

Electrochemical Oxidative Cyclization of Olefinic Carbonyls with Diselenides

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Supporting Information

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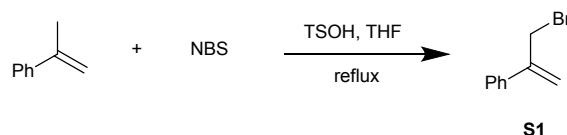
General information

All glassware was oven dried at 110 °C for hours and cooled down under vacuum. Unless otherwise noted, all reagents were purchased from commercial suppliers and used without further purification. The instrument for electrolysis was dual display potentiostat (DJS-292B) (made in China). Cyclic voltammograms were obtained on a CHI 605E potentiostat. The anodic electrode was graphite rod (ϕ 6 mm, **hard**) and cathodic electrode was platinum sheet (1.5 cm $\times$ 1.5 cm $\times$ 0.3 mm). These electrodes were commercially available from GaossUnion, China. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 °C). GC-MS spectra were recorded on a Varian GC-MS 3900-2100T. The known compounds were characterized by ^1H NMR, ^{13}C NMR and ^{19}F NMR. ^1H , ^{19}F and ^{13}C NMR data were recorded with ADVANCE III 400 MHz with tetramethylsilane as an internal standard. High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument. All chemical shifts (δ) were reported in ppm and coupling constants (J) in Hz. All chemical shifts were reported relative to tetramethylsilane (0 ppm for ^1H), Chloroform-*d* (77.16 ppm for ^{13}C), respectively.

Experimental Section

1) General procedure for preparation of olefinic carbonyl compounds

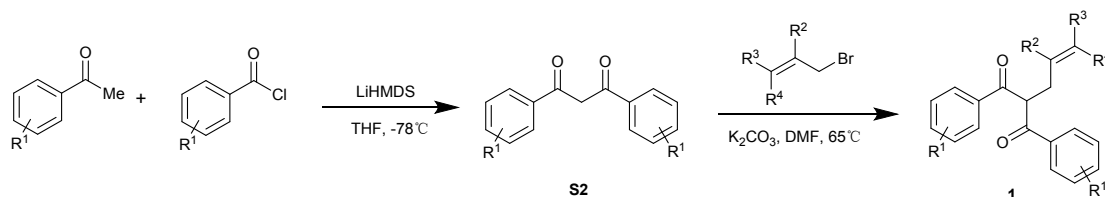
Preparation of (3-bromoprop-1-en-2-yl)benzene¹. To a solution of α -methylstyrene (20 mmol) in THF (30 mL) was added N-bromosuccinimide (NBS, 25 mmol) and TsOH (2 mmol), and the mixture was heated to reflux for 8 h. After cooling the reaction mixture to room temperature, then quenched with water (100 mL), extracted with EtOAc (3 $\times$ 30 mL). The combined organic layer was dried over Na_2SO_4 , filtered and concentrated under reduced pressure to afford the crude product, which was purified by flash column chromatography (PE/EA) to give (3-bromoprop-1-en-2-yl)benzene **S1**.



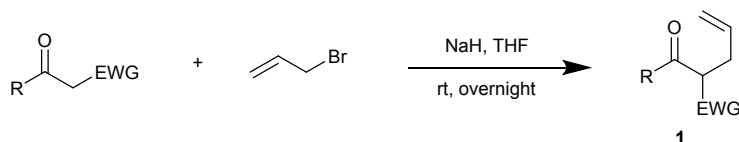
Preparation of **1a-1l**, **1p**¹. The substituted acetophenones (10 mmol) was dissolved in THF (30 mL) in a dried round bottom flask under an N_2 atmosphere. The solution was cool down to -78 °C, followed by addition of lithium bis(trimethylsilyl)amide (LiHDMS) (20 mL, 1 M in THF). This solution was stirred at -78 °C for 1 h before the corresponding benzoyl chloride (10 mmol, 1.0 equiv) was added dropwise. The mixture was allowed to warm to room temperature stirred overnight. Then quenched with 1 M HCl (30 mL, 1 M) and water (100 mL), extracted with EtOAc (3 $\times$ 50 mL). The combined organic layer was dried over Na_2SO_4 , filtered and concentrated under reduced pressure to afford the crude product, which was purified by flash column chromatography (PE/EA) to give the corresponding products **S2**.

The obtained **S2** (10 mmol) was dissolved in DMF (20 mL) in a dried round bottom flask, followed by addition of the corresponding allyl bromide **S1** (11 mmol) and K_2CO_3 (2.07 g, 15mmol). The mixture was stirred at 65 °C for 6 h under an N_2 atmosphere. Then diluted with Water (70 mL).

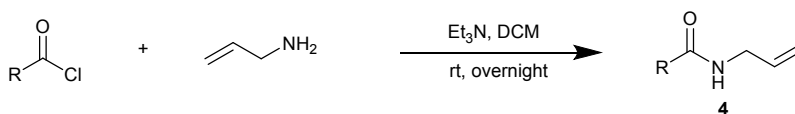
extracted with EtOAc (3 × 50 mL). The combined organic layer was dried over Na₂SO₄, filtered and concentrated under reduced pressure to afford the crude product, which was purified by flash column chromatography (PE/EA) to give the corresponding product **1**.



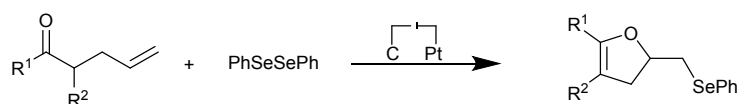
Preparation of **1m-1o**, **1q-1v**². To a solution of NaH (12 mmol, 1.2 equiv) in THF (20 mL) at 0 °C was added corresponding olefinic carbonyl compounds (10 mmol, 1.0 equiv) in THF (10 mL) dropwisely, and the mixture was stirred at 0 °C for 1 h. The corresponding allyl bromide **S1** (12 mmol, 1.2 equiv) was added to the solution over 5 min and the reaction mixture was further stirred overnight at room temperature. The reaction was quenched with saturated NH₄Cl and extracted with ethyl acetate. The combined organic layer was dried over Na₂SO₄, filtered and concentrated under reduced pressure to afford the crude product, which was purified by flash column chromatography (PE/EA) to give the corresponding products **1**.



Preparation of **4a-4q**³. To a solution of benzoyl chloride (1.45 mL, 12.5 mmol) in DCM (20 mL) was added dropwise a solution of allylamine (0.75 mL, 10 mmol) and Et₃N (1.39 mL, 10 mmol) in DCM (20 mL) at 0 °C. After the addition, the reaction was allowed to warm to room temperature and stirred overnight. The reaction was quenched with water and the aqueous layer was washed with DCM. The organic layers were combined and evaporated under vacuum. The residue was purified by a flash chromatograph (PE/EA) on silica gel to give desired products **4**.



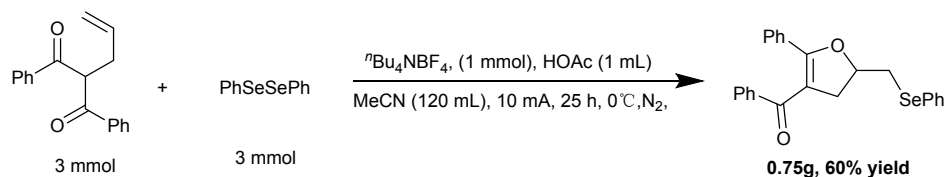
2) General procedure for preparation electrochemical oxidative cyclization of olefinic carbonyls with diselenides



In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, olefinic carbonyl compounds **1** (0.3 mmol), diselenides **2** (0.3 mmol), and *n*Bu₄NBF₄ (0.1 mmol) were combined and added. The bottle was equipped with graphite rod (ϕ 6 mm, about 18 mm immersion depth in solution) as the anode and platinum plate (1.5 cm × 1.5 cm × 1 mm) as the cathode and was then charged with nitrogen. Under the protection of N₂, HOAc (0.1 mL), MeCN (12.0 mL) were injected respectively into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a

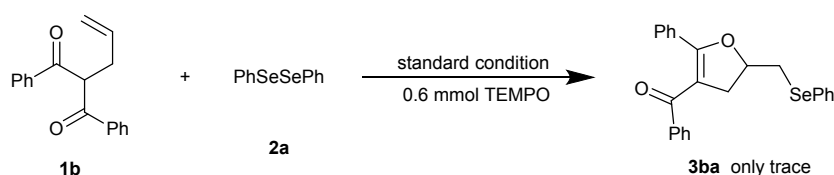
constant current of 10 mA at 0°C for 3 h. When the reaction was finished, the pure product was purified by flash column chromatography (PE/EA) on silica gel.

3) Gram-scale experiments



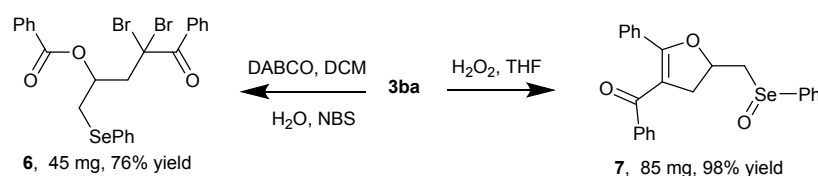
In an oven-dried undivided three-necked bottle (150 mL) equipped with a stir bar, olefinic carbonyl compounds **1b** (3 mmol), diselenides **2** (3 mmol), and $t\text{Bu}_4\text{NBF}_4$ (1 mmol) were combined and added. The bottle was equipped with graphite rod (ϕ 6 mm) as the anode and platinum plate (1.5 cm $\times$ 1.5 cm $\times$ 1 mm) as the cathode and was then charged with nitrogen. Under the protection of N_2 , HOAc (1 mL), MeCN (120 mL) were injected respectively into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA at 0°C for 25 h. When the reaction was finished, the pure product was purified by flash column chromatography (PE/EA) on silica gel.

4) Control experiment



In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, olefinic carbonyl compounds **1b** (0.3 mmol), diselenides **2** (0.3 mmol), TEMPO (0.5 mmol) and $t\text{Bu}_4\text{NBF}_4$ (0.1 mmol) were combined and added. The bottle was equipped with graphite rod (ϕ 6 mm, about 18 mm immersion depth in solution) as the anode and platinum plate (1.5 cm $\times$ 1.5 cm $\times$ 1 mm) as the cathode and was then charged with nitrogen. Under the protection of N_2 , HOAc (0.1 mL), MeCN (12.0 mL) were injected respectively into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA at 0°C for 3 h.

5) Derivatization of products

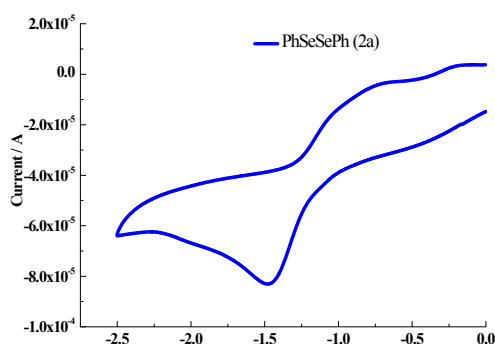
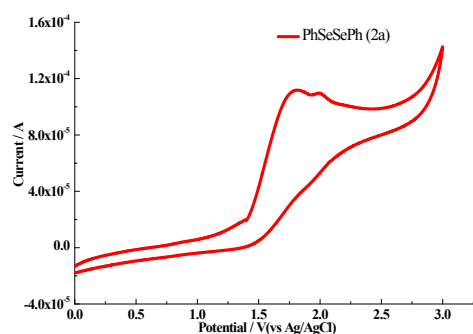


Preparation of **6**. To a solution of **3ba** (0.1 mmol, 1 equiv), DABCO (0.02 mmol, 0.2 equiv) and 30 μL H_2O in dichloromethane (AR grade, 2 mL) was added NBS (0.25 mmol, 2.5 equiv) under an N_2 atmosphere. The resulting mixture was stirred for 3 h in the absence of light at room temperature. When the reaction was finished, the pure product was purified by flash column chromatography (PE/EA) on silica gel.

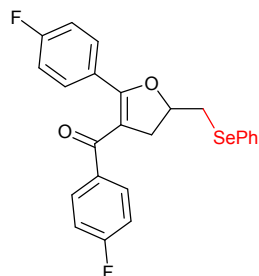
Preparation of **7**. A mixture of **3ba** (0.2 mmol, 1 equiv) and H₂O₂ (30% in H₂O, 2 equiv) in anhydrous THF (2 mL) was stirred at room temperature until complete consumption of the starting material, as monitored by TLC. After the evaporation of the solvent, the residual crude product was purified by flash chromatography.

6) Procedure for cyclic voltammetry (CV)

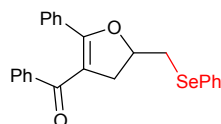
Cyclic voltammetry was performed in a three-electrode cell connected to a schlenk line under nitrogen at room temperature. The working electrode was a steady glassy carbon disk electrode, the counter electrode a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution, and separated from reaction by a salt bridge. 12 mL of MeCN containing 0.04 M *n*Bu₄NBF₄ were poured into the electrochemical cell in all experiments. The CV of substrates (**2a**) were measured at the concentration of 0.01M. The scan rate of **2a** is 0.05 V/s, ranging from 0 V to 3.0 V and 0 V to -2.5 V.



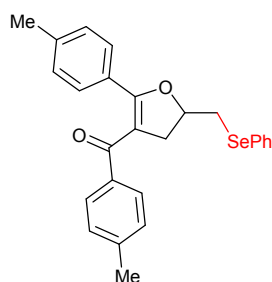
Detail descriptions for products



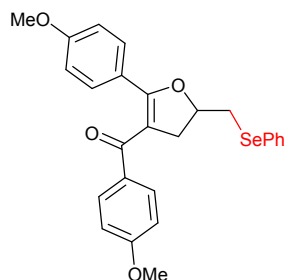
(4-fluorophenyl)(2-(4-fluorophenyl)-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)methanone (3aa). colorless oil was obtained in 90% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.54 (m, 2H), 7.47 (m, 2H), 7.31 – 7.22 (m, 3H), 7.15 – 7.07 (m, 2H), 6.77 (dt, J = 12.7, 8.6 Hz, 4H), 5.01 (m, 1H), 3.44 (dd, J = 15.2, 9.9 Hz, 1H), 3.36 (dd, J = 12.7, 5.5 Hz, 1H), 3.22 (dd, J = 12.7, 6.8 Hz, 1H), 3.10 (dd, J = 15.2, 7.4 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 191.51, 165.29 (d, J = 101.4 Hz), 164.06, 162.78 (d, J = 100.6 Hz), 135.08 (d, J = 3.0 Hz), 133.23, 131.50 (d, J = 8.7 Hz), 131.33 (d, J = 8.9 Hz), 129.31, 129.17, 127.50, 125.95 (d, J = 3.3 Hz), 115.02 (d, J = 4.1 Hz), 114.80 (d, J = 4.3 Hz), 111.42, 81.08, 38.62, 32.53. ^{19}F NMR (377 MHz, CDCl_3) δ -107.34, -108.58. HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{19}\text{F}_2\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 457.0513 found 457.0506.



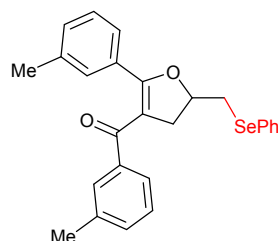
phenyl(2-phenyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)methanone (3ba)⁴. colorless oil was obtained in 91% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.59 (m, 2H), 7.50 – 7.38 (m, 2H), 7.31 – 7.24 (m, 3H), 7.24 – 7.10 (m, 4H), 7.09 – 6.99 (m, 4H), 5.01 (m, 1H), 3.51 – 3.32 (m, 2H), 3.22 (dd, J = 12.6, 7.1 Hz, 1H), 3.12 (dd, J = 15.2, 7.3 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.41, 165.47, 138.97, 133.30, 131.22, 130.06, 129.90, 129.38, 129.32, 129.23, 128.94, 127.70, 127.63, 127.50, 111.70, 81.04, 38.60, 32.62.



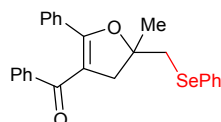
(5-((phenylselanyl)methyl)-2-(p-tolyl)-4,5-dihydrofuran-3-yl)(p-tolyl)methanone (3ca). colorless oil was obtained in 75% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.63 – 7.52 (m, 2H), 7.42 – 7.35 (m, 2H), 7.31 – 7.23 (m, 3H), 7.10 – 7.02 (m, 2H), 6.90 (d, J = 7.9 Hz, 2H), 6.85 (d, J = 7.9 Hz, 2H), 4.97 (m, 1H), 3.48 – 3.34 (m, 2H), 3.20 (dd, J = 12.6, 7.2 Hz, 1H), 3.09 (dd, J = 15.2, 7.3 Hz, 1H), 2.24 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.26, 164.73, 141.80, 140.27, 136.36, 133.29, 129.32, 129.15, 128.44, 128.35, 127.47, 127.14, 110.89, 80.74, 38.97, 32.60, 21.52, 21.46. HRMS (ESI) calculated for $\text{C}_{26}\text{H}_{25}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 449.1014 found 449.1007.



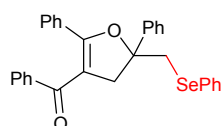
(4-methoxyphenyl)(2-(4-methoxyphenyl)-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)methanone (3da). colorless oil was obtained in 56% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.58 (m, 2H), 7.57 – 7.50 (m, 2H), 7.34 – 7.27 (m, 3H), 7.23 – 7.15 (m, 2H), 6.70 – 6.59 (m, 4H), 4.99 (m, 1H), 3.77 (s, 3H), 3.75 (s, 3H), 3.51 – 3.37 (m, 2H), 3.24 (dd, J = 12.6, 7.1 Hz, 1H), 3.12 (dd, J = 15.1, 7.3 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 192.30, 163.78, 162.27, 160.88, 133.31, 131.69, 131.31, 131.09, 129.39, 129.34, 127.48, 122.47, 113.19, 113.13, 110.05, 80.52, 55.41, 55.35, 39.21, 32.63. HRMS (ESI) calculated for $\text{C}_{26}\text{H}_{25}\text{O}_4\text{Se}^+$ $[\text{M}+\text{H}]^+$ 481.0913 found 481.0905.



(5-((phenylselanyl)methyl)-2-(m-tolyl)-4,5-dihydrofuran-3-yl)(m-tolyl)methanone (3ea). colorless oil was obtained in 69% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.59 (m, 2H), 7.31 – 7.16 (m, 5H), 7.04 – 6.90 (m, 5H), 6.86 (m, 1H), 5.00 (m, 1H), 3.50 – 3.33 (m, 2H), 3.22 (dd, J = 12.6, 7.2 Hz, 1H), 3.11 (dd, J = 15.2, 7.3 Hz, 1H), 2.10 (s, 3H), 2.06 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.69, 165.92, 139.05, 137.26, 137.23, 133.25, 131.73, 130.75, 130.18, 129.89, 129.60, 129.31, 129.28, 127.59, 127.54, 127.48, 126.22, 125.95, 111.91, 81.01, 38.42, 32.60, 21.03, 20.99. HRMS (ESI) calculated for $\text{C}_{26}\text{H}_{25}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 449.1014 found 449.1005.

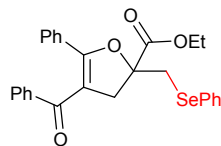


(5-methyl-2-phenyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (3fa). colorless oil was obtained in 78% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.53 (m, 2H), 7.47 – 7.41 (m, 2H), 7.27 – 7.21 (m, 3H), 7.21 – 6.95 (m, 8H), 3.46 – 3.27 (m, 3H), 3.18 (d, J = 15.1 Hz, 1H), 1.66 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.50, 164.88, 139.12, 132.92, 131.10, 130.63, 130.15, 129.95, 129.36, 129.27, 128.96, 127.66, 127.59, 127.24, 111.86, 87.63, 44.04, 39.23, 26.89. HRMS (ESI) calculated for $\text{C}_{25}\text{H}_{23}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 430.0858 found 430.0853.



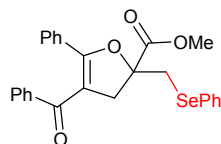
(2,5-diphenyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (3ga). white solid was obtained in 71% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.41 (m, 6H), 7.36 (dd, J = 8.4, 6.7 Hz, 2H), 7.32 – 7.25 (m, 1H), 7.18 (m, 7H), 7.04 (td, J = 7.6, 4.7 Hz, 4H), 3.80 –

3.55 (m, 4H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.19, 164.46, 144.24, 138.95, 133.01, 131.21, 130.57, 130.09, 129.86, 129.49, 129.13, 128.99, 128.60, 127.87, 127.70, 127.64, 127.16, 124.93, 112.00, 89.73, 45.10, 41.48. HRMS (ESI) calculated for $\text{C}_{30}\text{H}_{25}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 497.1014 found 497.1009.



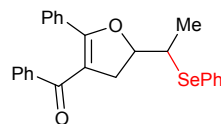
ethyl 4-benzoyl-5-phenyl-2-((phenylselanyl)methyl)-2,3-dihydrofuran-2-carboxylate (3ha).

colorless oil was obtained in 68% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.56 (m, 2H), 7.51 – 7.43 (m, 2H), 7.31 – 7.23 (m, 4H), 7.19 (dt, J = 8.6, 1.6 Hz, 3H), 7.15 – 7.02 (m, 4H), 4.25 (m, 2H), 3.71 – 3.56 (m, 3H), 3.51 (d, J = 15.7 Hz, 1H), 1.31 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.01, 170.86, 164.63, 138.53, 133.62, 131.48, 130.26, 129.83, 129.57, 129.26, 129.19, 129.01, 127.76, 127.62, 127.56, 111.25, 88.07, 62.23, 42.72, 34.92, 14.18. HRMS (ESI) calculated for $\text{C}_{27}\text{H}_{25}\text{O}_4\text{Se}^+$ $[\text{M}+\text{H}]^+$ 493.0913 found 493.0906.

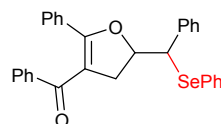


methyl 4-benzoyl-5-phenyl-2-((phenylselanyl)methyl)-2,3-dihydrofuran-2-carboxylate (3ia).

colorless oil was obtained in 55% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.64 – 7.55 (m, 2H), 7.49 – 7.40 (m, 2H), 7.23 (m, 4H), 7.19 – 7.11 (m, 3H), 7.11 – 6.99 (m, 4H), 3.74 (s, 3H), 3.66 – 3.52 (m, 3H), 3.46 (d, J = 15.8 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 192.99, 171.38, 164.47, 138.53, 133.69, 131.55, 130.32, 129.71, 129.59, 129.25, 129.23, 129.05, 127.82, 127.67, 127.65, 111.24, 88.09, 53.04, 42.71, 35.00. HRMS (ESI) calculated for $\text{C}_{25}\text{H}_{23}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 435.0858 found 435.0851.



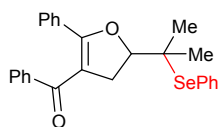
phenyl(2-phenyl-5-(1-(phenylselanyl)ethyl)-4,5-dihydrofuran-3-yl)methanone (3ja). colorless oil was obtained in 70% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.67 (m, 2H), 7.48 (m, 2H), 7.38 – 7.28 (m, 3H), 7.28 – 7.15 (m, 4H), 7.14 – 7.02 (m, 4H), 5.03 – 4.84 (m, 1H), 3.77 – 3.54 (m, 1H), 3.46 (m, 1H), 3.29 (m, 1H), 1.60 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.41, 193.39, 165.78, 165.74, 139.06, 135.73, 135.13, 131.15, 130.03, 130.01, 129.98, 129.95, 129.36, 129.31, 129.23, 129.14, 128.95, 128.93, 128.30, 128.10, 127.98, 127.69, 127.65, 127.60, 112.23, 112.00, 85.22, 84.52, 43.52, 42.65, 37.34, 35.59, 18.07, 16.60. HRMS (ESI) calculated for $\text{C}_{25}\text{H}_{23}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 430.0858 found 430.0851.



phenyl(2-phenyl-5-(phenyl(phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)methanone (3ka).

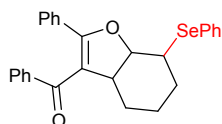
colorless oil was obtained in 37% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.41 (m, 2H), 7.36 – 7.16 (m, 11H), 7.16 – 7.07 (m, 3H), 7.06 – 6.96 (m, 4H), 5.31 (ddd, J = 10.2, 7.8, 6.5 Hz, 1H), 4.51 (d, J = 6.5 Hz, 1H), 3.50 (dd, J = 15.3, 10.1 Hz, 1H), 3.27 (dd, J = 15.4, 7.8 Hz, 1H). ^{13}C

NMR (101 MHz, CDCl₃) δ 193.39, 165.36, 138.97, 138.79, 135.77, 131.26, 130.07, 129.81, 129.43, 129.11, 128.96, 128.95, 128.48, 128.41, 128.35, 127.70, 127.64, 127.59, 111.94, 83.39, 52.71, 37.93. HRMS (ESI) calculated for C₃₀H₂₅O₂Se⁺ [M+H]⁺ 497.1014 found 497.1004.



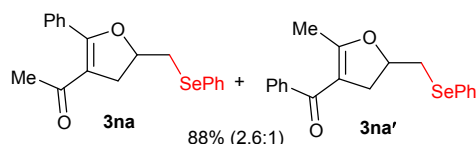
phenyl(2-phenyl-5-(2-(phenylselanyl)propan-2-yl)-4,5-dihydrofuran-3-yl)methanone (3la).

colorless oil was obtained in 26% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.76 – 7.65 (m, 2H), 7.47 – 7.34 (m, 3H), 7.34 – 7.27 (m, 2H), 7.24 – 7.13 (m, 4H), 7.10 – 7.00 (m, 4H), 4.73 (dd, *J* = 10.0, 9.0 Hz, 1H), 3.38 (dd, *J* = 9.4, 1.3 Hz, 2H), 1.51 (s, 3H), 1.48 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 193.56, 166.03, 139.19, 138.61, 131.18, 130.11, 130.06, 129.38, 129.06, 129.00, 128.96, 127.75, 127.69, 126.45, 112.39, 88.49, 48.94, 35.47, 26.34, 24.16. HRMS (ESI) calculated for C₂₆H₂₅O₂Se⁺ [M+H]⁺ 449.1014 found 449.1008.



phenyl(2-phenyl-7-(phenylselanyl)-3a,4,5,6,7,7a-hexahydrobenzofuran-3-yl)methanone (3ma).

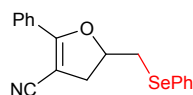
colorless oil was obtained in 52% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.65 (m, 2H), 7.53 – 7.45 (m, 2H), 7.39 – 7.29 (m, 3H), 7.26 – 7.18 (m, 1H), 7.16 – 7.10 (m, 1H), 7.10 – 7.04 (m, 4H), 7.03 – 6.96 (m, 2H), 4.80 (dd, *J* = 7.4, 5.8 Hz, 1H), 3.76 (ddd, *J* = 7.9, 5.8, 4.4 Hz, 1H), 3.68 (q, *J* = 6.9 Hz, 1H), 2.21 – 2.00 (m, 2H), 1.79 (m, 2H), 1.65 – 1.52 (m, 1H), 1.47 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 193.60, 165.48, 138.98, 135.48, 131.53, 130.16, 130.05, 129.54, 129.29, 129.17, 128.61, 128.09, 127.80, 127.67, 117.53, 85.29, 44.20, 43.11, 28.92, 26.37, 21.06. HRMS (ESI) calculated for C₂₇H₂₅O₂Se⁺ [M+H]⁺ 461.1014 found 461.1006.



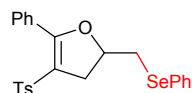
1-(2-phenyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)ethan-1-one (3na) and (2-methyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (3na'). colorless oil was obtained in 88% isolated yield.

3na: ¹H NMR (400 MHz, Chloroform-*d*) δ 7.55 (m, 4H), 7.50 – 7.44 (m, 1H), 7.43 – 7.36 (m, 2H), 7.30 – 7.22 (m, 3H), 4.84 (m, 1H), 3.29 – 3.17 (m, 2H), 3.10 (dd, *J* = 12.7, 6.9 Hz, 1H), 2.97 – 2.86 (m, 1H), 1.76 (t, *J* = 1.5 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 193.12, 168.49, 140.85, 133.24, 131.10, 129.29, 129.25, 128.32, 127.83, 127.50, 112.27, 81.31, 36.94, 32.68, 15.52. HRMS (ESI) calculated for C₁₉H₁₉O₂Se⁺ [M+H]⁺ 359.0545 found 359.0541.

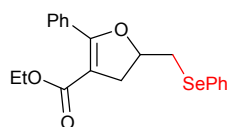
3na': ¹H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.53 (m, 2H), 7.51 – 7.37 (m, 5H), 7.30 – 7.23 (m, 3H), 4.91 (m, 1H), 3.40 – 3.20 (m, 2H), 3.13 (dd, *J* = 12.6, 7.3 Hz, 1H), 2.95 (dd, *J* = 15.2, 7.2 Hz, 1H), 1.94 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 194.71, 165.83, 133.39, 130.78, 130.73, 129.36, 129.29, 129.20, 128.41, 127.58, 114.42, 81.23, 37.18, 32.75, 29.07. HRMS (ESI) calculated for C₁₉H₁₉O₂Se⁺ [M+H]⁺ 359.0545 found 359.0541.



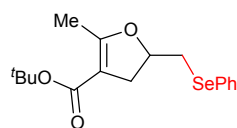
2-phenyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-carbonitrile (30a)⁴. colorless oil was obtained in 76% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.92 – 7.83 (m, 2H), 7.64 – 7.57 (m, 2H), 7.52 – 7.40 (m, 3H), 7.36 – 7.26 (m, 3H), 5.03 (m, 1H), 3.34 (dd, *J* = 12.8, 5.4 Hz, 1H), 3.25 (dd, *J* = 14.9, 10.1 Hz, 1H), 3.14 (dd, *J* = 12.8, 7.4 Hz, 1H), 2.92 (dd, *J* = 14.8, 7.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 166.48, 133.48, 131.40, 129.38, 128.66, 128.63, 127.81, 127.73, 127.07, 117.65, 82.13, 79.00, 37.16, 32.08.



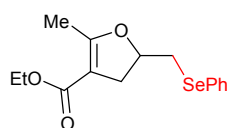
5-phenyl-2-((phenylselanyl)methyl)-4-tosyl-2,3-dihydrofuran (3pa). colorless oil was obtained in 50% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.64 – 7.55 (m, 4H), 7.50 – 7.45 (m, 2H), 7.45 – 7.41 (m, 1H), 7.40 – 7.32 (m, 2H), 7.29 – 7.20 (m, 5H), 4.87 (m, 1H), 3.34 – 3.16 (m, 2H), 3.05 (dd, *J* = 12.7, 7.4 Hz, 1H), 2.94 (dd, *J* = 14.7, 7.2 Hz, 1H), 2.39 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 163.10, 143.78, 138.89, 133.38, 130.98, 129.67, 129.55, 129.36, 128.79, 128.42, 127.82, 127.65, 127.10, 110.32, 80.60, 37.75, 32.34, 21.67. HRMS (ESI) calculated for C₂₄H₂₃O₃SSe⁺ [M+H]⁺ 471.0528 found 457.0514.



