–Supporting Information –

Radical Cascade Reaction of Aryl Alkynoates at Room Temperature: Synthesis of Fully Substituted α,β-Unsaturated Acids with Chalcogen Functionality

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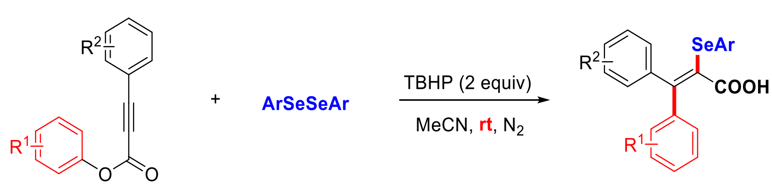
General Information:

All non-aqueous reactions were carried out under an atmosphere of nitrogen in flame-dried glass ware and were stirred using a magnetic stir plate. All reactions were carried out using anhydrous solvent unless otherwise noted. DCE, MeCN, and DMSO were dried over calcium hydride. Dry toluene, and THF were prepared by distilling over sodium ketyl. Dried DMF and MeOH were purchased from FINAR. TBHP and DTBP were procured from Sigma Aldrich Company.

All reactions were monitored by thin layer chromatography (TLC) on WhatmanPartisil® K6F TLC plates (silica gel 60 Å, 0.25 mm thickness) and visualized using a UV lamp (366 or 254 nm) or by use of one of the following visualization reagents: PMA: 10 g phosphomolybdic acid/ 100 mL ethanol, $KMnO_4$: 0.75 g potassium permanganate, 5 g K_2CO_3,/100mL water. Products were isolated by column chromatography (Merck silica gel 100-200μm). Yields refer to chromatographically and spectroscopically homogenous materials unless noted otherwise. ^{13}C and ^{1}H NMR spectra were recorded on a Bruker 400 or Bruker 500 MHz spectrometers. Chemical shift values (δ) are reported in ppm and calibrated to the residual solvent peak $CDCl_3$ δ = 7.2600 ppm for ^{1}H, δ = 77.16 ppm for ^{13}C and DMSO-d_6 δ = 2.500 ppm for ^{1}H; δ = 39.51ppm for ^{13}C or calibrated to tetramethylsilane (δ = 0.00). All NMR spectra were recorded at ambient temperature (290 K) unless otherwise noted. ^{1}H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constant, integration). The following abbreviations are used to indicate multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet, sext, sextet, sept, septet, m, multiplet; dd, doublet of doublet; dt, doublet of triplet; dq, doublet of quartet; td, triplet of doublet; tt, triplet of triplet; dq, doublet of quartet; br, broad; app, apparent. Mass spectra were recorded by electron spray ionization (ESI) method on a Q-TOF Micro with lock spray source.

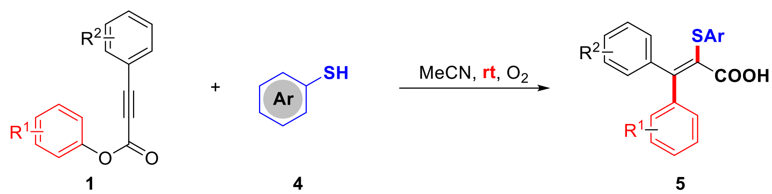
Arylalkynoates **1** were synthesized following previously published procedures (*Chem. Commun*. **2017***, 53,* 10136). Diselenide derivatives **2** were prepared following the know procedure (*Org. Biomol. Chem*. **2014**, *12*, 9557).

General Procedure for Selenium Radical Based Smile Rearrangement of Aryl Alkynoates:



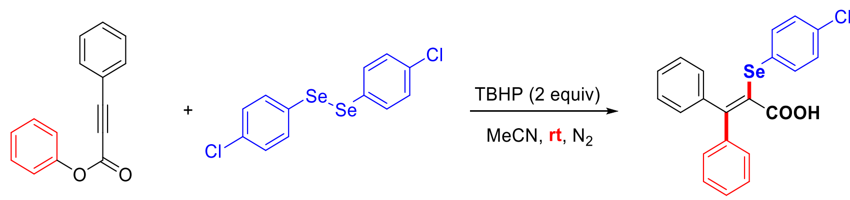
The aryl alkynoates **1** (0.20 mmol), diaryl diselenides **2** (0.40 mmol) and TBHP in decane solution (0.40 mmol) were taken in an oven dried reaction tube with a magnetic stir. The reaction tube was purged with nitrogen and then, dry CH_3CN (1.5 mL) was added via a syringe. The reaction mixture was allowed to stir at room temperature for 24 h. After completion of the reaction (TLC monitored), it was transferred to a round bottom flask after dilution with CH_2Cl_2. Volatiles were evaporated under reduced pressure and the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate to get pure products **3**.

General Procedure for Sulfur Radical Based Smile Rearrangement of Aryl Alkynoates:



The aryl alkynoates **1** (0.20 mmol) and aryl thiols **4** (0.40 mmol) were taken in an oven dried reaction tube with a magnetic stir. Then, dry CH_3CN (1.5 mL) was added with a syringe and the mixture was allowed to stir under oxygen atmosphere (oxygen balloon) for 24 h at room temperature. After completion of the reaction (TLC monitored), it was transferred to a round bottom flask after dilution with CH_2Cl_2. Volatiles were evaporated under reduced pressure and the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate to get pure products **5**.

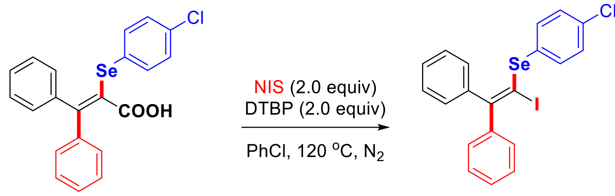
Gram Scale Synthesis of Product 3y:



The phenyl 3-phenylpropiolate **1b** (1.45 g, 6.5 mmol), bis(4-chlorophenyl) diselenide **2b** (5.0 g, 13.0 mmol) and TBHP in decane solution (2.0 equiv) were taken in an oven dried round bottom flask with a magnetic stir. The reaction flask was purged with nitrogen and then, dry CH_3CN (40 mL) was added via a syringe. The reaction mixture was allowed to stir under nitrogen atmosphere for 24 h at room temperature. After completion of the reaction (TLC monitored), the solvent was evaporated to dryness. The resulting residue was purified by silica gel column chromatography (hexane : ethyl acetate, 70 : 30) to provide pure product **3y** in 78% yield (2.1 g).

Post-functionalization:

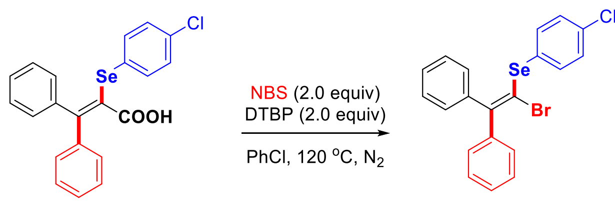
Synthesis of compound 6:



3y **6**

The product **3y** (0.2 mmol), *N*-iodosuccinimide (0.4 mmol) and DTBP (0.4 mmol) were taken in an oven dried reaction tube equipped with a magnetic stir. Then, PhCl (1.5 mL) was added and the mixture was allowed to stir at 120 °C for 24 h. After completion of the reaction (TLC monitored), it was transferred to a round bottom flask after dilution with CH_2Cl_2. The volatiles were evaporated to dryness under reduced pressure and the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate to get pure product **6** (78%, 77 mg) as white solid.

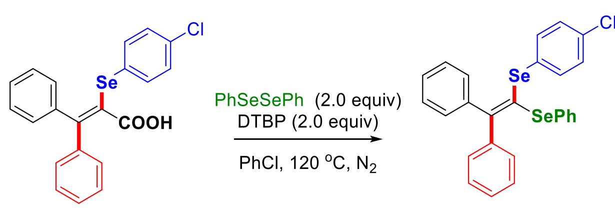
Synthesis of compound 7:



3y **7**

The product **3y** (0.2 mmol), *N*-bromosuccinimide (0.4 mmol) and DTBP (0.4 mmol) were taken in an oven dried reaction tube equipped with a magnetic stir. Then, PhCl (1.5 mL) was added and the mixture was allowed to stir at 120 °C for 24 h. After completion of the reaction (TLC monitored), it was transferred to a round bottom flask after dilution with CH_2Cl_2. The volatiles were evaporated to dryness under reduced pressure and the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate to get pure product **7** (70%, 63 mg) as white solid.

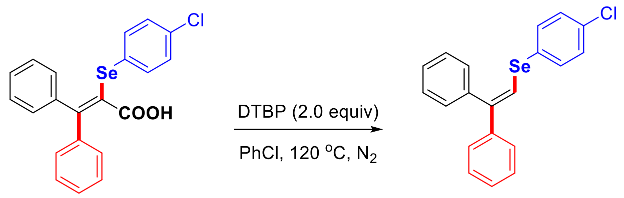
Synthesis of compound 8:



3y **8**

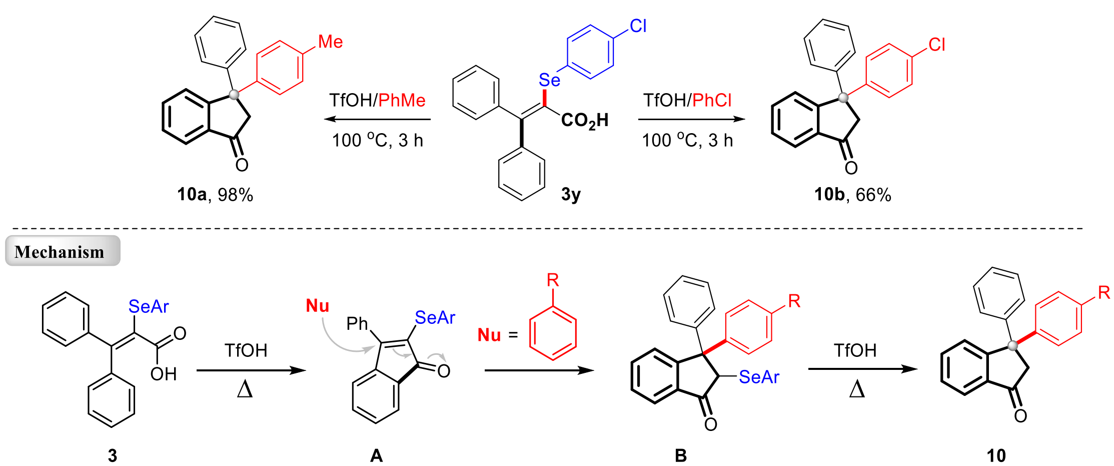
The product **3y** (0.2 mmol), diphenyldiselenide **2a** (0.4 mmol) and DTBP (0.4 mmol) were taken in an oven dried reaction tube equipped with a magnetic stir. Then, PhCl (1.5 mL) was added and the mixture was allowed to stir at 120 °C for 24 h. After completion of the reaction (TLC monitored), it was transferred to a round bottom flask after dilution with CH_2Cl_2. The volatiles were evaporated to dryness under reduced pressure and the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate to get pure product **8** (75%, 79 mg) as white solid.

Synthesis of compound 9:



The product **3y** (0.2 mmol), and DTBP (0.4 mmol) were taken in an oven dried reaction tube equipped with a magnetic stir. Then, PhCl (1.5 mL) was added and the mixture was allowed to stir at 120 °C for 24 h. After completion of the reaction (TLC monitored), it was transferred to a round bottom flask after dilution with CH_2Cl_2. The volatiles were evaporated to dryness under reduced pressure and the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate to get pure product **9** (84%, 62 mg) as white solid.

Synthesis of 3,3-Disubstituted Indanones:



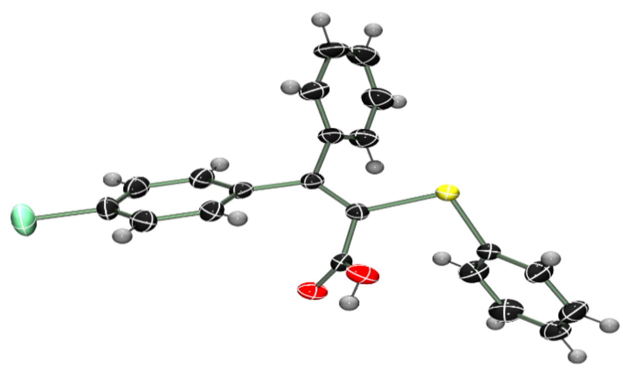
The product **3y** (0.2 mmol) was taken in an oven dried reaction tube equipped with a magnetic stir. Triflic acid (0.1 mL) and dry solvent (PhMe, 1 mL) was added. The mixture was allowed to stir at 100 °C for 3 h. After that, it was allowed to cool to room temperature and 5 mL water was added. The reaction mixture was extracted with EtOAc (5 mL, three times). The organic layer was washed with saturated $NaHCO_3$ solution, dried over anhydrous magnesium sulfate, and concentrated under reduced pressure. The resulting residue was directly purified by silica gel column chromatography to get the desired product **10a** (58 mg, 98% yield).

Compound **10b** (42 mg, 66% yield) was prepared in the same way using PhCl (1 mL).

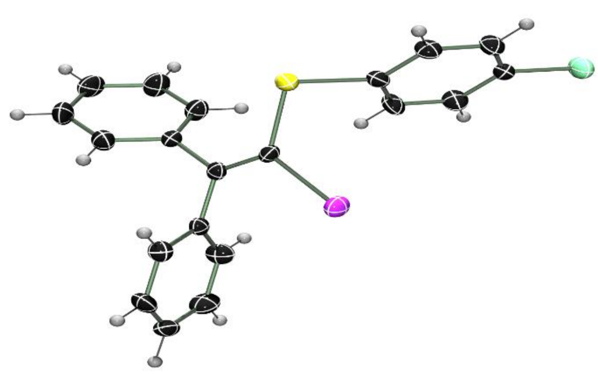
*This reaction proceeded through an acid promoted intramolecular cyclization flowed by 1,4-addition reaction of nucleophile solvent to give the intermediate **B**, which undergo deselenylation upon heating under acidic condition. These observations are in line with previous literature findings (Totu, T.; Kawai, S.; Ueno, Y. Synlett, **1996**, 539; Ramulu, B. V.; Niharika, P.; Satyanarayana, G. Synthesis **2015**; 47, 1255).*

Crystallographic Experimental Section:

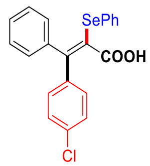
*ORTEP diagram of **3a:** CCDC **1825820** (Ellipsoid probability 30%)*



*ORTEP diagram of **6:** CCDC 1825821 (Ellipsoid probability 30%)*

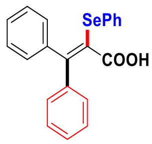


Spectroscopic Data:



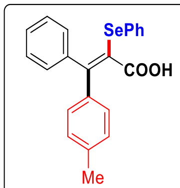
3a

3a: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 95% (79 mg), Mp (196-198 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 12.80 (s, 1H), 7.56 – 7.48 (m, 2H), 7.42 – 7.27 (m, 10H), 7.23 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, DMSO) δ 167.58, 144.61, 140.82, 139.65, 133.41, 132.75, 130.14, 129.25, 128.82, 128.71, 128.54, 128.28, 128.20, 127.97, 126.05. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{21}H_{15}ClO_2SeNa^+$ 436.9823; Found 436.9832.



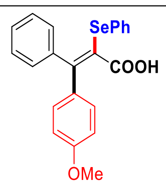
3b

3b: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 93% (71 mg); **^{1}H NMR** (400 MHz, DMSO) δ 12.73 (s, 1H), 7.53 – 7.51 (m, 2H), 7.44 – 7.19 (m, 13H). **^{13}C NMR** (101 MHz, DMSO) δ 167.85, 146.31, 141.28, 140.81, 133.18, 129.25, 129.12, 128.70, 128.44, 128.34, 128.22, 128.02, 127.83, 124.89. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{21}H_{16}O_2SeH^+$ 381.0394; Found 381.0371.



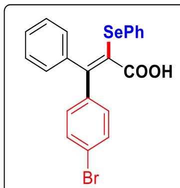
3c

3c: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 91% (72 mg), Mp (181-183 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 12.64 (s, 1H), 7.50 (s, 2H), 7.40 – 7.21 (m, 8H), 7.11 (s, 4H), 2.27 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 167.90, 146.55, 141.36, 137.91, 137.44, 132.93, 129.24, 129.13, 128.69, 128.66, 128.25, 127.88, 127.64, 123.95. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{22}H_{18}O_2SeH^+$ 395.0550; Found 395.0533.



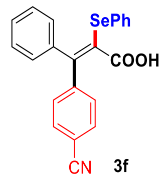
3d

3d: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 85% (70 mg), Mp (172-174 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 12.64 (s, 1H), 7.57 – 7.47 (m, 2H), 7.42 – 7.28 (m, 6H), 7.28 – 7.21 (m, 2H), 7.15 (d, *J* = 8.8 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 2H), 3.74 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 168.18, 159.06, 146.82, 141.54, 133.07, 132.68, 129.78, 129.52, 129.14, 128.73, 128.23, 127.89, 127.53, 122.99, 113.56. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{22}H_{18}O_3SeNa^+$ 433.0319; Found 433.0305.



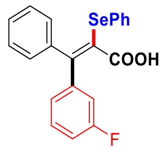
3e

3e: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 72% (66 mg), Mp (173-175 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 12.80 (s, 1H), 7.51 (s, 4H), 7.45 – 7.25 (m, 8H), 7.17 (d, *J* = 6.9 Hz, 2H). **^{13}C NMR** (101 MHz, DMSO) δ 167.47, 144.58, 140.70, 139.96, 133.36, 131.12, 130.36, 129.17, 128.76, 128.64, 128.46, 128.13, 127.90, 125.99, 121.33. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{21}H_{15}BrO_2SeH^+$ 458.9499; Found 458.9493.



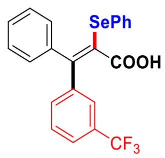
3f

3f: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 61% (49 mg); **^{1}H NMR** (400 MHz, DMSO) δ 12.80 (s, 1H), 7.51 (s, 4H), 7.45 – 7.25 (m, 8H), 7.17 (d, *J* = 6.9 Hz, 2H). **^{13}C NMR** (126 MHz, DMSO) δ 167.17, 145.48, 143.36, 140.29, 133.91, 132.23, 129.31, 129.20, 128.74, 128.42, 128.36, 128.27, 118.60, 110.48. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{22}H_{15}NO_2SeNa^+$ 428.0166; Found 428.0147.



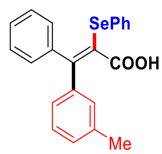
3g

3g: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 88% (69 mg), Mp (142-144 °C); **^{1}H NMR** (400 MHz, DMSO) δ 12.87 (s, 1H), 7.55 – 7.51 (m, 2H), 7.44 – 7.28 (m, 9H), 7.13 (td, *J* = 8.6, 2.1 Hz, 1H), 7.07 – 7.03 (m, 2H). **^{13}C NMR** (101 MHz, DMSO) δ 167.41, 161.67 (d, *J* = 244.2 Hz), 143.90, 142.96 (d, *J* = 7.7 Hz), 140.61, 133.60, 130.23 (d, *J* = 8.5 Hz), 129.23, 128.58 (d, *J* = 7.0 Hz), 128.20, 128.05, 126.63, 124.54 (d, *J* = 2.5 Hz), 115.08, 114.87 (d, *J* = 2.6 Hz), 114.68. **^{19}F NMR** (471 MHz, DMSO) δ -113.23. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{21}H_{15}FO_2SeNa^+$ 421.0119; Found 421.0114.



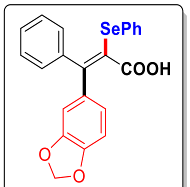
3h

3h: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 70% (62 mg); **^{1}H NMR** (400 MHz, DMSO) δ 12.90 (s, 1H), 7.72 – 7.50 (m, 6H), 7.44 – 7.23 (m, 8H). **^{13}C NMR** (101 MHz, DMSO) δ 167.35, 143.55, 141.70, 140.47, 133.74, 132.39, 129.41, 129.23, 128.96 (d, *J* = 31.5 Hz), 128.69, 128.63, 128.51, 128.31, 128.12, 127.53, 124.57 (d, *J* = 3.7 Hz), 123.96 (q, *J* = 273.81 Hz). **^{19}F NMR** (471 MHz, DMSO) δ -61.21. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{22}H_{15}F_3O_2SeNa^+$ 471.0087; Found 471.0103.



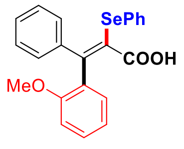
3i

3i: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 78% (61 mg), Mp (111-113 °C); **^{1}H NMR** (400 MHz, DMSO) δ 12.72 (s, 1H), 7.56 – 7.47 (m, 2H), 7.43 – 7.24 (m, 8H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.10 – 7.03 (m, 3H), 2.23 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 167.91, 146.65, 141.30, 140.82, 137.27, 133.05, 129.25, 129.22, 128.78, 128.73, 128.66, 128.41, 128.12, 128.00, 127.77, 125.54, 124.54, 20.99. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{22}H_{18}O_2SeH^+$ 395.0550; Found 395.0568.



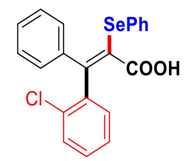
3j

3j: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 72% (61 mg), Mp (148-150 °C); **^{1}H NMR** (400 MHz, DMSO) δ 12.74 (s, 1H), 7.55 – 7.47 (m, 2H), 7.41 – 7.26 (m, 8H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.71– 6.70 (m, 2H), 6.02 (s, 2H). **^{13}C NMR** (101 MHz, DMSO) δ 168.05, 147.17, 147.02, 146.21, 141.30, 134.69, 132.95, 129.28, 129.24, 128.74, 128.38, 128.05, 127.73, 123.92, 122.53, 108.60, 108.07, 101.32. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{22}H_{16}O_4SeH^+$ 425.0292; Found 425.0273.



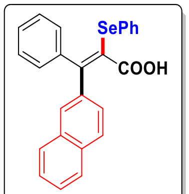
3k

3k: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 62% (51 mg), Mp (139-141 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 12.47 (s, 1H), 7.52 (d, *J* = 6.9 Hz, 2H), 7.40 – 7.20 (m, 10H), 7.03 – 6.86 (m, 2H), 3.66 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 167.70, 156.45, 146.31, 141.23, 132.39, 130.27, 130.19, 130.07, 129.71, 129.43, 128.44, 128.09, 127.88, 127.55, 124.91, 120.32, 111.91, 55.75. **HRMS** (ESI/TOF-Q) m/z: [M+K]+ Calcd for $C_{22}H_{18}O_3SeK^+$ 449.0058; Found 449.0072.



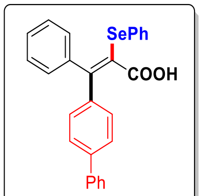
3l

3l: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 55% (46 mg); **^{1}H NMR** (400 MHz, DMSO) δ 12.67 (s, 1H), 7.56 – 7.49 (m, 3H), 7.47 – 7.25 (m, 11H). **^{13}C NMR** (101 MHz, DMSO) δ 166.92, 144.70, 139.55, 139.20, 132.85, 131.95, 131.03, 129.64, 129.43, 129.32, 129.28, 128.24, 128.14, 127.78, 127.13, 126.94. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{21}H_{15}ClO_2SeH^+$ 415.0004; Found 415.0025.



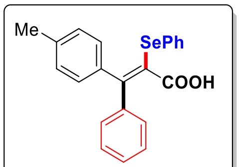
3m

3m: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 66% (57 mg);**^{1}H NMR** (500 MHz, DMSO) δ 12.72 (s, 1H), 7.91 – 7.78 (m, 4H), 7.59 – 7.46 (m, 4H), 7.44 – 7.37 (m, 2H), 7.37 – 7.25 (m, 7H).**^{13}C NMR** (126 MHz, DMSO) δ 167.87, 146.58, 141.10, 138.49, 133.12, 132.50, 132.32, 129.26, 129.15, 128.81, 128.45, 128.14, 128.08, 127.82, 127.65, 127.51, 127.24, 126.59, 126.52, 126.34, 125.39. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{25}H_{18}O_2SeNa^+$ 453.0370; Found 453.0379.



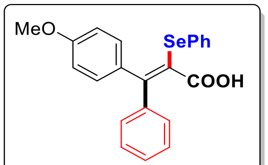
3n

3n: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 70% (64 mg); **^{1}H NMR** (400 MHz, DMSO) δ 12.86 (s, 1H), 7.69– 7.63 (m, 4H), 7.58 – 7.52 (m, 2H), 7.50 – 7.27 (m, 13H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.92, 145.80, 141.25, 139.87, 139.68, 139.38, 133.24, 129.28, 129.12, 129.01, 128.81, 128.52, 128.11, 127.88, 127.72, 126.65, 126.48, 125.11. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{27}H_{20}O_2SeNa^+$ 479.0526; Found 479.0502.



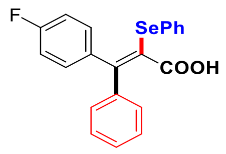
3o

3o: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 92% (73 mg); **^{1}H NMR** (400 MHz, DMSO) δ 7.52 (d, *J* = 3.2 Hz, 2H), 7.31– 7.29 (m, 6H), 7.25 – 7.11 (m, 6H), 2.31 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 167.95, 146.59, 141.02, 138.45, 137.51, 133.05, 129.26, 128.98, 128.71, 128.40, 128.18, 128.01, 127.78, 124.35, 20.86. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{22}H_{18}O_2SeH^+$ 395.0550; Found 395.0533.



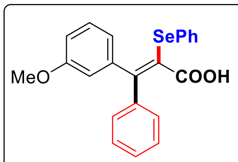
3p

3p: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 79% (65 mg); **^{1}H NMR** (400 MHz, DMSO) δ 12.61 (s, 1H), 7.59 – 7.47 (m, 2H), 7.32 – 7.28 (m, 6H), 7.29 –7.17 (m, 4H), 6.93 (d, *J* = 8.6 Hz, 2H), 3.76 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 168.02, 158.98, 146.63, 141.19, 133.47, 132.82, 130.31, 129.47, 129.21, 128.46, 128.11, 127.96, 127.64, 123.77, 113.66, 55.10. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{22}H_{18}O_3SeNa^+$ 433.0319; Found 433.0305.



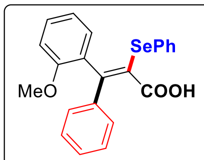
3q

3q: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 65% (52 mg); **^{1}H NMR** (400 MHz, DMSO) δ 7.54 – 7.44 (m, 2H), 7.39 – 7.26 (m, 8H), 7.25 – 7.14 (m, 4H). **^{13}C NMR** (101 MHz, DMSO) δ 167.78, 161.66 (d, J = 245.1 Hz), 145.48, 140.65, 137.57, 133.11, 130.99 (d, J = 8.4 Hz), 129.24, 129.01, 128.29 (d, J = 8.5 Hz), 128.11, 127.85, 125.24, 115.32 (d, J = 21.5 Hz). **^{19}F NMR** (471 MHz, DMSO) δ -113.52. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{21}H_{15}FO_2SeNa^+$ 421.0119; Found 421.0114.



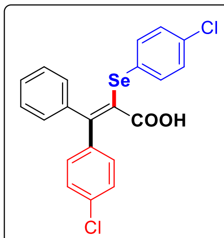
3r

3r: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 62% (51 mg); **^{1}H NMR** (500 MHz, DMSO) δ 7.52 (dd, J = 5.7, 2.3 Hz, 2H), 7.36 – 7.27 (m, 7H), 7.26 – 7.22 (m, 2H), 6.93 – 6.88 (m, 1H), 6.81 (d, J = 6.8 Hz, 2H), 3.71 (s, 3H). **^{13}C NMR** (126 MHz, DMSO) δ 167.74, 159.05, 145.98, 142.53, 140.54, 133.15, 129.65, 129.22, 129.18, 128.23, 128.17, 127.99, 127.80, 124.88, 120.82, 114.17, 113.35, 55.05. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{22}H_{18}O_3SeH^+$ 411.0499; Found 411.0510.



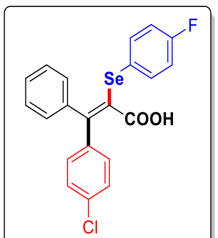
3s

3s: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 57% (47 mg); **^{1}H NMR** (400 MHz, DMSO) δ 7.52 – 7.44 (m, 2H), 7.36 – 7.22 (m, 9H), 7.16 (dd, J = 7.4, 1.6 Hz, 1H), 7.04 (d, J = 8.1 Hz, 1H), 6.97 (t, J = 7.4 Hz, 1H), 3.69 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 167.92, 155.75, 144.51, 140.46, 132.86, 130.37, 129.57 (2×C), 129.35, 129.12, 128.01, 127.75, 127.54 (2×C), 125.78, 120.48, 111.83, 55.54. **HRMS** (ESI/TOF-Q) m/z: [M+K]+ Calcd for $C_{22}H_{18}O_3SeK^+$ 449.0058; Found 449.0072.



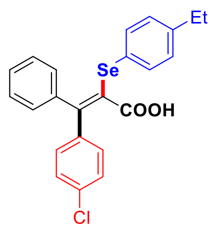
3t

3t: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 89% (80 mg), Mp (154-156 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 12.91 (s, 1H), 7.53 (d, J = 8.5 Hz, 2H), 7.43 – 7.32 (m, 7H), 7.28 (d, J = 6.8 Hz, 2H), 7.23 (d, J = 8.5 Hz, 2H). **^{13}C NMR** (101 MHz, DMSO) δ 167.43, 144.85, 140.65, 139.47, 135.29, 133.08, 132.81, 130.11, 129.17, 128.66, 128.55, 128.28, 127.56, 125.78. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{21}H_{14}Cl_2O_2SeNa^+$ 470.9434; Found 470.9418.



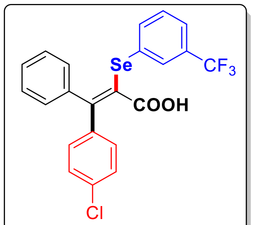
3u

3u: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 65% (56 mg); **^{1}H NMR** (500 MHz, DMSO) δ 7.59– 7.54 (m, 2H), 7.43 – 7.34 (m, 6H), 7.29 (d, J = 7.0 Hz, 2H), 7.24 – 7.16 (m, 4H). **^{13}C NMR** (126 MHz, DMSO) δ 167.28, 162.34 (d, J = 245.7 Hz), 143.08, 140.62, 139.54, 136.69 (d, J = 8.2 Hz), 132.70, 130.11, 128.67 (d, J = 11.7 Hz), 128.29, 128.26, 126.74, 123.40, 123.38, 116.35 (d, J = 21.7 Hz). **^{19}F NMR** (471 MHz, DMSO) δ -113.36. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{21}H_{14}ClFO_2SeNa^+$ 454.9729; Found 454.9706.



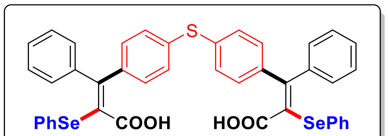
3v

3v: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 71% (63 mg); **^{1}H NMR** (400 MHz, DMSO) δ 7.46 – 7.33 (m, 7H), 7.32 – 7.27 (m, 2H), 7.26 – 7.20 (m, 2H), 7.17 (d, *J* = 8.1 Hz, 2H), 2.59 (q, *J* = 7.6 Hz, 2H), 1.16 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO) δ 167.42, 144.01, 143.23, 140.80, 139.68, 134.07, 132.64, 130.13, 128.75, 128.58, 128.26, 128.17, 126.77, 125.01, 27.77, 15.35. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{23}H_{19}ClO_2SeH^+$ 443.0317; Found 443.0324.



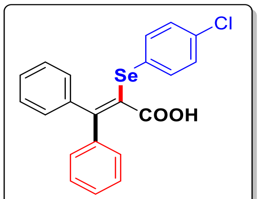
3w

3w: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 55% (53 mg); **^{1}H NMR** (500 MHz, DMSO) δ 7.85 – 7.75 (m, 2H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.43 – 7.32 (m, 5H), 7.27 – 7.23 (m, 4H). **^{13}C NMR** (126 MHz, DMSO) δ 167.65, 146.47, 140.61, 139.39, 136.81, 132.96, 130.79, 130.13, 130.09, 129.68 (d, *J* = 31.8 Hz), 128.96 (d, *J* = 3.7 Hz), 128.60, 128.52, 128.32, 124.91, 124.46 (d, *J* = 3.5 Hz), 123.70 (d, *J* = 273.54 Hz). **^{19}F NMR** (471 MHz, DMSO) δ -61.27. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{22}H_{14}ClF_3O_2SeH^+$ 482.9878; Found 482.9893.



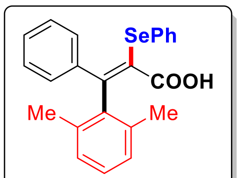
3x

3x: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 52% (82 mg); **^{1}H NMR** (400 MHz, DMSO) δ 7.53 – 7.49 (m, 2H), 7.43 – 7.14 (m, 12H). **^{13}C NMR** (101 MHz, DMSO) δ 167.80, 145.42, 140.94, 140.01, 134.19, 133.24, 130.30, 129.50, 129.28, 129.02, 128.75, 128.55, 128.19, 127.91, 125.74. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{42}H_{31}O_4SSe_2H^+$ 791.0273; Found 791.0252.



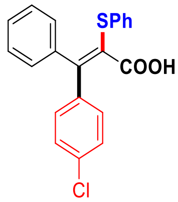
3y

3y: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 86% (71 mg), Mp (145-147 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 12.84 (s, 1H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.47 – 7.15 (m, 12H). **^{13}C NMR** (101 MHz, DMSO) δ 167.74, 146.54, 141.13, 140.67, 135.11, 132.99, 129.20, 128.68, 128.49, 128.34, 128.25, 128.13, 127.86, 124.67. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{21}H_{15}ClO_2SeNa^+$ 436.9823; Found 436.9832.



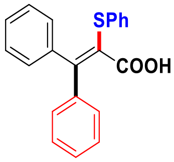
3z

3z: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 44% (36 mg); **^{1}H NMR** (400 MHz, DMSO) δ 7.56 – 7.51 (m, 2H), 7.38 – 7.30 (m, 9H), 7.03 – 7.01 (m, 2H), 2.27 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.52, 143.86, 140.22, 138.26, 135.75, 133.43, 129.28, 129.13, 128.81, 128.39, 128.13, 127.98, 127.61, 127.40, 124.34, 20.09. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{23}H_{20}O_2SeNa^+$ 431.0526; Found 431.0511.



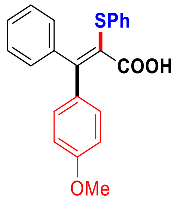
5a

5a: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 77% (56 mg), Mp (208-210 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 7.56 – 7.53 (m, 2H), 7.44 – 7.22 (m, 9H), 7.03 (d, *J* = 7.0 Hz, 2H), 2.27 (s, 6H). **^{13}C NMR** (126 MHz, DMSO) δ 167.25, 147.79, 140.26, 139.84, 133.74, 133.05, 130.32, 129.57, 129.22, 128.87, 128.48, 128.33, 128.29, 127.58, 127.08. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{21}H_{15}ClO_2SH^+$ 367.0560; Found 367.0555.



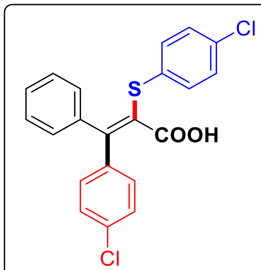
5b

5b: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 78% (50 mg), Mp (189-191 ºC); **^{1}H NMR** (500 MHz, DMSO) δ 7.42 – 7.30 (m, 10H), 7.29 – 7.24 (m, 3H), 7.23 – 7.21 (m, 2H). **^{13}C NMR** (101 MHz, DMSO) δ 167.54, 149.52, 140.97, 140.68, 134.07, 129.37, 129.22, 128.82, 128.51, 128.39, 128.35, 128.26, 128.14, 126.96, 126.52. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{21}H_{16}O_2SNa^+$ 355.0769; Found 355.0761.



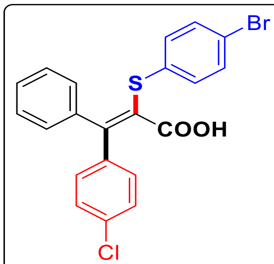
5c

5c: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 75% (69 mg), Mp (198-200 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 12.77 (s, 1H), 7.41 – 7.29 (m, 7H), 7.26 – 7.22 (m, 3H), 7.13 (d, *J* = 8.3 Hz, 2H), 6.90 (d, *J* = 8.3 Hz, 2H), 3.75 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 167.92, 159.40, 149.97, 140.94, 134.54, 133.20, 130.06, 129.12, 128.89, 128.85, 128.24, 128.07, 126.62, 124.56, 113.63, 55.14. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{22}H_{18}O_3SH^+$ 363.1055; Found 363.1061.



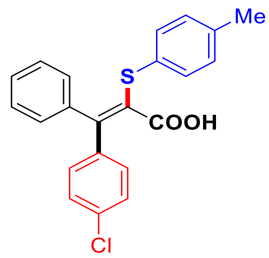
5d

5d: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 81% (65 mg), Mp (169-171 ºC); **^{1}H NMR** (400 MHz, DMSO) δ 13.05 (s, 1H), 7.47 – 7.33 (m, 9H), 7.29 (d, *J* = 6.9 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H). **^{13}C NMR** (101 MHz, DMSO) δ 167.09, 148.31, 140.08, 139.67, 133.16, 132.82, 131.95, 131.38, 130.29, 129.17, 128.82, 128.51, 128.38, 128.35, 127.08. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{21}H_{14}Cl_2O_2SH^+$ 401.0170; Found 401.0152.



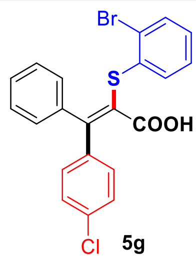
5e

5e: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 72% (64 mg); **^{1}H NMR** (500 MHz, DMSO) δ 7.54 (d, *J* = 8.2 Hz, 2H), 7.43 – 7.30 (m, 7H), 7.28 (d, *J* = 7.1 Hz, 2H), 7.22 (d, *J* = 8.1 Hz, 2H). **^{13}C NMR** (126 MHz, DMSO) δ 167.03, 148.49, 140.04, 139.63, 133.41, 133.14, 132.01, 131.53, 130.25, 128.76, 128.47, 128.35, 128.30, 126.90, 120.28. **HRMS** (ESI/TOF-Q) m/z: [M+H]+Calcd for $C_{21}H_{14}BrClO_2SH^+$ 444.9665; Found 444.9653.



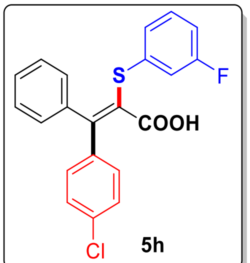
5f

5f: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 68% (52 mg); **^{1}H NMR** (400 MHz, DMSO) δ 7.49 – 7.26 (m, 9H), 7.21 – 7.15 (m, 4H), 2.27 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 167.03, 145.87, 140.20, 139.85, 137.04, 132.91, 130.53, 130.27, 129.80, 129.59, 128.92, 128.61, 128.46, 128.27, 128.15, 20.60. **HRMS** (ESI/TOF-Q) m/z: [M+K]+Calcd for $C_{22}H_{17}ClO_2SK^+$ 419.0275; Found 419.0289.



