–Supporting Information –

Ruthenium(II)-Catalyzed *ortho*-C–H Chalcogenation of Benzoic Acids *via* Weak *O*-Coordination: Synthesis of Chalcogenoxanthones

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General information

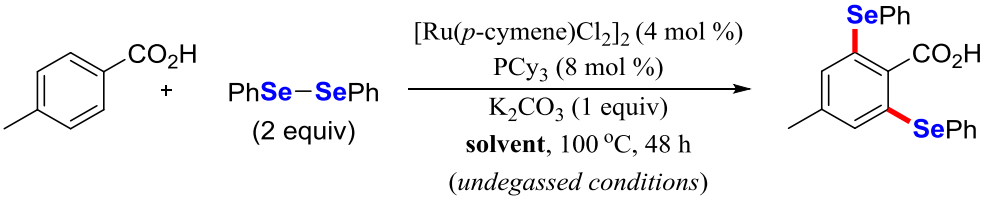
All non-aqueous reactions were carried out under an air atmosphere in flame-dried glassware and were stirred using a magnetic stir plate. All reactions were carried out using anhydrous solvent unless otherwise noted. DMSO and DMF were purchased from Acros Organic Company. Dry toluene, xylene, tetrahydrofuran and 1,4-dioxane were prepared by distilling over sodium ketyl. [Ru(*p*-cymene)Cl_2]$_2$ was purchased from Alfa-Aesar 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 = 7.260 ppm for ^{1}H, δ = 77.160 ppm for ^{13}C, DMSO-d_6 δ = 2.500 ppm for ^{1}H, δ = 39.500 ppm 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 spry ionization (ESI) method on a Q-TOF Micro with lock spray source. The crystal data were collected and integrated using a BrukerAxs kappa apex2 CCD diffractometer, with graphite monochromated Mo-Kα radiation.

Screening of the reaction conditions:

Table S1: Solvent optimization

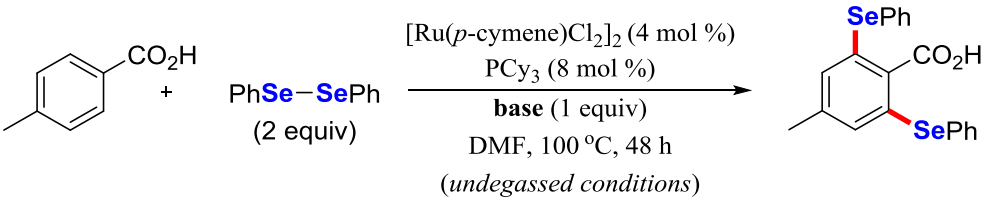


entry	solvent	yield (%)
1	**DMF**	**40**
2	DMSO	-
3	Xylene	trace
4	Toluene	trace
5	1,4-Dioxane	14 (27)[a]
6	CH_3OH	-

7	THF	-
8	DCE	-
9	DME	-
10	CH_3CN	-
11	DMAc	-
12	Trifluorotoluene	12 (20)[a]
13	1,3-Bis(trifluoromethyl)benzene	8

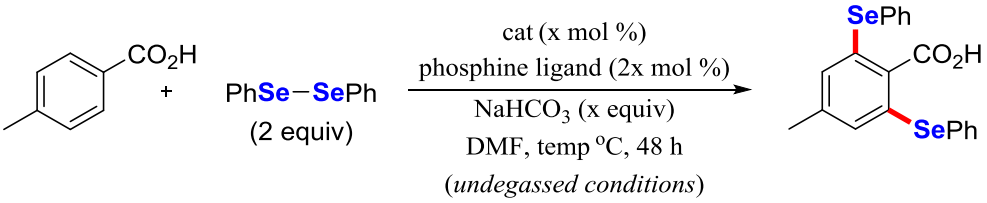
[a]$NaHCO_3$ was used instead of K_2CO_3 and yields are given in parenthesis.

Table S2: Optimization of **bases**



Entry	base	yield (%)
1	Na_2CO_3	90
2	Guanidine carbonate	-
3	Li_2CO_3	trace
4	Mn_2CO_3	trace
5	Cupric carbonate	-
6	Ag_2CO_3	trace
7	$KHCO_3$	56
8	**$NaHCO_3$**	**96**
9	NH_4HCO_3	-
10	K_3PO_4	80
11	Na_2HPO_4	trace
12	K_2HPO_4	51
13	LiO^tBu	45

