Ruthenium Catalyzed Dolye-Kirmse Rearrangement Reaction of Sulfoxonium Ylides with Sulfides or Selenides

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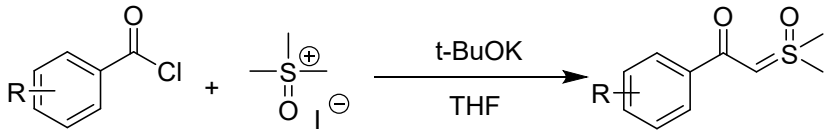
1. General information

Unless noted, all reactions were carried out in flame-dried glassware with magnetic stirring under an atmosphere of air. Solvents used were of analytical purity. All the reactions were monitored by thinlayer chromatography (TLC) and were visualized using UV light. The product purification was done using silica gel column chromatography. Thin-layer chromatography (TLC) characterization was performed with precoated silica gel GF254 (0.2 mm), while column chromatography characterization was performed with silica gel (100-200 mesh). NMR spectra were recorded on a Varian spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C and 376 MHz for ^{19}F). Chemical shifts are reported in δ ppm referenced to an internal SiMe4 standard for ^{1}H NMR and chloroform-d (δ 77.16) for ^{13}C NMR. Coupling constants were given in Hz. HRMS spectra were recorded on a Waters Q-TOF Premier.

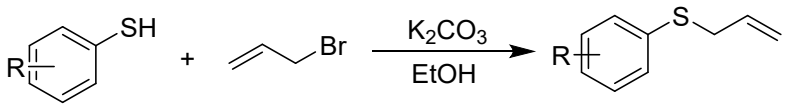
2. Experimental section

2.1. Preparation of sulfoxonium ylide[1]



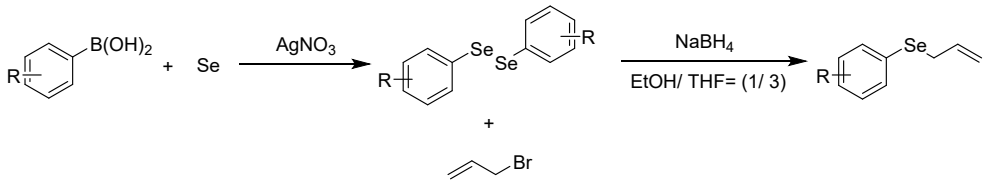
Under N_2, trimethylsulfoxonium iodide (42.7 mmol, 3.0 equiv) was suspended in dry THF (50 mL) in a flame-dried round bottom flask that was protected from light with aluminium foil. Potassium tert-butoxide (42.7 mmol, 3.0 equiv) was added and the mixture was stirred at reflux for 2 hours. After cooling to 0 °C, benzoyl chloride (14 mmol, 1.0 equiv) in THF (10 mL) was added dropwise to the mixture via a dropping funnel. After stirring at room temperature for 4 hour, the mixture was filtered through a plug of celite (elution DCM). After evaporation of all volatiles, purification by flash chromatography (100% ethyl acetate) gave sulfoxonium ylide (64-92% white solid).

2.2 Preparation of allyl sulfides[2]



Allyl sulfide was synthesized by addition of allyl/propargyl bromide (1.2 mmol) to the benzenethiol (1.0 mmol) in EtOH in the presence of potassium carbonate (3.0 mmol) at roomtemperature with constant stirring overnight. The crude was extracted with DCM/H_2O. The organic solution was dried over anhydrous Na_2SO_4 and evaporated under vacuum. The residue was purified by column chromatography on silica gel (68-83% colorless oil).

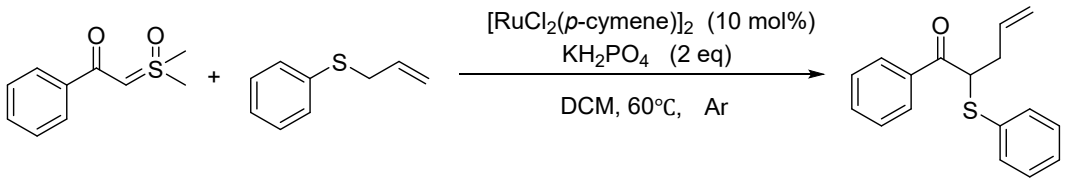
2.3 Preparation of allyl selenide[3]



Phenylboric acid (5 mmol) and selenium powder (15 mmol) were added to DMSO solution (15 ml) of silver nitrate (5 mmol) and reacted in air at 130 ℃ for three hours. After three times of extraction with EA/H_2O, no further purification was required for the next step of synthesis .

Under the condition of N_2 protection, $NaBH_4$ (2.0 mmol) was dissolved in EtOH (8 ml) and added into the double-neck flask. Add the THF solution (16 ml) from the product obtained in the previous step to the flask drop by drop at 0 ℃. A THF solution (8 ml) of allyl bromide (2 mmol) is then added drop by drop to the flask. Reaction at 0 ℃ for 30 min, quenched with water, DCM/H_2O extraction and silica gel column purification to obtain the product (52-80%, yellow oil).

2.4 Optimization of the reaction conditions



1a **2a** **3aa**

entry	catalyst	addition	1a:2a	solvent	t (h)	T (℃)	3aa(%)[b]
1	$Rh_2(OAc)_4$	none	1:2	DCE	12	60	NR
2	$[Ir(cod)Cl]_2$	none	1:2	DCE	12	60	13
3	$[Ru(p\text{-cymene})Cl_2]_2$	none	1:2	DCE	12	60	28
4	$Rh_2(esp)_4$	none	1:2	DCE	12	60	NR
5	CuI	none	1:2	DCE	12	60	NR
6	Au(PPh3)Cl	none	1:2	DCE	12	60	NR
7	$[CP^*RhCl2]_2$	none	1:2	DCE	12	60	NR
8	$Cu(MeCN)_4PF_6$	none	1:2	DCM	12	60	NR
9	CuOTf	none	1:2	DCM	12	60	NR
10	$[Ru(p\text{-cymene})Cl_2]_2$	none	1:3	DCE	12	60	28
11	$[Ru(p\text{-cymene})Cl_2]_2$	none	1:4	DCE	12	60	29
12	$[Ru(p\text{-cymene})Cl_2]_2$	none	1:5	DCE	12	60	29
13	$[Ru(p\text{-cymene})Cl_2]_2$	CuF_2	1:2	DCE	12	60	28
14	$[Ru(p\text{-cymene})Cl_2]_2$	CuCN	1:2	DCE	12	60	trace
15	$[Ru(p\text{-cymene})Cl_2]_2$	AgNTf	1:2	DCE	12	60	NR
16	$[Ru(p\text{-cymene})Cl_2]_2$	$AlCl_3$	1:2	DCE	12	60	trace
17	$[Ru(p\text{-cymene})Cl_2]_2$	KH_2PO_5	1:2	DCE	12	60	72
18	$[Ru(p\text{-cymene})Cl_2]_2$	KH_2PO_5	1:2	DCM	12	60	81
19	$[Ru(p\text{-cymene})Cl_2]_2$	KH_2PO_5	1:2	MeCN	12	60	68
20	$[Ru(p\text{-cymene})Cl_2]_2$	KH_2PO_5	1:2	EA	12	60	65
21	$[Ru(p\text{-cymene})Cl_2]_2$	KH_2PO_5	1:2	Tol	12	60	77
22	$[Ru(p\text{-cymene})Cl_2]_2$	KH_2PO_5	1:2	PhCl	12	60	74
23[e]	$[Ru(p\text{-cymene})Cl_2]_2$	KH_2PO_5	1:2	PhCl	12	60	68

24	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	PhF	12	60	73
25[e]	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	PhF	12	60	66
26	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	DCM	1.5	60	14
27	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	DCM	3	60	32
28	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	DCM	24	60	82
29	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	DCM	12	rt	trace
30	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	DCM	12	40	45
31	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	DCM	12	80	63
32	[Ru(*p*-cymene)Cl_2]$_2$	KH_2PO_5	1:2	DCM	12	60	78
33[e]	$Cu(MeCN)_4PF_6$	none	1:2	DCM	12	60	58
34[e]	$Cu(MeCN)_4PF_6$	KH_2PO_5	1:2	DCM	12	60	61
35[e]	CuOTf	none	1:2	DCM	12	60	49
36[e]	CuOTf	KH_2PO_5	1:2	DCM	12	60	52

Reaction condtions: [a] **1a** (0.1 mmol scale, 1 equiv), catalyst (0.1 equiv), and additive (2 equiv) were dissolved in solvent (2.0 mL) and were stirred under Ar. [b] Isolated yield. [c] NR = not reaction. [d] reaction under air. [e] **1a** reacted with allyl selenide instead of allyl sulfide.

2.5 Typical procedure for Rh-catalyzed Doyle−Kirmse Rearrangement Reactions

To a flame-dried 15 mL thick-walled pressure bottle equipped with a magnetic stir bar was added the sulfoxonium ylide **1a** (0.1 mmol), allyl compounds **2a**/**4a** (0.2 mmol), [$RuCl_2$(*p*-cymene)]$_2$ (10 mol %), KH_2PO_4 (0.2 mmol). Then 2 mL DCM was added and the mixture was stirred at 60℃ for 12h under Ar. (Warning: Explosion-proof cover should be used due to the potential risk of explosion). Afterwards, it was diluted with EA and solvent was removed under reduced pressure. The residue was purified by silica gel chromatography using PE/EA.

2.6 Reference

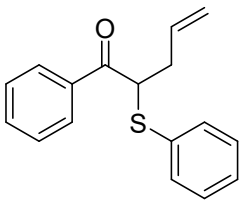
[1] Jianglian Li, Hua He, Mengyi Huang, Yuncan Chen, Yi Luo, Kaichuan Yan, Qiantao Wang, Yong Wu, Org. Lett. 2019, 21, 22, 9005–9008.

[2] Xinyu Zhang, Bo Lin, Jianhui Chen, Jiajia Chen, Yanshu Luo, Yuanzhi Xia, Org. Lett. 2021, 23, 3, 819–825.

[3] (1) Tao Leng, Ge Wu,, Yun-Bing Zhou, Wenxia Gao, Jinchang Ding, Xiaobo Huang, Miaochang Liu, Huayue Wua, Adv. Synth. Catal. 2018, 360, 4336 – 4340. (2) Sripati Jana, Rene M. Koenigs, Org. Lett. 2019, 21, 10, 3653–3657.

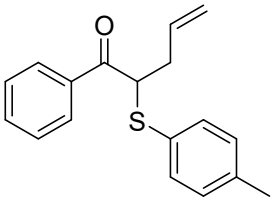
3. Characterization data for the products

1-phenyl-2-(phenylthio)pent-4-en-1-one (3aa)



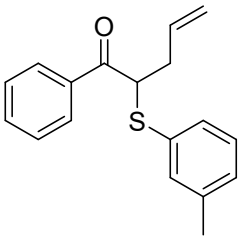
Yield: 81% (21.9 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.95 – 7.90 (m, 2H), 7.59 – 7.52 (m, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.34 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.31 – 7.25 (m, 3H), 5.88 (ddt, *J* = 17.1, 10.3, 6.8 Hz, 1H), 5.15 – 5.05 (m, 2H), 4.53 – 4.47 (m, 1H), 2.80 – 2.55 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.2, 136.1, 134.8, 134.8, 133.1, 131.5, 129.0, 128.8, 128.6, 128.6, 117.8, 50.8, 35.1. **HRMS (ESI)** calculated for $[C_{17}H_{16}NaOS, M+Na]^+$: 291.0814; Found: 291.0815.

1-phenyl-2-(p-tolylthio)pent-4-en-1-one (3ab)



Yield: 75% (21.1 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.96 – 7.91 (m, 2H), 7.58 – 7.53 (m, 1H), 7.47 – 7.42 (m, 2H), 7.22 (dt, *J* = 8.6, 2.4 Hz, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 5.87 (ddt, *J* = 17.0, 10.1, 6.8 Hz, 1H), 5.15 – 5.05 (m, 2H), 4.45 – 4.40 (m, 1H), 2.77 – 2.51 (m, 2H), 2.33 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.0, 139.2, 136.2, 135.4, 135.0, 133.0, 129.8, 128.6, 128.6, 127.4, 117.6, 50.8, 34.9, 21.3. **HRMS (ESI)** calculated for $[C_{18}H_{18}NaOS, M+Na]^+$: 305.0971; Found: 305.0973.

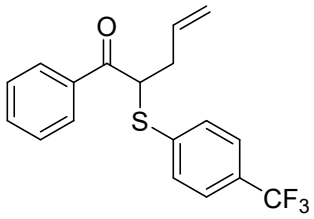
phenyl-2-(m-tolylthio)pent-4-en-1-one (3ac)



Yield: 76% (21.4 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.91 (dd, *J* = 7.3, 1.9 Hz, 2H), 7.58 – 7.52 (m, 1H), 7.47 – 7.40 (m, 2H), 7.19 – 7.09 (m, 4H), 5.88 (ddt, *J* = 17.1, 10.3, 6.8 Hz, 1H), 5.15 – 5.05 (m, 2H), 4.52 – 4.46 (m, 1H), 2.68 (ddt, *J* = 72.3, 14.2, 7.5 Hz, 2H), 2.28 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ

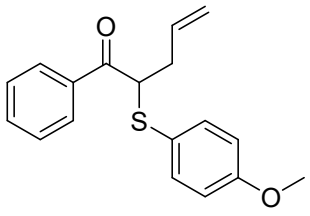
195.4, 138.7, 136.2, 135.4, 134.9, 133.1, 131.7, 131.3, 129.6, 128.8, 128.6, 128.6, 117.7, 50.9, 35.2, 21.2. **HRMS (ESI)** calculated for [$C_{18}H_{18}NaOS$, M+Na]$^+$: 305.0971; Found: 305.0970.

1-phenyl-2-((4-(trifluoromethyl)phenyl)thio)pent-4-en-1-one (3ad)



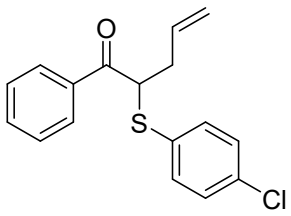
Yield: 65% (21.7 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.95 – 7.89 (m, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.45 (q, *J* = 7.9 Hz, 4H), 5.86 (ddt, *J* = 17.0, 10.1, 6.8 Hz, 1H), 5.17 – 5.08 (m, 2H), 4.61 (t, *J* = 7.2 Hz, 1H), 2.71 (ddt, *J* = 78.7, 14.4, 7.2 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.04, 136.05, 134.73, 133.15, 132.44, 132.40, 129.20 (q, J_{C-F} = 33.3 Hz), 127.71, 127.51, 124.74 (q, J_{C-F} = 3.7 Hz), 122.73 (q, J_{C-F} = 260.0 Hz), 117.22, 49.46, 34.15. **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -62.72. **HRMS (ESI)** calculated for [$C_{18}H_{15}F_3NaOS$, M+Na]$^+$: 359.0688; Found: 359.0685.

2-((4-methoxyphenyl)thio)-1-phenylpent-4-en-1-one (3ae)



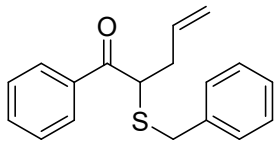
Yield: 93% (27.7 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.94 (dd, *J* = 7.1, 1.5 Hz, 2H), 7.59 – 7.53 (m, 1H), 7.48 – 7.43 (m, 2H), 7.26 – 7.22 (m, 2H), 6.82 – 6.77 (m, 2H), 5.88 (ddt, *J* = 17.1, 10.3, 6.8 Hz, 1H), 5.15 – 5.05 (m, 2H), 4.37 (t, *J* = 7.3 Hz, 1H), 3.79 (s, 3H), 2.72 – 2.50 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.9, 160.6, 137.7, 136.2, 135.0, 133.0, 128.6, 121.1, 117.6, 114.5, 55.3, 50.8, 34.6. **HRMS (ESI)** calculated for [$C_{18}H_{18}NaO_2S$, M+Na]$^+$: 321.0920; Found: 321.0918.

2-((4-chlorophenyl)thio)-1-phenylpent-4-en-1-one (3af)



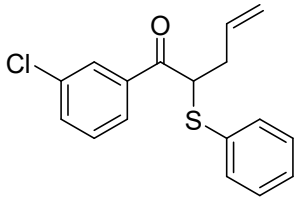
Yield: 62% (18.7 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.95 – 7.89 (m, 2H), 7.57 (tt, *J* = 6.8, 1.4 Hz, 1H), 7.48 – 7.43 (m, 2H), 7.25 (s, 3H), 5.86 (ddt, *J* = 17.1, 10.3, 6.8 Hz, 1H), 5.15 – 5.04 (m, 2H), 4.47 (t, *J* = 7.3 Hz, 1H), 2.77 – 2.51 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.9, 136.4, 135.9, 135.4, 134.5, 133.3, 129.6, 129.2, 128.7, 128.6, 118.0, 50.7, 34.8. **HRMS (ESI)** calculated for [$C_{17}H_{15}ClNaOS$, M+Na]$^+$: 325.0424; Found: 325.0427.

2-(benzylthio)-1-phenylpent-4-en-1-one (3ag)



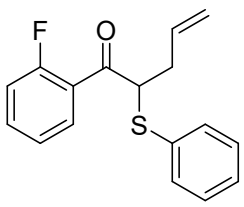
Yield: 78% (22.0 mg). Colorless wax. **^{1}H NMR** (400 MHz, Dimethyl sulfoxide-d_6) δ 7.92 – 7.86 (m, 2H), 7.66 – 7.61 (m, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.31 – 7.22 (m, 5H), 5.78 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H), 5.10 – 4.99 (m, 2H), 4.58 (dd, *J* = 8.2, 6.4 Hz, 1H), 3.79 (d, *J* = 12.6 Hz, 1H), 3.64 (d, *J* = 12.6 Hz, 1H), 2.79 – 2.70 (m, 1H), 2.54 (d, *J* = 7.0 Hz, 1H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 195.3, 137.1, 136.0, 134.8, 133.1, 129.2, 128.6, 128.6, 128.5, 127.3, 117.6, 46.7, 34.8, 34.2. **HRMS (ESI)** calculated for [$C_{18}H_{18}NaOS$, M+Na]$^+$: 305.0971; Found: 305.0972.

1-(3-chlorophenyl)-2-(phenylthio)pent-4-en-1-one (3ba)



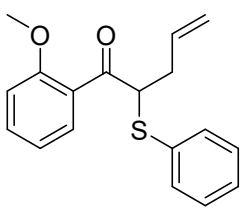
Yield: 74% (22.3 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.79 (t, *J* = 2.0 Hz, 1H), 7.72 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.51 – 7.47 (m, 1H), 7.43 (dd, *J* = 6.8, 1.7 Hz, 2H), 7.35 (t, *J* = 8.1 Hz, 2H), 7.30 – 7.26 (m, 2H), 5.86 (ddt, *J* = 17.0, 10.1, 6.7 Hz, 1H), 5.15 – 5.06 (m, 2H), 4.48 – 4.43 (m, 1H), 2.84 – 2.59 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.7, 137.8, 136.8, 135.3, 134.8, 132.8, 131.5, 129.8, 129.3, 129.2, 128.5, 126.4, 117.7, 44.9, 35.0. **HRMS (ESI)** calculated for [$C_{17}H_{15}ClNaOS$, M+Na]$^+$: 325.0424; Found: 325.0426.

1-(2-fluorophenyl)-2-(phenylthio)pent-4-en-1-one (3ca)



Yield: 58% (16.5 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 7.8 Hz, 1H), 7.60 (dt, *J* = 9.6, 2.3 Hz, 1H), 7.41 (td, *J* = 8.1, 5.5 Hz, 1H), 7.33 (dd, *J* = 7.0, 2.3 Hz, 3H), 7.30 – 7.25 (m, 3H), 5.87 (ddt, *J* = 17.1, 10.3, 6.9 Hz, 1H), 5.16 – 5.07 (m, 2H), 4.41 (dd, *J* = 7.9, 6.6 Hz, 1H), **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.8 (d, *J* = 2.02 Hz), 162.8 (d, *J* = 240.0 Hz), 138.3 (d, *J* = 6.3 Hz), 135.0, 134.6, 131.0, 130.2 (d, *J* = 7.5 Hz), 129.1, 124.2 (d, *J* = 3.2 Hz), 120.2, 120.0, 118.0, 115.4 (d, *J* = 22.5 Hz), 51.0, 34.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -111.73. **HRMS (ESI)** calculated for [$C_{17}H_{15}FNaOS$, M+Na]$^+$: 309.0720; Found: 309.0723.

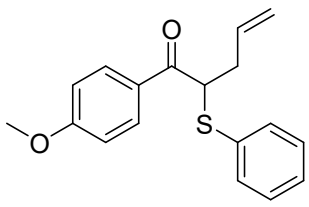
1-(2-methoxyphenyl)-2-(phenylthio)pent-4-en-1-one (3da)



Yield: 48% (14.3 mg). Yellow wax. **^{1}H NMR** (400 MHz,

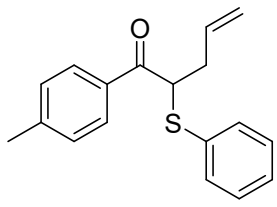
Chloroform-*d*) δ 7.70 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.44 (ddd, *J* = 8.3, 7.3, 1.8 Hz, 1H), 7.29 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.26 – 7.20 (m, 3H), 7.02 (td, *J* = 7.5, 1.0 Hz, 1H), 6.88 (dd, *J* = 8.4, 1.0 Hz, 1H), 5.94 (ddt, *J* = 17.1, 10.2, 6.8 Hz, 1H), 5.17 – 5.07 (m, 2H), 4.79 (t, *J* = 7.3 Hz, 1H), 3.77 (s, 3H), 2.81 – 2.46 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 197.4, 158.0, 135.4, 134.1, 133.4, 132.5, 131.4, 128.7, 128.1, 127.4, 120.9, 117.2, 111.4, 55.4, 55.2, 34.6. **HRMS (ESI)** calculated for $[C_{18}H_{18}NaO_2S, M+Na]^+$: 321.0920; Found: 321.0921.

1-(4-methoxyphenyl)-2-(phenylthio)pent-4-en-1-one (3ea)



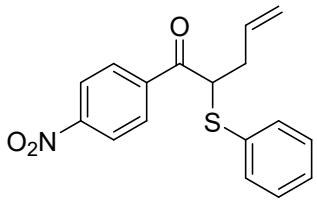
Yield: 82% (24.5 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.85 (dt, *J* = 9.2, 2.4 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.36 – 7.31 (m, 1H), 7.26 (d, *J* = 2.2 Hz, 2H), 6.89 (dt, *J* = 9.2, 2.6 Hz, 2H), 5.92 – 5.79 (m, 1H), 5.13 – 5.01 (m, 2H), 4.55 – 4.48 (m, 1H), 3.86 (s, 3H), 2.72 (ddt, *J* = 81.9, 13.8, 6.8 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.2, 163.4, 136.6, 135.7, 130.7, 129.1, 128.9, 127.1, 123.9, 117.3, 113.7, 55.5, 44.6, 35.5. **HRMS (ESI)** calculated for $[C_{18}H_{18}NaO_2S, M+Na]^+$: 321.0920; Found:321.0918.

2-(phenylthio)-1-(p-tolyl)pent-4-en-1-one (3fa)



Yield: 82% (25.7 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.84 – 7.80 (m, 2H), 7.34 (dt, *J* = 6.3, 1.9 Hz, 2H), 7.31 – 7.26 (m, 3H), 7.23 (d, *J* = 8.3 Hz, 2H), 5.87 (ddt, *J* = 17.0, 10.3, 6.9 Hz, 1H), 5.14 – 5.04 (m, 2H), 4.48 (dd, *J* = 7.9, 6.6 Hz, 1H), 2.79 – 2.54 (m, 2H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.0, 144.0, 134.9, 134.7, 133.5, 131.7, 129.3, 129.0, 128.7, 128.7, 117.7, 50.8, 35.2, 21.7. **HRMS (ESI)** calculated for $[C_{18}H_{18}NaOS, M+Na]^+$: 305.0971; Found: 305.0968.

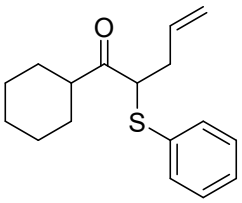
1-(4-nitrophenyl)-2-(phenylthio)pent-4-en-1-one (3ga)



Yield: 52% (16.2 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.27 (d, *J* = 8.8 Hz, 2H), 8.04 (d, *J* = 8.4 Hz, 2H), 7.37 – 7.27 (m, 5H), 5.89 (ddt, *J* = 17.0, 10.2, 6.8 Hz, 1H), 5.18 – 5.09 (m, 2H), 4.43 (t, *J* = 7.4 Hz, 1H), 2.69 (ddt, *J* = 58.4, 14.4, 7.1 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.2, 150.2, 140.9,

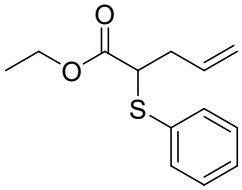
135.1, 134.3, 130.5, 129.6, 129.4, 129.2, 123.8, 118.3, 51.4, 34.6. **HRMS (ESI)** calculated for $[C_{17}H_{15}NNaO_3S, M+Na]^+$: 336.0665; Found: 336.0666.

1-cyclohexyl-2-(phenylthio)pent-4-en-1-one (3ha)



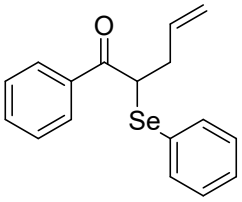
Yield: 52% (16.2 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.38 (dd, *J* = 6.4, 3.2 Hz, 2H), 7.34 – 7.27 (m, 3H), 5.82 – 5.70 (m, 1H), 5.12 – 5.03 (m, 2H), 3.74 (t, *J* = 7.4 Hz, 1H), 2.70 – 2.37 (m, 3H), 1.78 (d, *J* = 11.7 Hz, 4H), 1.66 (d, *J* = 11.5 Hz, 1H), 1.53 – 1.41 (m, 1H), 1.25 – 1.19 (m, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 208.4, 134.6, 133.7, 132.2, 129.0, 128.3, 117.8, 54.4, 48.7, 34.6, 29.5, 28.3, 25.9, 25.8, 25.4. **HRMS (ESI)** calculated for $[C_{17}H_{22}NaOS, M+Na]^+$: 297.1284; Found: 297.1282.

ethyl 2-(phenylthio)pent-4-enoate (3ia)



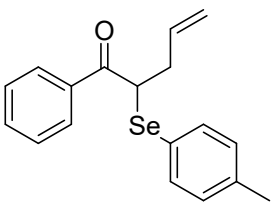
Yield: 56% (13.2 mg). Colorless wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 7.2, 2.4 Hz, 2H), 7.30 (dd, *J* = 5.0, 2.4 Hz, 3H), 5.81 (ddt, *J* = 17.1, 10.2, 6.8 Hz, 1H), 5.21 – 5.07 (m, 2H), 4.11 (qd, *J* = 7.1, 1.7 Hz, 2H), 3.70 (dd, *J* = 8.7, 6.4 Hz, 1H), 2.69 – 2.47 (m, 2H), 1.17 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 171.7, 133.9, 133.2, 133.1, 128.9, 128.0, 118.0, 61.2, 50.3, 35.8, 14.1. **HRMS (ESI)** calculated for $[C_{13}H_{16}NaO_2S, M+Na]^+$: 259.0763; Found: 259.0761.

1-phenyl-2-(phenylselanyl)pent-4-en-1-one (5aa)



Yield: 82% (25.8 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.42 (q, *J* = 7.7 Hz, 4H), 7.35 (t, *J* = 7.3 Hz, 1H), 7.28 – 7.24 (m, 2H), 5.87 (ddt, *J* = 17.0, 10.1, 6.7 Hz, 1H), 5.14 – 5.04 (m, 2H), 4.54 (t, *J* = 7.4 Hz, 1H), 2.72 (ddt, *J* = 76.8, 14.4, 7.2 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.2, 136.7, 136.2, 135.6, 132.9, 131.6, 129.1, 128.5, 128.4, 126.8, 117.4, 44.7, 35.2. **HRMS (ESI)** calculated for $[C_{17}H_{16}NaOSe, M+Na]^+$: 339.0259; Found: 339.0261.

