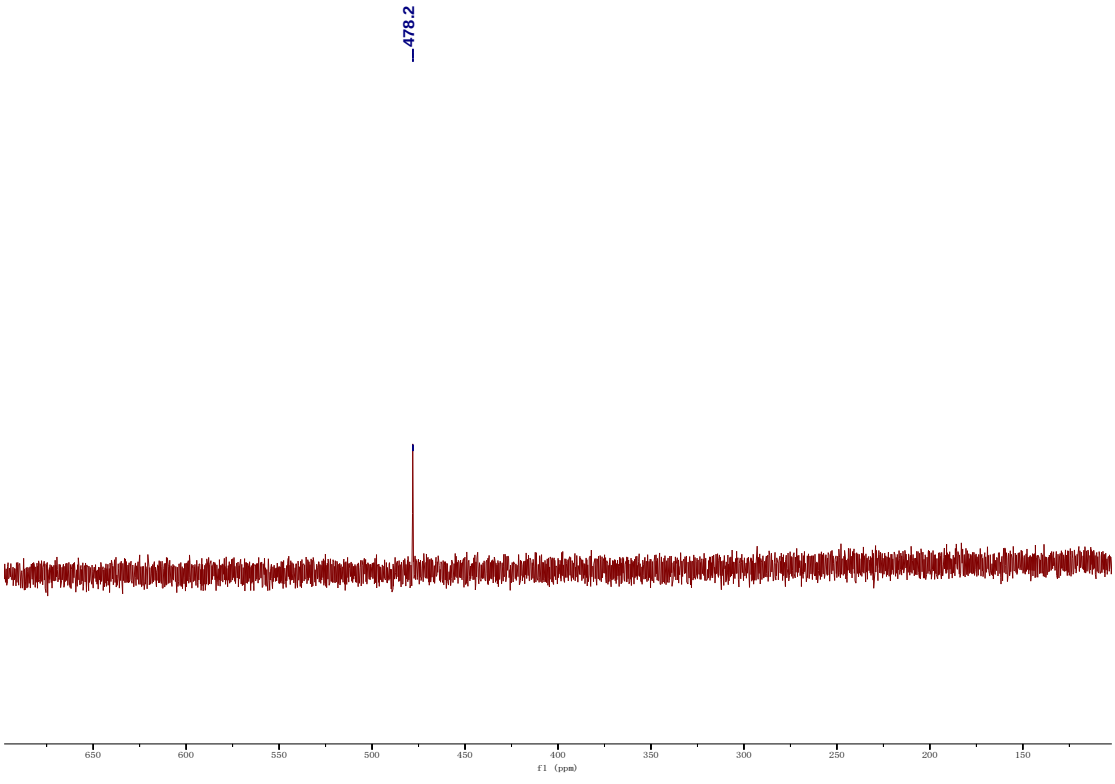

491.77
50
800
750
700
650
600
550
500
450
400
35
f1 (ppm)

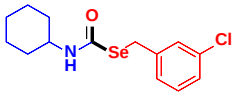

O
N
H
Se

3p

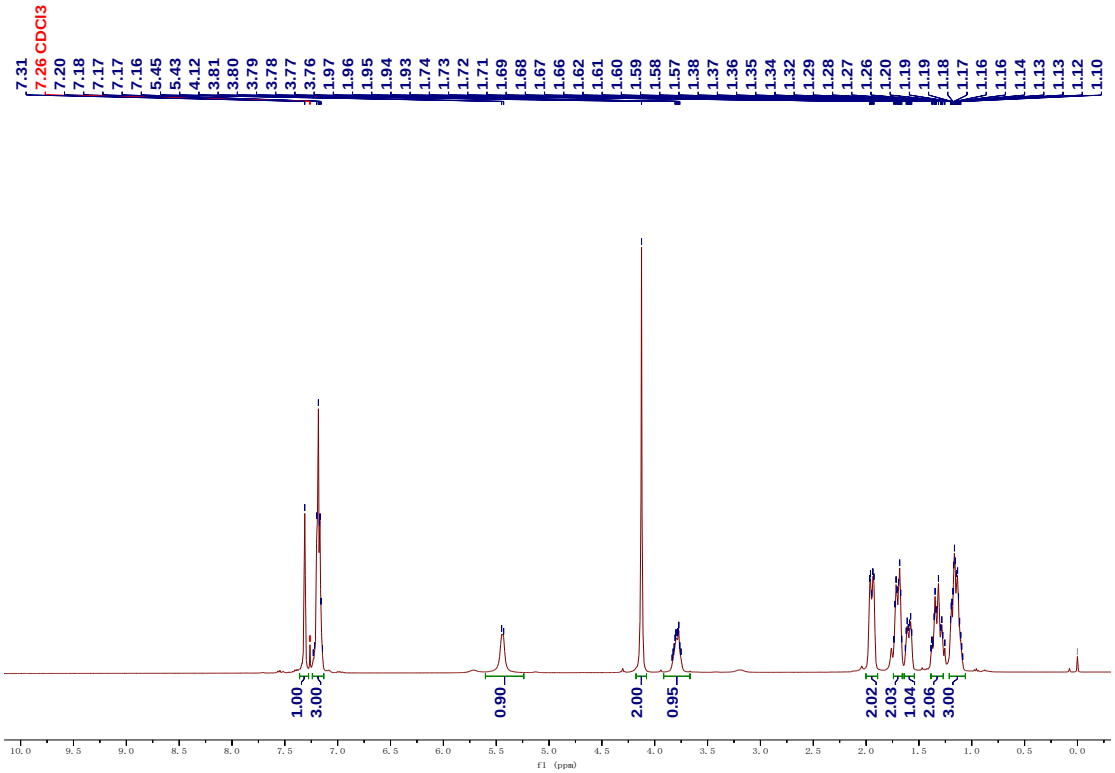

7.25 CDCl3
7.22
7.22
7.21
7.20
7.08
7.06
5.35
4.16
3.80
3.79
3.78
3.78
3.77
3.76
2.30
1.97
1.96
1.95
1.94
1.93
1.92
1.91
1.73
1.72
1.71
1.70
1.68
1.67
1.66
1.65
1.62
1.61
1.60
1.59
1.58
1.57
1.56
1.37
1.34
1.31
1.29
1.28
1.27
1.19
1.18
1.17
1.16
1.15
1.14
1.13
1.12
1.11
1.10
1.09
1.08
-0.00
1.97
2.00
0.90
2.05
0.94
3.02
2.00
2.13
1.06
2.05
3.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

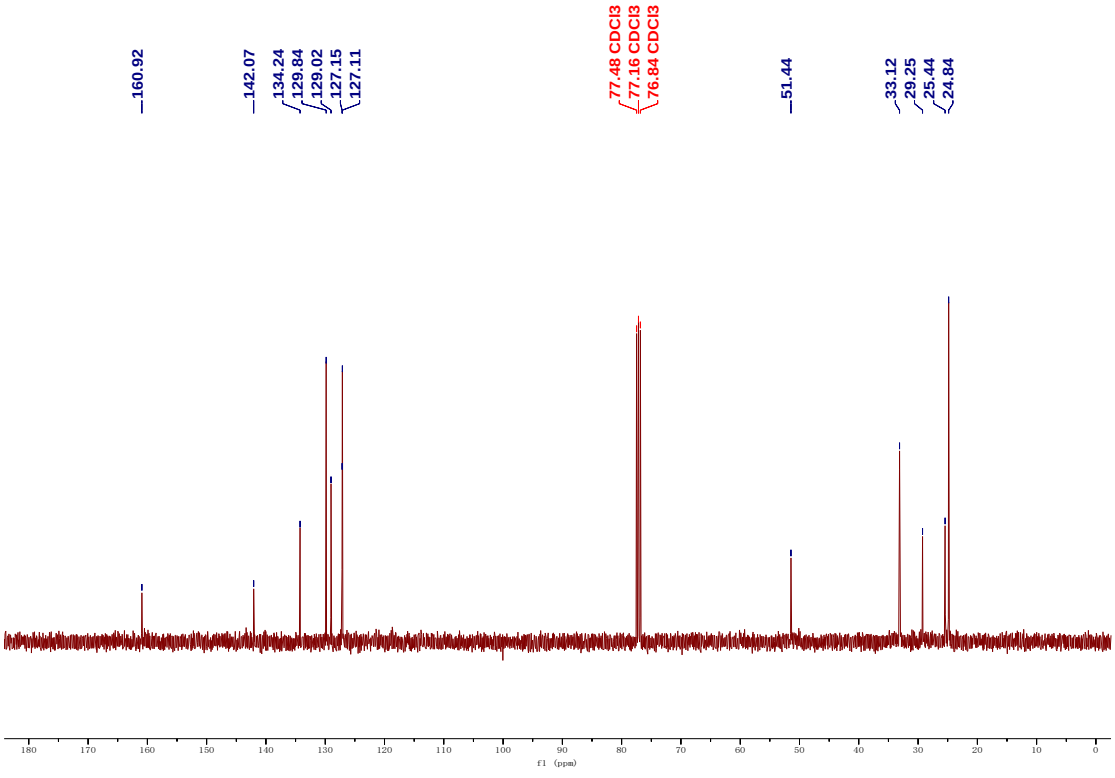

161.56
136.66
136.62
129.35
128.85
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
51.26
33.16
29.84
25.48
24.86
21.20
f1 (ppm)