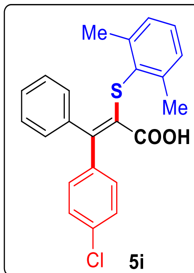
5g

5g: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 73% (65 mg), Mp (161-163 °C); **^{1}H NMR** (400 MHz, DMSO) δ 13.10 (s, 1H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.55 – 7.34 (m, 7H), 7.25 (d, *J* = 8.0 Hz, 4H), 7.17 (t, *J* = 7.3 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO) δ 167.30, 152.09, 140.13, 139.71, 136.11, 133.39, 132.97, 130.34, 129.04, 128.64, 128.55, 128.47, 128.37, 128.02, 125.30, 121.58. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+Calcd for $C_{21}H_{14}BrClO_2SNa^+$ 466.9484; Found 466.9456.



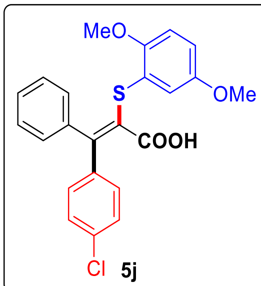
5h

5h: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 71% (55 mg), Mp (211-213 °C); **^{1}H NMR** (400 MHz, DMSO) δ 7.48 – 7.32 (m, 6H), 7.32 – 7.17 (m, 6H), 7.1 – 7.05 (m, 1H). **^{13}C NMR** (101 MHz, DMSO) δ 167.28, 162.20 (d, *J* = 246.3 Hz), 149.92, 140.14, 139.68, 136.80 (d, *J* = 8.0 Hz), 133.30, 131.03 (d, *J* = 8.6 Hz), 130.34, 128.78, 128.50, 128.47, 128.38, 126.23, 124.91, 115.46 (d, *J* = 23.5 Hz), 113.78 (d, *J* = 21.0 Hz). **^{19}F NMR** (471 MHz, DMSO) δ -111.91. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{21}H_{14}ClFO_2SNa^+$ 407.0285; Found 407.0308.



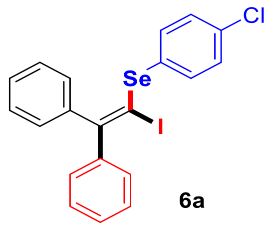
5i

5i: Yellow solid, eluent (30% ethyl acetate in hexane). **Yield**: 76% (60 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.45 (t, *J* = 7.6 Hz, 2H), 7.39 – 7.32 (m, 5H), 7.23 (d, *J* = 8.3 Hz, 2H), 7.19 – 7.14 (m, 1H), 7.10 (d, *J* = 7.4 Hz, 2H), 2.47 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 166.05, 143.23, 139.74, 139.47, 138.00, 132.33, 131.16, 130.15, 129.37, 129.21, 128.61, 128.57, 128.14, 128.03, 127.91, 21.78. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{23}H_{19}ClO_2SNa^+$ 417.0692; Found 417.0709.



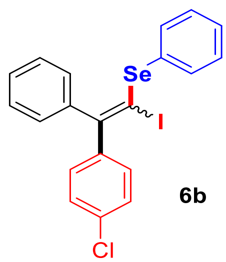
5j

5j: Yellow liquid, eluent (30% ethyl acetate in hexane). **Yield**: 81% (69 mg); **^{1}H NMR** (400 MHz, DMSO) δ 7.42 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.29 (m, 3H), 7.27 – 7.20 (m, 4H), 6.93 – 6.89 (m, 2H), 6.77 (dd, *J* = 8.9, 2.7 Hz, 1H), 3.70 (d, *J* = 8.4 Hz, 6H). **^{13}C NMR** (101 MHz, DMSO) δ 167.79, 153.43, 150.29, 150.25, 140.40, 139.97, 133.20, 130.35, 128.79, 128.40, 128.38, 125.99, 123.94, 114.61, 112.10, 111.79, 56.22, 55.39. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{23}H_{19}ClO_4SNa^+$ 449.0590; Found 449.0586.



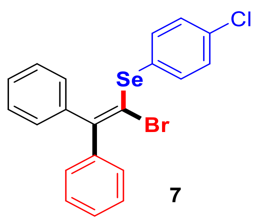
6a

6a: Yellow solid, eluent (4% ethyl acetate in hexane). **Yield**: 78% (77 mg), Mp (138-140 °C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.36 – 7.23 (m, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.72, 146.07, 141.56, 135.46, 134.70, 132.24, 129.52, 128.82, 128.70, 128.47, 128.38, 128.24, 127.98, 81.91. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{20}H_{14}ClISeH^+$ 496.9072; Found 496.9068.



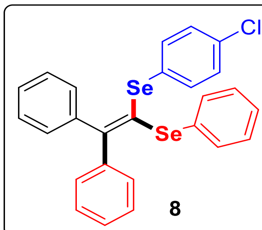
6b

6b: Yellow solid, eluent (4% ethyl acetate in hexane). **Yield**: 72% (71 mg), (**E**/**Z** = 1:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.50 – 7.49 (m, 2H), 7.38 – 7.19 (m, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.89, 154.57, 145.98, 144.56, 141.36, 139.98, 134.40, 134.10, 134.02, 134.00, 133.87, 133.78, 130.41, 130.20, 129.37, 129.32, 128.88, 128.79, 128.63, 128.60, 128.54, 128.51, 128.46, 128.32, 128.08, 83.81, 83.26. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{20}H_{14}ClISeH^+$ 496.9072; Found 496.9068.



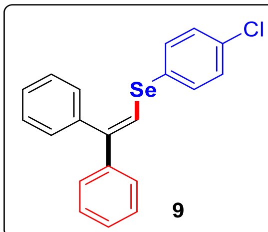
7

7: Yellow solid, eluent (4% ethyl acetate in hexane). **Yield**: 70% (63 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.3 Hz, 2H), 7.35 – 7.23 (m, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 151.07, 142.48, 141.95, 135.40, 134.70, 129.68, 129.49, 129.16, 129.04, 128.48, 128.31, 128.28, 127.95, 108.11. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{20}H_{14}ClBrSeH^+$ 448.9211; Found 448.9229.



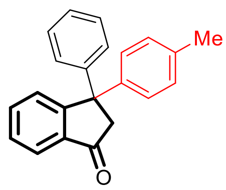
8

8: Yellow solid, eluent (4% ethyl acetate in hexane). **Yield**: 75% (79 mg), Mp (128-130 °C); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.31 – 7.25 (m, 6H), 7.24 – 7.19 (m, 7H), 7.17 – 7.13 (m, 2H), 7.12 – 7.06 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.58, 143.06, 143.04, 135.12, 133.65, 133.48, 132.27, 130.49, 129.36, 128.70, 128.20, 128.17, 127.94, 127.44, 122.09. **HRMS** (ESI/TOF-Q) m/z: [M+K]+ Calcd for $C_{26}H_{19}ClSe_2K^+$ 564.9143; Found 564.9178.



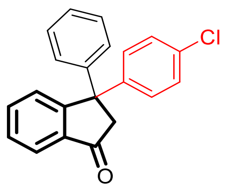
9

9: Yellow solid, eluent (4% ethyl acetate in hexane). **Yield**: 84% (62 mg), Mp (96-98 °C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.45 – 7.35 (m, 3H), 7.34 – 7.21 (m, 9H), 7.03 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.81, 141.46, 140.27, 133.93, 133.79, 129.88, 129.58, 129.39, 128.69, 128.46, 128.19, 127.54, 127.30, 121.91. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{20}H_{15}ClSeNa^+$ 392.9925; Found 392.9946.



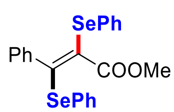
10a

10a: White solid, eluent (5% ethyl acetate in hexane). **Yield**: 98% (58 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.5 Hz, 1H), 7.63 – 7.51 (m, 1H), 7.45 – 7.32 (m, 2H), 7.28 – 7.19 (m, 3H), 7.19 – 7.13 (m, 2H), 7.07 (q, *J* = 8.3 Hz, 4H), 3.47 (d, *J* = 2.2 Hz, 2H), 2.31 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 205.26, 160.18, 146.98, 143.82, 136.27, 135.77, 134.86, 129.15, 128.44, 128.05, 127.96, 127.93, 126.58, 123.68, 56.15, 55.85, 20.94. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{22}H_{18}OH^+$ 299.1436; Found 299.1453.



10b

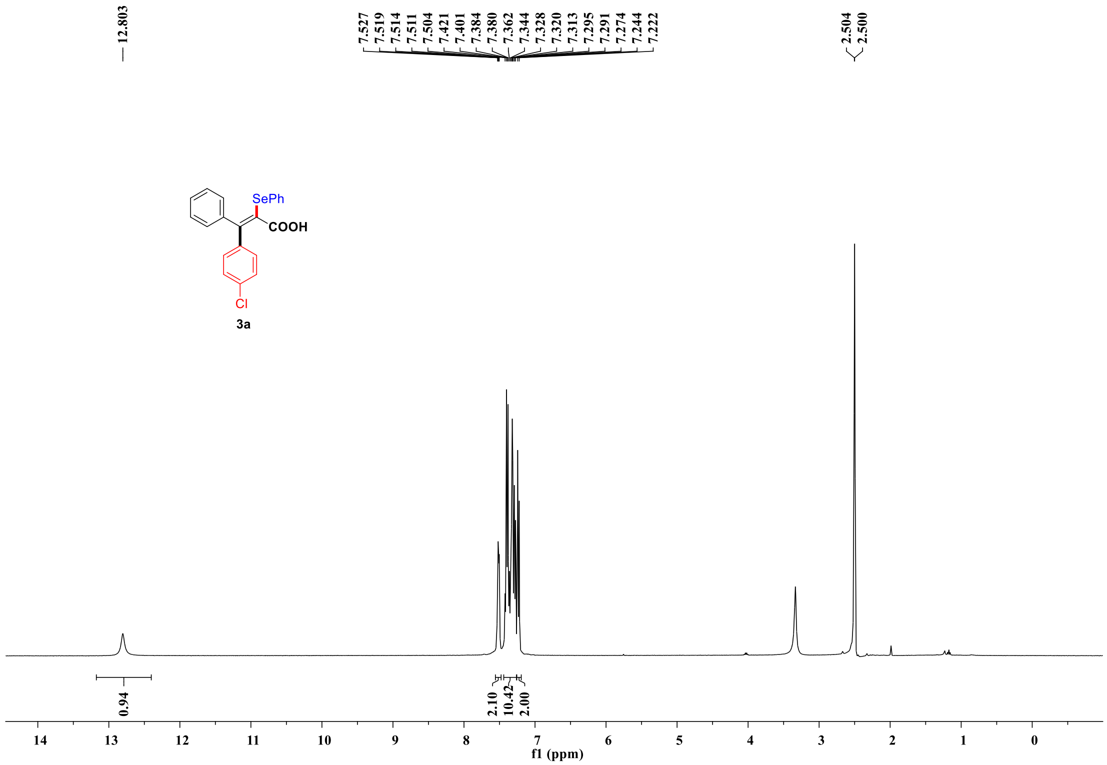
10b: Yellow solid, eluent (5% ethyl acetate in hexane). **Yield**: 66% (42 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 – 7.76 (m, 1H), 7.61 (td, *J* = 7.8, 1.2 Hz, 1H), 7.44 (td, *J* = 7.6, 0.9 Hz, 1H), 7.36 – 7.22 (m, 6H), 7.15 – 7.08 (m, 4H), 3.45 (q, *J* = 19.0 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 204.71, 159.54, 146.36, 145.52, 135.84, 135.14, 132.72, 129.55, 128.71, 128.36, 128.02, 127.98, 126.96, 123.97, 56.06, 55.85. **HRMS** (ESI/TOF-Q) m/z: [M+H]+ Calcd for $C_{21}H_{15}ClOH^+$ 319.0890; Found 319.0893.



3za'

3za': Yellow solid, eluent (4% ethyl acetate in hexane). **Yield**: 20% (19 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38 – 7.30 (m, 2H), 7.26 – 7.18 (m, 5H), 7.11 – 6.96 (m, 6H), 6.93 – 6.90 (m, 2H), 3.62 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.04, 156.01, 139.62, 136.31, 132.34, 131.70, 130.13, 129.08, 128.46, 128.20, 127.86, 127.59, 127.33, 118.53, 52.70. **HRMS** (ESI/TOF-Q) m/z: [M+Na]+ Calcd for $C_{22}H_{18}O_2Se_2Na^+$ 496.9535; Found 496.9527.