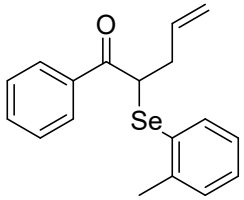
1-phenyl-2-(p-tolylselanyl)pent-4-en-1-one (5ab)



Yield: 83% (27.4 mg). Yellow wax. **^{1}H NMR** (400 MHz,

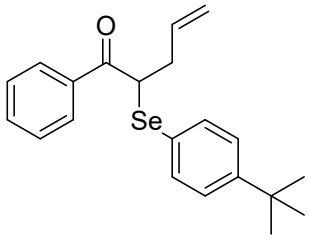
Chloroform-*d*) δ 7.88 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.53 (td, *J* = 6.3, 5.3, 3.4 Hz, 1H), 7.45 – 7.40 (m, 2H), 7.35 – 7.29 (m, 2H), 7.07 (d, *J* = 7.9 Hz, 2H), 5.86 (ddt, *J* = 17.0, 10.1, 6.8 Hz, 1H), 5.14 – 5.03 (m, 2H), 4.52 – 4.46 (m, 1H), 2.82 – 2.56 (m, 2H), 2.34 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.0, 139.4, 136.9, 136.2, 135.7, 132.8, 129.9, 128.5, 128.4, 122.9, 117.3, 44.6, 35.1, 21.3. **HRMS (ESI)** calculated for [$C_{18}H_{18}NaOSe$, M+Na]$^+$: 353.0415; Found: 353.0412.

1-phenyl-2-(o-tolylselanyl)pent-4-en-1-one (5ac)



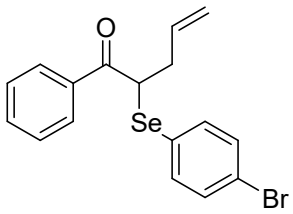
Yield: 79% (26.1 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.71 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.45 – 7.37 (m, 2H), 7.32 – 7.25 (m, 2H), 7.17 – 7.08 (m, 2H), 6.98 (td, *J* = 7.3, 2.1 Hz, 1H), 5.79 (ddt, *J* = 17.0, 10.1, 6.7 Hz, 1H), 5.08 – 4.95 (m, 2H), 4.51 – 4.45 (m, 1H), 2.87 – 2.57 (m, 2H), 2.21 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.7, 142.5, 137.2, 136.2, 135.6, 132.9, 130.2, 129.2, 128.8, 128.4, 128.3, 126.5, 117.4, 44.8, 35.5, 23.1. **HRMS (ESI)** calculated for [$C_{18}H_{18}NaOSe$, M+Na]$^+$: 353.0415; Found: 353.0419.

2-((4-(tert-butyl)phenyl)selanyl)-1-phenylpent-4-en-1-one (5ad)



Yield: 87% (32.3 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.82 – 7.74 (m, 2H), 7.44 (tt, *J* = 6.8, 1.3 Hz, 1H), 7.35 – 7.26 (m, 4H), 7.22 – 7.17 (m, 2H), 5.80 (ddt, *J* = 17.0, 10.1, 6.8 Hz, 1H), 5.07 – 4.96 (m, 2H), 4.44 (dd, *J* = 8.3, 6.5 Hz, 1H), 2.79 – 2.51 (m, 2H), 1.23 (s, 9H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.4, 151.3, 135.5, 135.3, 134.6, 131.8, 127.4, 127.4, 127.3, 125.2, 122.2, 116.3, 43.6, 34.1, 30.2. **HRMS (ESI)** calculated for [$C_{21}H_{24}NaOSe$, M+Na]$^+$: 395.0885; Found: 395.0887.

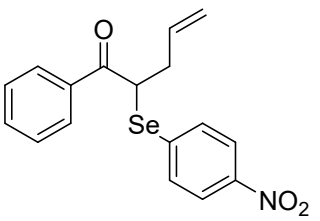
2-((4-bromophenyl)selanyl)-1-phenylpent-4-en-1-one (5ae)



Yield: 86% (33.7 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.88 – 7.84 (m, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.44 (d, *J* = 7.9 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 5.85 (ddt, *J* = 17.0, 10.3, 6.8 Hz, 1H), 5.14 – 5.05 (m, 2H), 4.56 – 4.51 (m, 1H), 2.83 – 2.55 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ

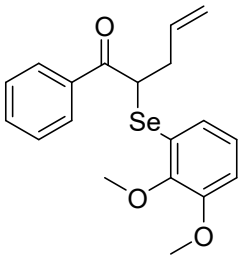
194.9, 138.4, 136.0, 135.3, 133.1, 132.3, 128.6, 128.3, 125.2, 124.1, 117.7, 44.6, 35.1. **HRMS (ESI)** calculated for $[C_{17}H_{15}BrNaOSe, M+Na]^+$: 416.9364; Found: 416.9360.

2-((4-nitrophenyl)selanyl)-1-phenylpent-4-en-1-one (5af)



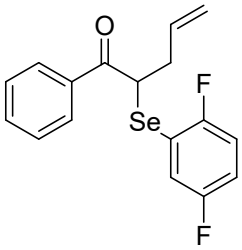
Yield: 78% (28.2 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-d) δ 8.12 – 7.98 (m, 2H), 7.91 – 7.72 (m, 2H), 7.61 – 7.45 (m, 3H), 7.37 (t, J = 7.7 Hz, 2H), 5.78 (ddt, J = 17.0, 10.1, 6.8 Hz, 1H), 5.19 – 4.95 (m, 2H), 4.63 (dd, J = 8.0, 6.7 Hz, 1H), 2.90 – 2.49 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 193.91, 146.91, 135.19, 134.91, 134.62, 133.67, 132.39, 127.73, 127.29, 122.76, 117.17, 44.11, 34.37. **HRMS (ESI)** calculated for $[C_{17}H_{15}NO_3Se, M+Na]^+$: 384.0109; Found: 384.0110.

2-((2,3-dimethoxyphenyl)selanyl)-1-phenylpent-4-en-1-one (5ag)



Yield: 71% (36.7 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.29 (t, *J* = 7.7 Hz, 2H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.89 – 6.81 (m, 2H), 5.76 (dtd, *J* = 16.9, 6.5, 3.4 Hz, 1H), 4.97 (dd, *J* = 29.8, 13.7 Hz, 2H), 4.78 – 4.71 (m, 1H), 3.80 (s, 3H), 3.70 (s, 3H), 2.95 – 2.61 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 196.6, 153.0, 149.4, 136.2, 135.6, 132.9, 128.5, 128.4, 127.2, 124.7, 123.8, 117.2, 113.1, 60.6, 55.9, 44.3, 36.1. **HRMS (ESI)** calculated for $[C_{19}H_{20}NaO_3Se, M+Na]^+$: 399.0470; Found: 399.0467.

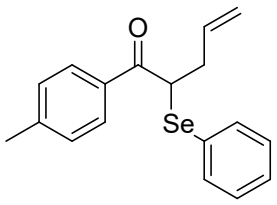
2-((2,5-difluorophenyl)selanyl)-1-phenylpent-4-en-1-one (5ah)



Yield: 78% (27.4 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.81 – 7.76 (m, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.28 (q, *J* = 7.6 Hz, 1H), 6.73 (dtd, *J* = 22.1, 8.4, 2.7 Hz, 2H), 5.77 (ddt, *J* = 17.0, 10.2, 6.8 Hz, 1H), 5.07 – 4.97 (m, 2H), 4.53 (dd, *J* = 8.4, 6.4 Hz, 1H), 2.65 (ddd, *J* = 64.3, 14.7, 7.5 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.1, 163.0 (dd, *J* = 251.0, 11.9 Hz) 162.8 (dd, *J* = 251.0, 11.9 Hz), 161.8 (dd, *J* = 50.8, 11.8 Hz), 139.2 (dd, *J* = 9.5, 2.8 Hz), 135.0, 134.1, 132.0, 127.5, 127.2, 116.6, 111.1 (dd, *J* = 21.2, 3.8 Hz), 107.4 (dd, *J* = 23.2, 4.0 Hz), 103.4 (dd, *J* = 28.5, 25.5 Hz), 43.2, 34.2. **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -94.42 (d, *J* = 3.0 Hz),-106.48 (d, *J* = 3.0 Hz). **HRMS (ESI)** calculated

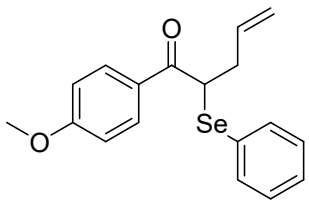
for $[C_{17}H_{14}F_2NaOSe, M+Na]^+$: 375.0070; Found: 375.0074.

2-(phenylselanyl)-1-(p-tolyl)pent-4-en-1-one (5ba)



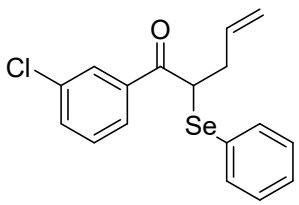
Yield: 88% (29.0 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.80 – 7.76 (m, 2H), 7.48 – 7.43 (m, 2H), 7.38 – 7.32 (m, 1H), 7.28 (s, 1H), 7.23 (t, *J* = 7.4 Hz, 3H), 5.86 (ddt, *J* = 17.1, 10.3, 6.8 Hz, 1H), 5.13 – 5.02 (m, 2H), 4.53 (dd, *J* = 8.2, 6.6 Hz, 1H), 2.86 – 2.57 (m, 2H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.9, 142.7, 135.6, 134.6, 132.5, 128.2, 128.0, 128.0, 127.4, 125.9, 116.3, 43.6, 34.3, 20.6. **HRMS (ESI)** calculated for $[C_{18}H_{18}NaOSe, M+Na]^+$: 353.0415; Found: 353.0412.

1-(4-methoxyphenyl)-2-(phenylselanyl)pent-4-en-1-one (5ca)



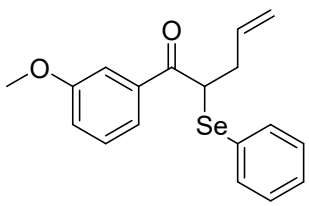
Yield: 89% (30.8 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.5 Hz, 2H), 7.37 – 7.25 (m, 5H), 6.91 (d, *J* = 8.5 Hz, 2H), 5.87 (ddt, *J* = 17.2, 10.6, 6.9 Hz, 1H), 5.08 (dd, *J* = 18.5, 13.7 Hz, 2H), 4.47 (t, *J* = 7.4 Hz, 1H), 3.86 (s, 3H), 2.67 (ddt, *J* = 73.4, 14.3, 7.1 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.0, 163.6, 135.0, 134.6, 131.9, 130.9, 129.0, 128.9, 128.6, 117.6, 113.8, 55.5, 50.6, 35.3. **HRMS (ESI)** calculated for $[C_{18}H_{18}NaO_2Se, M+Na]^+$: 369.0364; Found: 369.0365.

1-(3-chlorophenyl)-2-(phenylselanyl)pent-4-en-1-one (5da)



Yield: 75% (26.2 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.79 (t, *J* = 1.9 Hz, 1H), 7.72 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.49 (dd, *J* = 7.8, 2.1 Hz, 1H), 7.45 – 7.41 (m, 2H), 7.37 (t, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 5.86 (ddt, *J* = 17.0, 10.3, 6.8 Hz, 1H), 5.15 – 5.06 (m, 2H), 4.45 (dd, *J* = 8.2, 6.7 Hz, 1H), 2.84 – 2.59 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.7, 137.8, 136.8, 135.3, 134.8, 132.8, 131.5, 129.8, 129.3, 129.2, 128.5, 126.4, 117.7, 44.9, 35.0. **HRMS (ESI)** calculated for $[C_{17}H_{15}ClNaOSe, M+Na]^+$: 372.9869; Found: 372.9867.

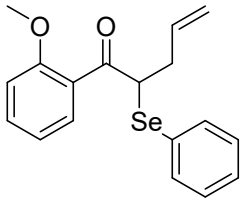
1-(3-methoxyphenyl)-2-(phenylselanyl)pent-4-en-1-one (5ea)



Yield: 77% (26.6 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 7.2 Hz, 2H), 7.43 – 7.39 (m, 2H), 7.38 – 7.29 (m, 2H), 7.28 (d, *J* = 7.7 Hz, 2H), 7.08 (dd, *J*

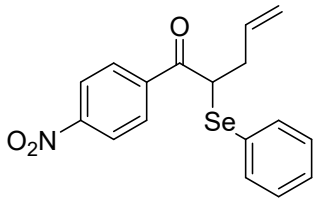
= 8.2, 2.6 Hz, 1H), 5.87 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H), 5.15 – 5.04 (m, 2H), 4.55 – 4.49 (m, 1H), 3.81 (s, 3H), 2.72 (ddt, *J* = 75.1, 14.4, 7.1 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.0, 159.8, 137.6 136.6, 135.5, 129.5, 129.1, 129.1, 126.9, 120.8, 119.4, 117.5, 112.8, 55.4, 44.9, 35.3. **HRMS (ESI)** calculated for [$C_{18}H_{18}NaO_2Se$, M+Na]$^+$: 369.0364; Found: 369.0366.

1-(2-methoxyphenyl)-2-(phenylselanyl)pent-4-en-1-one (5fa)



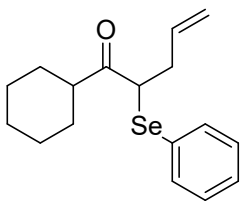
Yield: 77% (17.9 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.77 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.41 – 7.37 (m, 2H), 7.33 – 7.28 (m, 1H), 7.22 (dd, *J* = 8.1, 6.7 Hz, 2H), 7.03 (td, *J* = 7.5, 1.0 Hz, 1H), 6.87 (dd, *J* = 8.4, 1.0 Hz, 1H), 5.92 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H), 5.14 – 5.05 (m, 2H), 4.80 (t, *J* = 7.4 Hz, 1H), 3.77 (s, 3H), 2.82 – 2.49 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 196.7, 158.0, 136.4, 136.1, 133.3, 131.6, 128.8, 128.6, 127.2, 127.0, 120.9, 116.8, 111.4, 55.4, 49.9, 34.7. **HRMS (ESI)** calculated for [$C_{18}H_{18}NaO_2Se$, M+Na]$^+$: 369.0364; Found: 369.0363.

1-(4-nitrophenyl)-2-(phenylselanyl)pent-4-en-1-one (5ga)



Yield: 43% (15.5 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.33 – 8.20 (m, 2H), 8.01 – 7.93 (m, 2H), 7.43 – 7.32 (m, 3H), 7.30 – 7.22 (m, 2H), 5.89 (ddt, *J* = 17.1, 10.3, 6.8 Hz, 1H), 5.19 – 5.06 (m, 2H), 4.54 – 4.44 (m, 1H), 2.89 – 2.60 (m, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.0, 150.1, 141.1, 136.7, 135.0, 129.6, 129.3, 129.3, 126.2, 123.7, 118.0, 45.4, 34.7. **HRMS (ESI)** calculated for [$C_{17}H_{15}NNaO_3Se$, M+Na]$^+$: 384.0109; Found: 384.0112.

1-cyclohexyl-2-(phenylselanyl)pent-4-en-1-one (5ha)

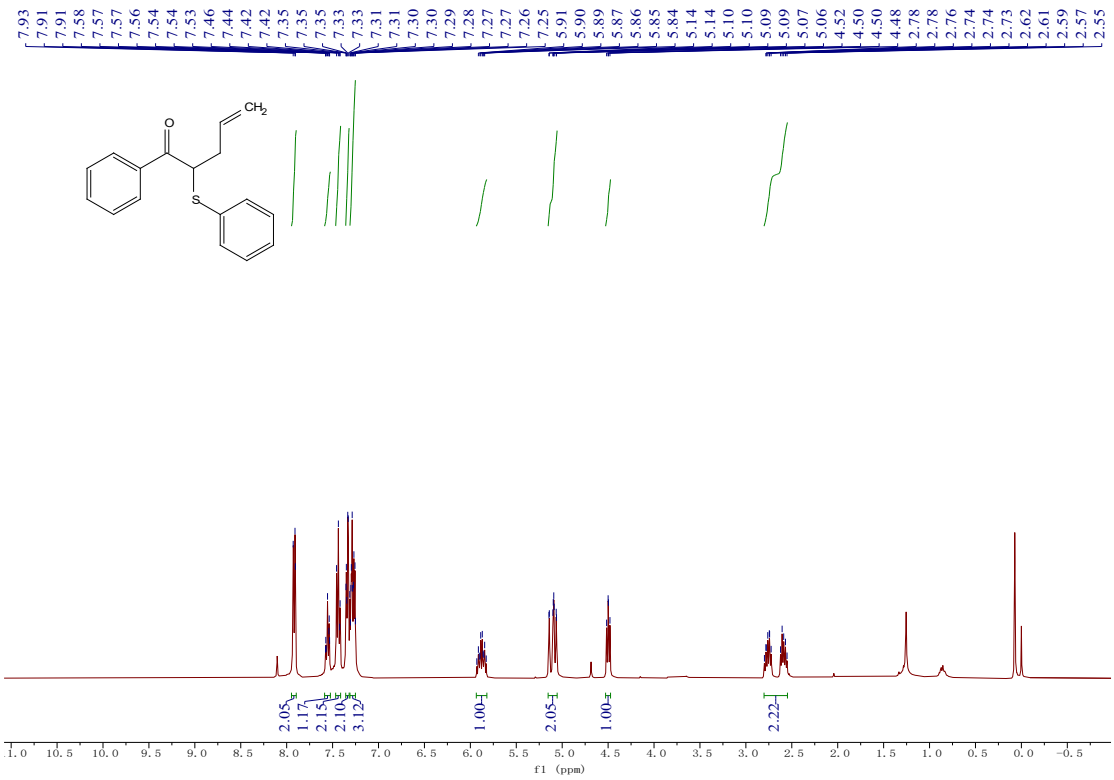


Yield: 32% (10.3 mg). Yellow wax. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 7.4 Hz, 2H), 7.31 (dt, *J* = 14.7, 7.2 Hz, 3H), 5.74 (ddt, *J* = 17.1, 10.4, 6.9 Hz, 1H), 5.05 (dd, *J* = 13.6, 9.3 Hz, 2H), 3.75 (dd, *J* = 8.7, 6.3 Hz, 1H), 2.65 – 2.55 (m, 2H), 2.42 (dt, *J* = 14.2, 6.8 Hz, 1H), 1.83 – 1.74 (m, 4H), 1.23 – 1.15 (m, 4H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 207.8, 136.2, 135.5, 129.1, 128.8, 117.4, 49.0, 48.8, 34.8, 29.8, 29.7, 28.4, 26.1, 25.8, 25.3. **HRMS (ESI)** calculated for [$C_{17}H_{22}NaOSe$, M+Na]$^+$: 345.0728;

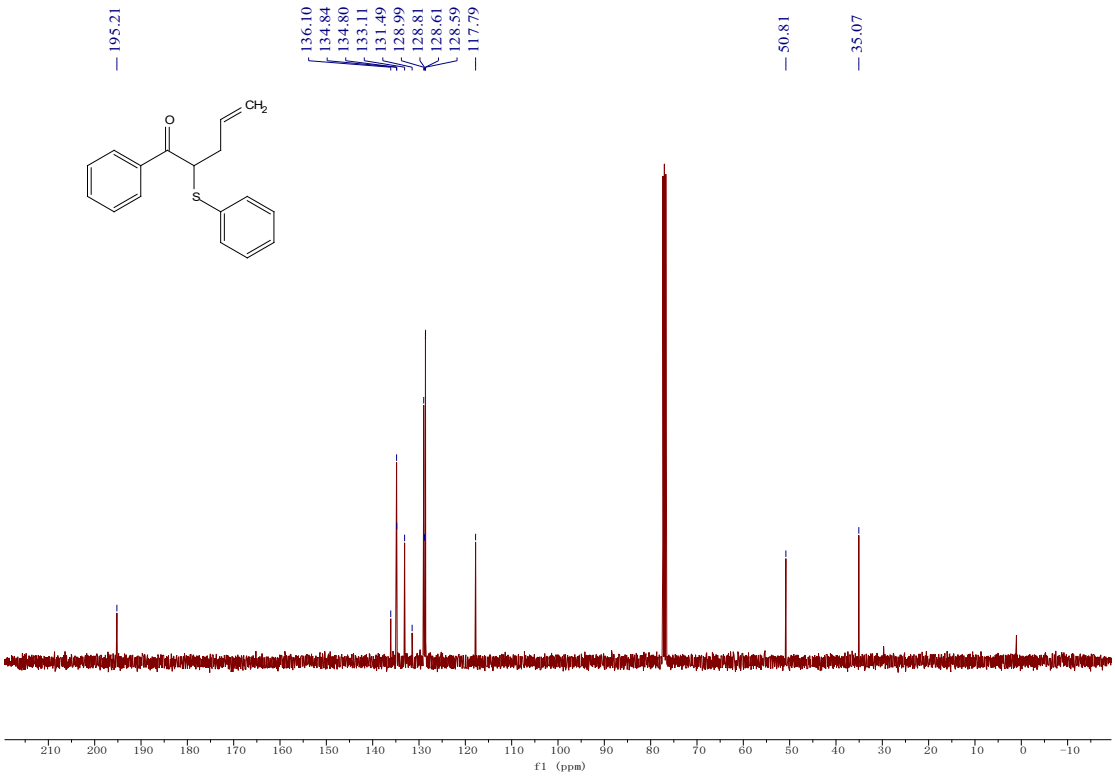
Found: 345.0725.

4. ^{1}H NMR , ^{13}C NMR and ^{19}F NMR spectra of new compounds

1-phenyl-2-(phenylthio)pent-4-en-1-one (3aa)

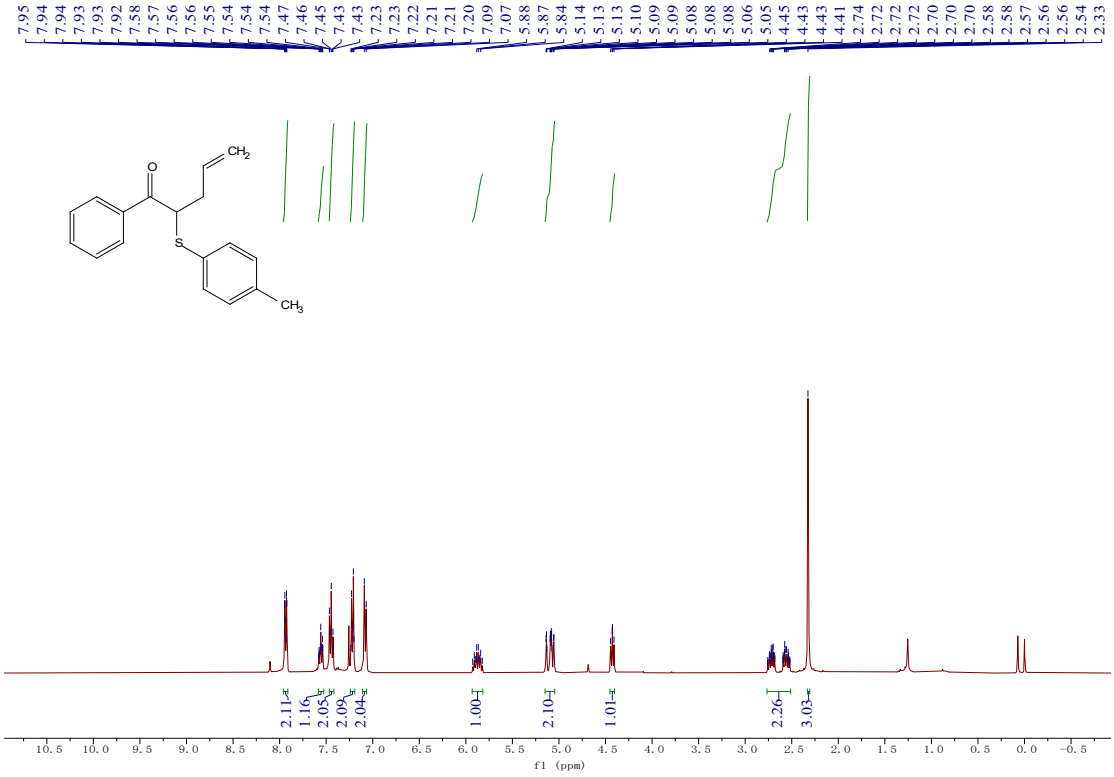


^{1}H NMR of 3aa (400 MHz, Chloroform-*d*)

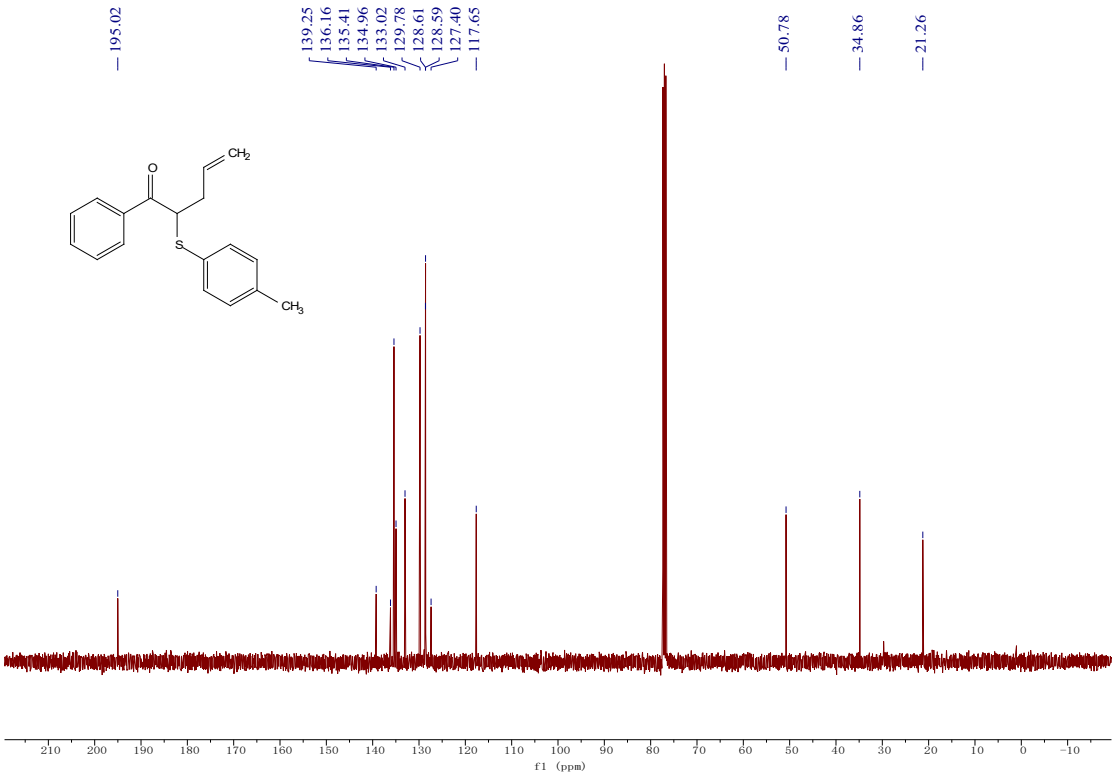


^{13}C NMR of 3aa (100 MHz, Chloroform-*d*)

phenyl-2-(p-tolylthio)pent-4-en-1-one (3ab)