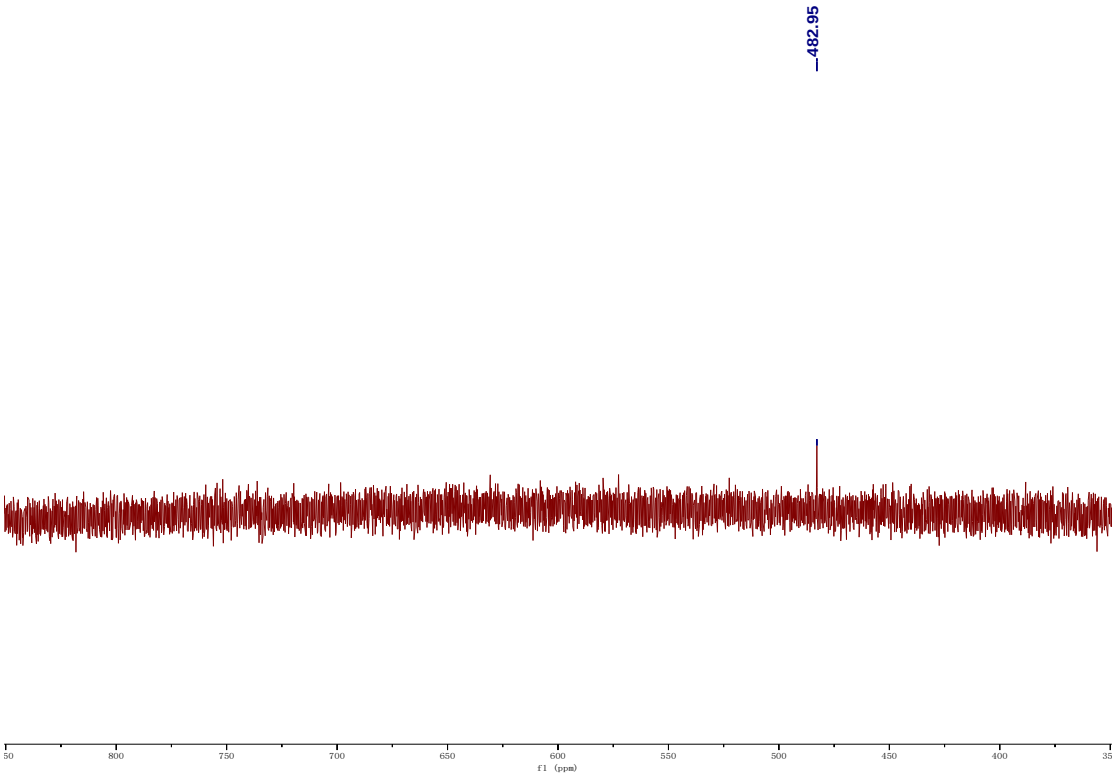

478.2
f1 (ppm)


O
N
H
Se
Cl

3q

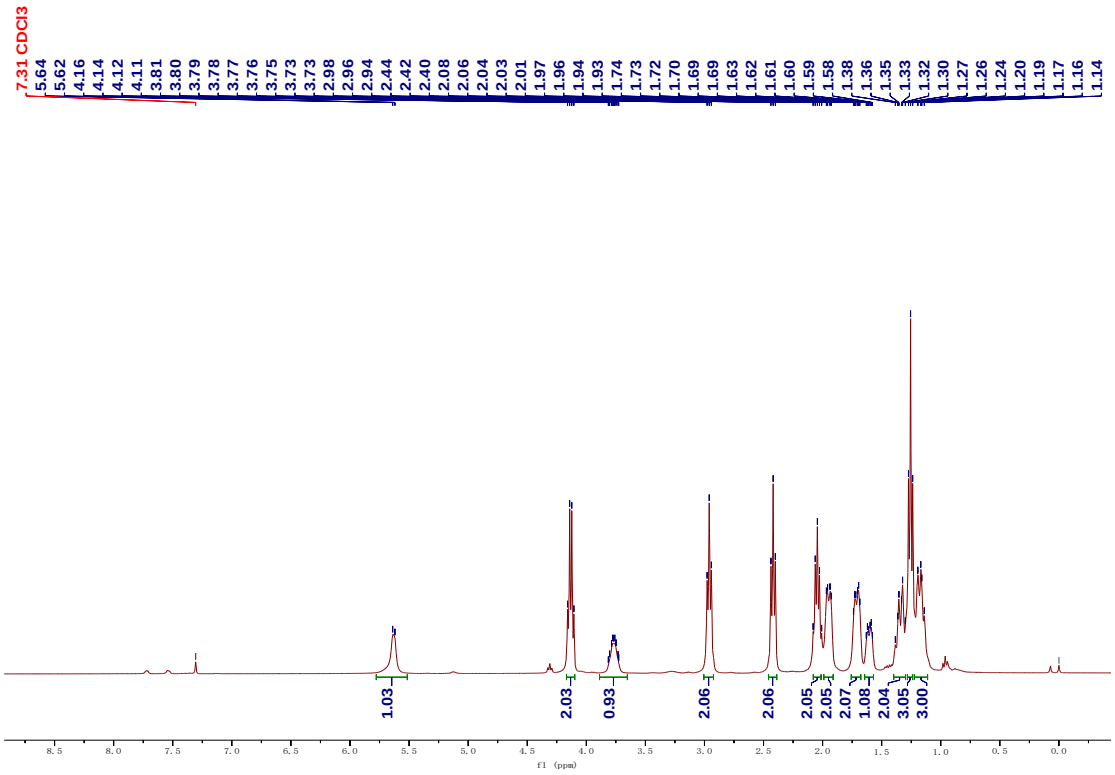

7.31
7.26 CDCl3
7.20
7.18
7.17
7.17
7.16
5.45
5.43
4.12
3.81
3.80
3.79
3.78
3.77
3.76
1.97
1.96
1.95
1.94
1.93
1.74
1.73
1.72
1.71
1.69
1.68
1.67
1.66
1.62
1.61
1.60
1.59
1.58
1.57
1.38
1.37
1.36
1.35
1.34
1.32
1.29
1.28
1.27
1.26
1.20
1.19
1.19
1.18
1.17
1.16
1.16
1.14
1.13
1.13
1.12
1.10
1.00
3.00
0.90
2.00
0.95
2.02
2.03
1.04
2.06
3.00
f1 (ppm)

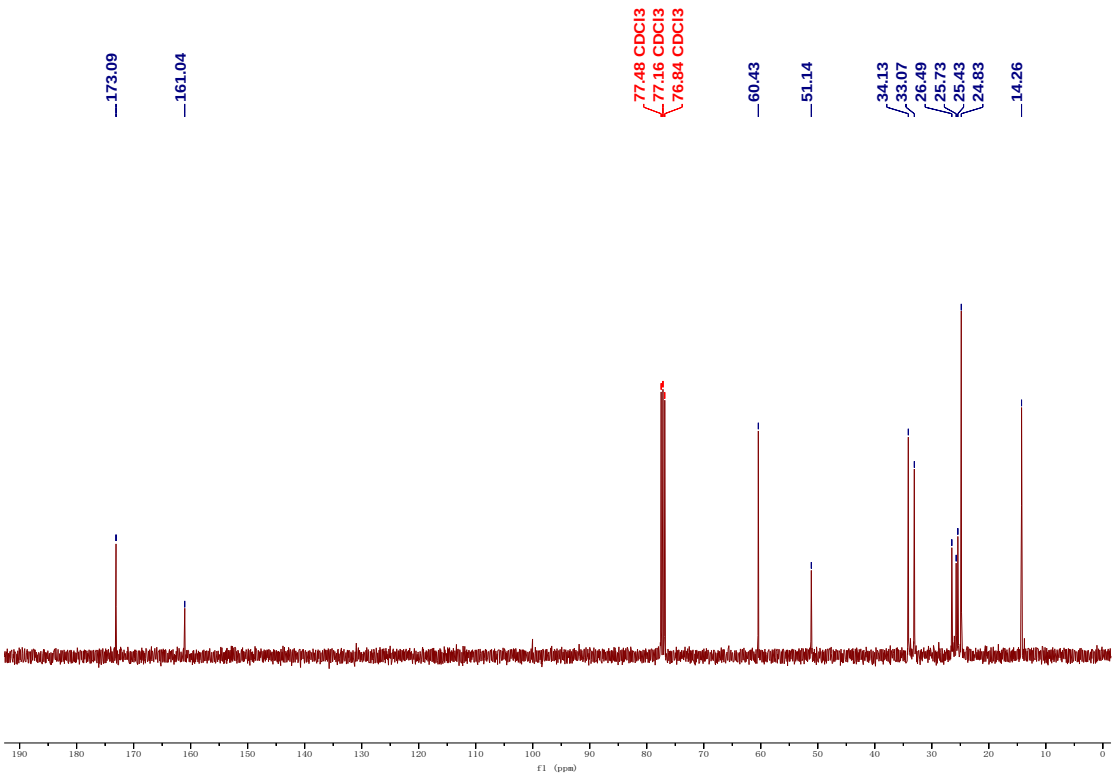

160.92
142.07
134.24
129.84
129.02
127.15
127.11
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
51.44
33.12
29.25
25.44
24.84
f1 (ppm)