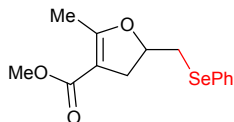
ethyl 2-phenyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-carboxylate (3qa)³. colorless oil was obtained in 65% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.67 (m, 2H), 7.60 – 7.52 (m, 2H), 7.45 – 7.31 (m, 3H), 7.29 – 7.21 (m, 3H), 4.89 (m, 1H), 4.12 (q, *J* = 7.1 Hz, 2H), 3.39 – 3.20 (m, 2H), 3.10 (dd, *J* = 12.6, 7.5 Hz, 1H), 2.93 (dd, *J* = 15.4, 7.1 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 165.27, 164.58, 133.34, 130.42, 129.91, 129.39, 129.31, 129.20, 127.65, 127.48, 102.07, 80.51, 59.89, 37.27, 32.65, 14.35.



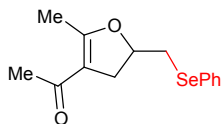
tert-butyl 2-methyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-carboxylate (3ra). colorless oil was obtained in 41% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.62 – 7.48 (m, 2H), 7.27 (dd, *J* = 4.8, 1.8 Hz, 3H), 4.72 (m, 1H), 3.19 (dd, *J* = 12.5, 5.8 Hz, 1H), 3.07 – 2.87 (m, 2H), 2.63 (m, 1H), 2.10 (m, 3H), 1.47 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ 166.23, 165.72, 133.26, 129.28, 127.45, 103.17, 80.72, 79.70, 35.90, 32.86, 28.52, 14.20. HRMS (ESI) calculated for C₂₆H₂₅O₂Se⁺ [M+H]⁺ 449.1014 found 449.1007. HRMS (ESI) calculated for C₁₇H₂₂O₃SeNa⁺ [M+Na]⁺ 377.0626 found 377.0620.



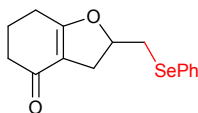
ethyl 2-methyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-carboxylate (3sa). colorless oil was obtained in 78% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.49 (m, 2H), 7.26 (m, 3H), 4.76 (m, 1H), 4.16 (q, J = 7.1 Hz, 2H), 3.20 (dd, J = 12.6, 5.7 Hz, 1H), 3.10 – 2.95 (m, 2H), 2.69 (m, 1H), 2.13 (t, J = 1.6 Hz, 3H), 1.27 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 167.46, 166.12, 133.20, 129.26, 129.24, 127.41, 101.70, 81.00, 59.57, 35.51, 32.76, 14.54, 14.14. HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{19}\text{O}_3\text{Se}^+$ $[\text{M}+\text{H}]^+$ 327.0494 found 327.0492.



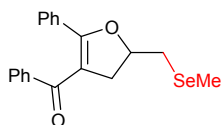
methyl 2-methyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-carboxylate (3ta)⁴. colorless oil was obtained in 82% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.49 (m, 2H), 7.33 – 7.19 (m, 3H), 4.76 (m, 1H), 3.69 (s, 3H), 3.19 (dd, J = 12.5, 5.7 Hz, 1H), 3.10 – 2.94 (m, 2H), 2.69 (m, 1H), 2.13 (t, J = 1.6 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 167.84, 166.51, 133.25, 129.29, 129.27, 127.46, 101.48, 81.13, 50.95, 35.50, 32.79, 14.13.



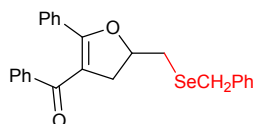
1-(2-methyl-5-((phenylselanyl)methyl)-4,5-dihydrofuran-3-yl)ethan-1-one (3ua)⁴. colorless oil was obtained in xx% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.50 (m, 2H), 7.27 (q, J = 2.7 Hz, 3H), 4.78 (m, 1H), 3.20 (dd, J = 12.6, 5.5 Hz, 1H), 3.14 – 2.99 (m, 2H), 2.82 – 2.69 (m, 1H), 2.17 (s, 3H), 2.15 (t, J = 1.5 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 194.59, 167.31, 133.28, 129.30, 129.18, 127.54, 111.84, 81.15, 36.20, 32.72, 29.57, 15.05.



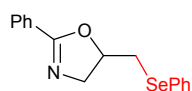
2-((phenylselanyl)methyl)-3,5,6,7-tetrahydrobenzofuran-4(2H)-one (3va). colorless oil was obtained in 93% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.54 (m, 2H), 7.28 (m, 3H), 4.95 (m, 1H), 3.22 (dd, J = 12.7, 5.9 Hz, 1H), 3.08 (dd, J = 12.8, 6.8 Hz, 1H), 3.03 – 2.91 (m, 1H), 2.64 (m, 1H), 2.44 – 2.23 (m, 4H), 2.07 – 1.93 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 195.56, 177.04, 133.35, 129.28, 129.02, 127.58, 112.95, 84.38, 36.45, 32.72, 31.82, 23.89, 21.69. HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{17}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 309.0388 found 309.0386.



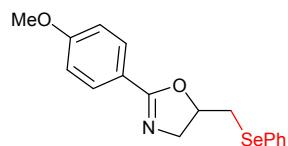
(5-((methylselanyl)methyl)-2-phenyl-4,5-dihydrofuran-3-yl)(phenyl)methanone (3ab). white solid was obtained in 60% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 7.42 (m, 2H), 7.25 – 7.14 (m, 4H), 7.11 – 7.01 (m, 4H), 5.07 (m, 1H), 3.46 (dd, J = 15.1, 9.8 Hz, 1H), 3.13 (dd, J = 15.1, 7.7 Hz, 1H), 3.01 (dd, J = 12.7, 5.6 Hz, 1H), 2.92 (dd, J = 12.8, 6.8 Hz, 1H), 2.11 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.52, 165.53, 139.04, 131.22, 130.09, 130.03, 129.40, 128.96, 127.72, 127.70, 111.86, 81.87, 38.79, 30.06, 5.35. HRMS (ESI) calculated for $\text{C}_{19}\text{H}_{19}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 359.0545 found 359.0541.



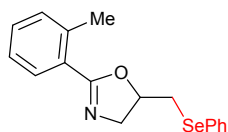
(5-((benzylselanyl)methyl)-2-phenyl-4,5-dihydrofuran-3-yl)(phenyl)methanone (3ac). colorless oil was obtained in 50% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.42 (m, 2H), 7.28 (d, J = 4.4 Hz, 4H), 7.24 – 7.13 (m, 5H), 7.06 (m, 4H), 4.96 (m, 1H), 3.88 (s, 2H), 3.39 (dd, J = 15.1, 9.8 Hz, 1H), 3.06 (dd, J = 15.2, 7.7 Hz, 1H), 2.98 – 2.82 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.50, 165.46, 139.05, 138.95, 131.25, 130.13, 130.03, 129.44, 129.06, 129.00, 128.70, 127.74, 127.73, 127.04, 111.90, 81.82, 38.80, 28.40, 27.95. HRMS (ESI) calculated for $\text{C}_{25}\text{H}_{23}\text{O}_2\text{Se}^+$ $[\text{M}+\text{H}]^+$ 435.0858 found 430.0853.



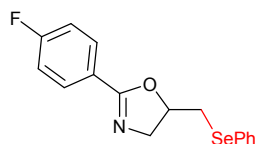
2-phenyl-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5aa)³. colorless oil was obtained in 88% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.78 (m, 2H), 7.56 (dd, J = 6.5, 3.0 Hz, 2H), 7.48 – 7.42 (m, 1H), 7.37 (dd, J = 8.3, 6.7 Hz, 2H), 7.25 (m, J = 3.6 Hz, 3H), 4.87 (m, 1H), 4.14 (dd, J = 15.0, 9.5 Hz, 1H), 3.81 (dd, J = 15.0, 6.9 Hz, 1H), 3.27 (dd, J = 12.7, 5.5 Hz, 1H), 3.03 (dd, J = 12.7, 7.5 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 163.72, 133.40, 131.38, 129.30, 128.95, 128.34, 128.18, 127.65, 127.54, 78.89, 60.28, 31.98.



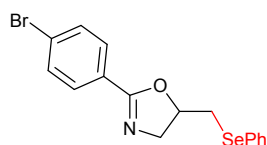
2-(4-methoxyphenyl)-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5ba)³. colorless oil was obtained in 82% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.75 (m, 2H), 7.62 – 7.50 (m, 2H), 7.27 (m, 3H), 6.94 – 6.83 (m, 2H), 4.86 (m, 1H), 4.13 (dd, J = 14.8, 9.4 Hz, 1H), 3.84 (s, 3H), 3.79 (dd, J = 14.8, 6.8 Hz, 1H), 3.28 (dd, J = 12.7, 5.5 Hz, 1H), 3.04 (dd, J = 12.7, 7.5 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 163.66, 162.15, 133.47, 129.99, 129.36, 129.06, 127.59, 120.21, 113.75, 78.87, 60.28, 55.48, 32.09.



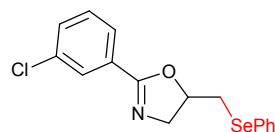
5-((phenylselanyl)methyl)-2-(o-tolyl)-4,5-dihydrooxazole (5ca). colorless oil was obtained in 74% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.69 (dd, J = 7.8, 1.5 Hz, 1H), 7.59 – 7.50 (m, 2H), 7.38 – 7.09 (m, 6H), 4.81 (m, 1H), 4.16 (dd, J = 14.9, 9.5 Hz, 1H), 3.84 (dd, J = 14.9, 6.8 Hz, 1H), 3.26 (dd, J = 12.6, 5.4 Hz, 1H), 3.03 (dd, J = 12.6, 7.5 Hz, 1H), 2.57 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.12, 138.80, 133.40, 131.26, 130.61, 129.90, 129.30, 128.96, 127.54, 126.98, 125.59, 77.88, 60.61, 32.04, 21.95. HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{18}\text{NOSe}^+$ $[\text{M}+\text{H}]^+$ 332.0548 found 332.0544.



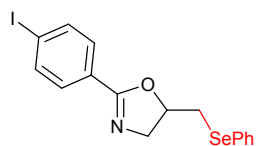
2-(4-fluorophenyl)-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5da)³. colorless oil was obtained in 70% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.83 (dd, J = 8.8, 5.5 Hz, 2H), 7.65 – 7.49 (m, 2H), 7.25 (dd, J = 5.0, 1.8 Hz, 3H), 7.04 (t, J = 8.7 Hz, 2H), 4.88 (m, 1H), 4.13 (dd, J = 14.9, 9.5 Hz, 1H), 3.80 (dd, J = 14.9, 6.9 Hz, 1H), 3.26 (dd, J = 12.8, 5.5 Hz, 1H), 3.04 (dd, J = 12.8, 7.2 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 164.73 (d, J = 251.7 Hz), 162.88, 133.44, 130.47 (d, J = 8.8 Hz), 129.34, 128.96, 127.61, 123.93 (d, J = 3.2 Hz), 115.50 (d, J = 22.0 Hz), 79.16, 60.33, 31.99. ¹⁹F NMR (377 MHz, CDCl₃) δ -108.11.



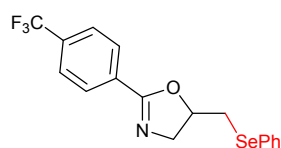
2-(4-bromophenyl)-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5ea)³. colorless oil was obtained in 58% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.64 (m, 2H), 7.60 – 7.45 (m, 4H), 7.26 (m, 3H), 4.88 (m, 1H), 4.14 (dd, J = 15.1, 9.5 Hz, 1H), 3.80 (dd, J = 15.1, 6.9 Hz, 1H), 3.26 (dd, J = 12.8, 5.4 Hz, 1H), 3.04 (dd, J = 12.8, 7.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 162.99, 133.44, 131.62, 129.74, 129.34, 128.92, 127.62, 126.61, 126.08, 79.22, 60.37, 31.96.



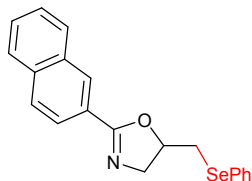
2-(3-chlorophenyl)-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5fa). colorless oil was obtained in 49% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.79 (t, J = 1.9 Hz, 1H), 7.73 (dt, J = 7.8, 1.4 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.42 (ddd, J = 8.1, 2.2, 1.1 Hz, 1H), 7.34 – 7.18 (m, 4H), 4.90 (m, 1H), 4.15 (dd, J = 15.1, 9.5 Hz, 1H), 3.83 (dd, J = 15.2, 6.9 Hz, 1H), 3.26 (dd, J = 12.8, 5.4 Hz, 1H), 3.06 (dd, J = 12.9, 7.2 Hz, 1H). HRMS (ESI) calculated for C₁₆H₁₅ClNOSe⁺ [M+H]⁺ 352.0002 found 351.9999.



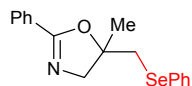
2-(4-iodophenyl)-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5ga). colorless oil was obtained in 79% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.71 (dd, J = 8.5, 1.8 Hz, 2H), 7.59 – 7.48 (m, 4H), 7.30 – 7.19 (m, 3H), 4.87 (m, 1H), 4.12 (dd, J = 15.1, 9.5, 1.6 Hz, 1H), 3.79 (dd, J = 15.1, 7.0, 1.2 Hz, 1H), 3.25 (dd, J = 12.8, 5.5, 1.6 Hz, 1H), 3.03 (dd, J = 12.8, 7.3, 1.6 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 163.08, 137.52, 133.37, 129.69, 129.28, 128.87, 127.55, 127.09, 98.46, 79.14, 60.29, 31.90. HRMS (ESI) calculated for C₁₆H₁₅IINOSe⁺ [M+H]⁺ 433.9358 found 433.9348.



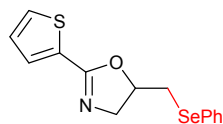
5-((phenylselanyl)methyl)-2-(4-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (5ha)³. colorless oil was obtained in 69% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 8.1 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.60 – 7.50 (m, 2H), 7.26 (dd, *J* = 4.9, 1.9 Hz, 3H), 4.93 (m, 1H), 4.18 (dd, *J* = 15.3, 9.5 Hz, 1H), 3.86 (dd, *J* = 15.2, 6.9 Hz, 1H), 3.27 (dd, *J* = 12.8, 5.4 Hz, 1H), 3.07 (dd, *J* = 12.8, 7.2 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 162.63, 133.49, 132.97 (d, *J* = 32.7 Hz), 131.03, 129.37, 128.88, 128.60, 127.68, 125.35 (q, *J* = 3.8 Hz), 123.87 (d, *J* = 272.5 Hz), 79.39, 60.42, 31.94. ¹⁹F NMR (377 MHz, CDCl₃) δ -62.90.



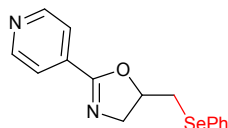
2-(naphthalen-2-yl)-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5ia)³. colorless oil was obtained in 65% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.28 (s, 1H), 7.96 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.84 (m, 3H), 7.67 – 7.41 (m, 4H), 7.37 – 7.16 (m, 3H), 4.94 (m, 1H), 4.21 (dd, *J* = 15.0, 9.5 Hz, 1H), 3.87 (dd, *J* = 15.0, 6.9 Hz, 1H), 3.32 (dd, *J* = 12.8, 5.4 Hz, 1H), 3.09 (dd, *J* = 12.8, 7.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 163.94, 134.76, 133.45, 132.67, 129.34, 129.02, 128.99, 128.78, 128.17, 127.85, 127.62, 127.60, 126.61, 124.94, 124.76, 79.14, 60.44, 32.07.



5-methyl-2-phenyl-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5ja). colorless oil was obtained in 69% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.78 (m, 2H), 7.56 – 7.50 (m, 2H), 7.47 – 7.40 (m, 1H), 7.39 – 7.31 (m, 2H), 7.24 – 7.16 (m, 3H), 4.01 (d, *J* = 14.8 Hz, 1H), 3.79 (d, *J* = 14.8 Hz, 1H), 3.27 (s, 2H), 1.57 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 163.07, 133.10, 131.28, 130.39, 129.20, 128.29, 128.16, 127.92, 127.26, 85.89, 65.61, 38.47, 26.05. HRMS (ESI) calculated for C₁₇H₁₈NOSe⁺ [M+H]⁺ 322.0548 found 322.0543.

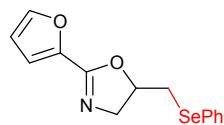


5-((phenylselanyl)methyl)-2-(thiophen-2-yl)-4,5-dihydrooxazole (5ka)³. colorless oil was obtained in 72% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.62 – 7.52 (m, 2H), 7.48 (dd, *J* = 3.7, 1.2 Hz, 1H), 7.42 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.32 – 7.19 (m, 3H), 7.04 (dd, *J* = 5.0, 3.7 Hz, 1H), 4.96 – 4.78 (m, 1H), 4.13 (dd, *J* = 14.9, 9.4 Hz, 1H), 3.79 (dd, *J* = 14.9, 6.8 Hz, 1H), 3.27 (dd, *J* = 12.7, 5.3 Hz, 1H), 3.03 (dd, *J* = 12.7, 7.8 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 159.55, 133.43, 130.32, 130.30, 129.92, 129.31, 128.81, 127.60, 79.45, 60.29, 31.76.

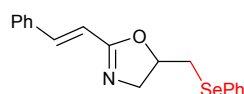


5-((phenylselanyl)methyl)-2-(pyridin-4-yl)-4,5-dihydrooxazole (5la). colorless oil was obtained in 49% isolated yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.74 – 8.60 (m, 2H), 7.68 – 7.61 (m, 2H), 7.60 – 7.53 (m, 2H), 7.27 (m, 3H), 4.94 (m, 1H), 4.19 (dd, *J* = 15.4, 9.6 Hz, 1H), 3.87 (dd, *J* = 15.5, 7.0 Hz, 1H), 3.26 (dd, *J* = 12.9, 5.3 Hz, 1H), 3.08 (dd, *J* = 12.9, 7.2 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃)

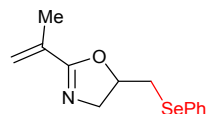
δ 162.11, 150.28, 134.98, 133.48, 129.37, 128.78, 127.71, 121.91, 79.48, 60.43, 31.83. HRMS (ESI) calculated for $C_{15}H_{15}N_2OSe^+$ $[M+H]^+$ 319.0344 found 319.0339.



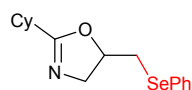
2-(furan-2-yl)-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5ma)³. colorless oil was obtained in 68% isolated yield. 1H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.46 (m, 3H), 7.33 – 7.20 (m, 3H), 6.86 (d, J = 3.4 Hz, 1H), 6.46 (dd, J = 3.5, 1.7 Hz, 1H), 4.85 (m, 1H), 4.15 (dd, J = 15.0, 9.4 Hz, 1H), 3.82 (dd, J = 15.0, 6.9 Hz, 1H), 3.27 (dd, J = 12.7, 5.2 Hz, 1H), 3.02 (dd, J = 12.7, 7.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.09, 145.27, 142.87, 133.40, 129.30, 128.74, 127.61, 114.39, 111.54, 79.16, 60.10, 31.59.



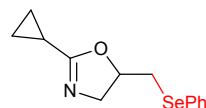
(E)-5-((phenylselanyl)methyl)-2-styryl-4,5-dihydrooxazole (5na). colorless oil was obtained in 54% isolated yield. 1H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.53 (m, 2H), 7.47 – 7.42 (m, 2H), 7.39 – 7.31 (m, 3H), 7.26 (qd, J = 3.9, 1.7 Hz, 3H), 7.20 (d, J = 16.3 Hz, 1H), 6.57 (d, J = 16.3 Hz, 1H), 4.86 – 4.72 (m, 1H), 4.08 (dd, J = 15.4, 9.4 Hz, 1H), 3.75 (dd, J = 15.3, 6.8 Hz, 1H), 3.24 (dd, J = 12.8, 5.5 Hz, 1H), 3.02 (dd, J = 12.8, 7.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.61, 140.00, 135.19, 133.36, 129.53, 129.29, 129.03, 128.87, 127.55, 127.53, 115.07, 78.63, 60.31, 31.97. HRMS (ESI) calculated for $C_{18}H_{18}NOSe^+$ $[M+H]^+$ 344.0548 found 344.0544.



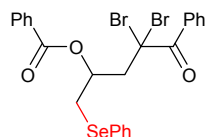
5-((phenylselanyl)methyl)-2-(prop-1-en-2-yl)-4,5-dihydrooxazole (5oa). colorless oil was obtained in 68% isolated yield. 1H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.50 (m, 2H), 7.26 (dt, J = 4.4, 1.6 Hz, 3H), 5.75 – 5.64 (m, 1H), 5.39 (q, J = 1.6 Hz, 1H), 4.74 (m, 1H), 4.05 (dd, J = 15.2, 9.4 Hz, 1H), 3.72 (dd, J = 15.3, 6.9 Hz, 1H), 3.21 (dd, J = 12.6, 5.3 Hz, 1H), 2.96 (dd, J = 12.6, 7.7 Hz, 1H), 1.98 (t, J = 1.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.76, 133.38, 132.61, 129.30, 128.97, 127.55, 122.02, 78.62, 60.40, 31.93, 19.29. HRMS (ESI) calculated for $C_{13}H_{16}NOSe^+$ $[M+H]^+$ 282.0392 found 282.0386.



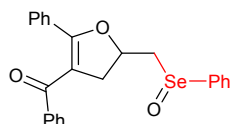
2-cyclohexyl-5-((phenylselanyl)methyl)-4,5-dihydrooxazole (5pa). colorless oil was obtained in 50% isolated yield. 1H NMR (400 MHz, Chloroform-*d*) δ 7.58 – 7.46 (m, 2H), 7.32 – 7.18 (m, 3H), 4.65 (m, 1H), 3.90 (ddd, J = 14.4, 9.5, 1.2 Hz, 1H), 3.57 (ddd, J = 14.4, 6.6, 1.1 Hz, 1H), 3.14 (dd, J = 12.6, 5.5 Hz, 1H), 2.93 (dd, J = 12.5, 7.4 Hz, 1H), 2.21 (m, 1H), 1.94 – 1.83 (m, 2H), 1.80 – 1.70 (m, 2H), 1.69 – 1.60 (m, 1H), 1.47 – 1.13 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.96, 133.31, 129.30, 129.11, 127.50, 78.00, 59.62, 37.47, 32.12, 29.82, 29.79, 25.92, 25.72, 25.71. HRMS (ESI) calculated for $C_{16}H_{22}NOSe^+$ $[M+H]^+$ 324.0861 found 324.0855.



2-cyclopropyl-5-((phenylselenanyl)methyl)-4,5-dihydrooxazole (5qa). colorless oil was obtained in 60% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.49 (m, 2H), 7.31 – 7.18 (m, 3H), 4.64 (m, 1H), 3.89 (dd, J = 14.2, 9.3 Hz, 1H), 3.55 (dd, J = 14.2, 6.7 Hz, 1H), 3.13 (dd, J = 12.6, 5.4 Hz, 1H), 2.93 (dd, J = 12.7, 7.4 Hz, 1H), 1.59 (m, 1H), 0.96 – 0.87 (m, 1H), 0.87 – 0.73 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 168.71, 133.31, 129.30, 129.03, 127.53, 78.40, 59.75, 31.93, 8.76, 6.90, 6.84. HRMS (ESI) calculated for $\text{C}_{13}\text{H}_{16}\text{NOSe}^+$ $[\text{M}+\text{H}]^+$ 282.0392 found 282.0386.



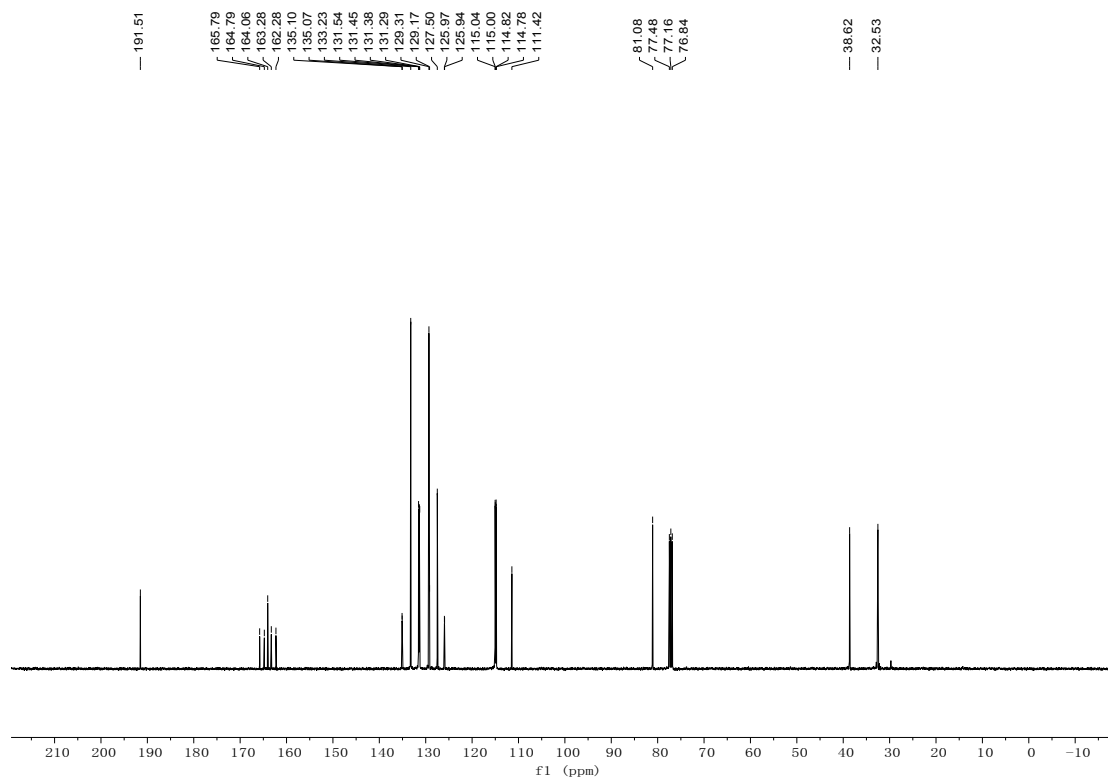
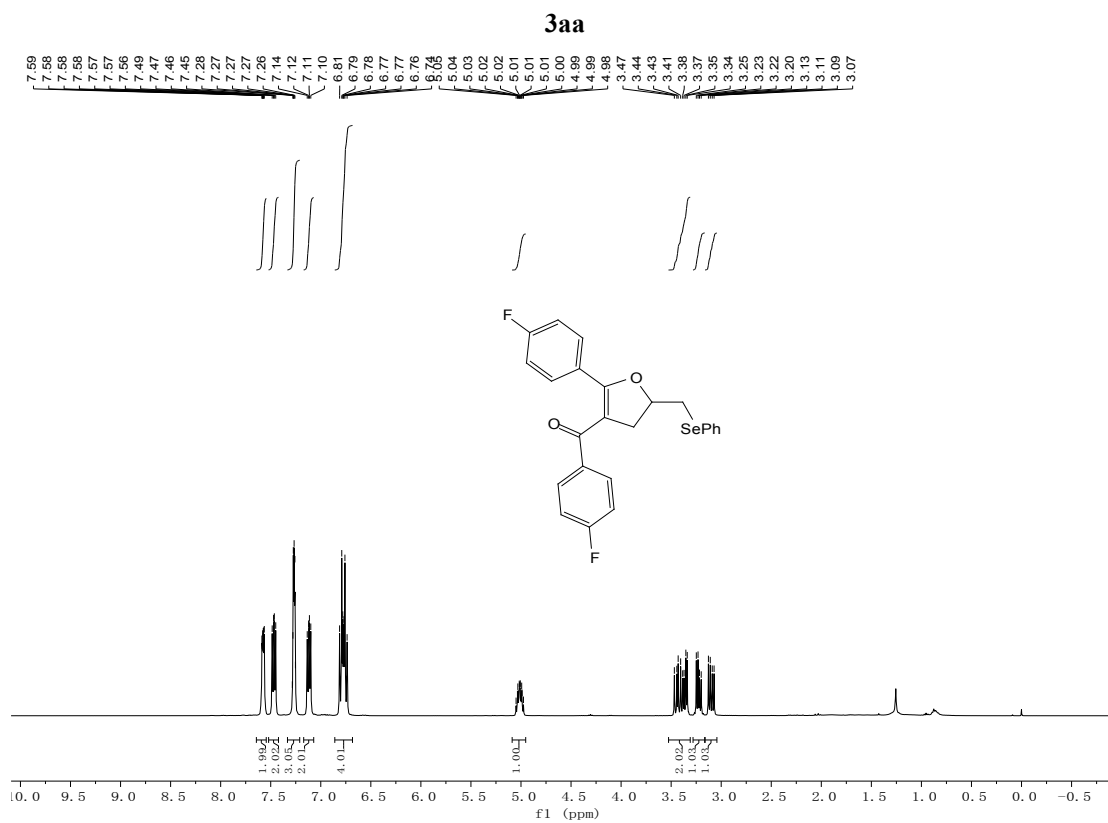
4,4-dibromo-5-oxo-2,5-diphenyl-1-(phenylselenanyl)pentan-2-yl benzoate (6). colorless oil was obtained in 76% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.19 (dt, J = 7.3, 1.3 Hz, 2H), 7.90 – 7.74 (m, 2H), 7.56 – 7.38 (m, 4H), 7.30 (dt, J = 13.5, 7.8 Hz, 4H), 7.19 – 7.01 (m, 3H), 5.68 (m, 1H), 3.49 – 3.22 (m, 4H). ^{13}C NMR (101 MHz, CDCl_3) δ 188.12, 165.61, 133.53, 133.12, 132.97, 132.03, 131.27, 129.91, 129.88, 129.52, 129.24, 128.33, 128.03, 127.29, 72.24, 61.43, 50.10, 32.42. HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{24}\text{Br}_2\text{O}_3\text{SeNa}^+$ $[\text{M}+\text{Na}]^+$ 618.8837 found 616.8837.