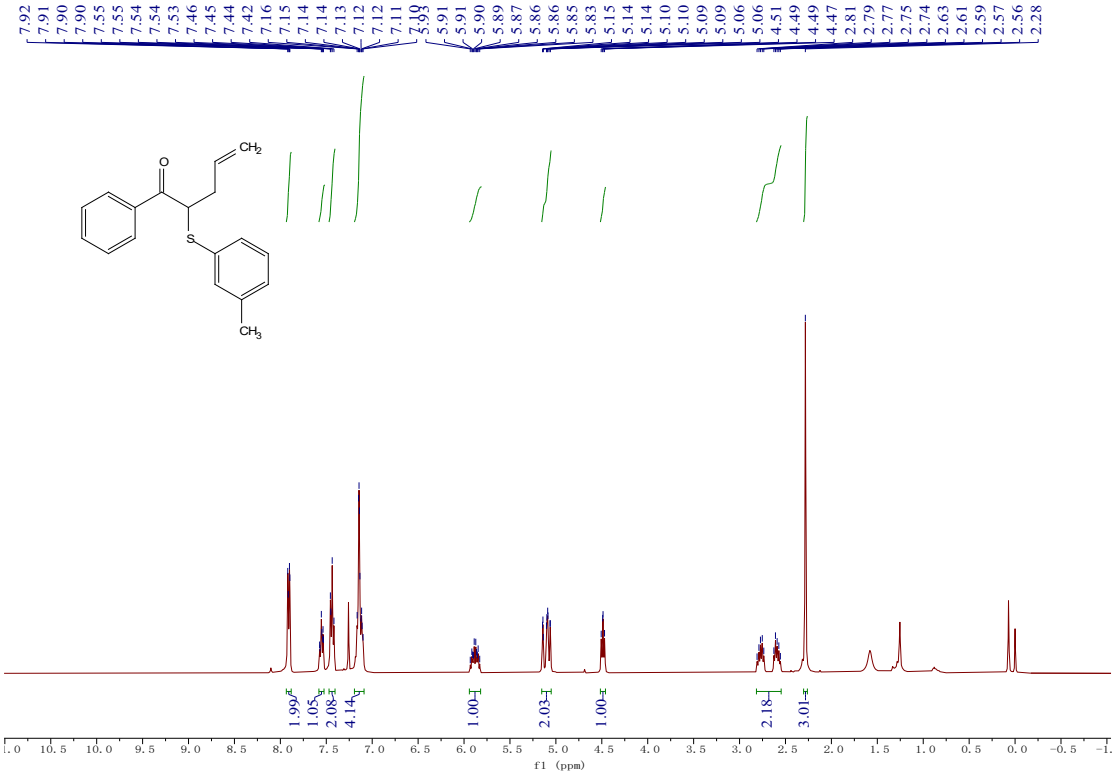


^{1}H NMR of 3ab (400 MHz, Chloroform-*d*)

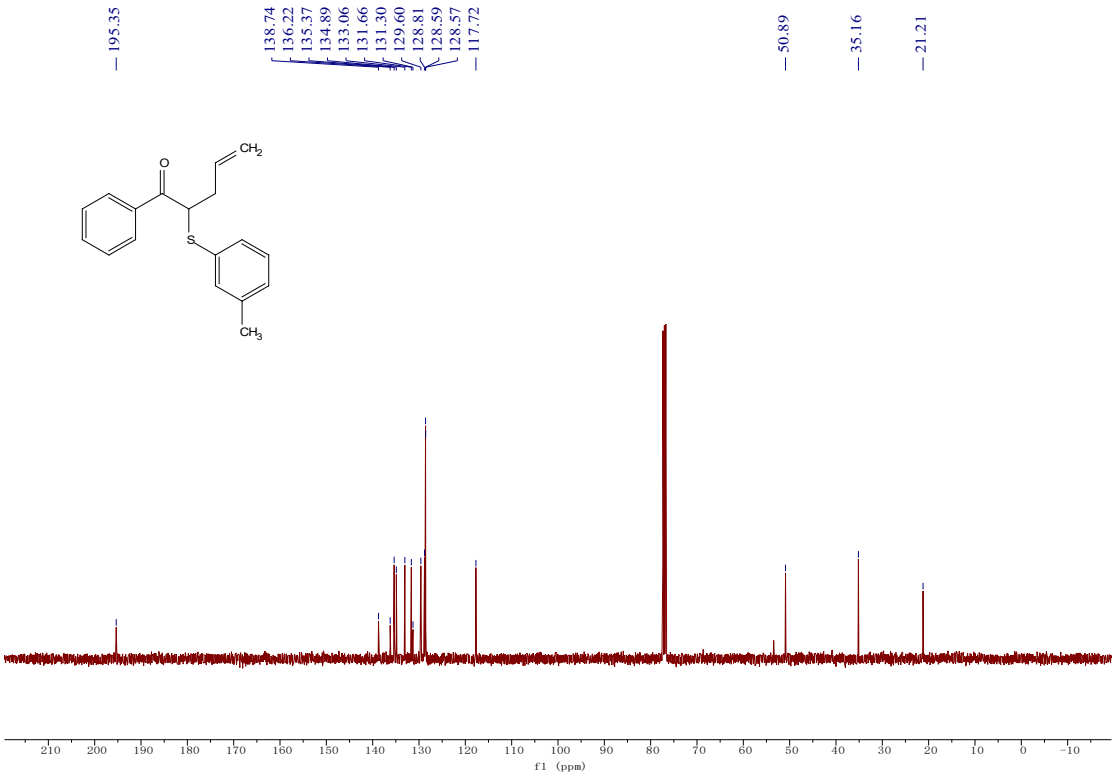


^{13}C NMR of 3ab (100 MHz, Chloroform-*d*)

phenyl-2-(m-tolylthio)pent-4-en-1-one (3ac)

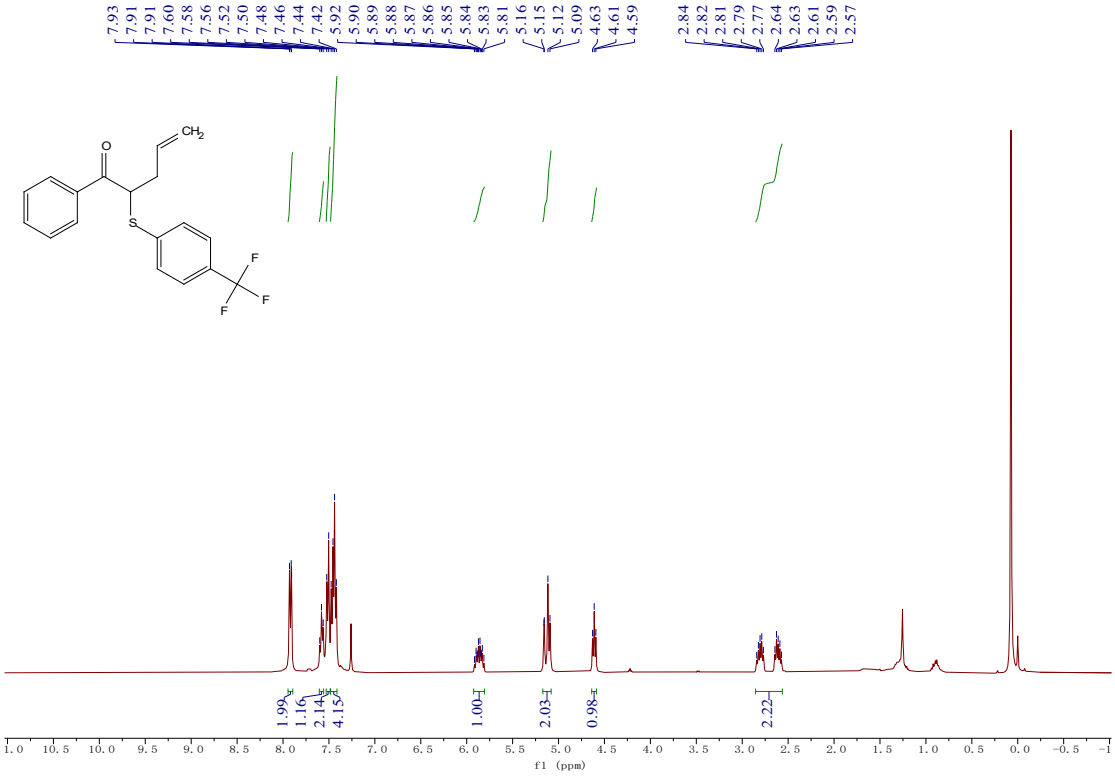


^{1}H NMR of 3ac (400 MHz, Chloroform-*d*)

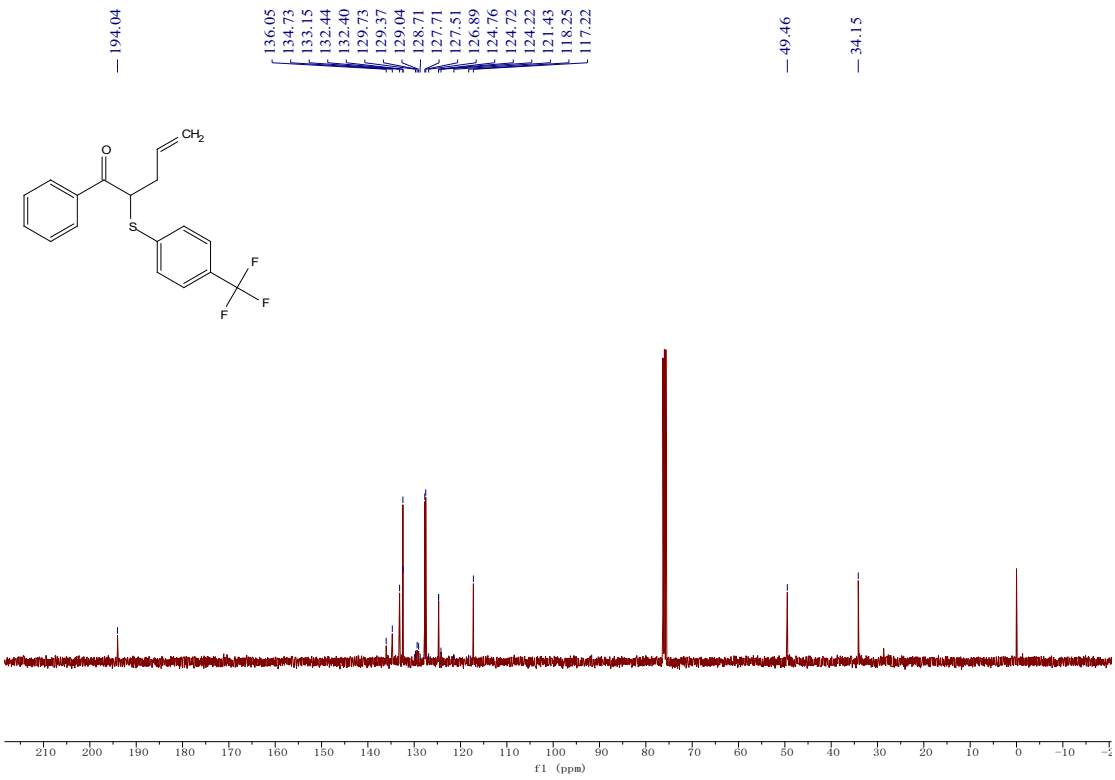


^{13}C NMR of 3ac (100 MHz, Chloroform-*d*)

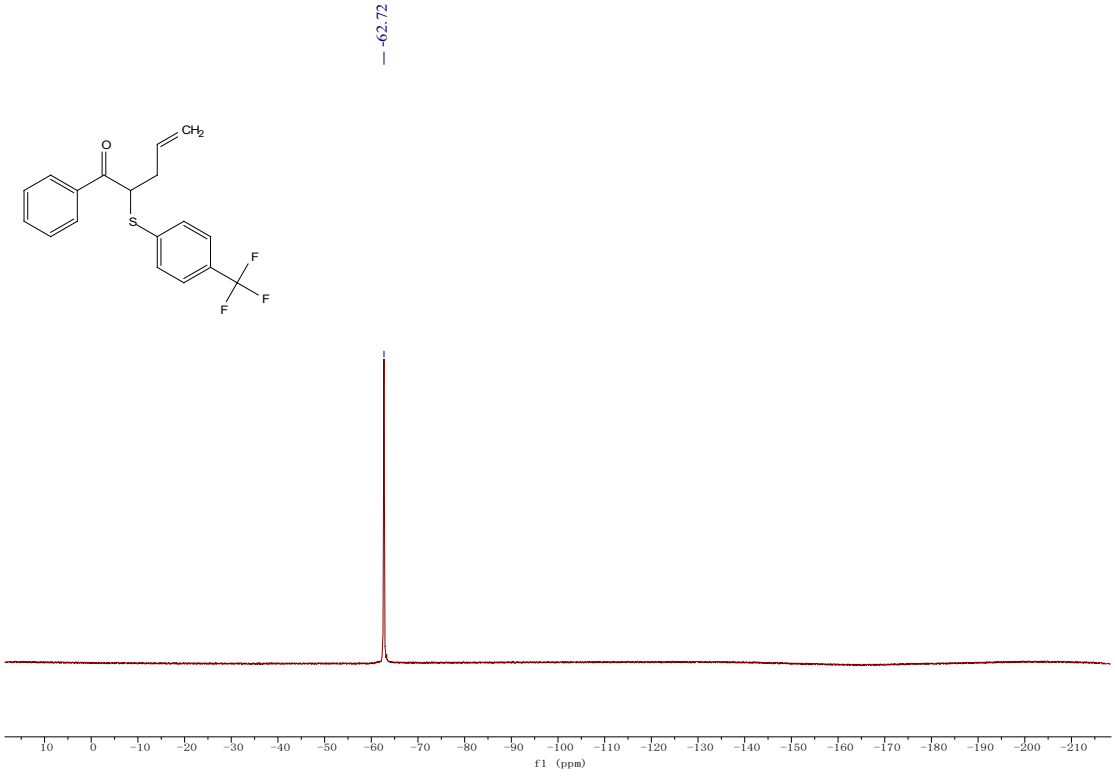
1-phenyl-2-((4-(trifluoromethyl)phenyl)thio)pent-4-en-1-one (3ad)



^{1}H NMR of 3ad (400 MHz, Chloroform-*d*)

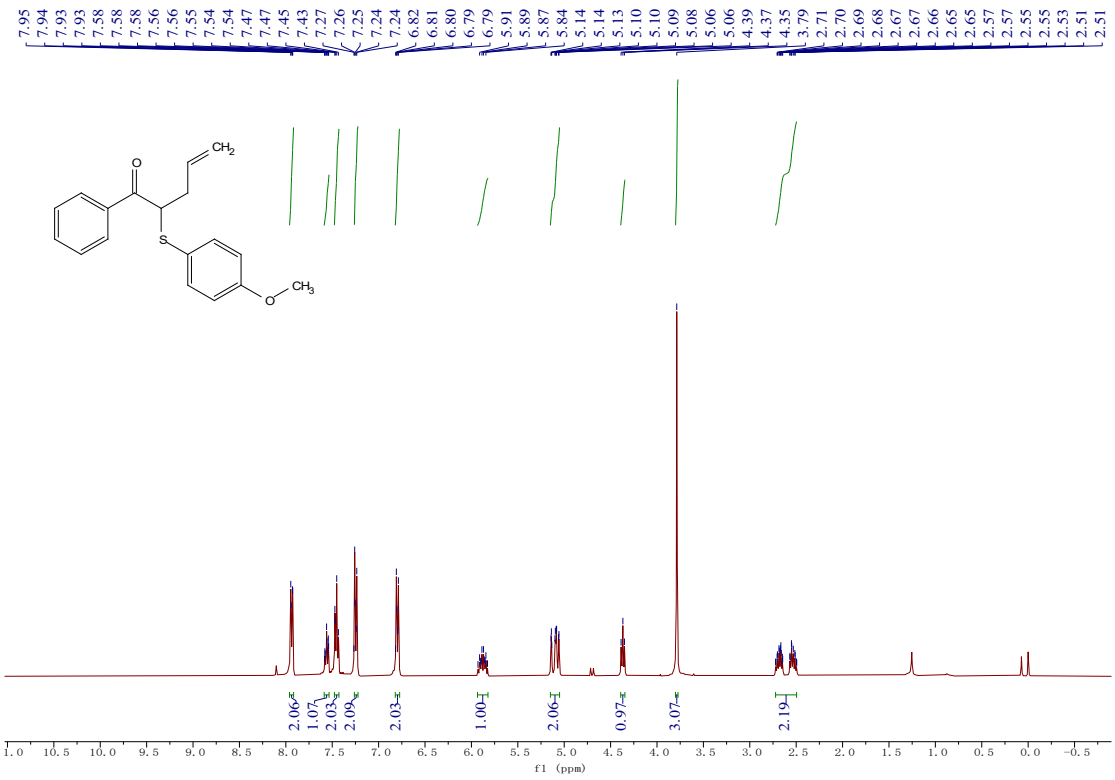


^{13}C NMR of 3ad (100 MHz, Chloroform-*d*)

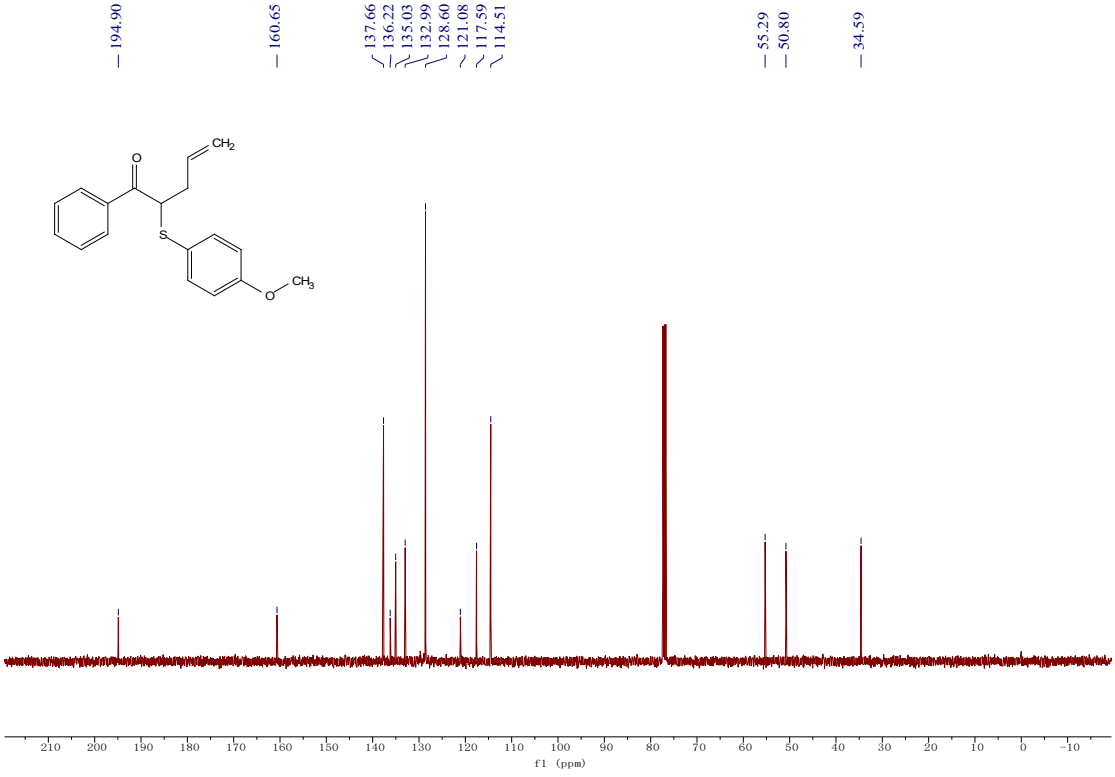


^{19}F NMR of 3ad (376 MHz, Chloroform-*d*)

2-((4-methoxyphenyl)thio)-1-phenylpent-4-en-1-one (3ae)

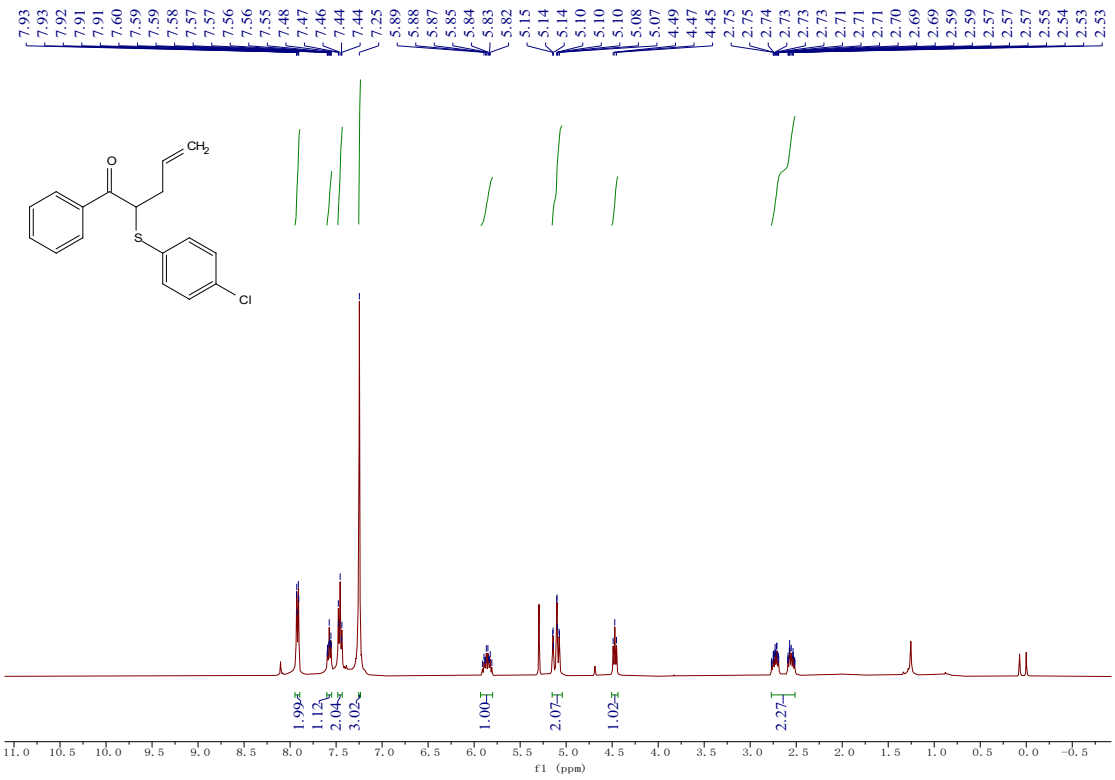


^{1}H NMR of 3ae (400 MHz, Chloroform-*d*)

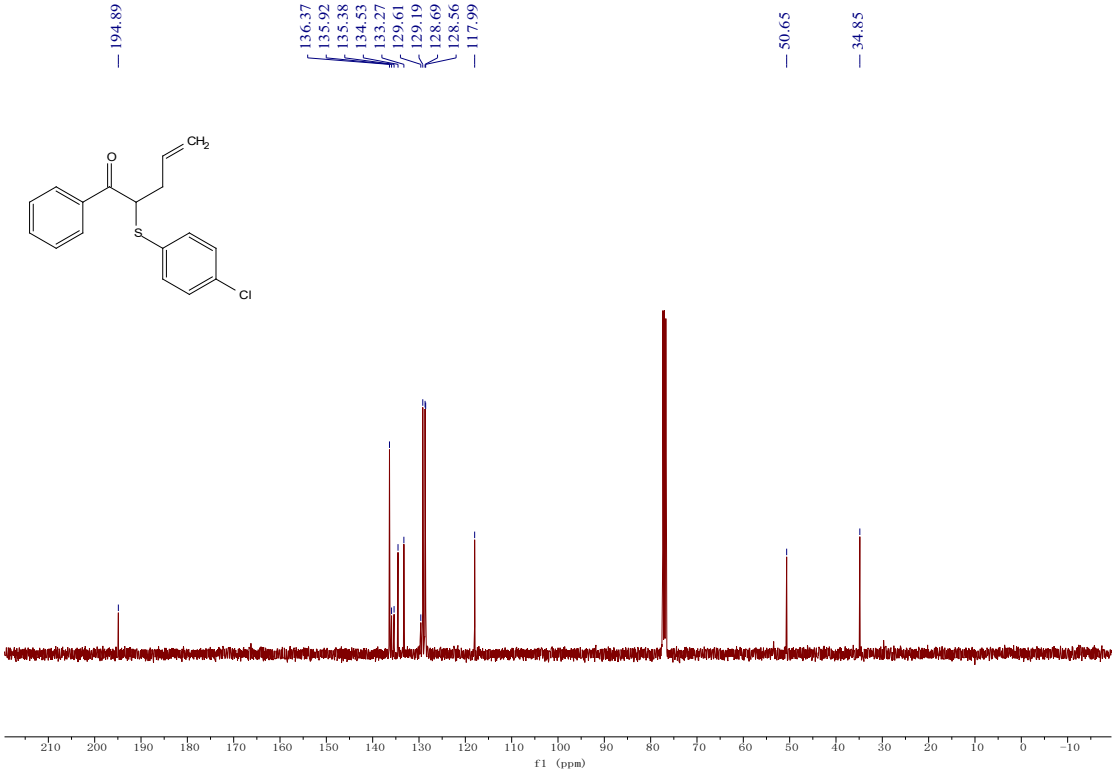


^{13}C NMR of 3ae (100 MHz, Chloroform-*d*)

2-((4-chlorophenyl)thio)-1-phenylpent-4-en-1-one (3af)

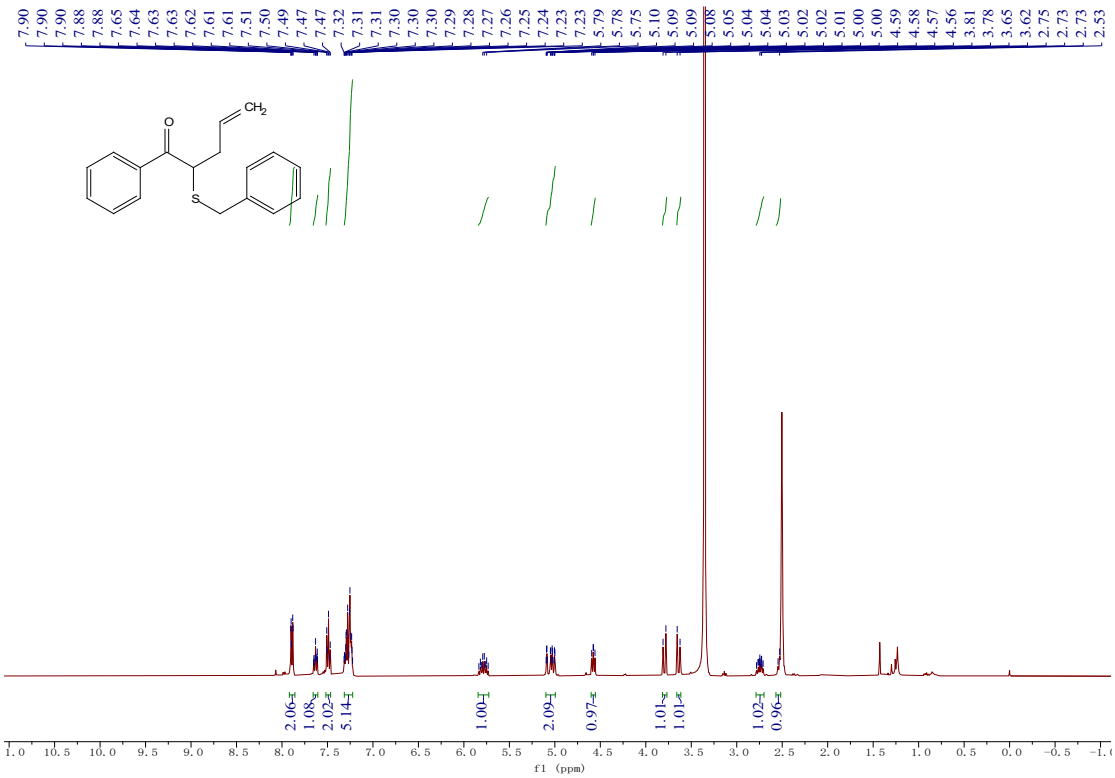


^{1}H NMR of 3af (400 MHz, Chloroform-*d*)