NMR Spectra: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7.320
7.313
7.295
7.291
7.274
7.244
7.222
2.504
2.500
SePh
COOH
Cl
3a
0.94
2.10
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2.00
14
13
12
11
10
9
8
7
6
5
4
3
2
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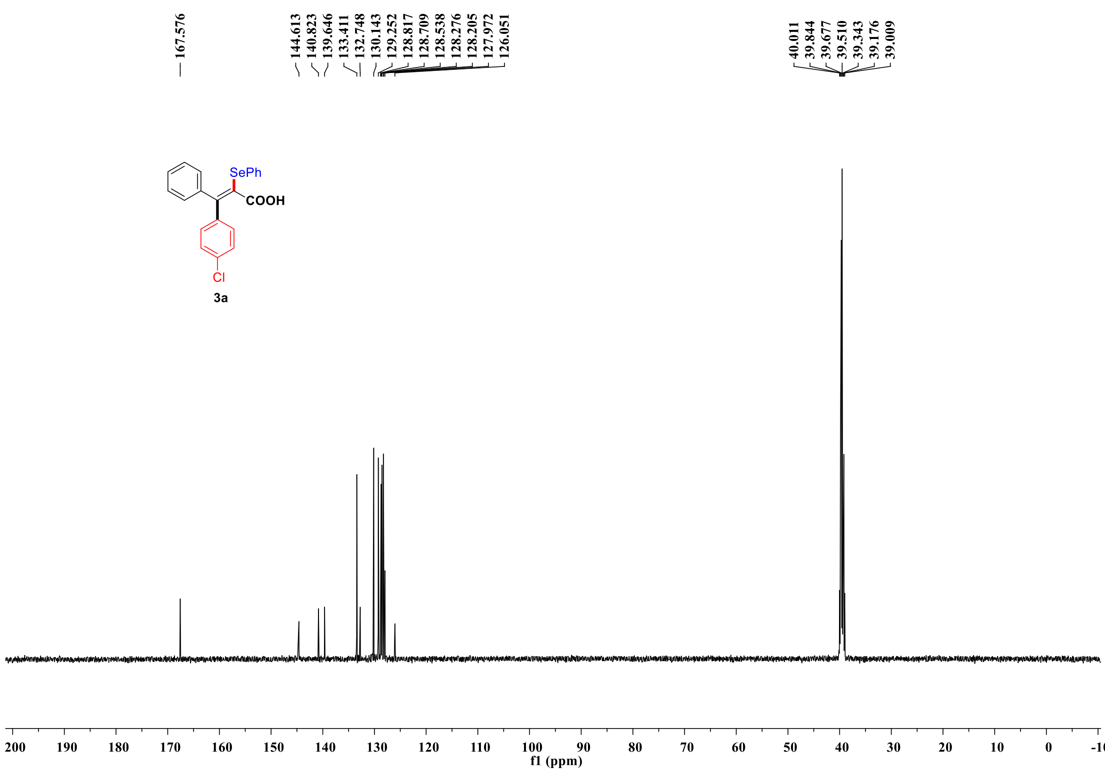
f1 (ppm)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40.011
39.844
39.677
39.510
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39.176
39.009
SePh
COOH
Cl
3a
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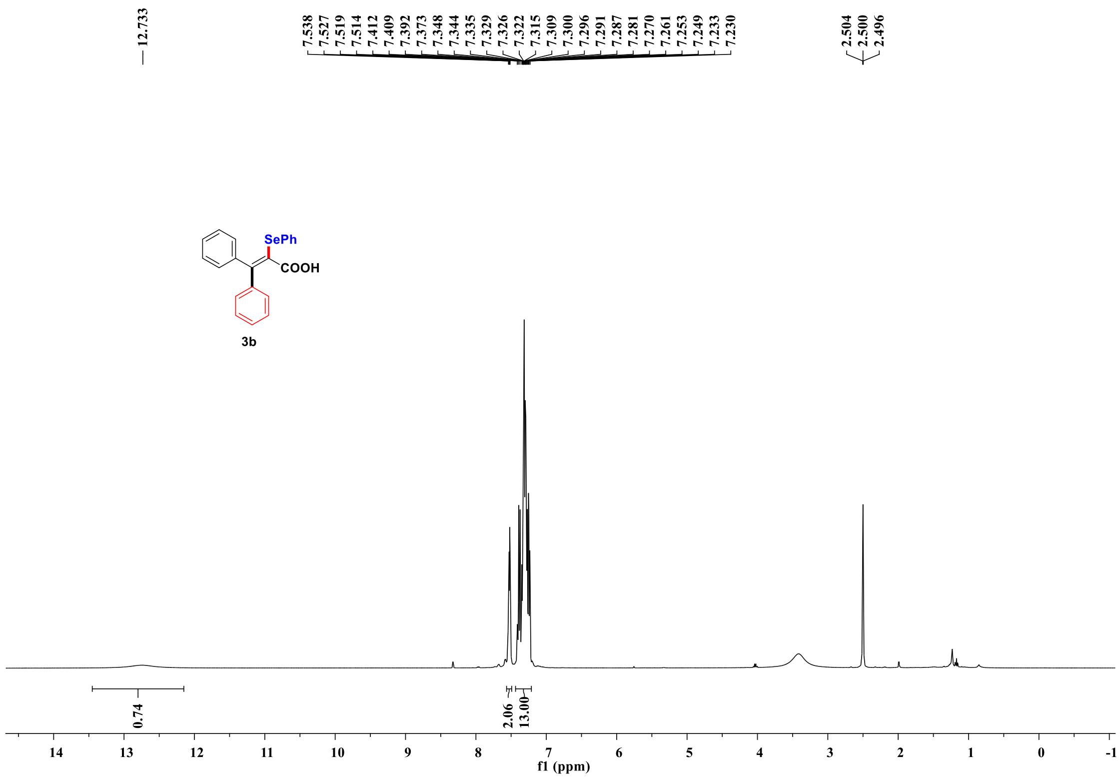
f1 (ppm)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2.504 2.500 2.496
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COOH
3b
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2.06
13.00
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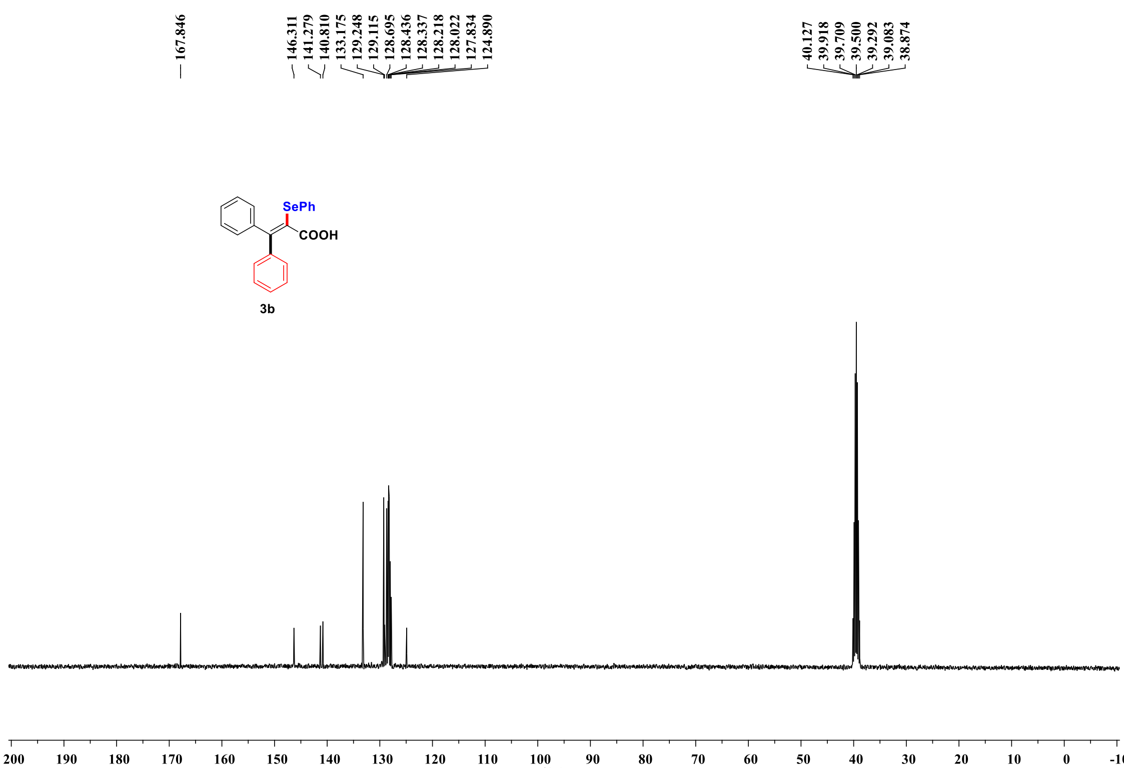
f1 (ppm)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40.127 39.918 39.709 39.500 39.292 39.083 38.874
SePh
COOH
3b
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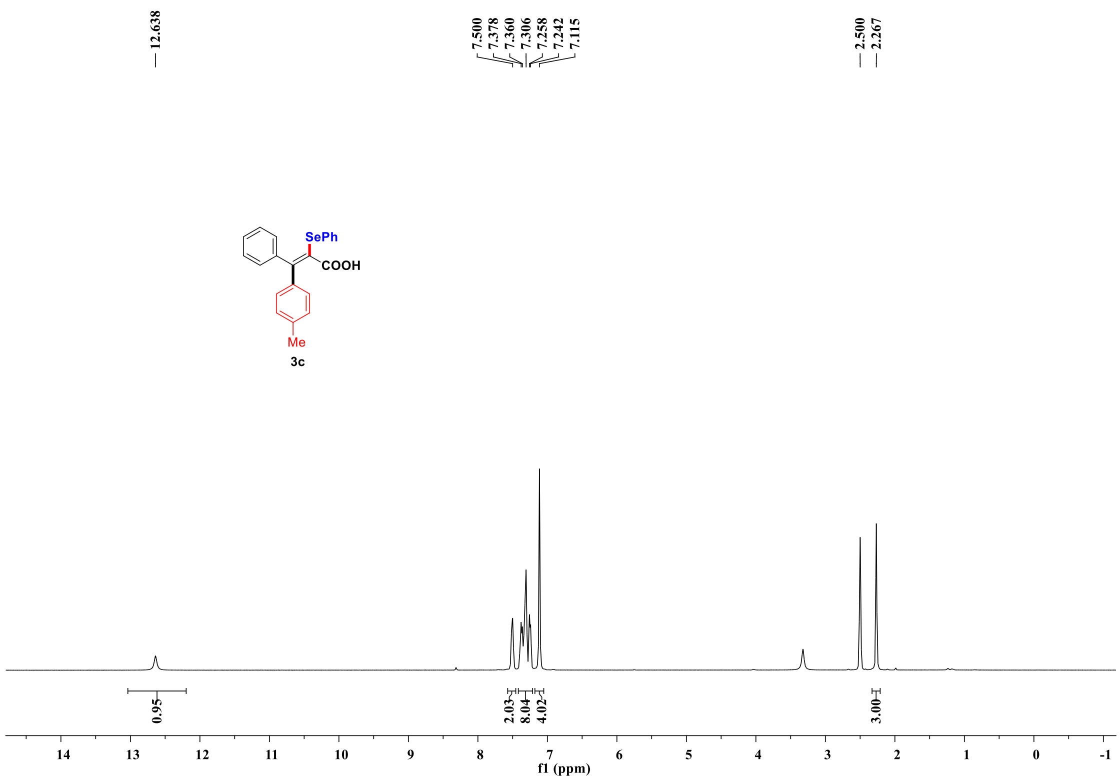
f1 (ppm)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4.02
3.00
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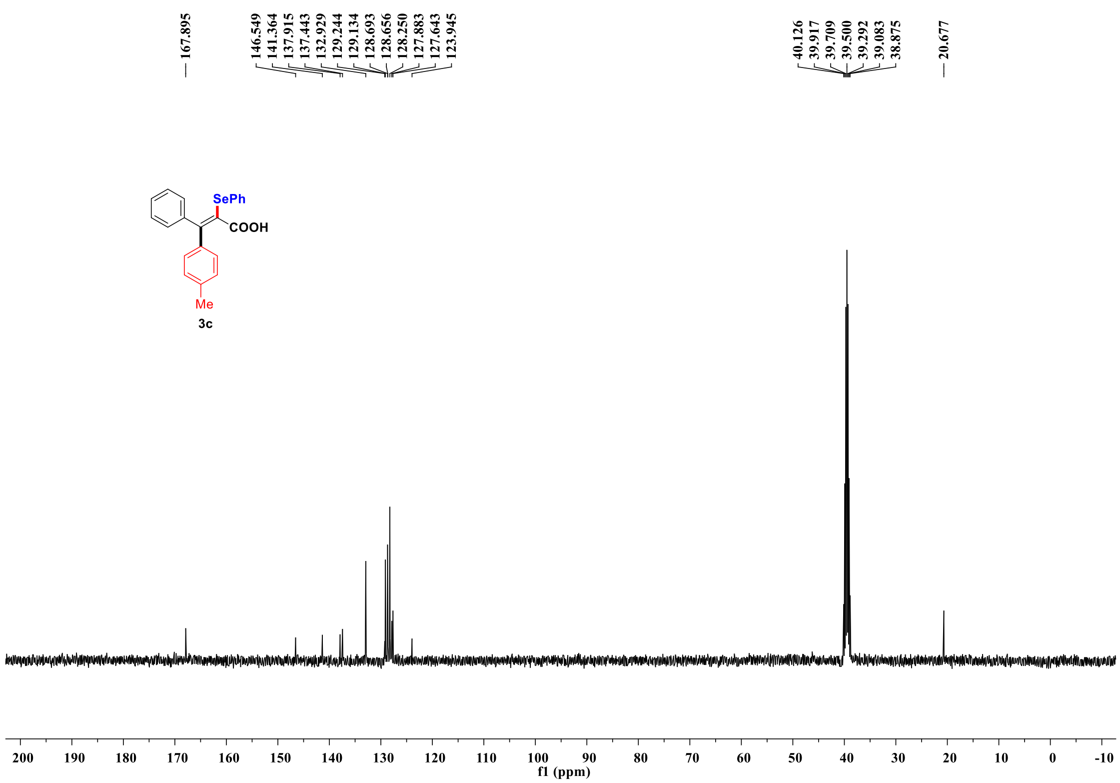
f1 (ppm)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39.917
39.709
39.500
39.292
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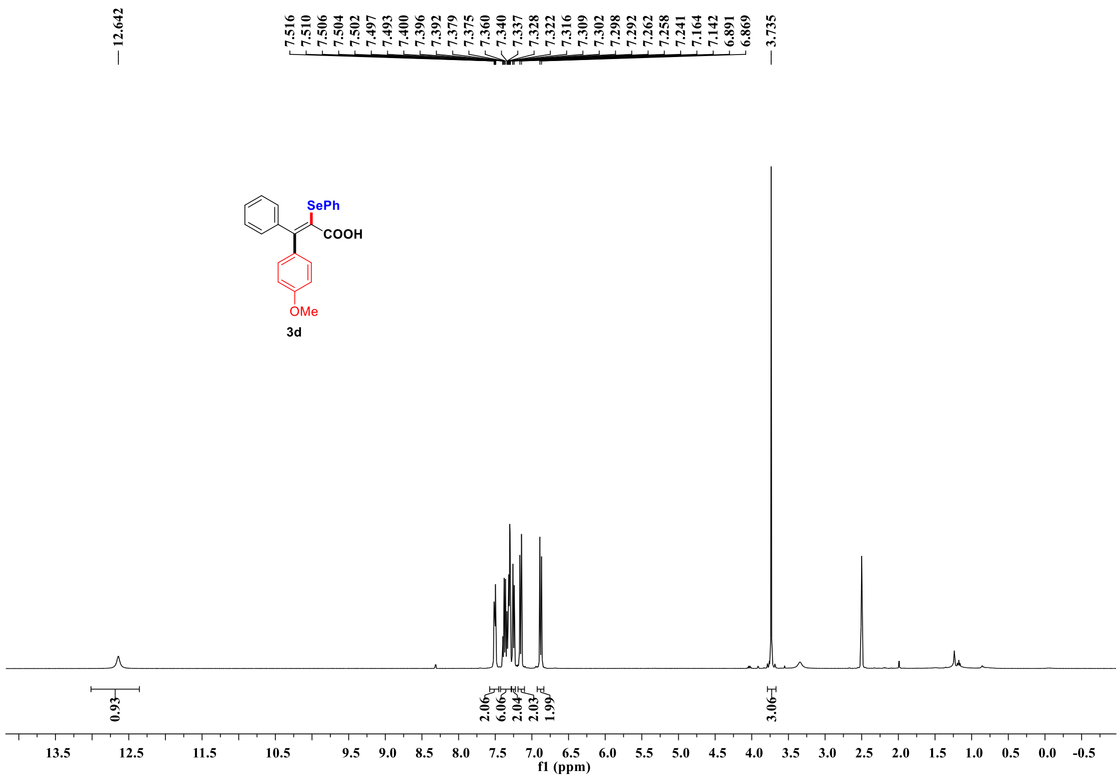
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COOH
OMe
3d
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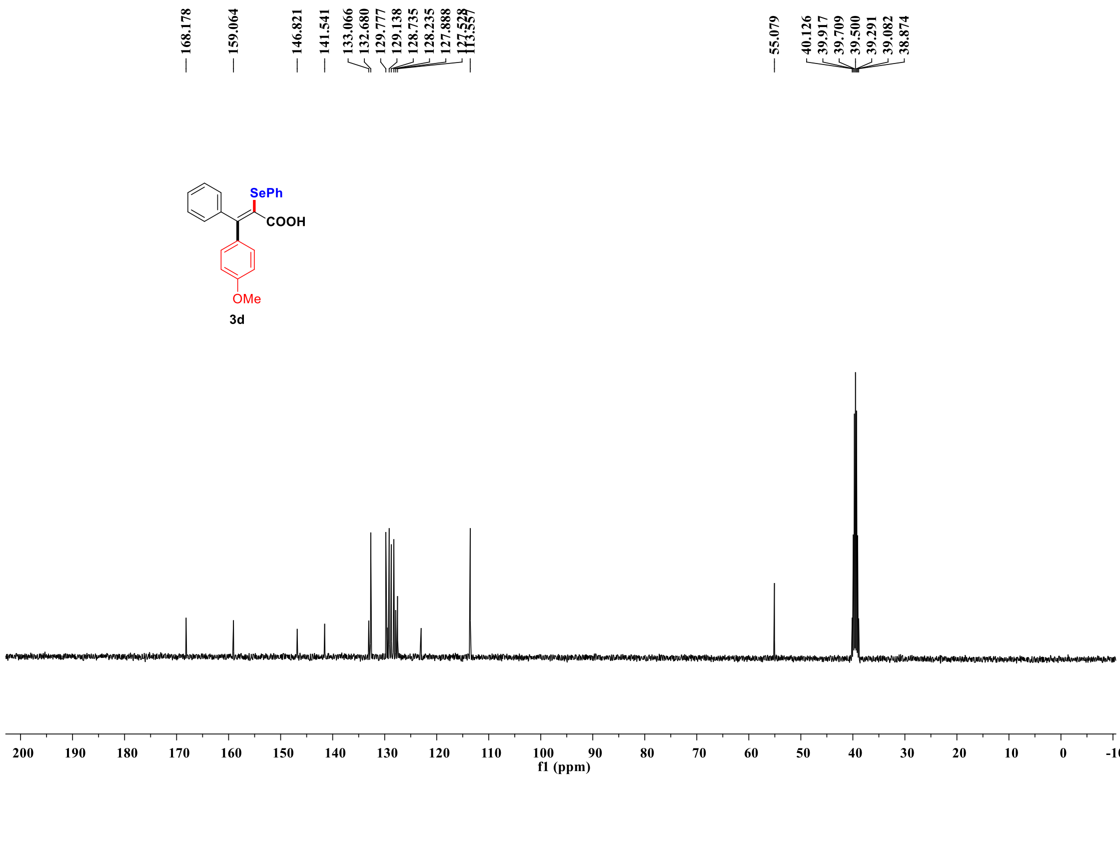
3.06
f1 (ppm)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141.541
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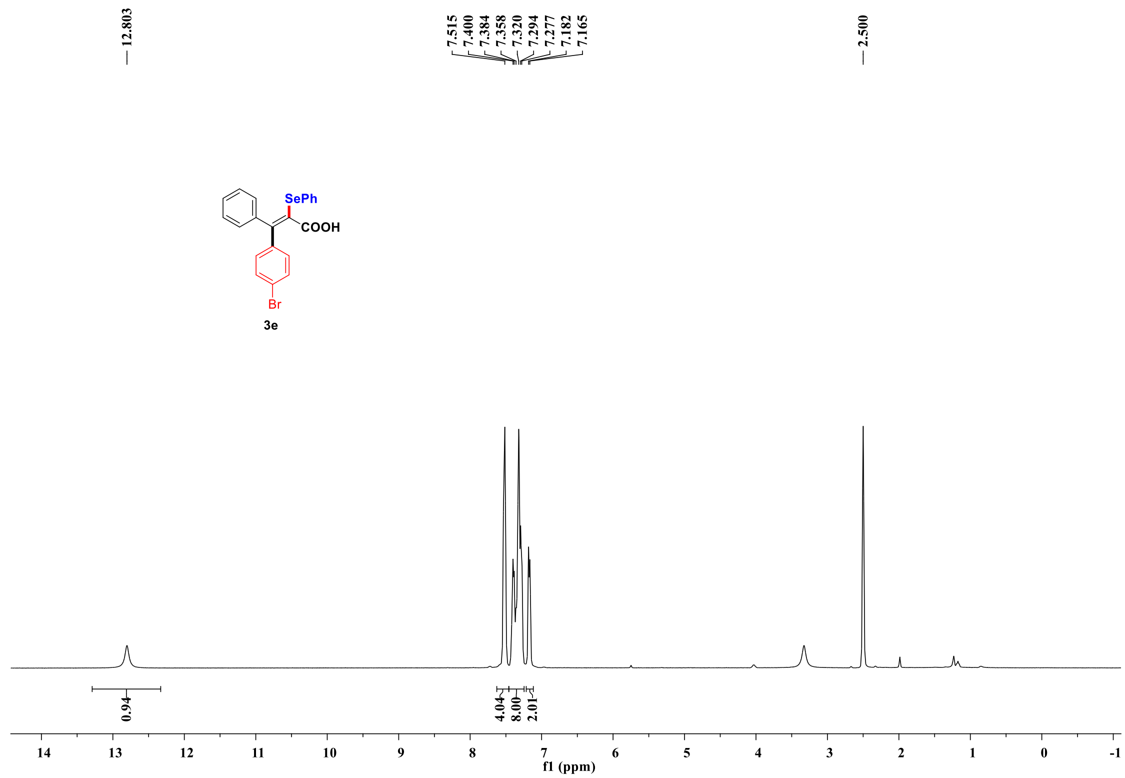
COOH
OMe
3d
f1 (ppm)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7.358
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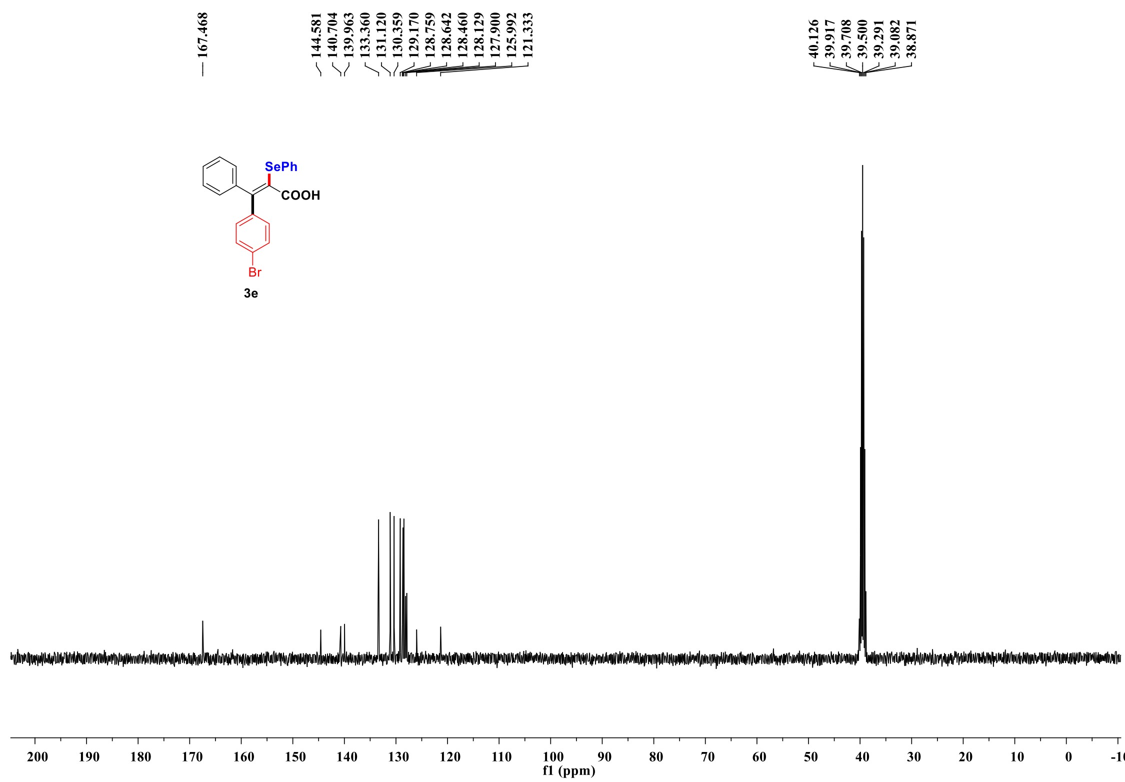
f1 (ppm)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125.992
121.333
40.126
39.917
39.708
39.500
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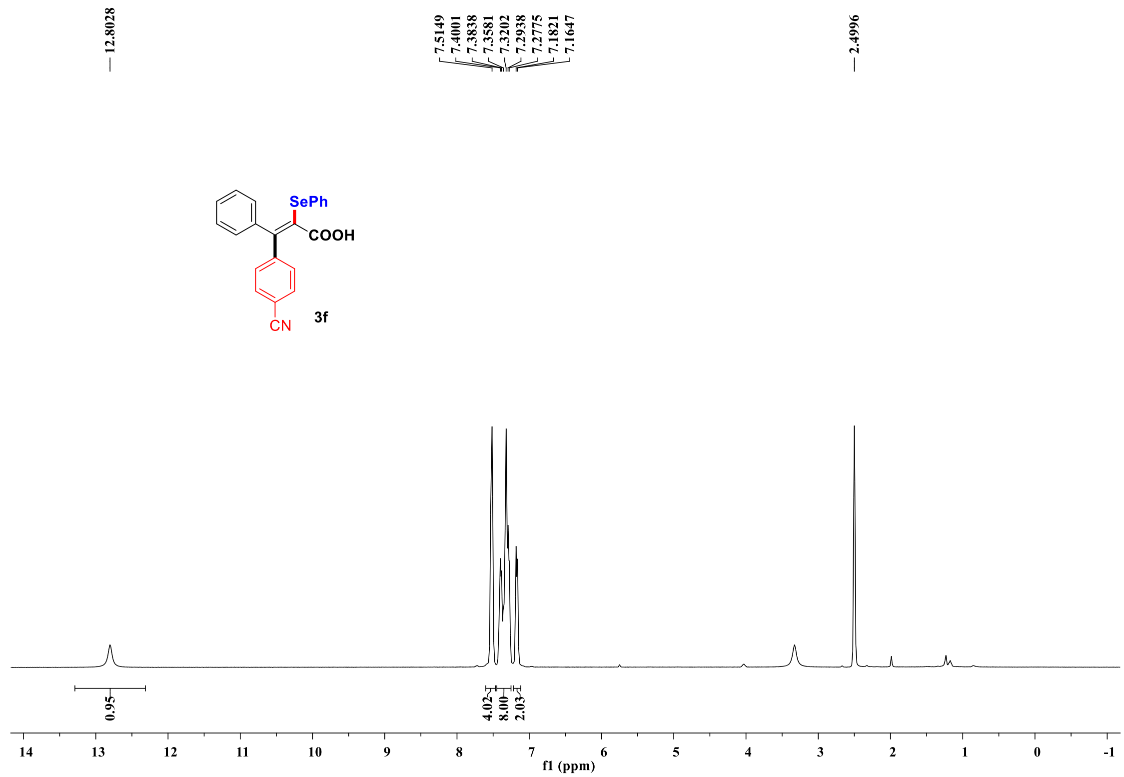
f1 (ppm)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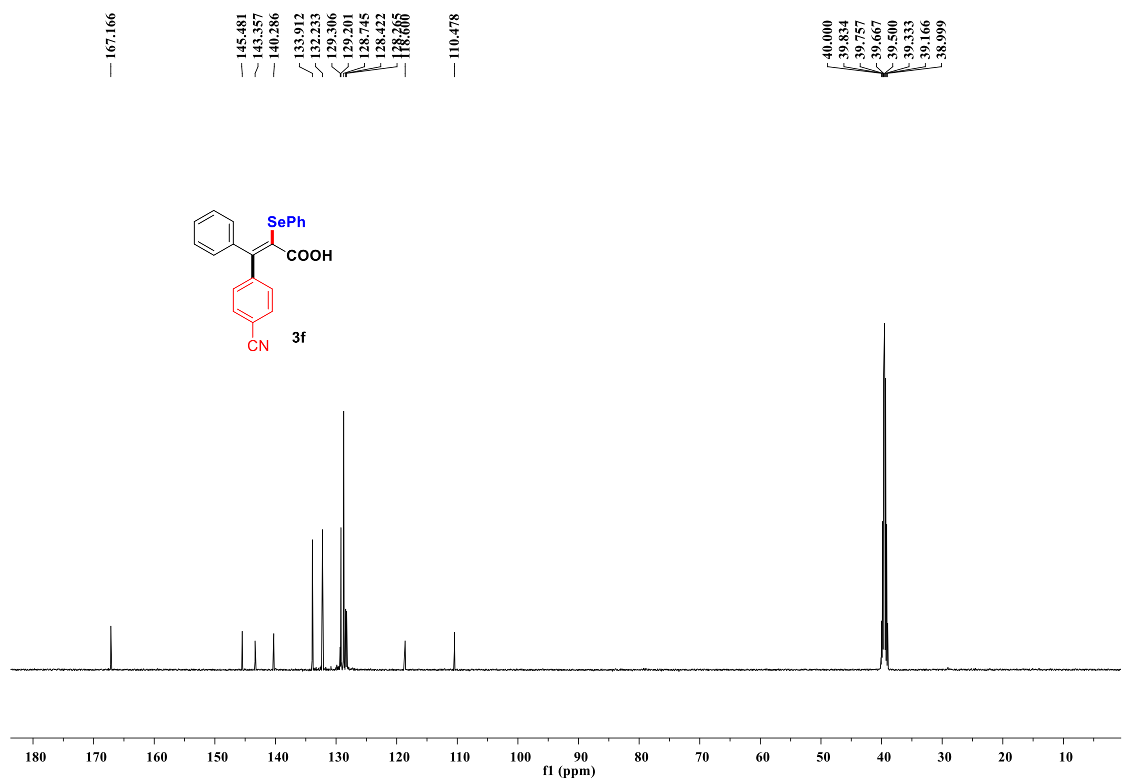
2.03
f1 (ppm)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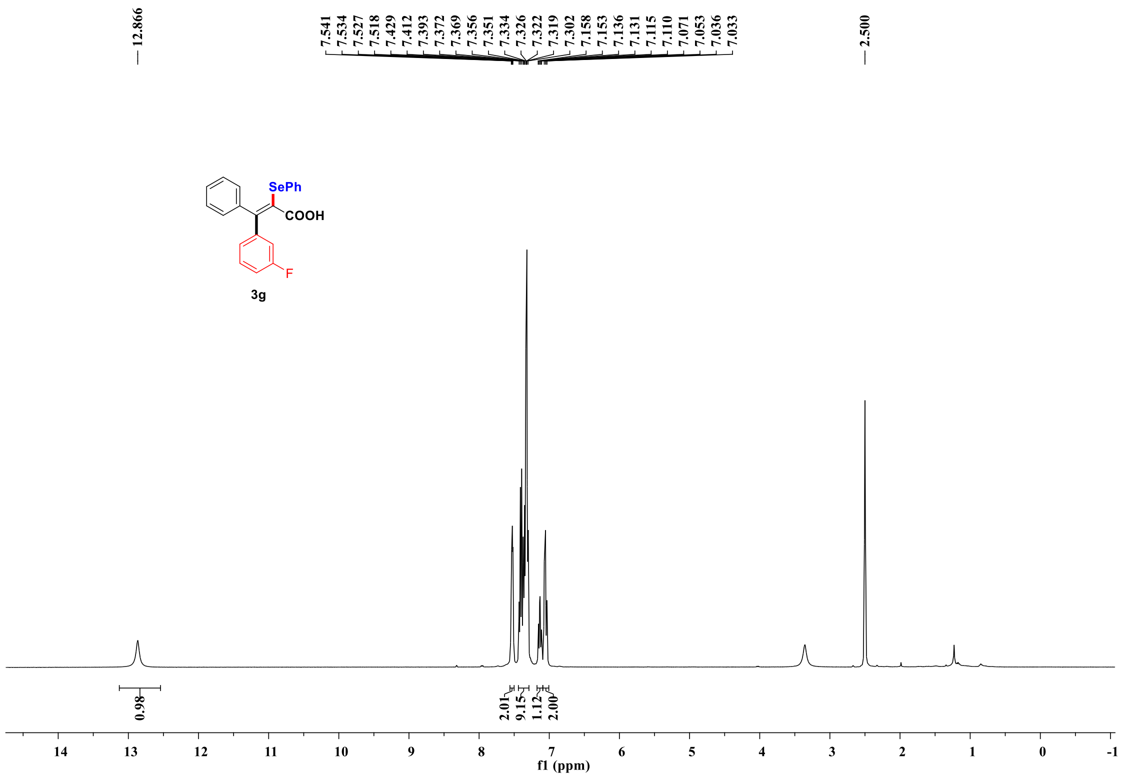
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7.322
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7.115
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7.053
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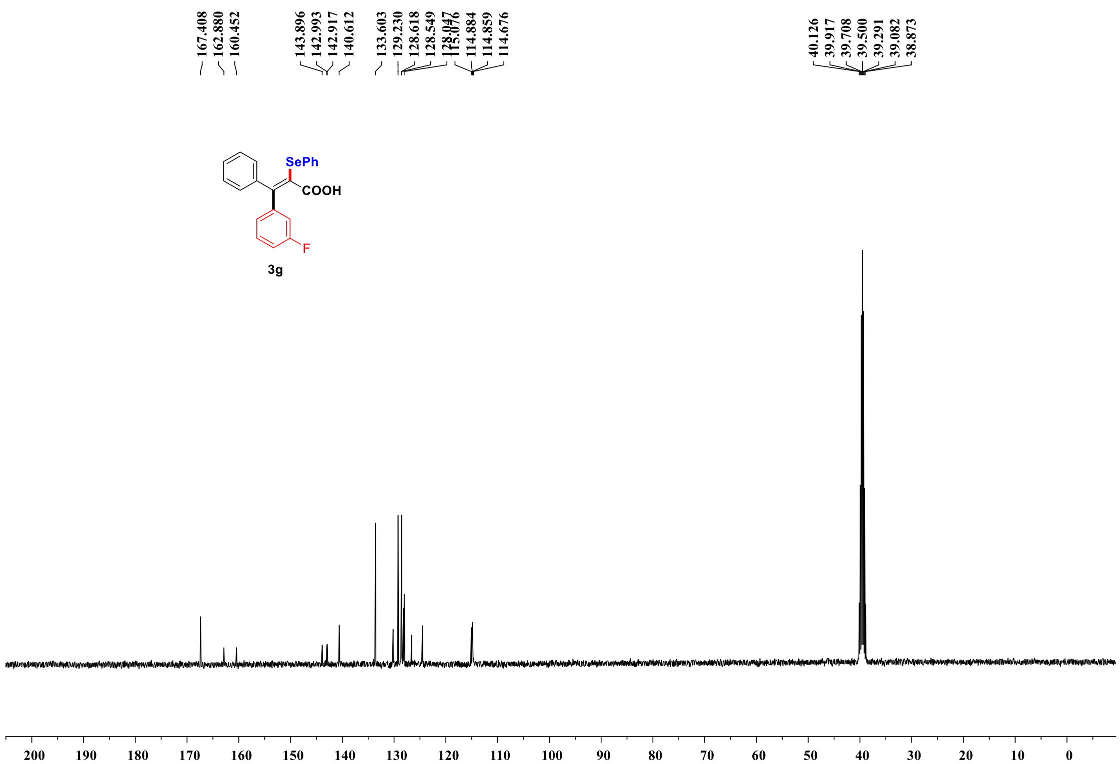
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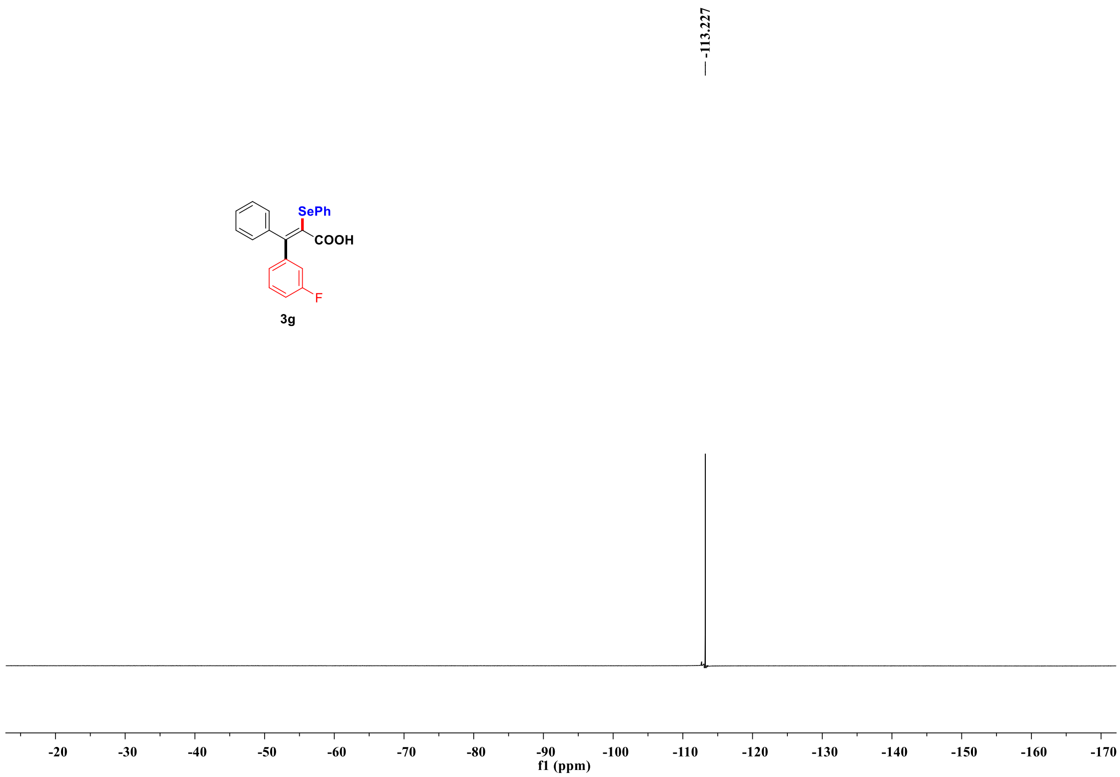
3g
f1 (ppm)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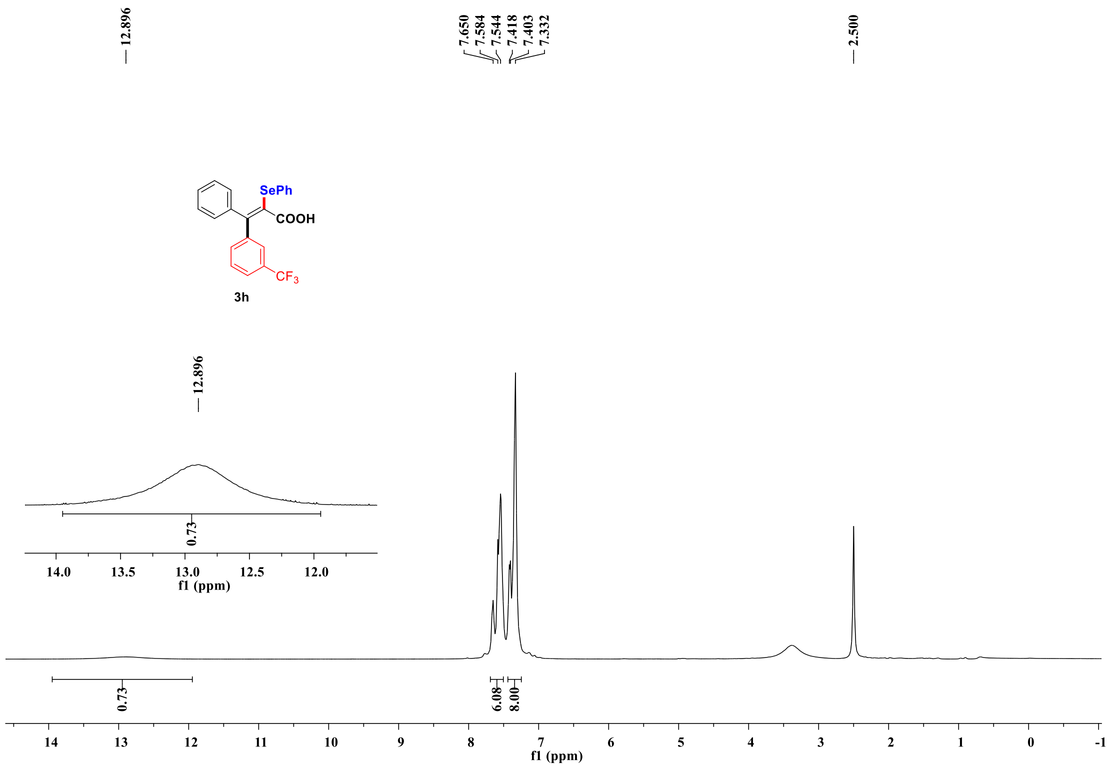
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8.00
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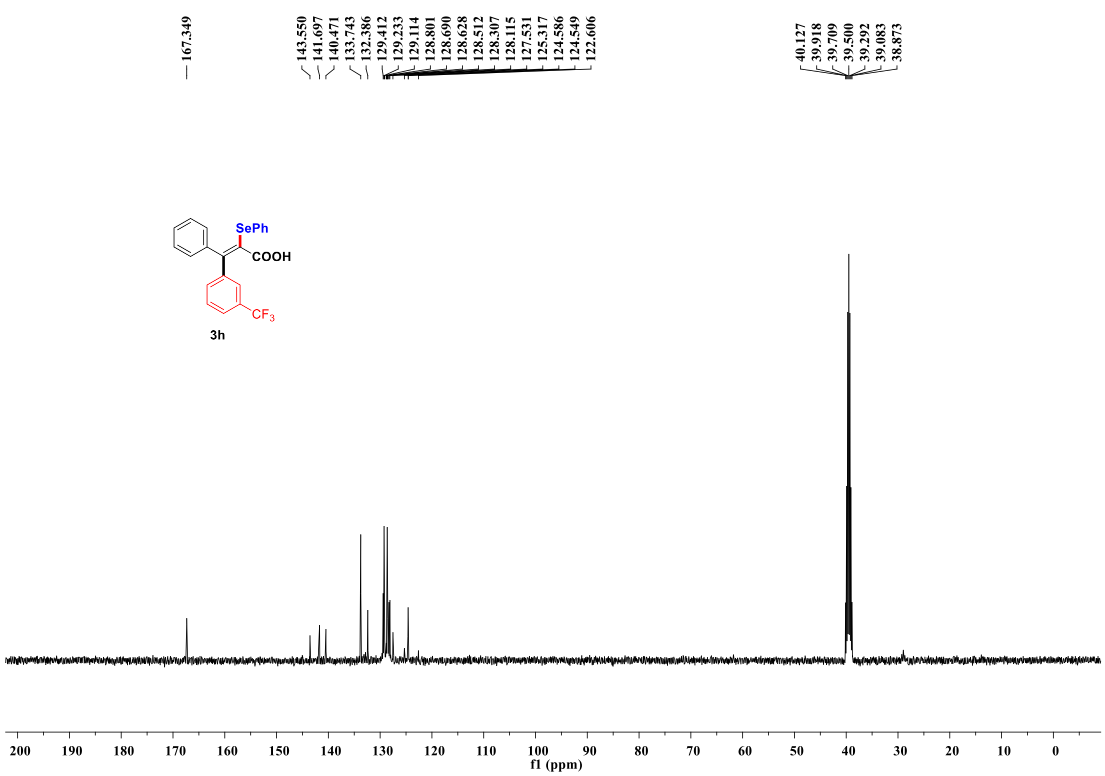
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COOH
CF3
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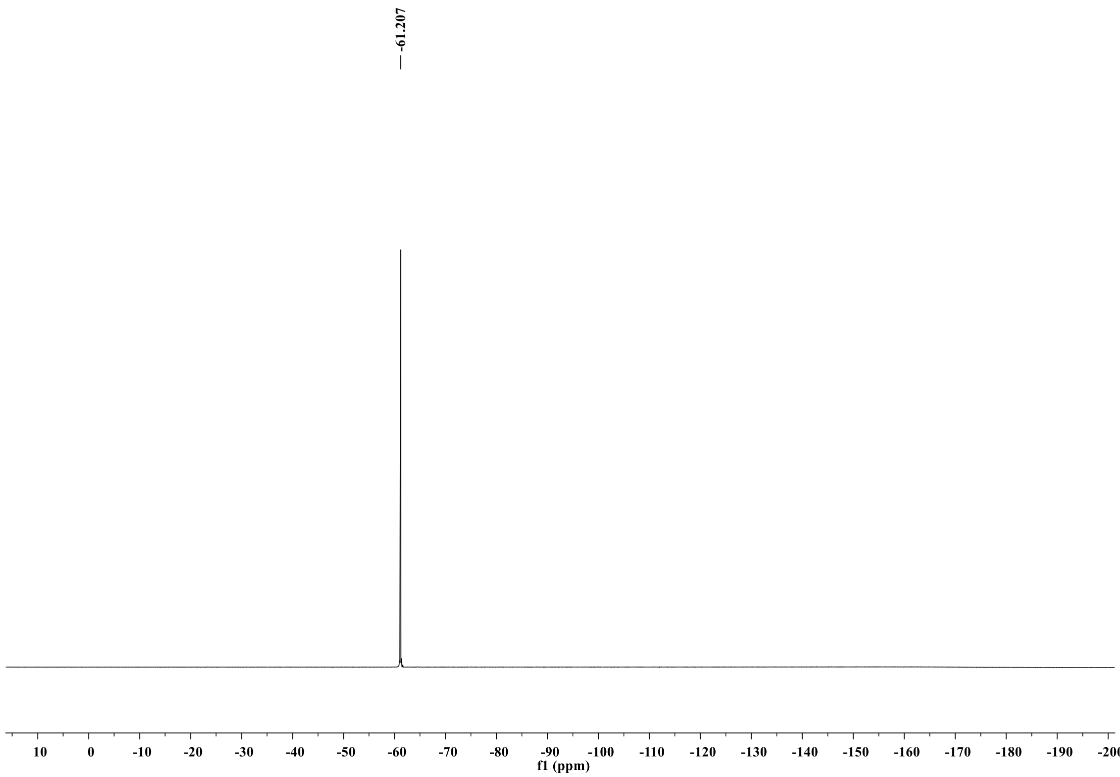
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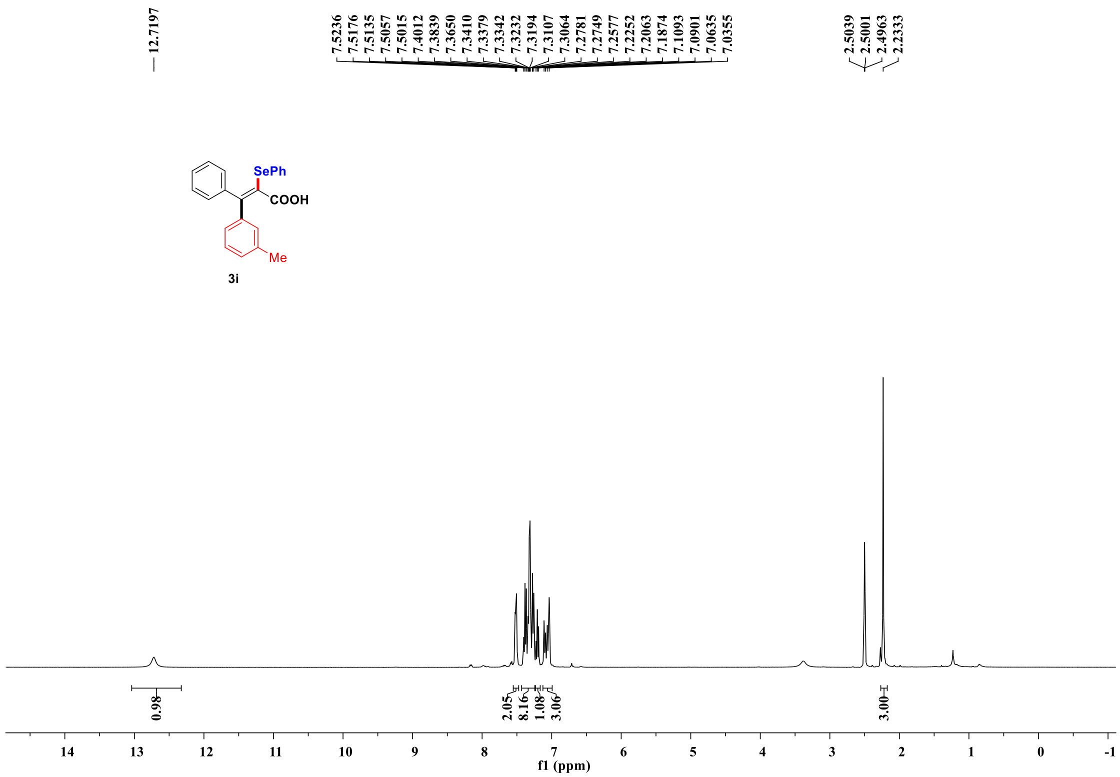
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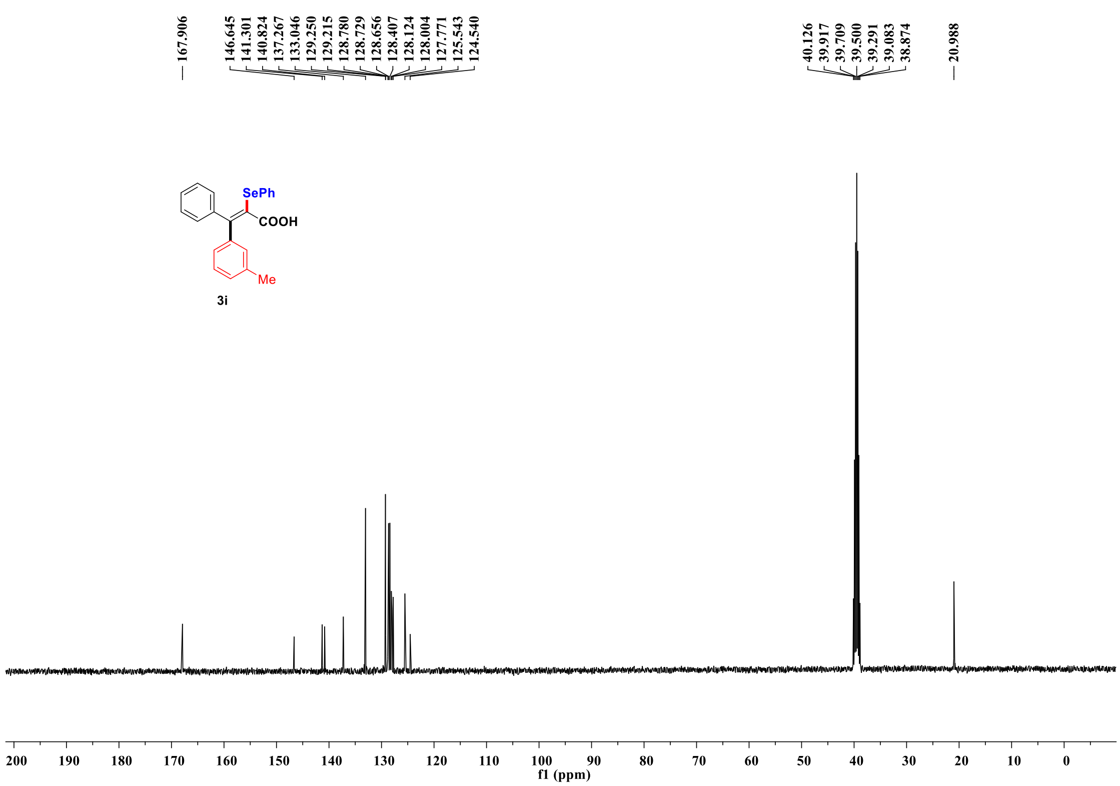
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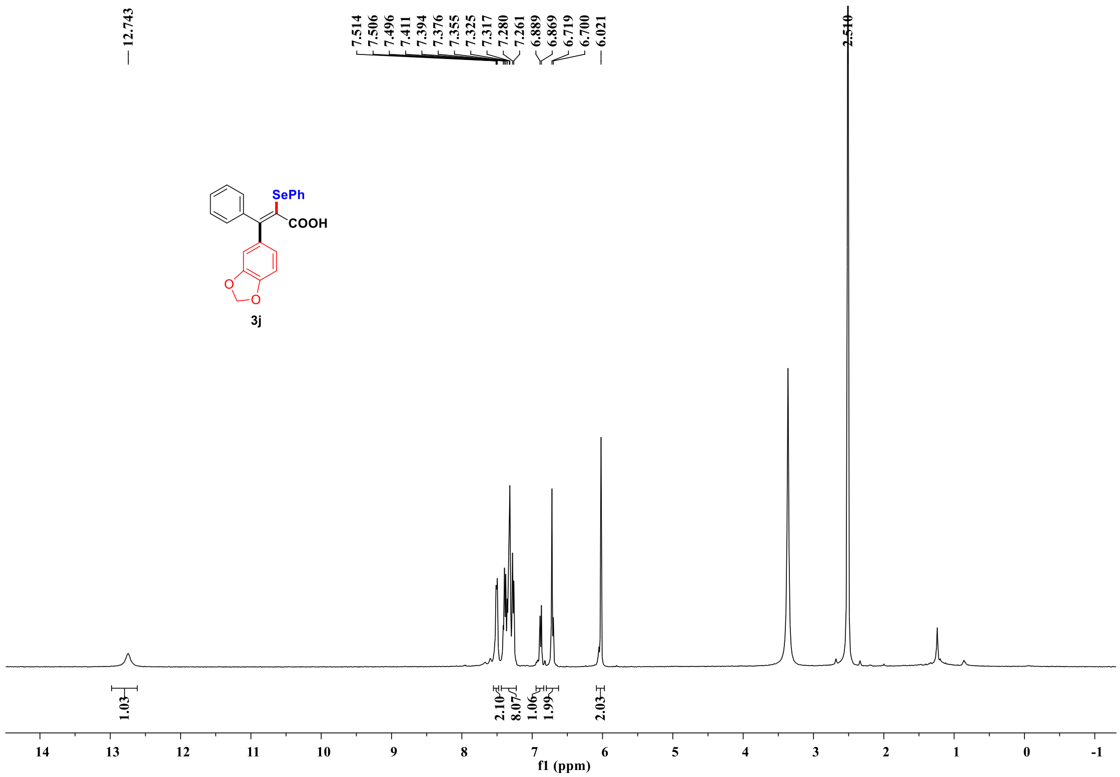
SePh
COOH
Me
3i
f1 (ppm)



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7.261
6.889
6.869
6.719
6.700
6.021
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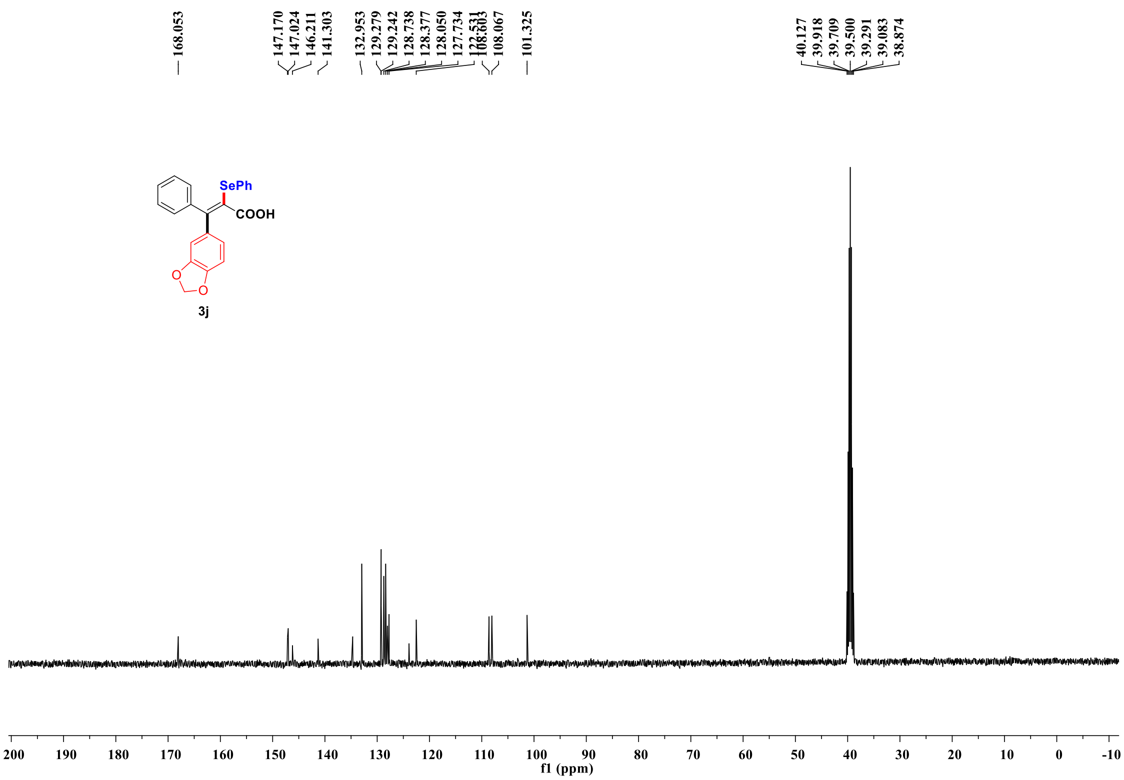
SePh
COOH
3j
1.03
2.10
8.07
1.06
1.99
2.03
f1 (ppm)