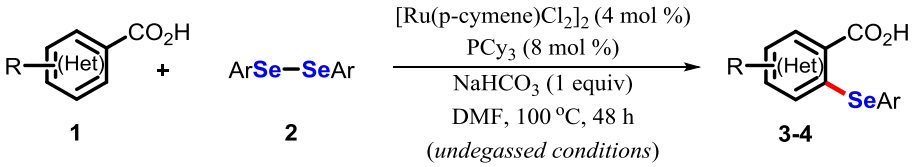
Table S3: Optimization of **other parameters**



entry	[Ru] (mol %)	$NaHCO_3$ (equiv)	ligands (mol %)	temp °C	yield (%)
1	[Ru(*p*-cymene)Cl_2]$_2$ (4 mol %)	1.0	P(*o*-tolyl)$_3$ (8 mol %)	100	81
2	"	"	PPh_3 (8 mol %)	"	72
3	"	"	-	"	83
4	[Ru(*p*-cymene)Cl_2]$_2$ (4 mol %)	"	PCy_3 (8 mol %)	"	48[a]
5	"	0.5	"	"	65
6	"	-	"	100	-
7	"	1.0	"	120	75
8	"	"	"	80	55
9	-	"	-	100	-
10	[Ru(*p*-cymene)Cl_2]$_2$ (2 mol %)	"	PCy_3 (4 mol %)	"	63
11	[Ru(*p*-cymene)Cl_2]$_2$ (4 mol %)	"	PCy_3 (8 mol %)	"	71[b]
12	(*p*-cymene)$RuCl_2PPh_3$ (4 mol%)	"	-	"	45
13	[Ru(*p*-cymene)Cl_2]$_2$ (4 mol %)	"	Cy_3PO (8 mol %)	"	94

[a]under N_2 atmosphere, [b]PhSeSePh (1.5 equiv)

General procedure: Ru(II)-catalyzed direct C–H selenylation of aromatic carboxylic acids



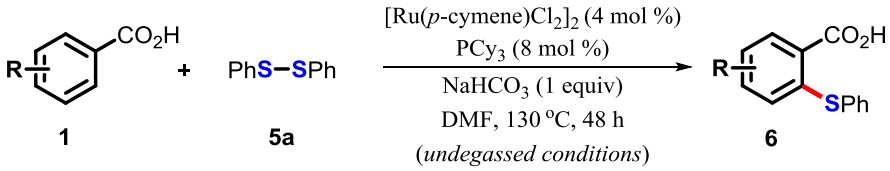
1 **2** **3-4**

The benzoic acids **1** (0.2 mmol), diselenide derivatives **2** (2 equiv), and [Ru(*p*-cymene)Cl_2]$_2$ (4 mol%), PCy_3 (8 mol%), and sodium bicarbonate (1 equiv) were taken in a dried screw cap reaction tube with a magnetic stir bar under open air. Then, dry DMF (1.5mL) was added with a syringe, the tube was capped,

and the resulting mixture was heated at 100 ºC for 48 h. After completion of the reaction, it was allowed to cool to room temperature, quenched with AcOH and diluted with brine solution and ethyl acetate. The mixture was extracted with ethyl acetate (10 mL, three times). The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography (hexane : ethyl acetate : acetic acid = 90 : 10 :1) to provide pure selenylation products **3-4**.

Ru(II)-catalyzed selenylation reaction of **1a** was also performed in 1.1 mmol scale. The benzoic acids **1a** (1.1 mmol, 150 mg, 1 equiv), diphenyl diselenide **2a** (2 equiv), and [Ru(*p*-cymene)Cl_2]$_2$ (4 mol%), PCy_3 (8 mol%), and sodium bicarbonate (1 equiv) were taken in a dried screw cap reaction tube with a magnetic stir bar under open air. Then, dry DMF (1.5mL) was added with a syringe, the tube was capped, and the resulting mixture was heated at 100 ºC for 48 h. After completion of the reaction, it was allowed to cool to room temperature, quenched with AcOH and diluted with brine solution and ethyl acetate. The mixture was extracted with ethyl acetate (10 mL, three times). The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography (hexane : ethyl acetate : acetic acid = 90 : 10 :1) to provide pure selenylation product **3a** as white solid (452 mg, 92% yield).

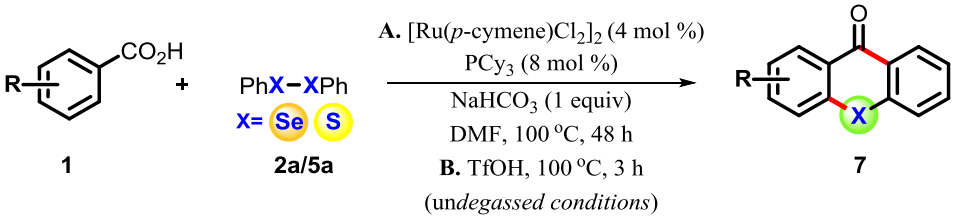
General procedure: Ru(II)-catalyzed direct C–H sulfenylation of aromatic carboxylic acids