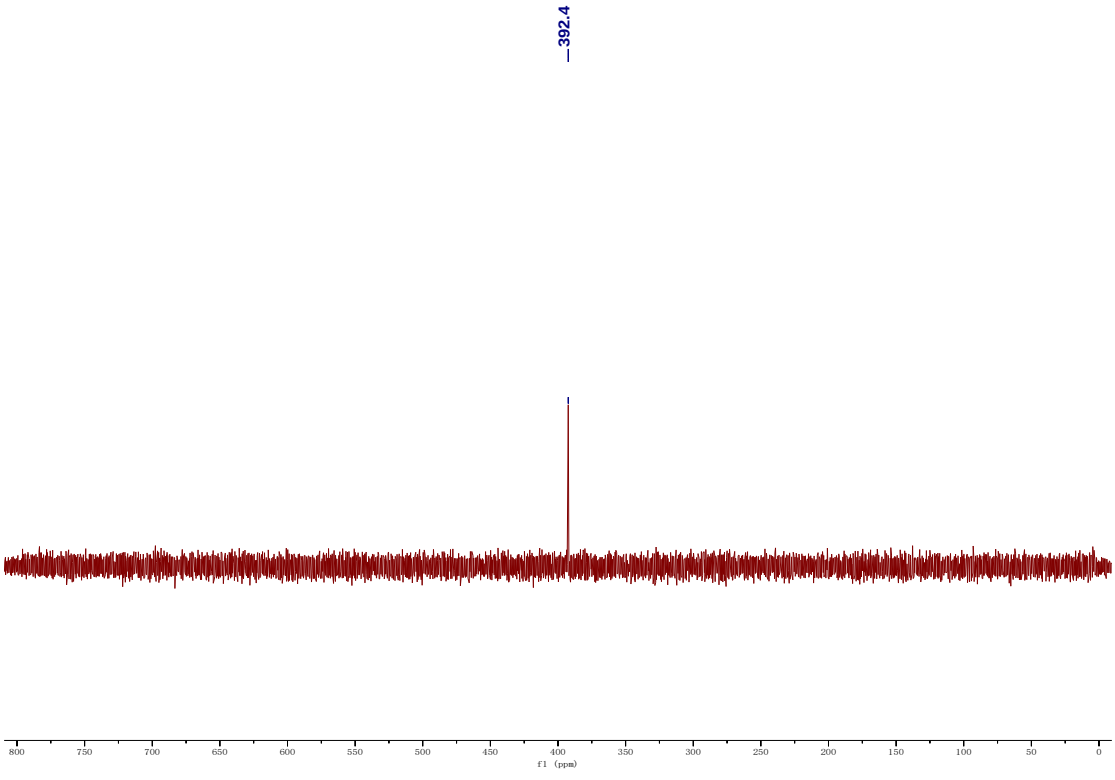

482.95
50
800
750
700
650
600
550
500
450
400
35
f1 (ppm)

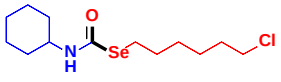

O
N
H
Se
CO2Et

3r

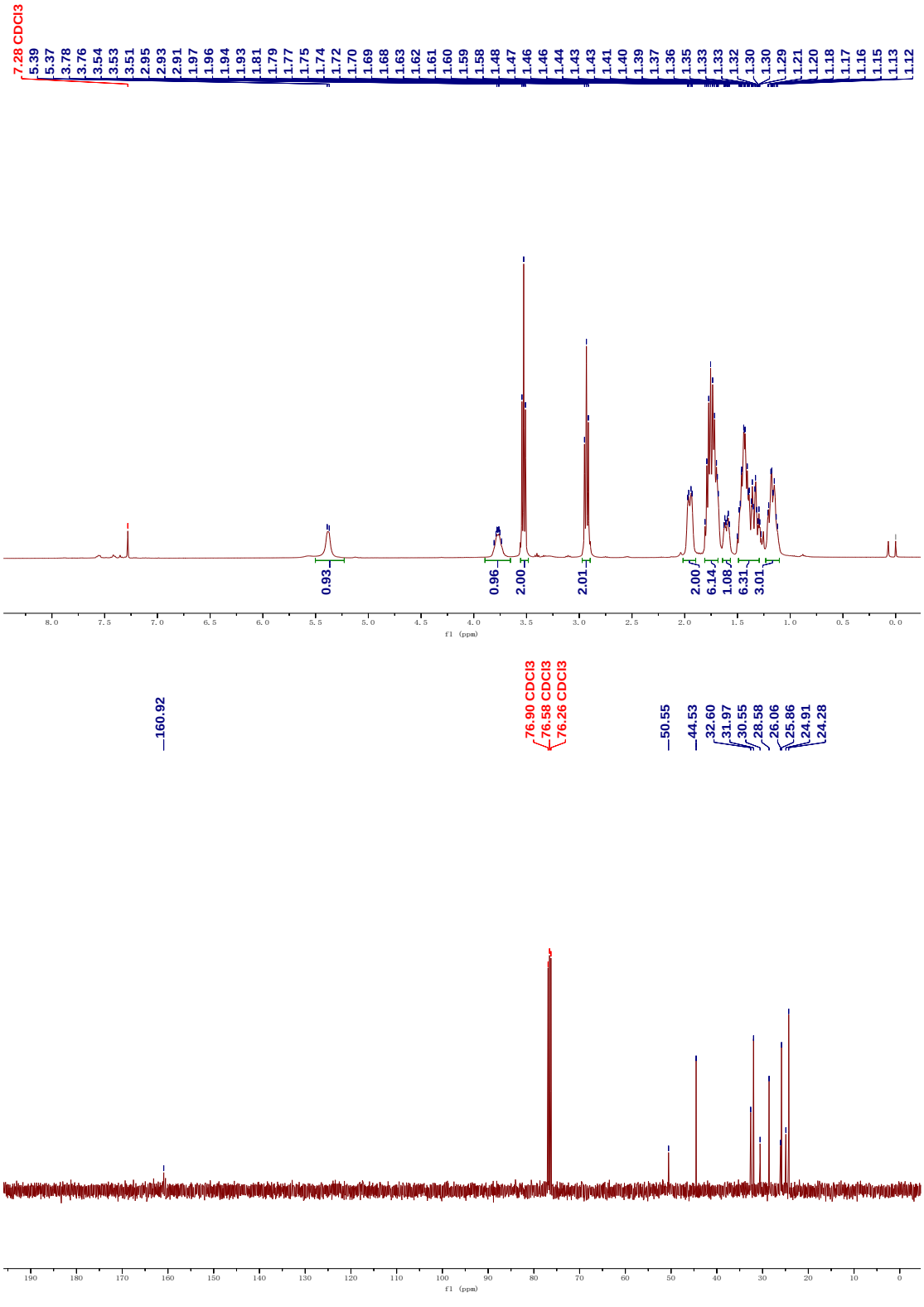

7.31 CDCl3
5.64
5.62
4.16
4.14
4.12
4.11
3.81
3.80
3.79
3.78
3.77
3.76
3.75
3.73
3.73
2.98
2.96
2.94
2.44
2.42
2.40
2.08
2.06
2.04
2.03
2.01
1.97
1.96
1.94
1.93
1.74
1.73
1.72
1.70
1.69
1.69
1.63
1.62
1.61
1.60
1.59
1.58
1.38
1.36
1.35
1.33
1.32
1.30
1.27
1.26
1.24
1.20
1.19
1.17
1.16
1.14
1.03
2.03
0.93
2.06
2.06
2.05
2.05
2.07
1.08
2.04
3.05
3.00
f1 (ppm)

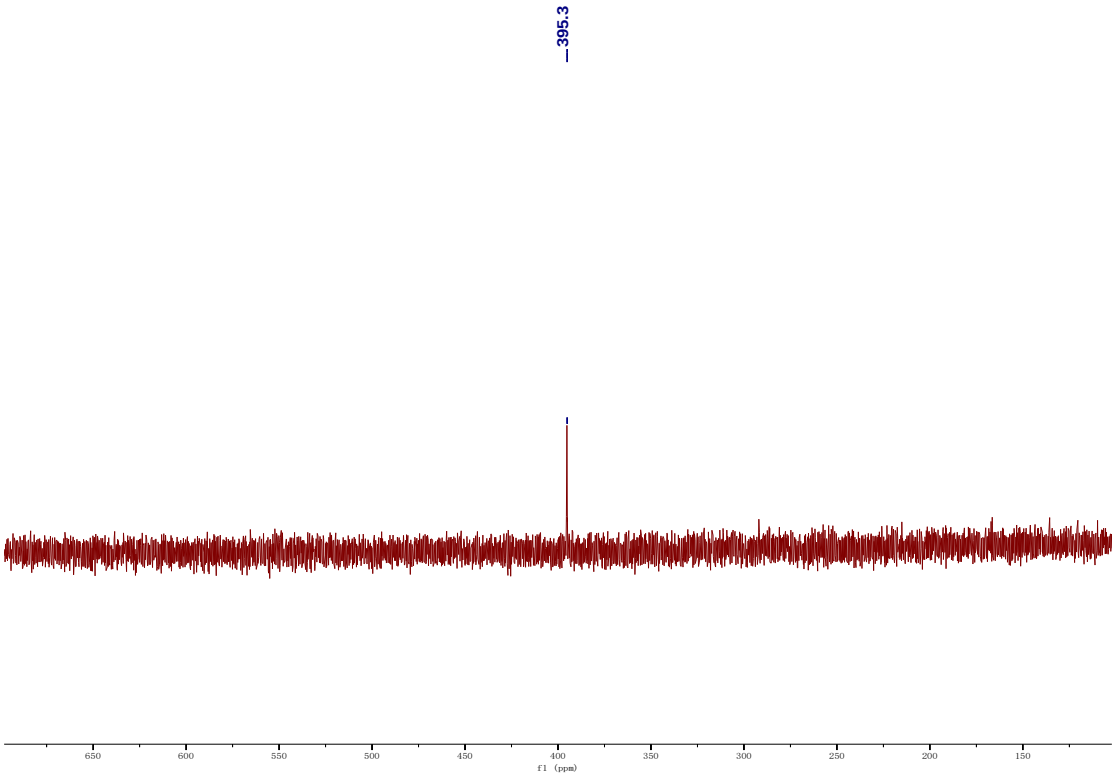

173.09
161.04
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
60.43
51.14
34.13
33.07
26.49
25.73
25.43
24.83
14.26
f1 (ppm)