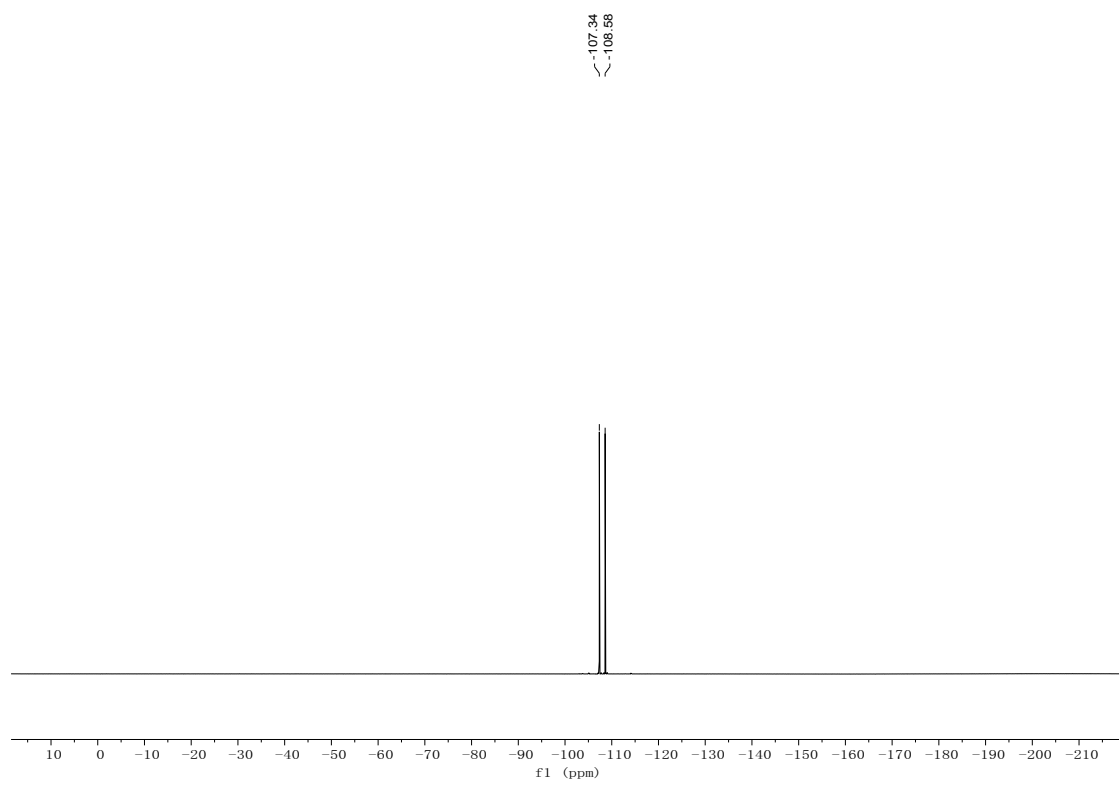


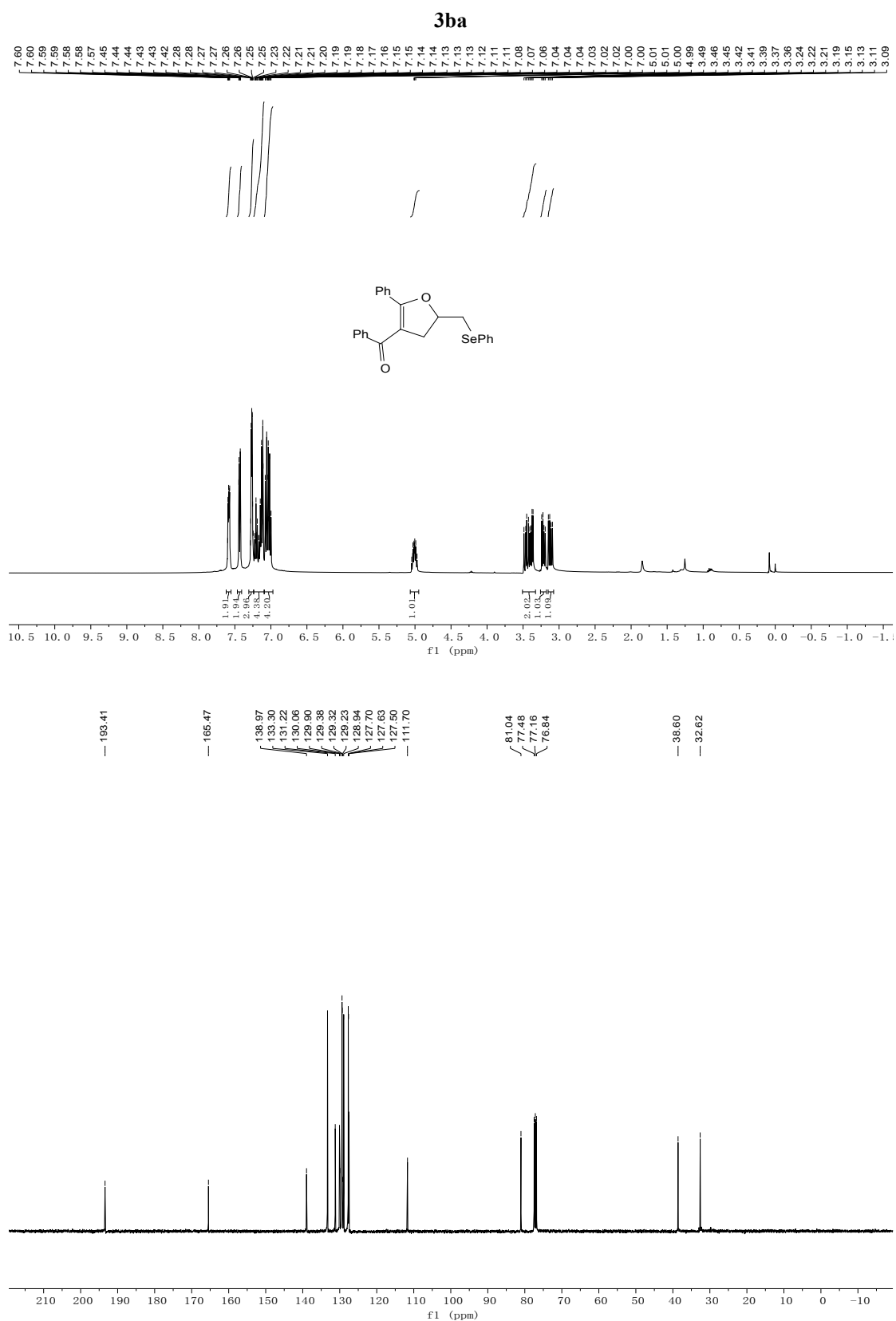
phenyl(2-phenyl-5-((phenylseleninyl)methyl)-4,5-dihydrofuran-3-yl)methanone (7). white solid. was obtained in 98% isolated yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.80 (m, 1H), 7.76 (dd, J = 6.5, 2.9 Hz, 1H), 7.60 – 7.49 (m, 3H), 7.48 – 7.41 (m, 2H), 7.28 – 7.15 (m, 3H), 7.15 – 7.00 (m, 5H), 5.44 (m, 0.5H), 5.04 (m, 0.5H), 3.46 (m, 2H), 3.27 – 2.95 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.15, 193.12, 164.46, 164.20, 140.36, 139.43, 138.44, 131.66, 131.62, 131.55, 130.37, 130.33, 129.91, 129.85, 129.44, 129.36, 129.32, 129.20, 128.91, 127.80, 127.76, 127.70, 126.24, 125.78, 111.64, 111.36, 76.03, 75.87, 58.95, 57.55, 39.03, 38.93. HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{21}\text{O}_3\text{Se}^+$ $[\text{M}+\text{H}]^+$ 437.0650 found 437.0632.

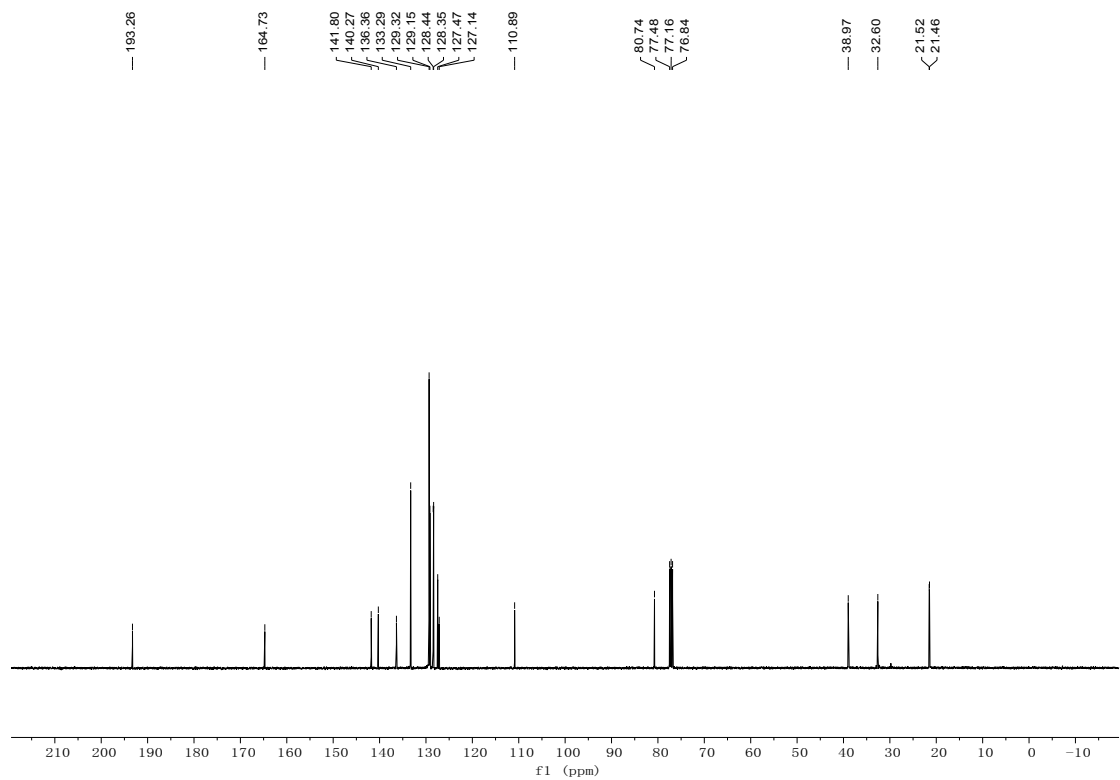
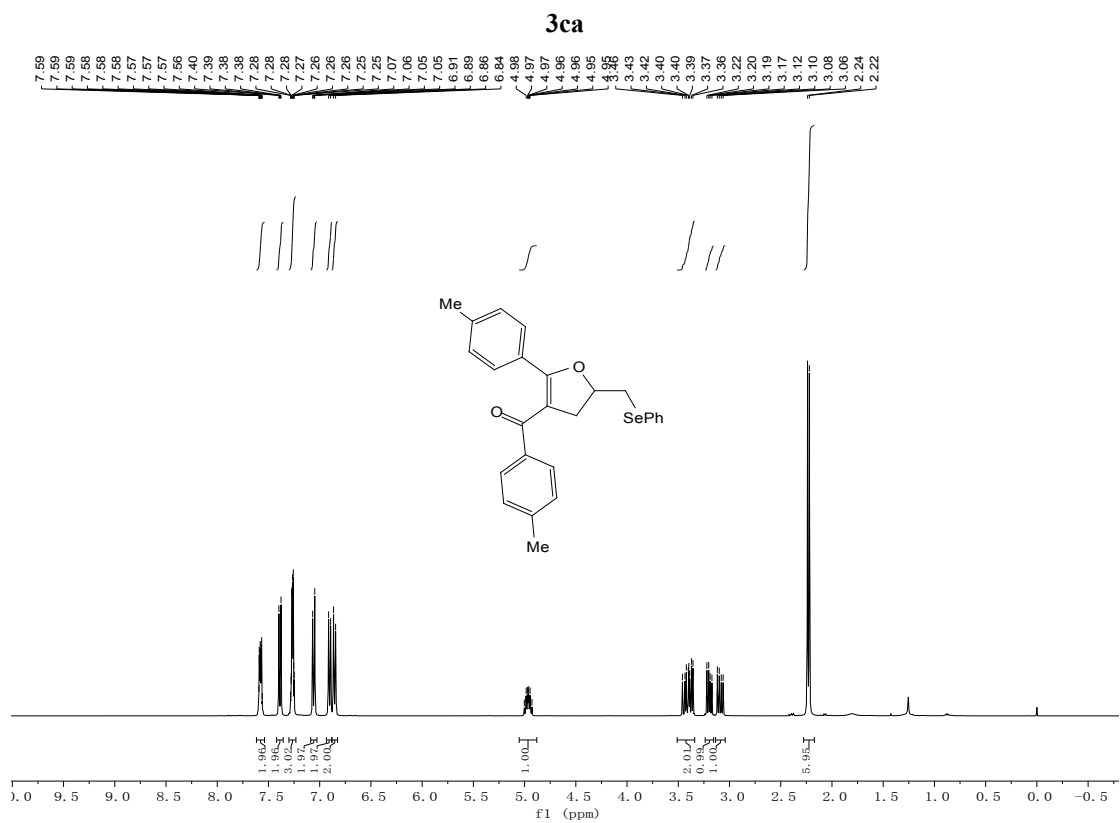
References

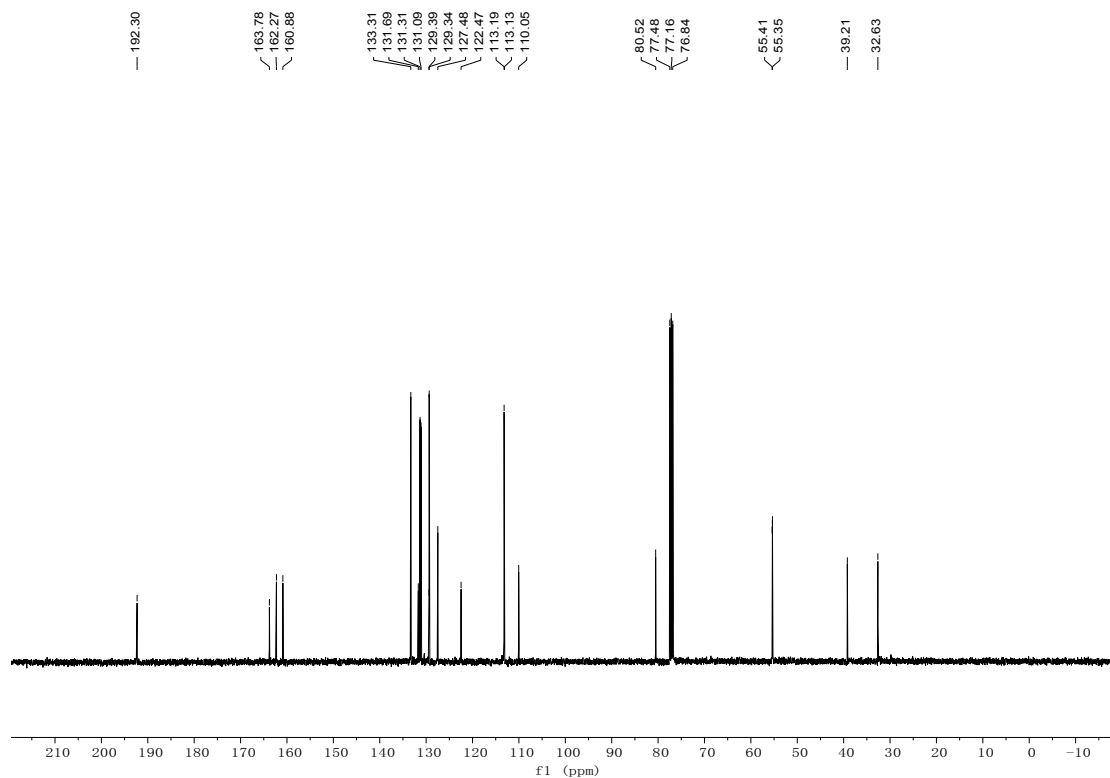
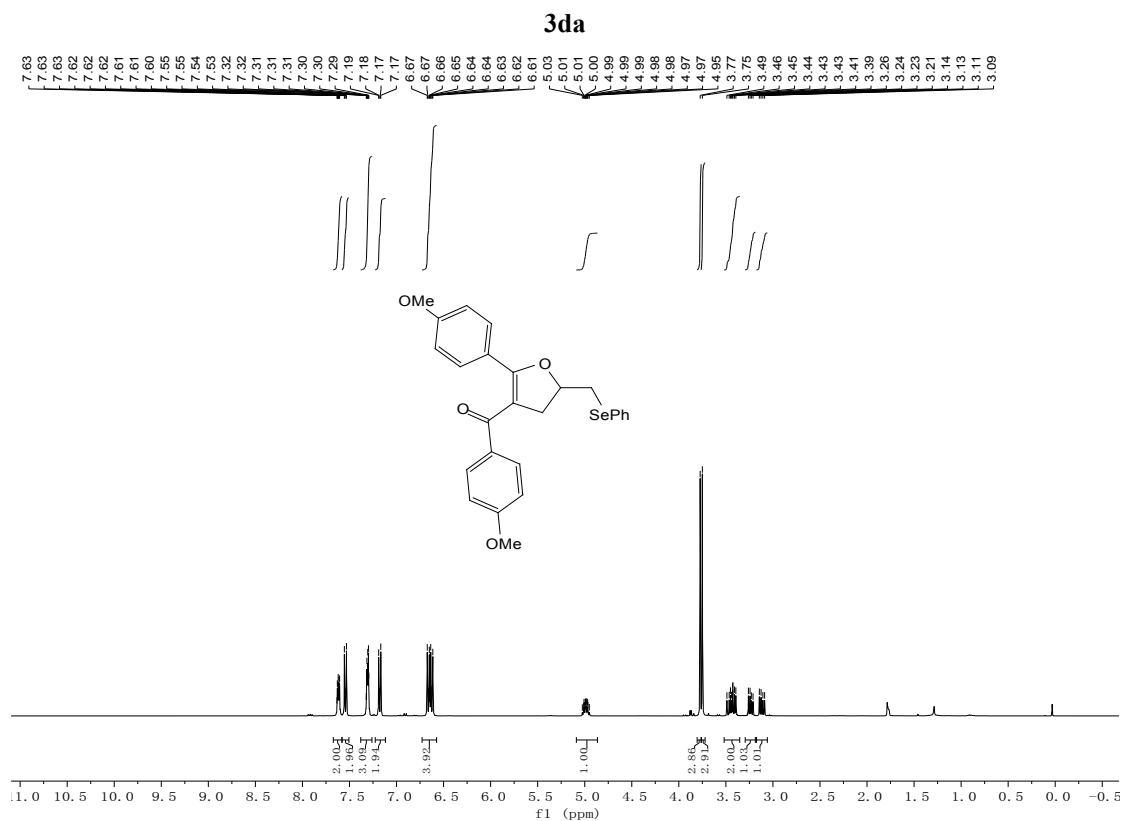
- (1) Yang, N. Y.; Li, Z. L.; Ye, L.; Tan, B.; Liu, X. Y. Organic base-catalysed solvent-tuned chemoselective carbotrifluoromethylation and oxytrifluoromethylation of unactivated alkenes. *Chem. Commun.* **2016**, 52, 9052–9055.
- (2) Jiang, Y.; Park, C. M.; Loh, T. P. Transition-Metal-Free Synthesis of Substituted Pyridines via Ring Expansion of 2-Allyl-2*H*-azirines. *Org. Lett.* **2014**, 16, 3432-3435.
- (3) Zhang, Q. B.; Yuan, P. F.; Kai, L. L.; Liu, K.; Ban, Y. L.; Wang, X. Y.; Wu, L. Z.; Liu, Q. Preparation of Heterocycles via Visible-Light-Driven Aerobic Selenation of Olefins with Diselenides. *Org. Lett.* **2019**, 21, 4885-889.
- (4) Tiecco, M.; Testaferri, L.; Tingoli, M.; Bartoli, D.; Balducci, R. Ring-closure reactions initiated by the peroxydisulfate ion oxidation of diphenyl diselenide. *J. Org. Chem.* **1990**, 55, 429-434.