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127.734
108.067
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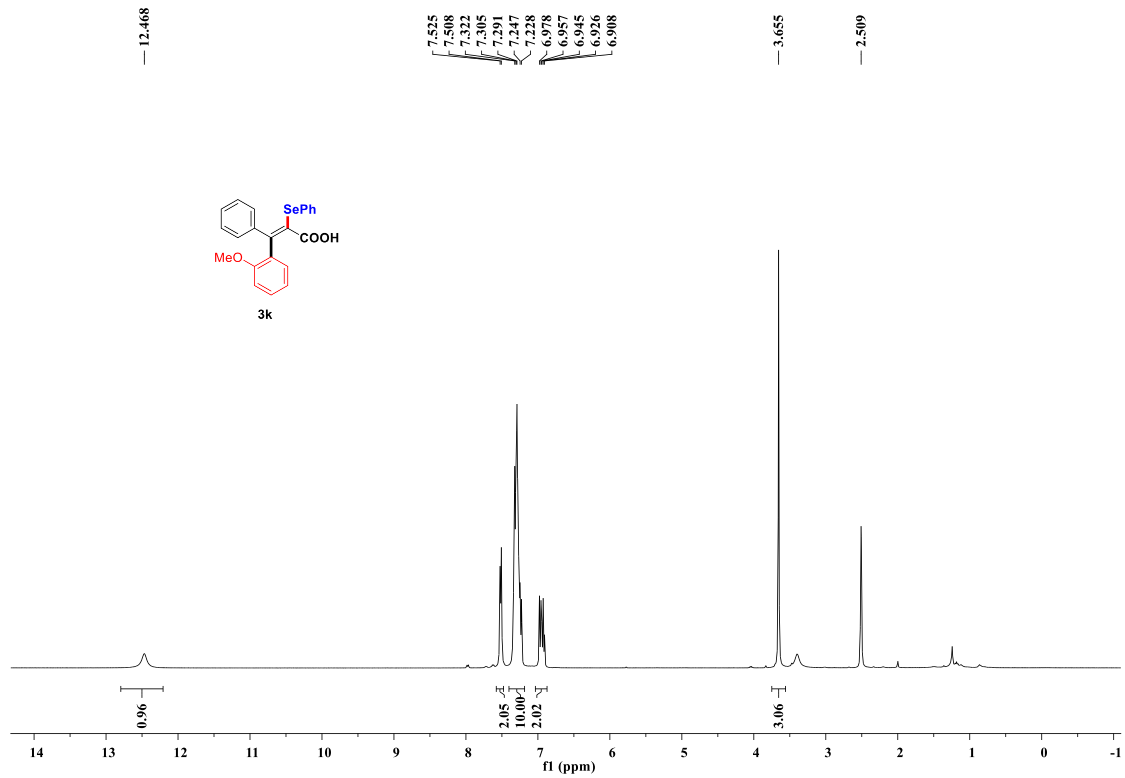
39.709
39.500
39.291
39.083
38.874
SePh
COOH
3j
f1 (ppm)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MeO
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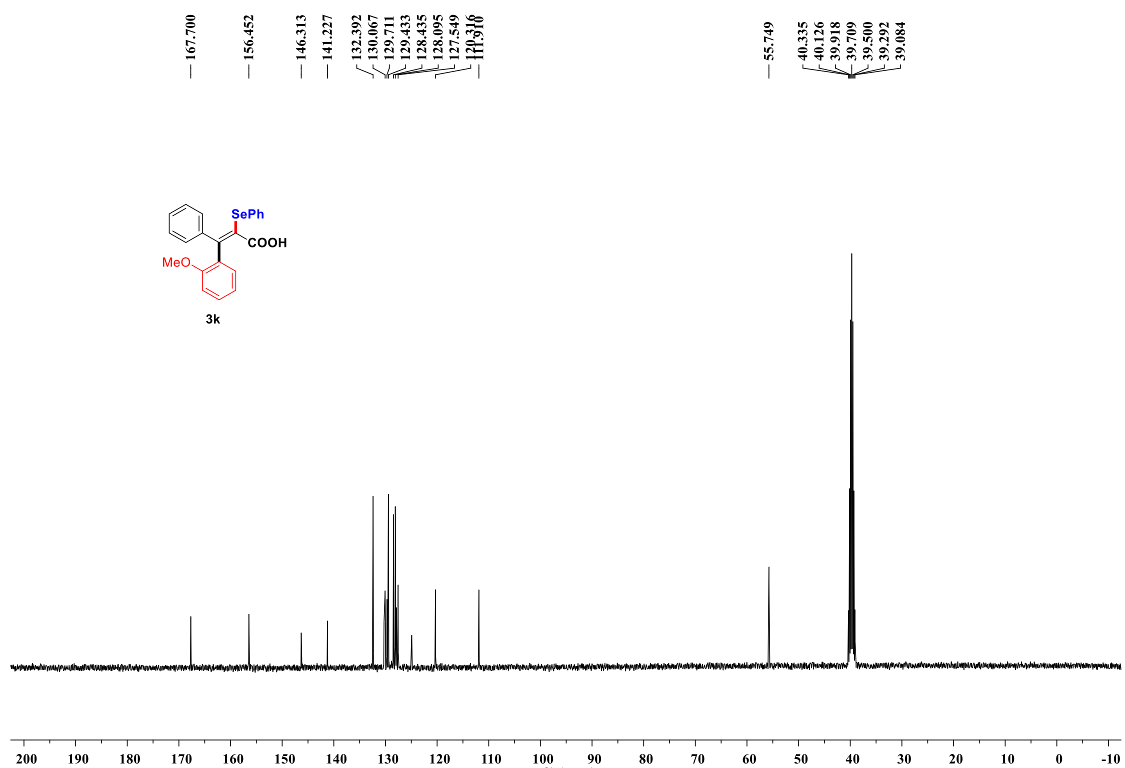
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COOH
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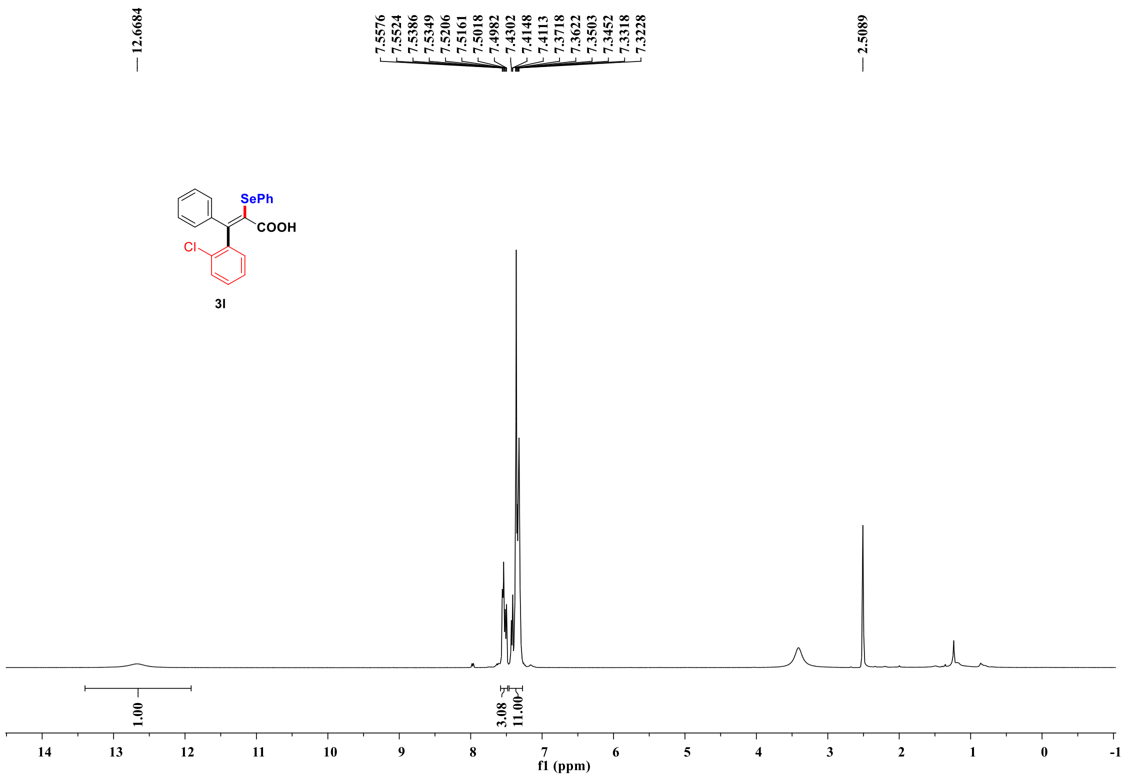
f1 (ppm)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7.4148
7.4113
7.3718
7.3622
7.3503
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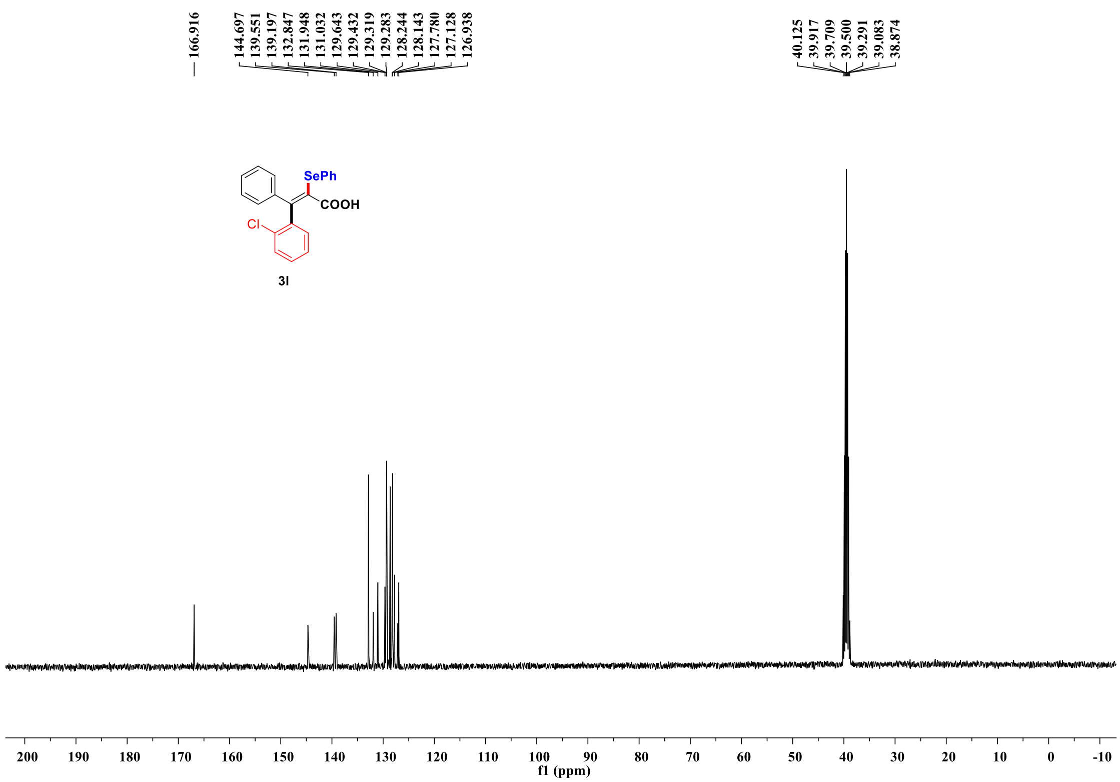
7.3228
2.5089
SePh
COOH
Cl
3l
1.00
3.08
11.00
f1 (ppm)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128.143
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127.128
126.938
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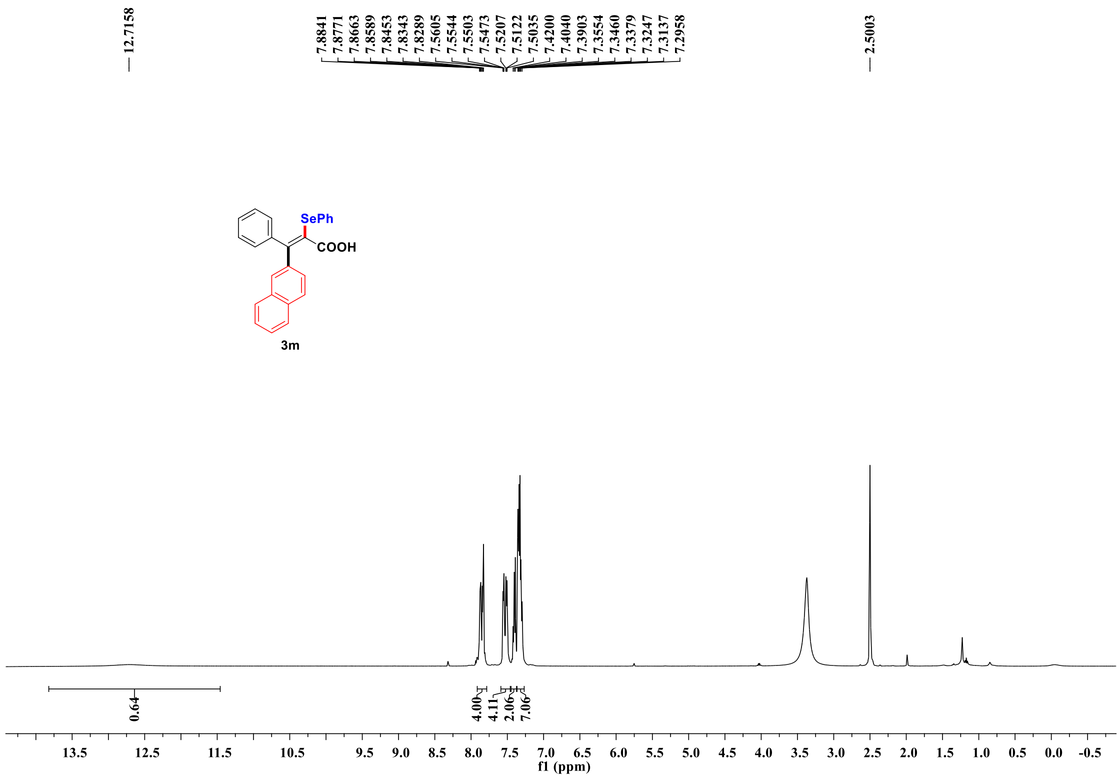
COOH
Cl
3l
f1 (ppm)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7.5473
7.5207
7.5122
7.5035
7.4200
7.4040
7.3903
7.3554
7.3460
7.3379
7.3247
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SePh
COOH
3m
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4.11
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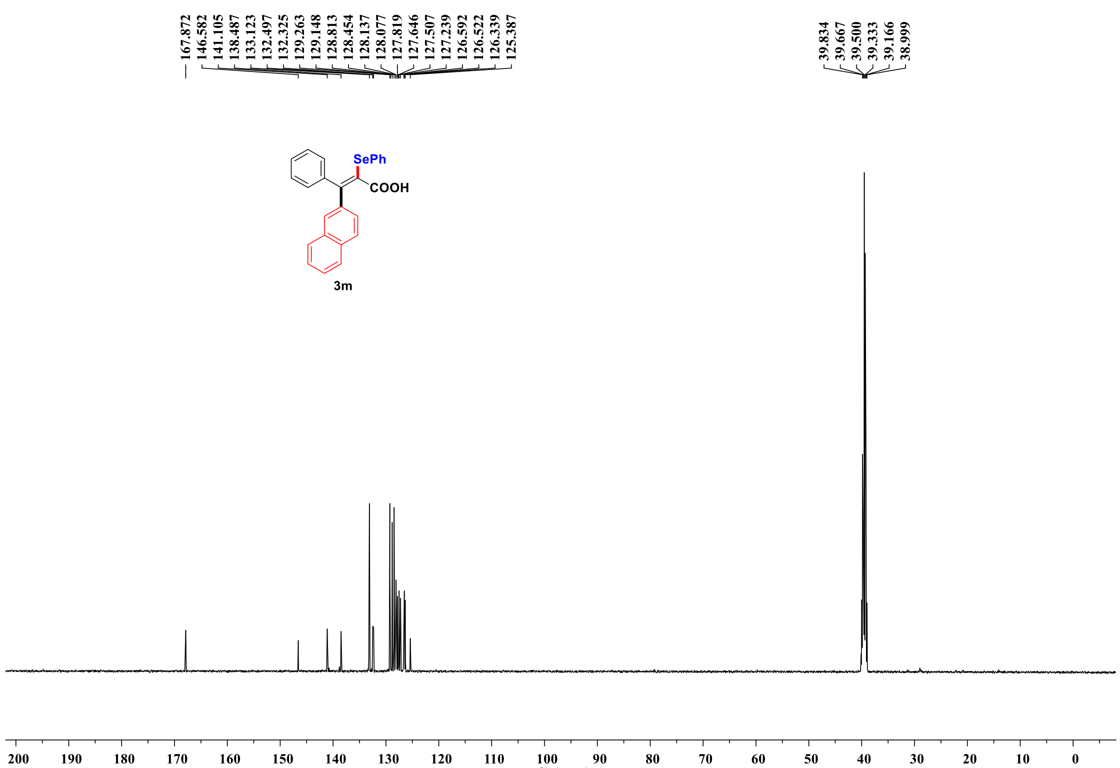
7.06
f1 (ppm)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127.819
127.646
127.507
127.239
126.592
126.522
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39.667
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39.333
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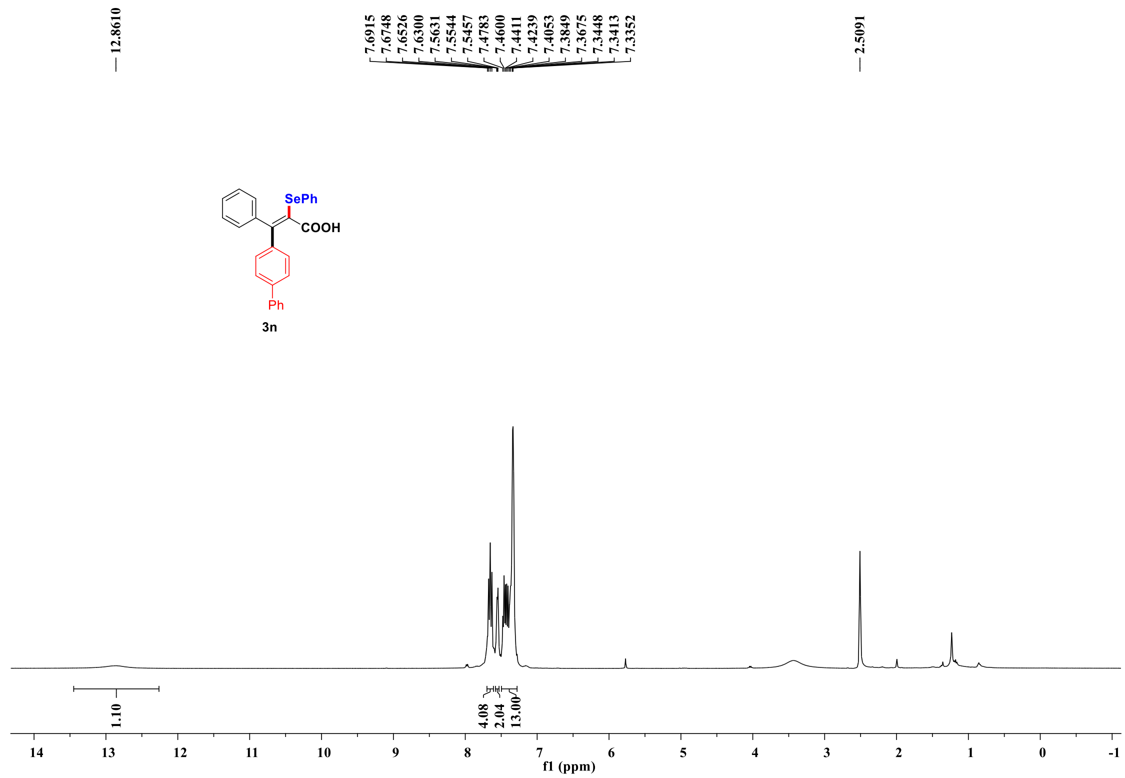
38.999
SePh
COOH
3m
f1 (ppm)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7.5544
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7.4783
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7.4411
7.4239
7.4053
7.3849
7.3675
7.3448
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SePh
COOH
Ph
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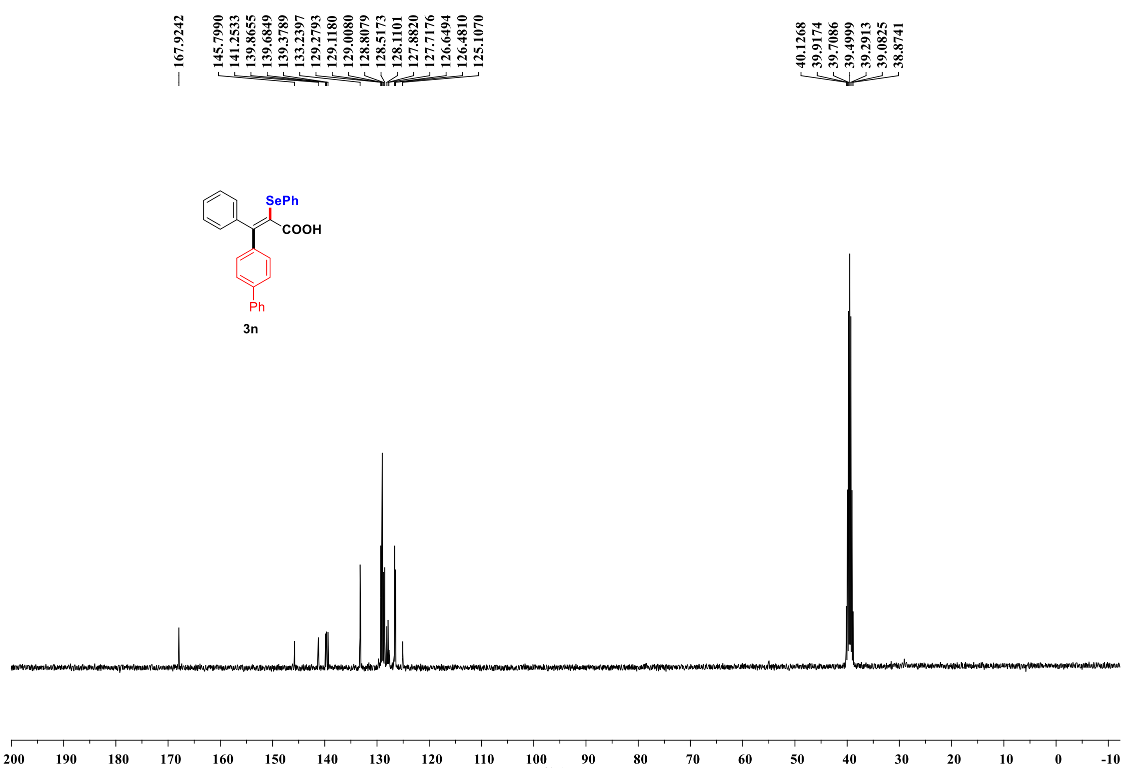
2.04
13.00
f1 (ppm)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128.8079
128.5173
128.1101
127.8820
127.7176
126.6494
126.4810
125.1070
40.1268
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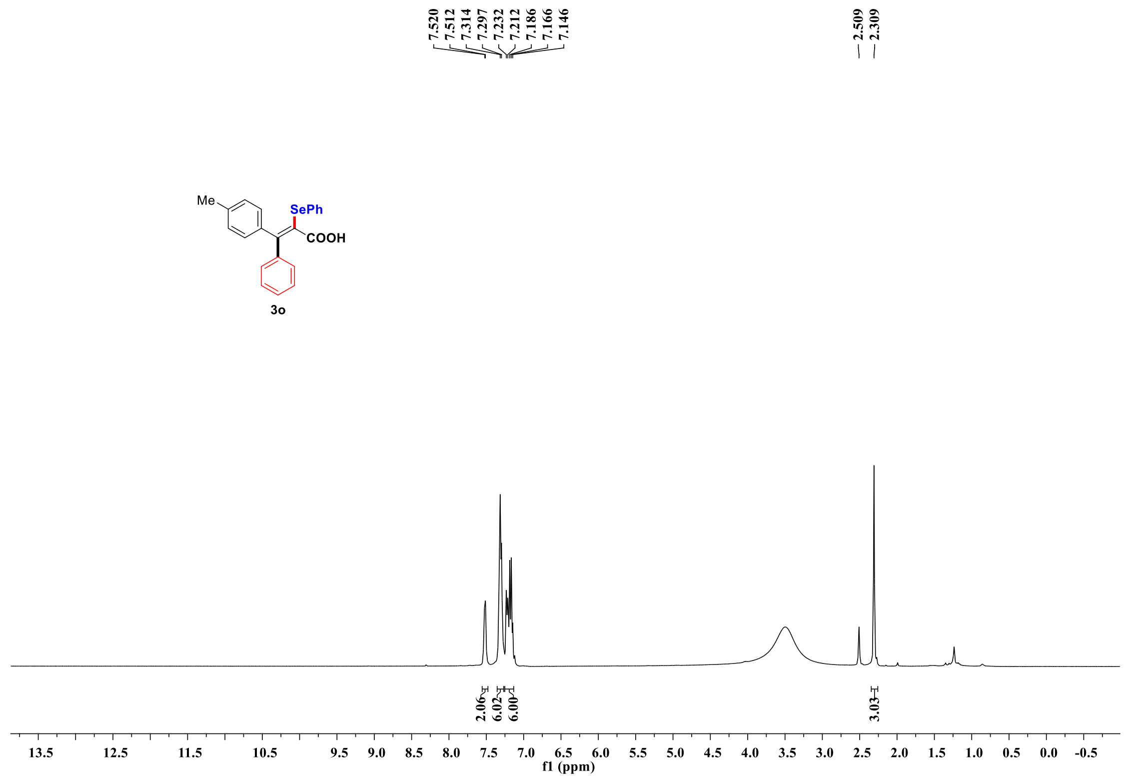
39.4999
39.2913
39.0825
38.8741
SePh
COOH
Ph
3n
f1 (ppm)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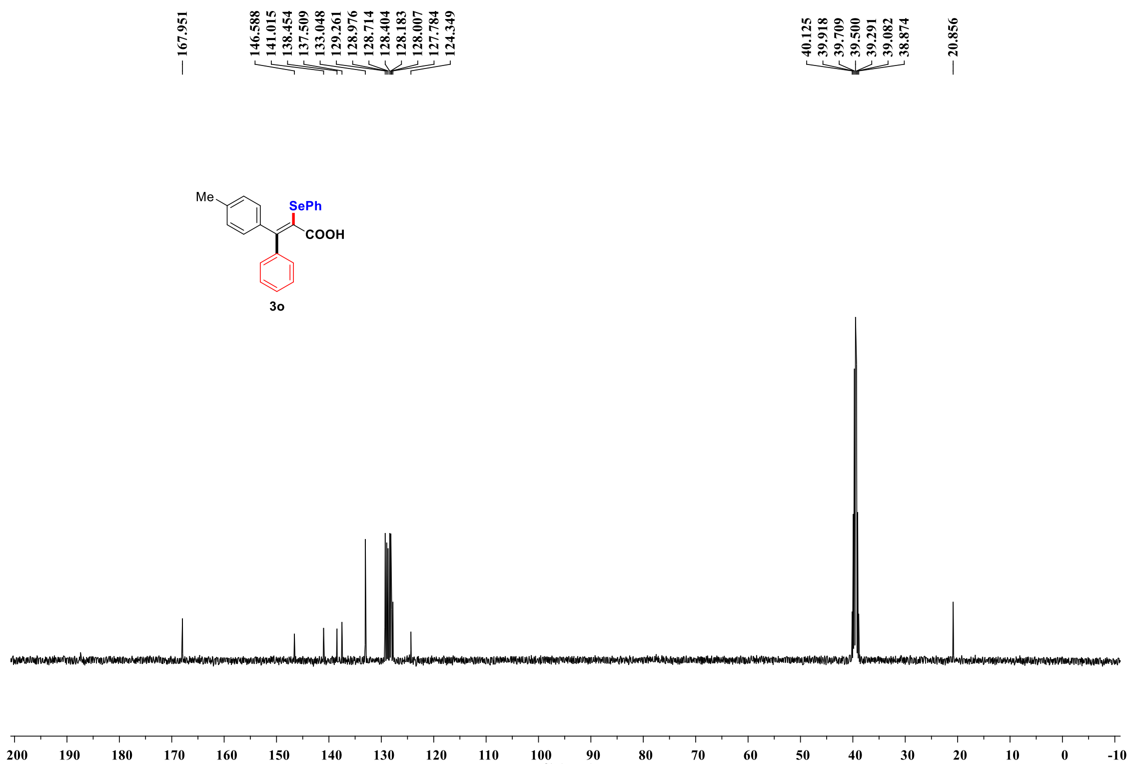
7.512
7.314
7.297
7.232
7.212
7.186
7.166
7.146
2.509
2.309
Me
SePh
COOH
3o
2.06
6.02
6.00
3.03
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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133.048
129.261
128.976
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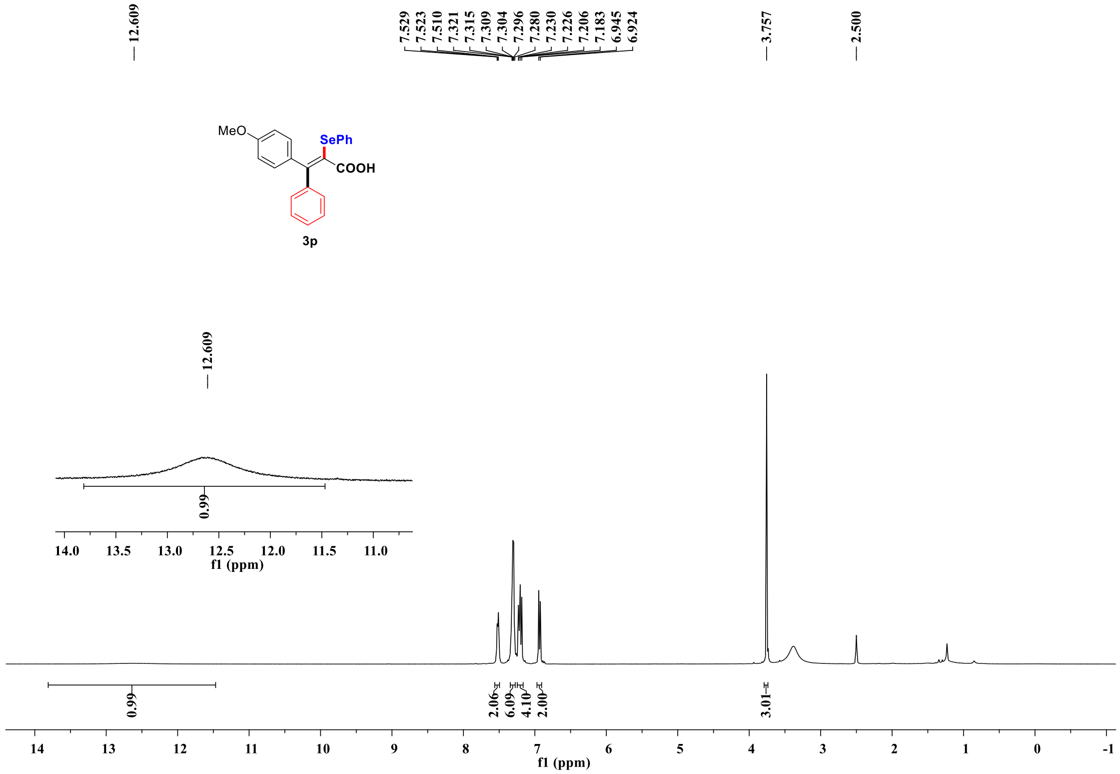
128.404
128.183
128.007
127.784
124.349
40.125
39.918
39.709
39.500
39.291
39.082
38.874
20.856
Me
SePh
COOH
3o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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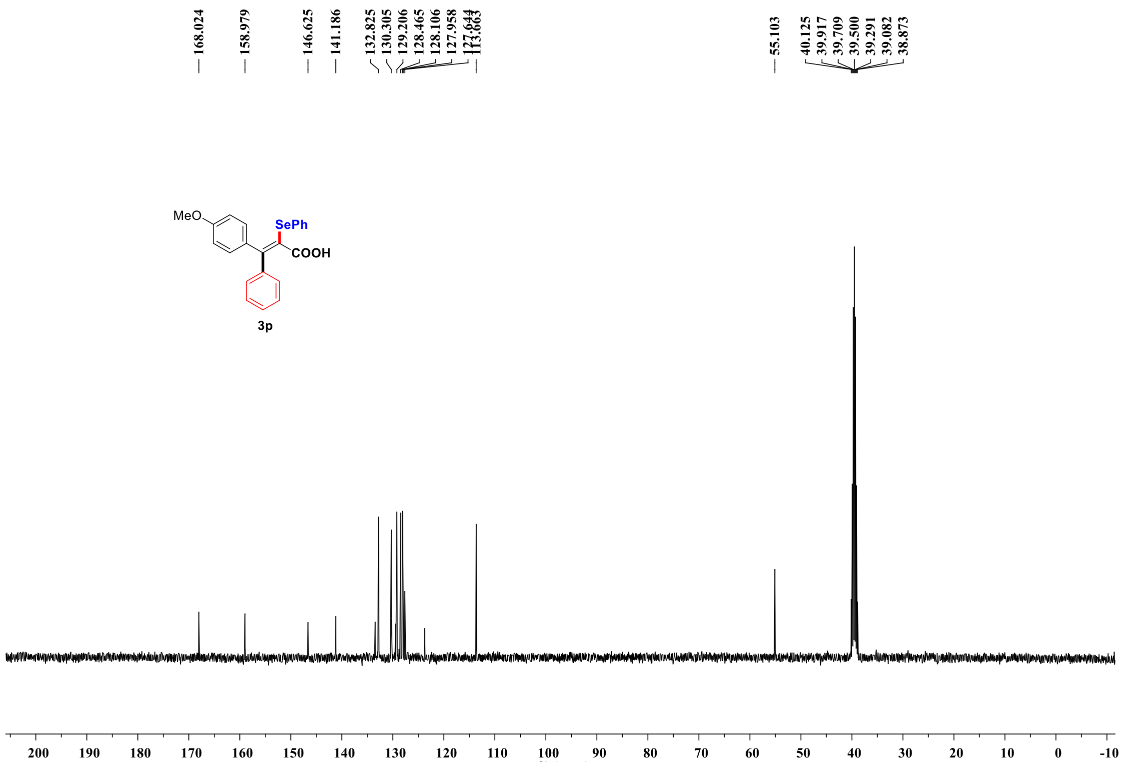
7.321
7.315
7.309
7.304
7.296
7.280
7.230
7.226
7.206
7.183
6.945
6.924
3.757
2.500
MeO
SePh
COOH
3p
0.99
2.06
6.09
4.10
2.00
3.01
f1 (ppm)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128.465
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39.709
39.500
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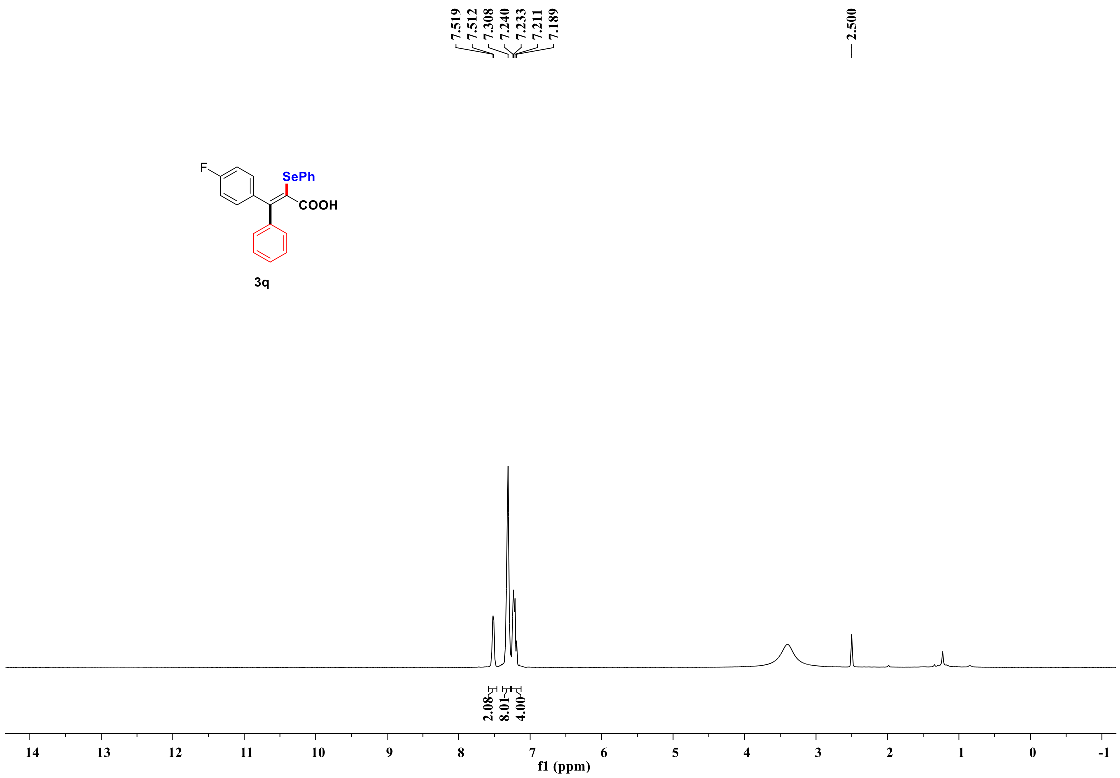
MeO
SePh
COOH
3p
f1 (ppm)


7.519
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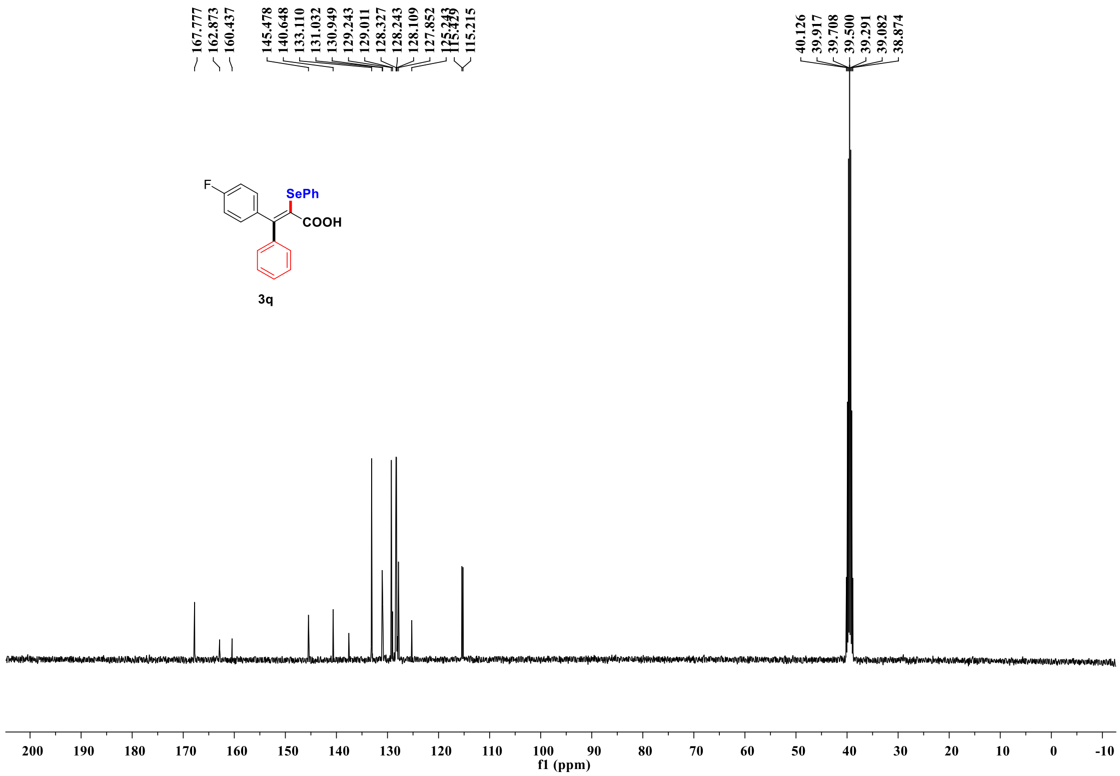
7.308
7.240
7.233
7.211
7.189
2.500
SePh
COOH
F
3q
2.08
8.01
4.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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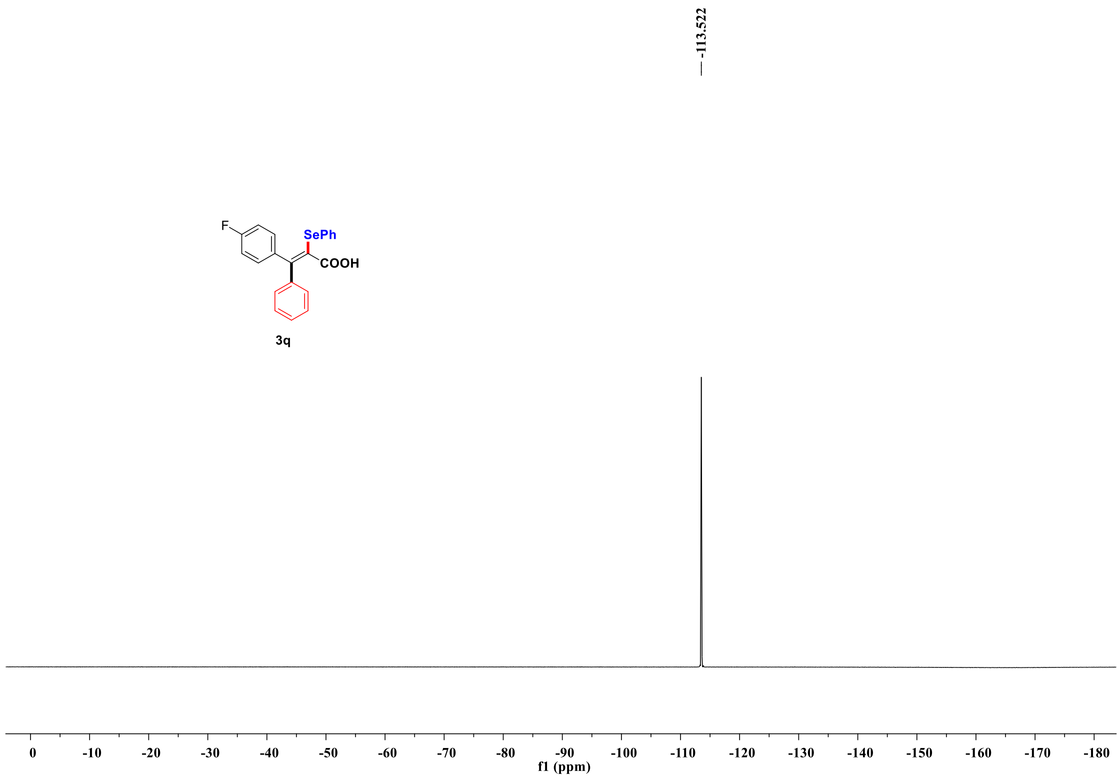
128.109
127.852
115.429
115.215
40.126
39.917
39.708
39.500
39.291
39.082
38.874
SePh
COOH
F
3q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-113.522
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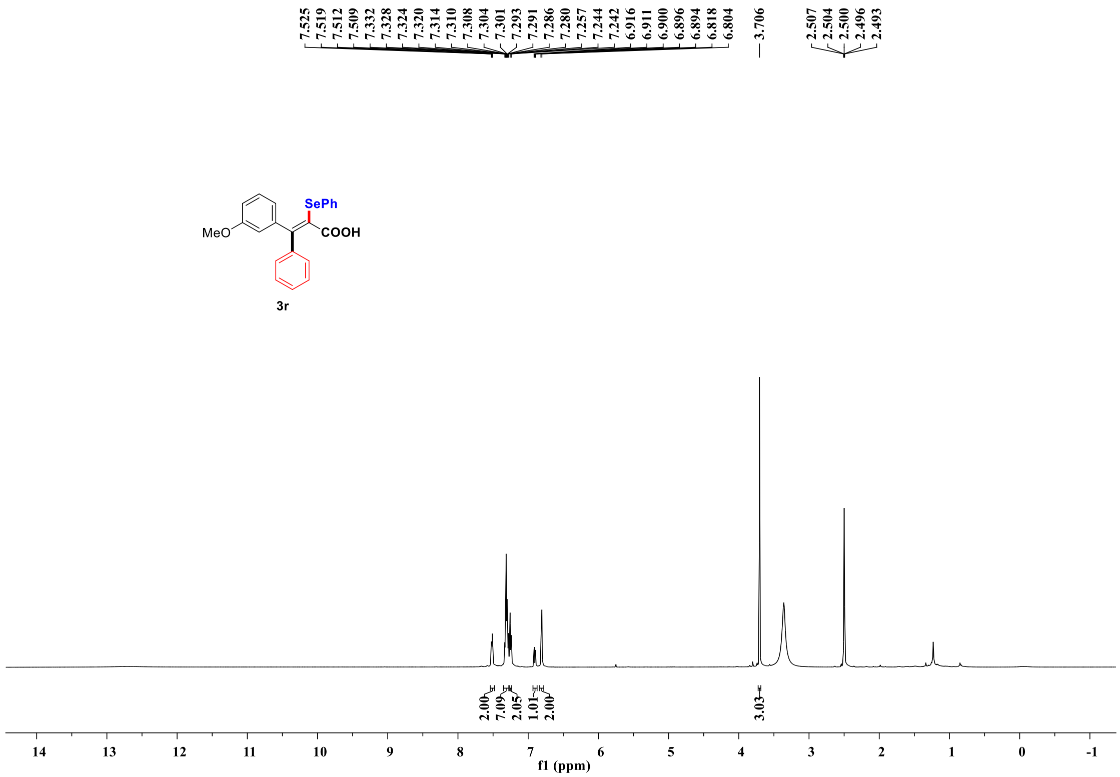
COOH
3q
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)