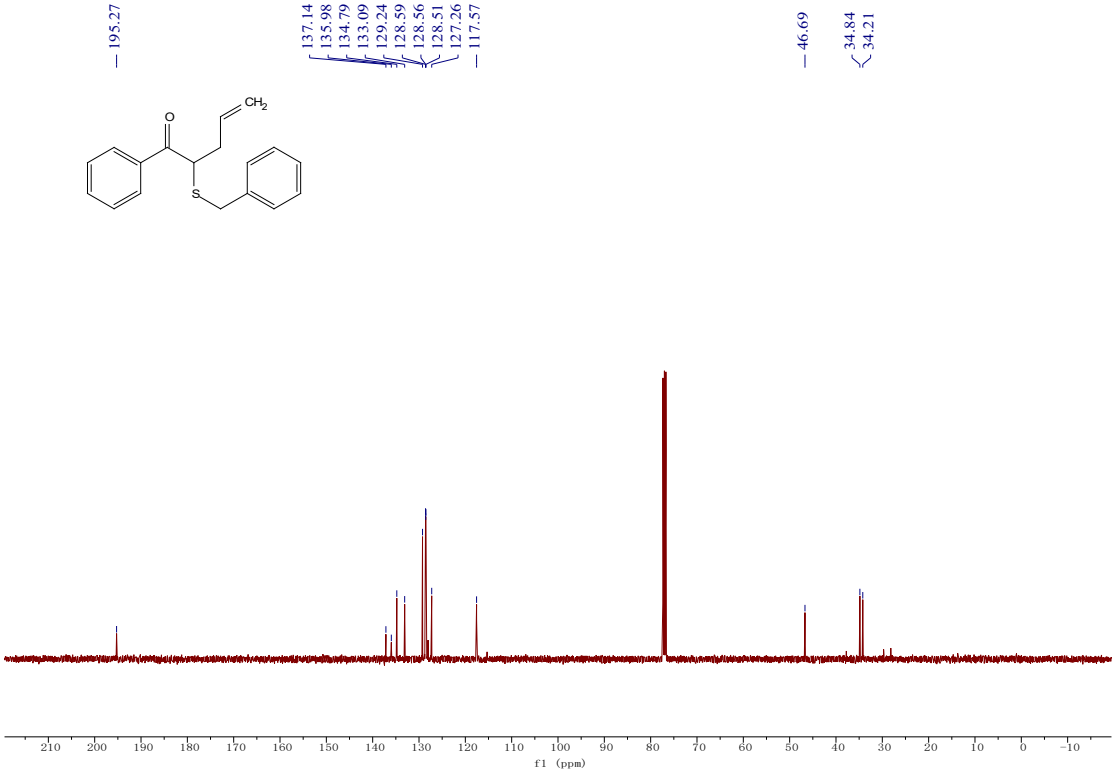


^{13}C NMR of 3af (100 MHz, Chloroform-*d*)

2-(benzylthio)-1-phenylpent-4-en-1-one (3ag)

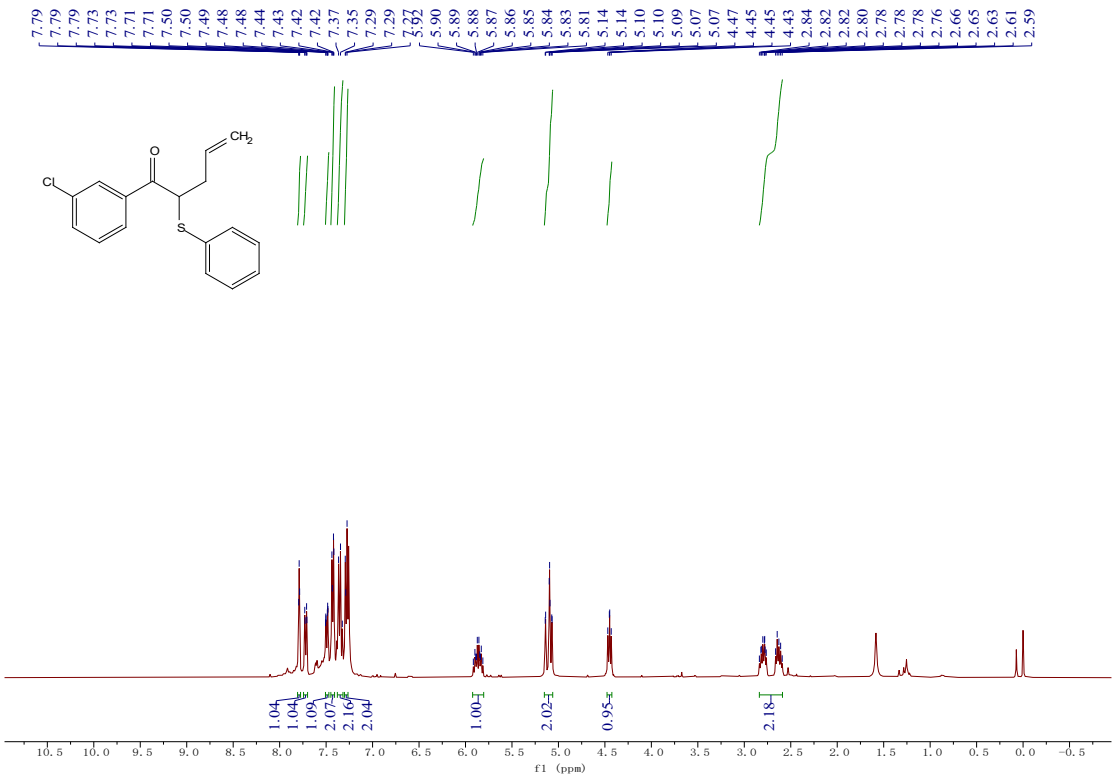


^{1}H NMR of 3ag (400 MHz, Dimethyl sulfoxide-d_6)

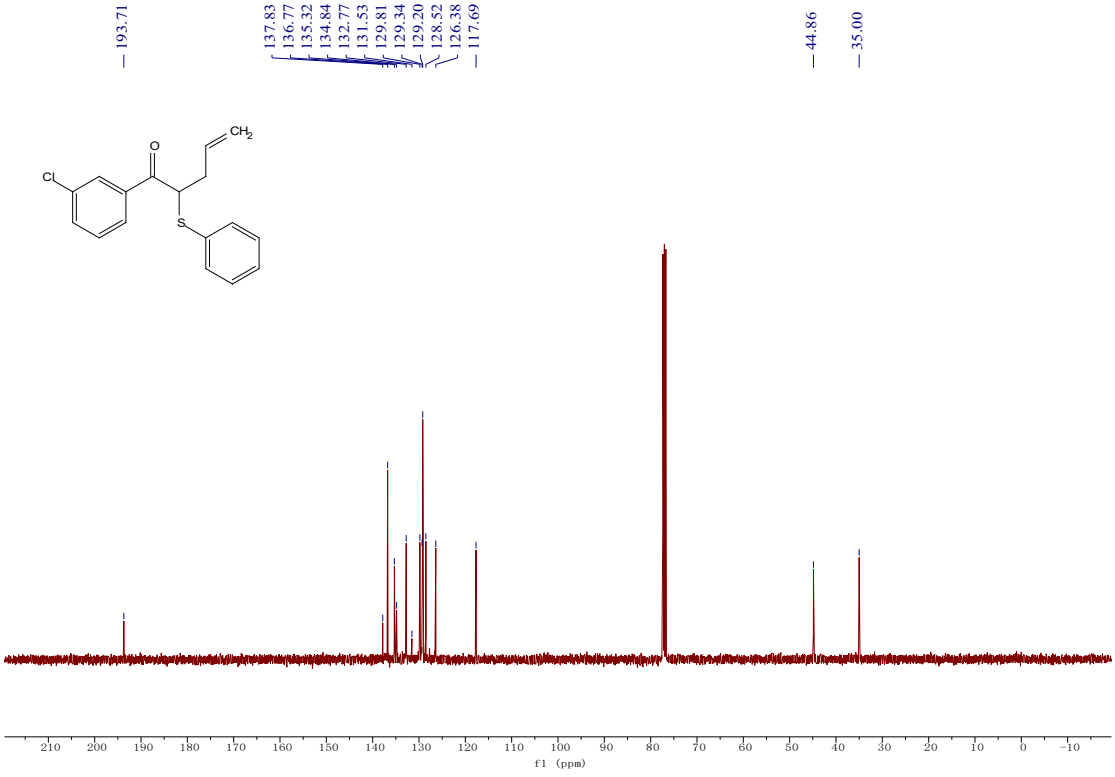


^{13}C NMR of 3ag (100 MHz, Chloroform-d)

1-(3-chlorophenyl)-2-(phenylthio)pent-4-en-1-one (3ba)

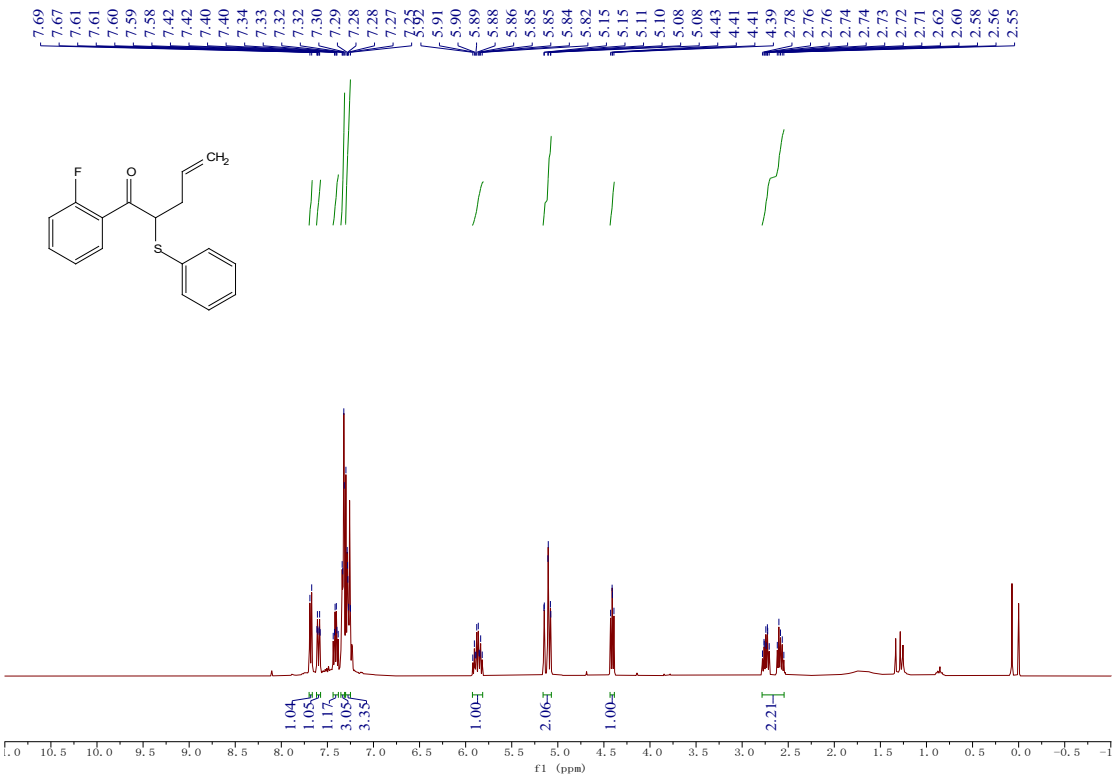


^{1}H NMR of 3ba (400 MHz, Chloroform-*d*)

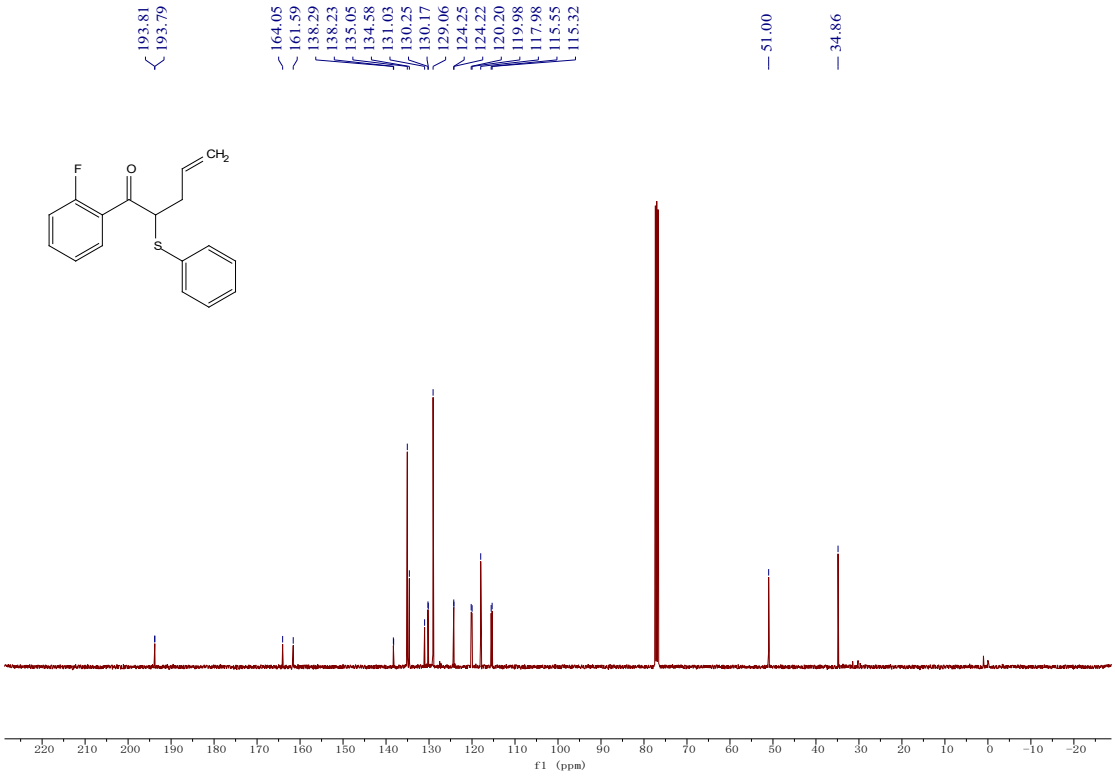


^{13}C NMR of 3ba (100 MHz, Chloroform-*d*)

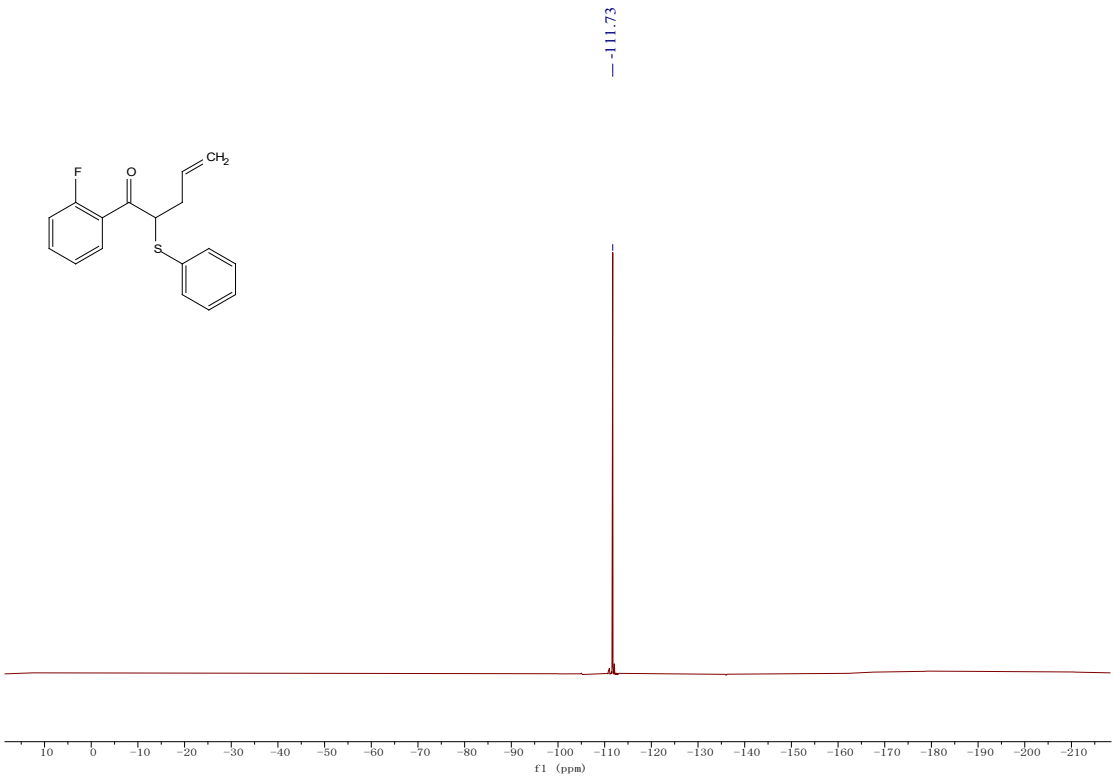
1-(2-fluorophenyl)-2-(phenylthio)pent-4-en-1-one (3ca)



^{1}H NMR of 3ca (400 MHz, Chloroform-*d*)

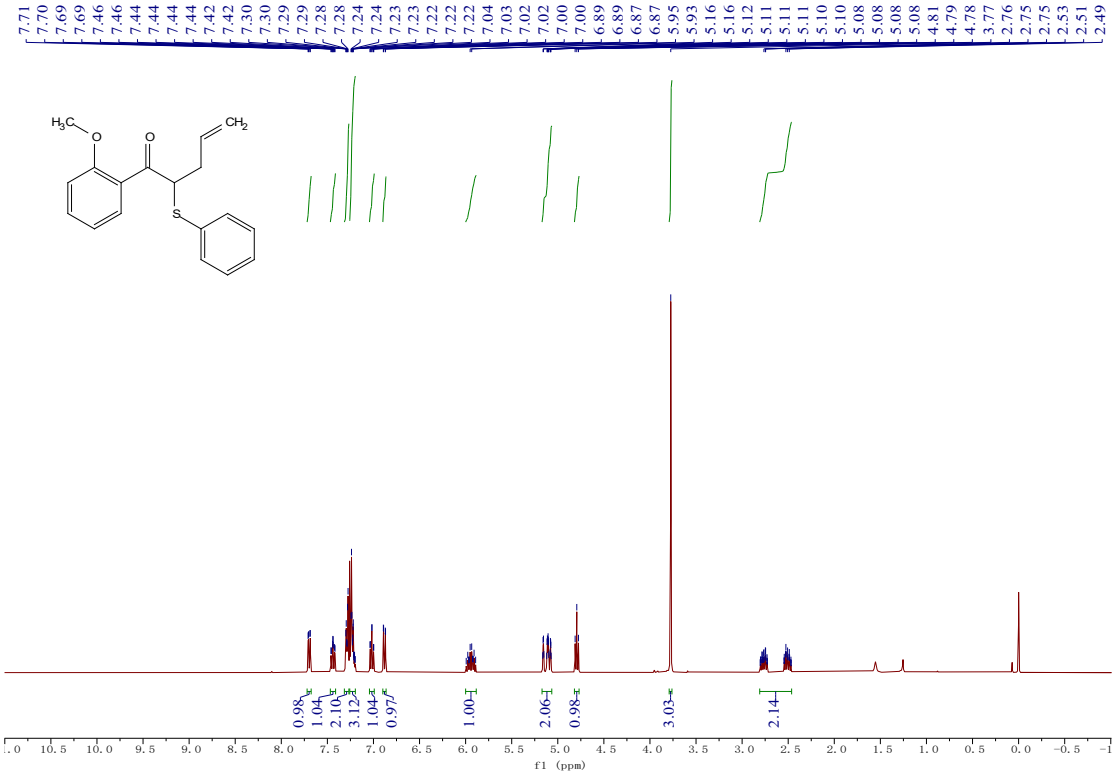


^{13}C NMR of 3ca (100 MHz, Chloroform-*d*)

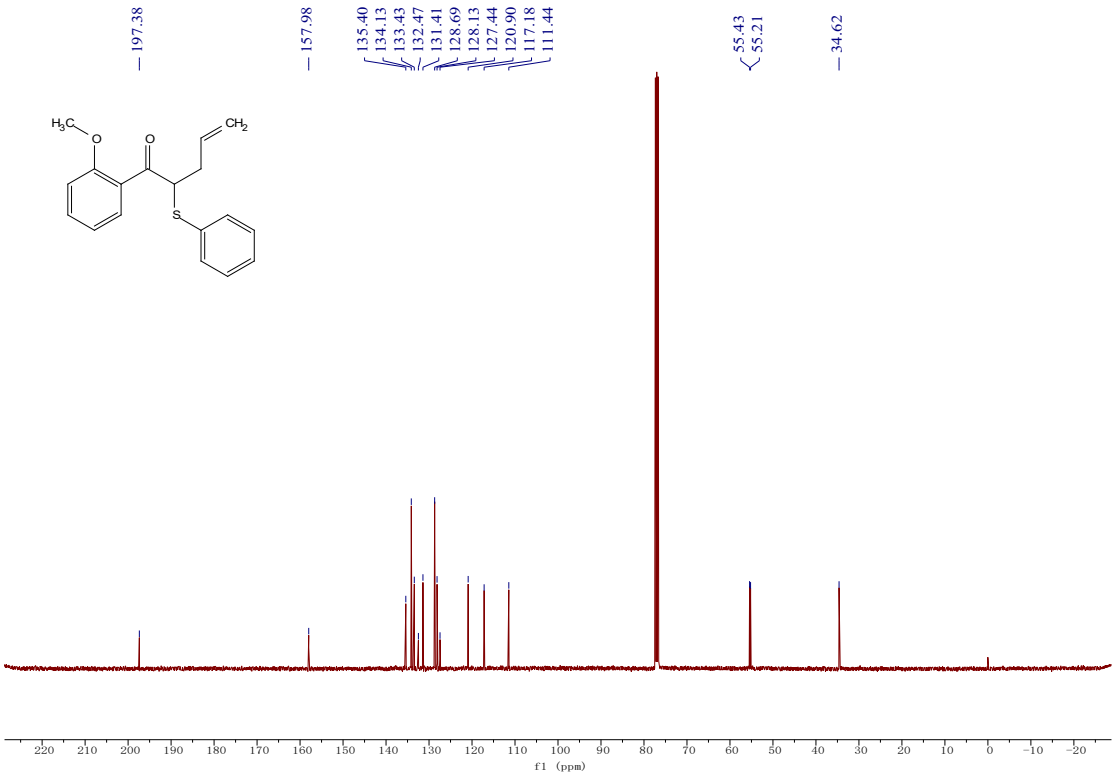


^{19}F NMR of 3ca (376 MHz, Chloroform-*d*)

1-(2-methoxyphenyl)-2-(phenylthio)pent-4-en-1-one (3da)

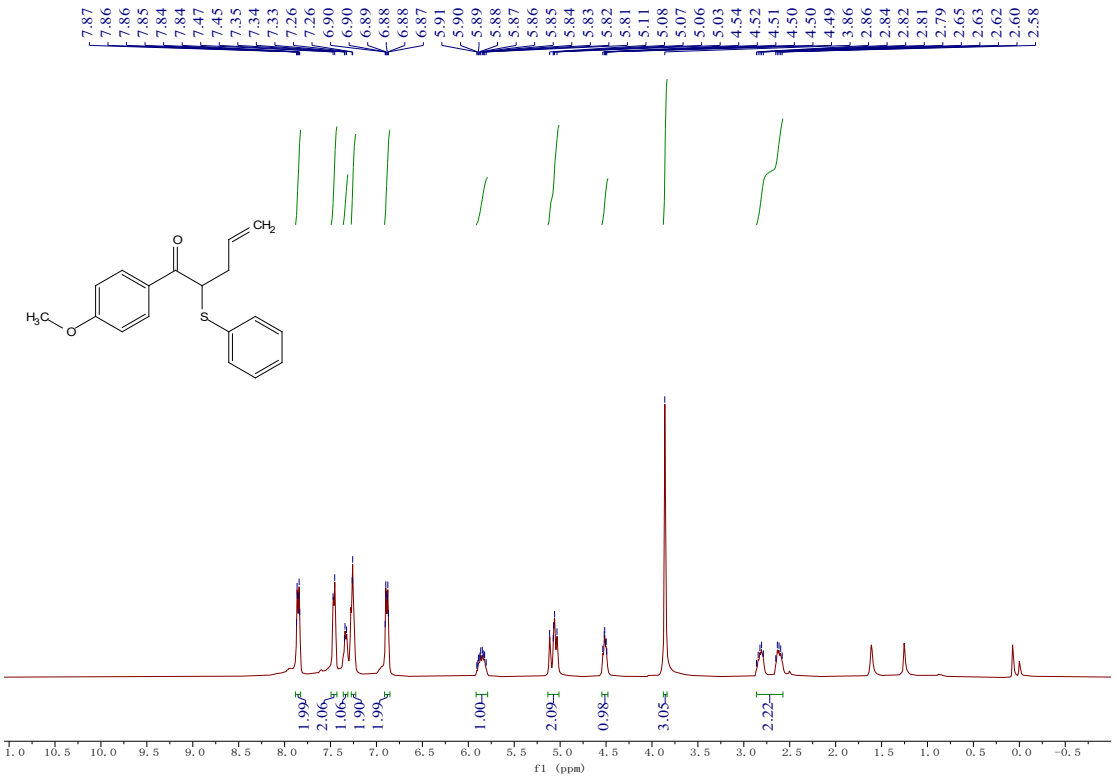


^{1}H NMR of 3da (400 MHz, Chloroform-*d*)

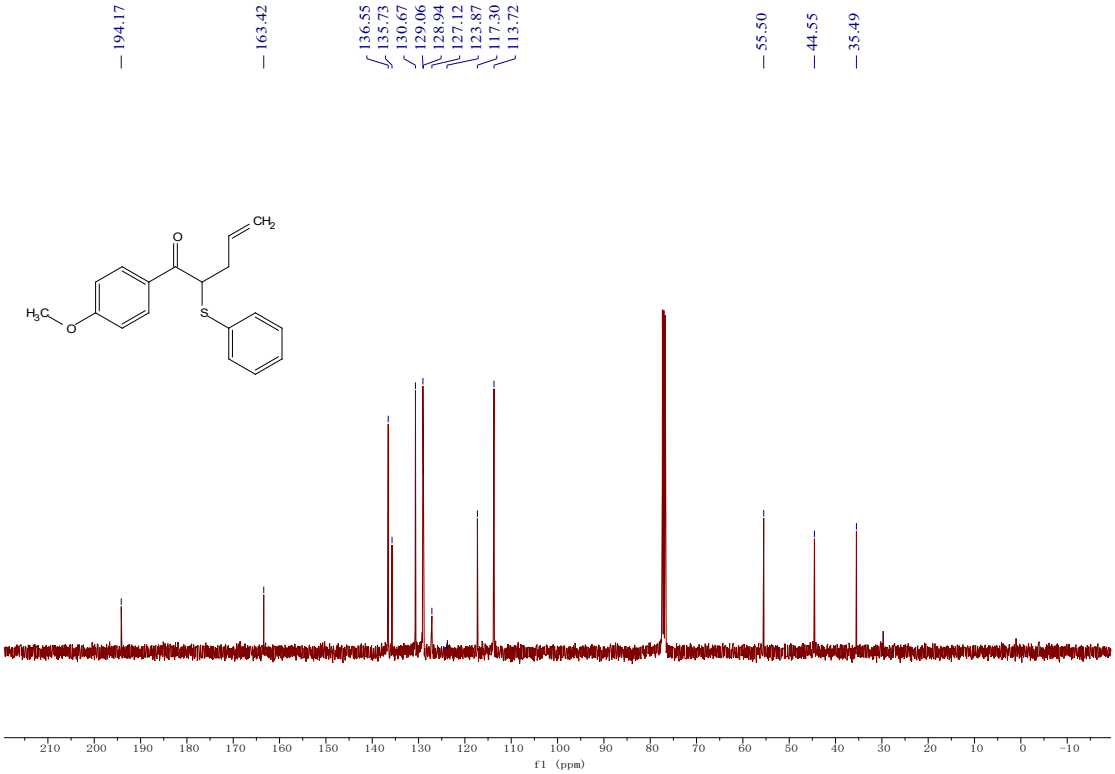


^{13}C NMR of 3da (100 MHz, Chloroform-*d*)