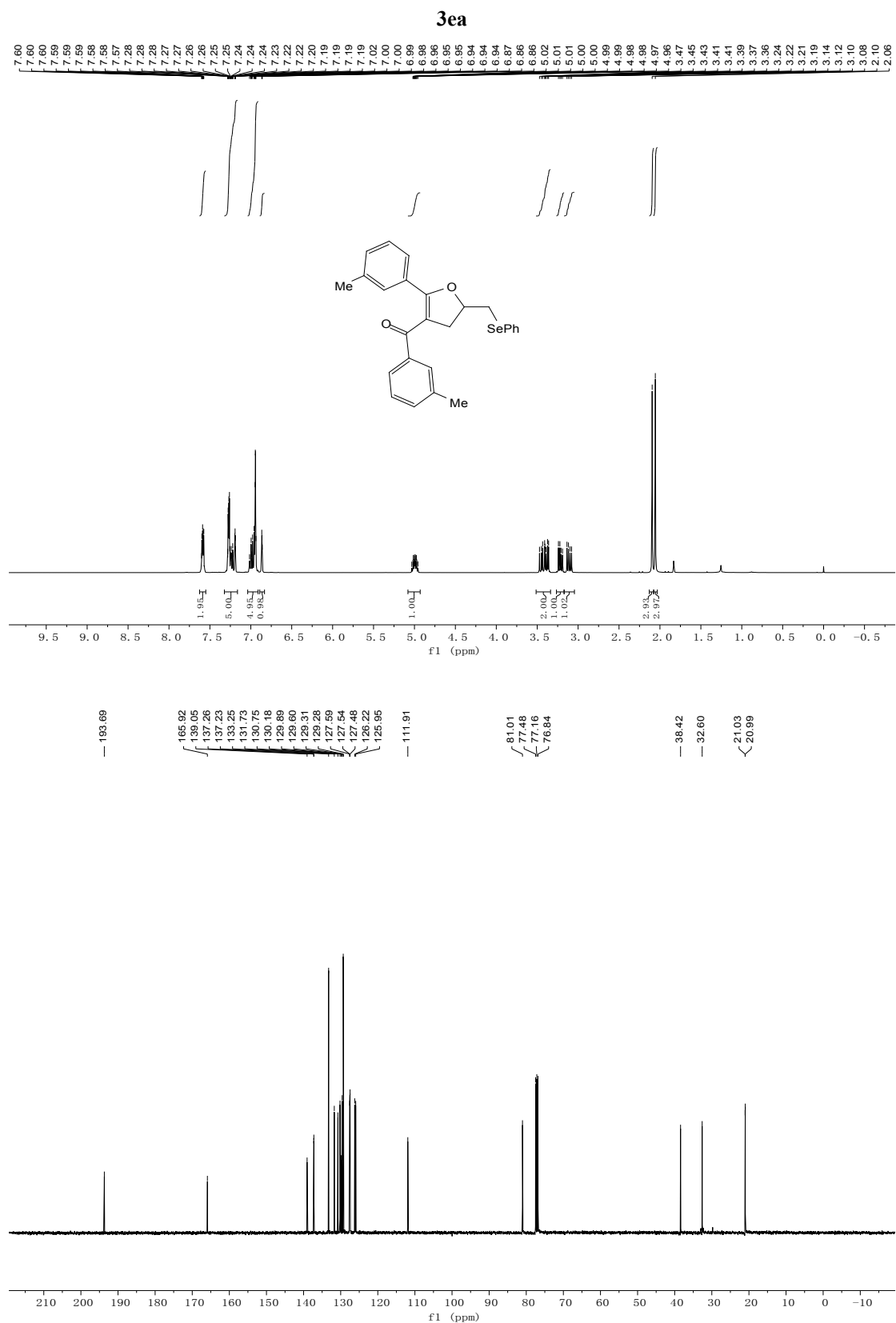


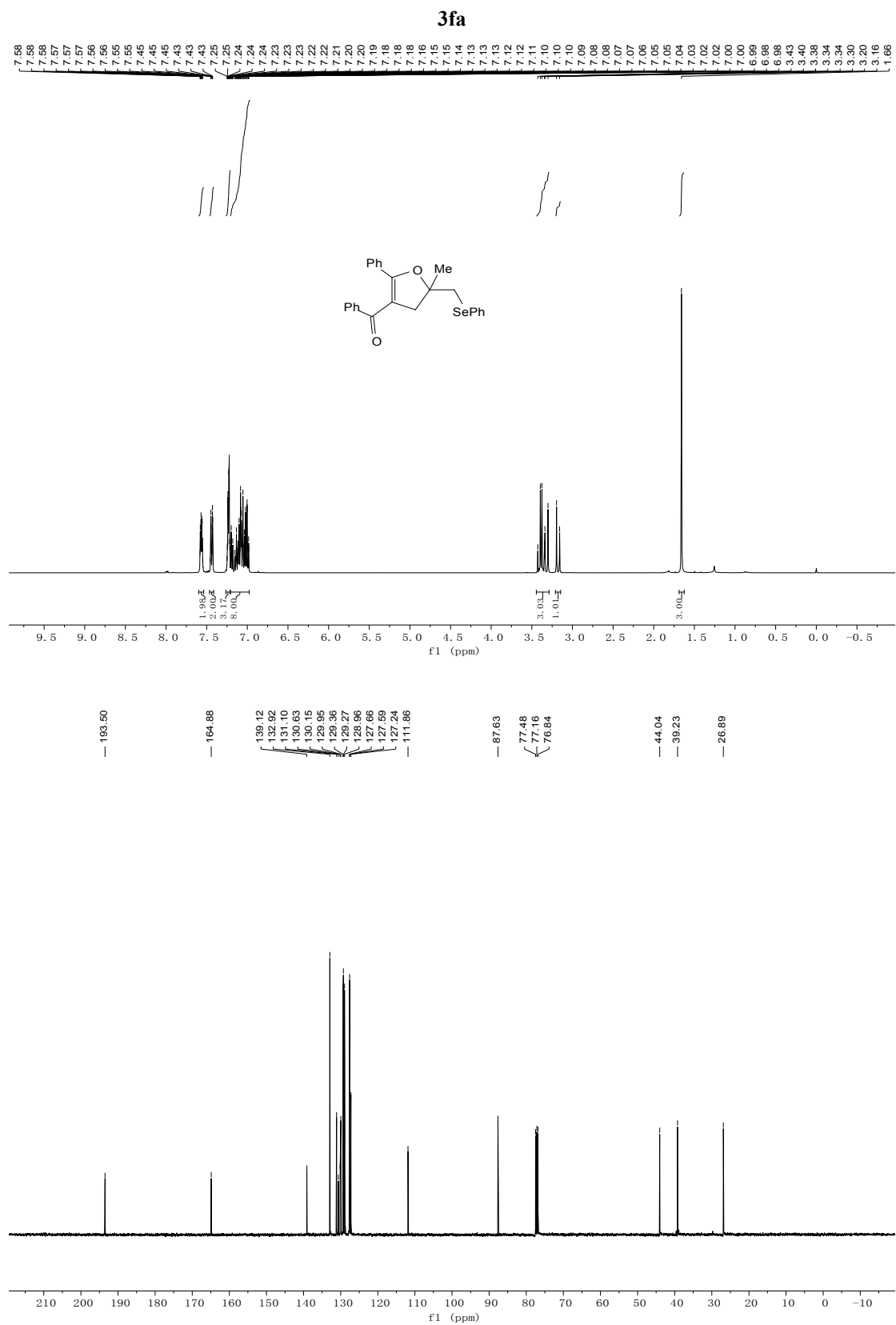


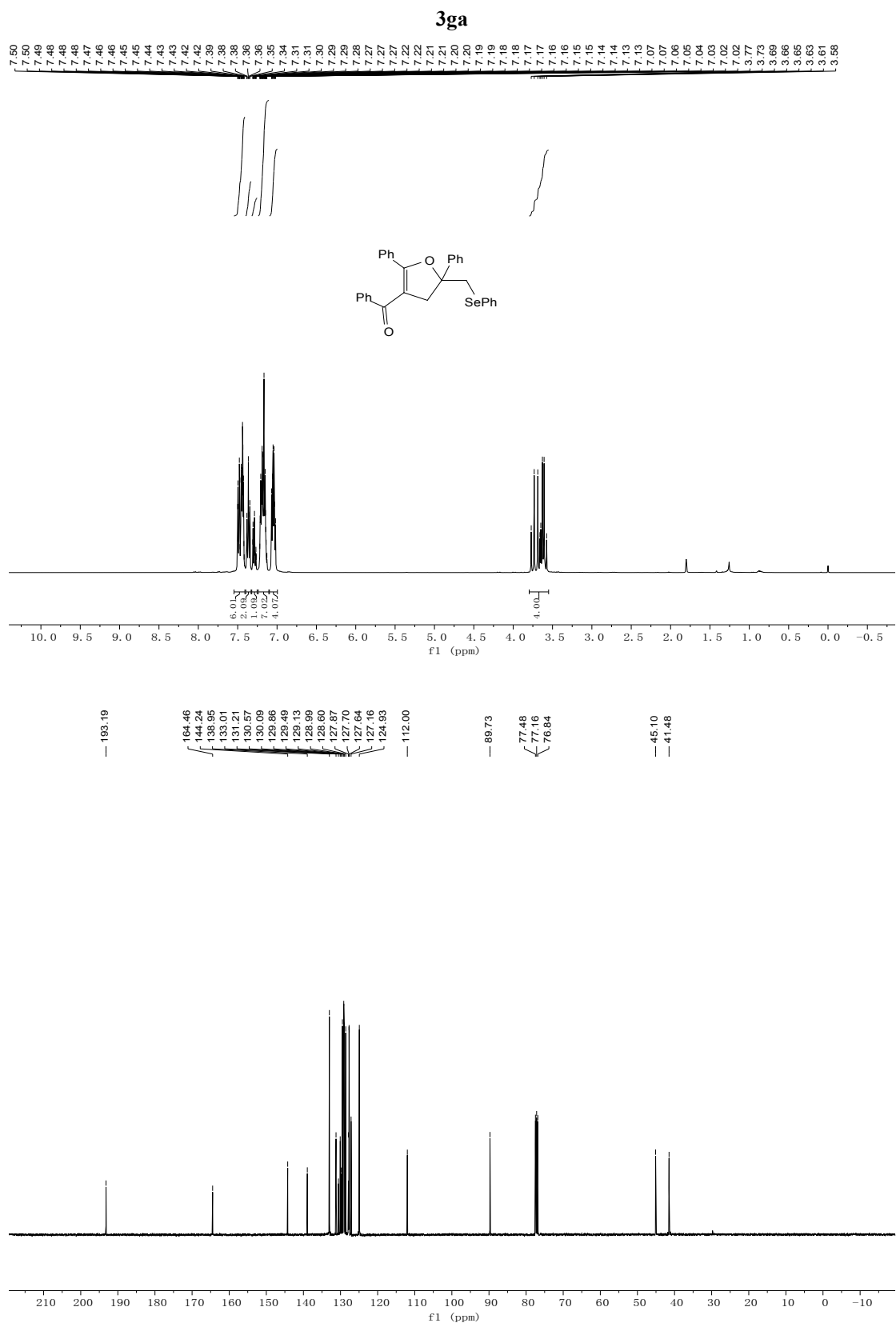




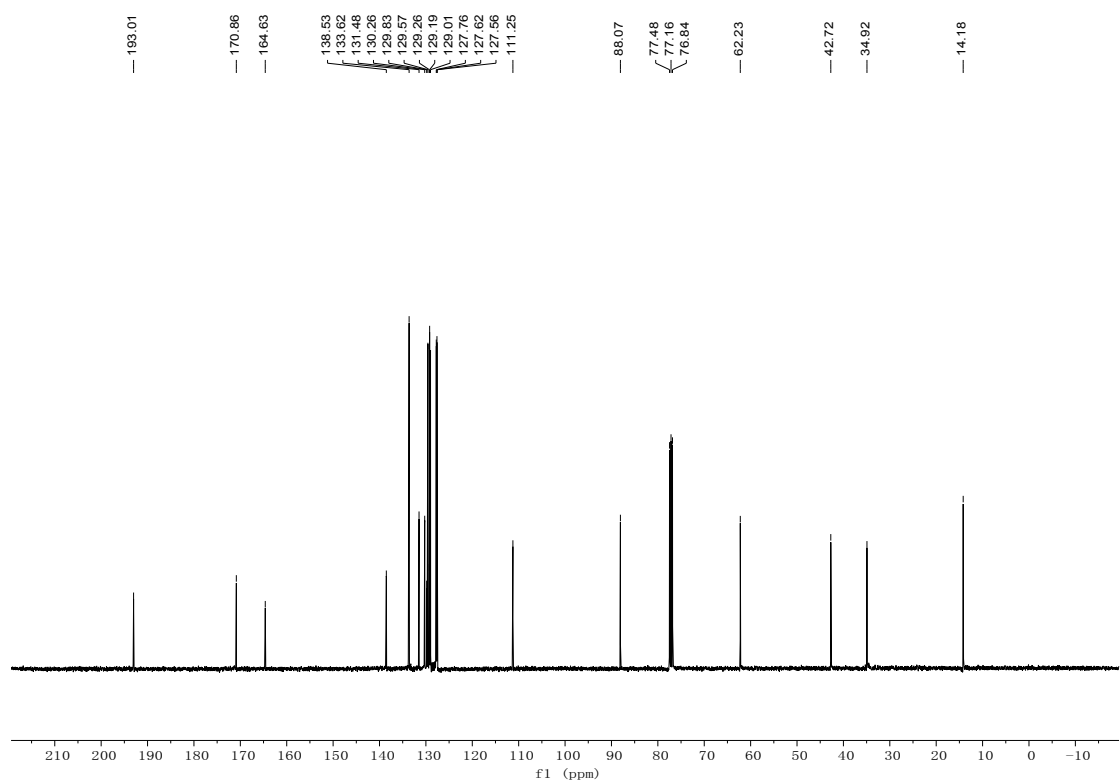
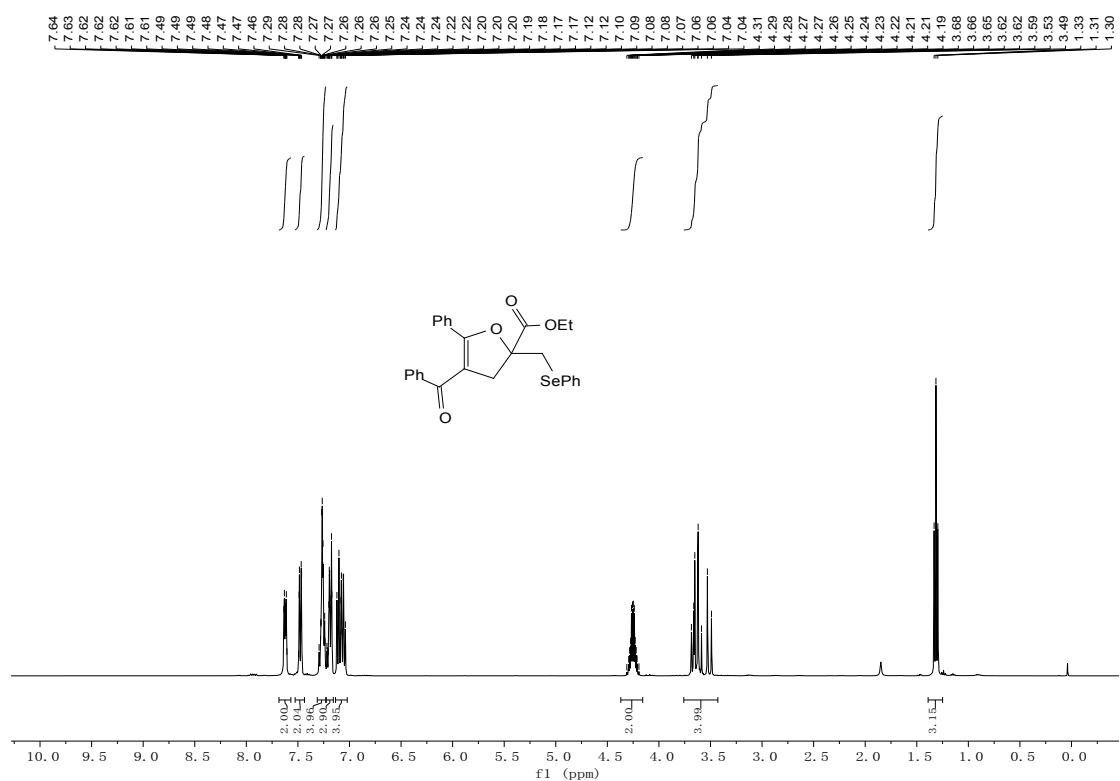




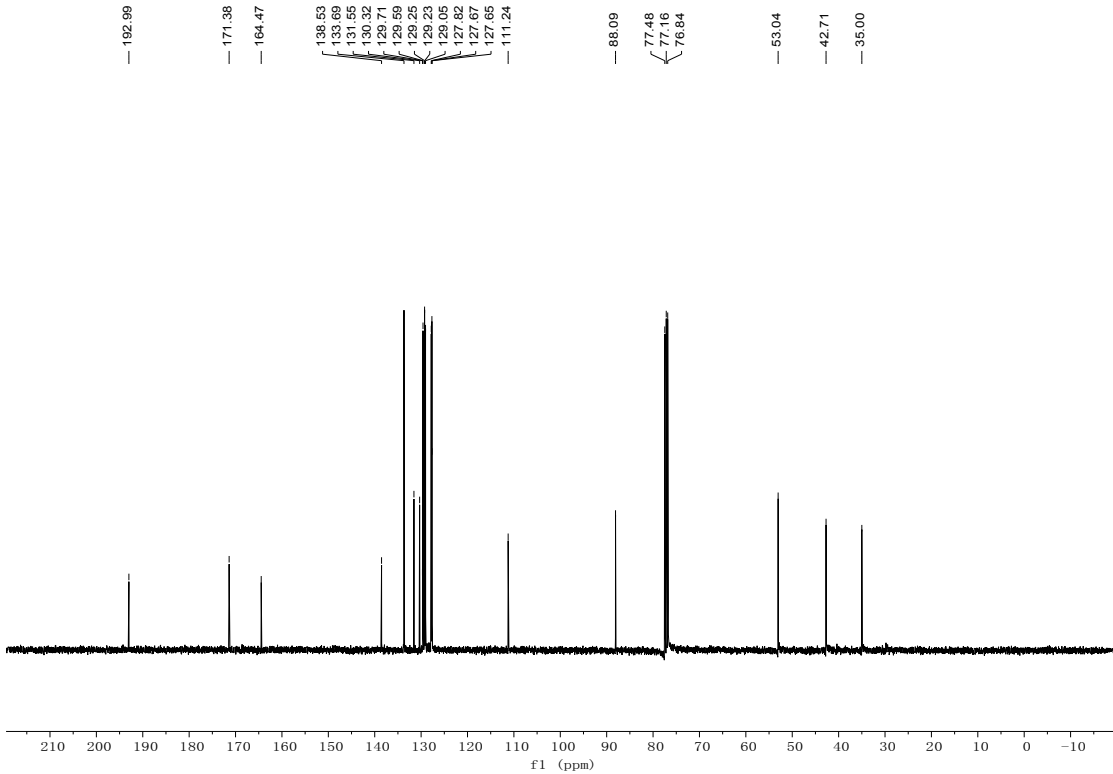
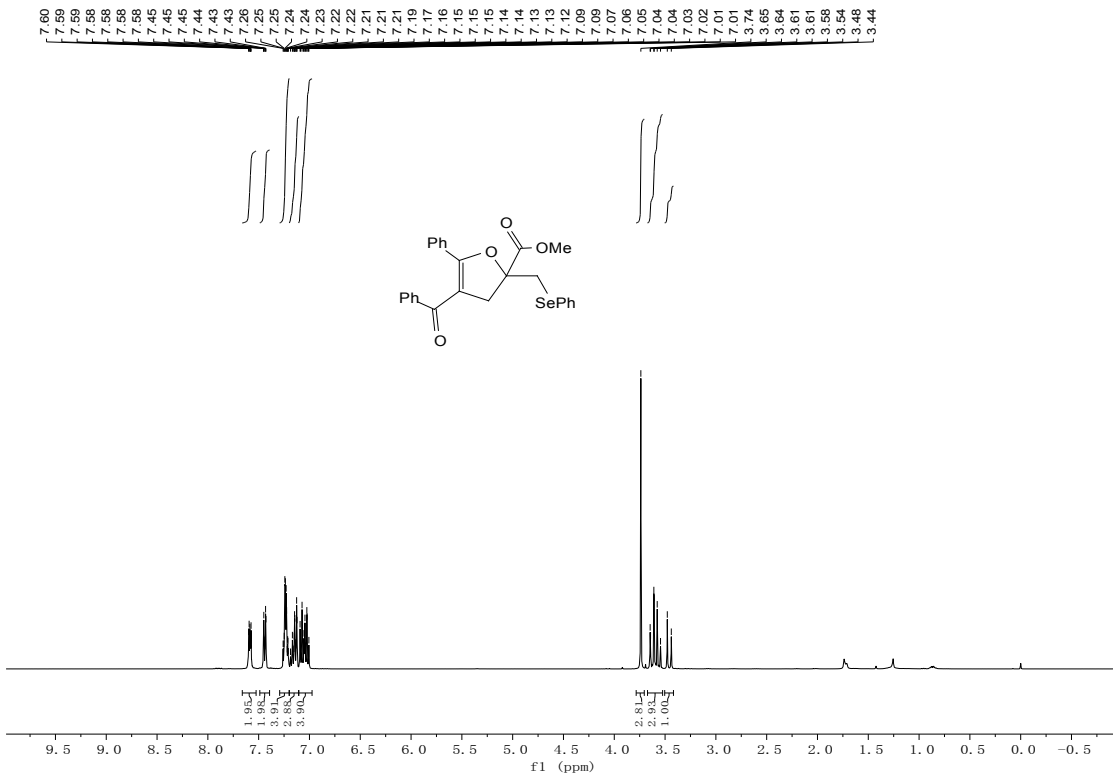


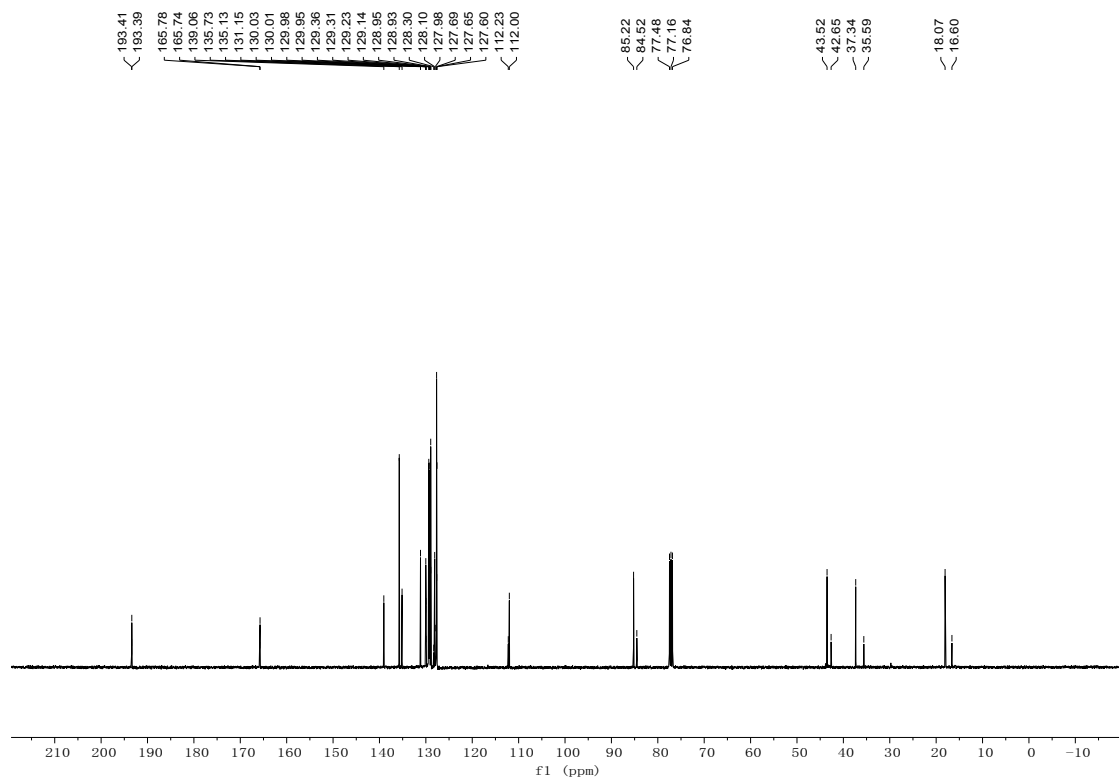
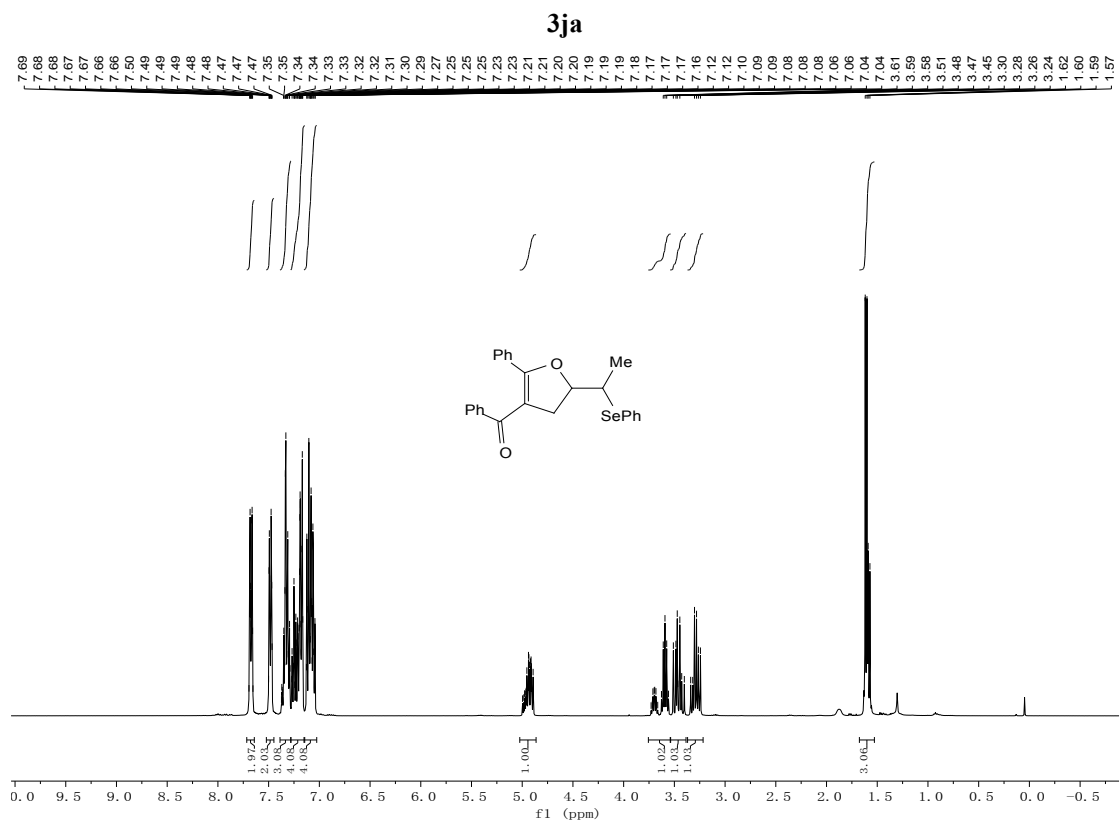


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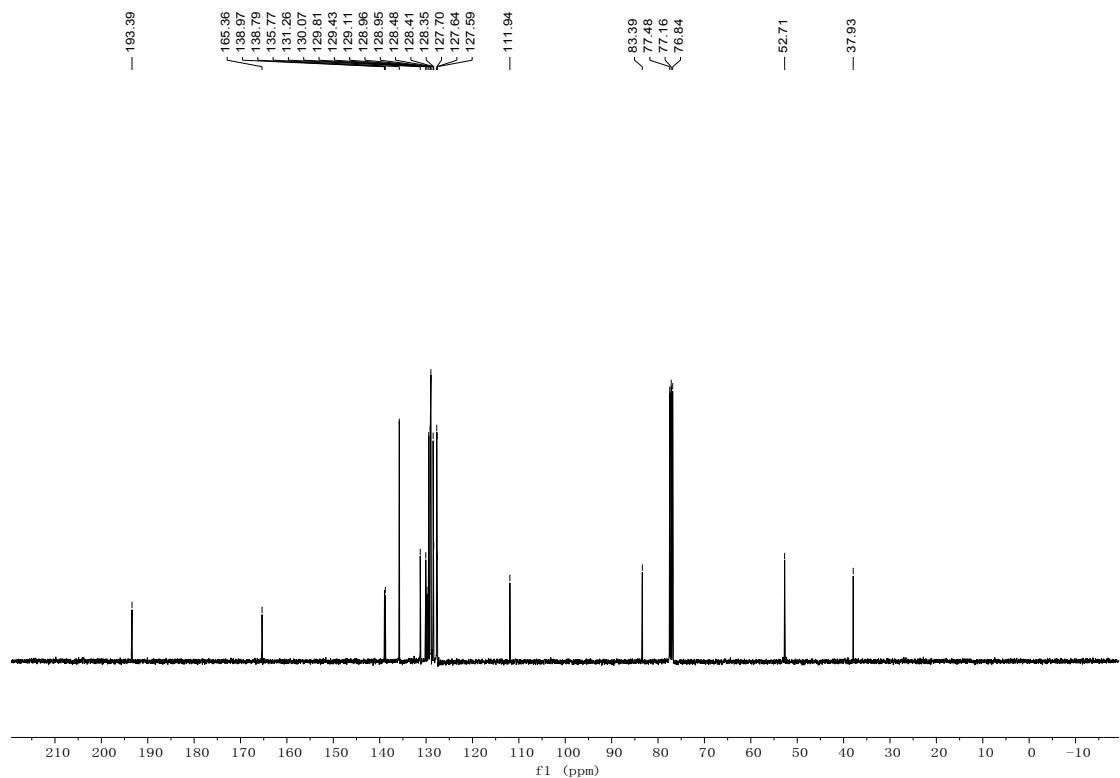
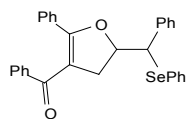
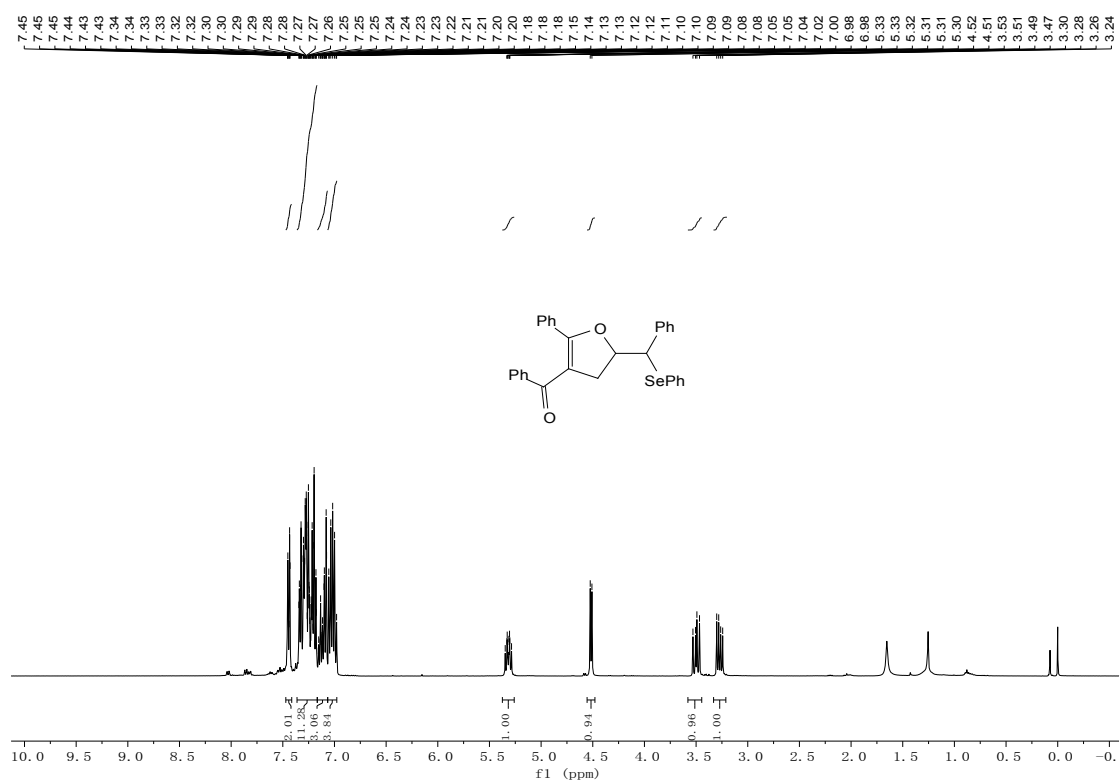


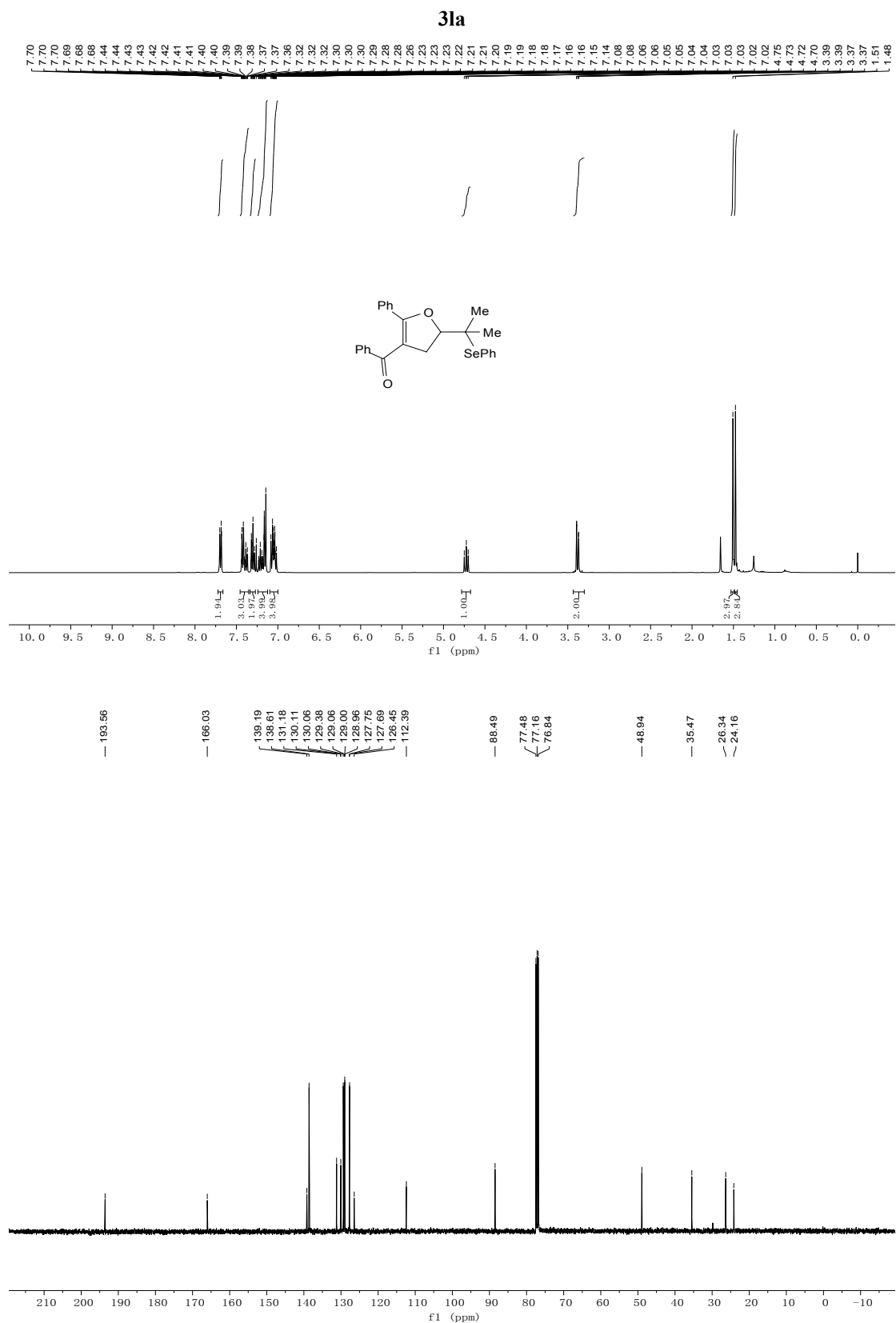
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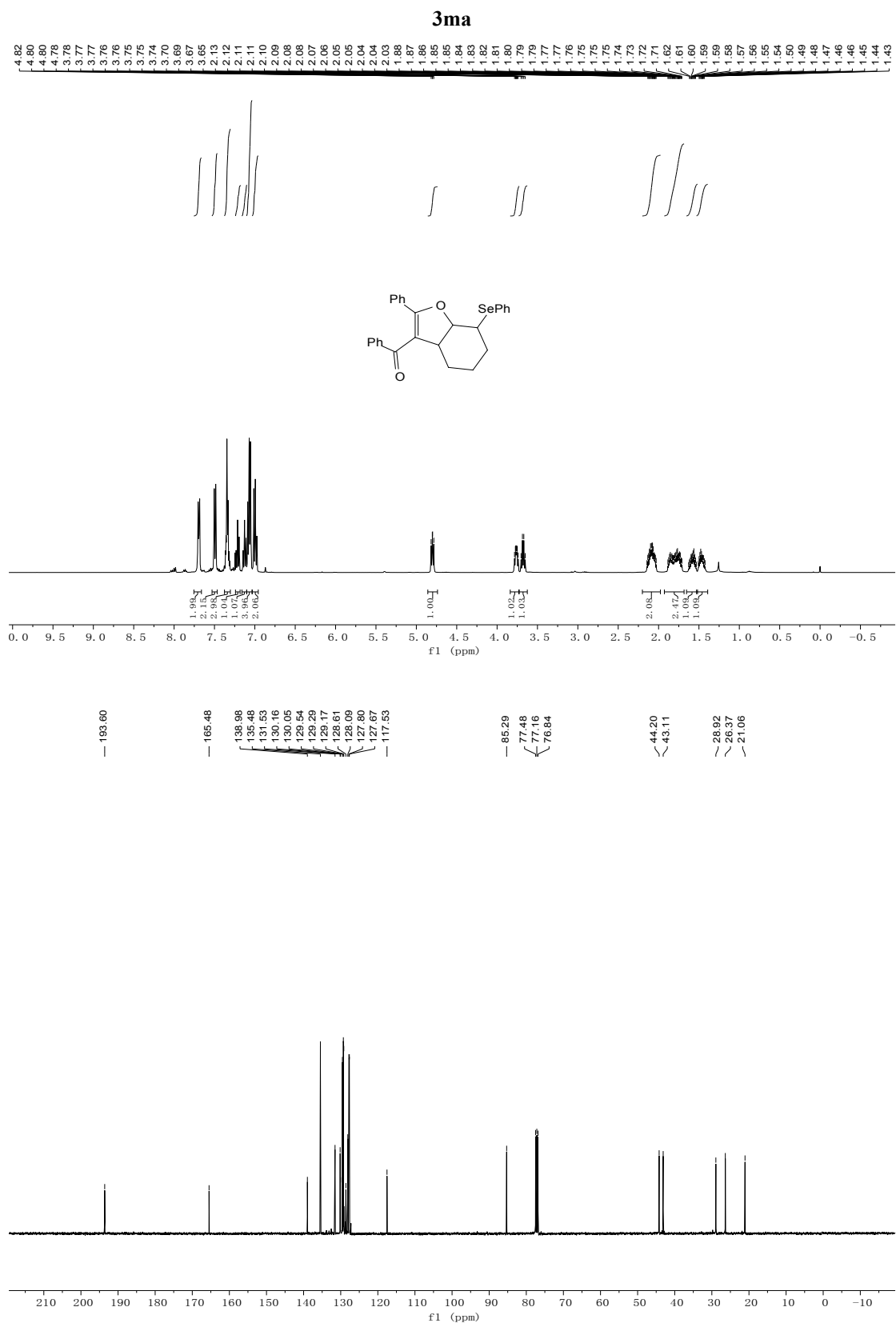