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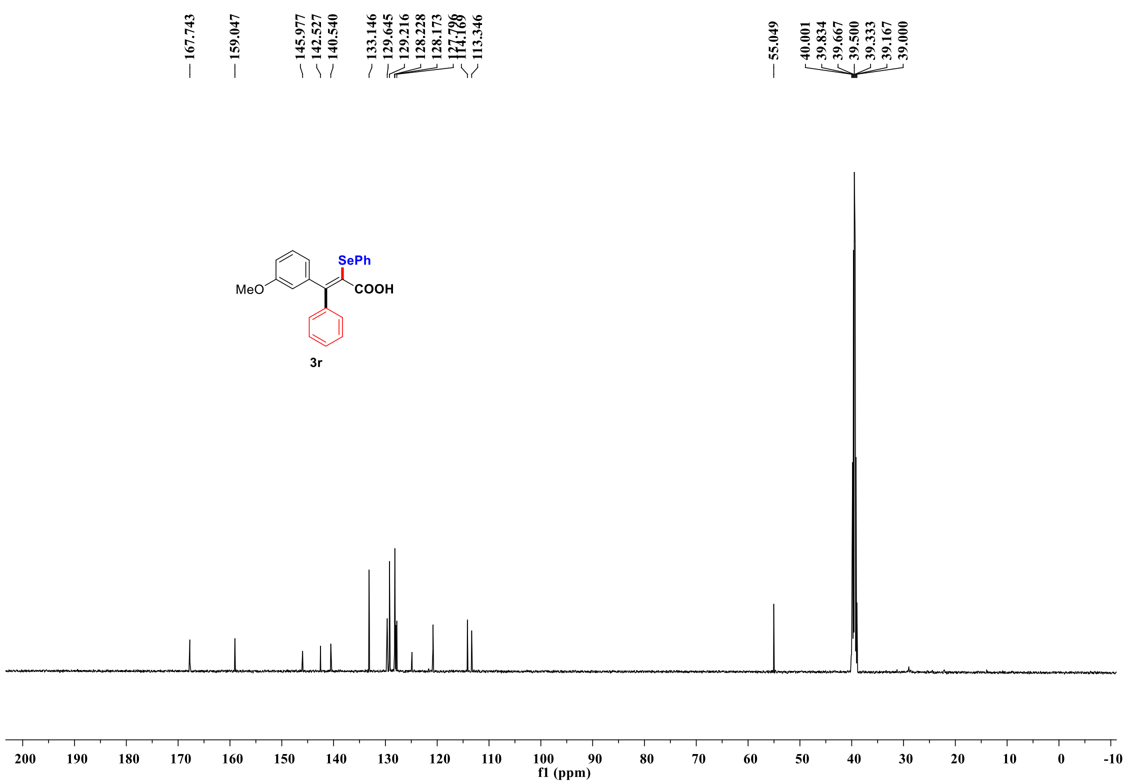
7.512
7.509
7.332
7.328
7.324
7.320
7.314
7.310
7.308
7.304
7.301
7.293
7.291
7.286
7.280
7.257
7.244
7.242
6.916
6.911
6.900
6.896
6.894
6.818
6.804
3.706
2.507
2.504
2.500
2.496
2.493
SePh
MeO
COOH
3r
2.00
7.09
2.05
1.01
2.00
3.03
f1 (ppm)



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145.977
142.527
140.540
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129.216
128.228
128.173
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114.169
113.346
55.049
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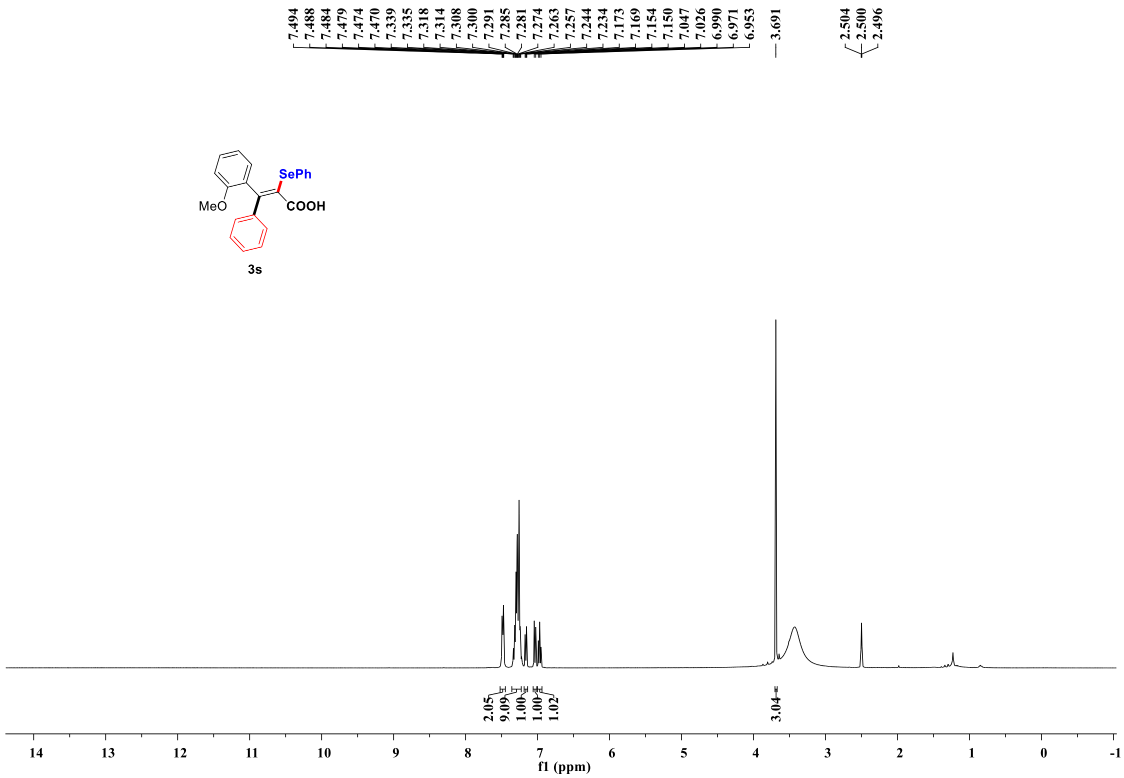
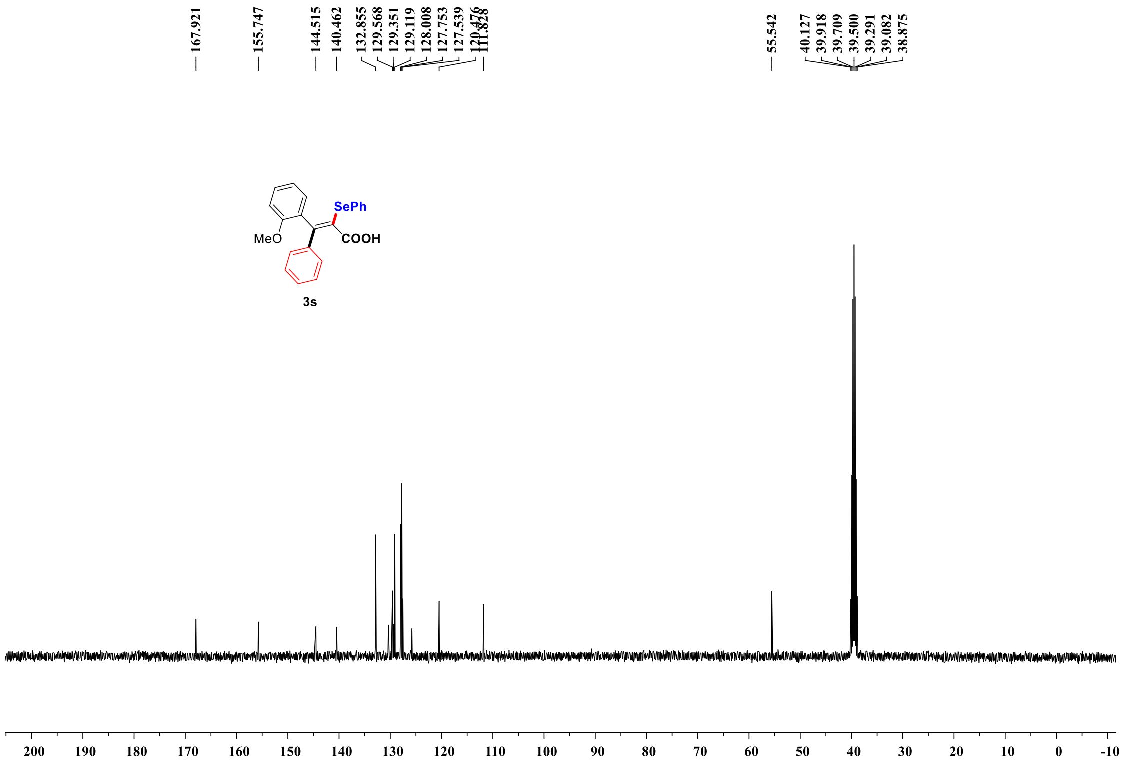
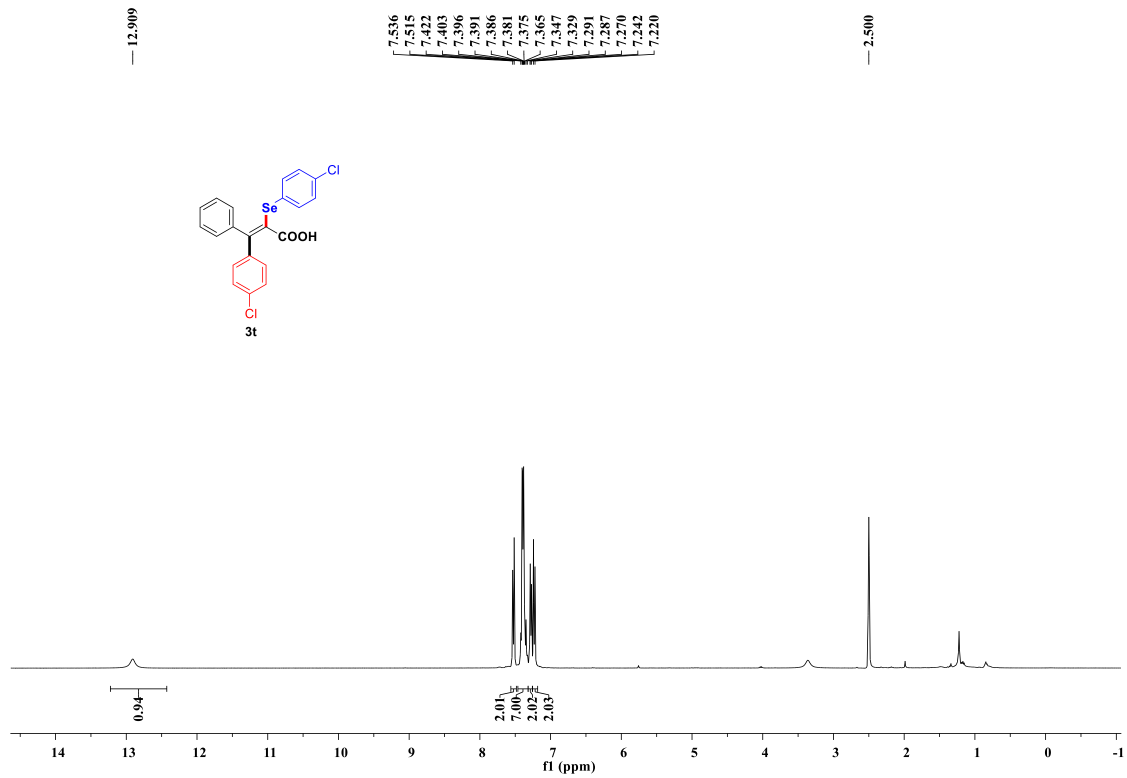
39.834
39.667
39.500
39.333
39.167
39.000
SePh
MeO
COOH
3r
f1 (ppm)



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7.291
7.287
7.270
7.242
7.220
2.500
Se
Cl
COOH
Cl
3t
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7.00
2.02
2.03
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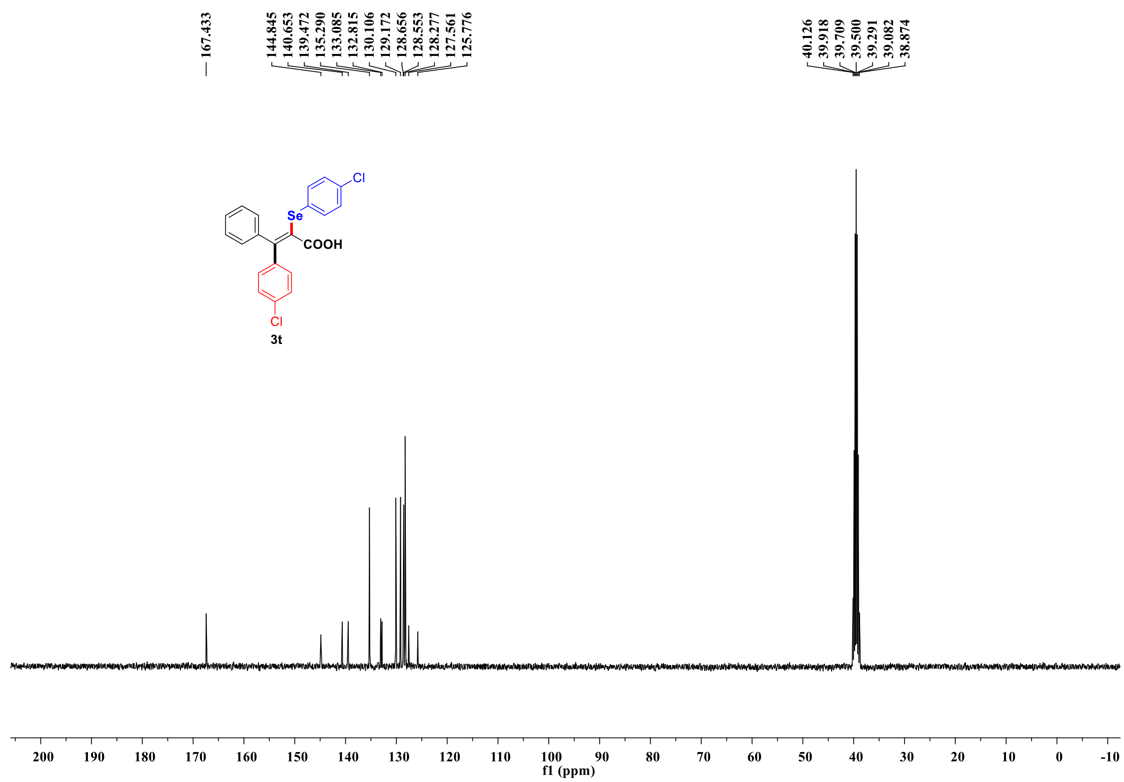
f1 (ppm)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127.561
125.776
40.126
39.918
39.709
39.500
39.291
39.082
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Se
Cl
COOH
Cl
3t
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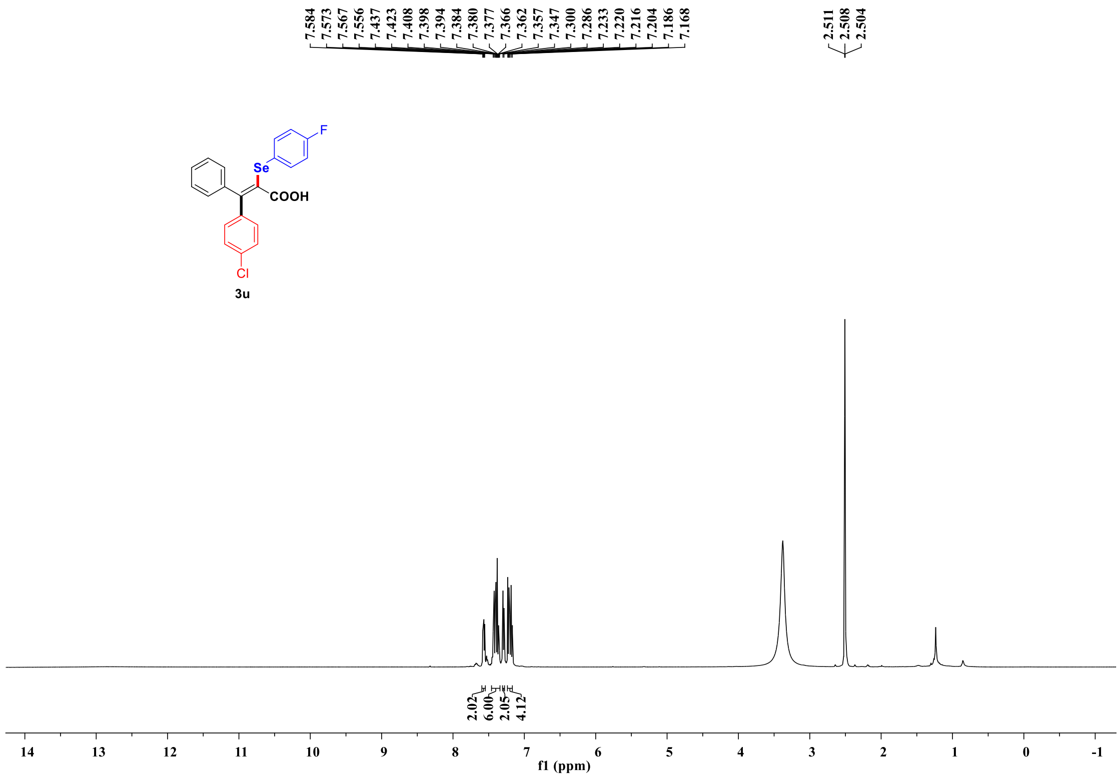
f1 (ppm)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7.204
7.186
7.168
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Cl
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6.00
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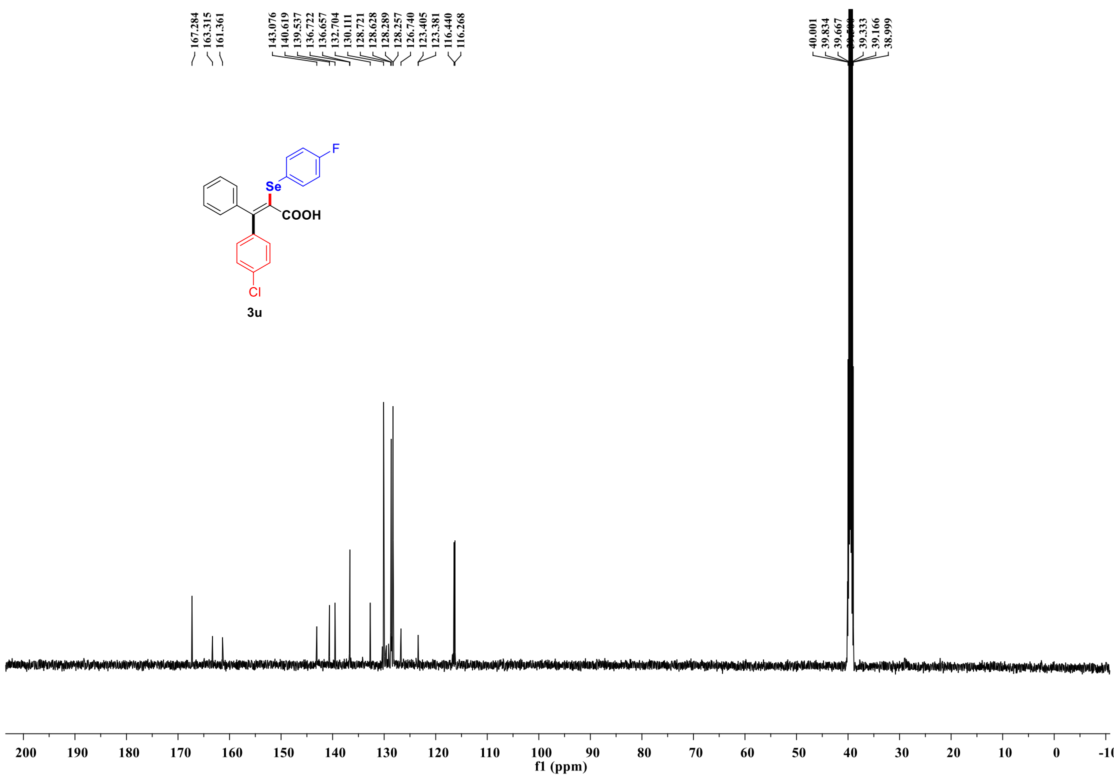
4.12
f1 (ppm)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128.289
128.257
126.740
123.405
123.381
116.440
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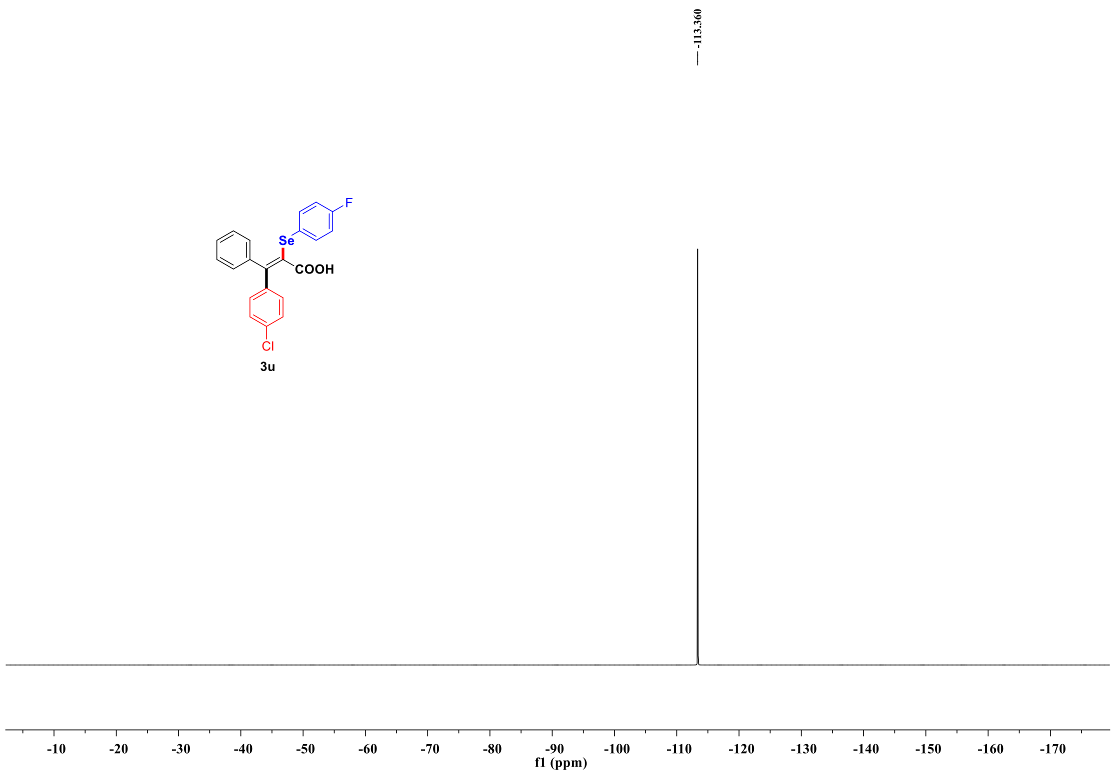
39.667
39.333
39.166
38.999
Se
F
COOH
Cl
3u
f1 (ppm)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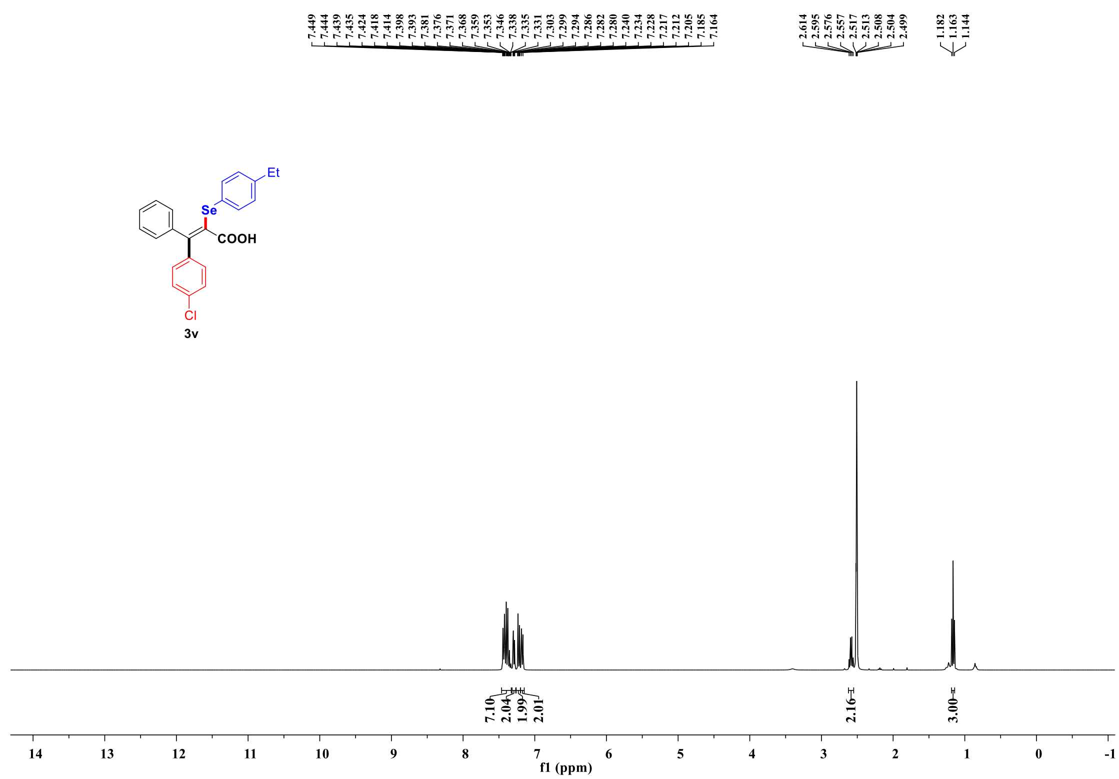
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7.164
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2.517
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1.182
1.163
1.144
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Et
COOH
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2.16
3.00
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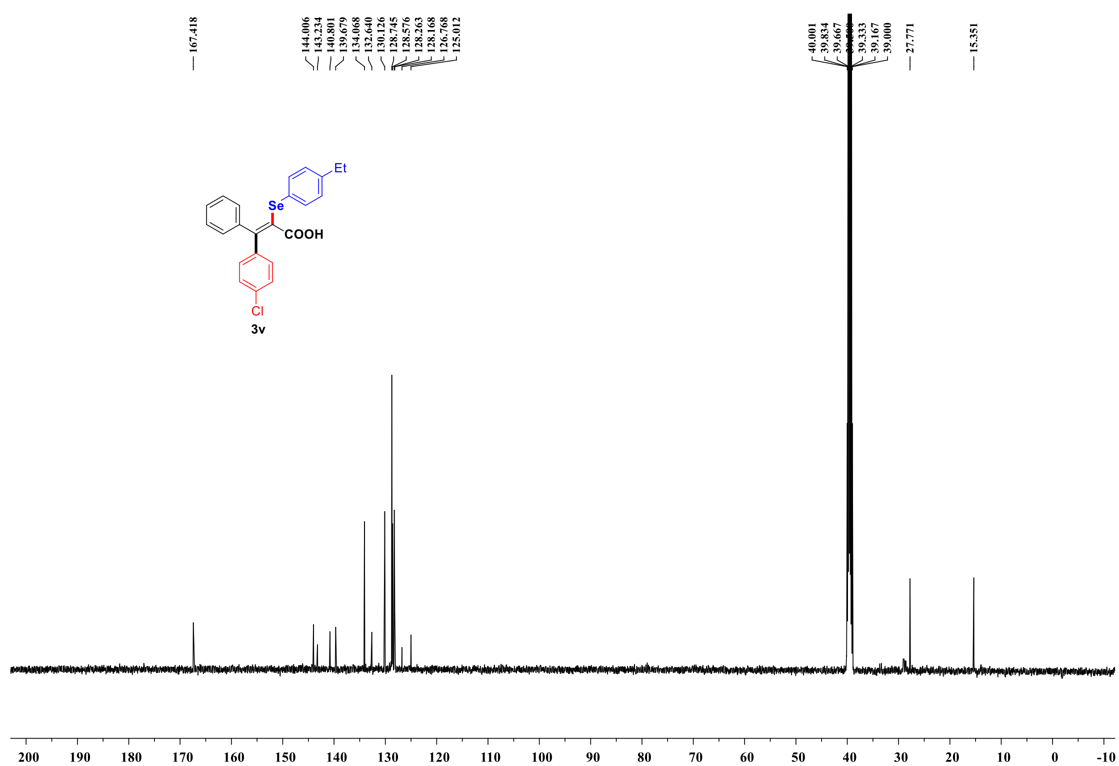
f1 (ppm)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125.012
40.001
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39.667
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39.167
39.000
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Et
COOH
Cl
3v
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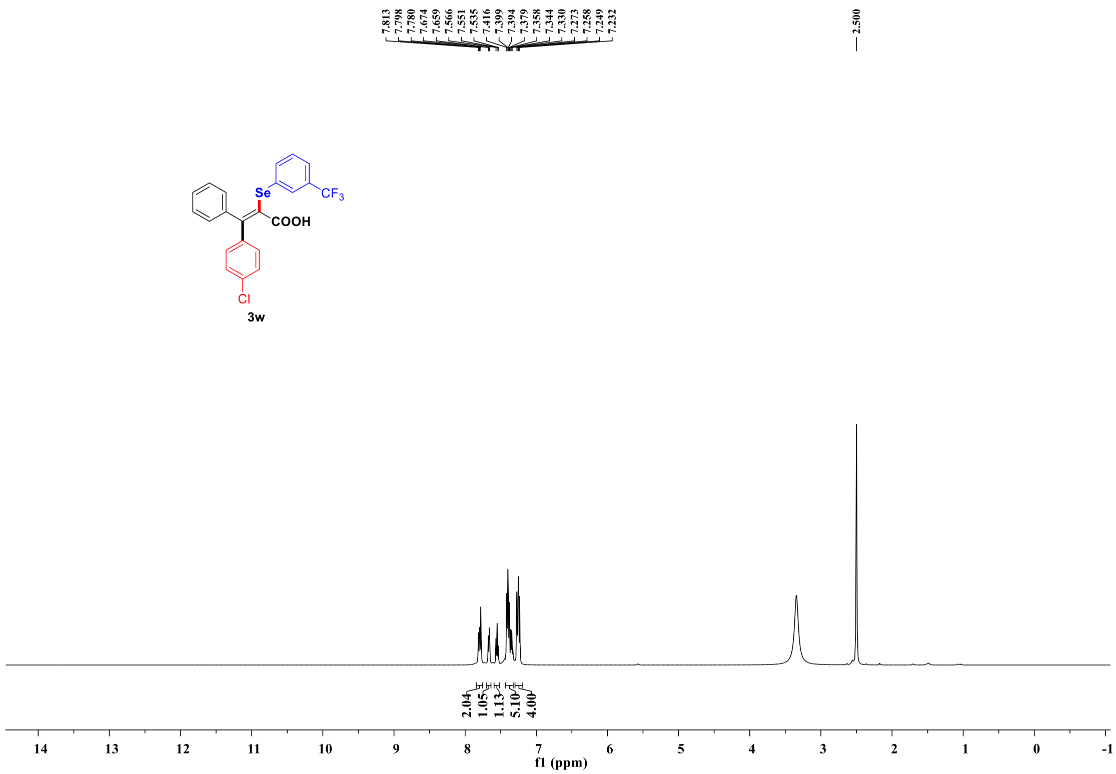
f1 (ppm)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CF3
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Cl
3w
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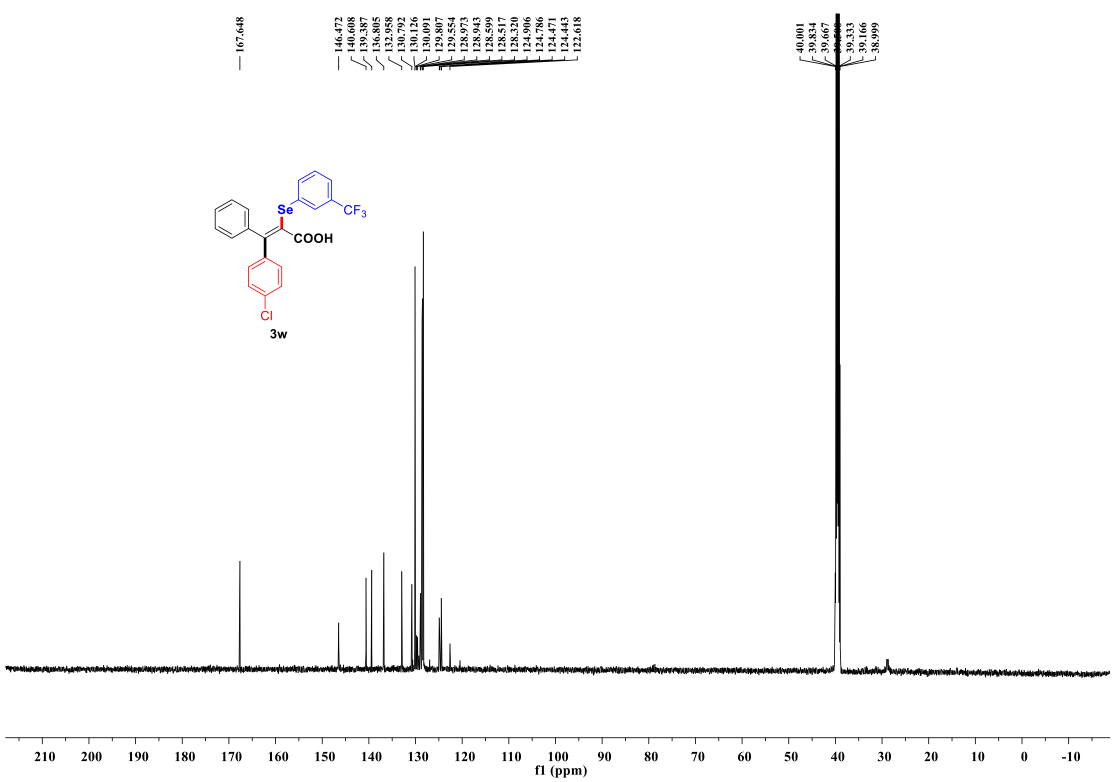
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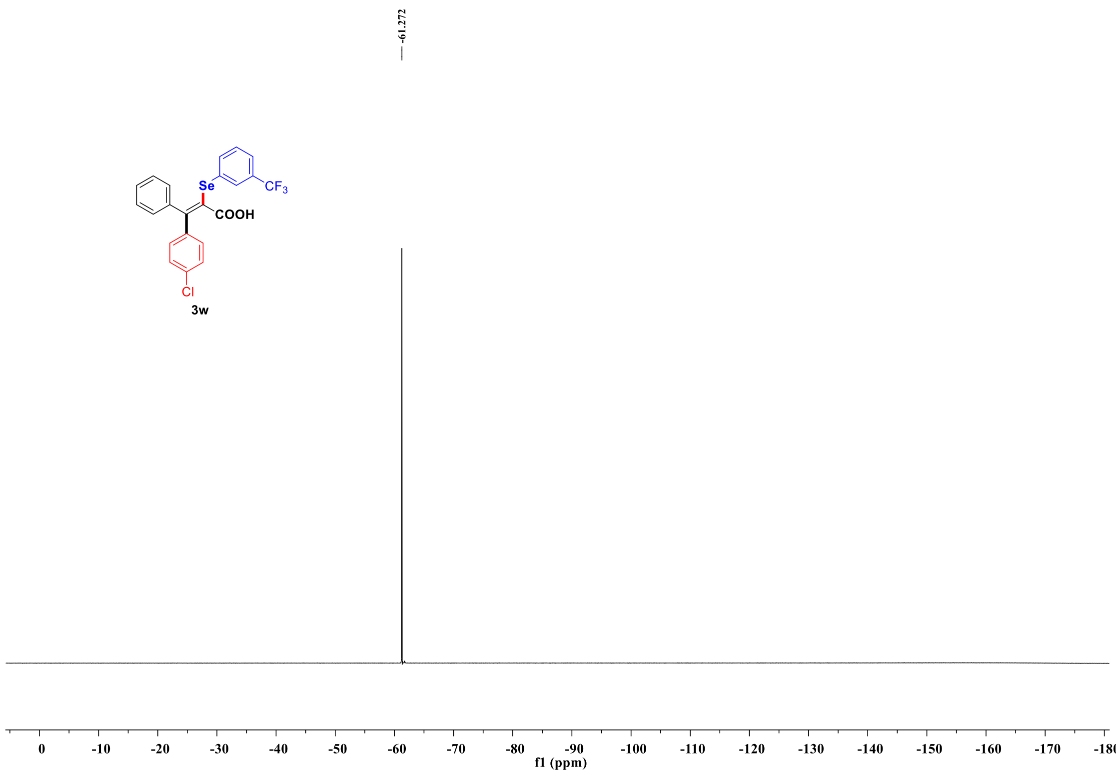
CF3
COOH
Cl
3w
f1 (ppm)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-100
-110
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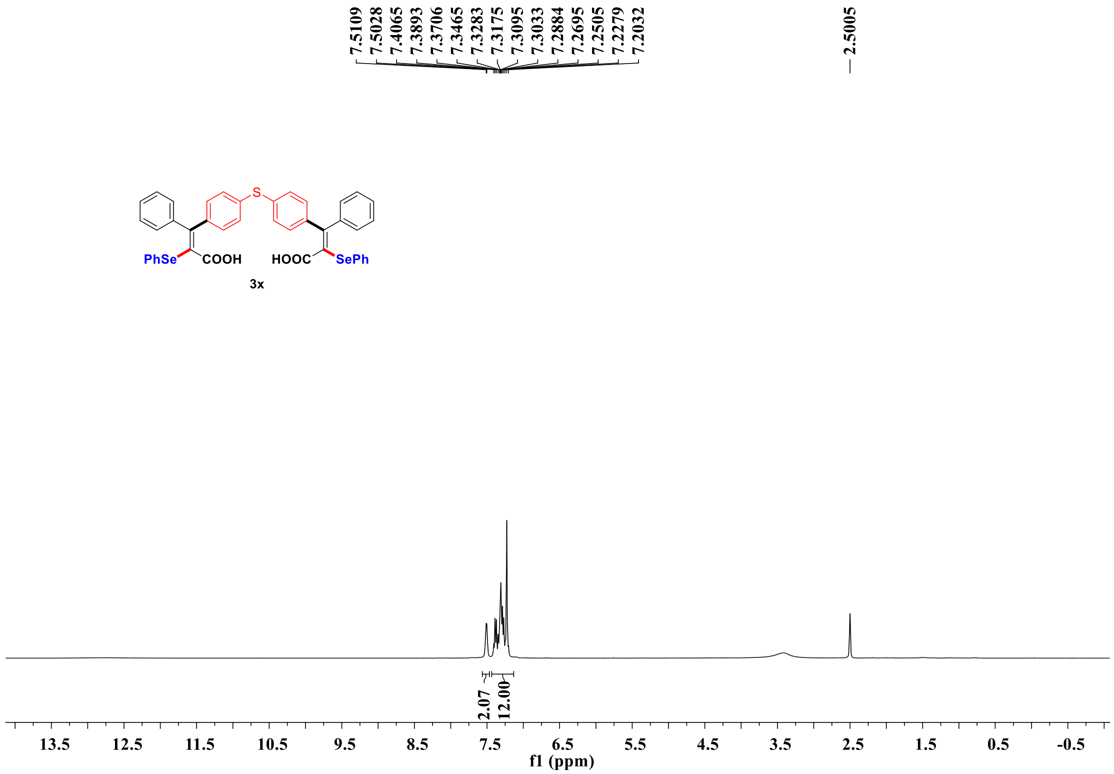
-130
-140
-150
-160
-170
-180
f1 (ppm)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7.2695
7.2505
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HOOC
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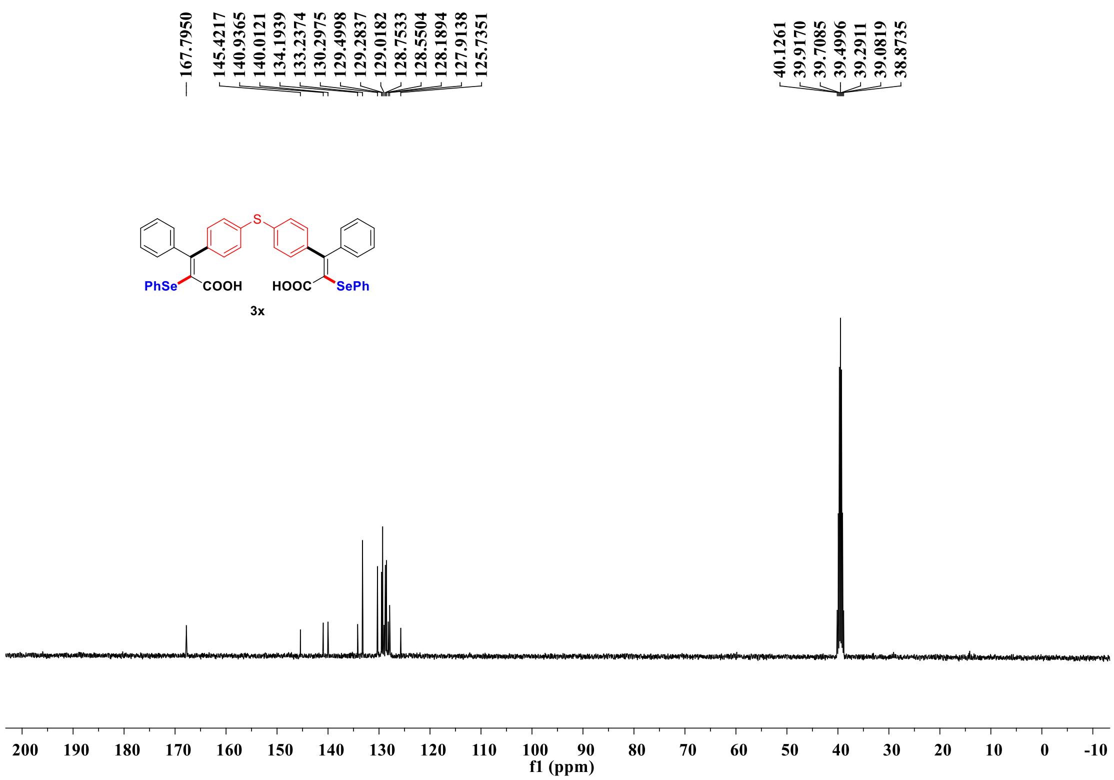
S
3x
2.07
12.00
f1 (ppm)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125.7351
40.1261
39.9170
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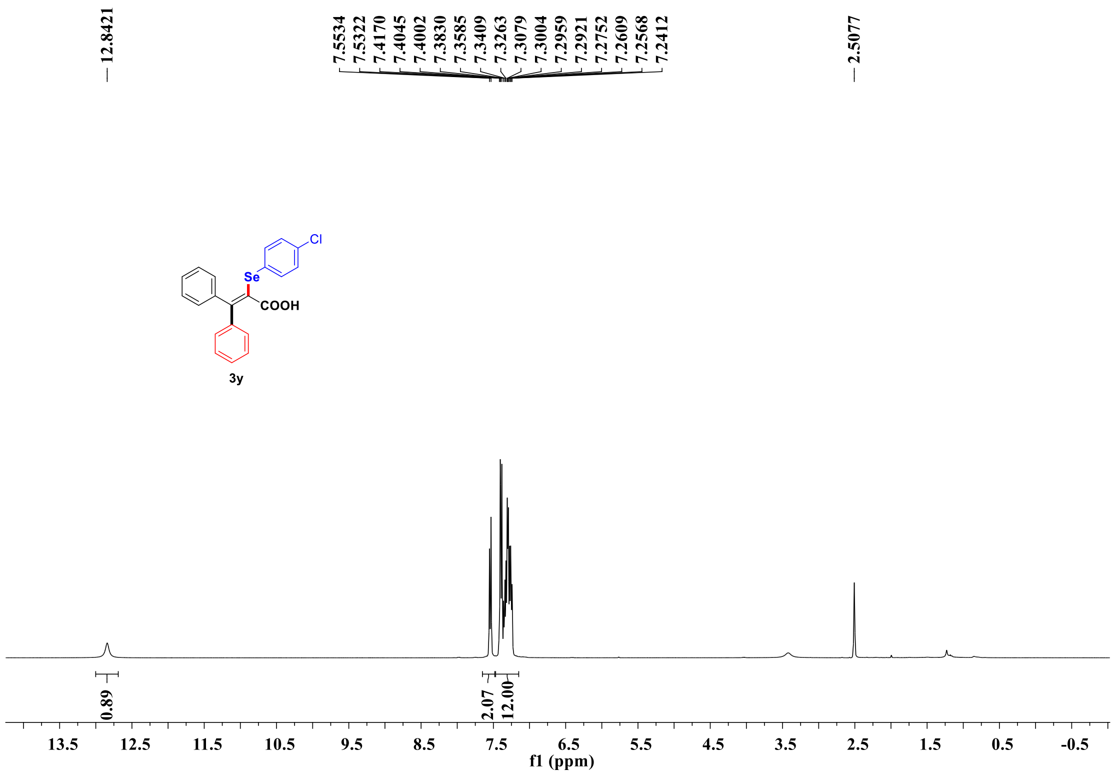
38.8735
PhSe
COOH
HOOC
SePh
S
3x
f1 (ppm)