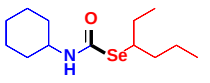

392.4
f1 (ppm)


O
N
H
Se
Cl

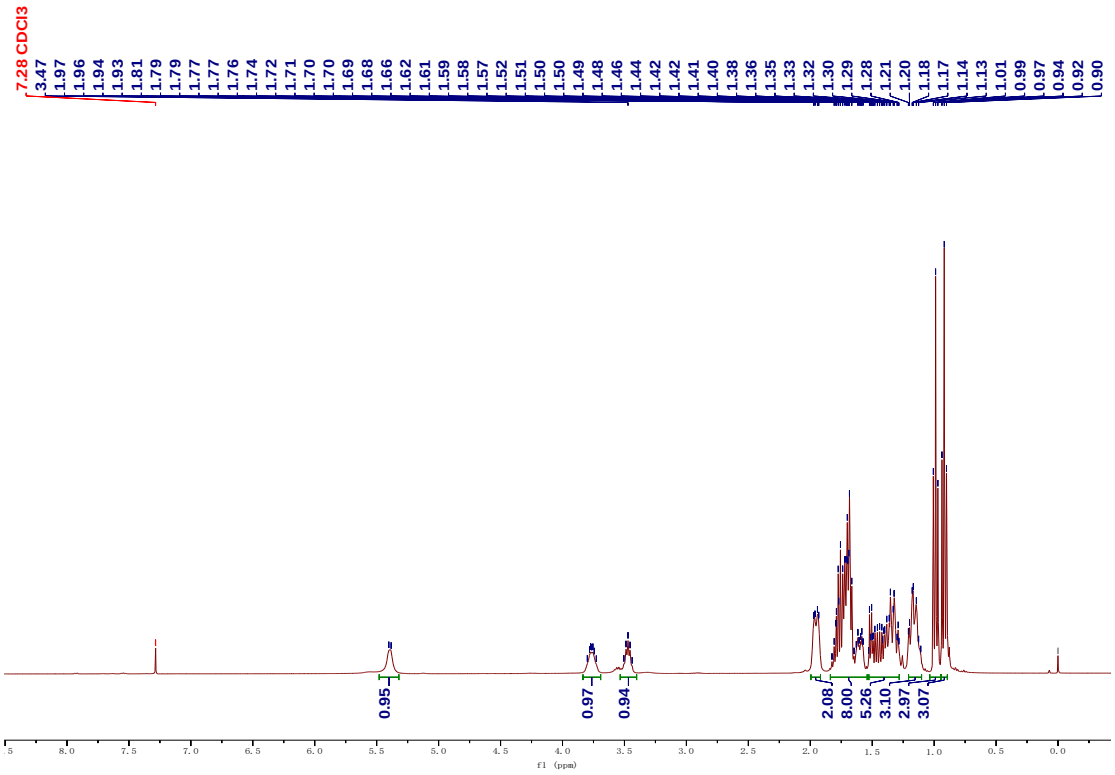
3s

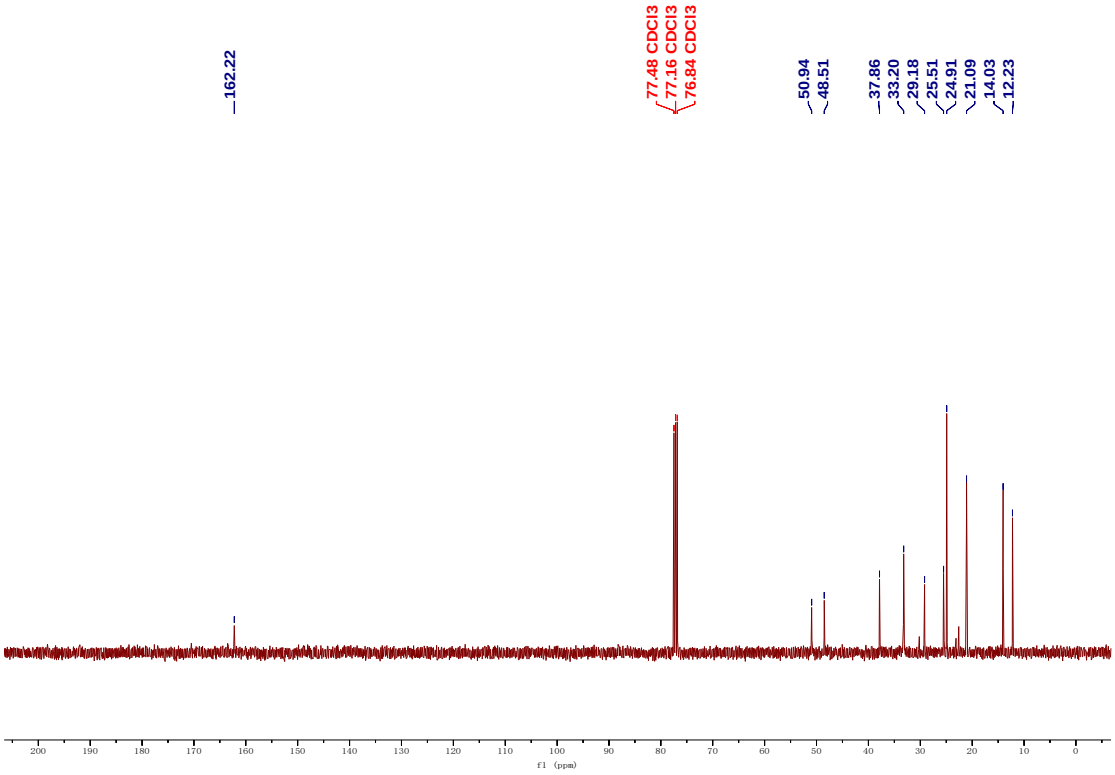

7.28 CDCl3
5.39
5.37
3.78
3.76
3.54
3.53
3.51
2.95
2.93
2.91
1.97
1.96
1.94
1.93
1.81
1.79
1.77
1.75
1.74
1.72
1.70
1.69
1.68
1.63
1.62
1.61
1.60
1.59
1.58
1.48
1.47
1.46
1.46
1.44
1.43
1.43
1.41
1.40
1.39
1.37
1.36
1.35
1.33
1.33
1.32
1.30
1.30
1.29
1.21
1.20
1.18
1.17
1.16
1.15
1.13
1.12
0.93
0.96
2.00
2.01
2.00
6.14
1.08
6.31
3.01
f1 (ppm)
160.92
76.90 CDCl3
76.58 CDCl3
76.26 CDCl3
50.55
44.53
32.60
31.97
30.55
28.58
26.06
25.86
24.91
24.28
f1 (ppm)

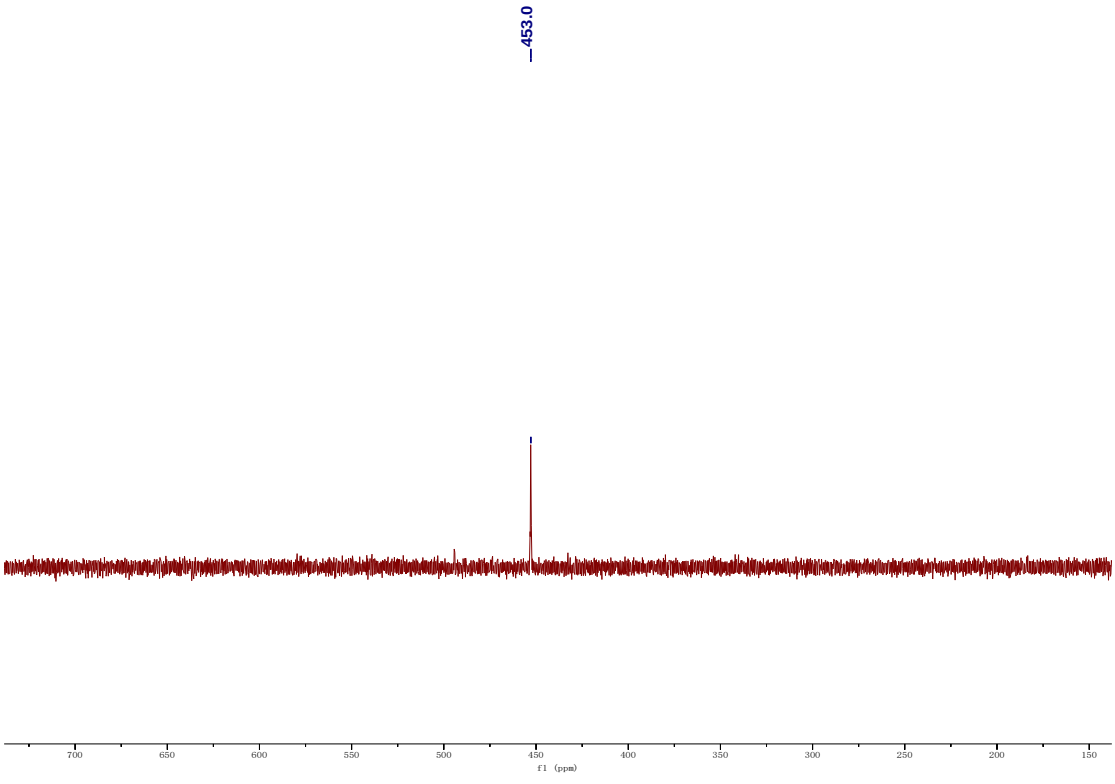

395.3
650
600
550
500
450
400
350
300
250
200
150
f1 (ppm)