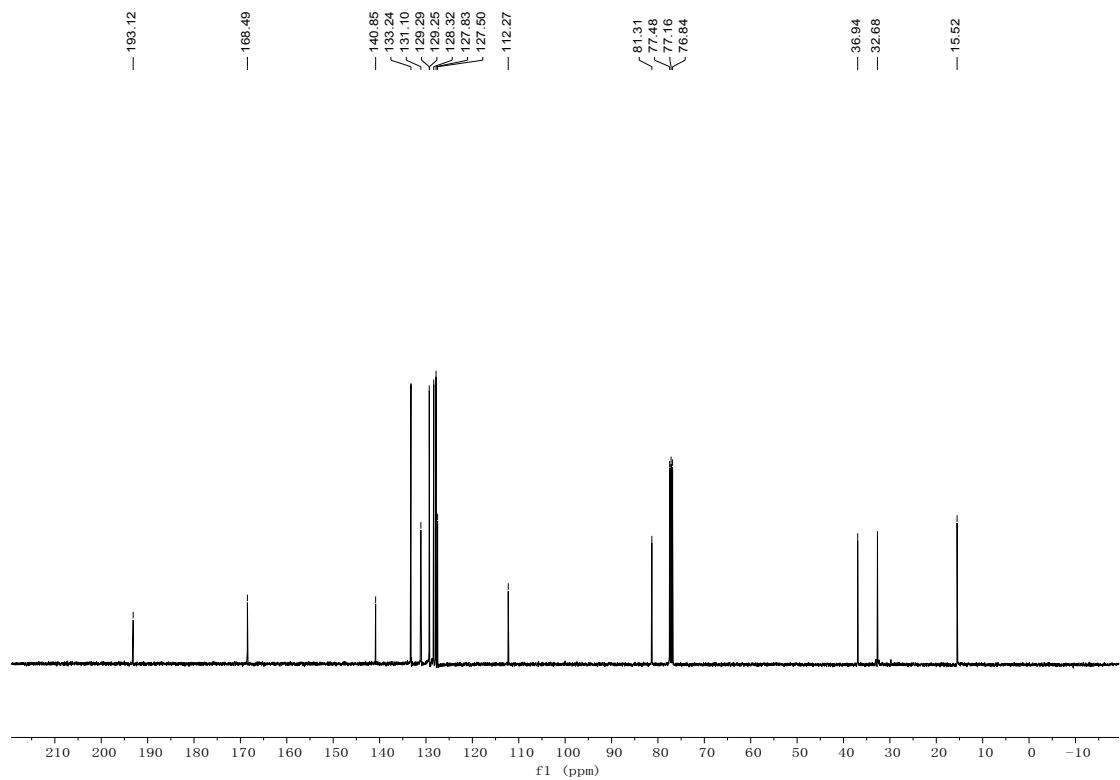
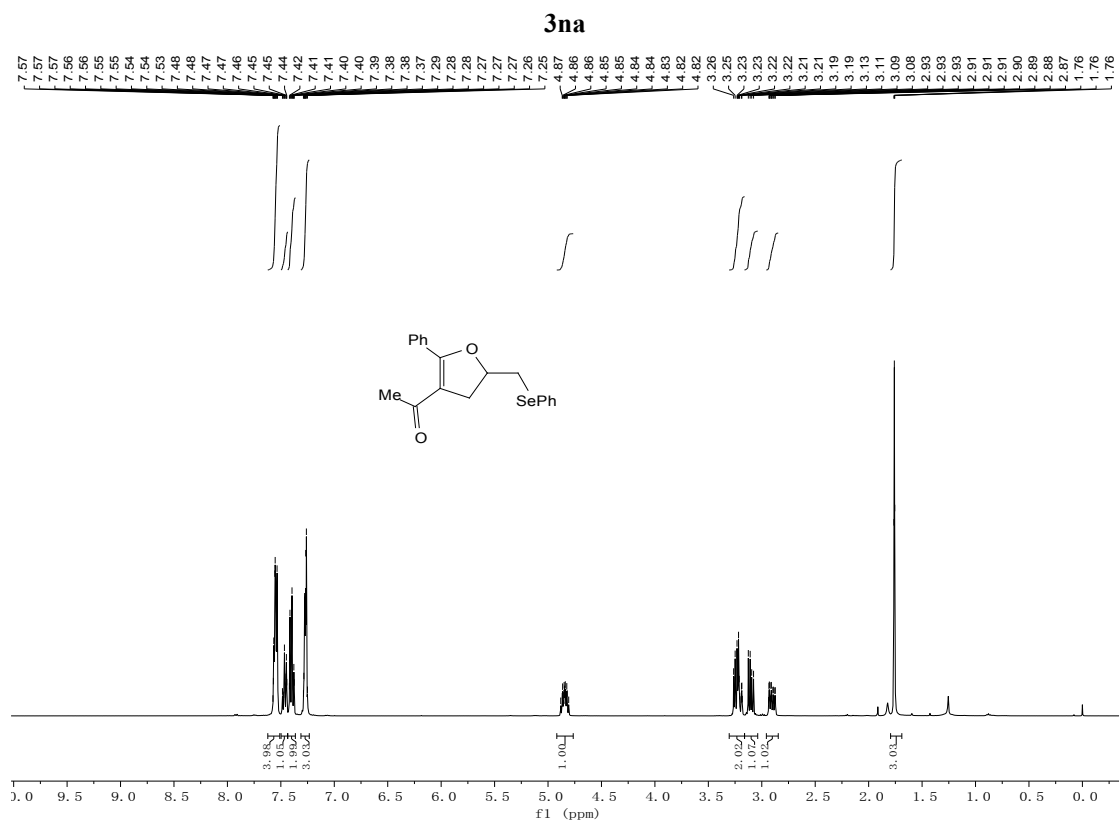


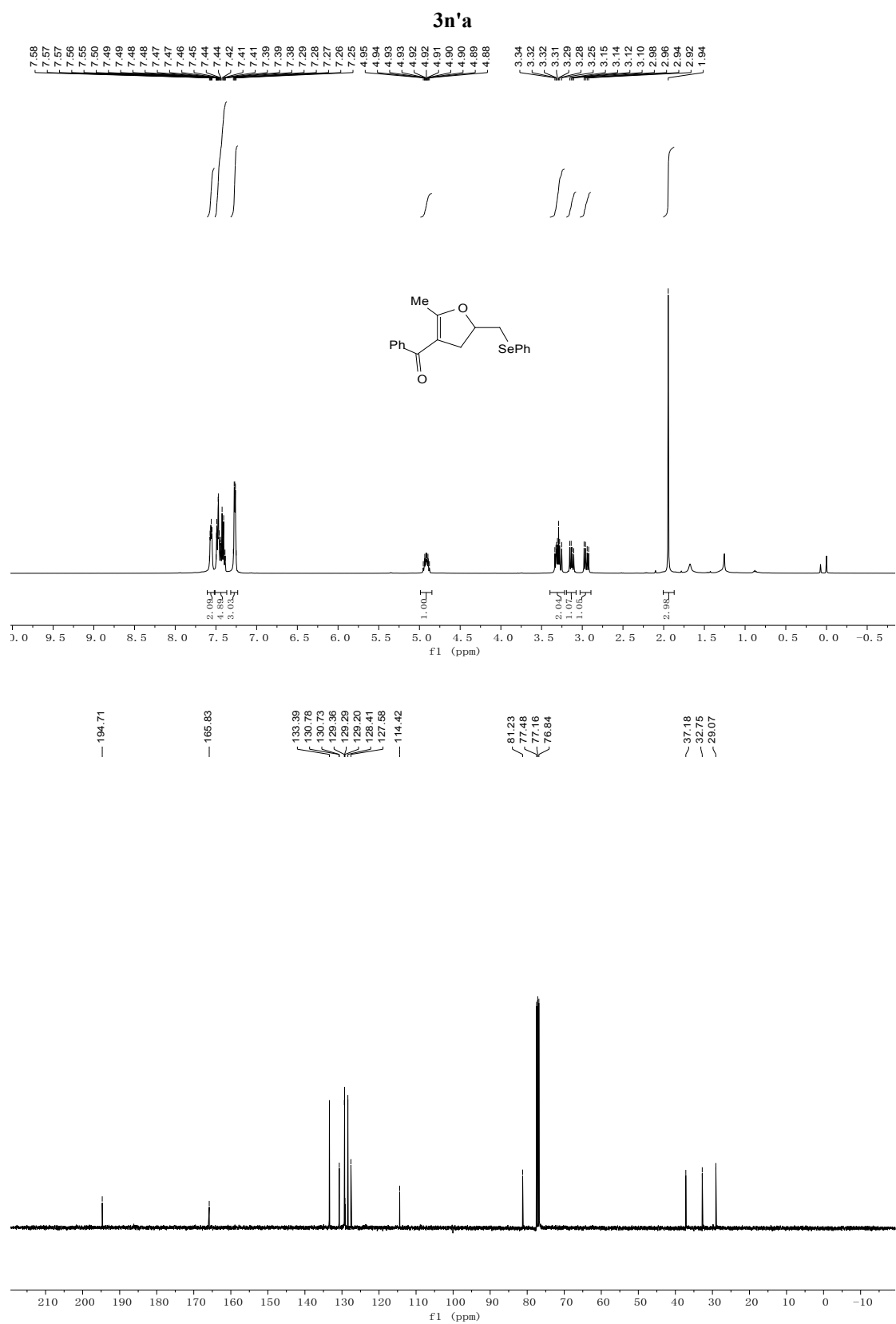
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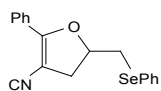


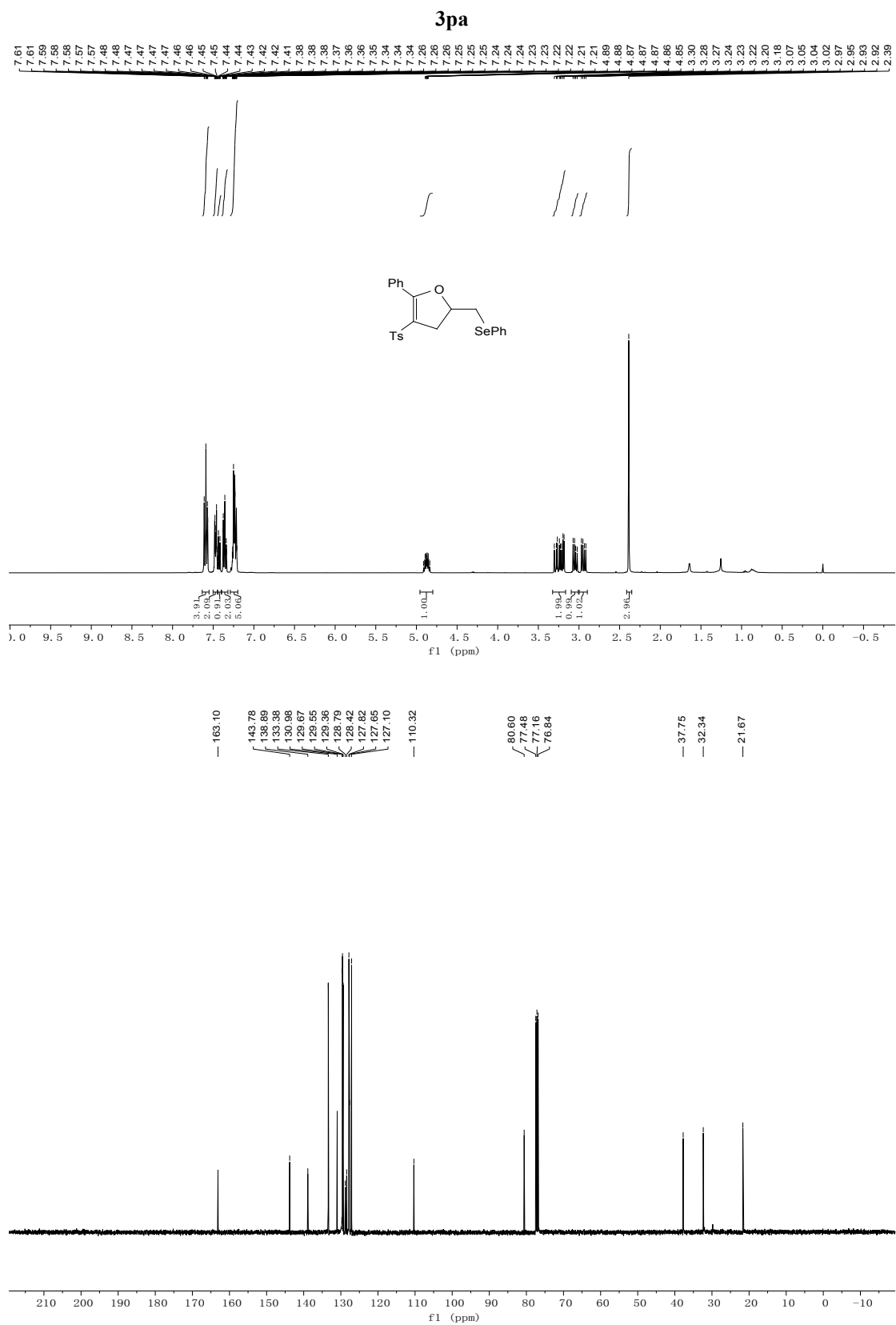


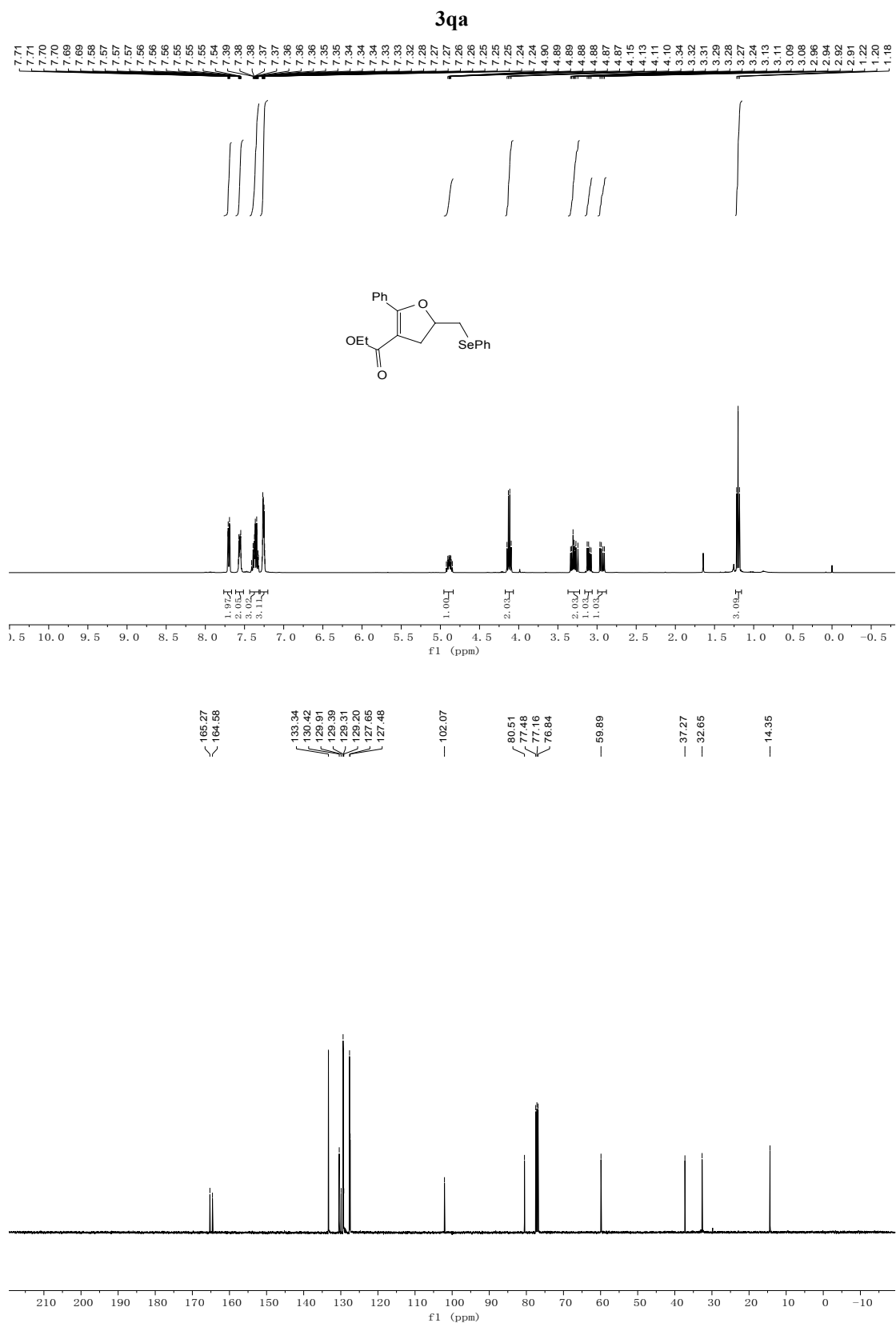




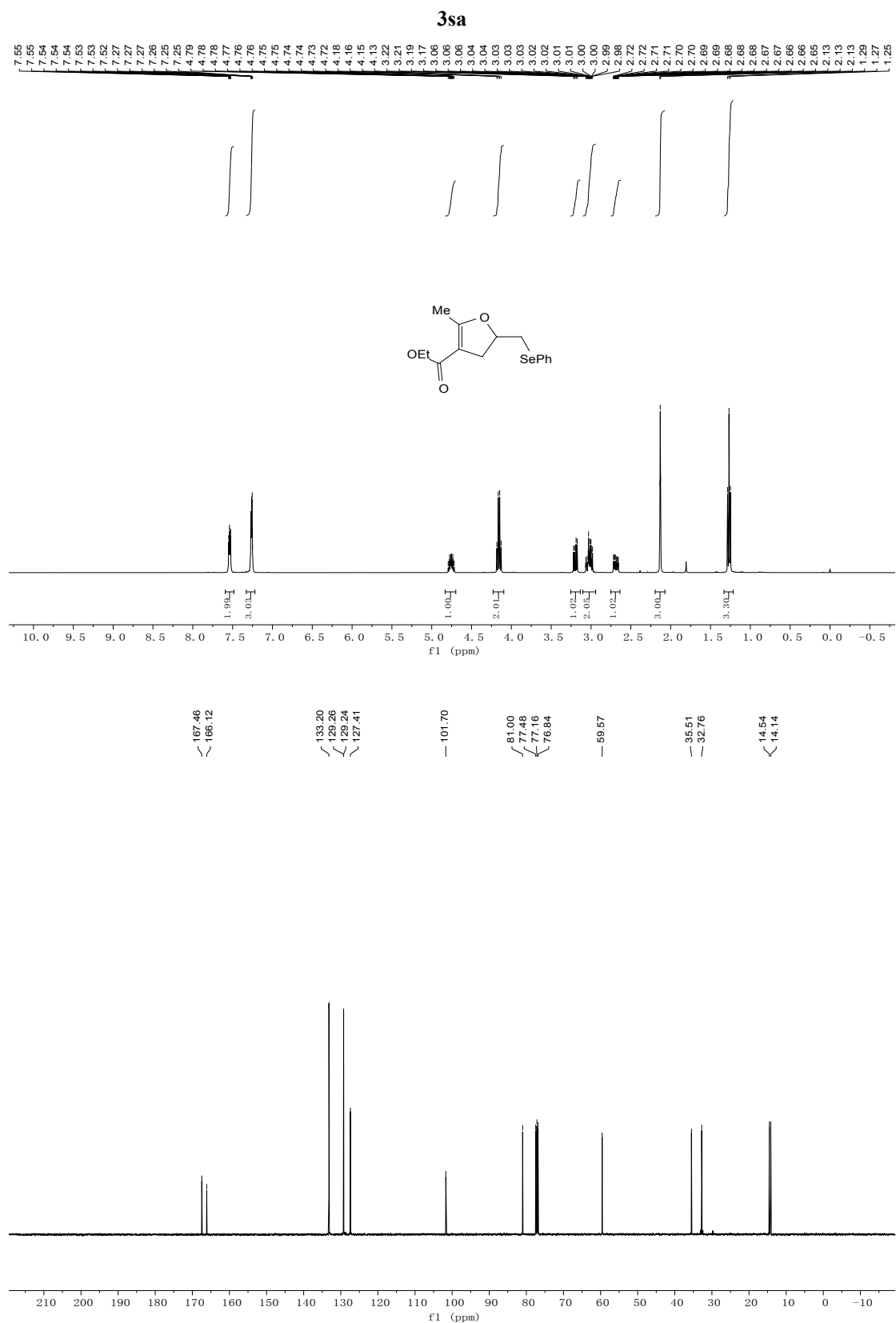
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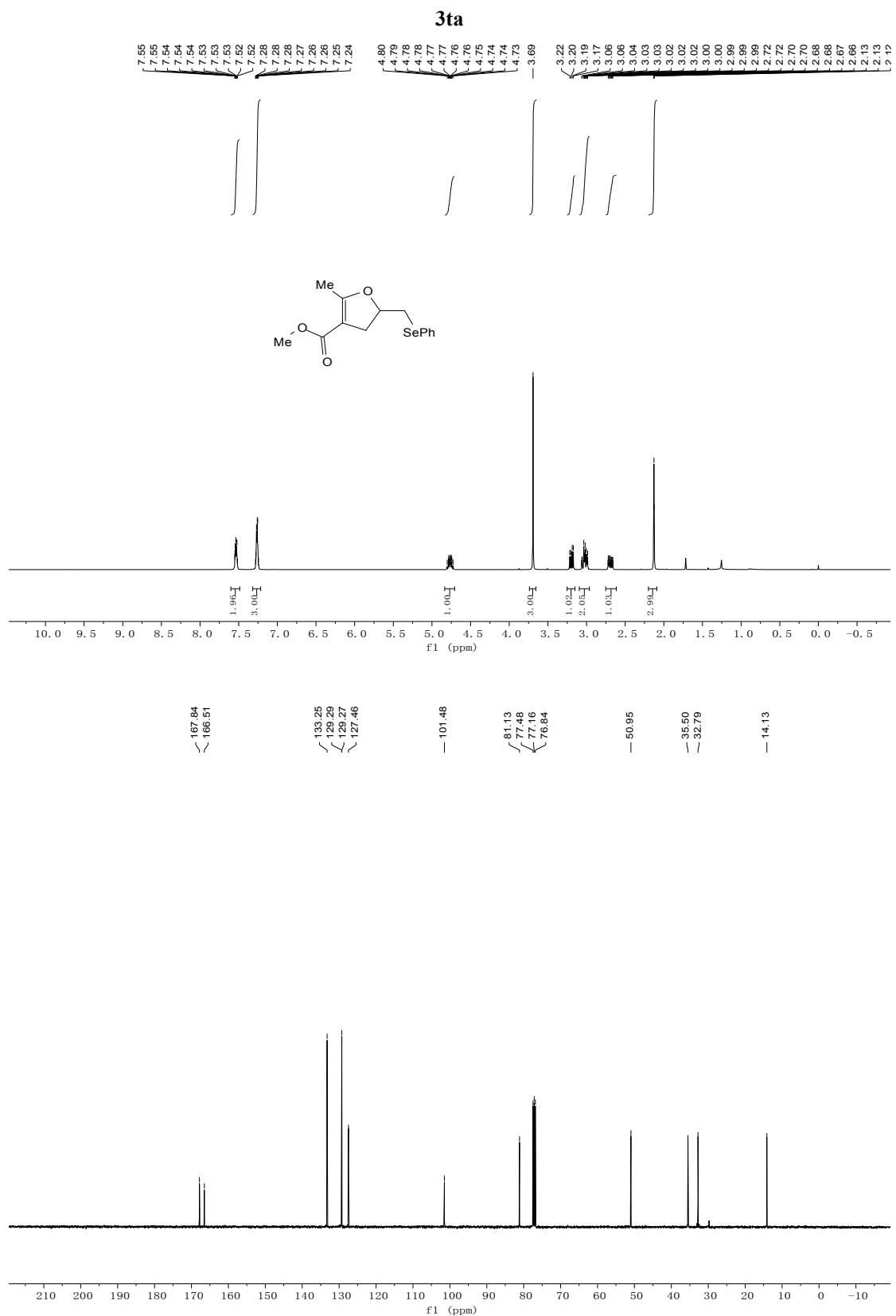


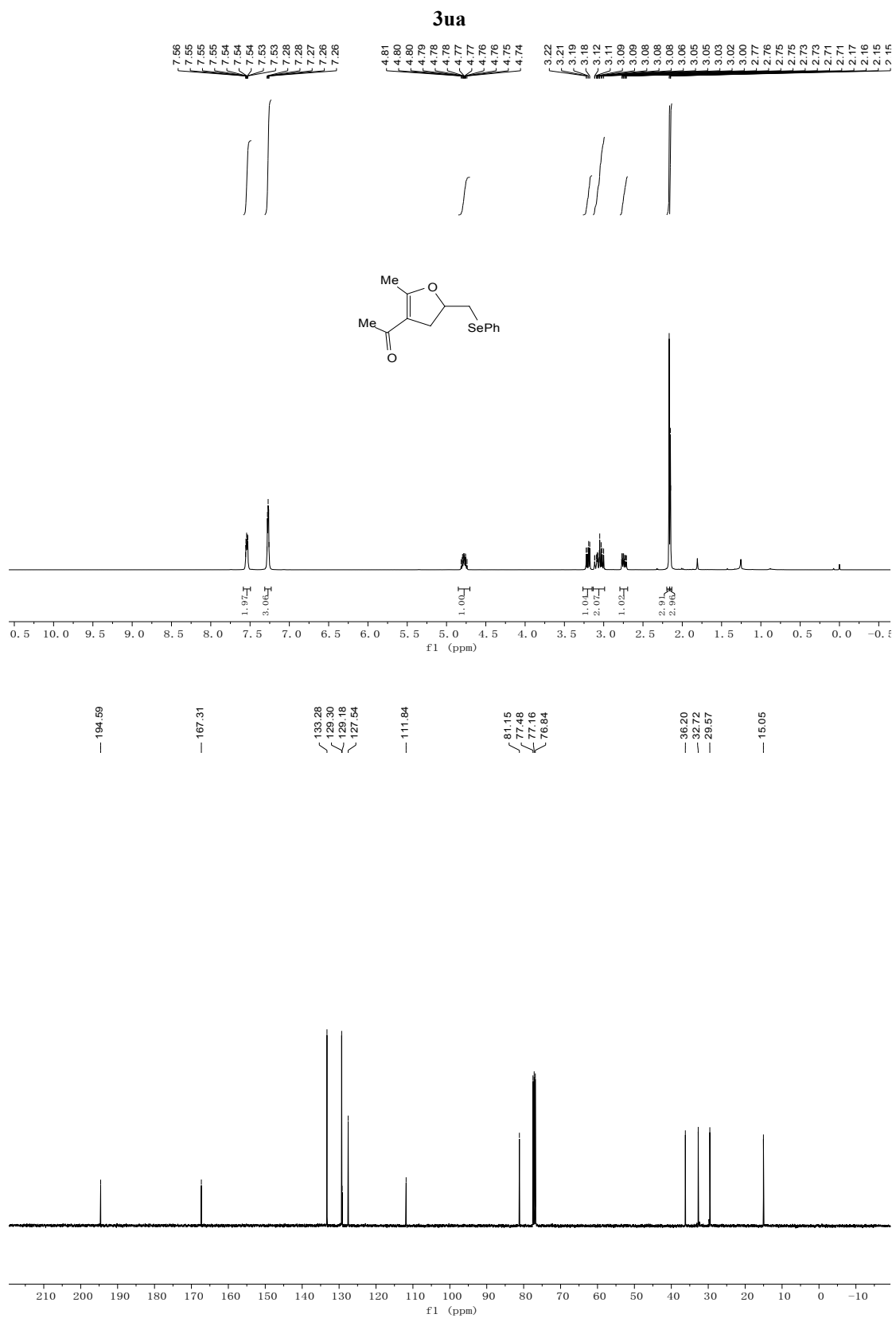


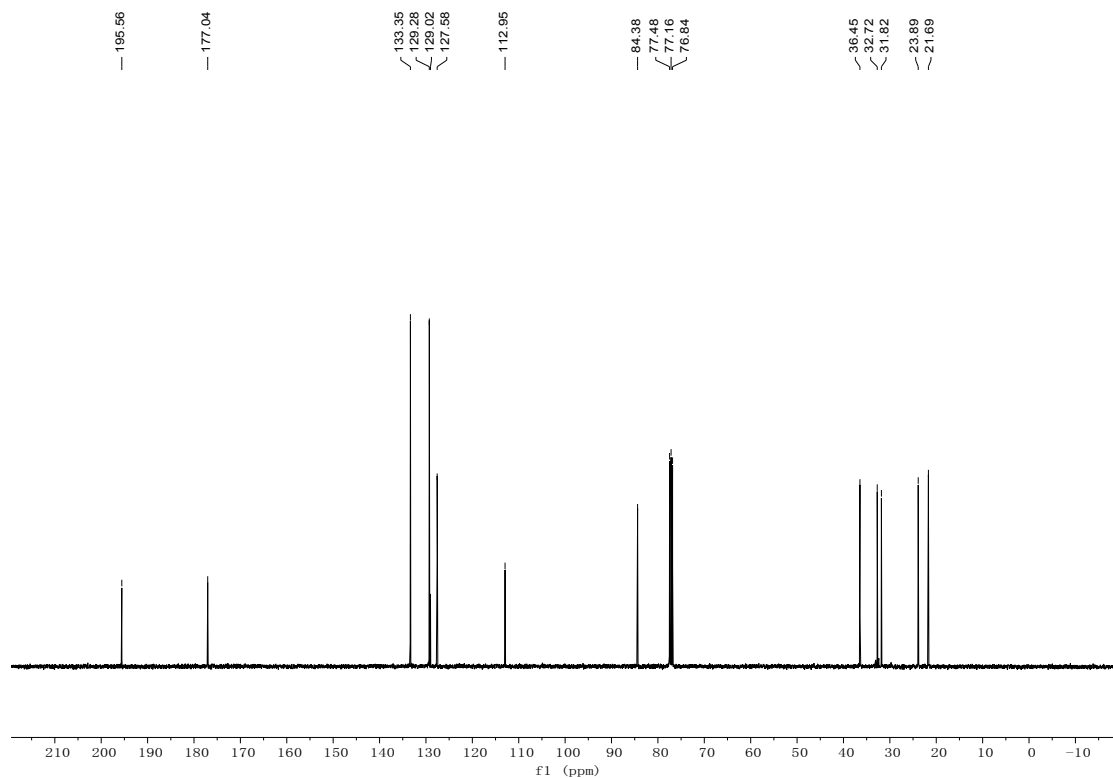
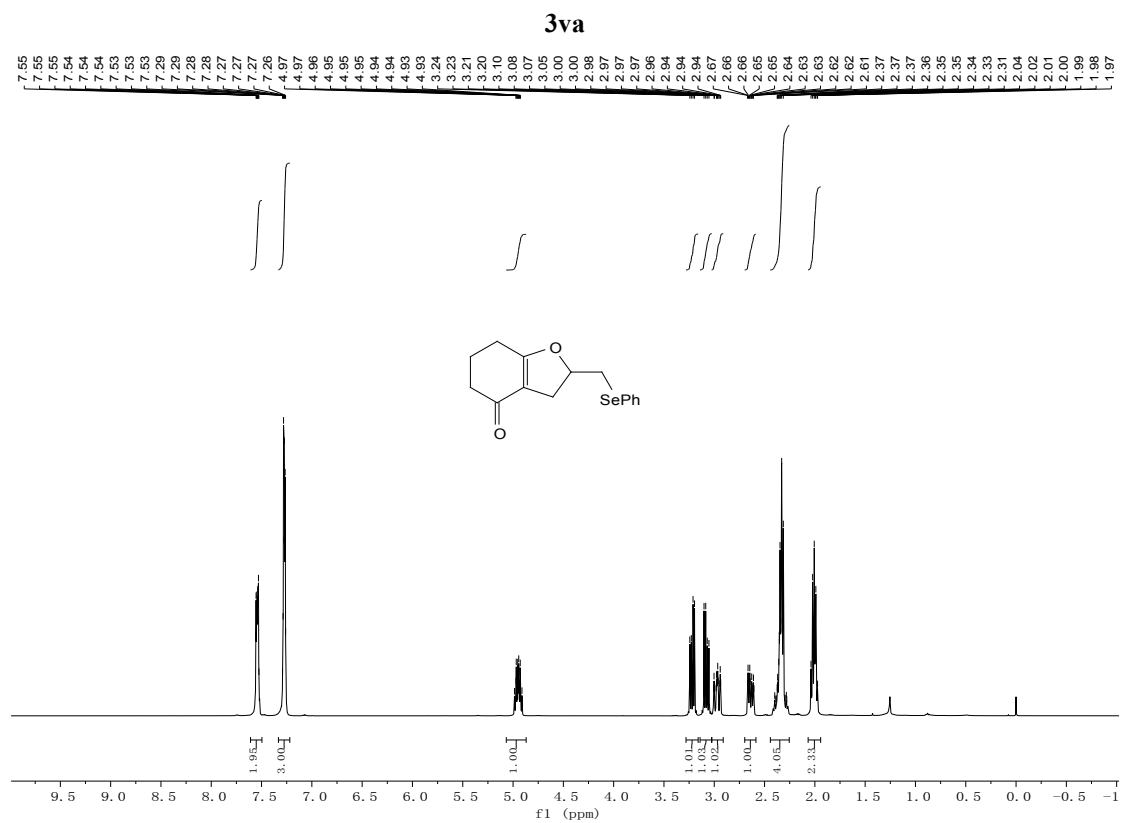