1-(4-methoxyphenyl)-2-(phenylthio)pent-4-en-1-one (3ea)

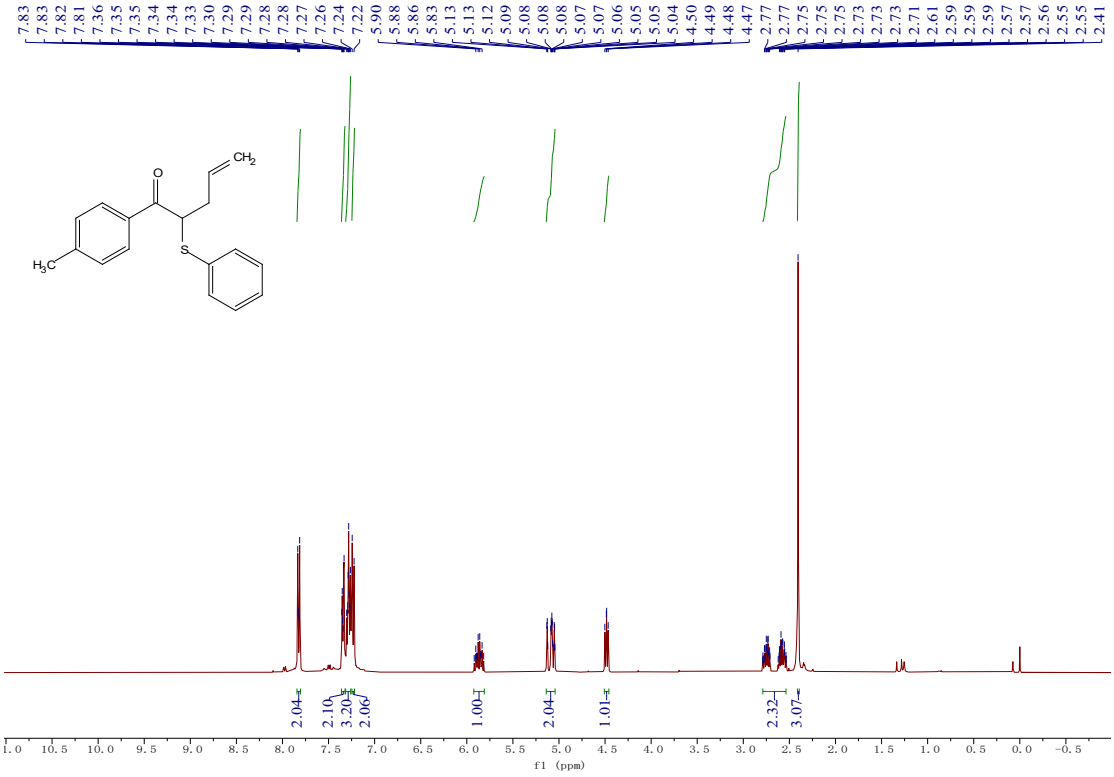


^{1}H NMR of 3ea (400 MHz, Chloroform-*d*)

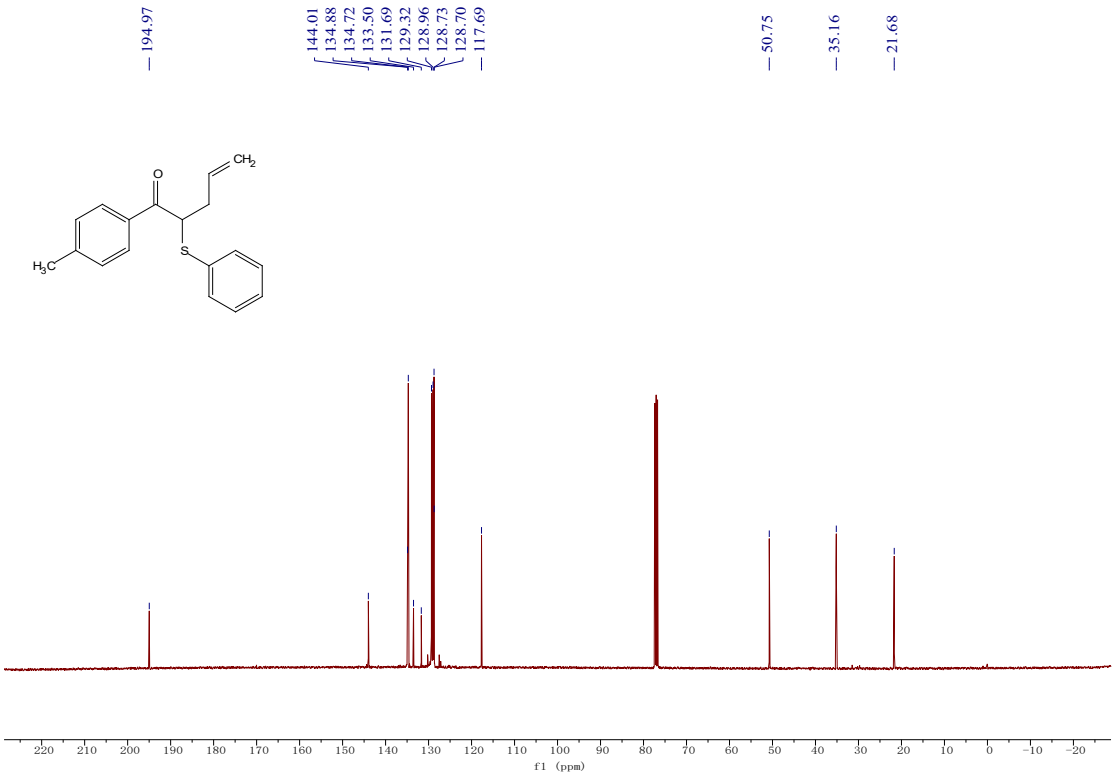


^{13}C NMR of 3ea (100 MHz, Chloroform-*d*)

2-(phenylthio)-1-(p-tolyl)pent-4-en-1-one (3fa)

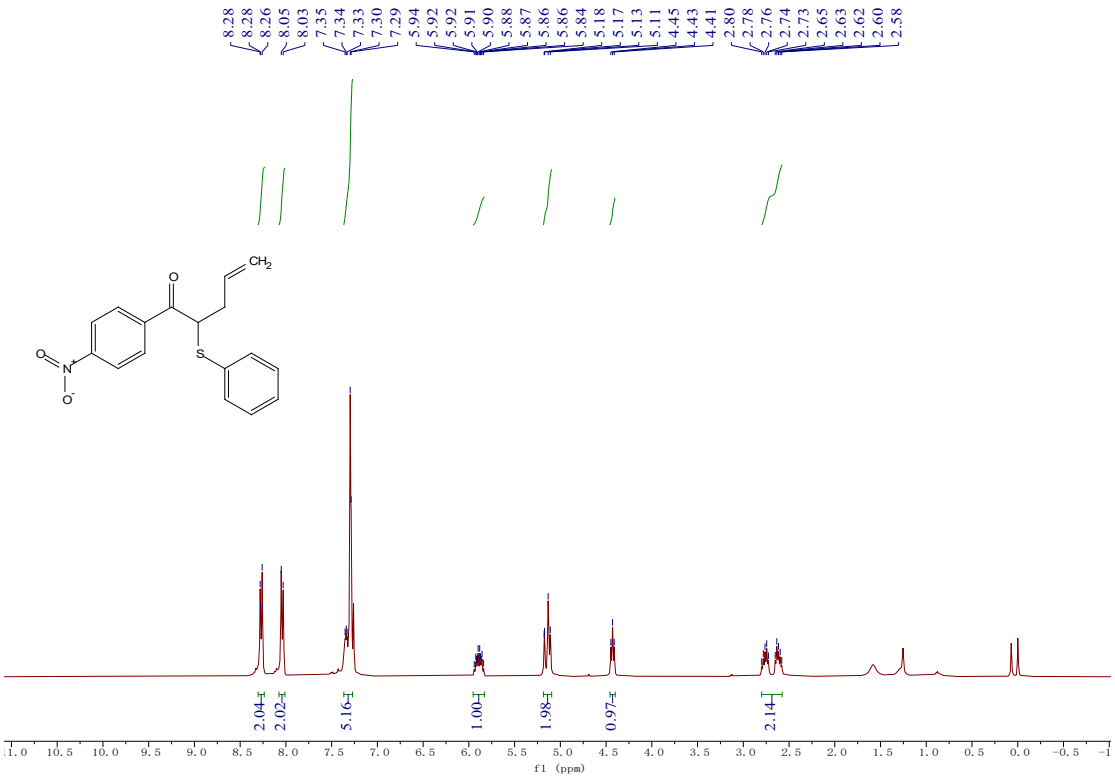


^{1}H NMR of 3fa (400 MHz, Chloroform-*d*)

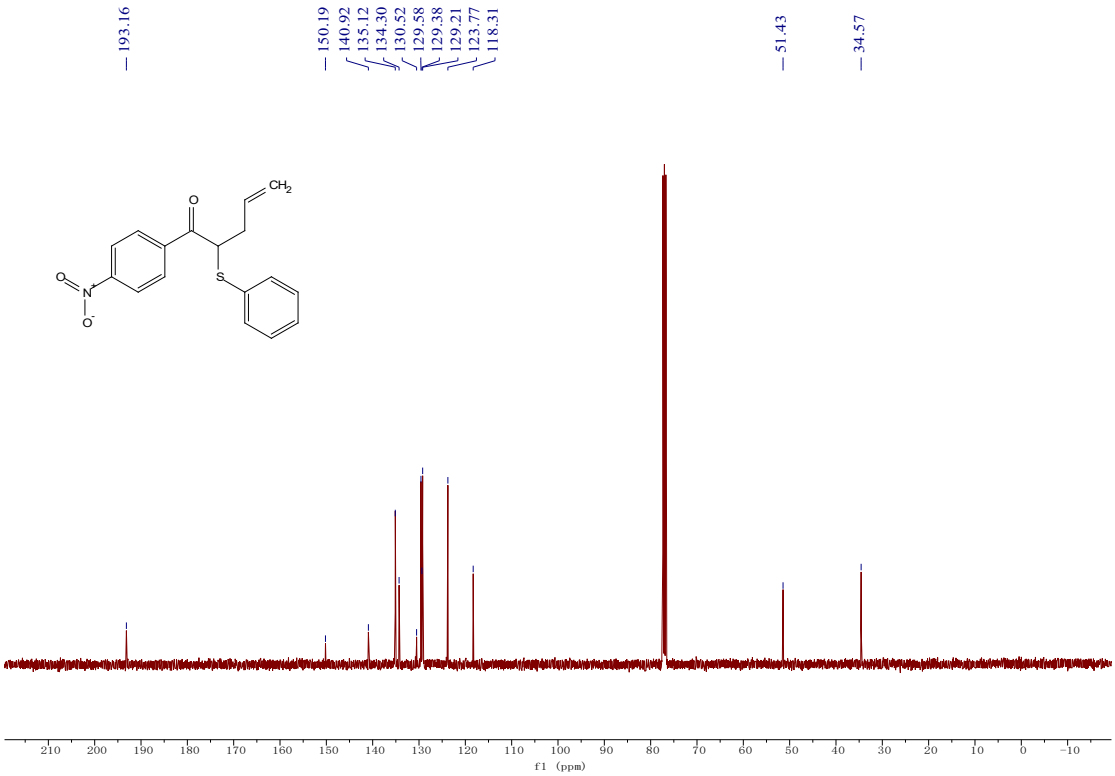


^{13}C NMR of 3fa (100 MHz, Chloroform-*d*)

1-(4-nitrophenyl)-2-(phenylthio)pent-4-en-1-one (3ga)

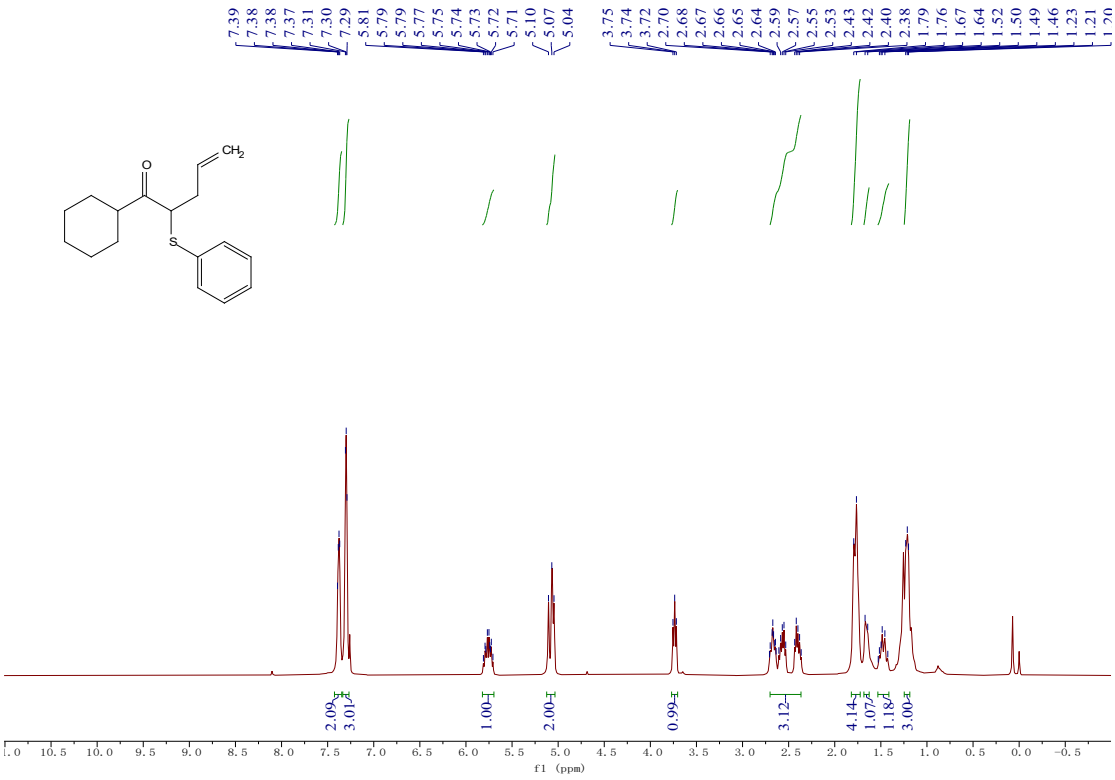


^{1}H NMR of 3ga (400 MHz, Chloroform-*d*)

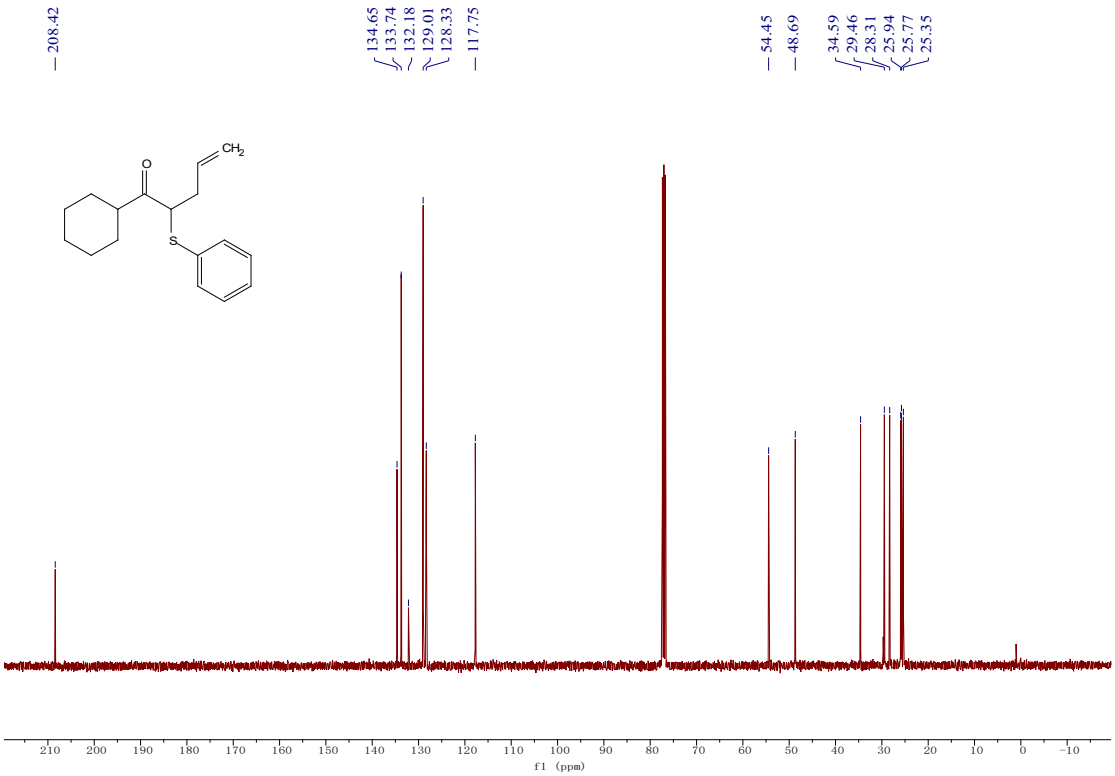


^{13}C NMR of 3ga (100 MHz, Chloroform-*d*)

1-cyclohexyl-2-(phenylthio)pent-4-en-1-one (3ha)

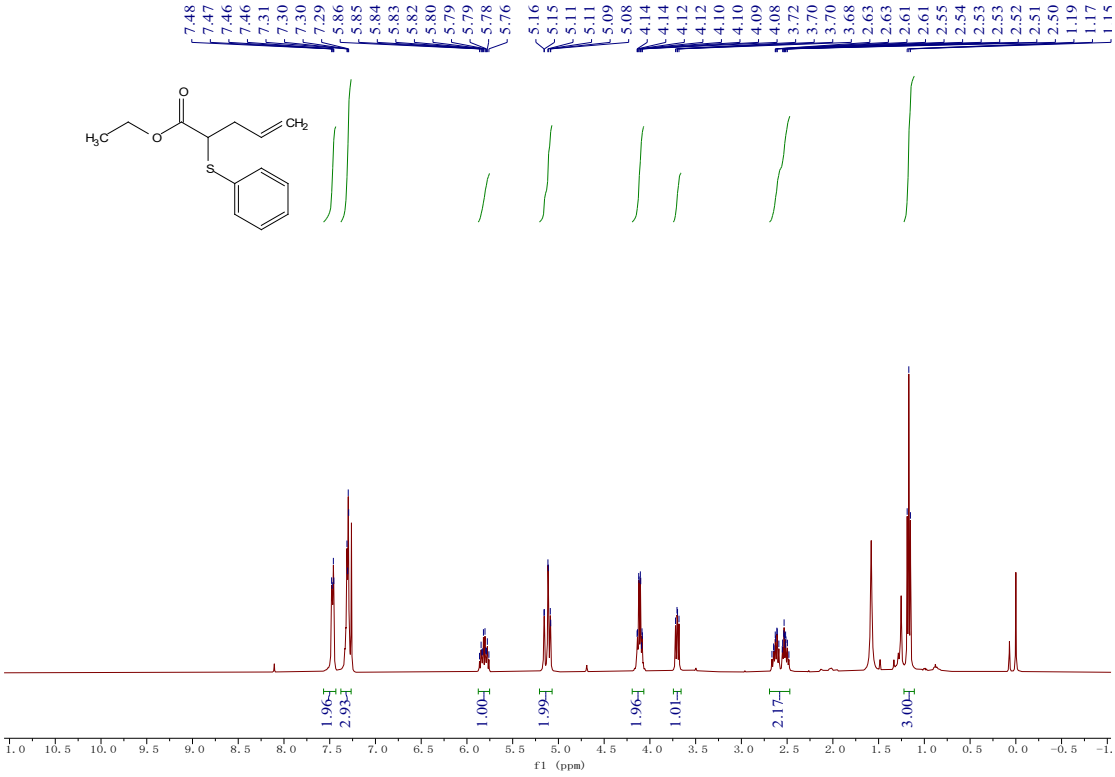


^{1}H NMR of 3ha (400 MHz, Chloroform-*d*)

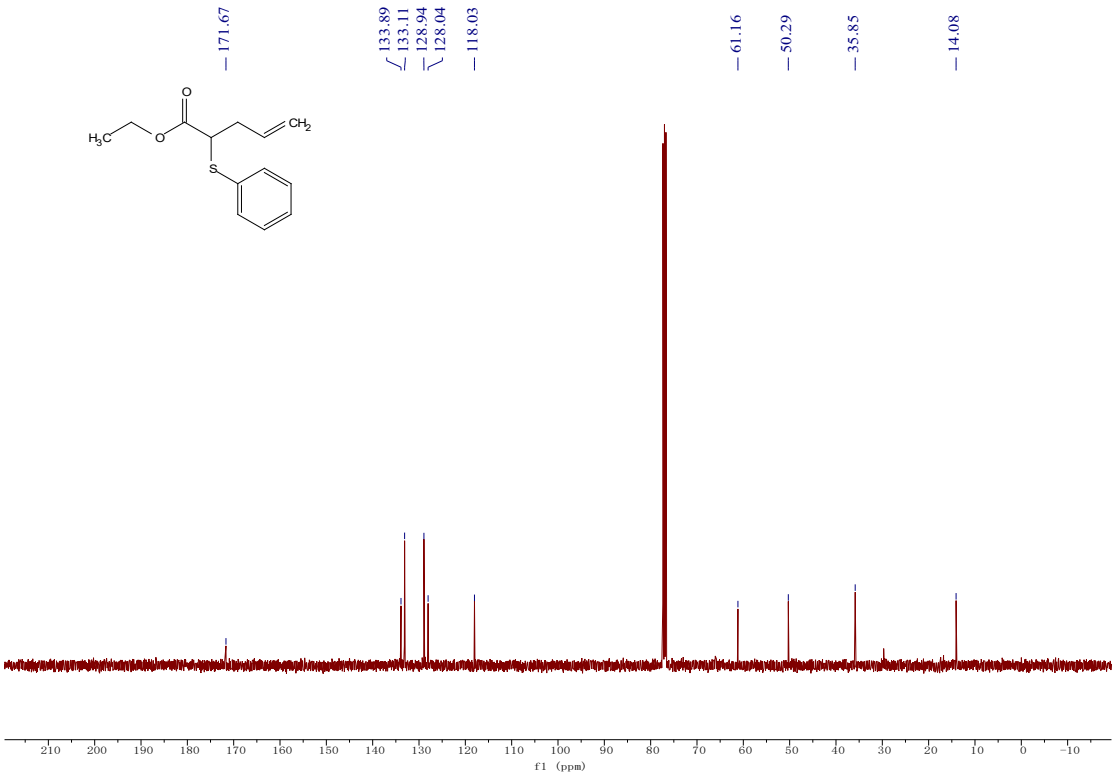


^{13}C NMR of 3ha (100 MHz, Chloroform-*d*)

ethyl 2-(phenylthio)pent-4-enoate (3ia)

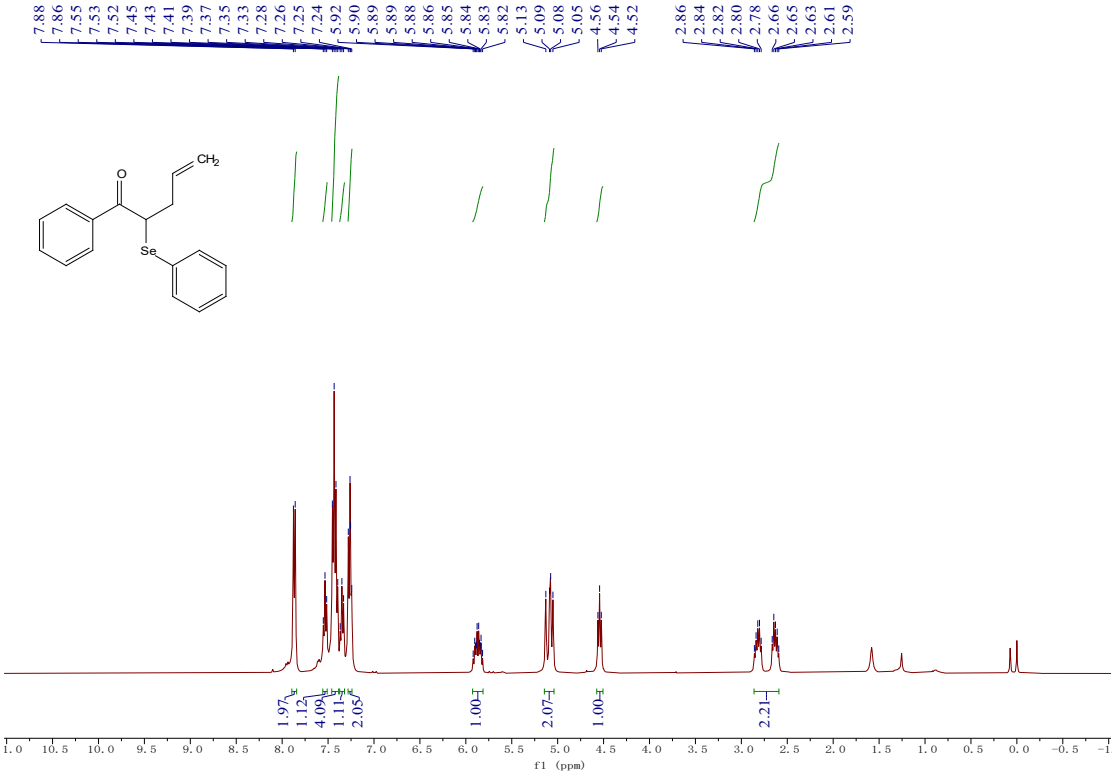


^{1}H NMR of 3ia (400 MHz, Chloroform-*d*)

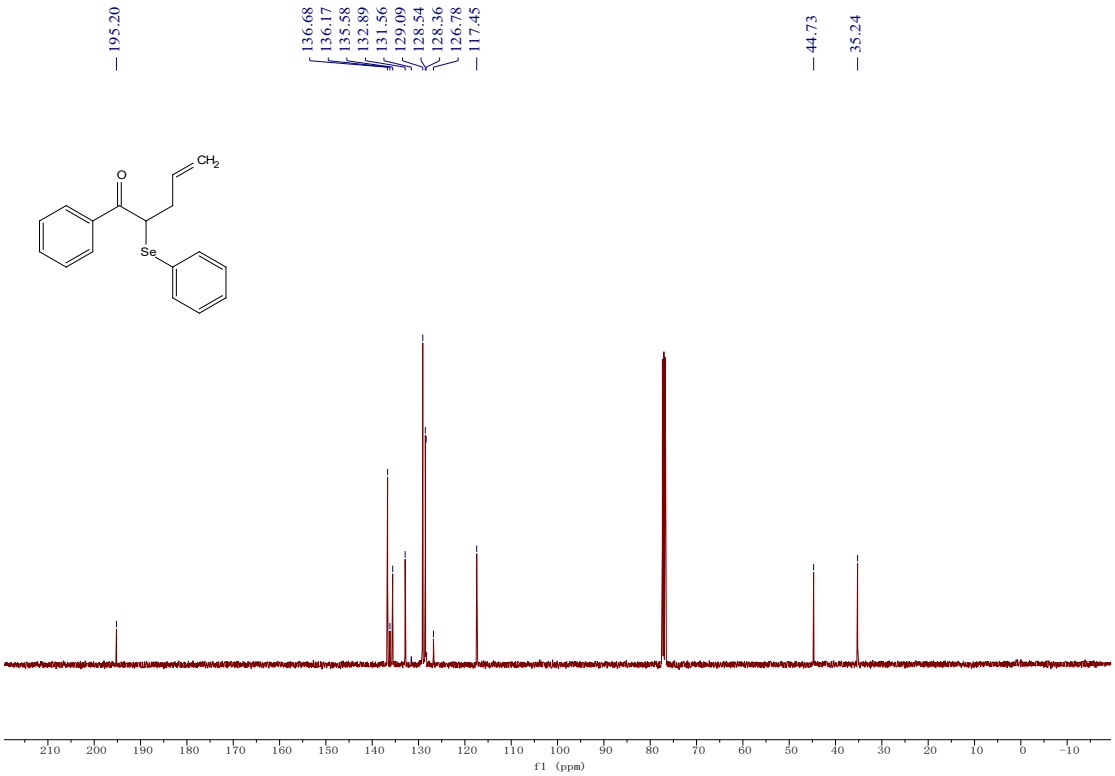


^{13}C NMR of 3ia (100 MHz, Chloroform-*d*)