O
N
H
Se

3t


7.28 CDCl3
3.47
1.97
1.96
1.94
1.93
1.81
1.79
1.79
1.77
1.77
1.76
1.74
1.72
1.71
1.70
1.70
1.69
1.68
1.66
1.62
1.61
1.59
1.58
1.57
1.52
1.51
1.50
1.50
1.49
1.48
1.46
1.44
1.42
1.42
1.41
1.40
1.38
1.36
1.35
1.33
1.32
1.30
1.29
1.28
1.21
1.20
1.18
1.17
1.14
1.13
1.01
0.99
0.97
0.94
0.92
0.90
0.95
0.97
0.94
2.08
8.00
5.26
3.10
2.97
3.07
f1 (ppm)

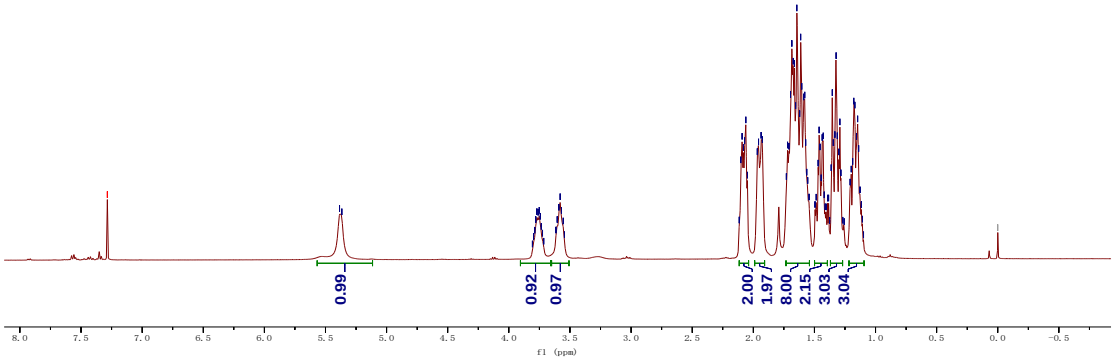

162.22
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
50.94
48.51
37.86
33.20
29.18
25.51
24.91
21.09
14.03
12.23
f1 (ppm)

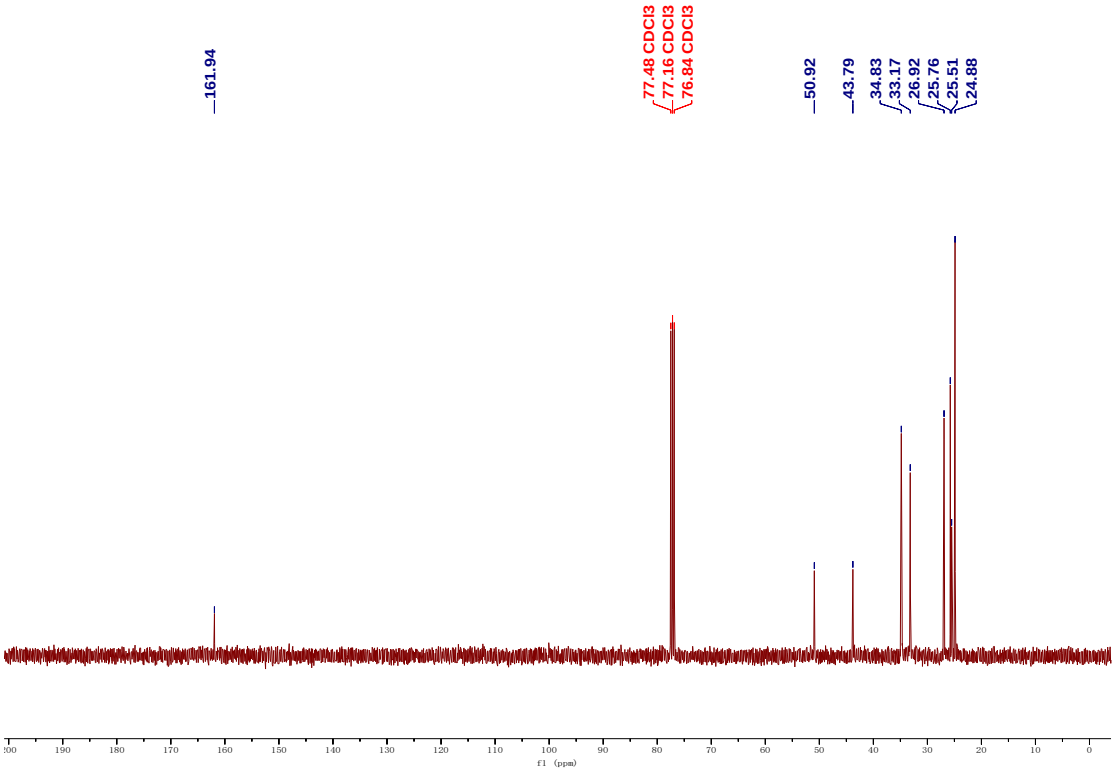

453.0
f1 (ppm)

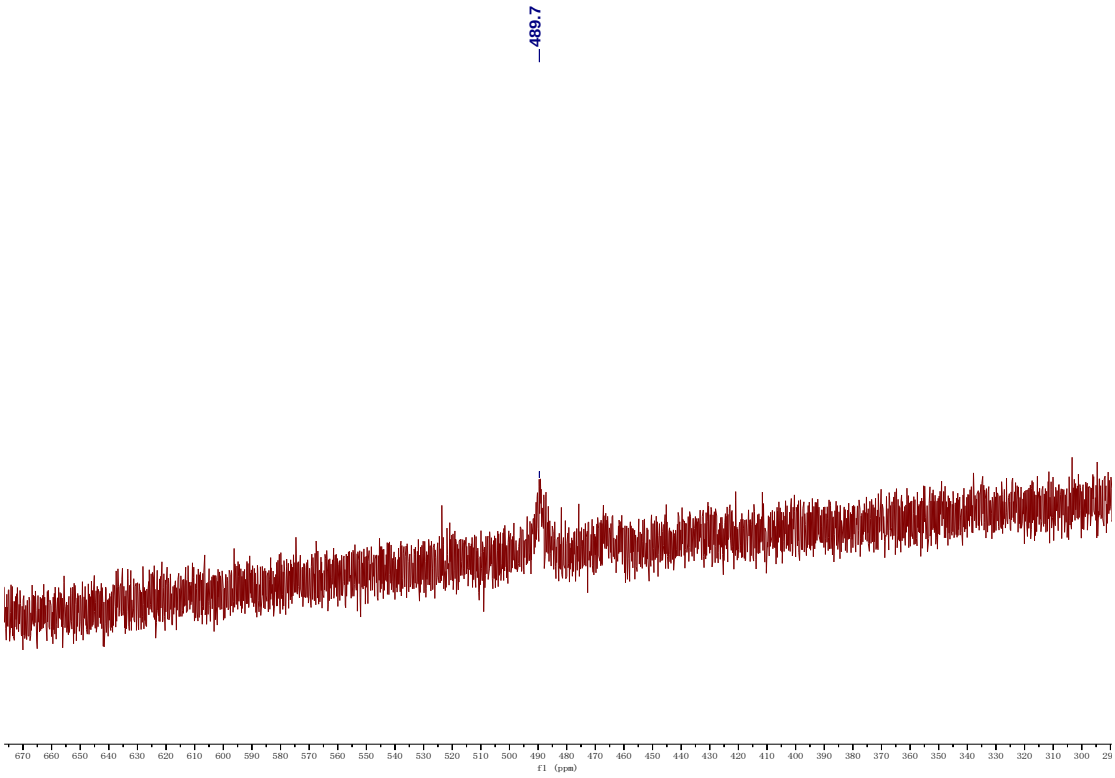

O
N
H
Se

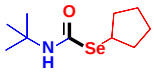
3u


7.28 CDCl3
3.58
2.10
2.09
2.08
2.07
2.06
2.05
1.97
1.96
1.94
1.93
1.73
1.72
1.71
1.70
1.68
1.67
1.66
1.65
1.64
1.62
1.61
1.60
1.59
1.58
1.57
1.56
1.55
1.54
1.49
1.47
1.46
1.45
1.44
1.44
1.43
1.42
1.38
1.36
1.35
1.35
1.33
1.32
1.31
1.30
1.29
1.28
1.21
1.20
1.19
1.18
1.17
1.16
1.15
1.14
1.13