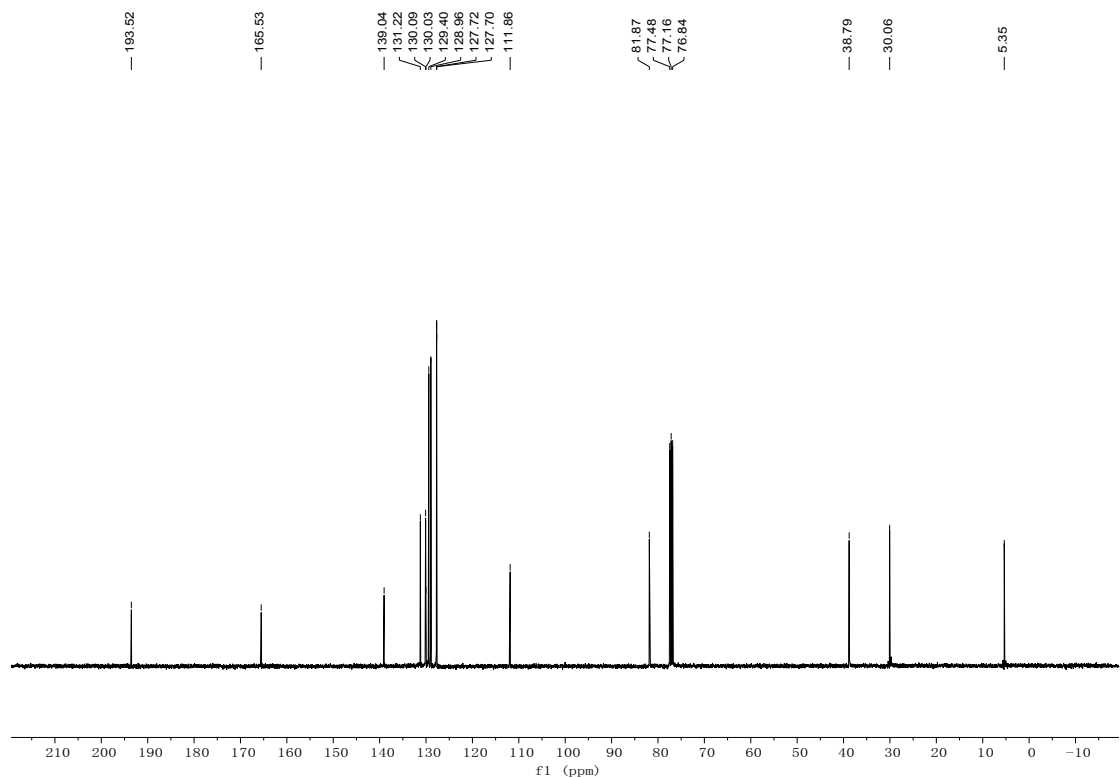
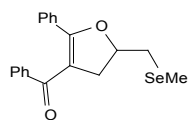
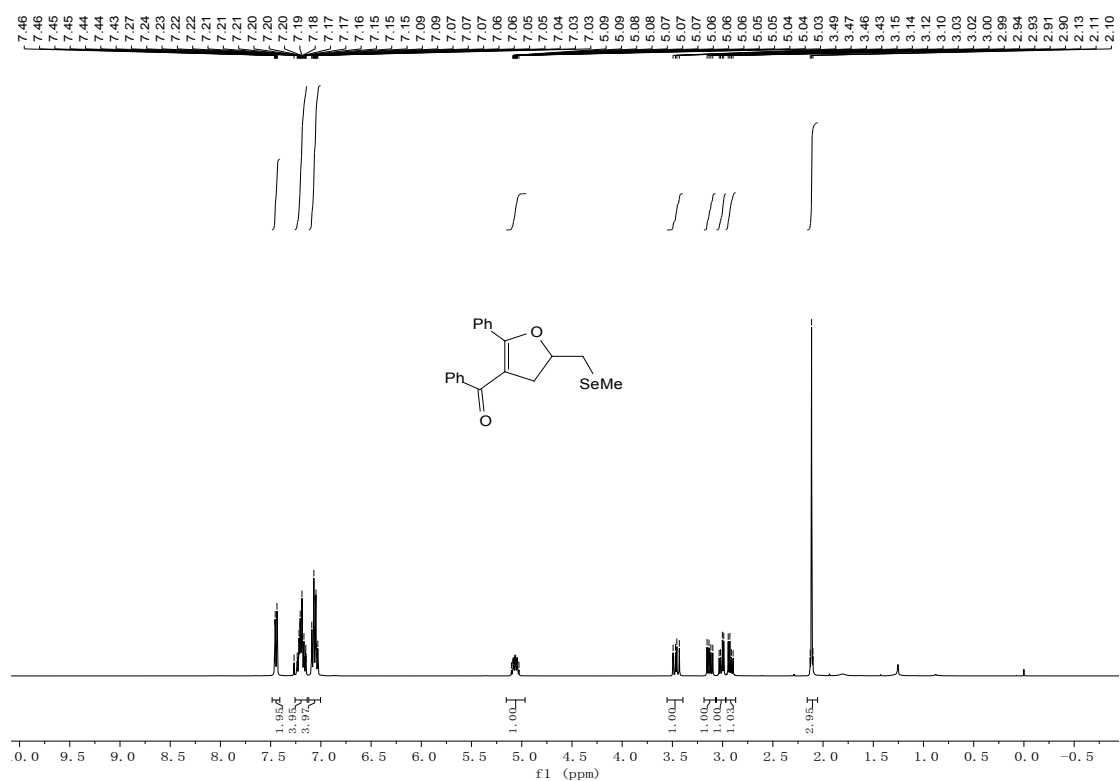


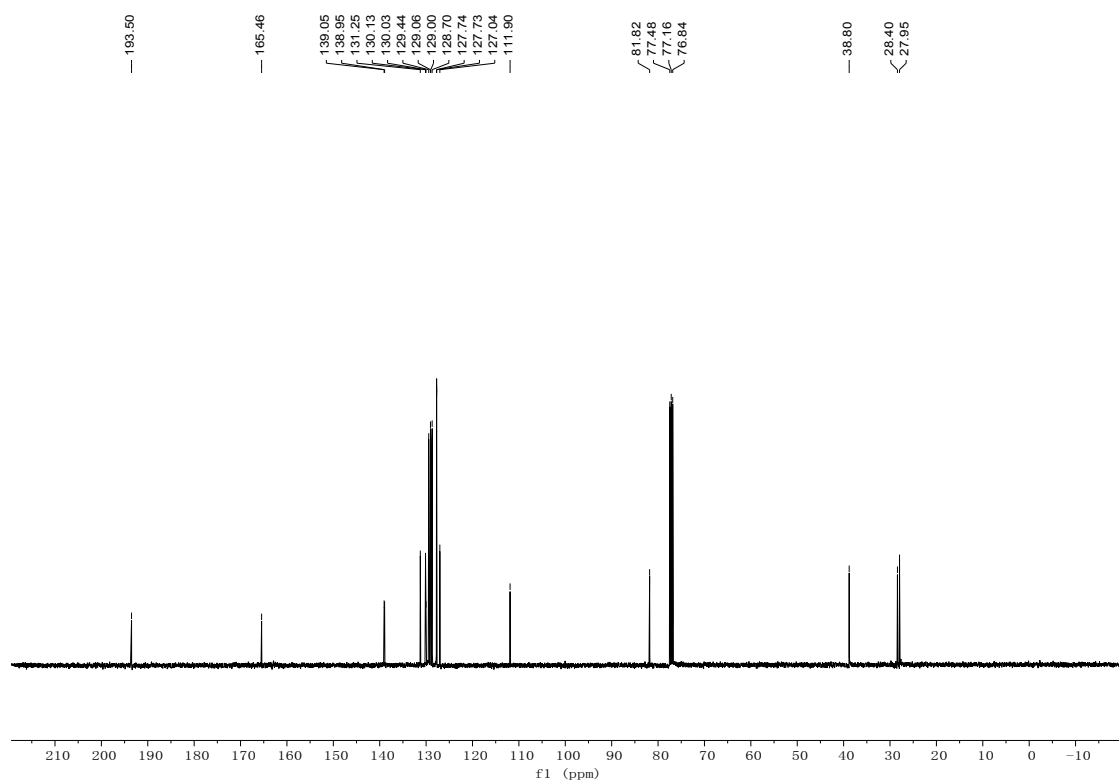
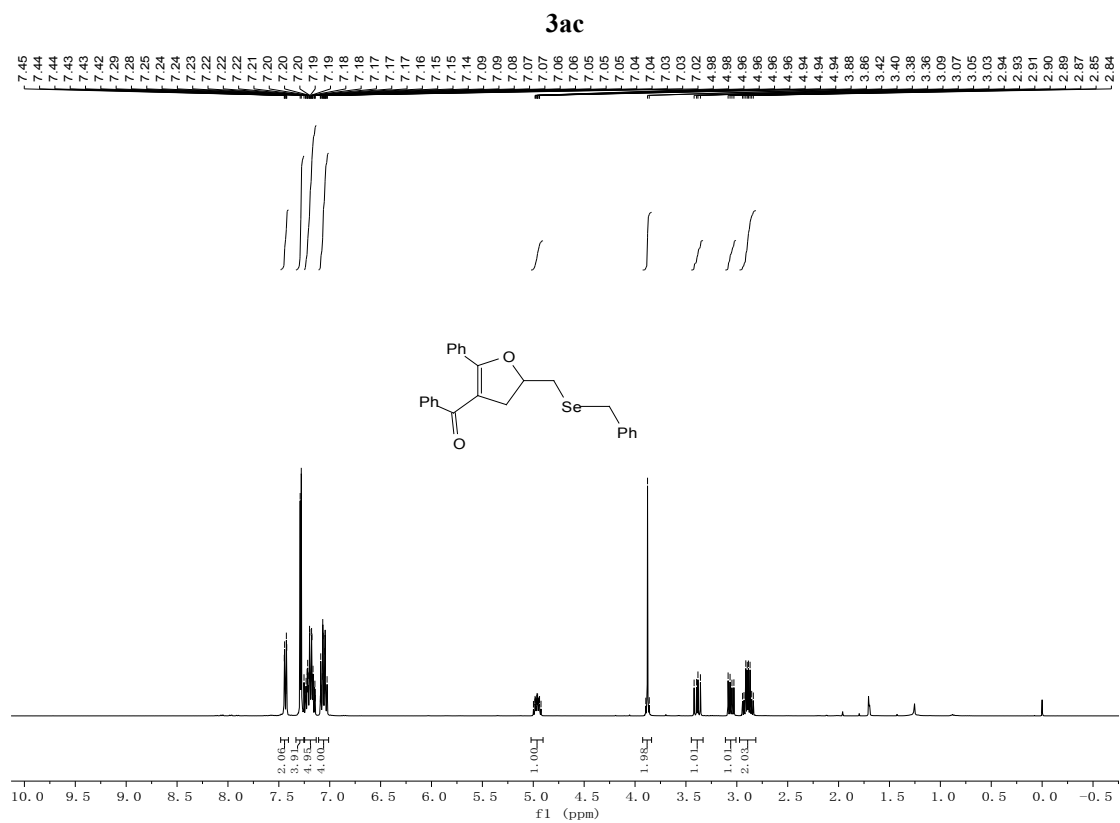




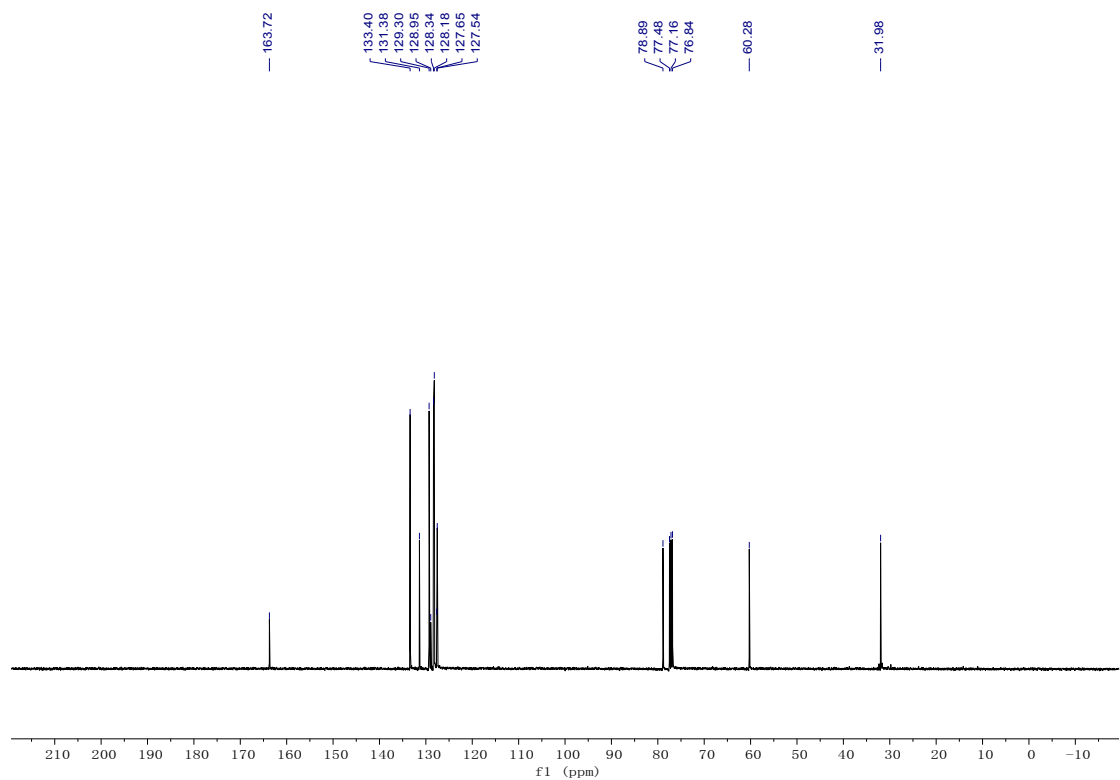
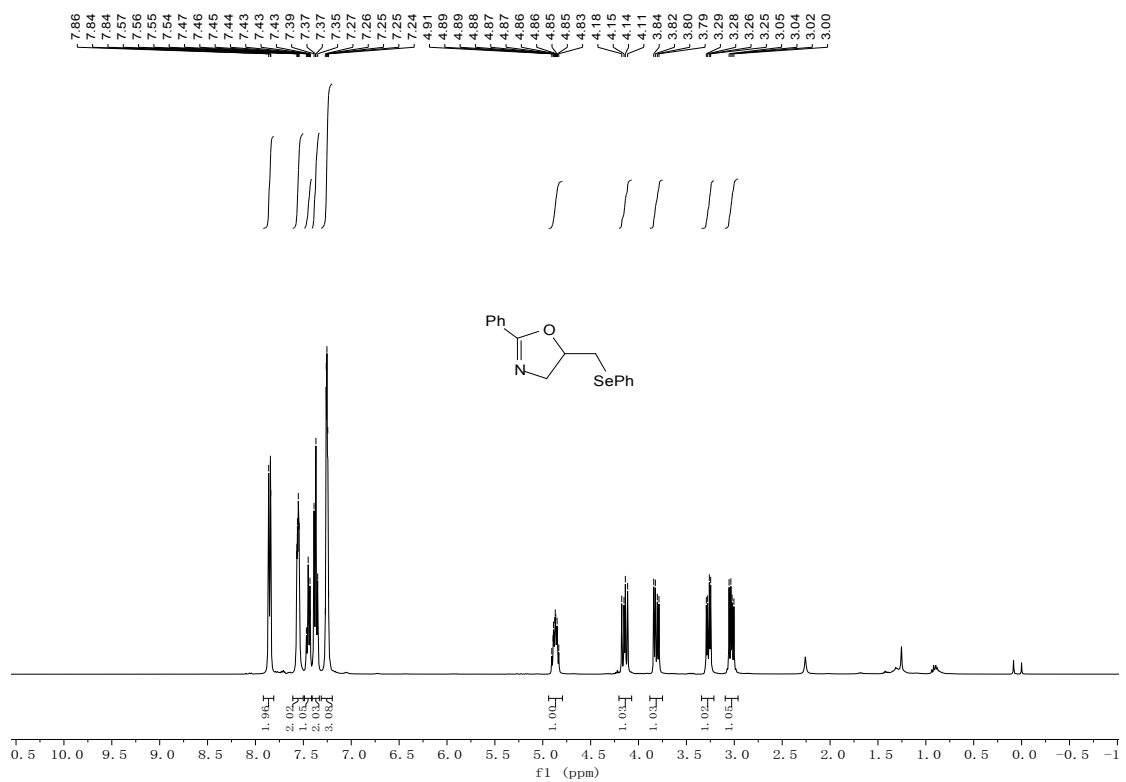


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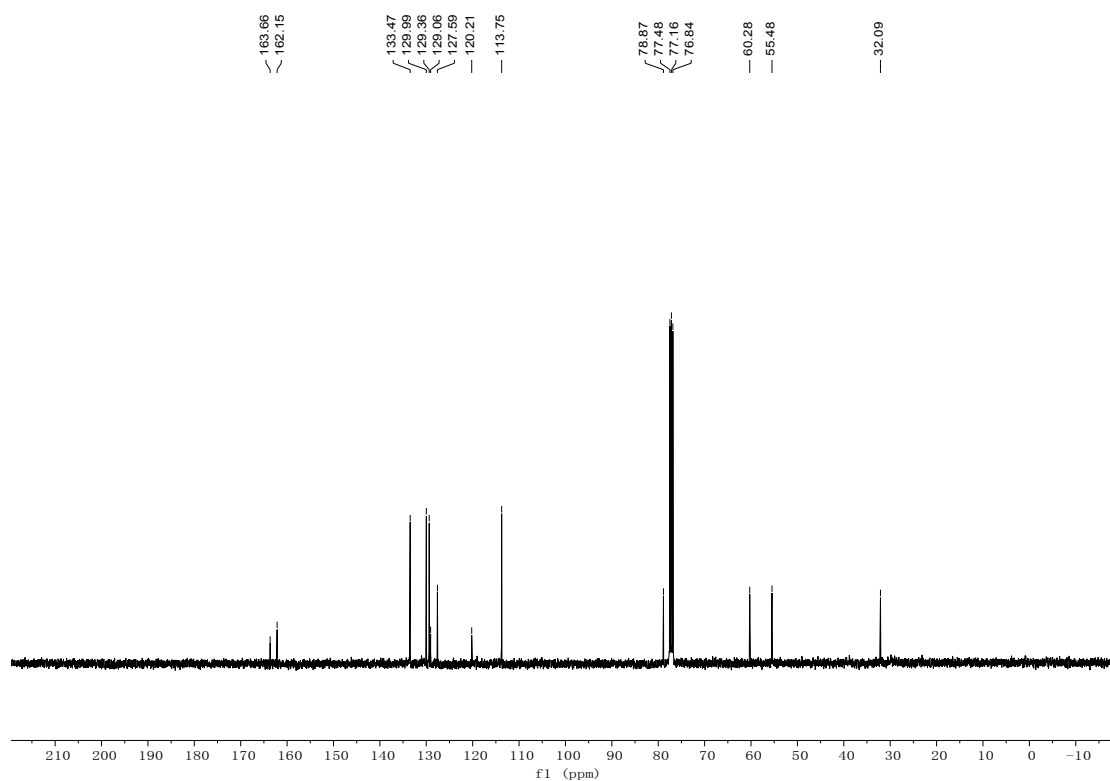
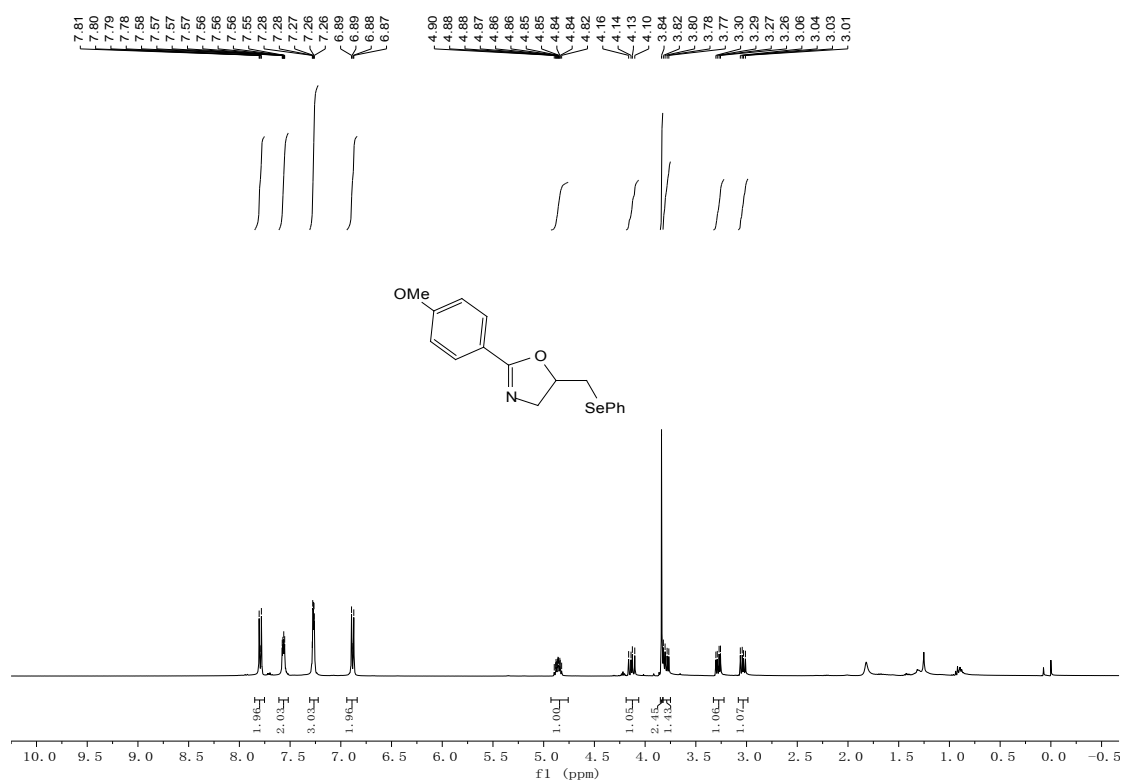


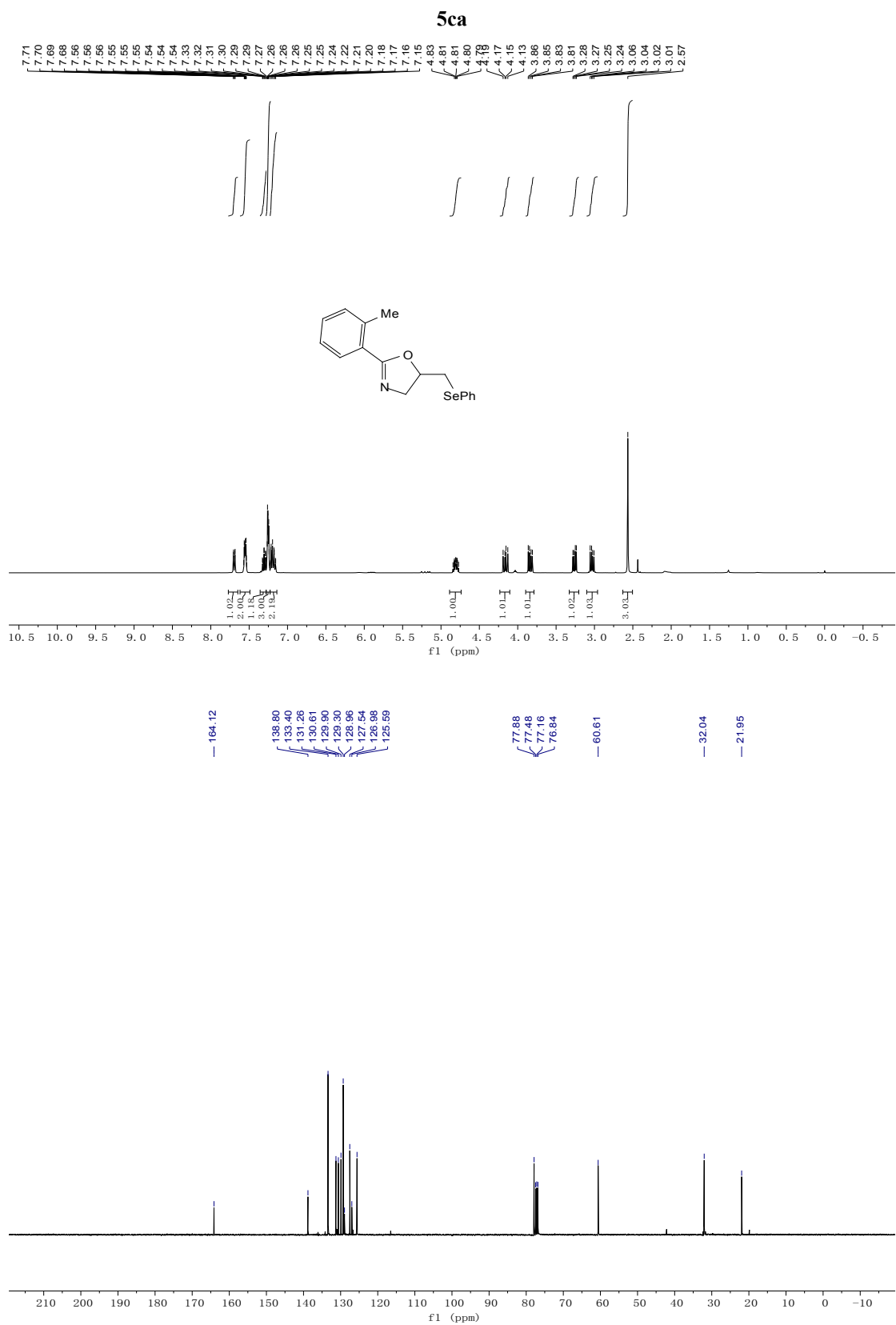


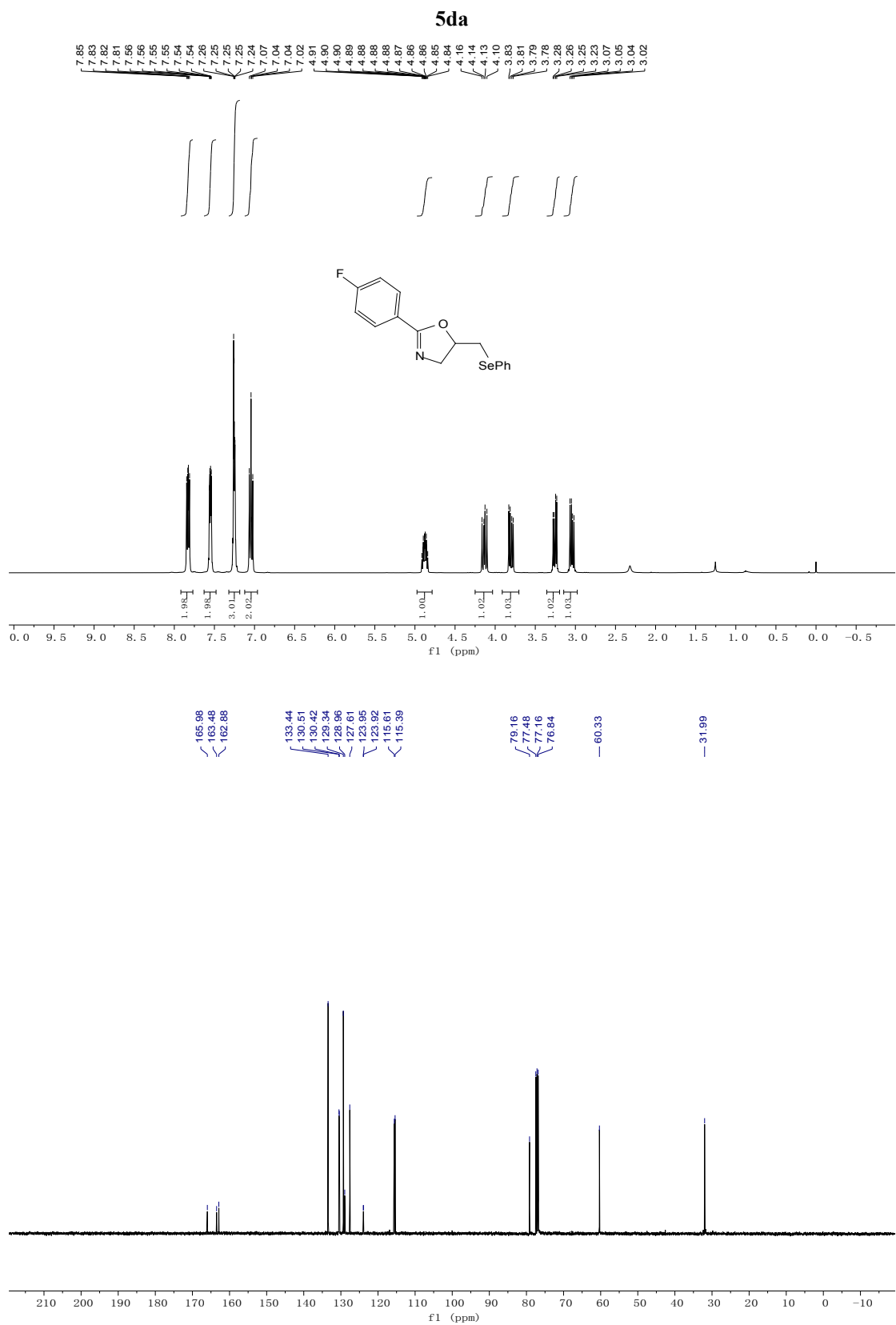
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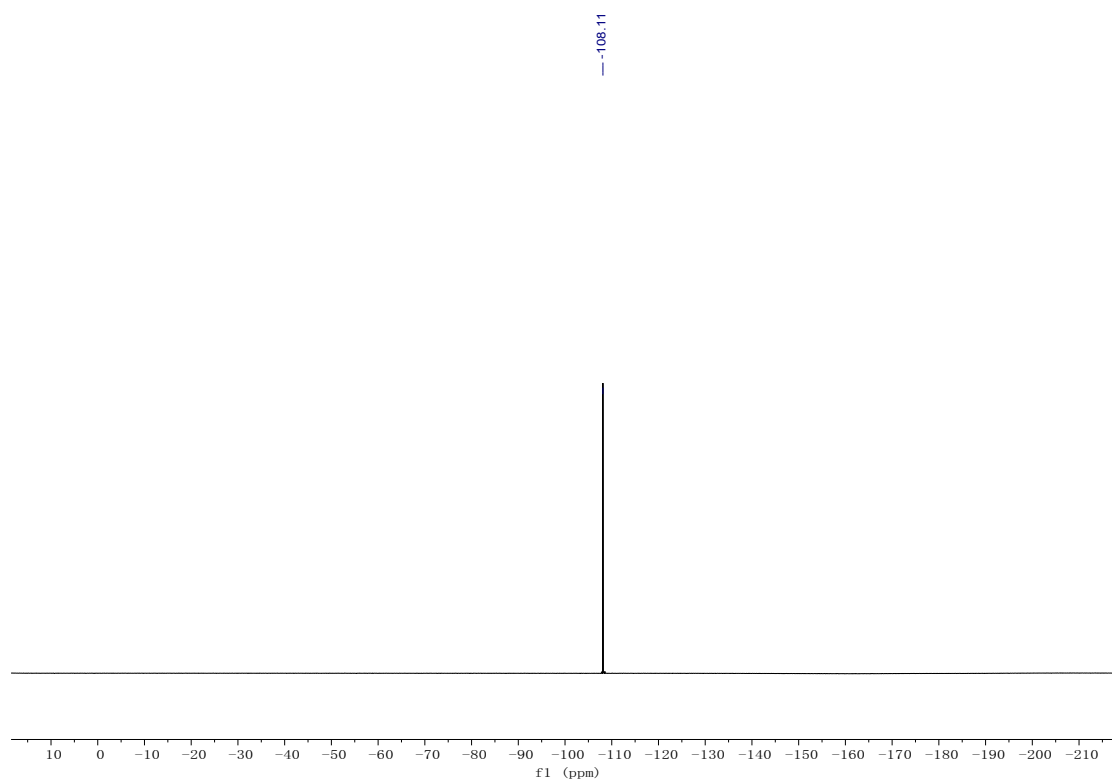