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7.2609
7.2568
7.2412
2.5077
Se
Cl
COOH
3y
0.89
2.07
12.00
13.5 12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
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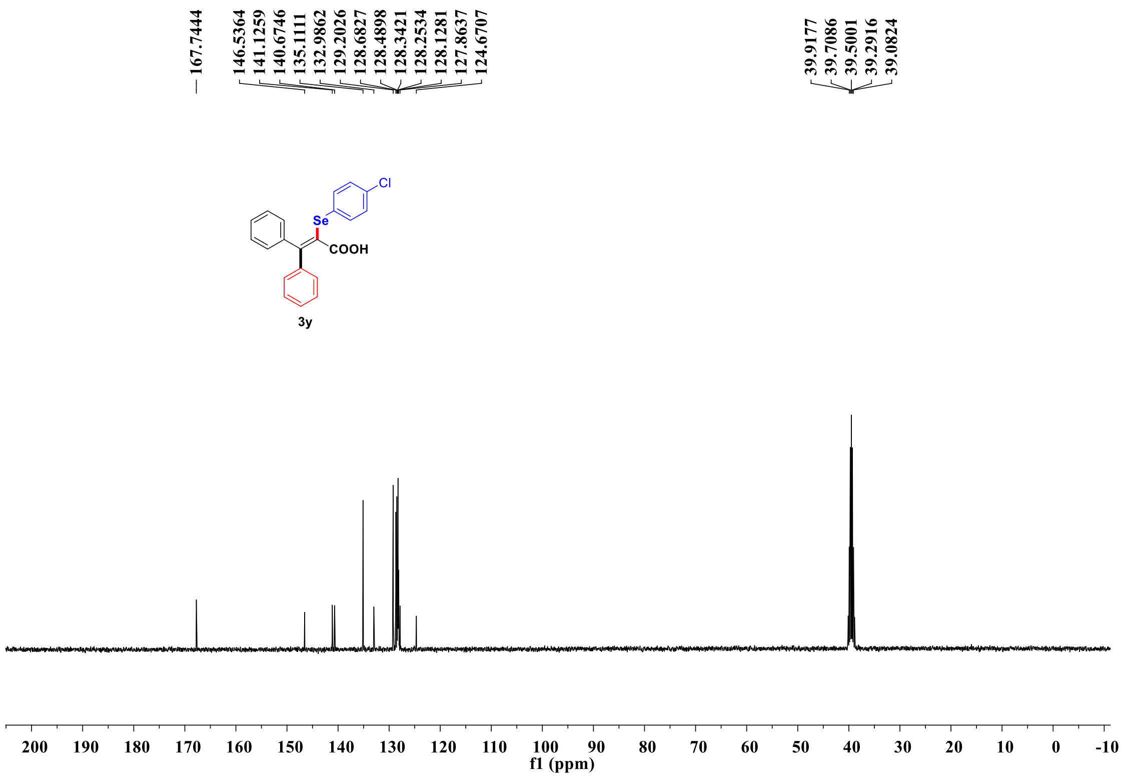

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Se
Cl
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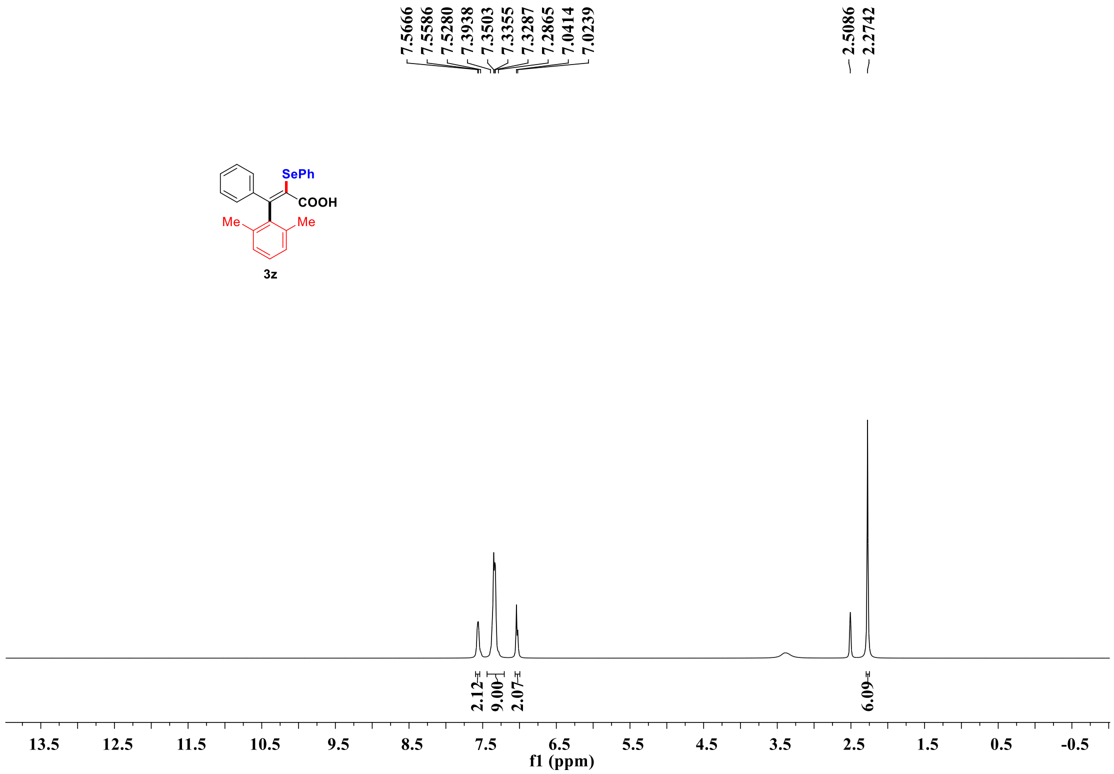
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COOH
Me
Me
3z
2.12
9.00
2.07
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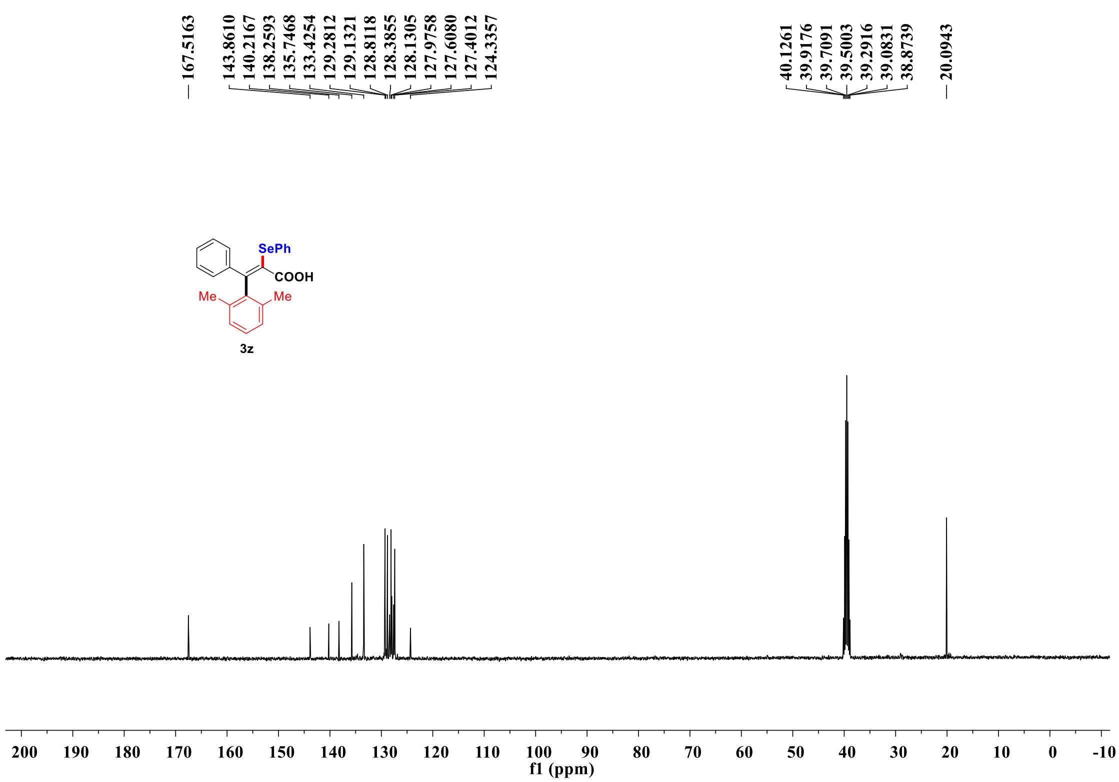
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127.4012
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39.0831
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COOH
Me
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3z
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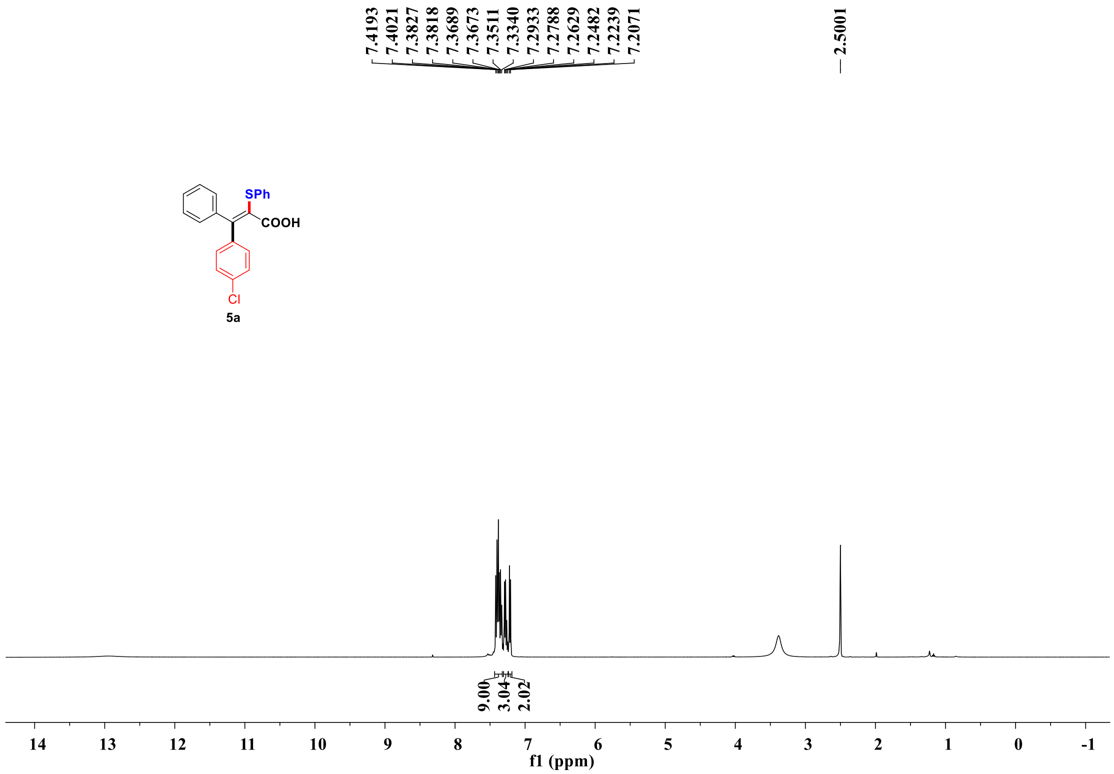
f1 (ppm)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7.2071
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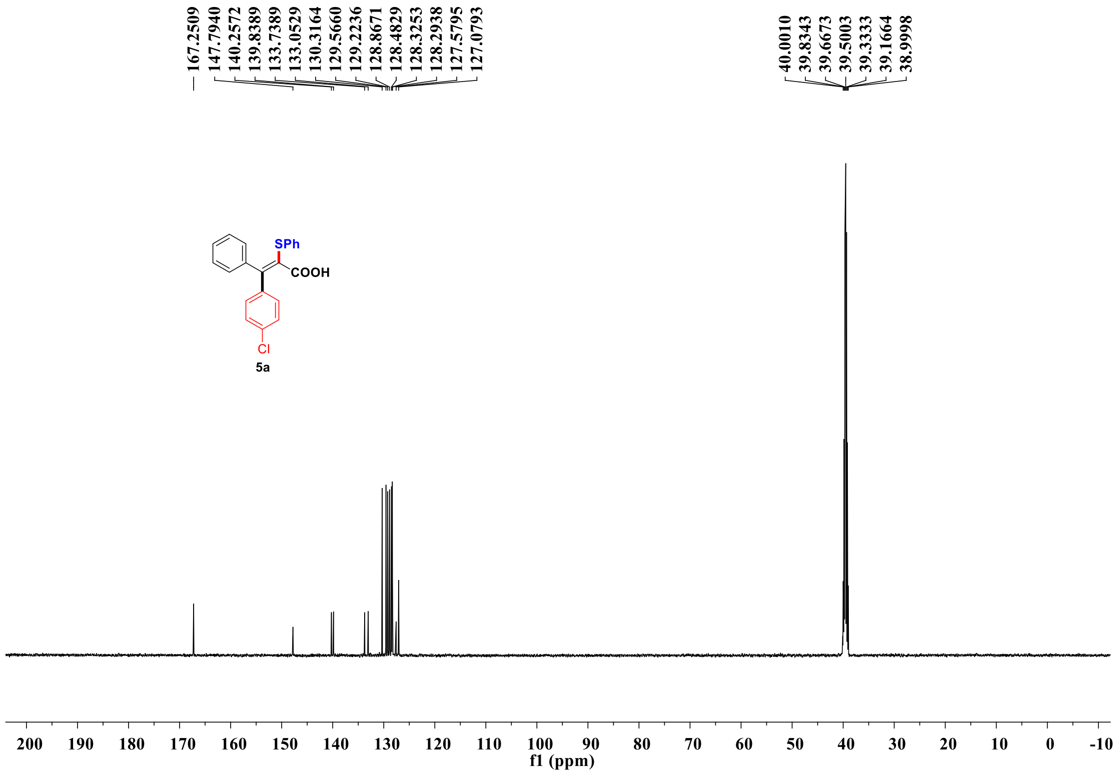
3.04
2.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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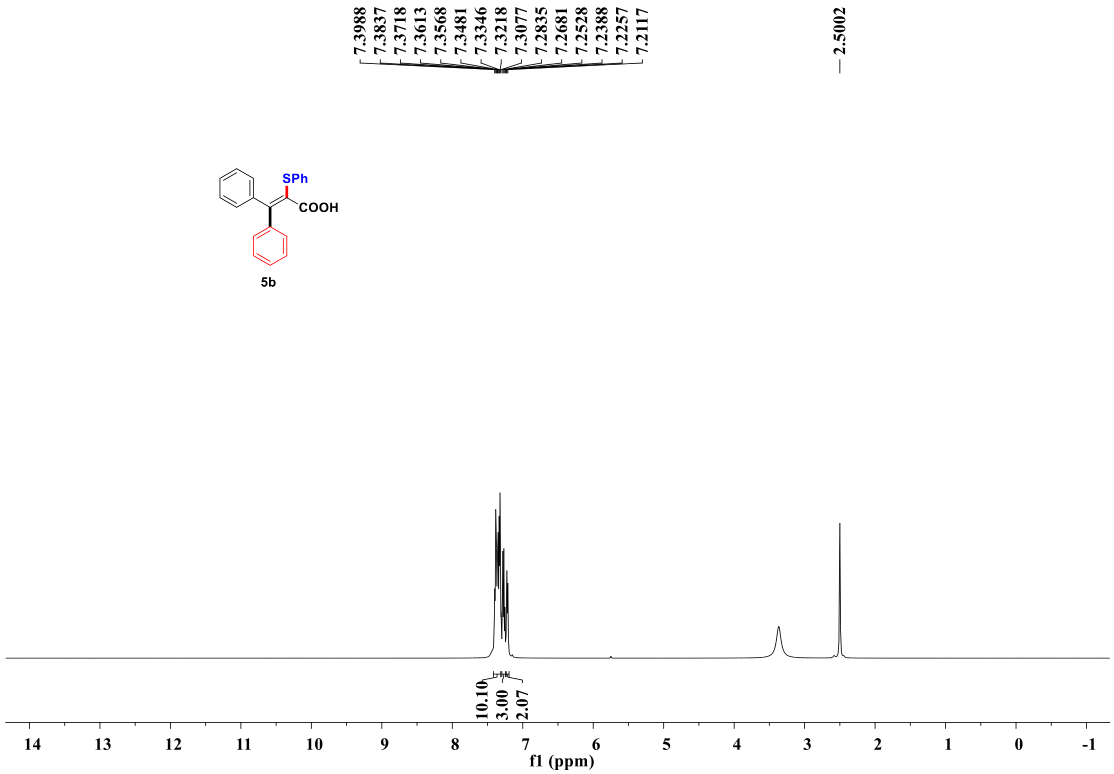
f1 (ppm)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7.2257
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3.00
2.07
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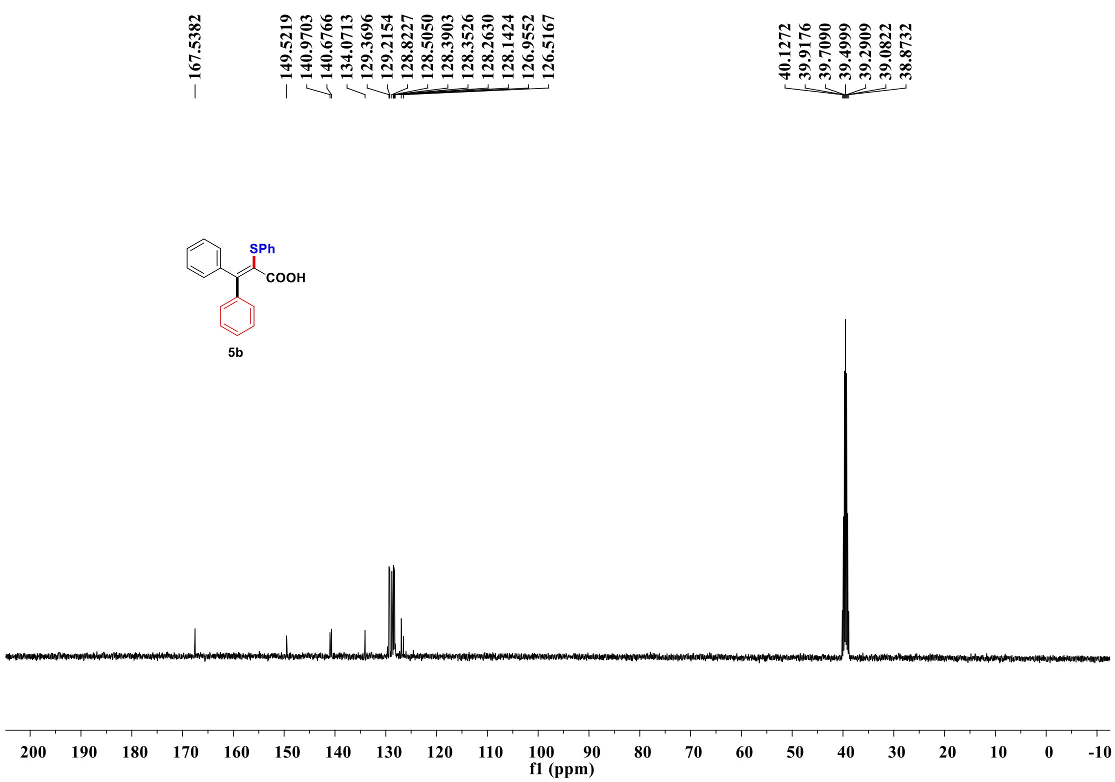
f1 (ppm)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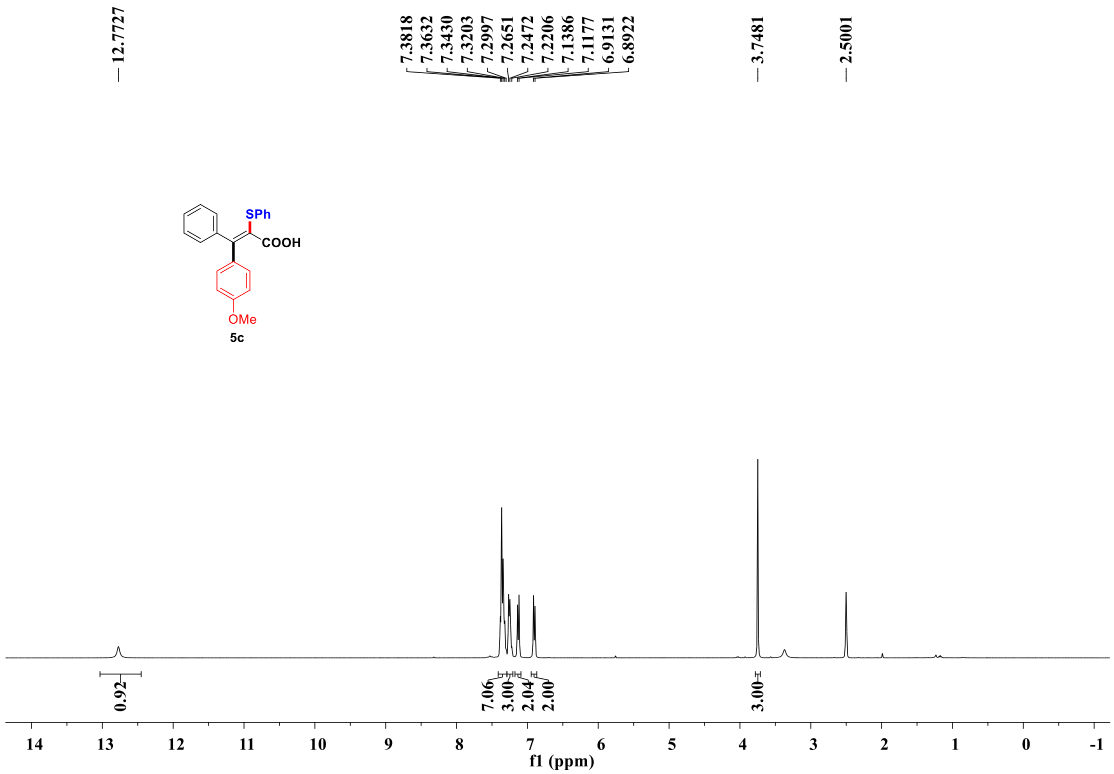