1-phenyl-2-(phenylselanyl)pent-4-en-1-one (5aa)

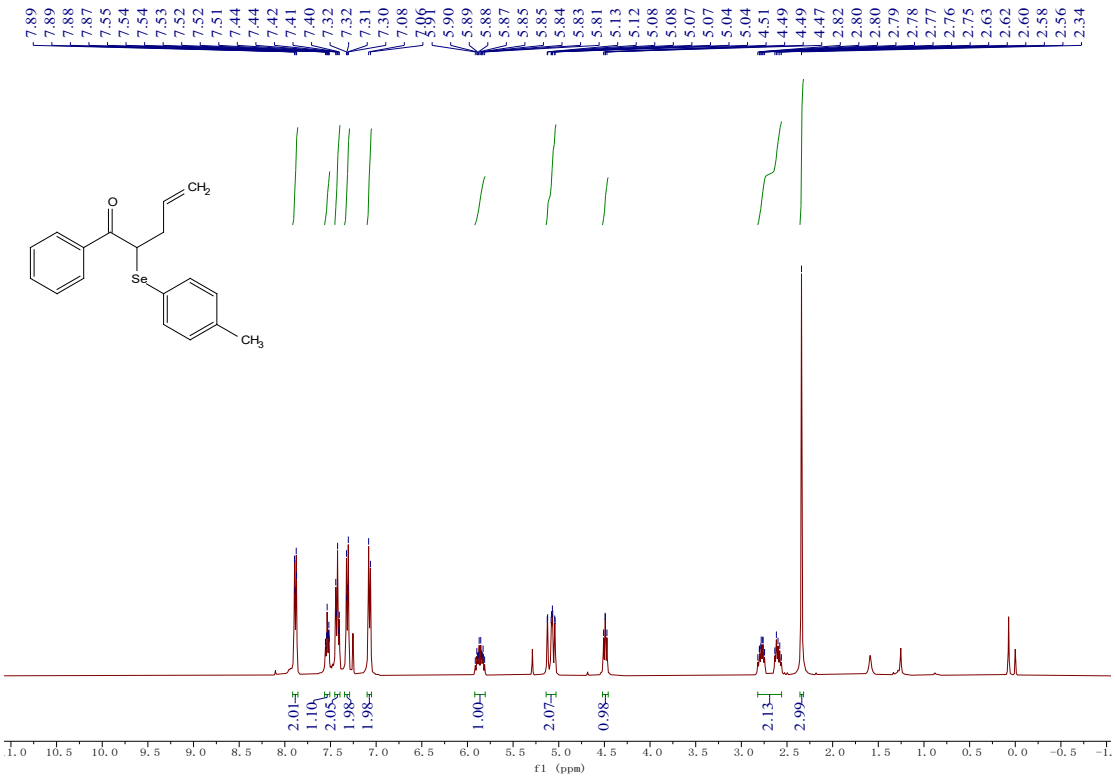


^{1}H NMR of 5aa (400 MHz, Chloroform-*d*)

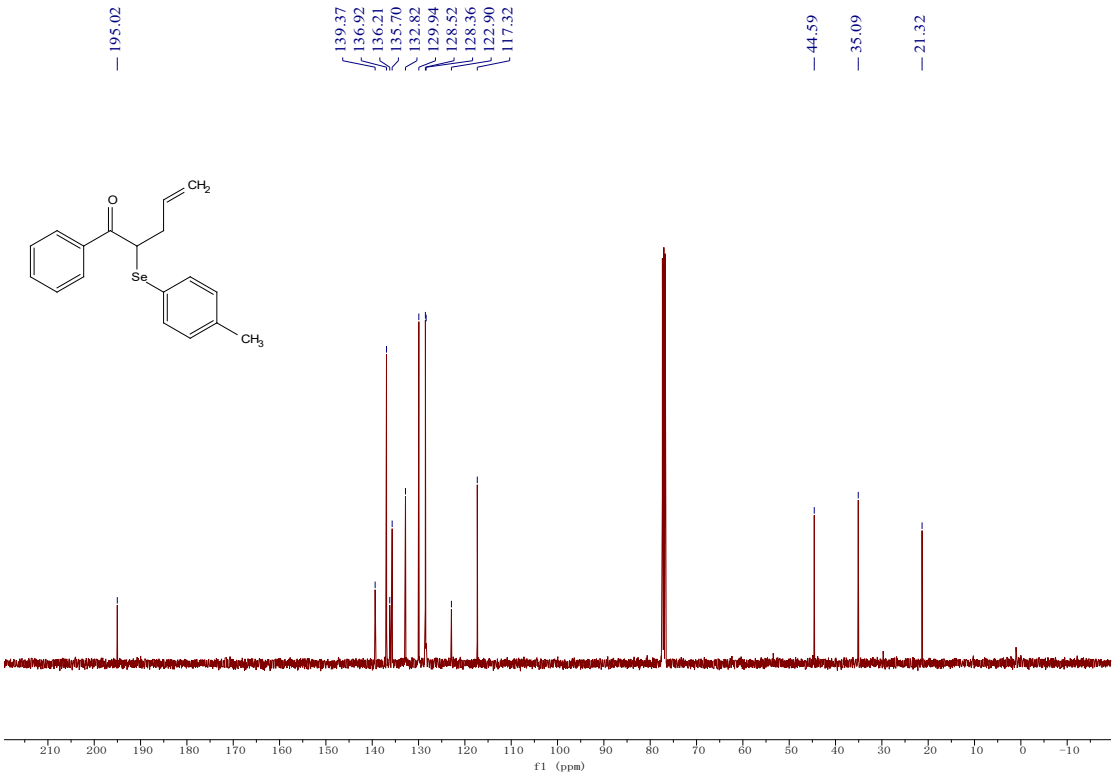


^{13}C NMR of 5aa (100 MHz, Chloroform-*d*)

1-phenyl-2-(p-tolylselanyl)pent-4-en-1-one (5ab)

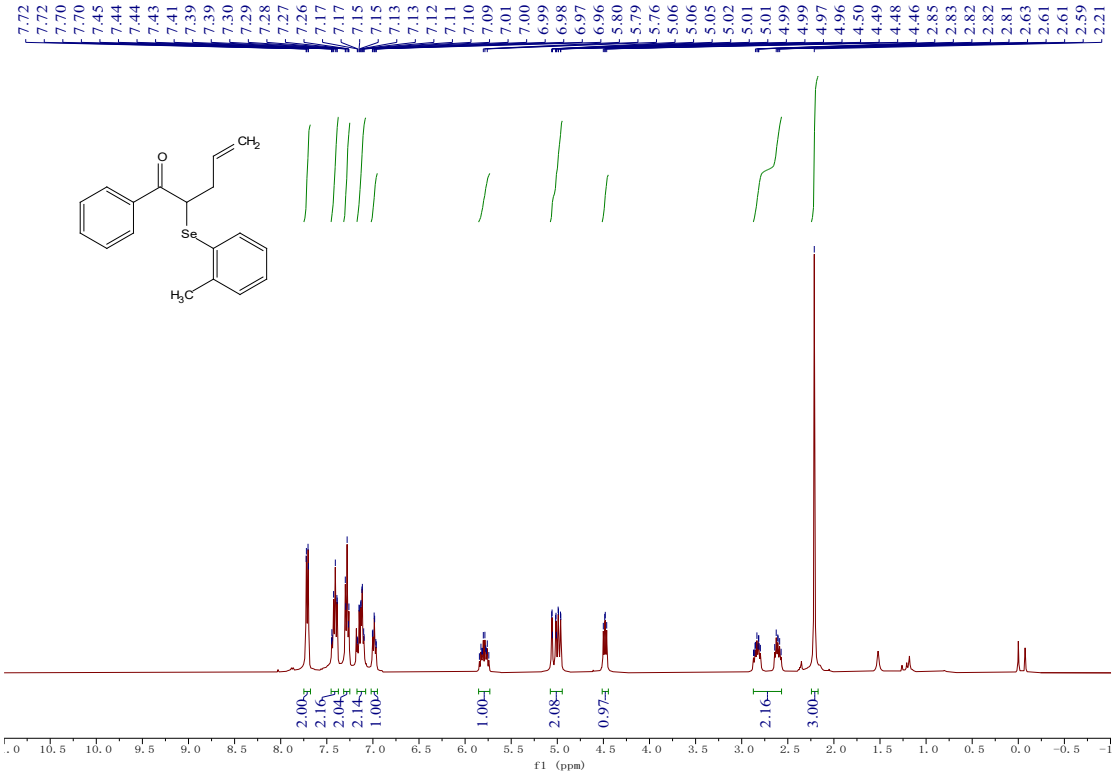


^{1}H NMR of 5ab (400 MHz, Chloroform-*d*)

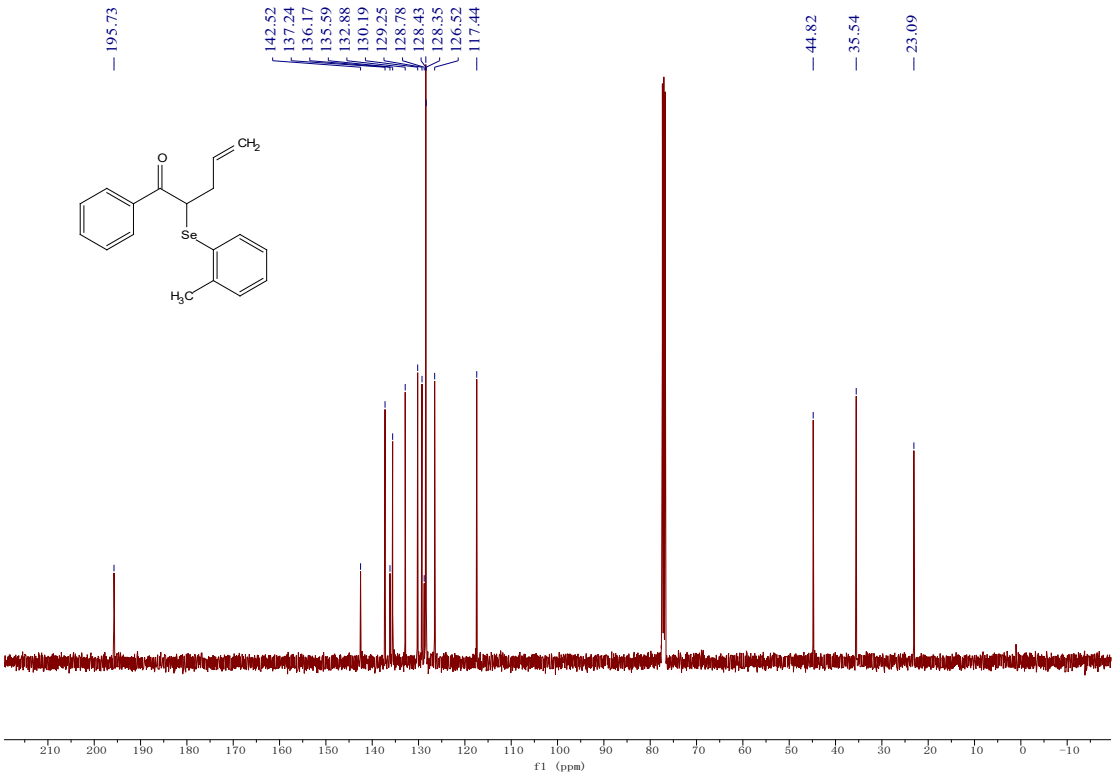


^{13}C NMR of 5ab (100 MHz, Chloroform-*d*)

1-phenyl-2-(o-tolylselanyl)pent-4-en-1-one (5ac)

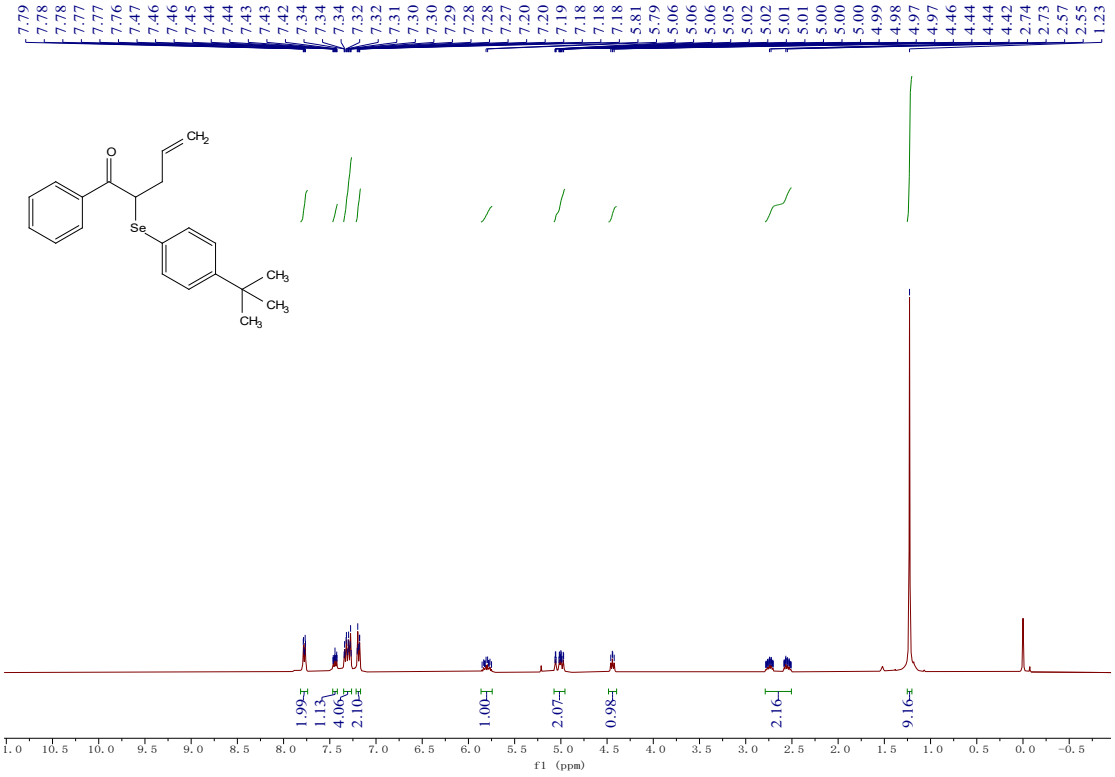


^{1}H NMR of 5ac (400 MHz, Chloroform-*d*)

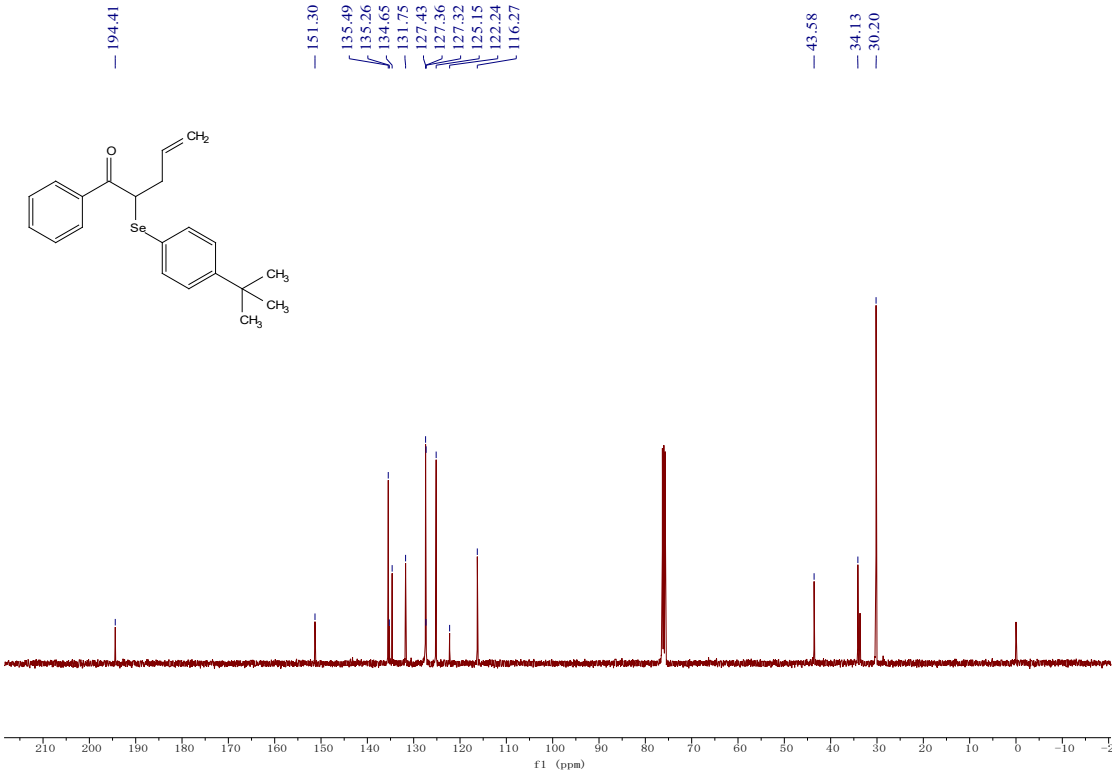


^{13}C NMR of 5ac (100 MHz, Chloroform-*d*)

2-((4-(tert-butyl)phenyl)selanyl)-1-phenylpent-4-en-1-one (5ad)

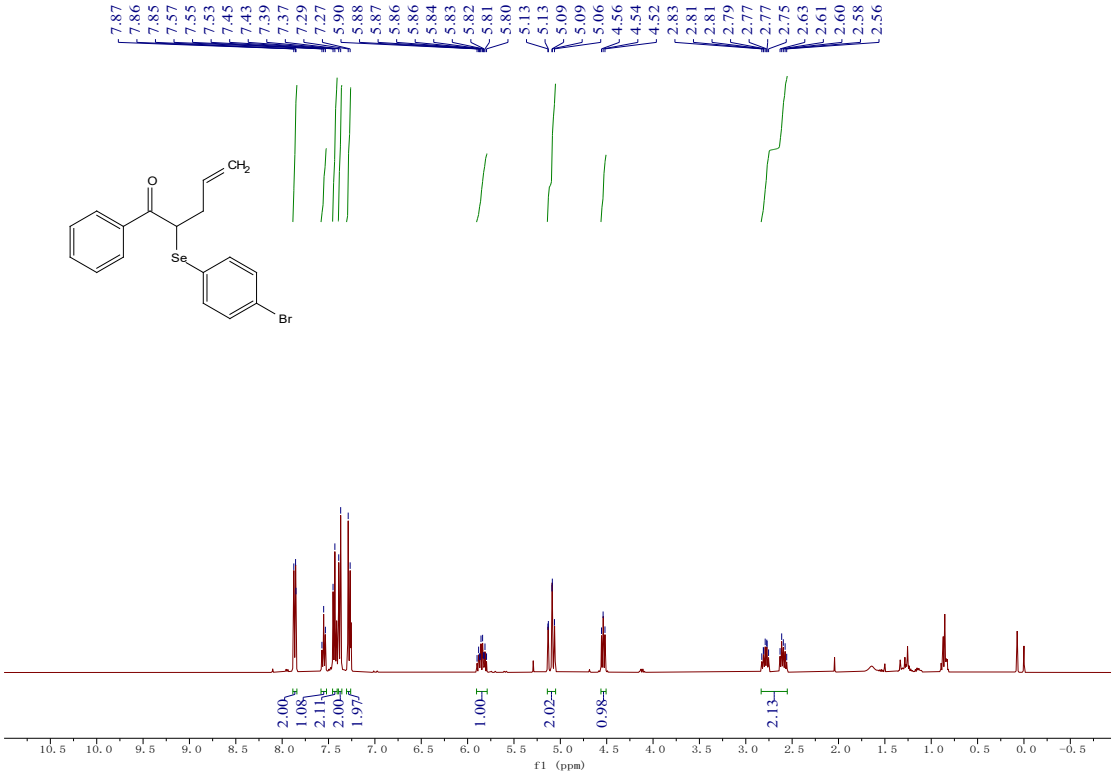


^{1}H NMR of 5ad (400 MHz, Chloroform-*d*)

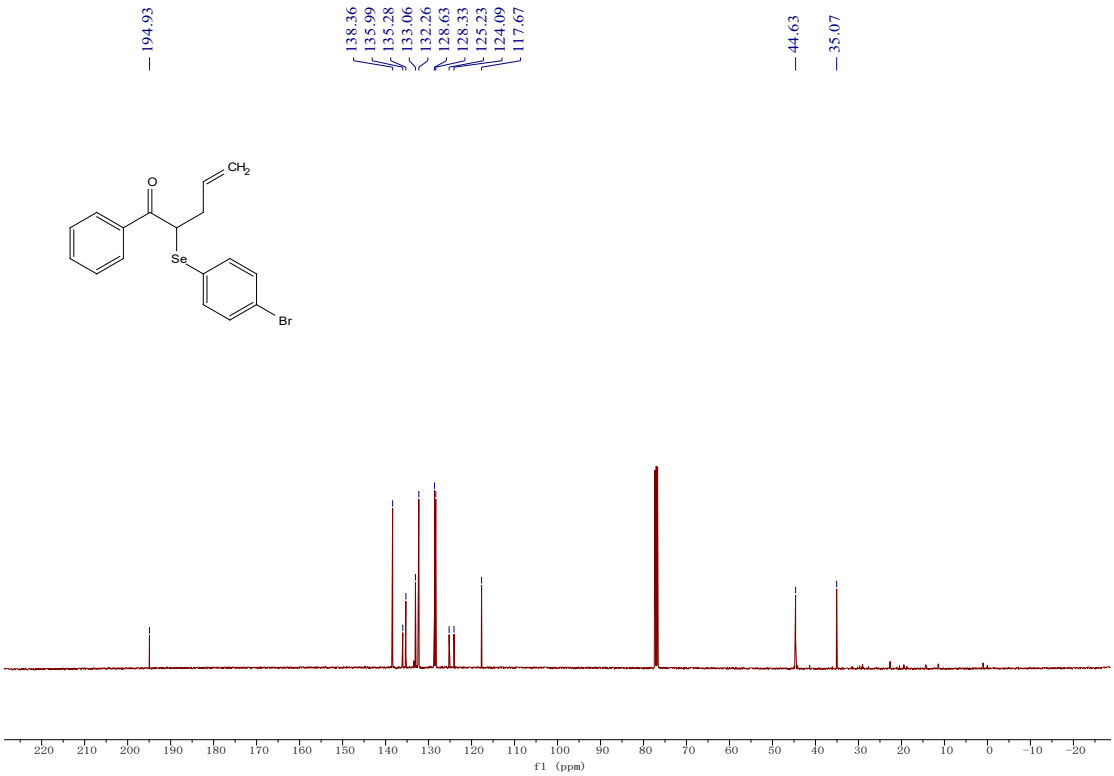


^{13}C NMR of 5ad (100 MHz, Chloroform-*d*)

2-((4-bromophenyl)selanyl)-1-phenylpent-4-en-1-one (5ae)

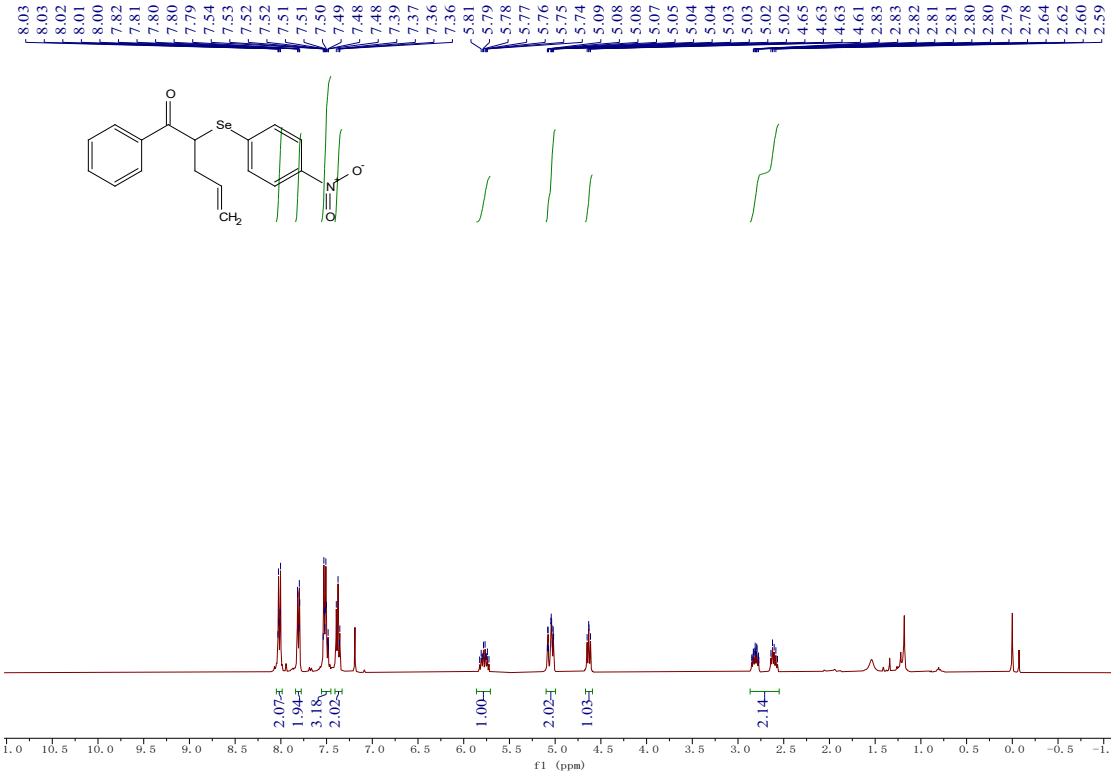


^{1}H NMR of 5ae (400 MHz, Chloroform-*d*)