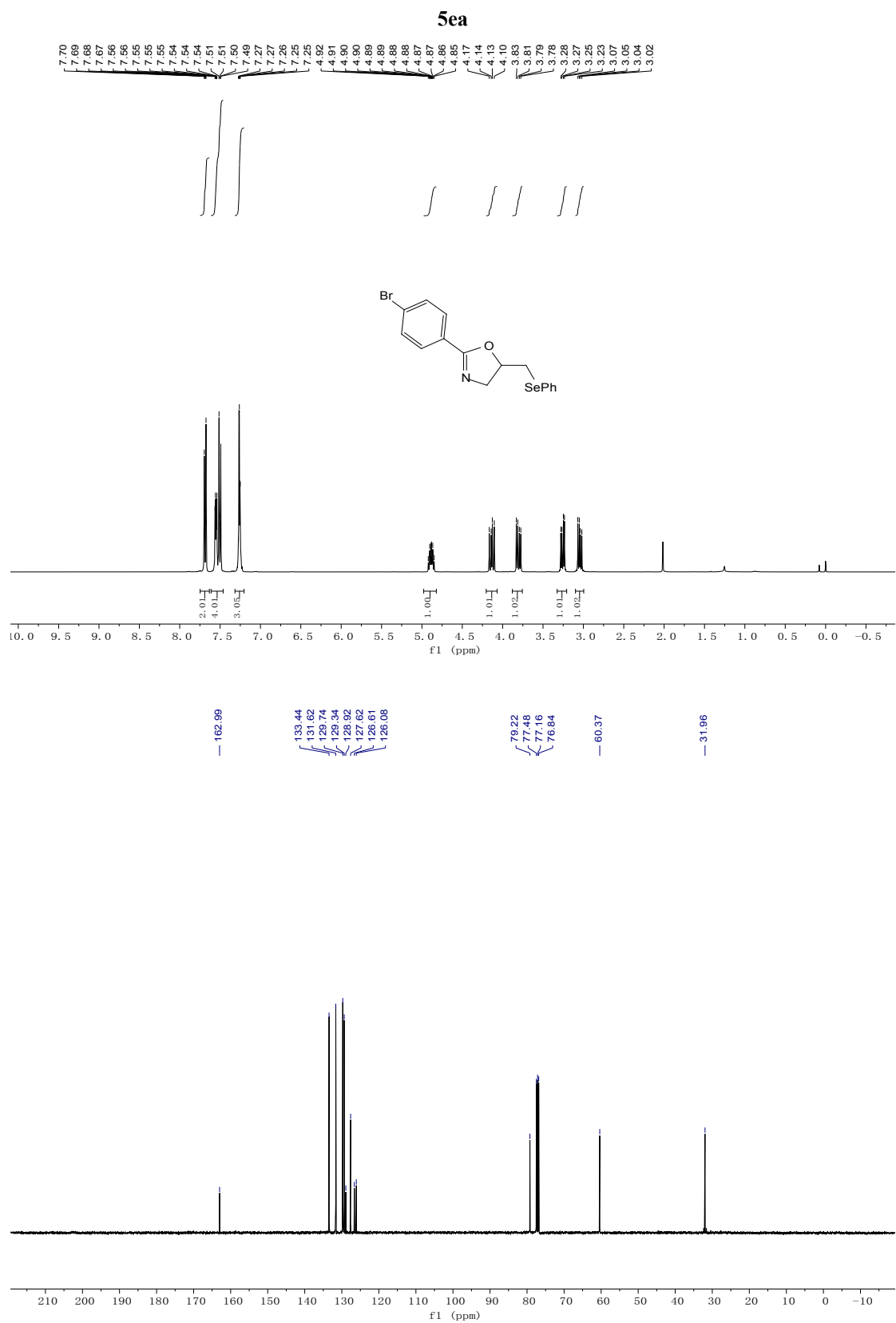
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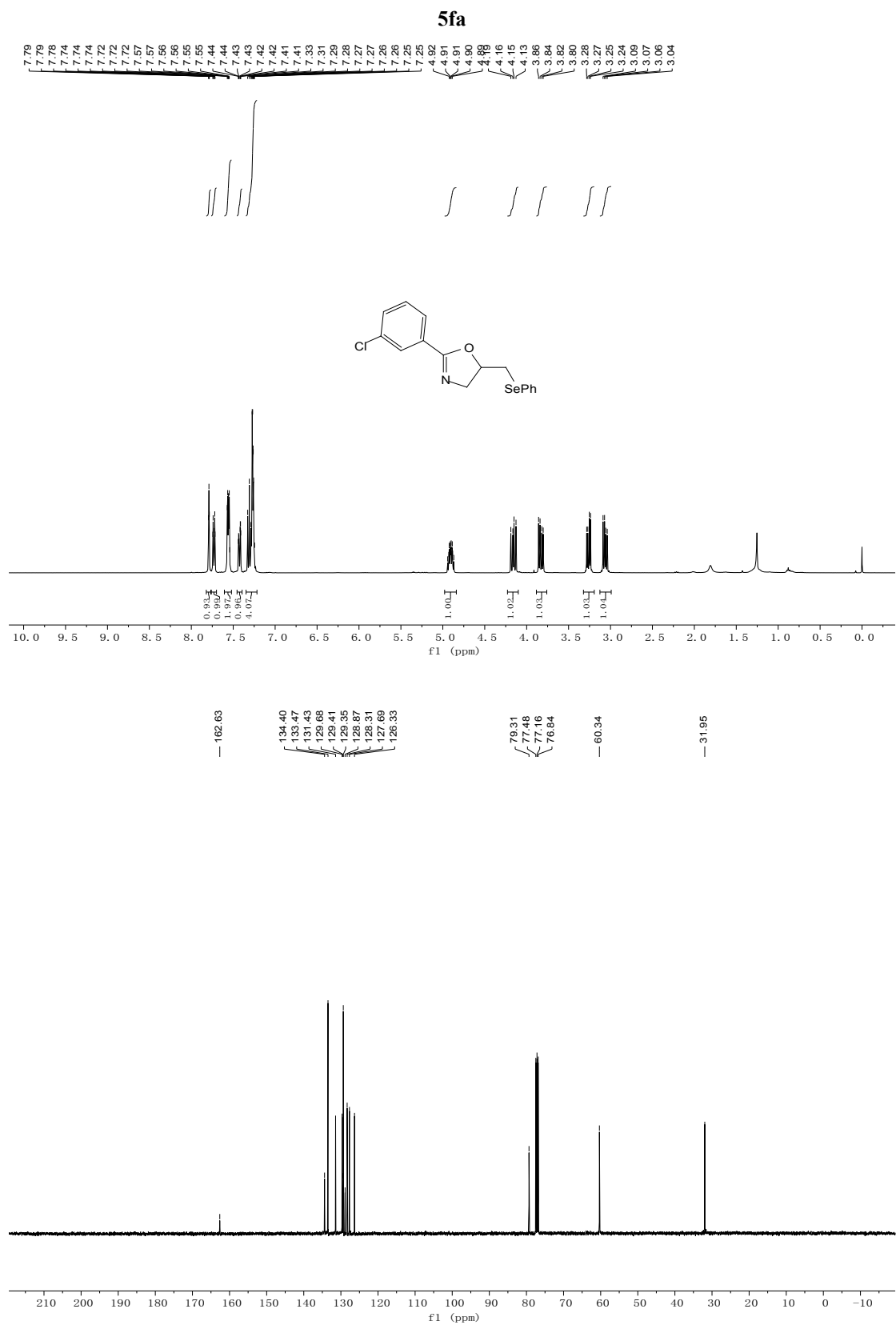


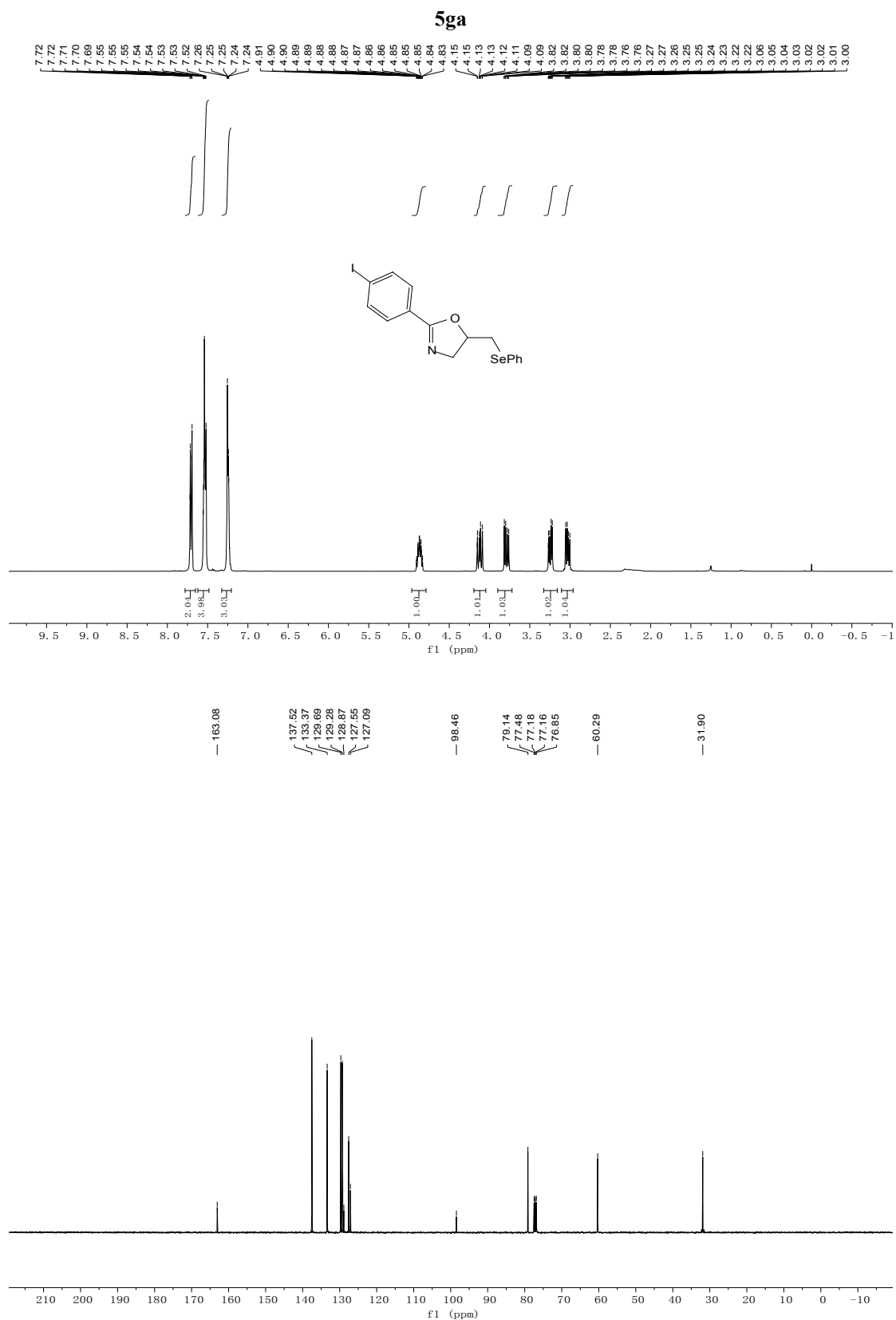


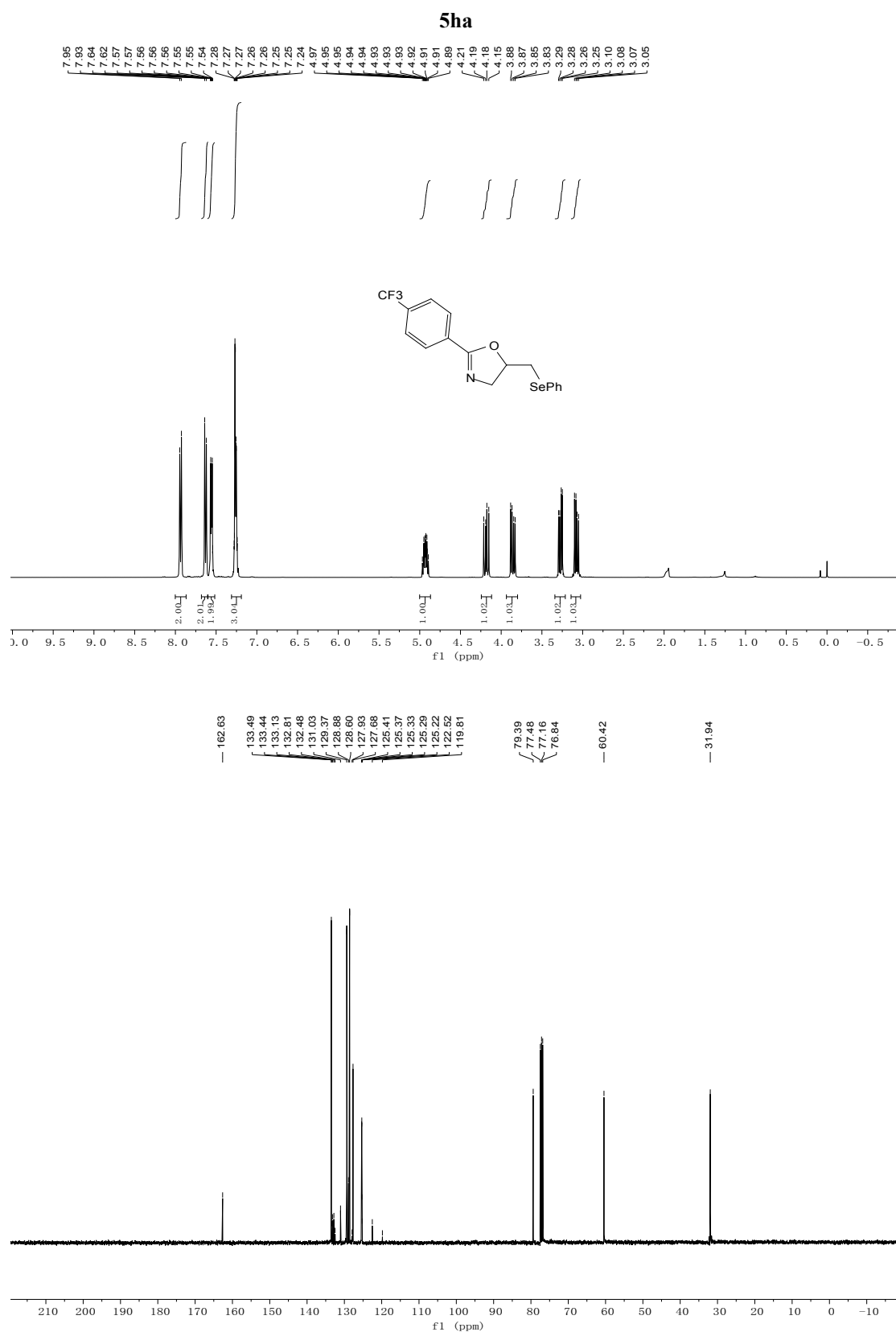


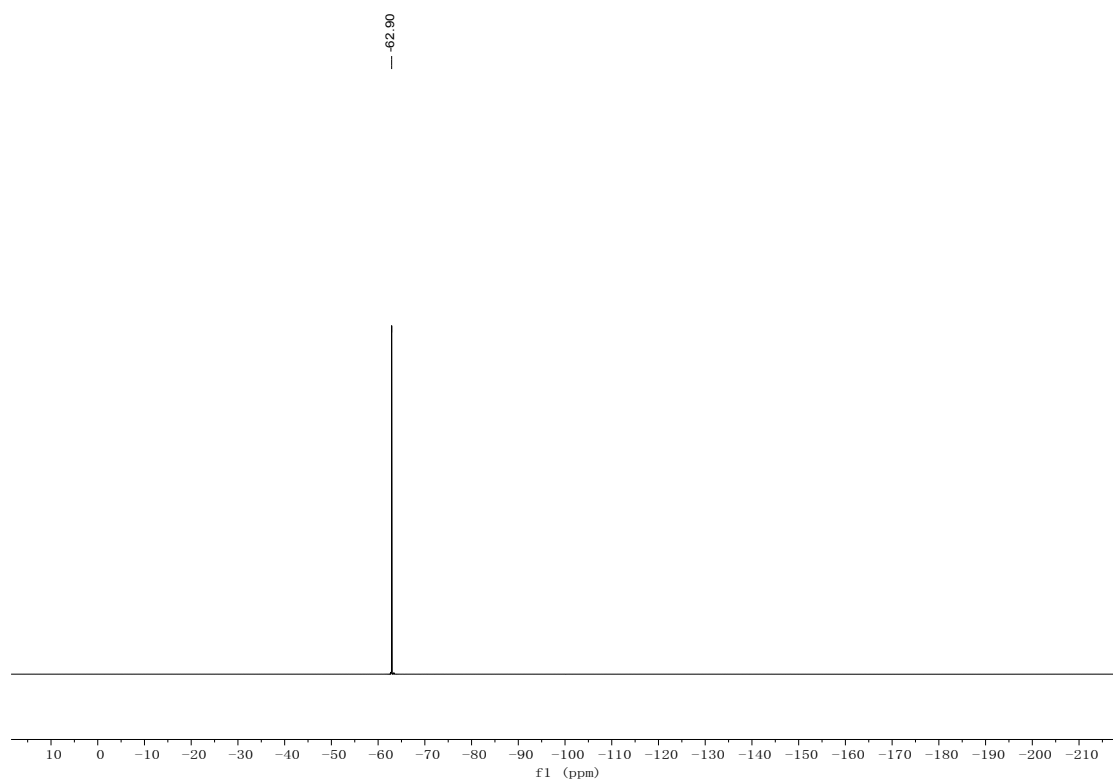


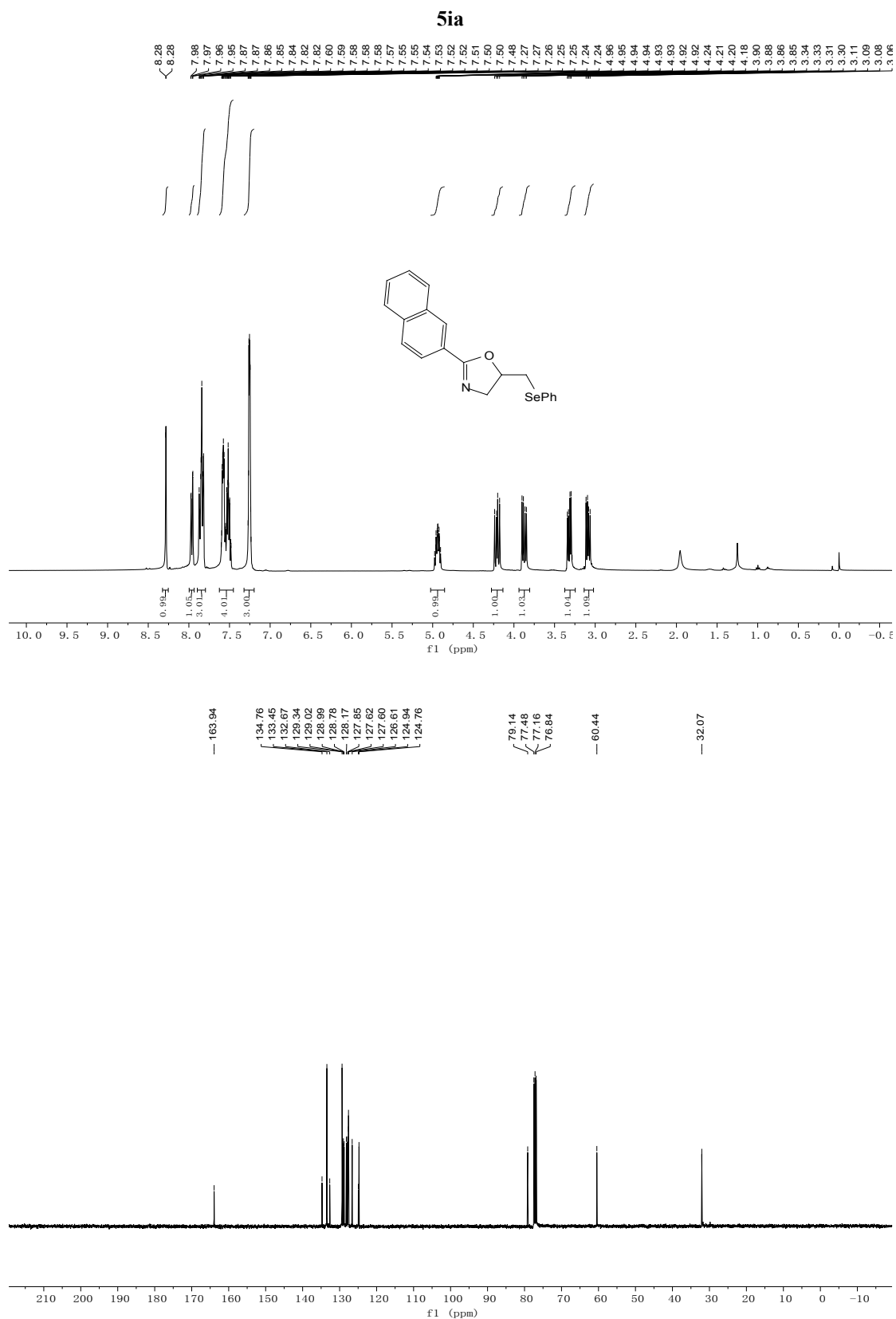


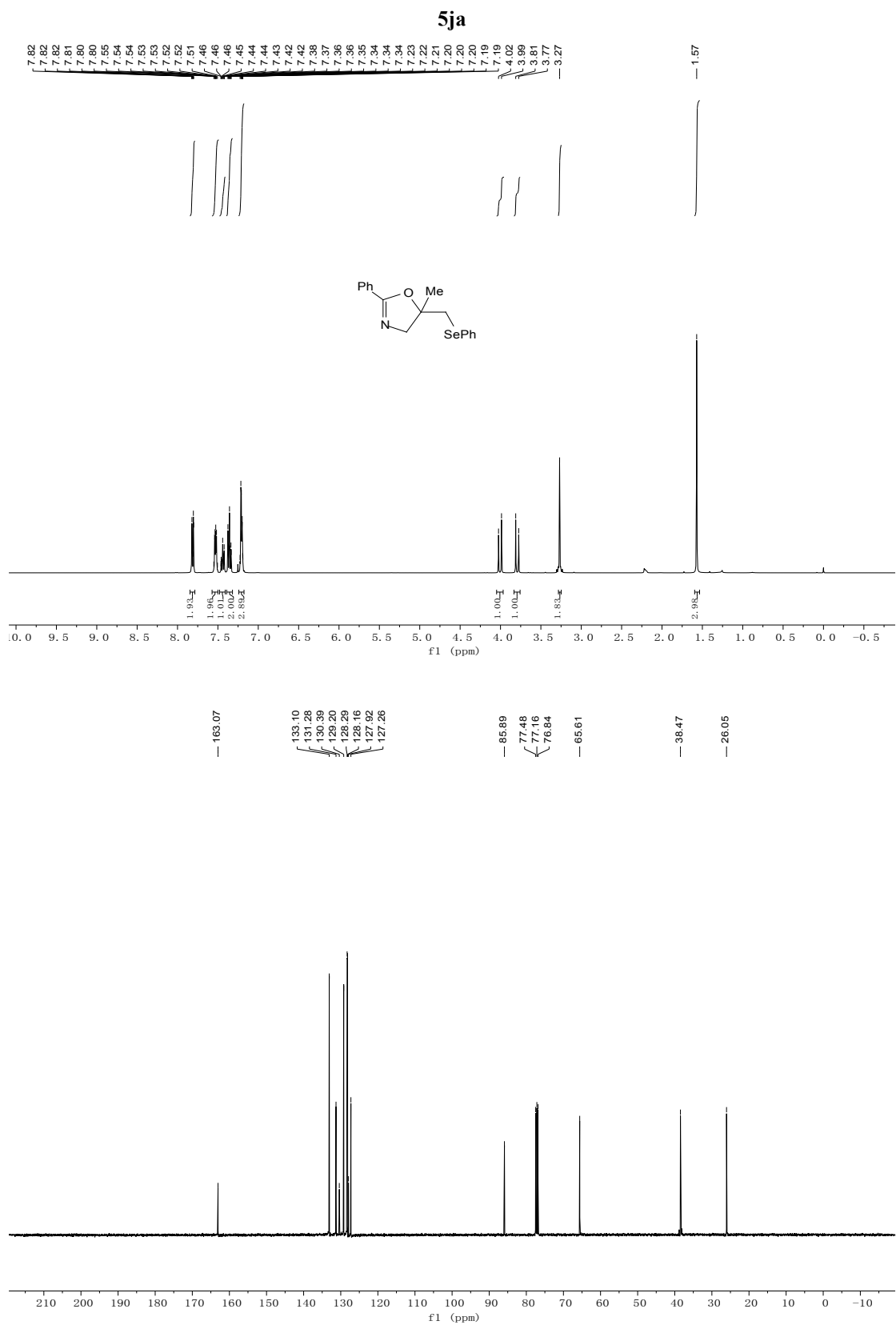


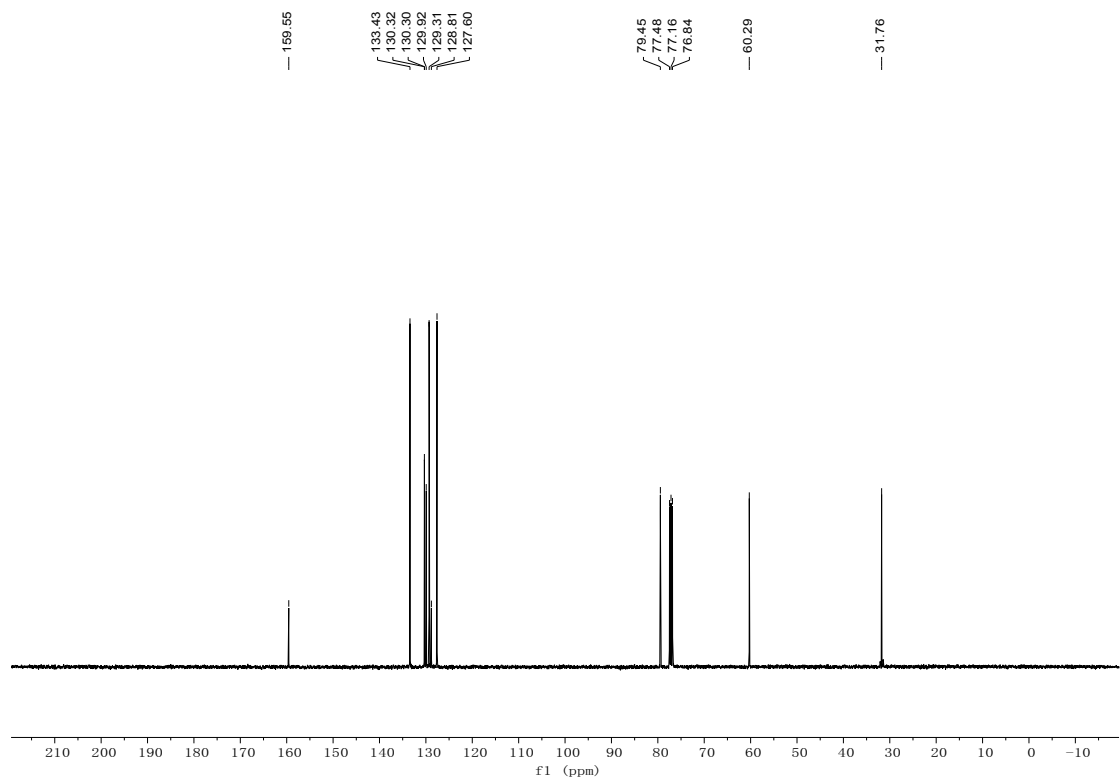
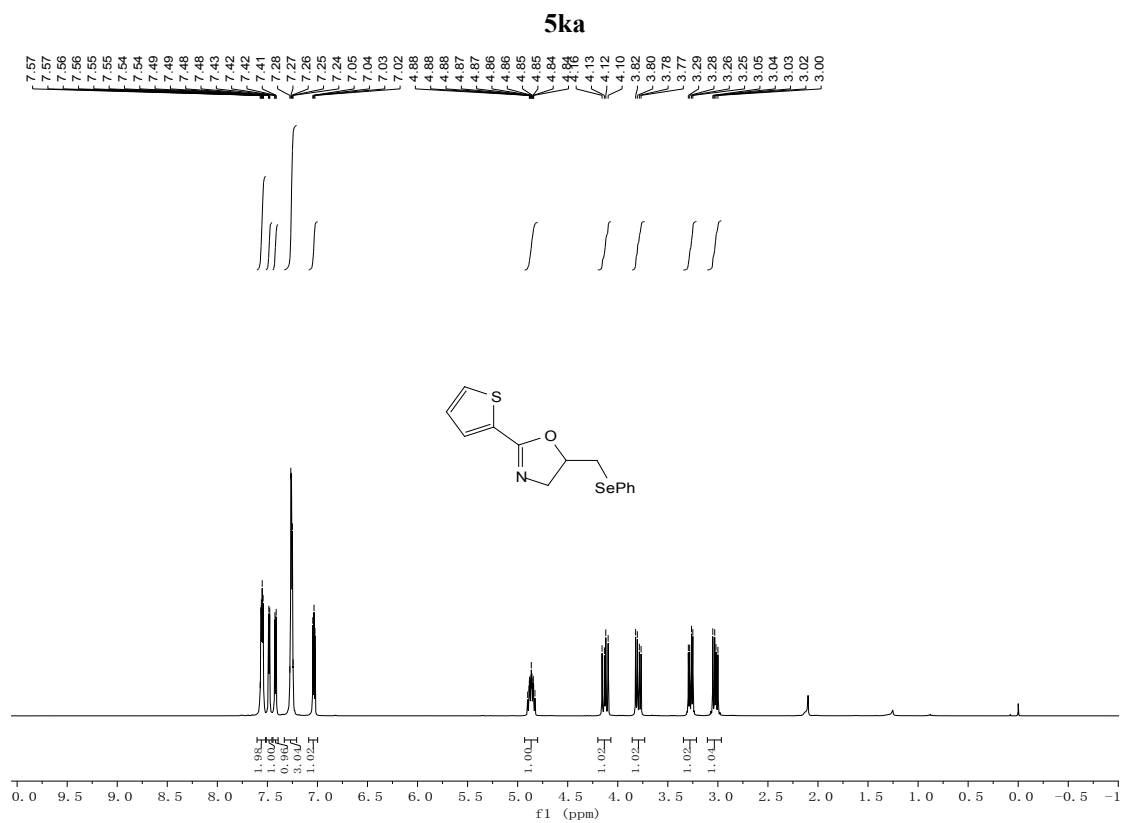