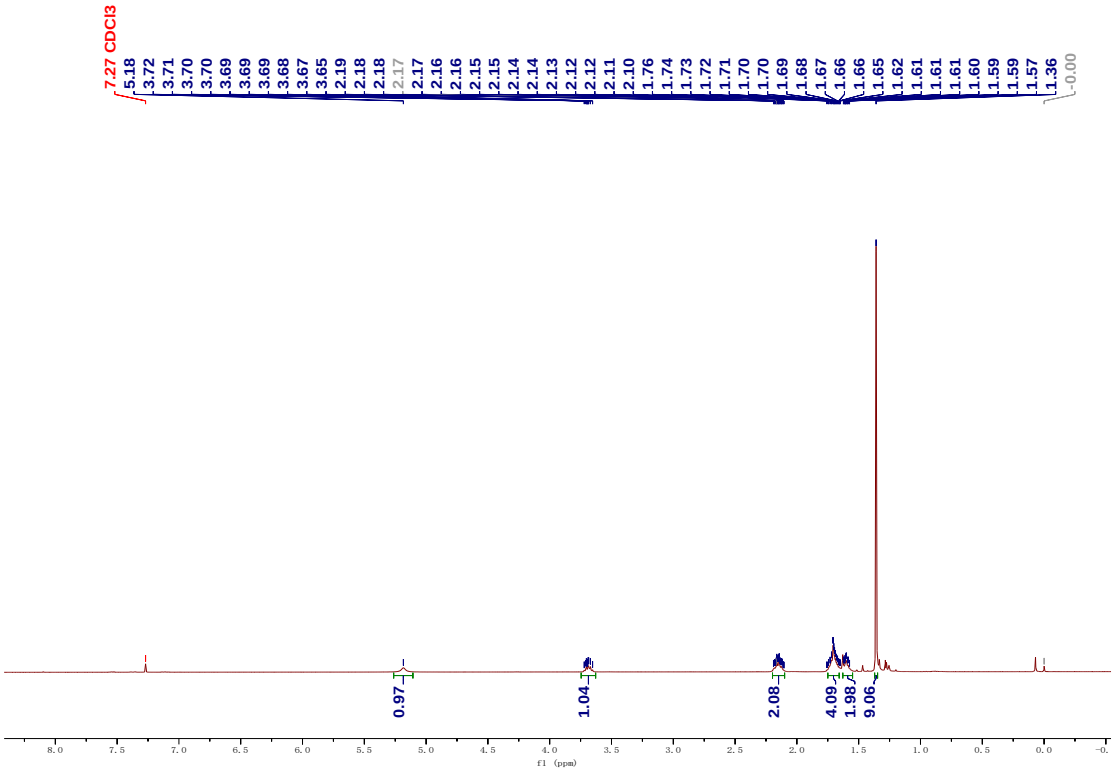

0.99
0.92
0.97
2.00
1.97
8.00
2.15
3.03
3.04
f1 (ppm)

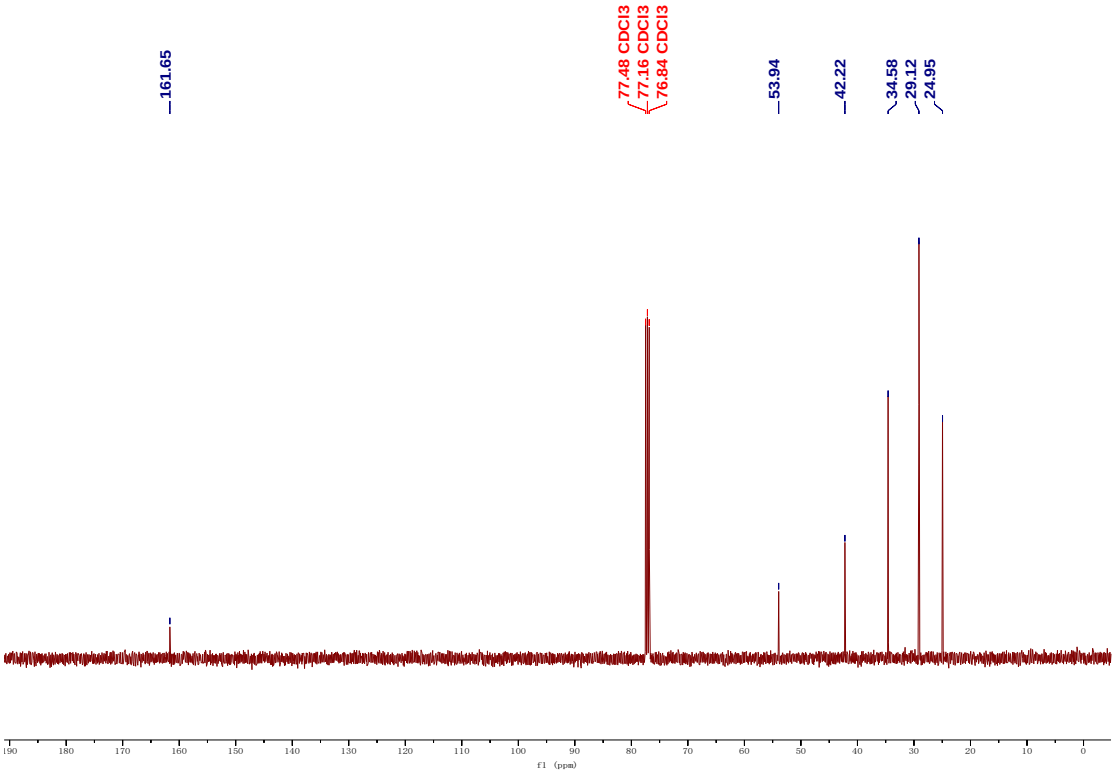

161.94
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
50.92
43.79
34.83
33.17
26.92
25.76
25.51
24.88
f1 (ppm)

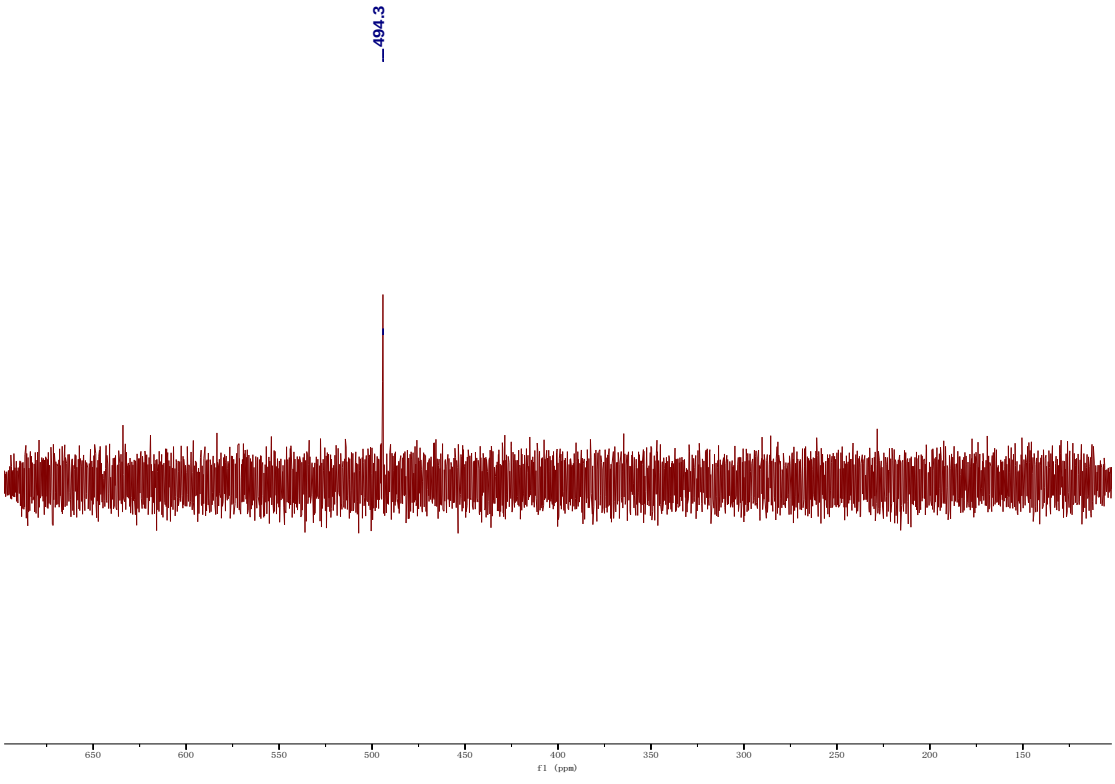

489.7
f1 (ppm)