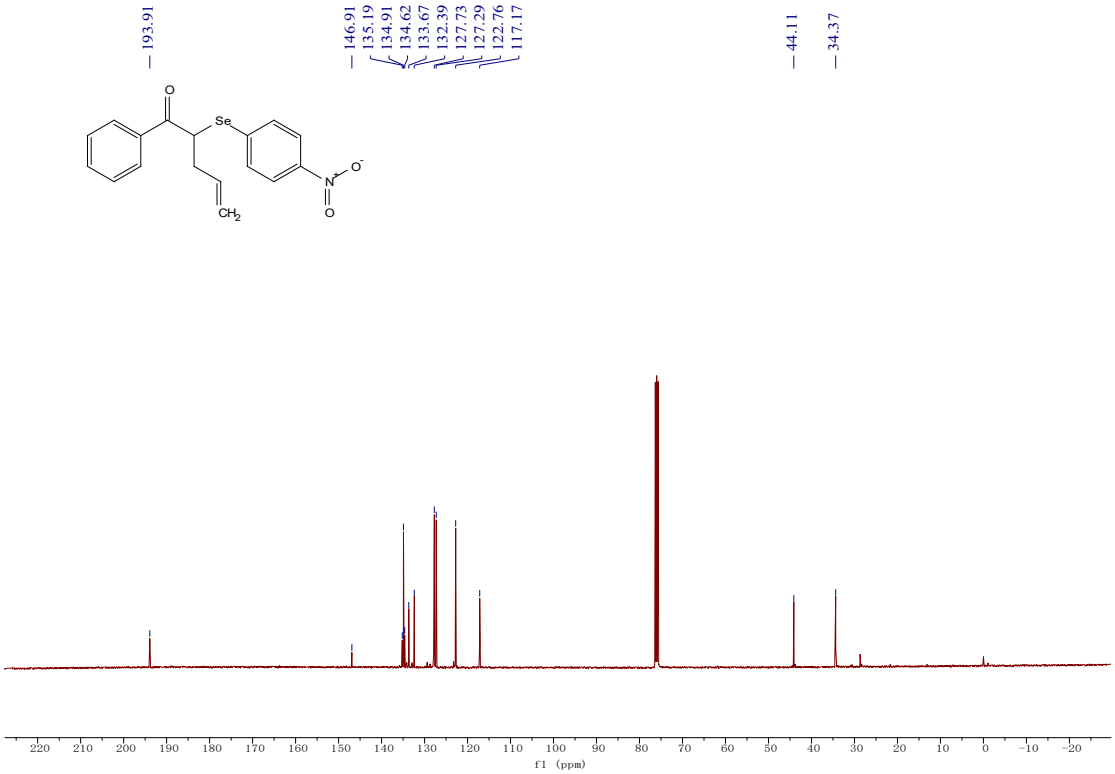


^{13}C NMR of 5ae (100 MHz, Chloroform-*d*)

2-((4-nitrophenyl)selanyl)-1-phenylpent-4-en-1-one (5af)

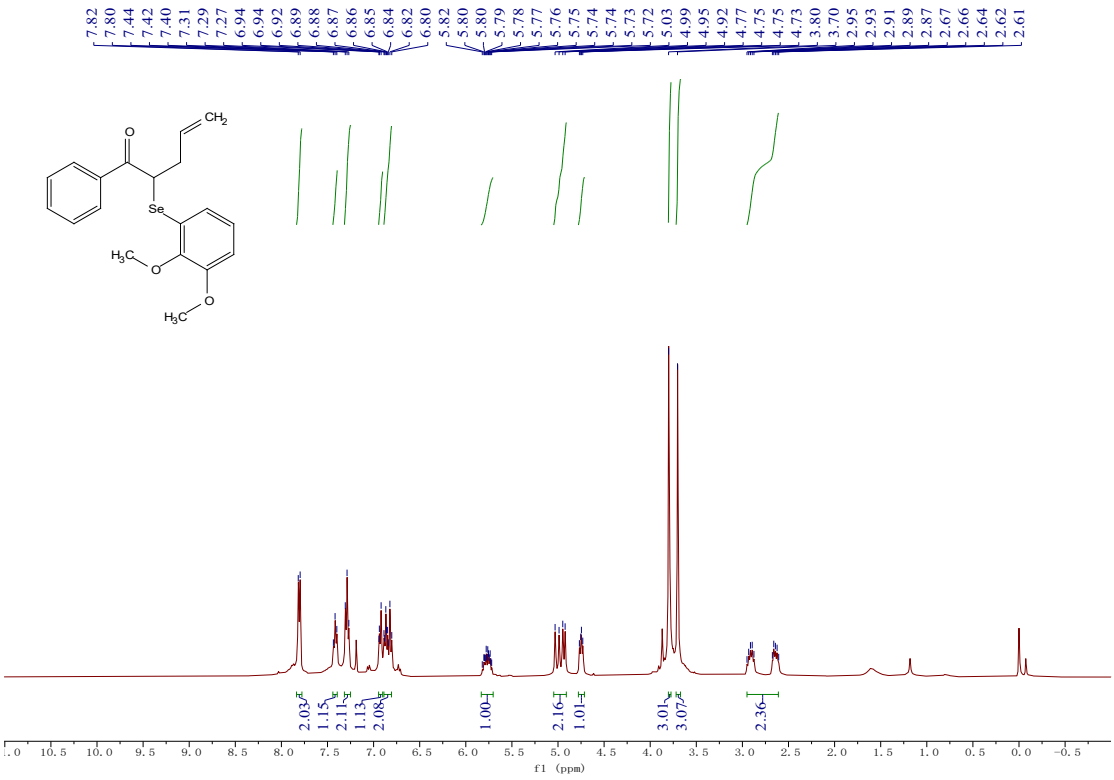


^{1}H NMR of 5af (400 MHz, Chloroform-*d*)

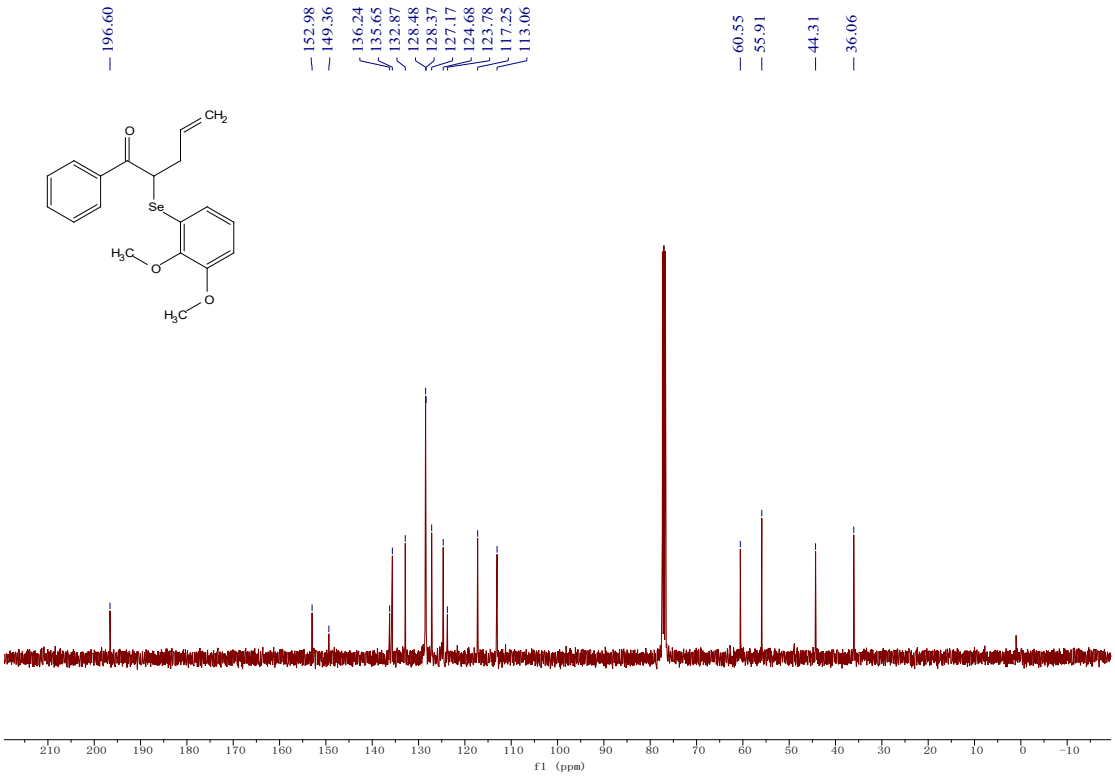


^{13}C NMR of 5af (100 MHz, Chloroform-*d*)

2-((2,3-dimethoxyphenyl)selanyl)-1-phenylpent-4-en-1-one (5ag)

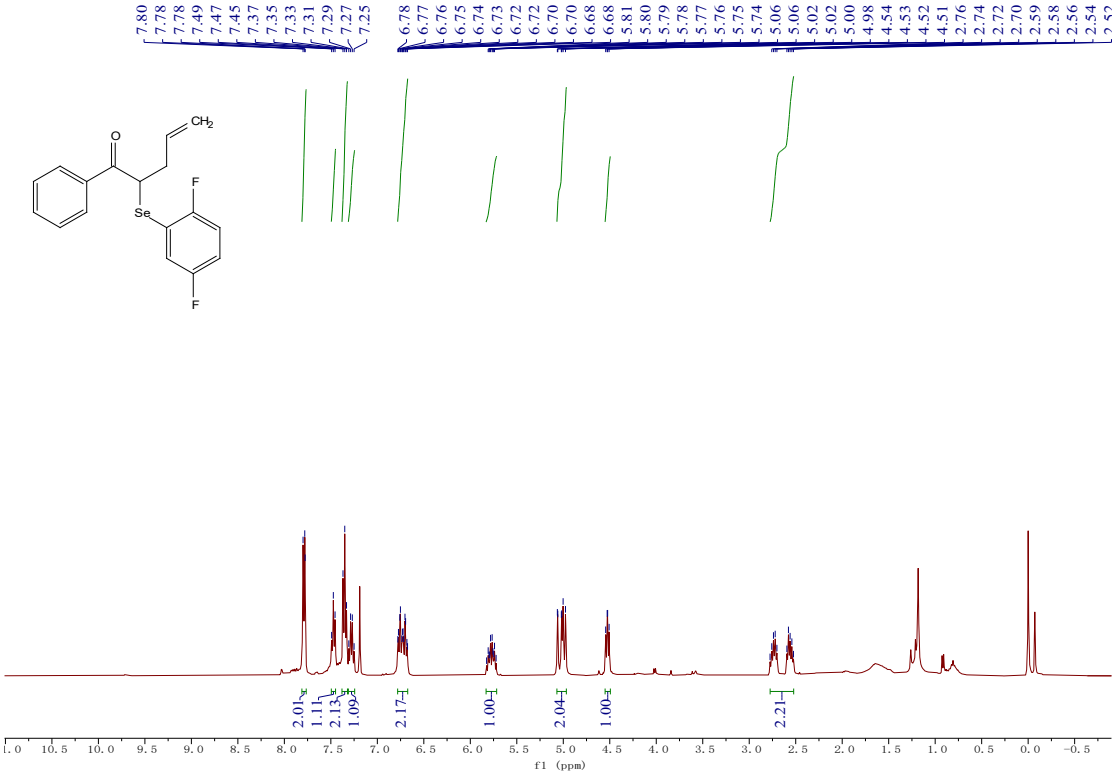


^{1}H NMR of 5ag (400 MHz, Chloroform-*d*)

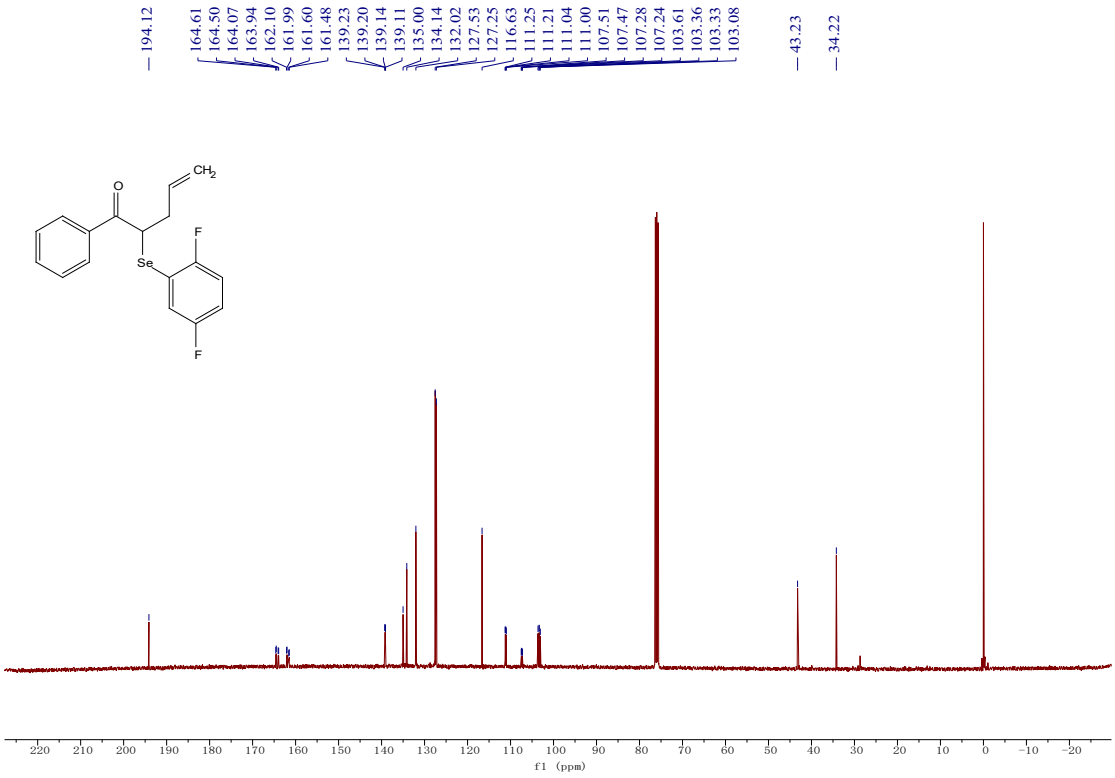


^{13}C NMR of 5ag (100 MHz, Chloroform-*d*)

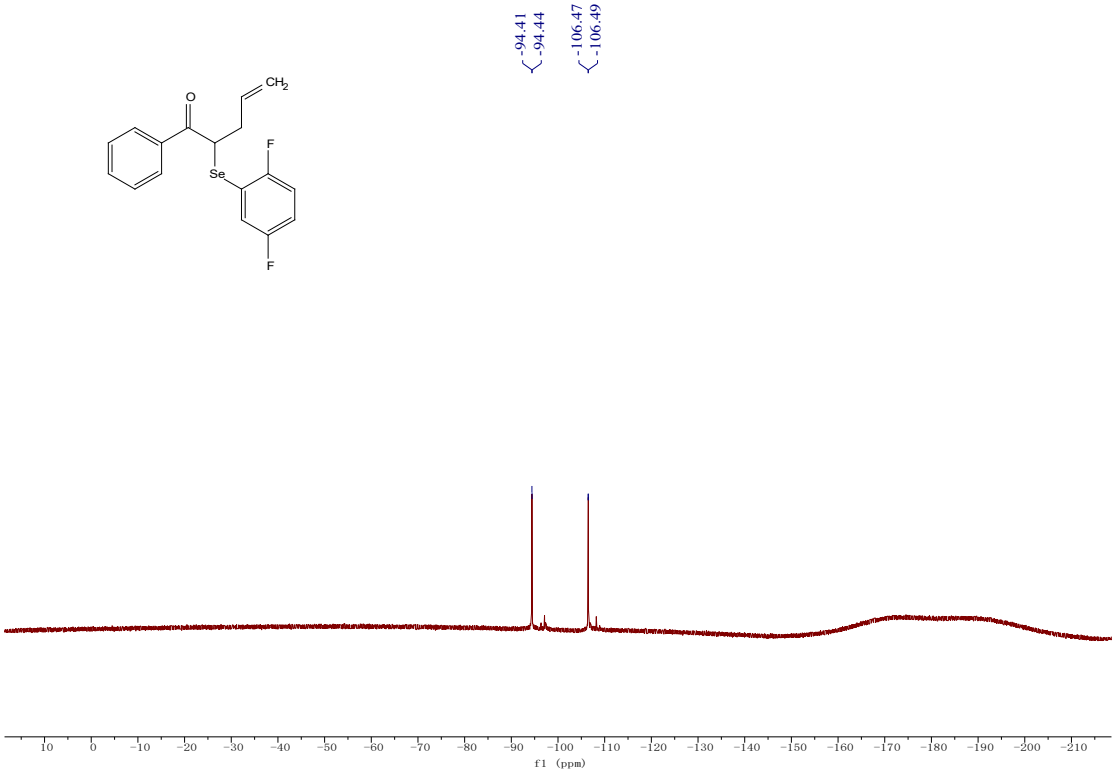
2-((2,5-difluorophenyl)selanyl)-1-phenylpent-4-en-1-one (5ah)



^{1}H NMR of 5ah (400 MHz, Chloroform-*d*)

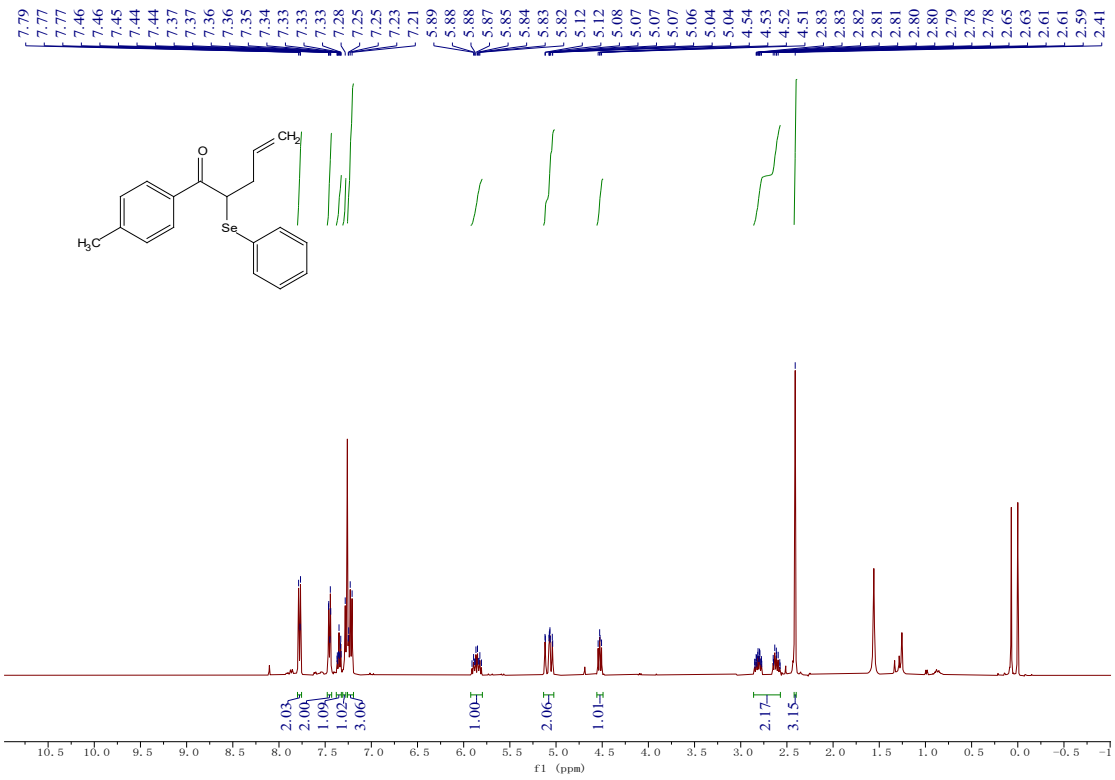


^{13}C NMR of 5ah (100 MHz, Chloroform-*d*)

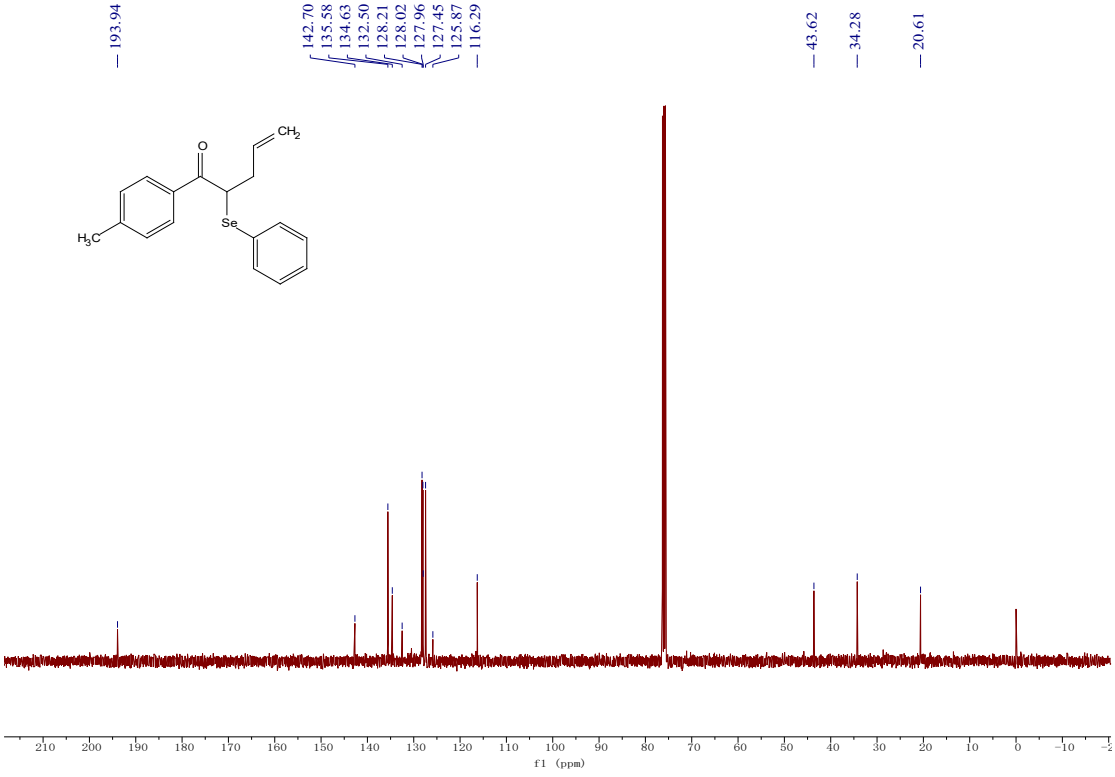


^{19}F NMR of 5ah (376 MHz, Chloroform-*d*)

2-(phenylselanyl)-1-(p-tolyl)pent-4-en-1-one (5ba)

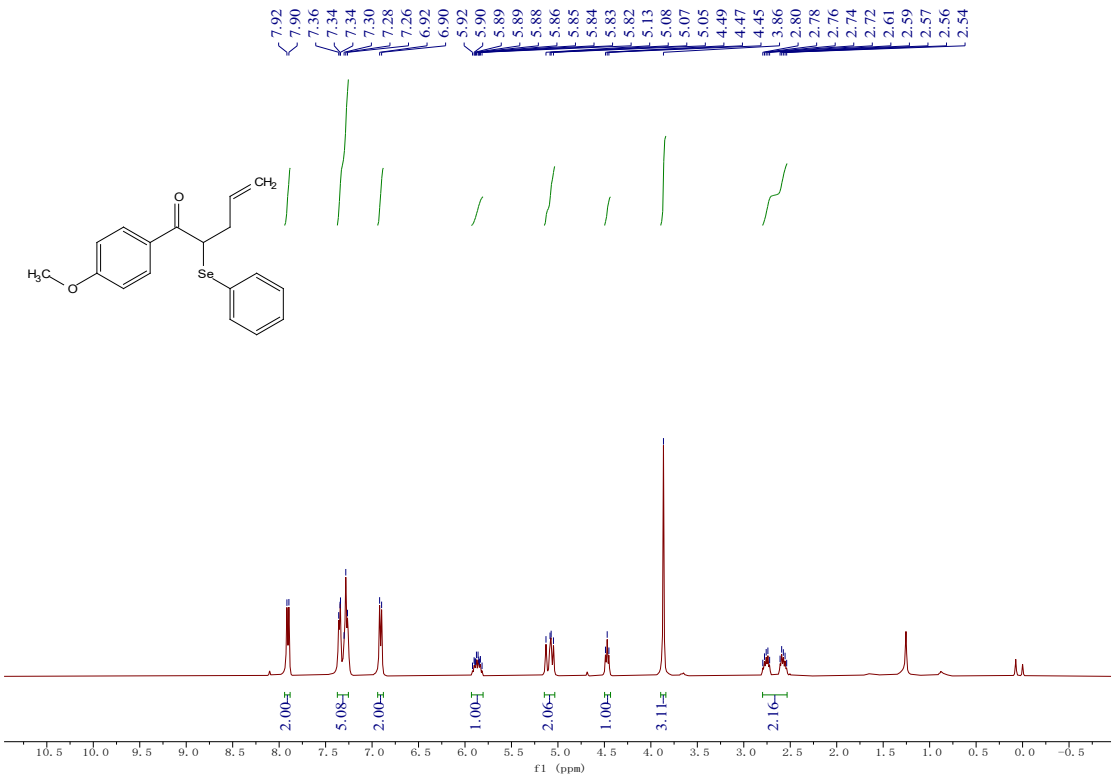


^{1}H NMR of 5ba (400 MHz, Chloroform-*d*)

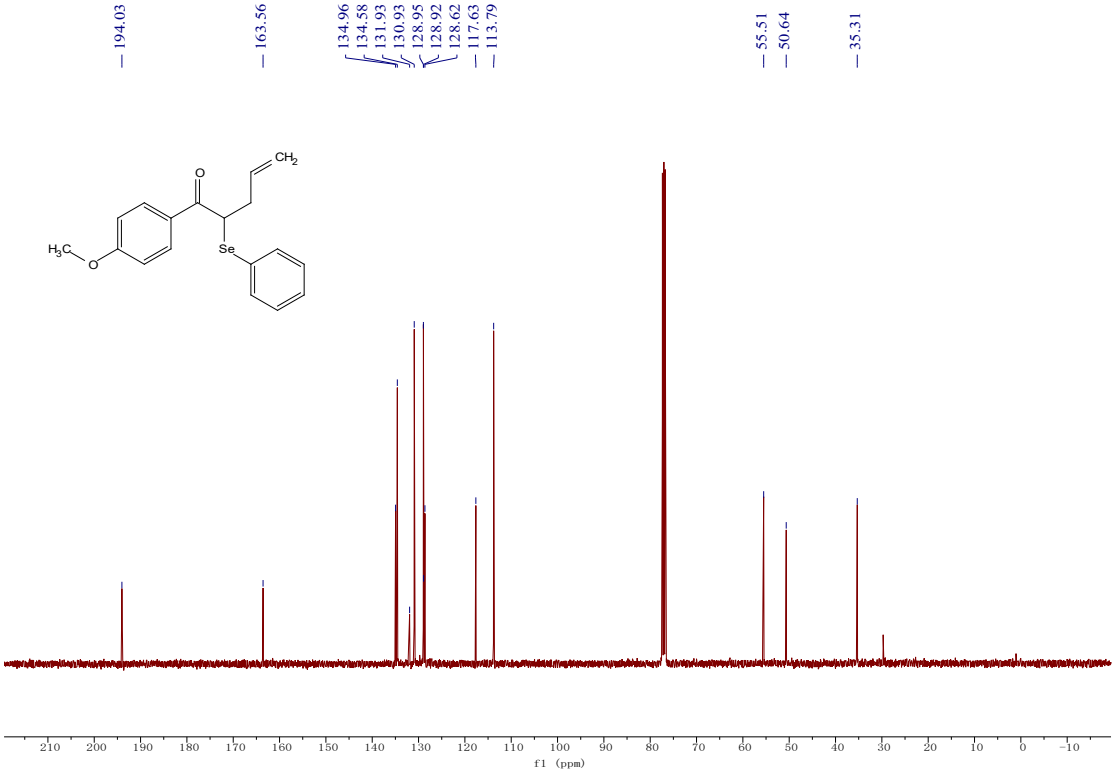


^{13}C NMR of 5ba (100 MHz, Chloroform-*d*)

1-(4-methoxyphenyl)-2-(phenylselanyl)pent-4-en-1-one (5ca)