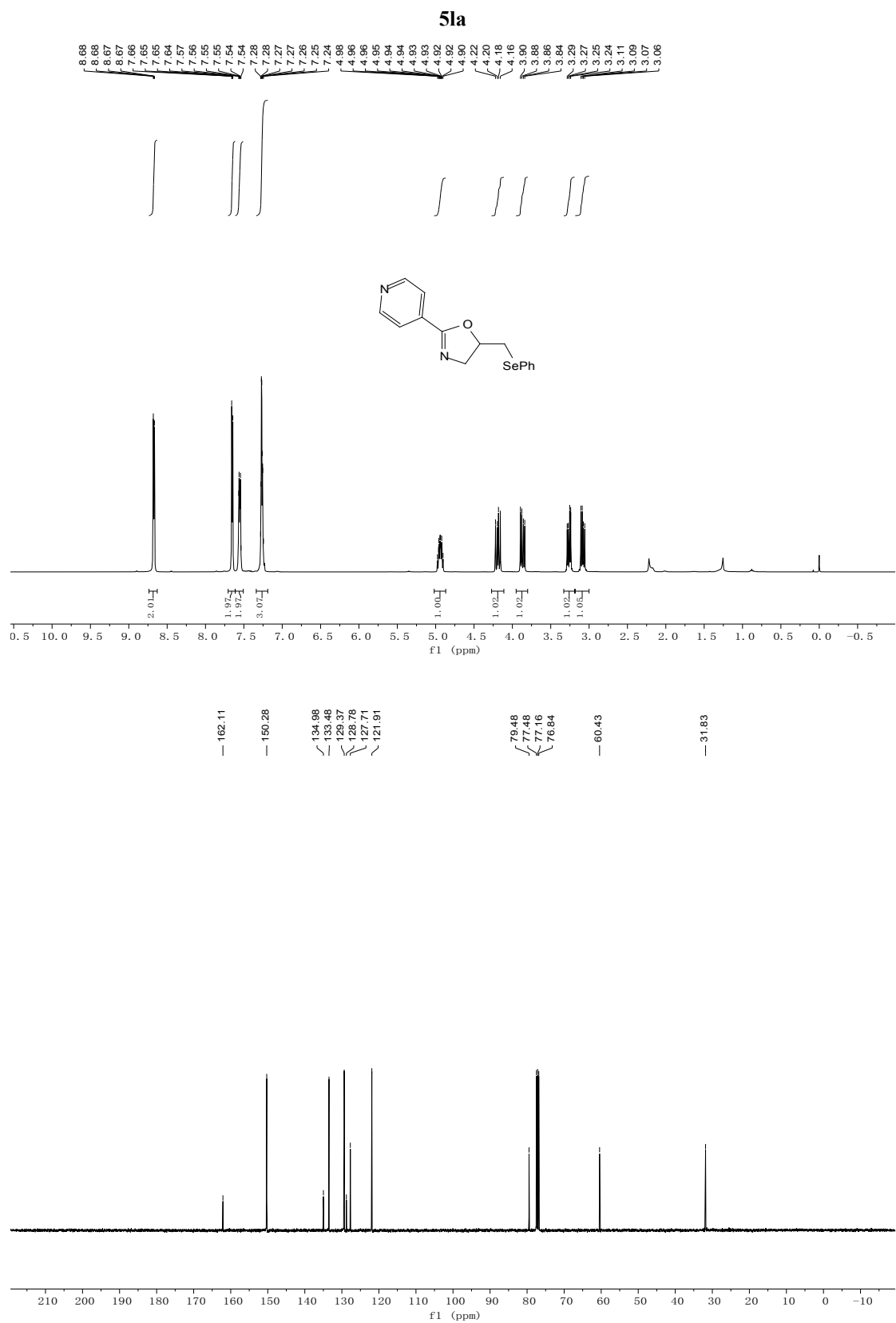


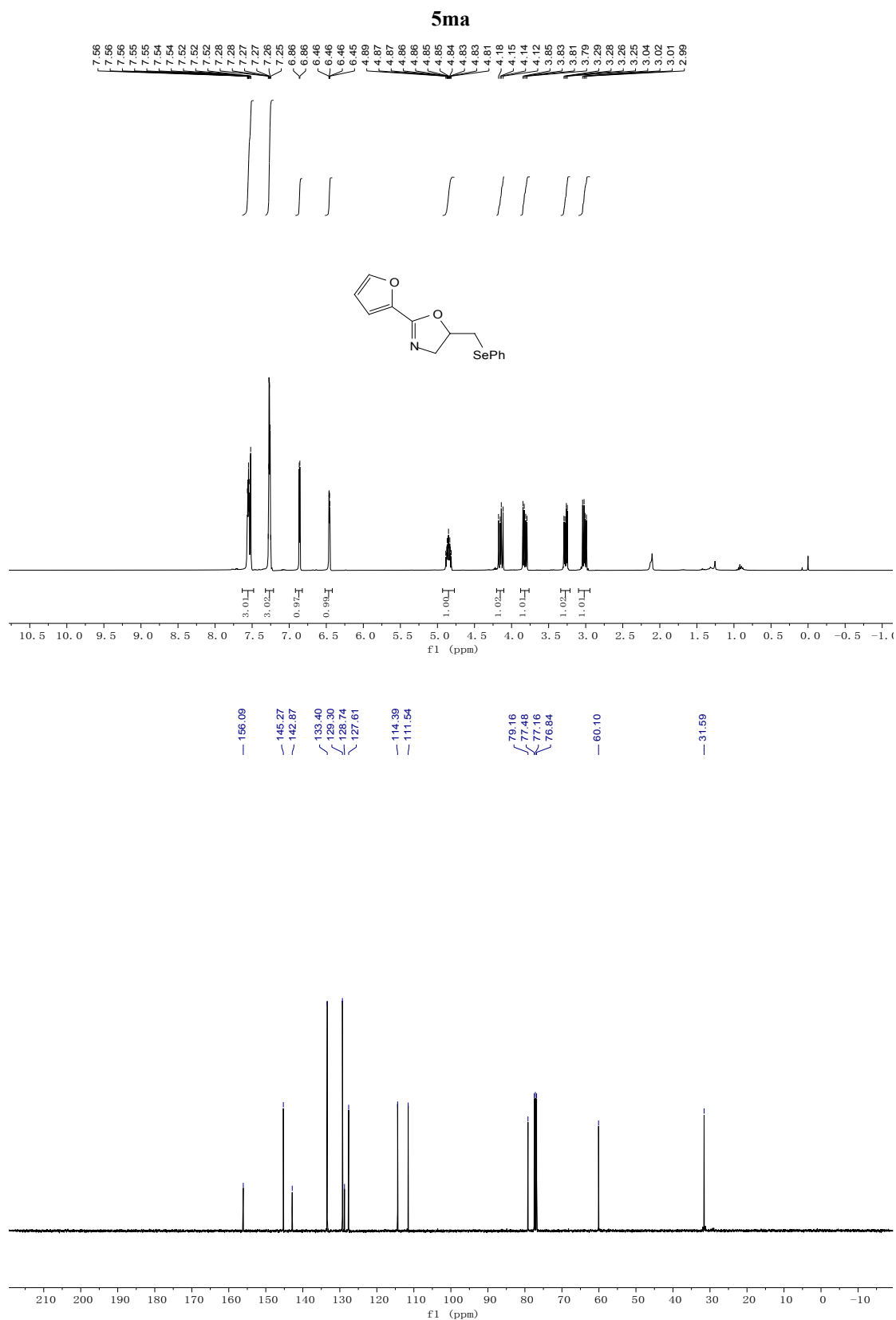




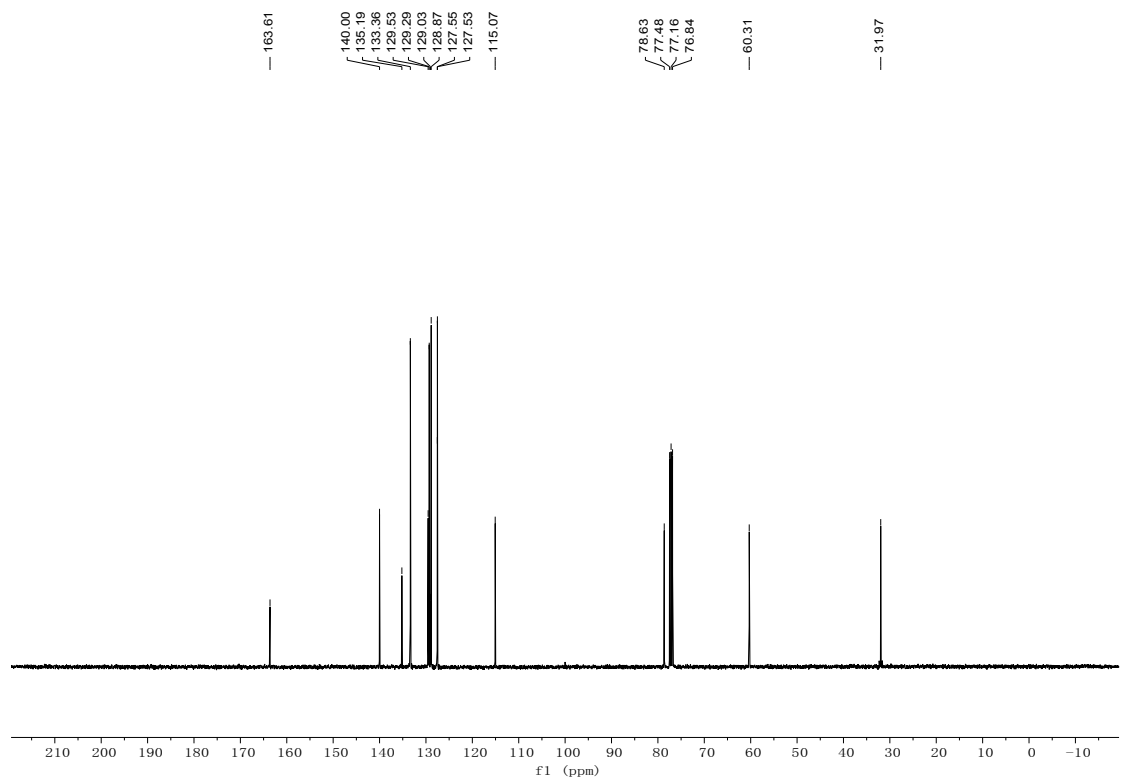
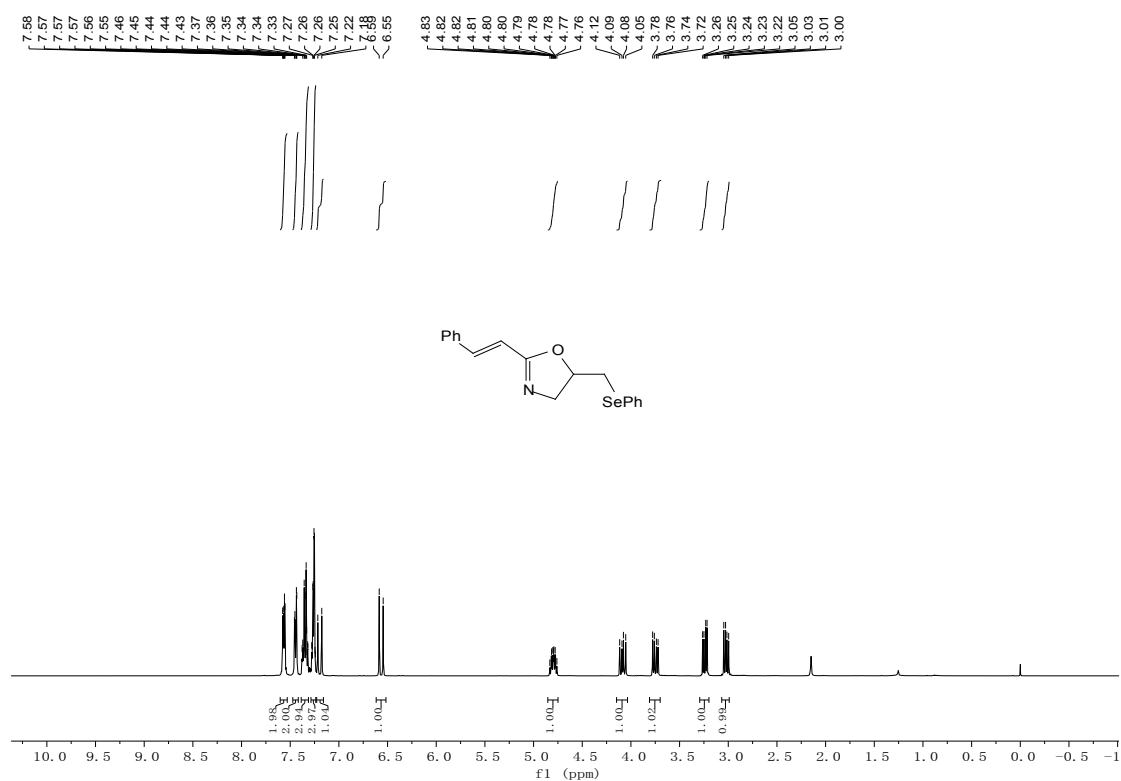




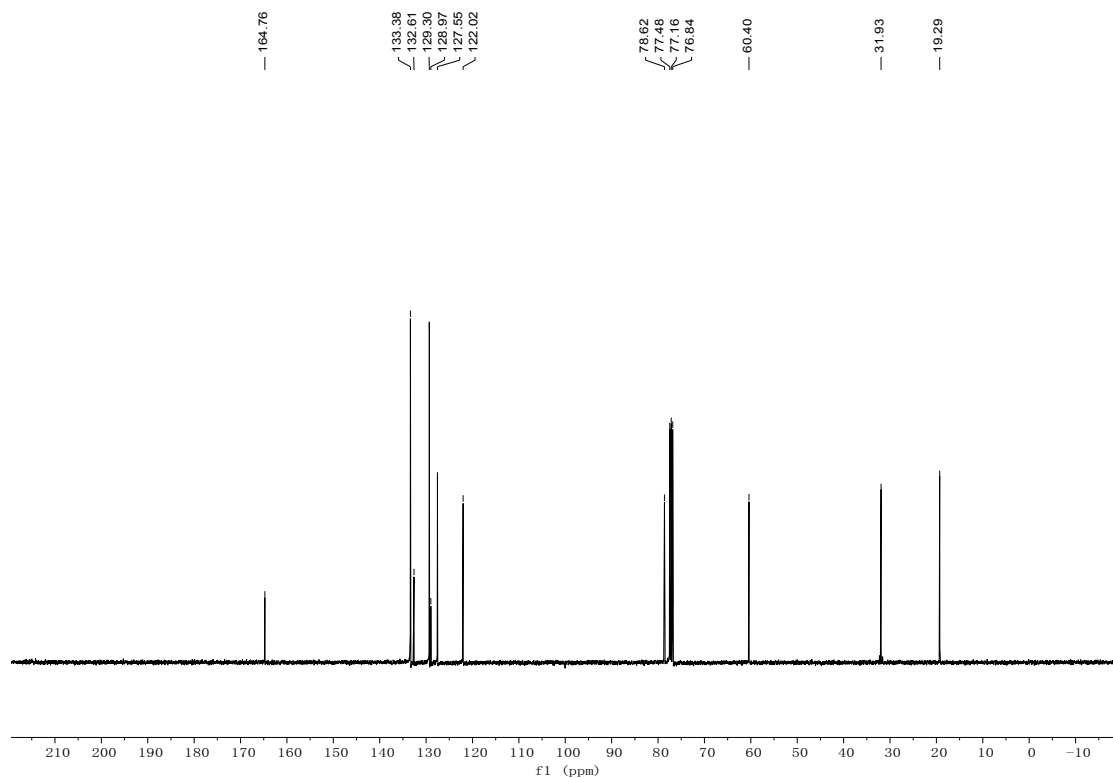
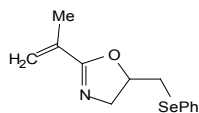
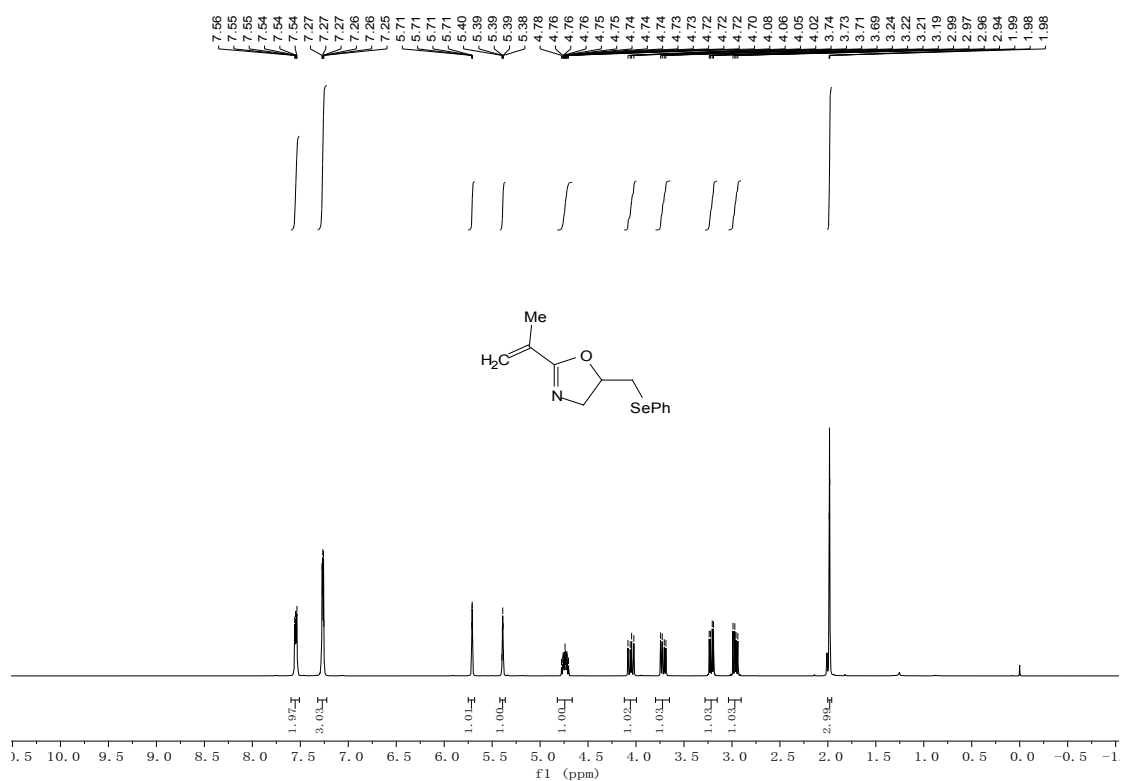


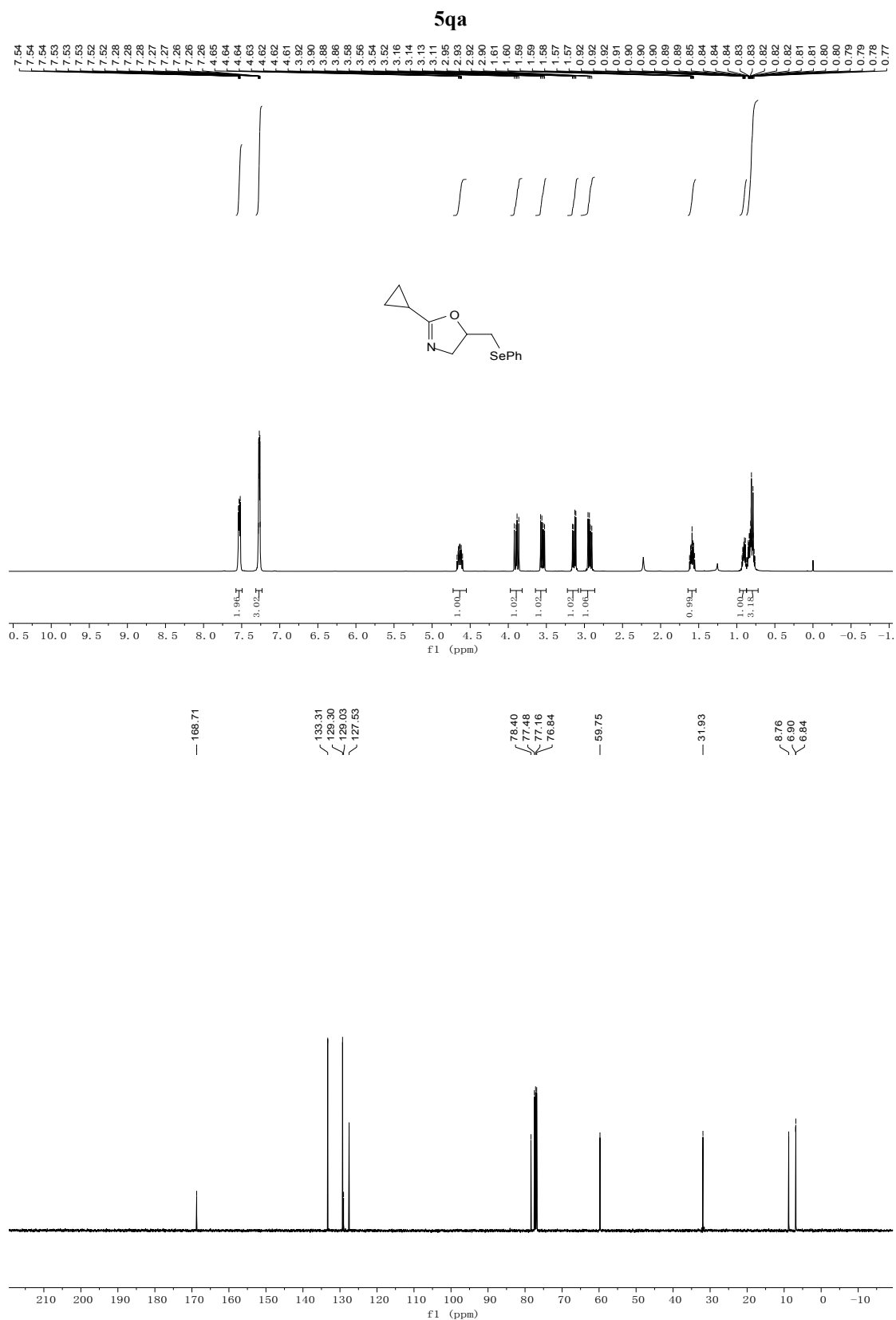


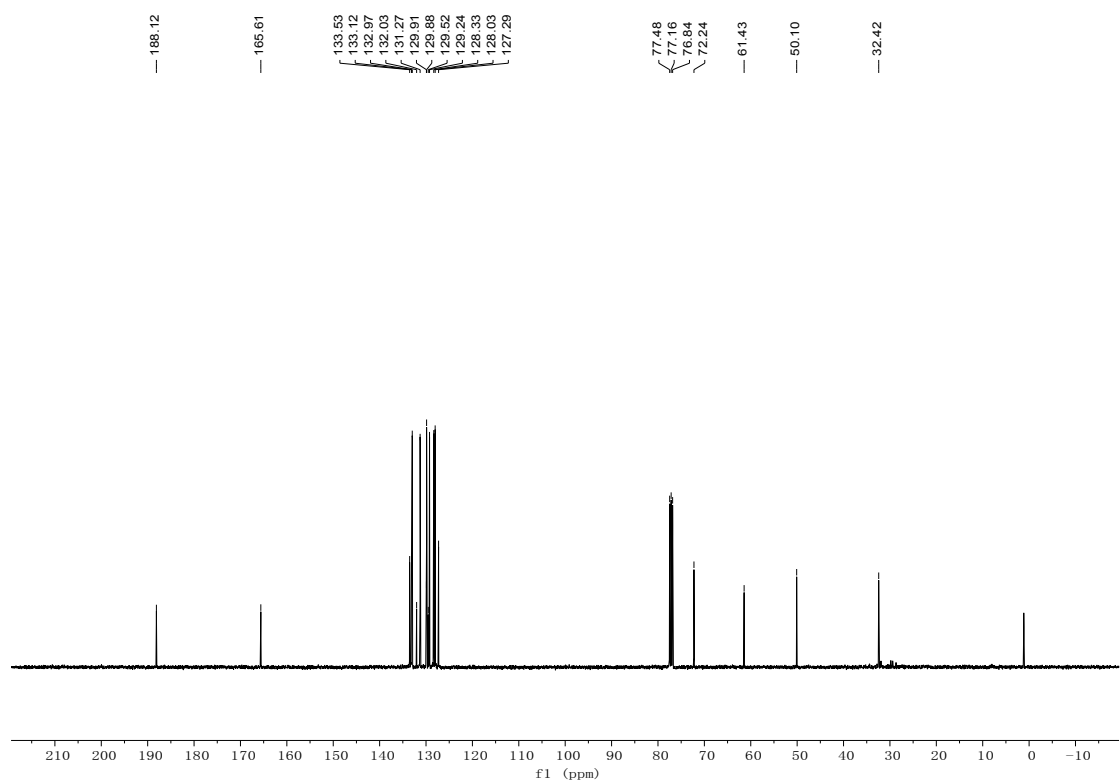
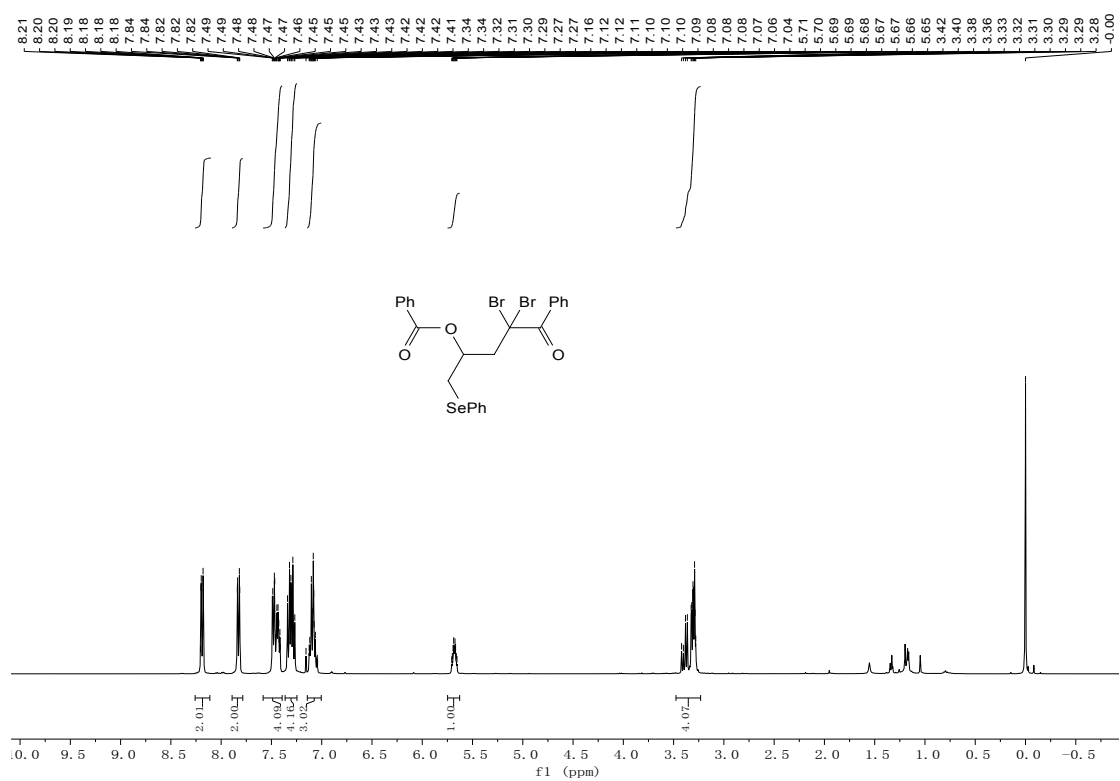
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