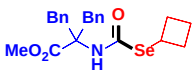

O
N
H
Se

3v

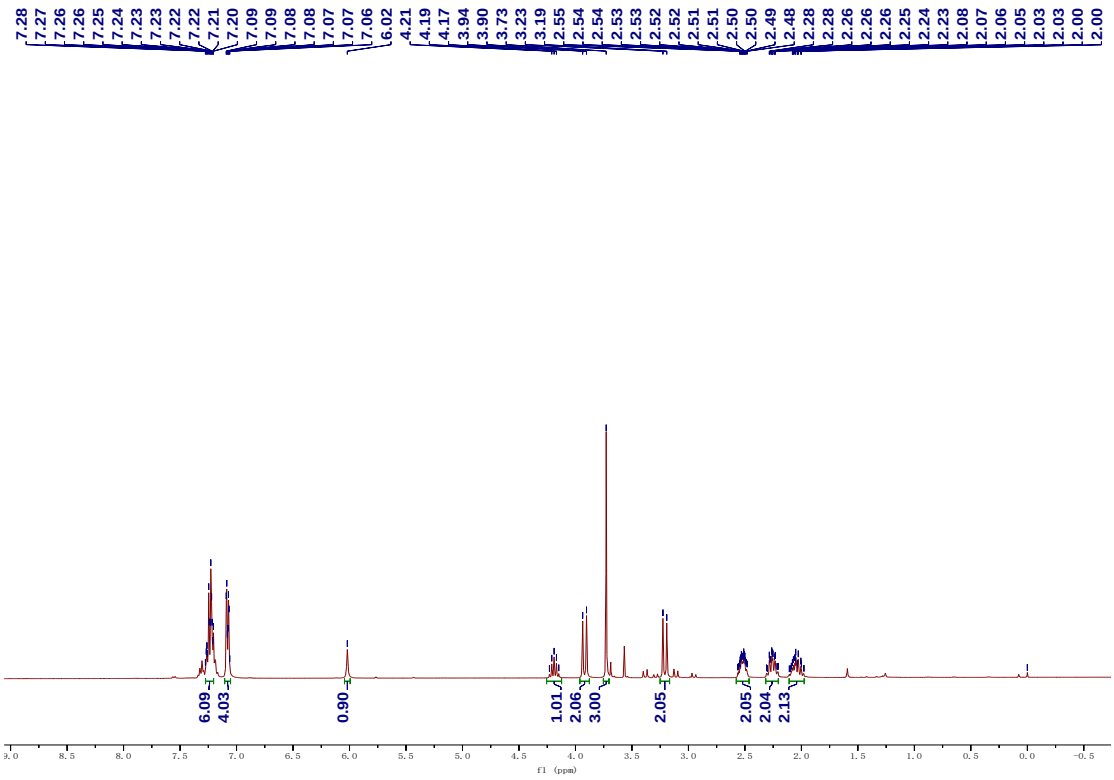

7.27 CDCl3
5.18
3.72
3.71
3.70
3.70
3.69
3.69
3.69
3.68
3.67
3.65
2.19
2.18
2.18
2.17
2.17
2.16
2.16
2.15
2.15
2.14
2.14
2.13
2.12
2.12
2.11
2.10
1.76
1.74
1.73
1.72
1.71
1.70
1.70
1.69
1.68
1.67
1.66
1.66
1.65
1.62
1.61
1.61
1.61
1.60
1.59
1.59
1.57
1.36
0.00
0.97
1.04
2.08
4.09
1.98
9.06
f1 (ppm)

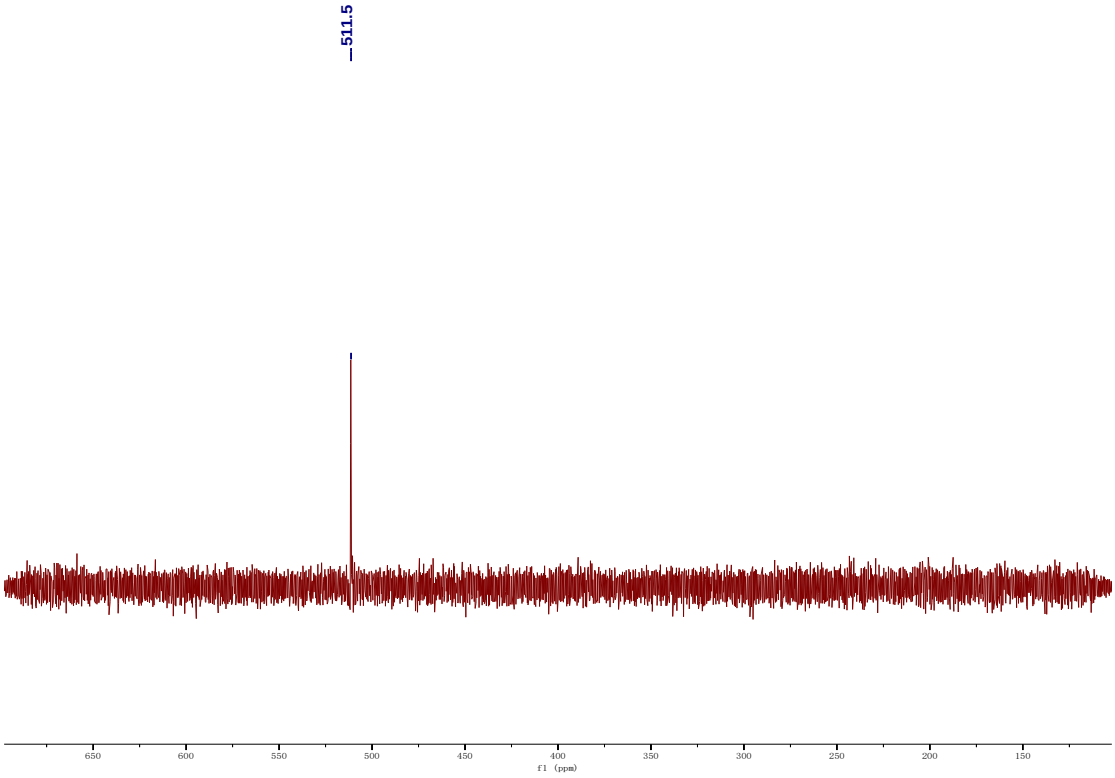

161.65
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
53.94
42.22
34.58
29.12
24.95
f1 (ppm)

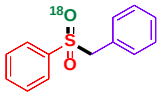

494.3
f1 (ppm)