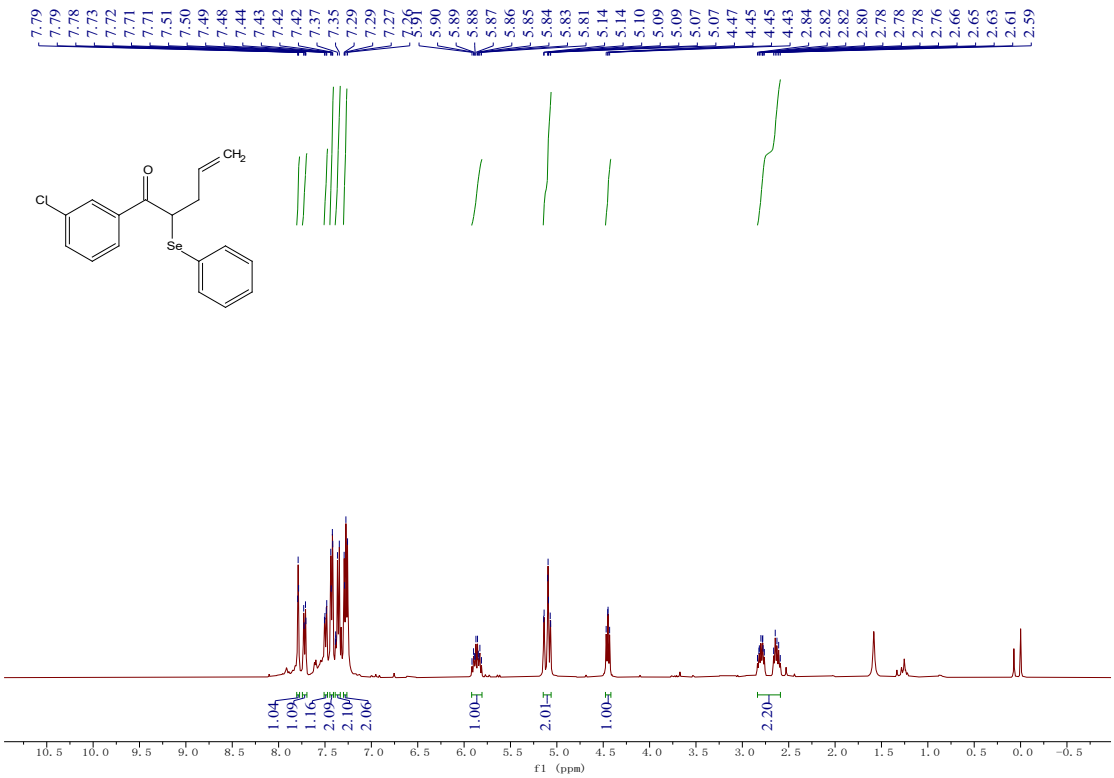


^{1}H NMR of 5ca (400 MHz, Chloroform-*d*)

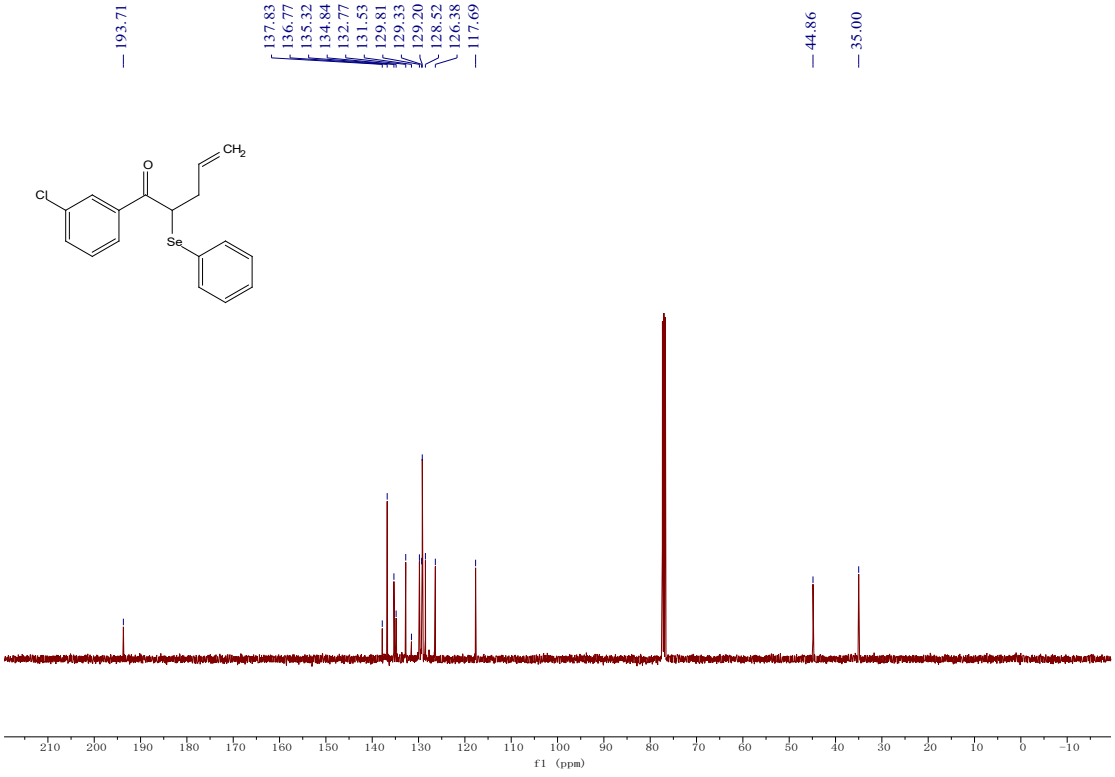


^{13}C NMR of 5ca (100 MHz, Chloroform-*d*)

1-(3-chlorophenyl)-2-(phenylselanyl)pent-4-en-1-one (5da)

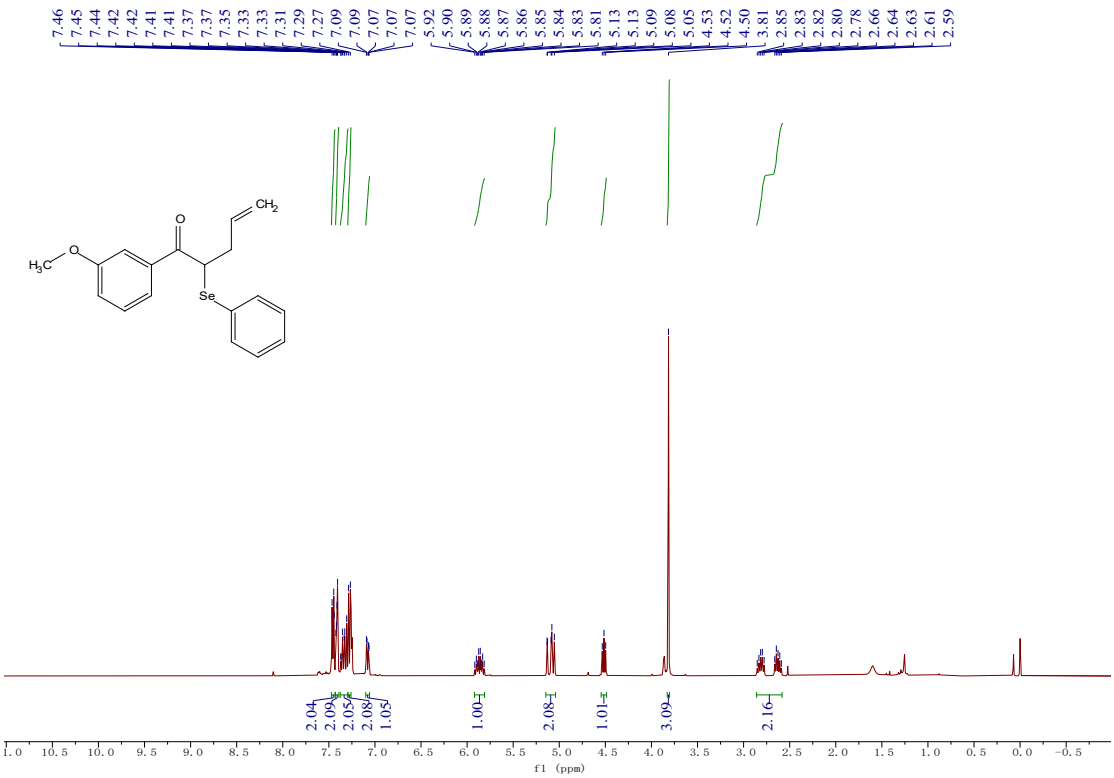


^{1}H NMR of 5da (400 MHz, Chloroform-*d*)

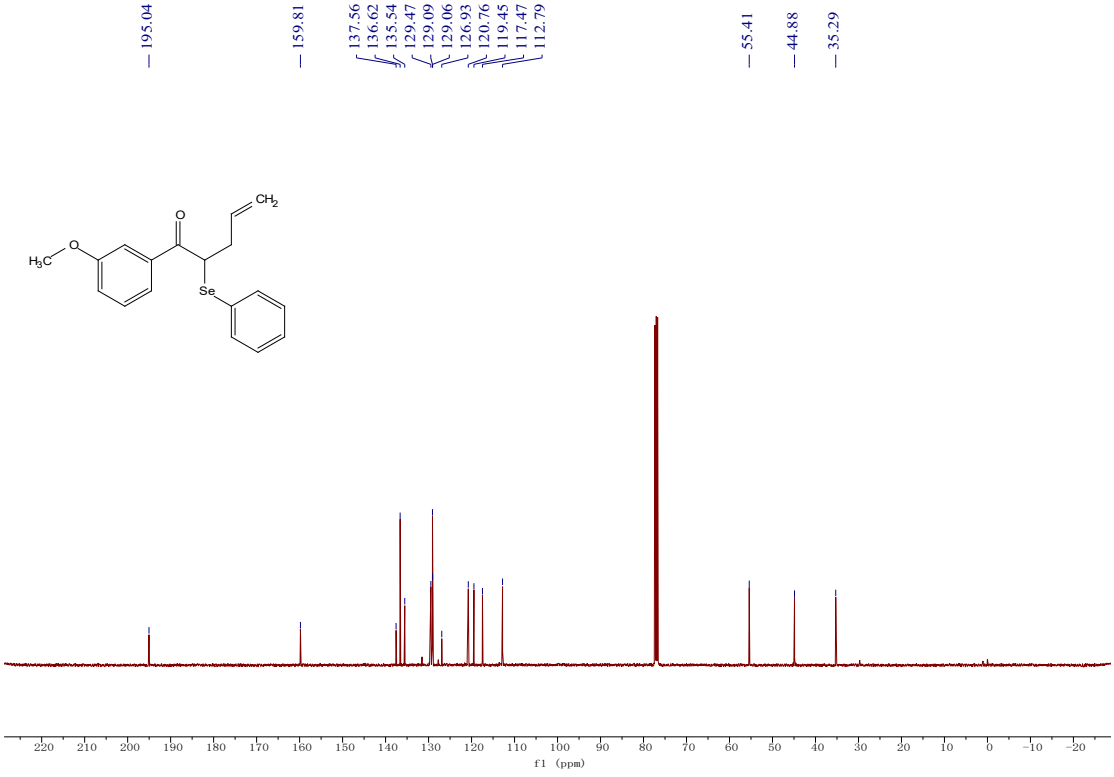


^{13}C NMR of 5da (100 MHz, Chloroform-*d*)

1-(3-methoxyphenyl)-2-(phenylselanyl)pent-4-en-1-one (5ea)

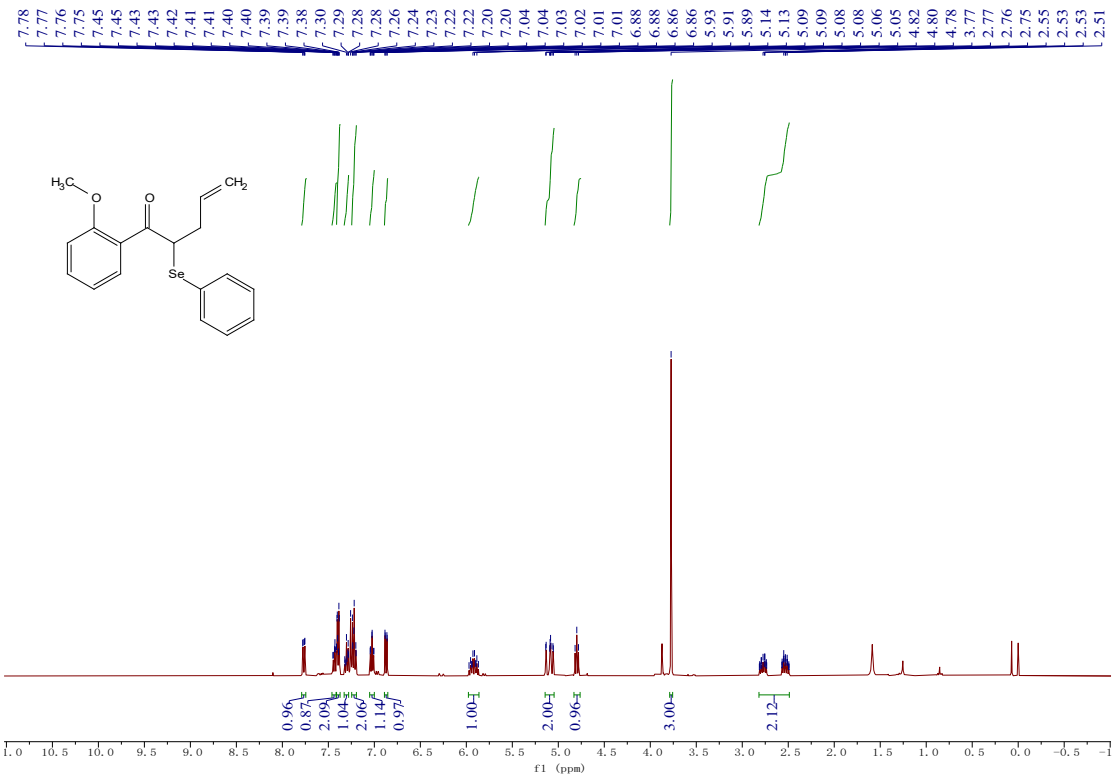


^{1}H NMR of 5ea (400 MHz, Chloroform-*d*)

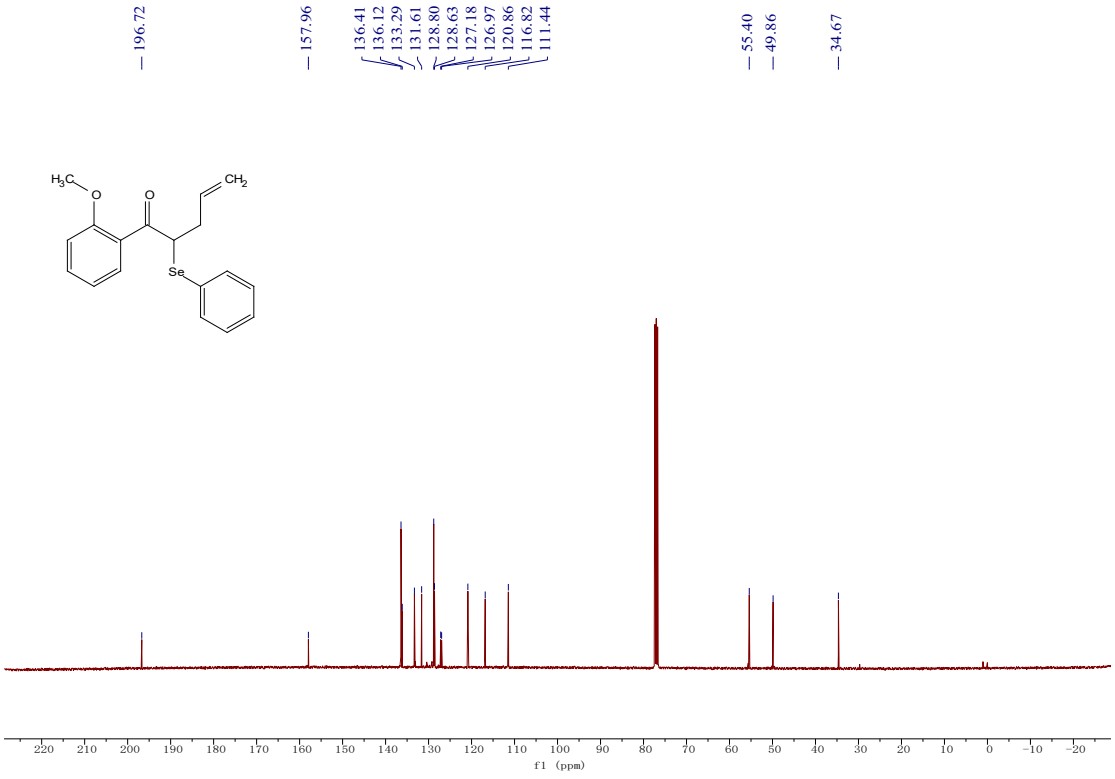


^{13}C NMR of 5ea (100 MHz, Chloroform-*d*)

1-(2-methoxyphenyl)-2-(phenylselanyl)pent-4-en-1-one (5fa)

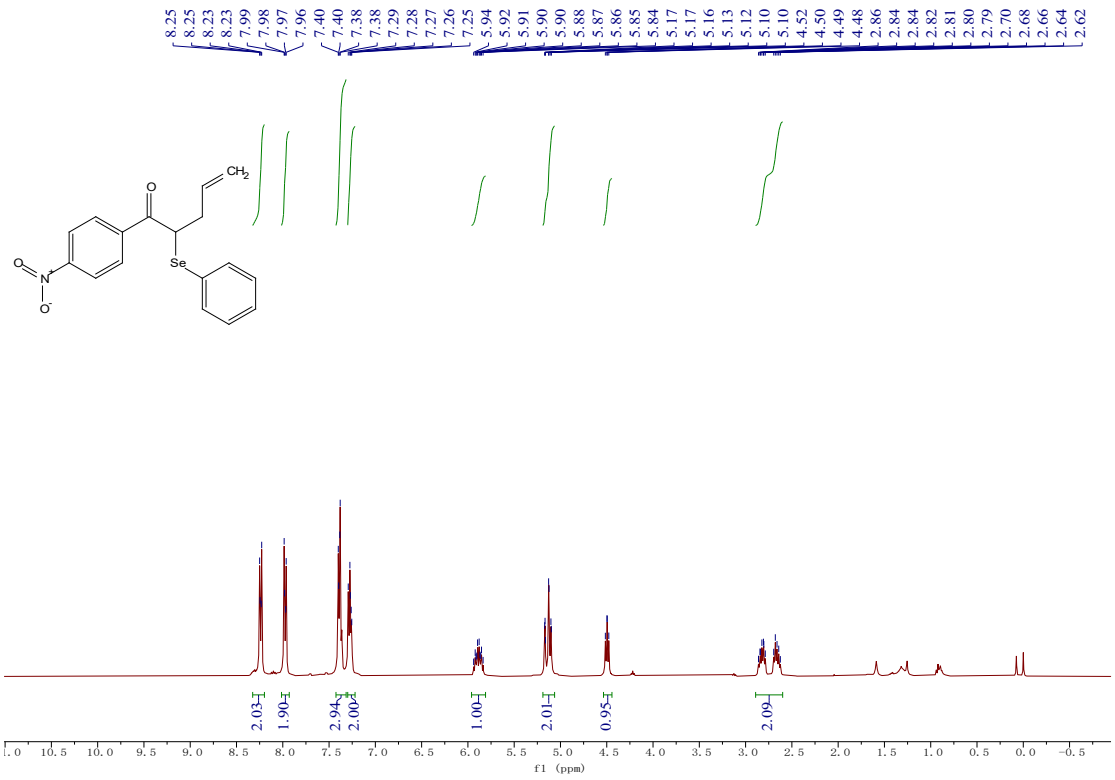


^{1}H NMR of 5fa (400 MHz, Chloroform-*d*)

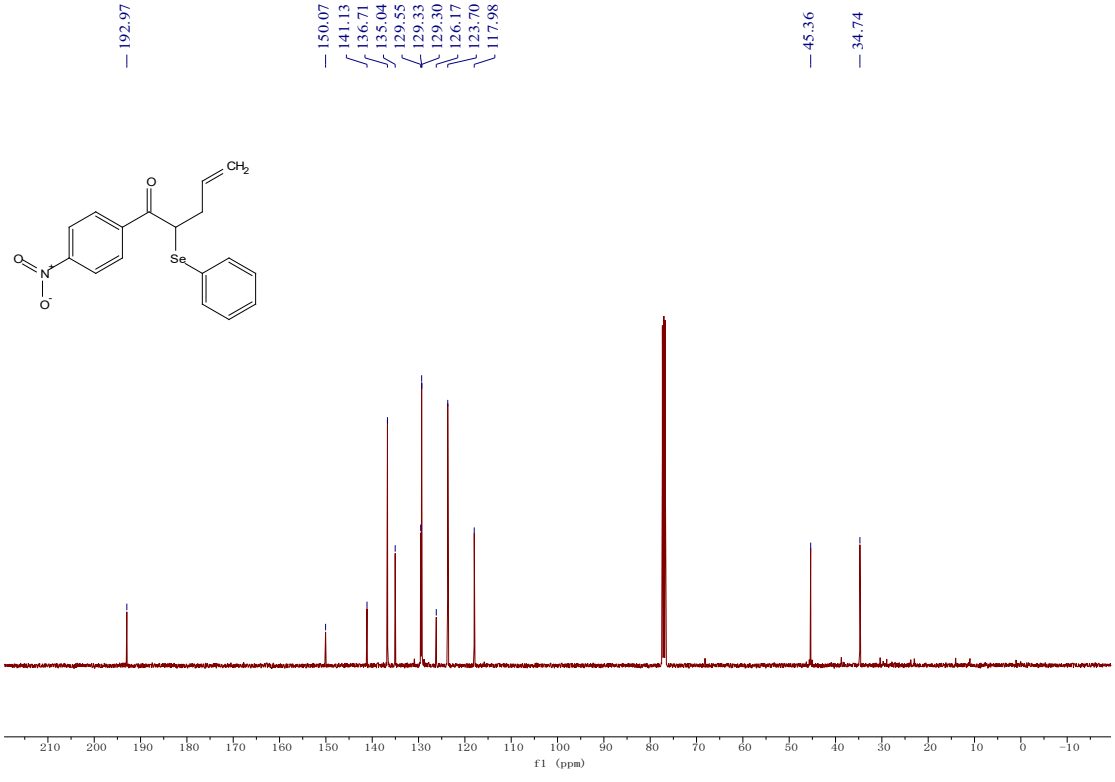


^{13}C NMR of 5fa (100 MHz, Chloroform-*d*)

1-(4-nitrophenyl)-2-(phenylselanyl)pent-4-en-1-one (5ga)

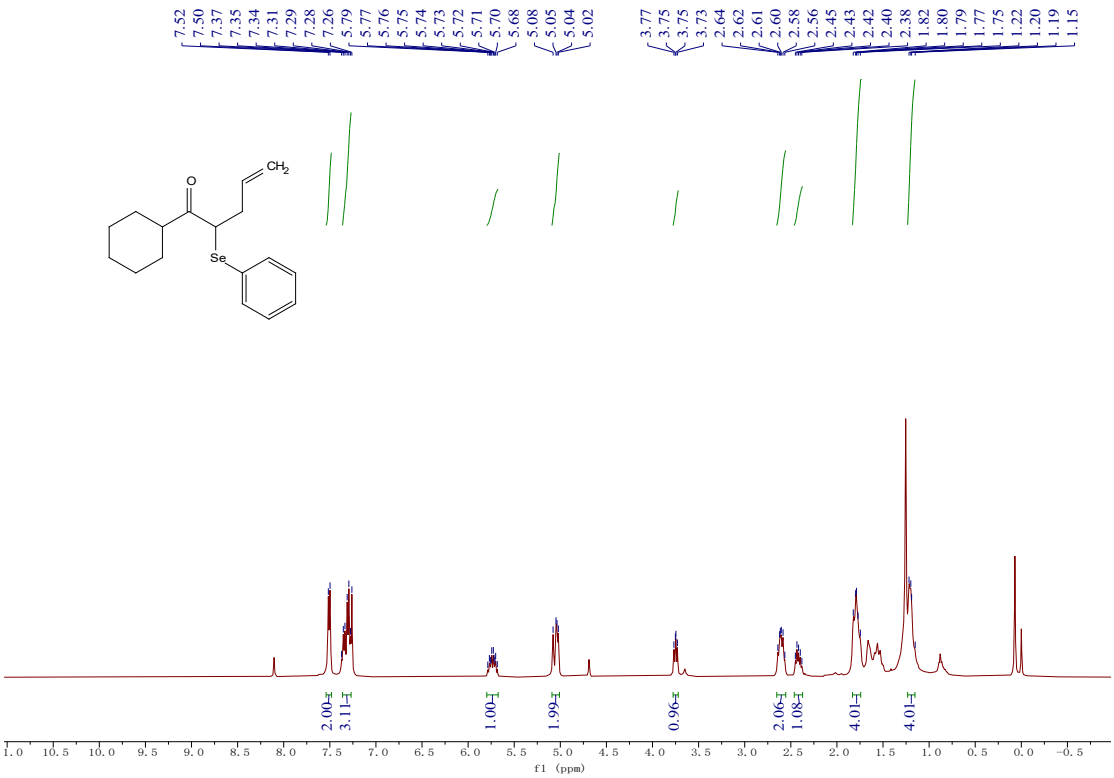


^{1}H NMR of 5ga (400 MHz, Chloroform-*d*)

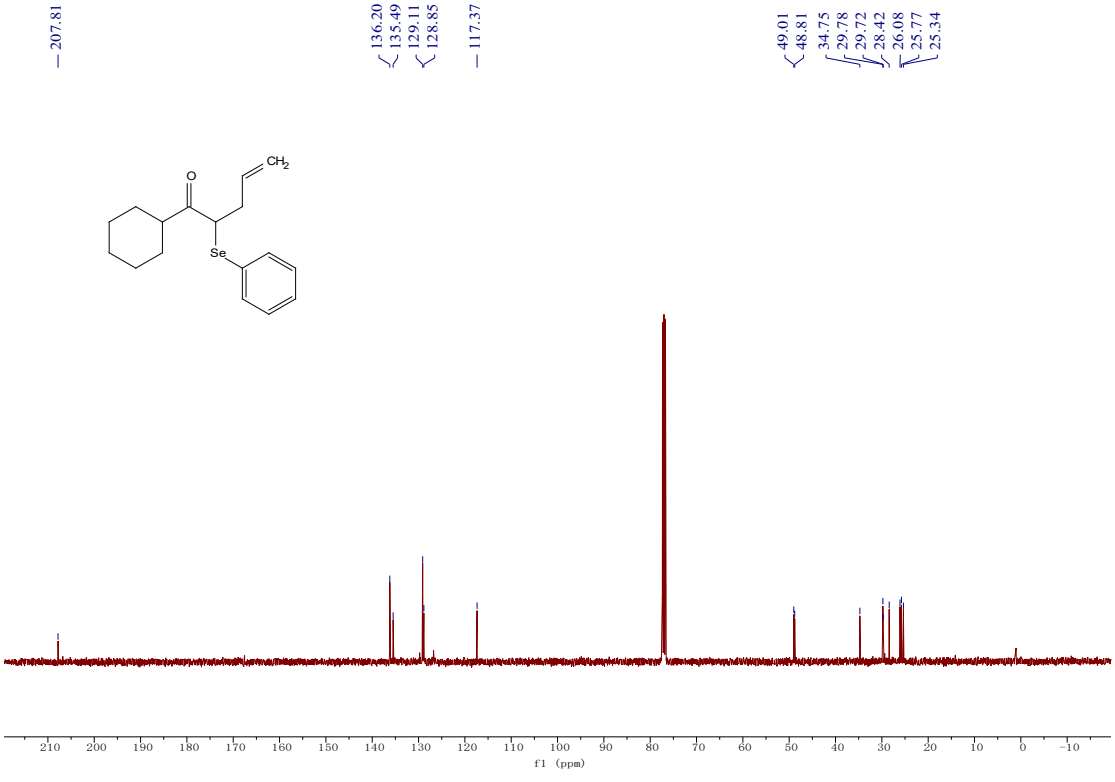


^{13}C NMR of 5ga (100 MHz, Chloroform-*d*)

1-cyclohexyl-2-(phenylselanyl)pent-4-en-1-one (5ha)



^{1}H NMR of 5ha (400 MHz, Chloroform-*d*)



^{13}C NMR of 5ha (100 MHz, Chloroform-*d*)