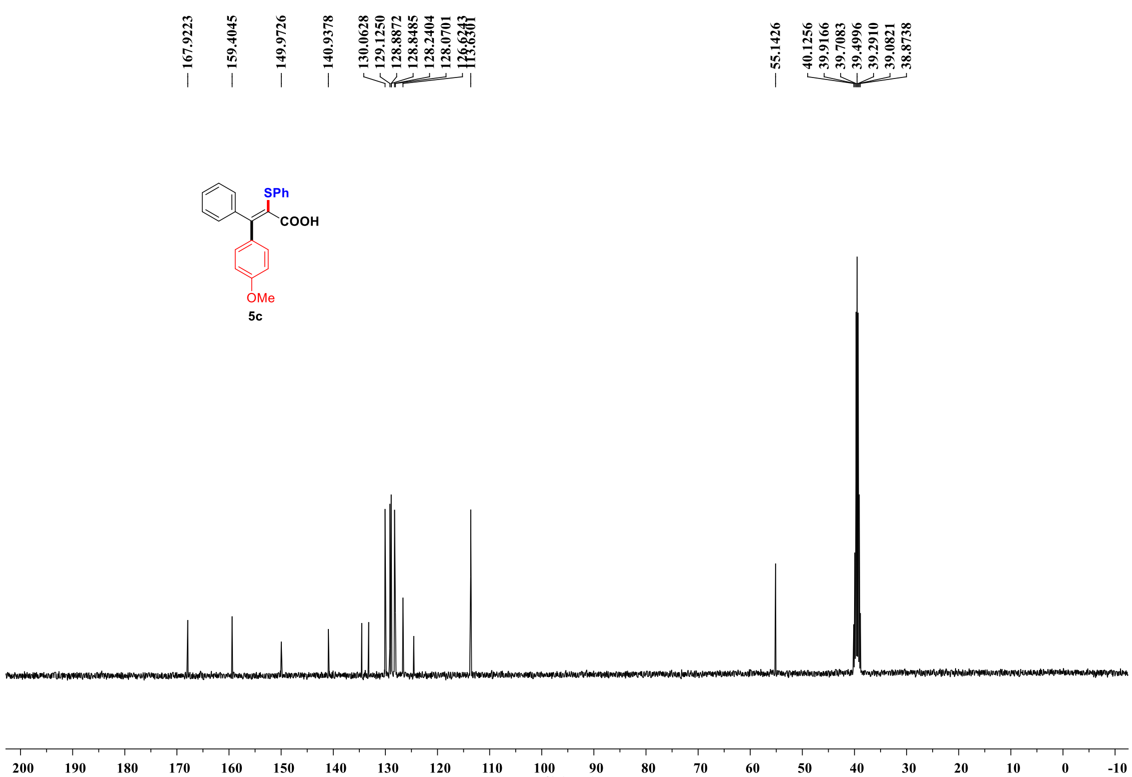

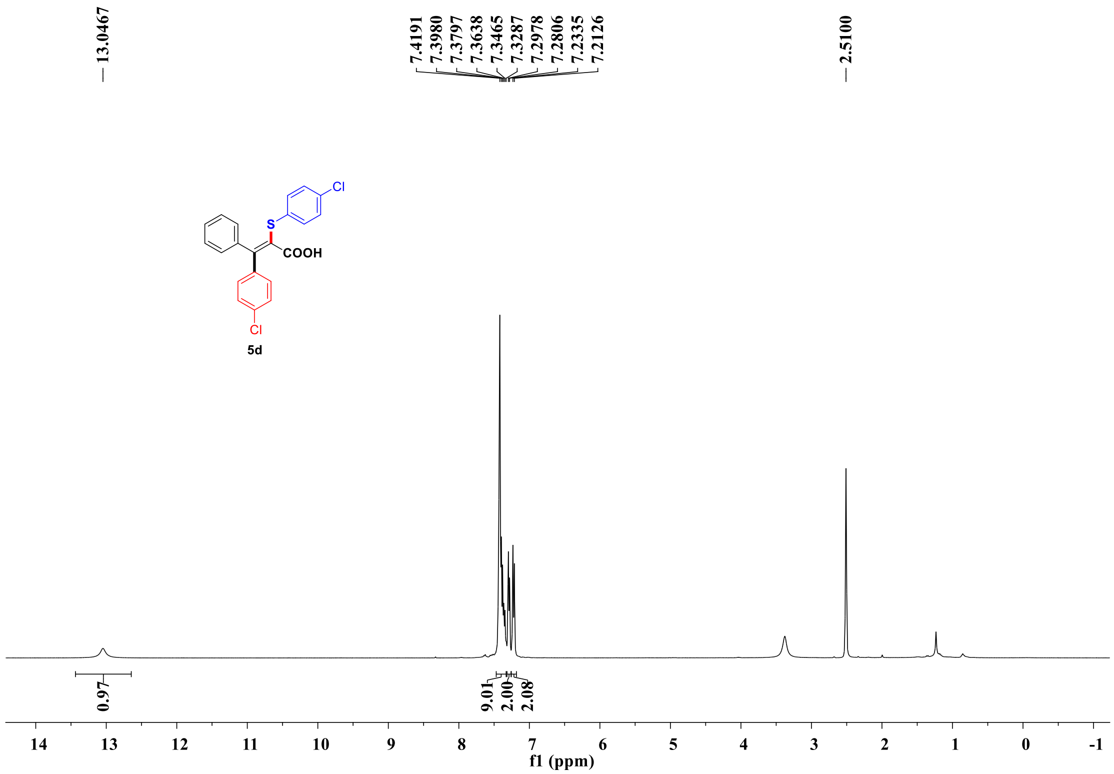
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Cl
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2.00
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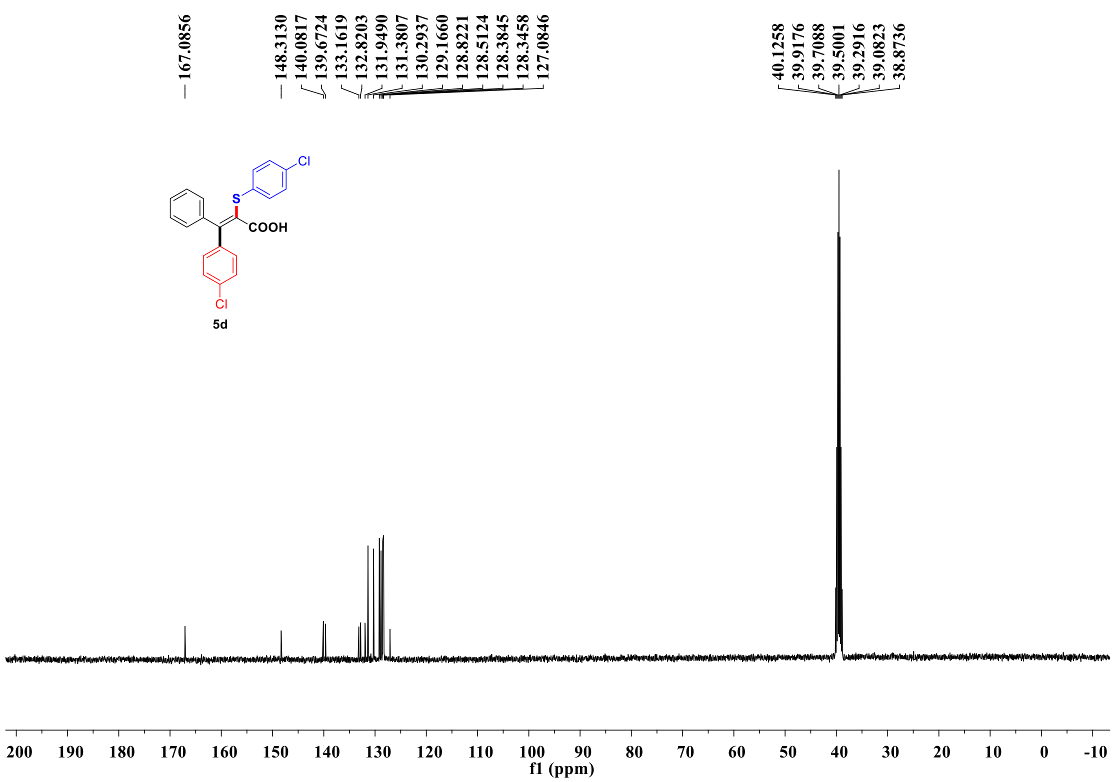
f1 (ppm)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128.3458
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40.1258
39.9176
39.7088
39.5001
39.2916
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Cl
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COOH
Cl
5d
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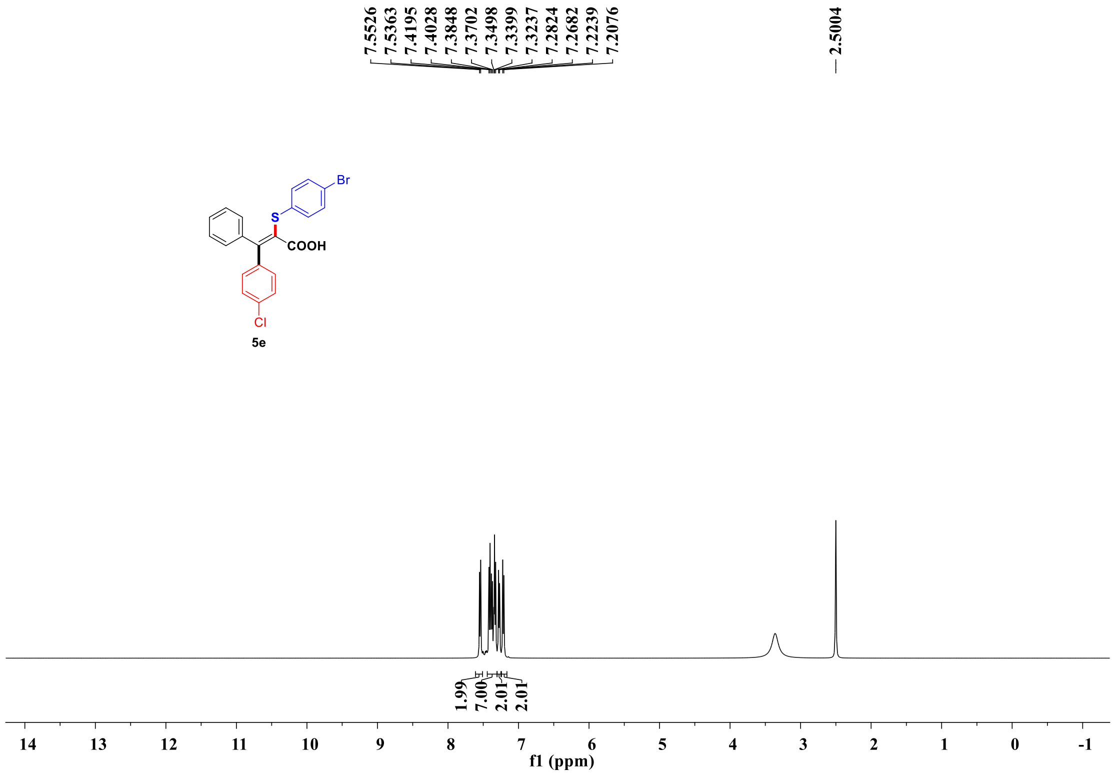
f1 (ppm)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Cl
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2.01
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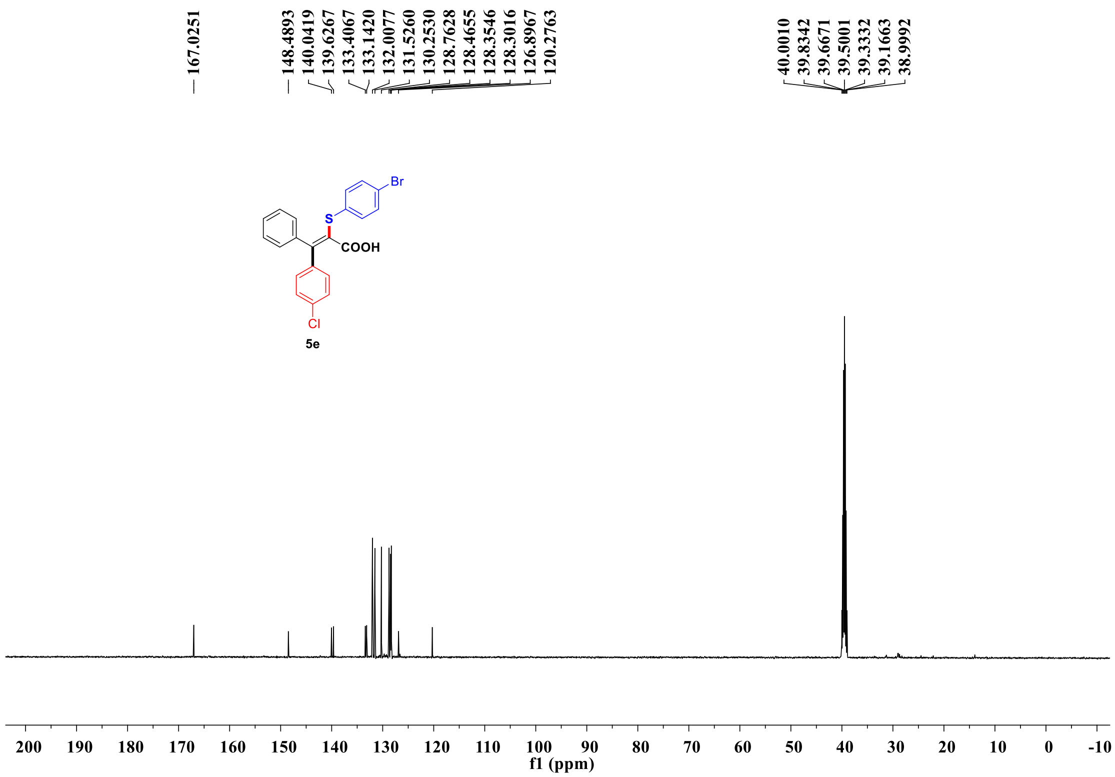
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Cl
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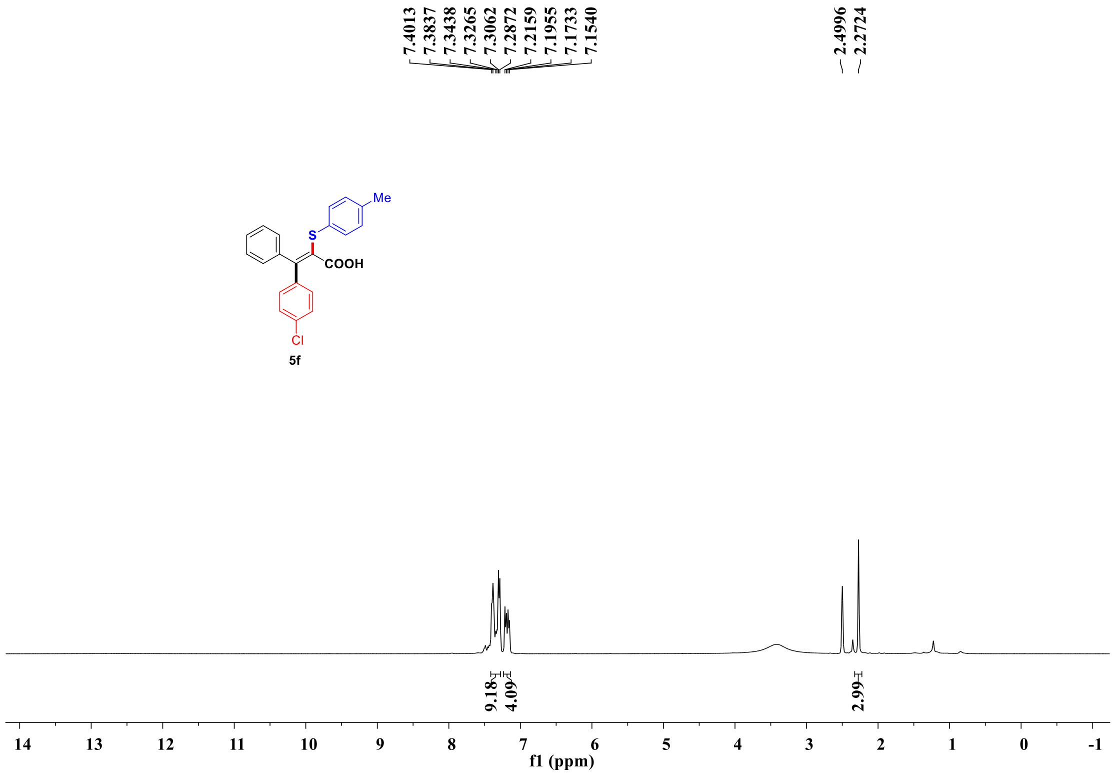
f1 (ppm)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2.4996
2.2724
Me
S
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Cl
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4.09
2.99
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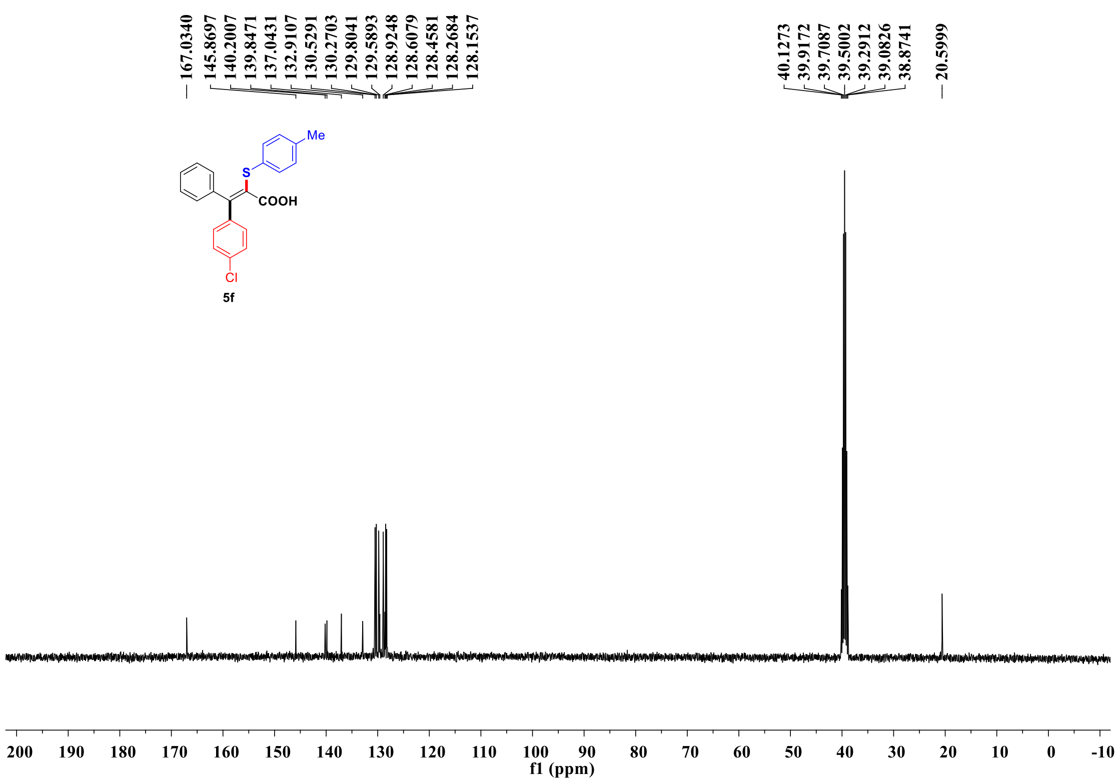
f1 (ppm)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39.0826
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Me
S
COOH
Cl
5f
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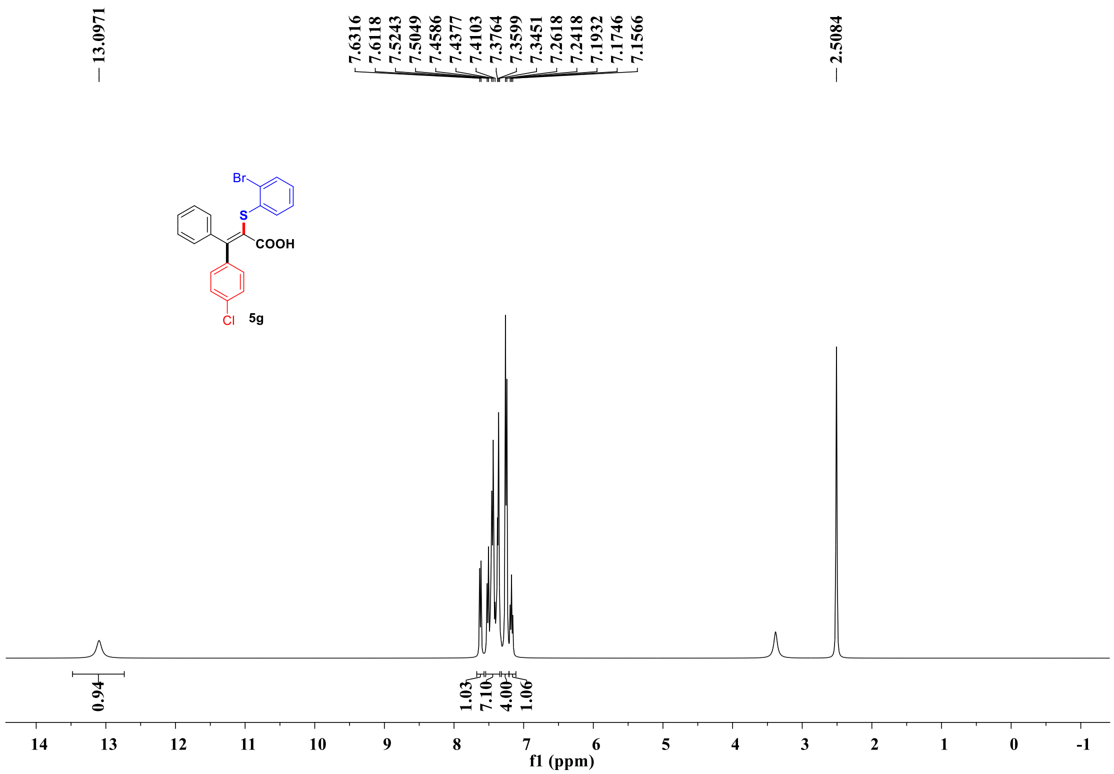
f1 (ppm)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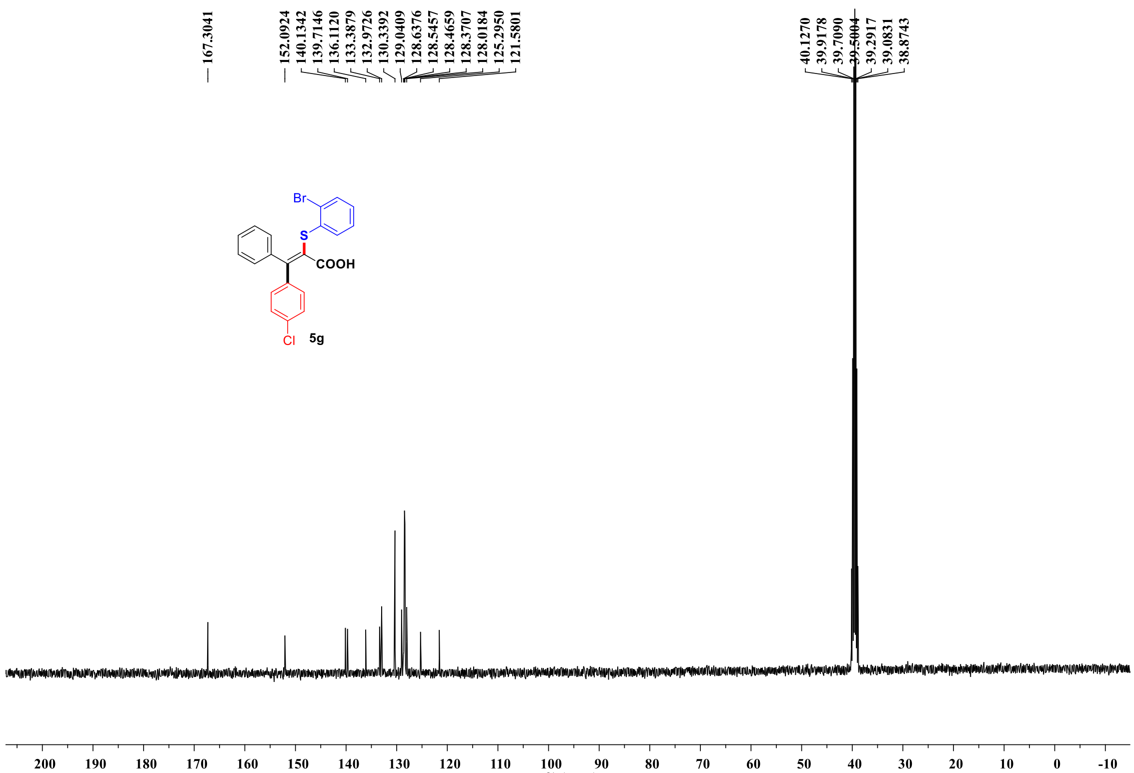
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S
COOH
Cl
5g
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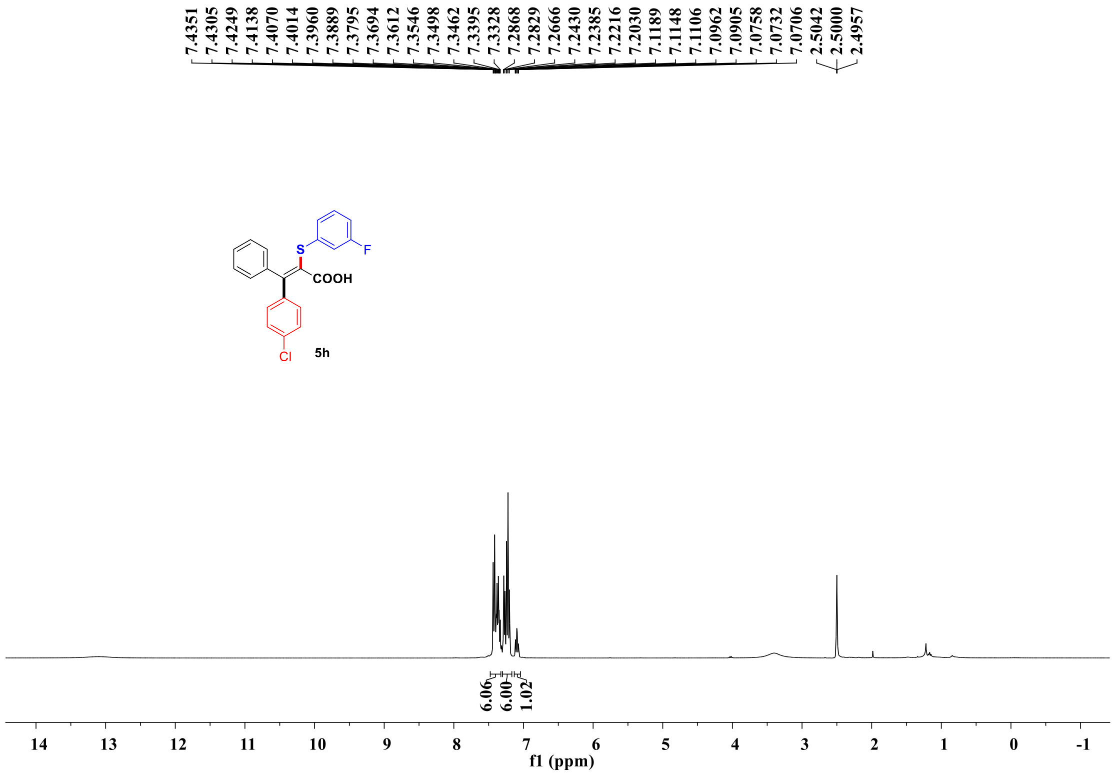
f1 (ppm)



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7.0706
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2.4957
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F
COOH
Cl
5h
6.06
6.00
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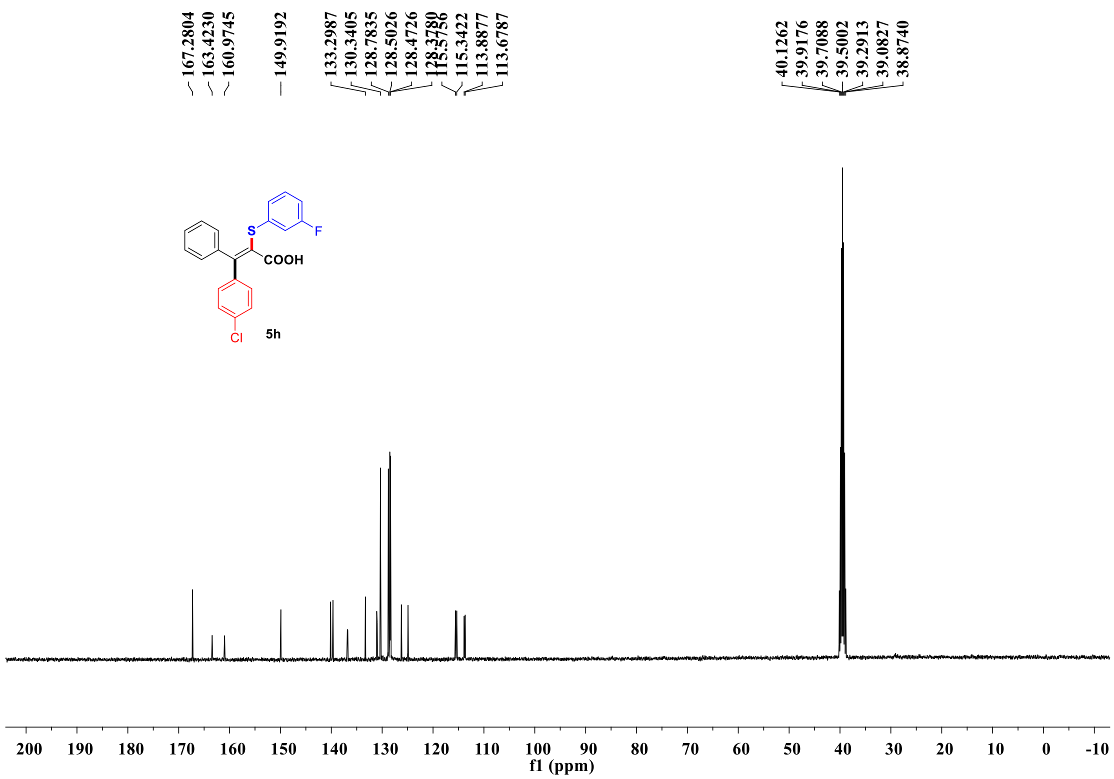