Bn
Bn
O
MeO2C
N
H
Se

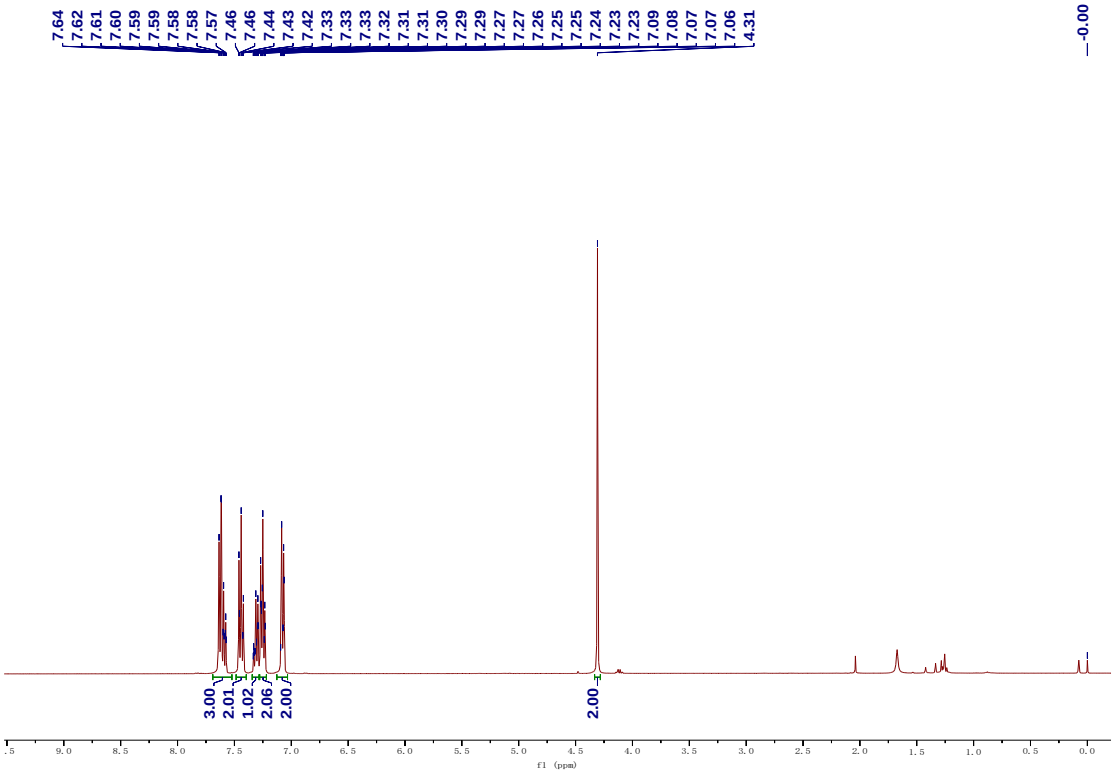
3w

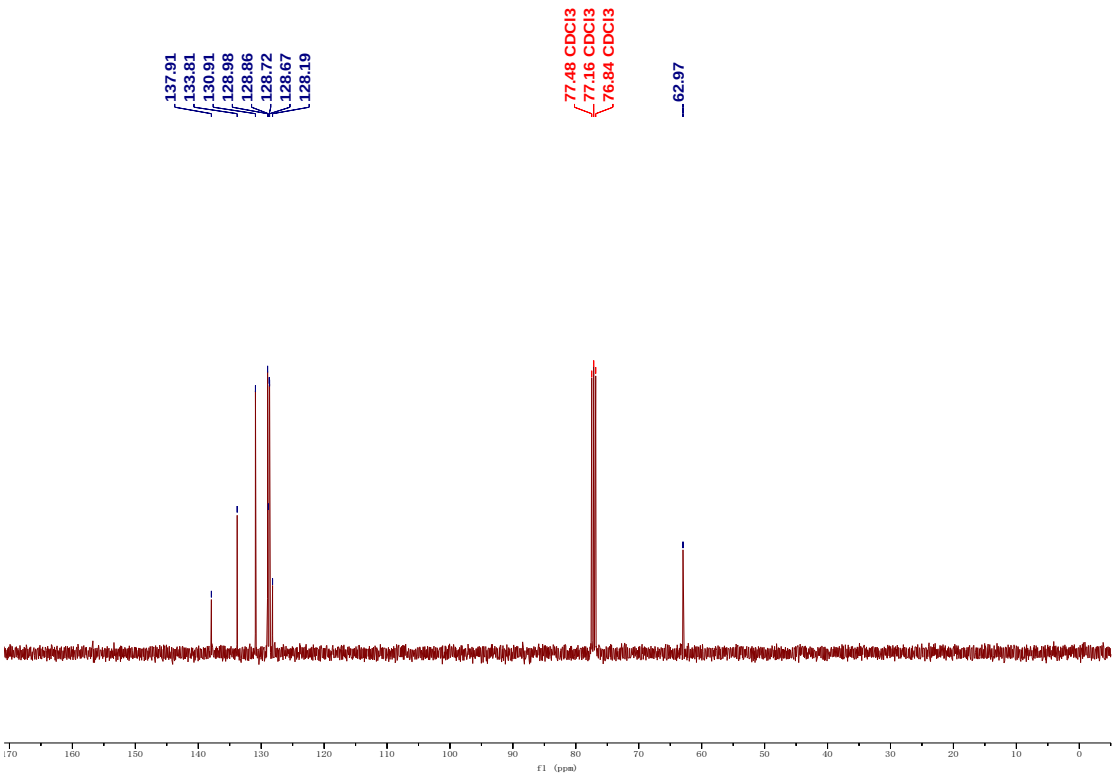

7.28 7.27 7.26 7.26 7.25 7.24 7.23 7.23 7.22 7.22 7.21 7.20 7.09 7.09 7.08 7.08 7.07 7.07 7.06 6.02
4.21 4.19 4.17 3.94 3.90 3.73 3.23 3.19 2.55 2.54 2.54 2.53 2.53 2.52 2.52 2.51 2.51 2.50 2.50 2.49 2.48 2.28 2.28 2.26 2.26 2.26 2.25 2.24 2.23 2.08 2.07 2.06 2.05 2.03 2.03 2.00 2.00
6.09 4.03 0.90 1.01 2.06 3.00 2.05 2.05 2.04 2.13
f1 (ppm)
172.02 163.10 135.90 129.73 128.43 127.18 77.48 CDCl3 77.16 CDCl3 76.84 CDCl3 69.62 52.65 41.41 35.57 31.81 20.65
f1 (ppm)

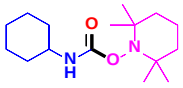

511.5
650
600
550
500
450
400
350
300
250
200
150
f1 (ppm)


18O
S
O

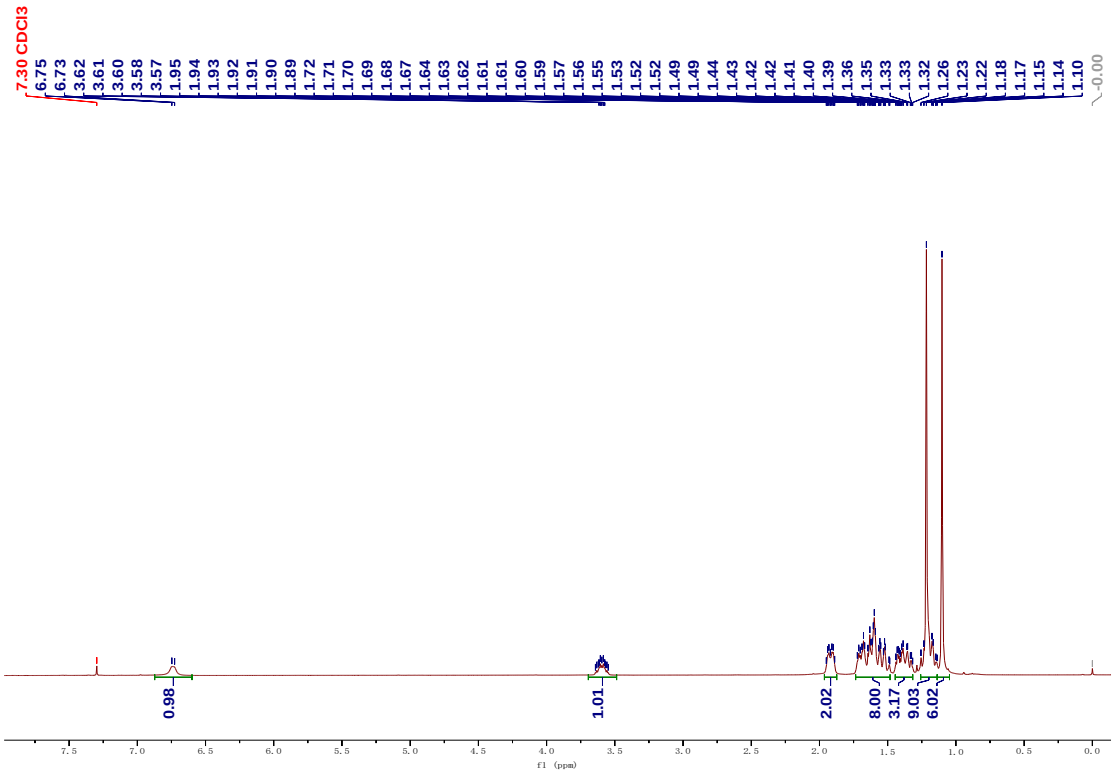
4a

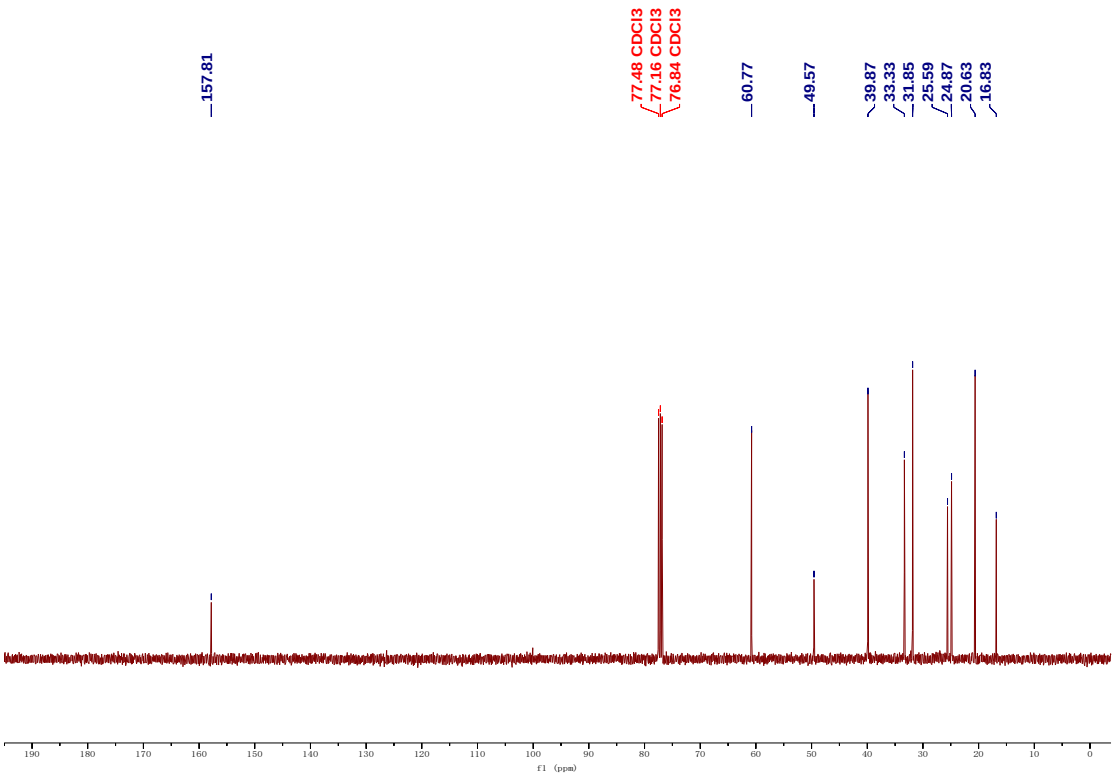

7.64
7.62
7.61
7.60
7.59
7.59
7.58
7.58
7.57
7.46
7.46
7.44
7.43
7.42
7.33
7.33
7.32
7.31
7.31
7.30
7.29
7.29
7.27
7.27
7.26
7.25
7.25
7.24
7.23
7.23
7.09
7.08
7.07
7.07
7.06
4.31
-0.00
3.00
2.01
1.02
2.06
2.00
2.00
f1 (ppm)


137.91
133.81
130.91
128.98
128.86
128.72
128.67
128.19
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
62.97
f1 (ppm)


O
N
H
O
N

4b


7.30 CDCl3
6.75
6.73
3.62
3.61
3.60
3.58
3.57
1.95
1.94
1.93
1.92
1.91
1.90
1.89
1.72
1.71
1.70
1.69
1.68
1.67
1.64
1.63
1.62
1.61
1.61
1.60
1.59
1.57
1.56
1.55
1.53
1.52
1.52
1.49
1.49
1.44
1.43
1.42
1.42
1.41
1.40
1.39
1.36
1.35
1.33
1.33
1.32
1.26
1.23
1.22
1.18
1.17
1.15
1.14
1.10
-0.00
0.98
1.01
2.02
8.00
3.17
9.03
6.02
f1 (ppm)


157.81
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
60.77
49.57
39.87
33.33
31.85
25.59
24.87
20.63
16.83
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)