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F
COOH
Cl
5h
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190
180
170
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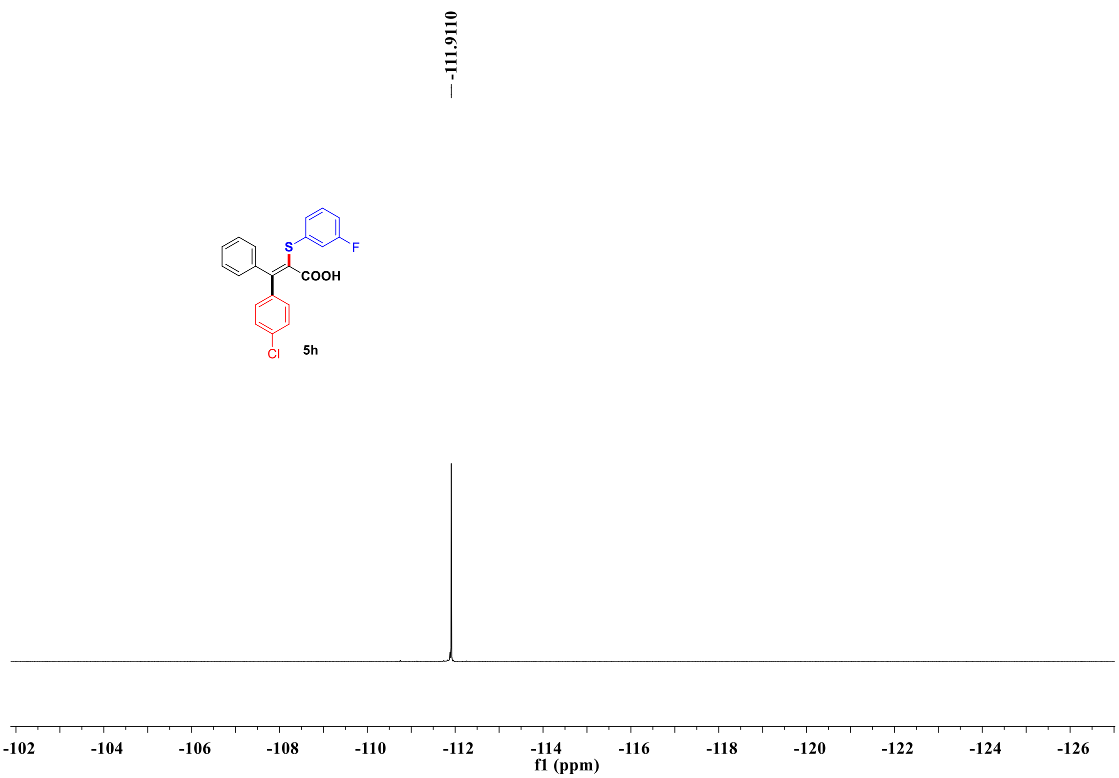
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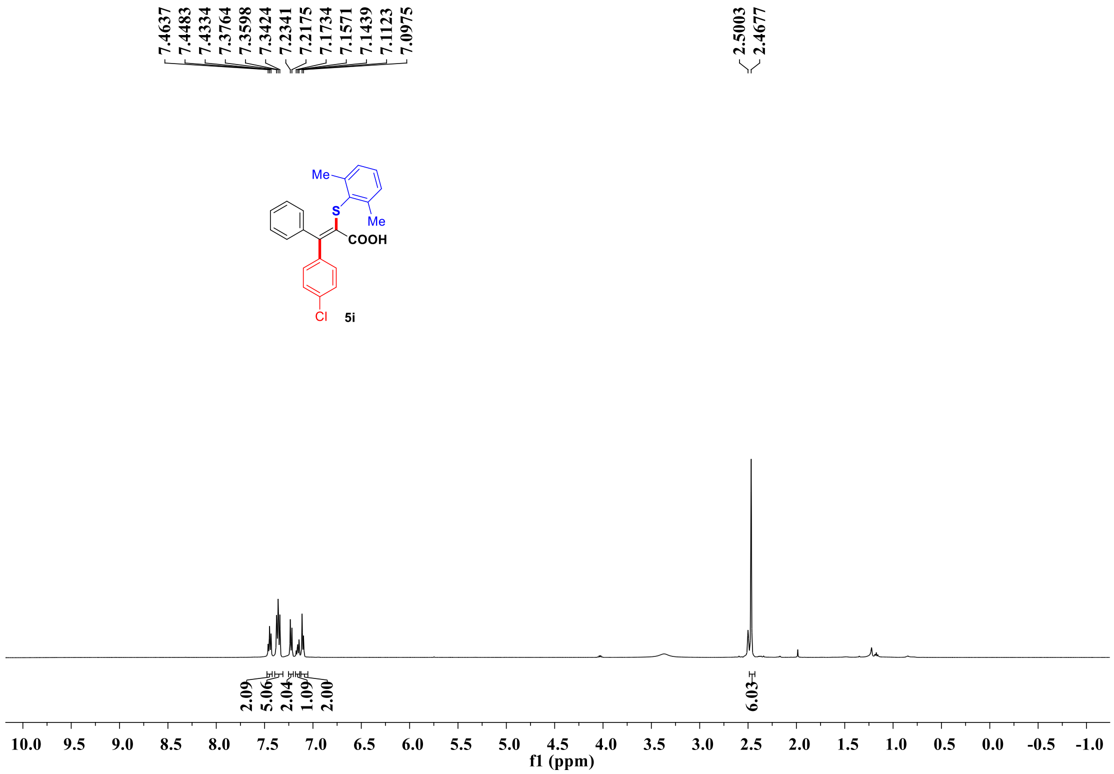
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2.04
1.09
2.00
6.03
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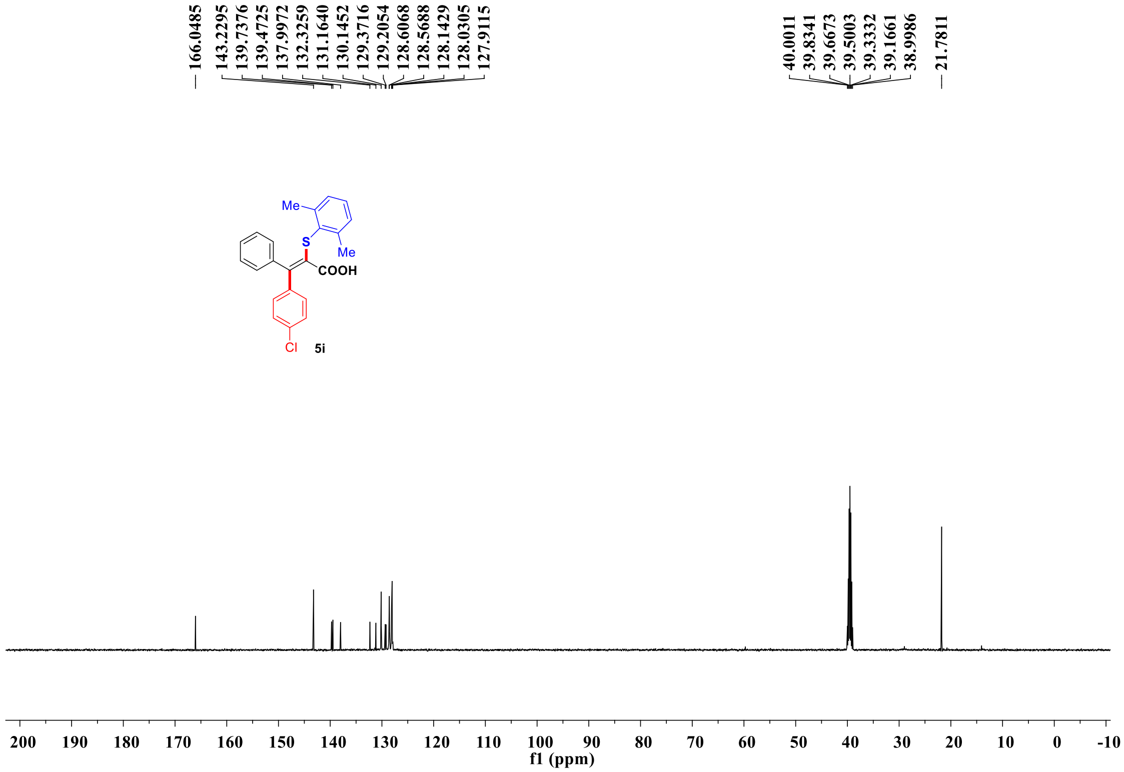
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Cl
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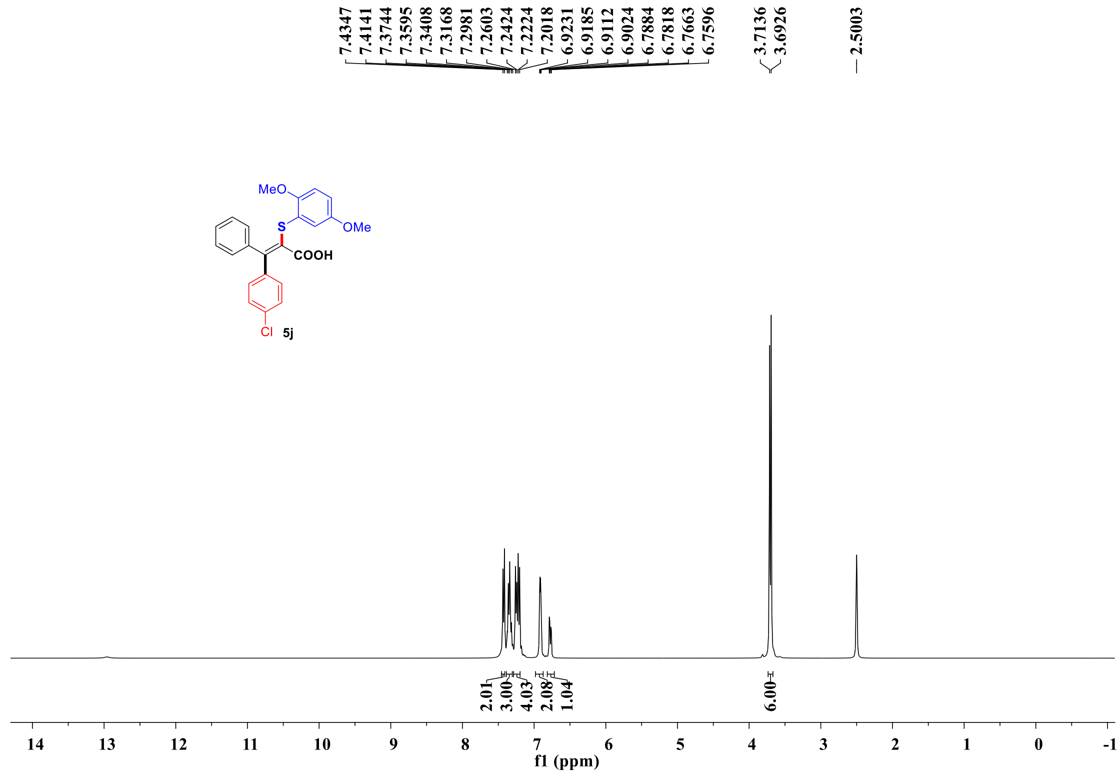
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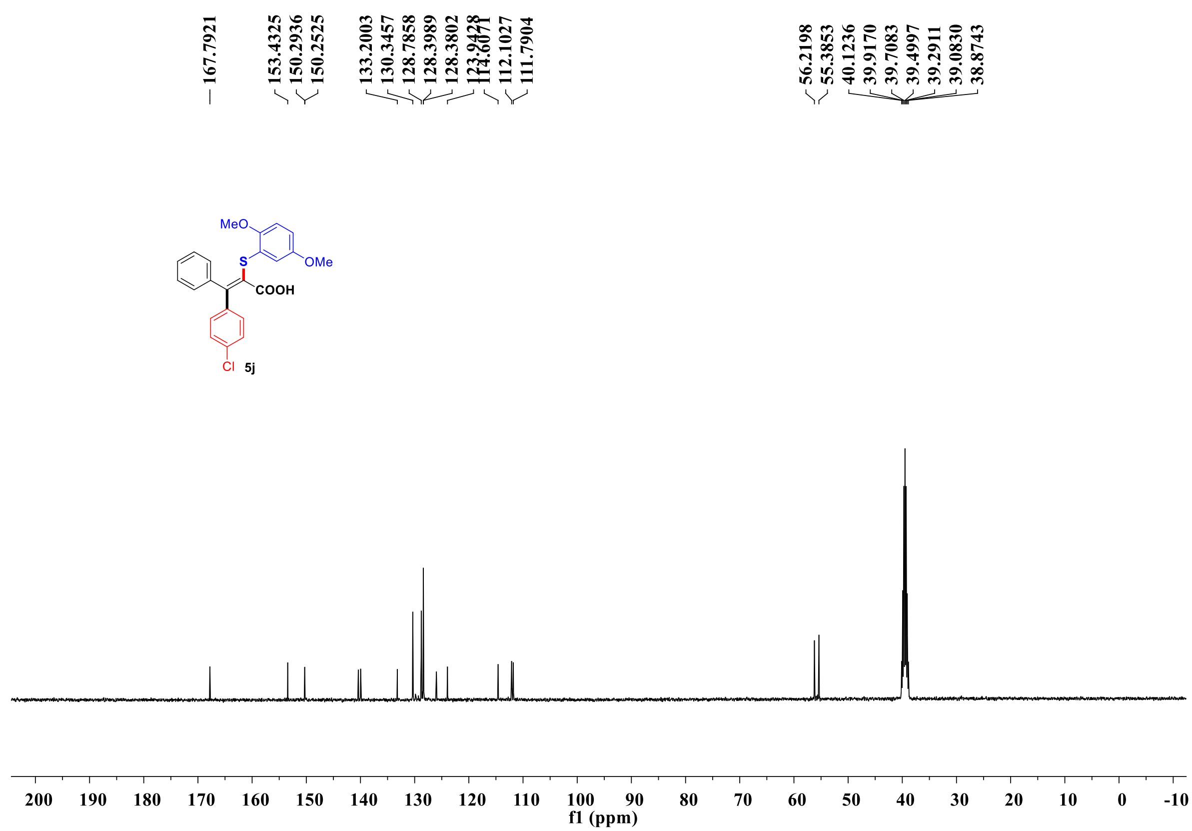
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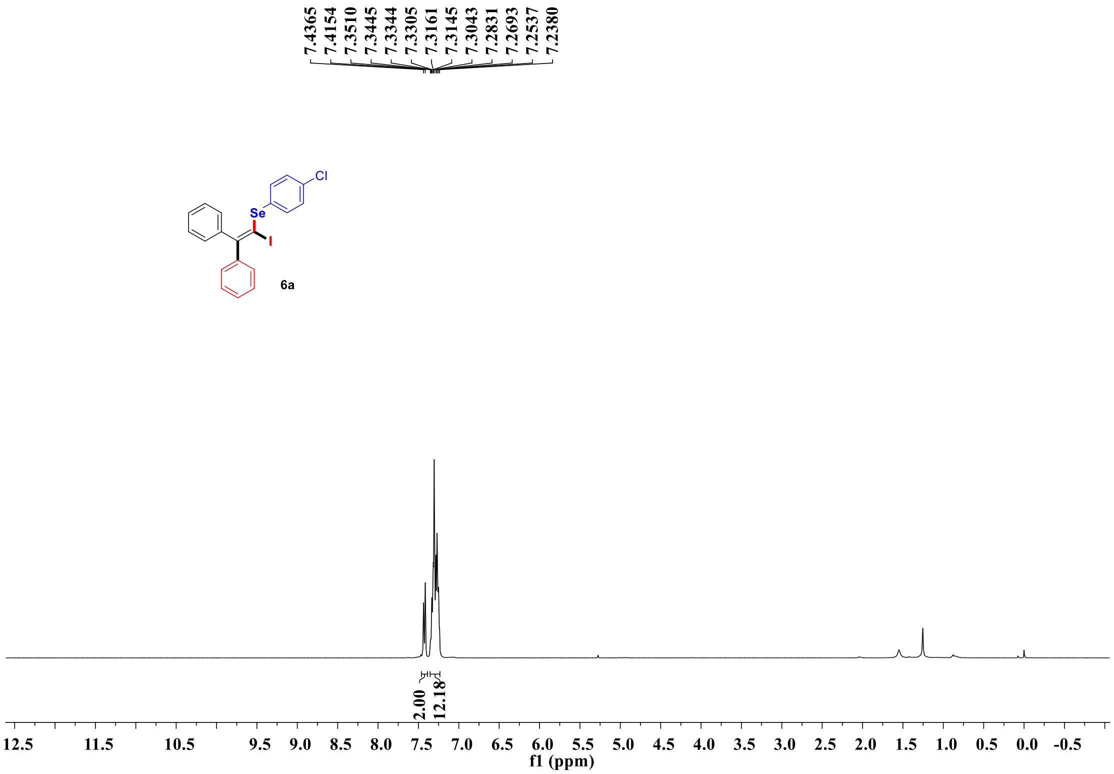
f1 (ppm)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Cl
Se
I
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2.00
12.18
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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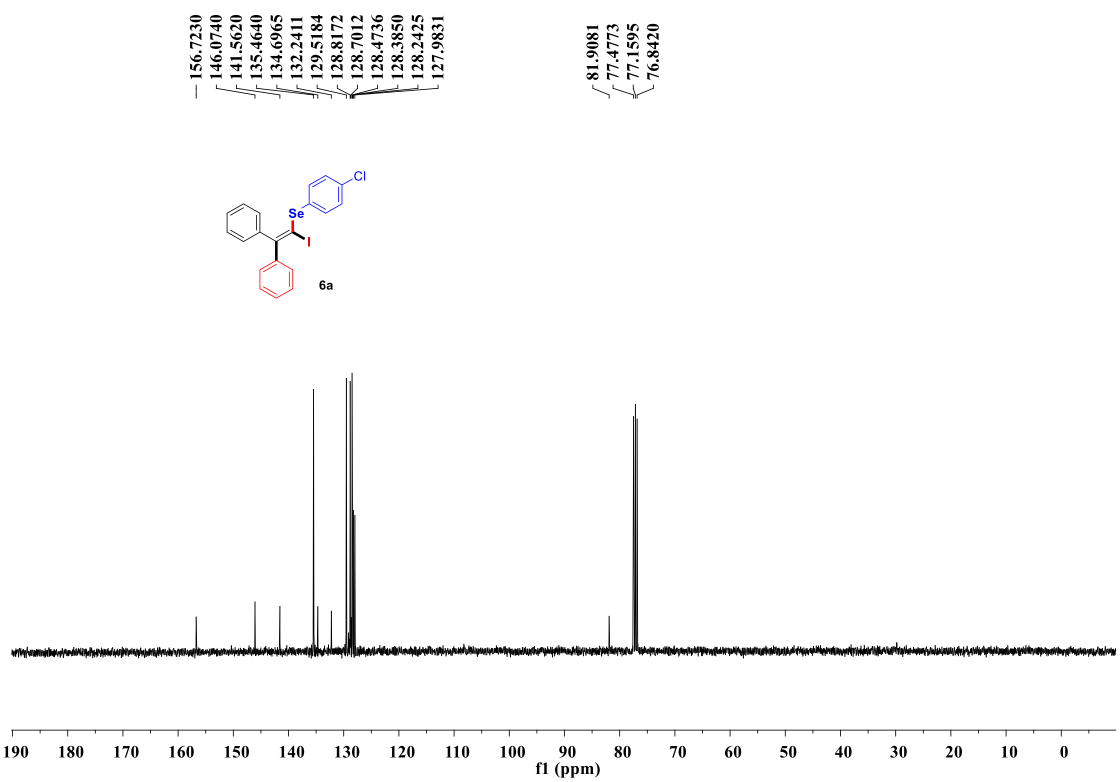
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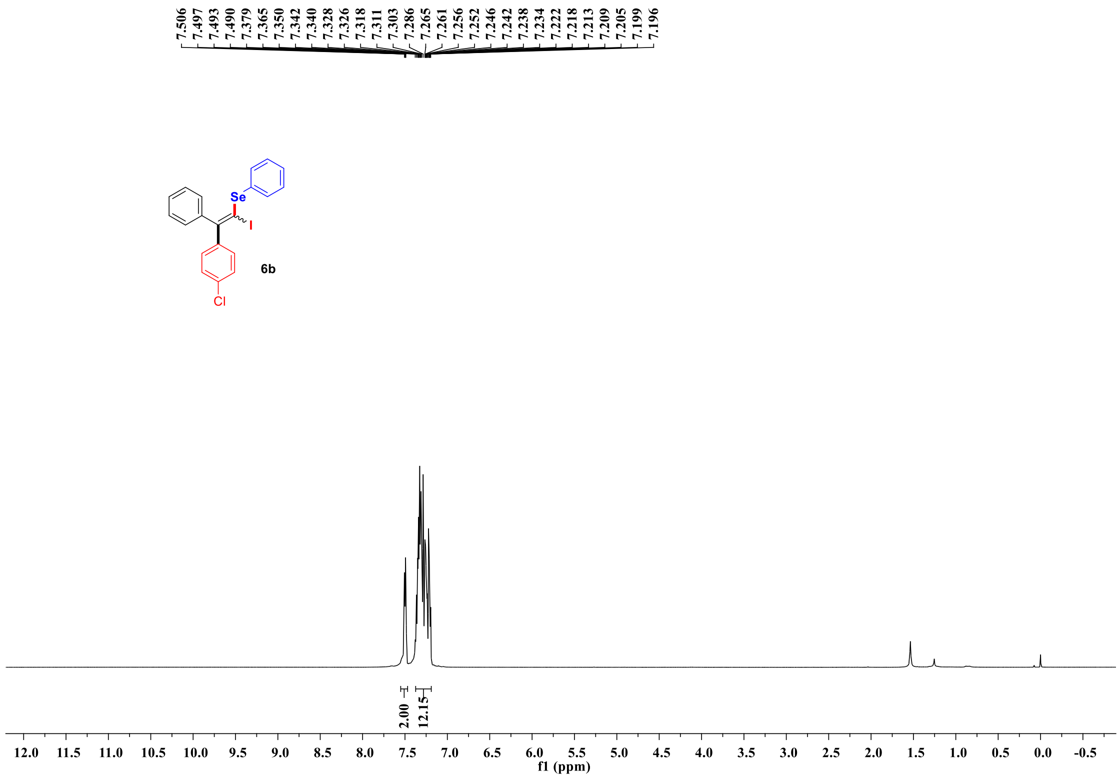
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I
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2.00
12.15
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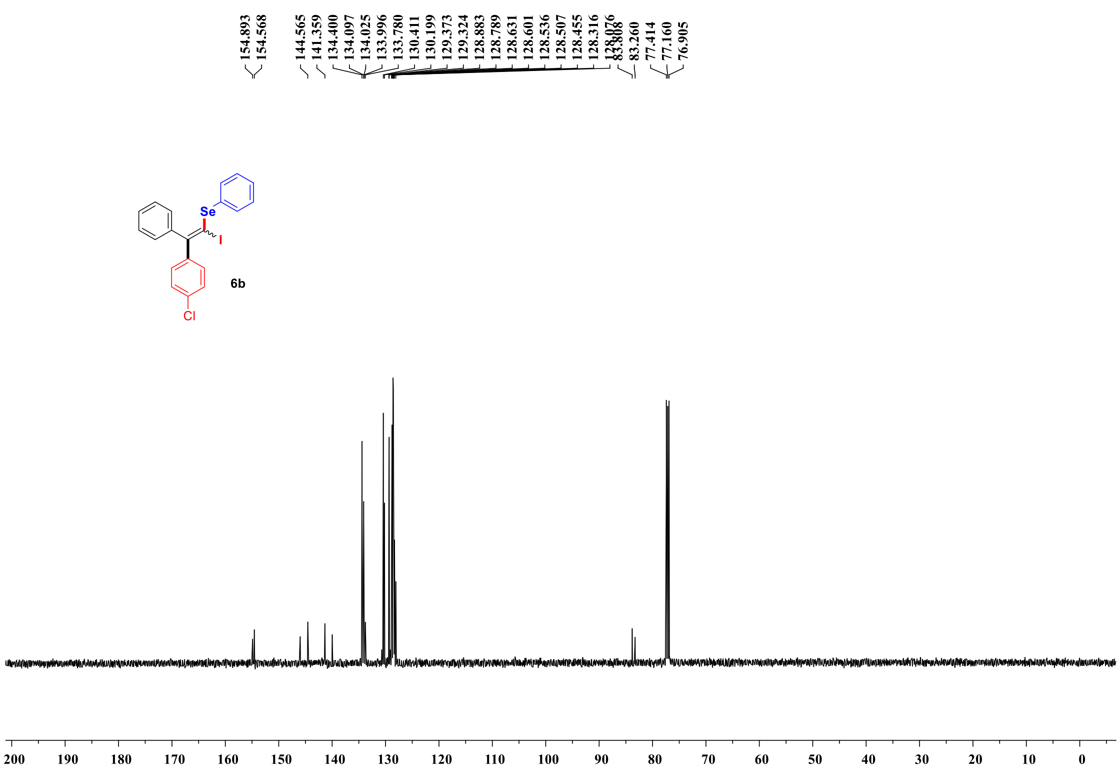
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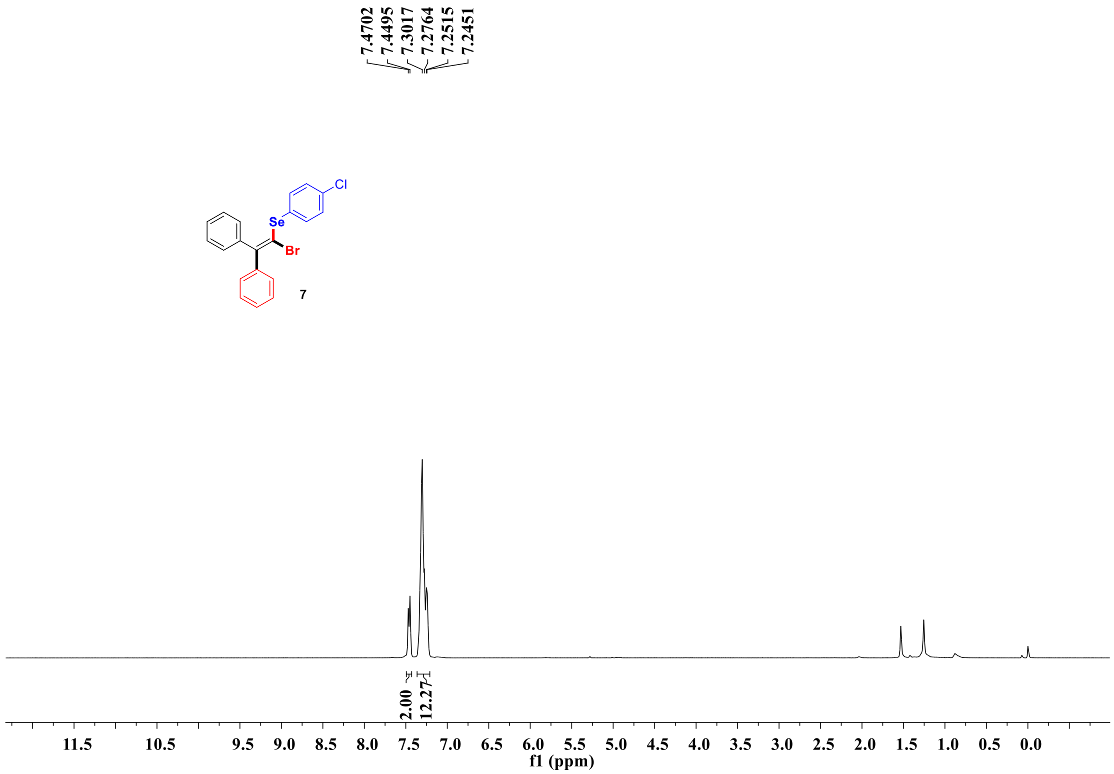
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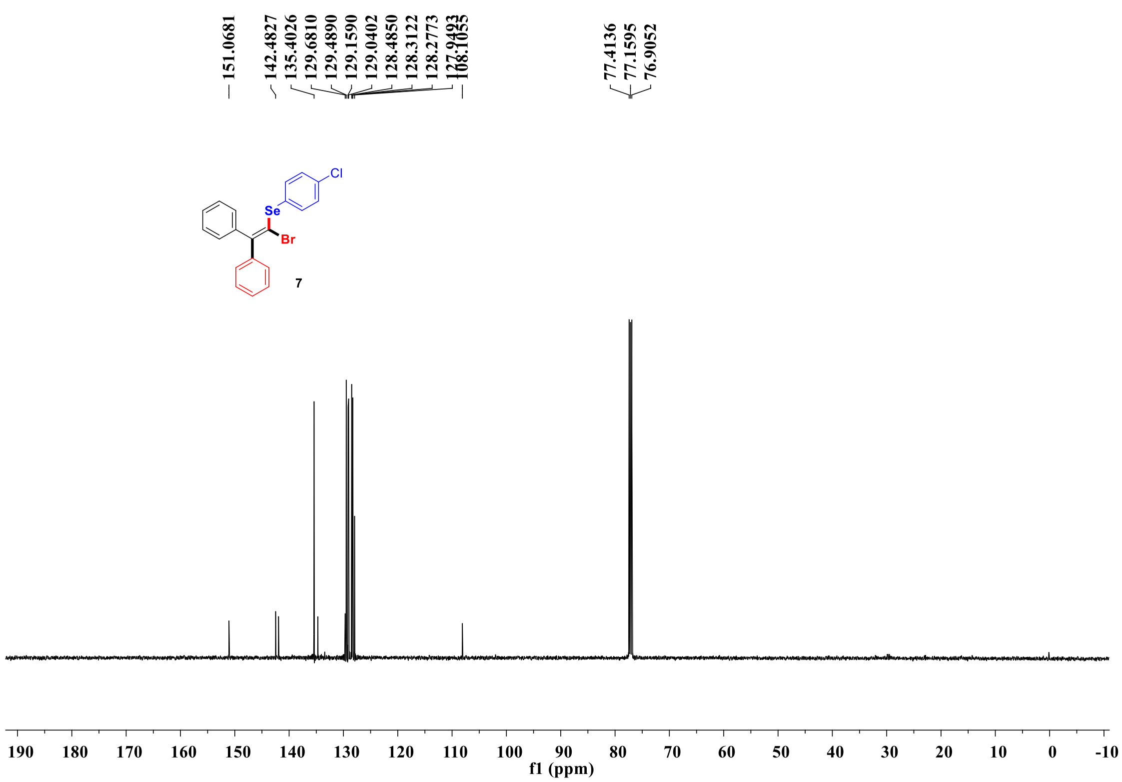
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Cl
Se
Br
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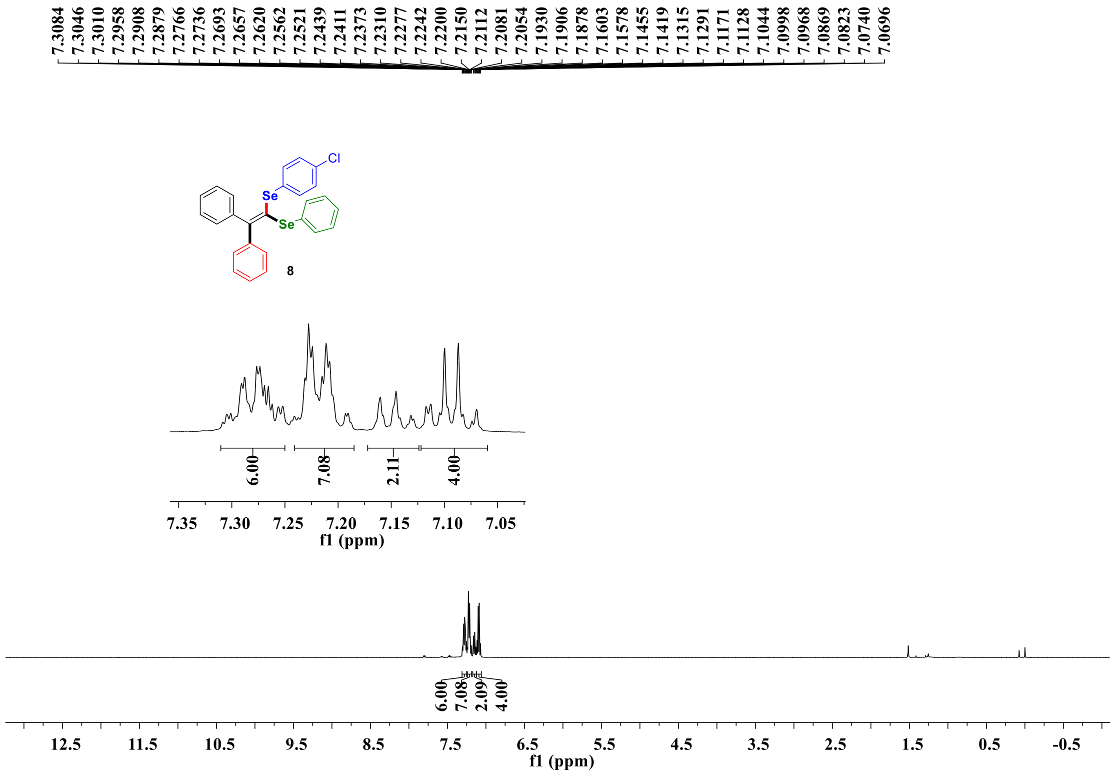
f1 (ppm)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7.0696
Se
Cl
Se
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7.08
2.11
4.00
7.35 7.30 7.25 7.20 7.15 7.10 7.05
f1 (ppm)
6.00
7.08
2.09
4.00
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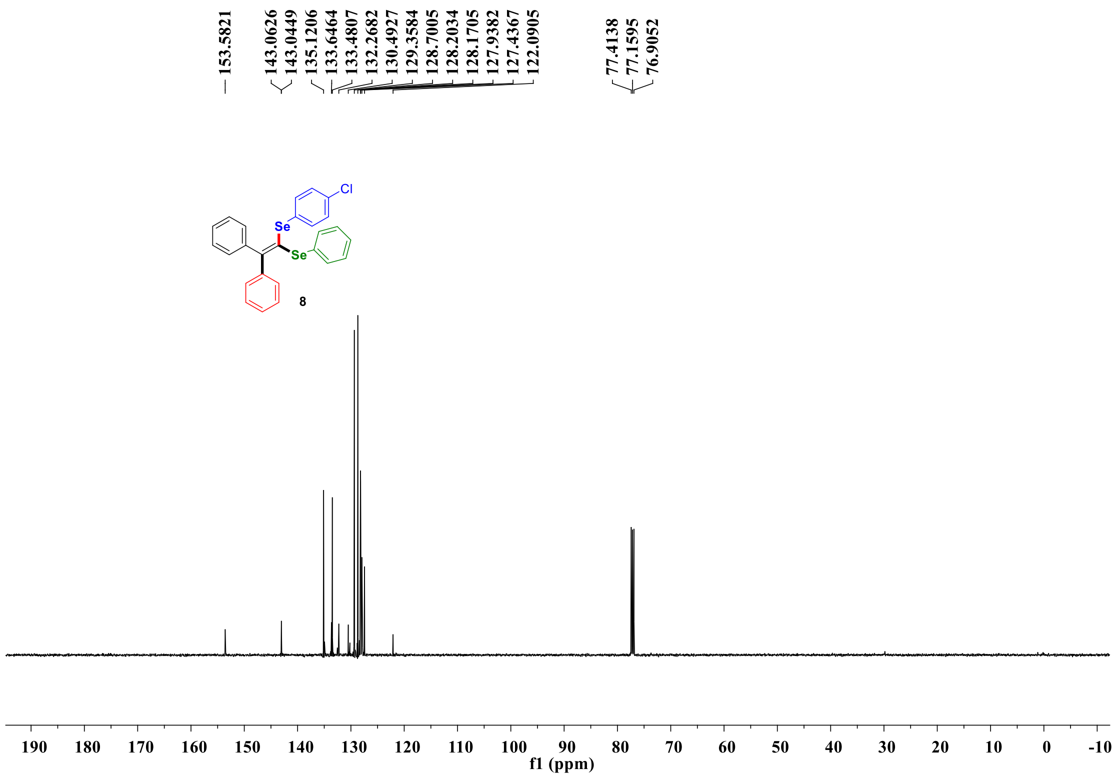
f1 (ppm)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128.2034
128.1705
127.9382
127.4367
122.0905
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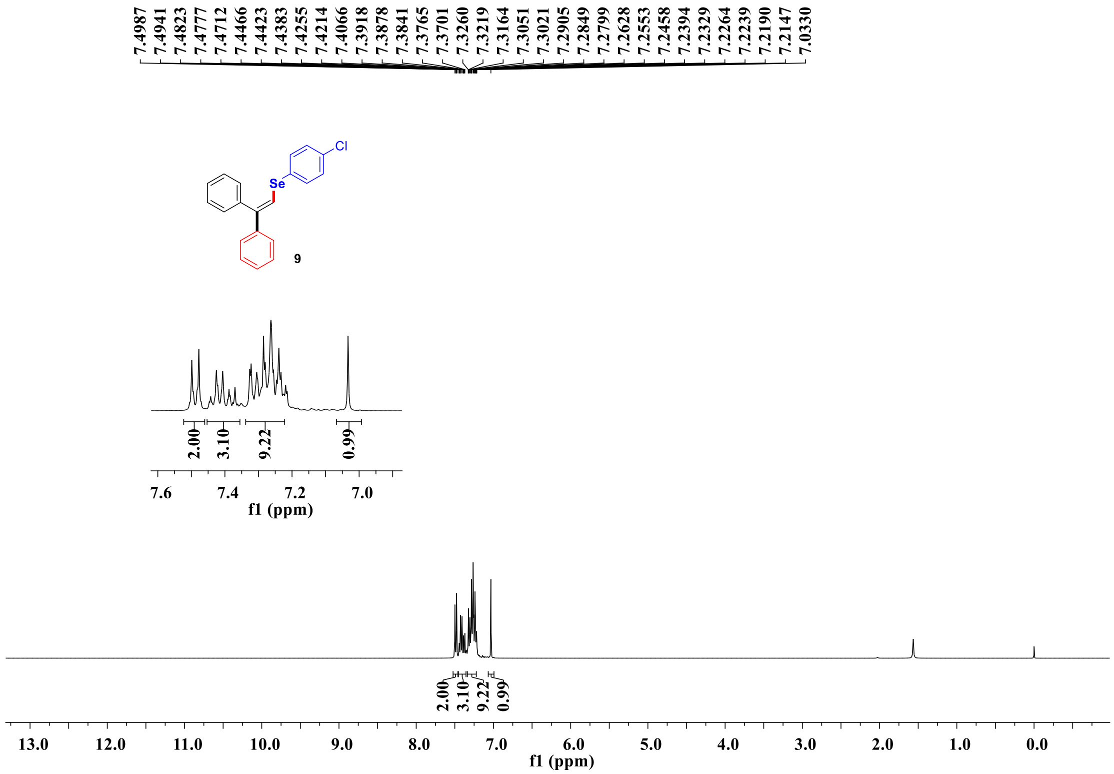
76.9052
Se
Cl
Se
8
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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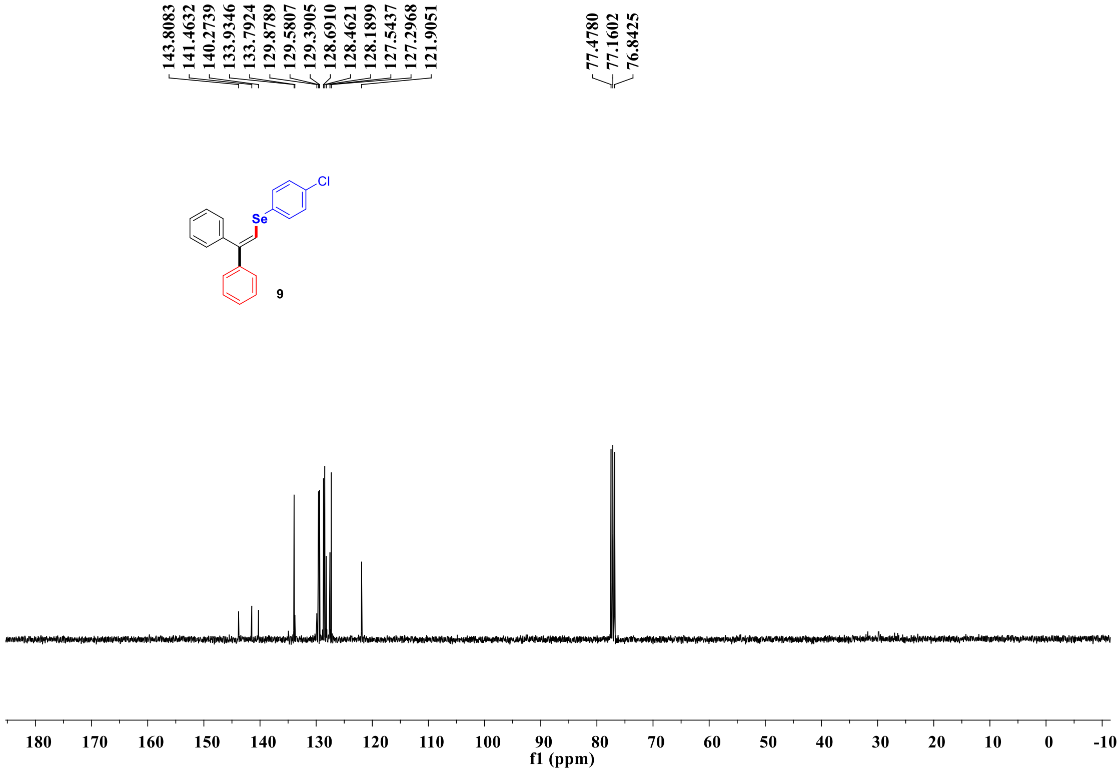
7.4066
7.3918
7.3878
7.3841
7.3765
7.3701
7.3260
7.3219
7.3164
7.3051
7.3021
7.2905
7.2849
7.2799
7.2628
7.2553
7.2458
7.2394
7.2329
7.2264
7.2239
7.2190
7.2147
7.0330
Se
Cl
9
2.00
3.10
9.22
0.99
7.6
7.4
7.2
7.0
f1 (ppm)
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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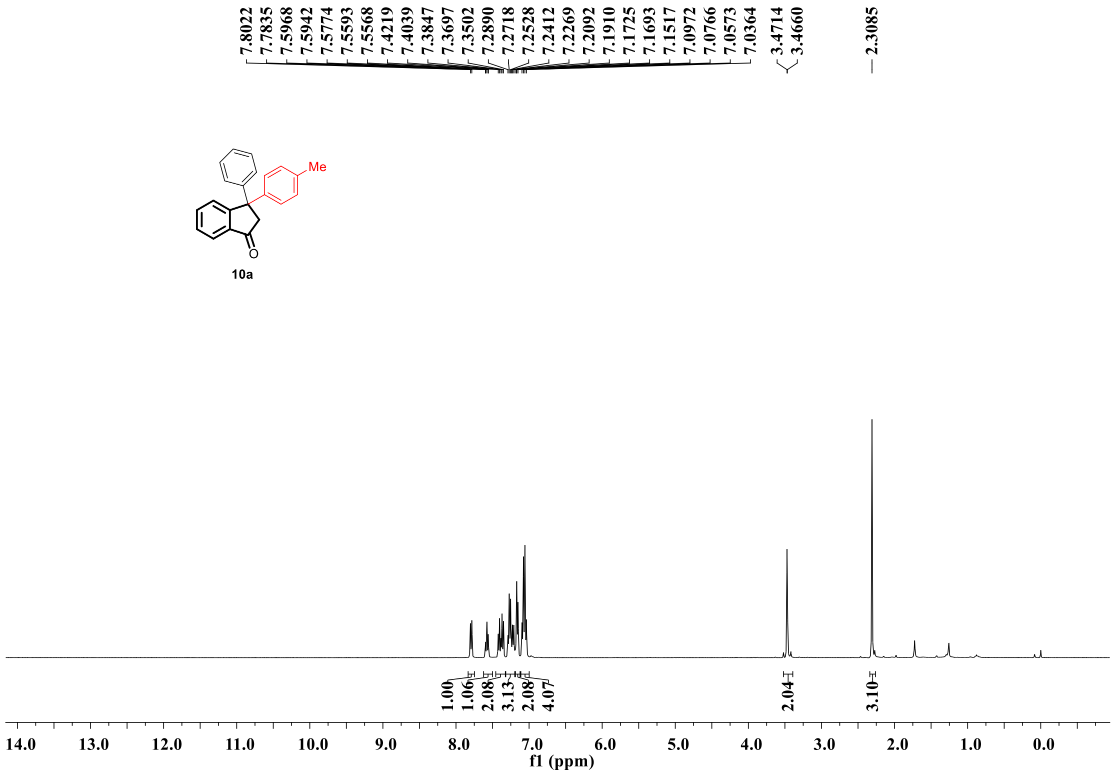
127.5437
127.2968
121.9051
77.4780
77.1602
76.8425
Se
Cl
9
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.3697
7.3502
7.2890
7.2718
7.2528
7.2412
7.2269
7.2092
7.1910
7.1725
7.1693
7.1517
7.0972
7.0766
7.0573
7.0364
3.4714
3.4660
2.3085
Me
10a
1.00
1.06
2.08
3.13
2.08
4.07
2.04
3.10
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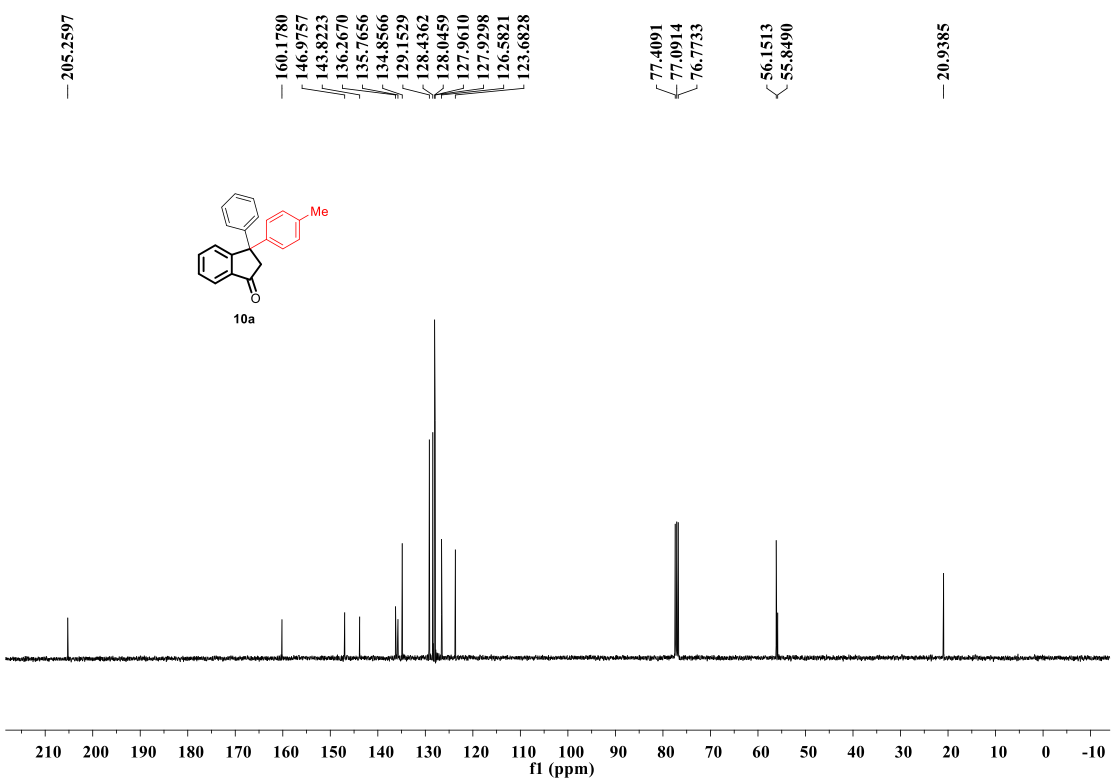
f1 (ppm)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127.9610
127.9298
126.5821
123.6828
77.4091
77.0914
76.7733
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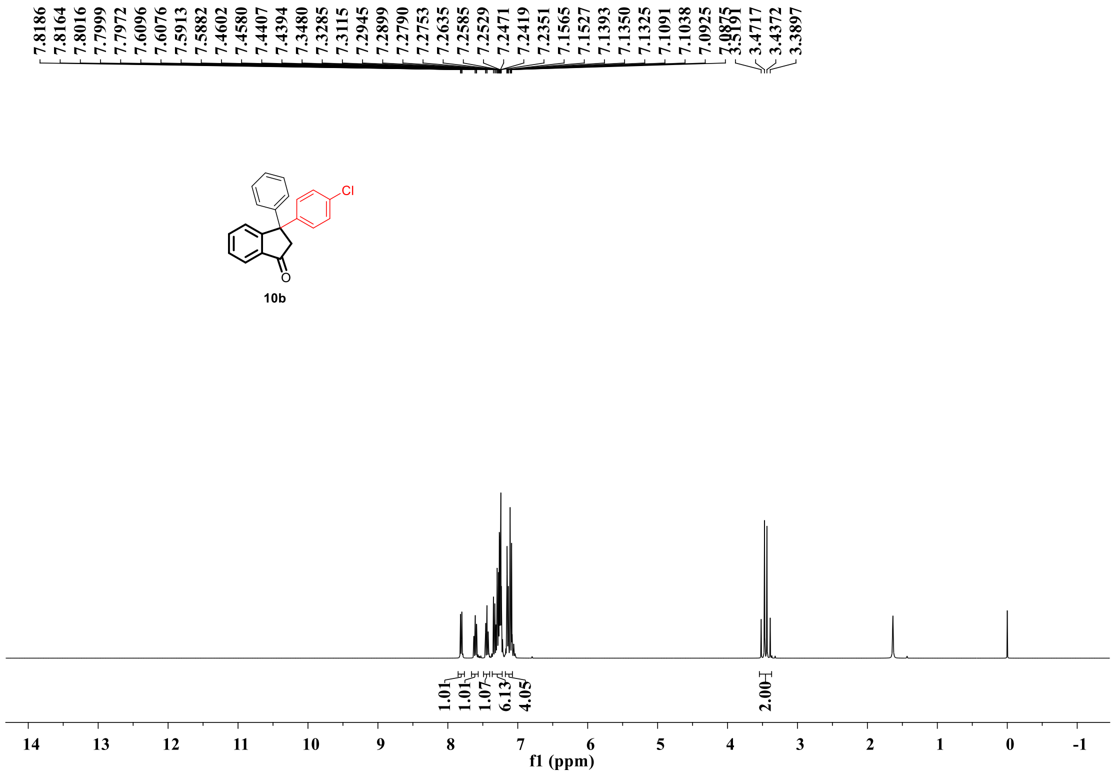
Me
10a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.6076
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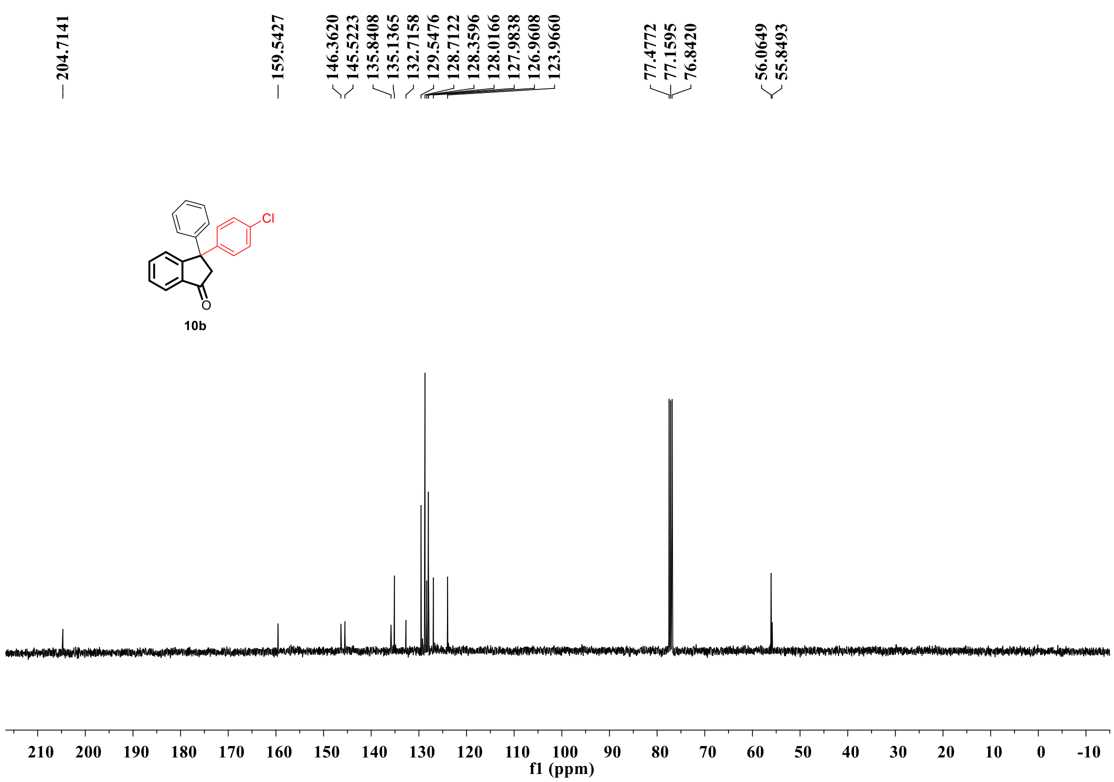
7.4580
7.4407
7.4394
7.3480
7.3285
7.3115
7.2945
7.2899
7.2790
7.2753
7.2635
7.2585
7.2529
7.2471
7.2419
7.2351
7.1565
7.1527
7.1393
7.1350
7.1325
7.1091
7.1038
7.0925
7.0875
3.5191
3.4717
3.4372
3.3897
Cl
O
10b
1.01
1.01
1.07
6.13
4.05
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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135.8408
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128.7122
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128.0166
127.9838
126.9608
123.9660
77.4772
77.1595
76.8420
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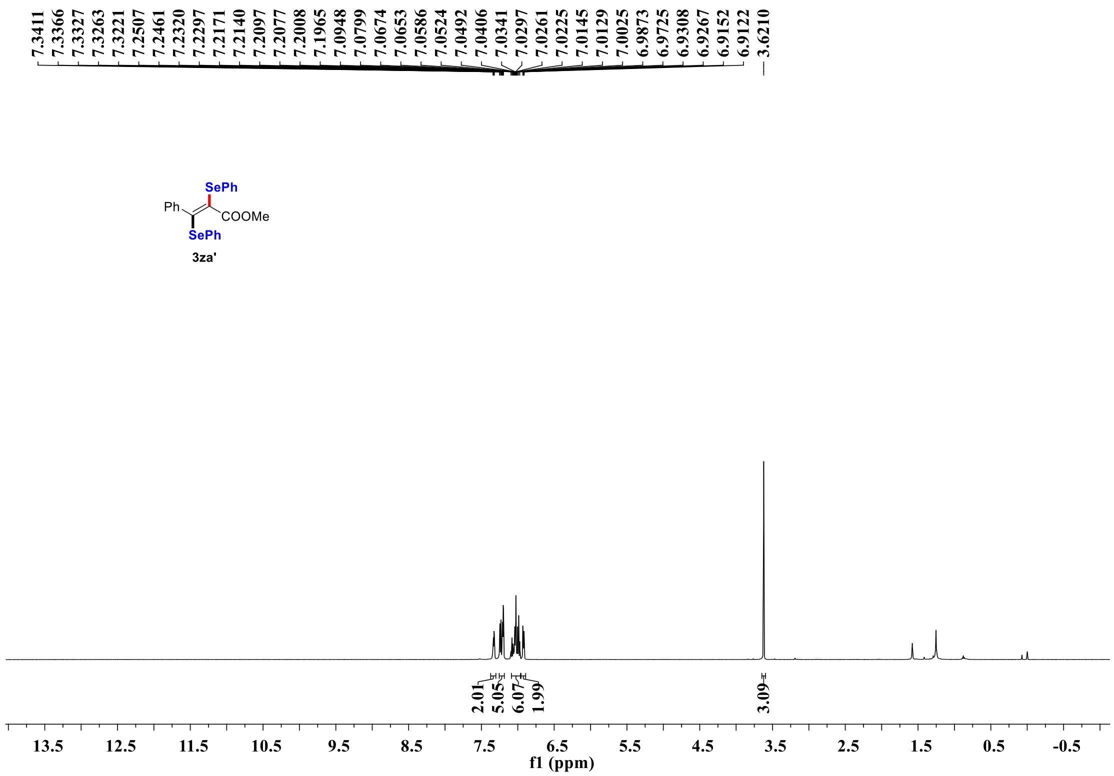
55.8493
Cl
O
10b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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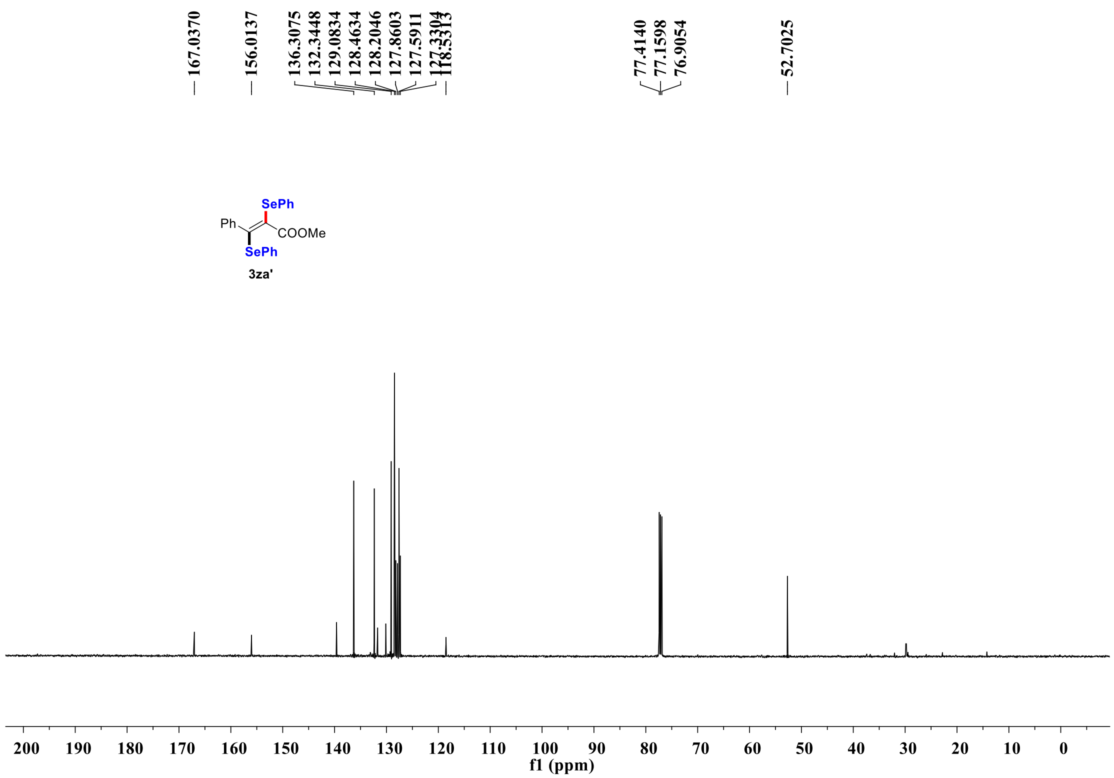
7.2297
7.2171
7.2140
7.2097
7.2077
7.2008
7.1965
7.0948
7.0799
7.0674
7.0653
7.0586
7.0524
7.0492
7.0406
7.0341
7.0297
7.0261
7.0225
7.0145
7.0129
7.0025
6.9873
6.9725
6.9308
6.9267
6.9152
6.9122
3.6210
SePh
Ph
COOMe
SePh
3za'
2.01
5.05
6.07
1.99
3.09
13.5 12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)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127.5911
127.3304
118.5313
77.4140
77.1598
76.9054
52.7025
SePh
Ph
COOMe
SePh
3za'
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)