1 5a 6

The benzoic acids **1** (0.2 mmol), diphenyl disulfide **5a** (2 equiv), and [Ru(*p*-cymene)Cl_2]$_2$ (4 mol%), PCy_3 (8 mol%), and sodium bicarbonate (1 equiv) were taken in a dried screw cap reaction tube with a magnetic stir bar under open air. Then, DMF (1.5mL) was added with a syringe, the tube was capped, and the resulting mixture was heated at 130 ºC for 48 h. After completion of the reaction, it was cooled to room temperature, quenched with AcOH and diluted with brine solution and ethyl acetate. The mixture was extracted with ethyl acetate (10 mL, three times). The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography (hexane : ethyl acetate : acetic acid = 90 : 10 :1) to provide pure sulfenylation products **6**.

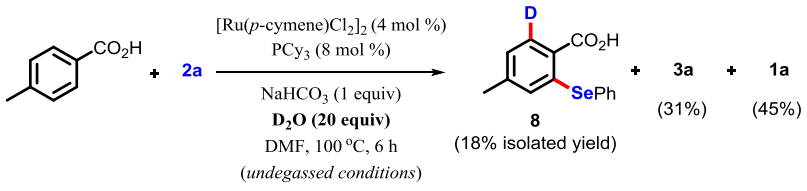
General procedure: Sequential synthesis of chalcogenoxanthones

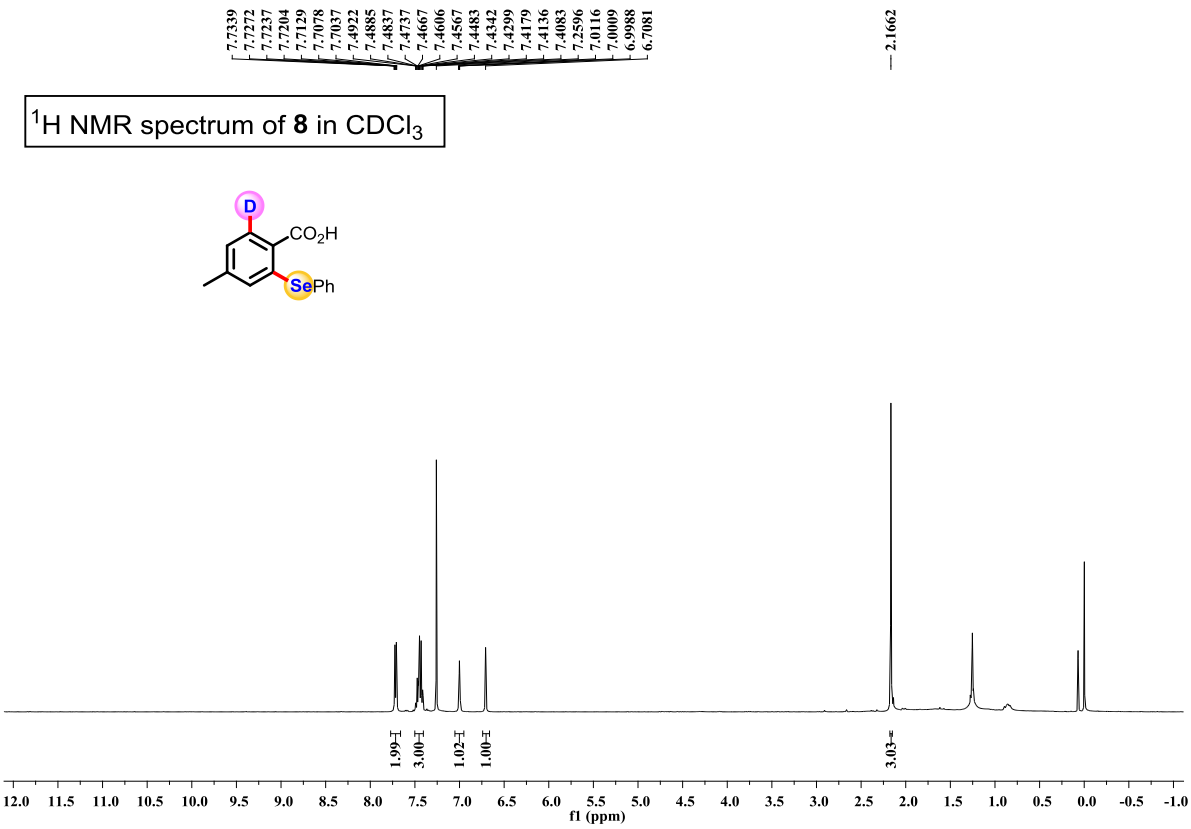


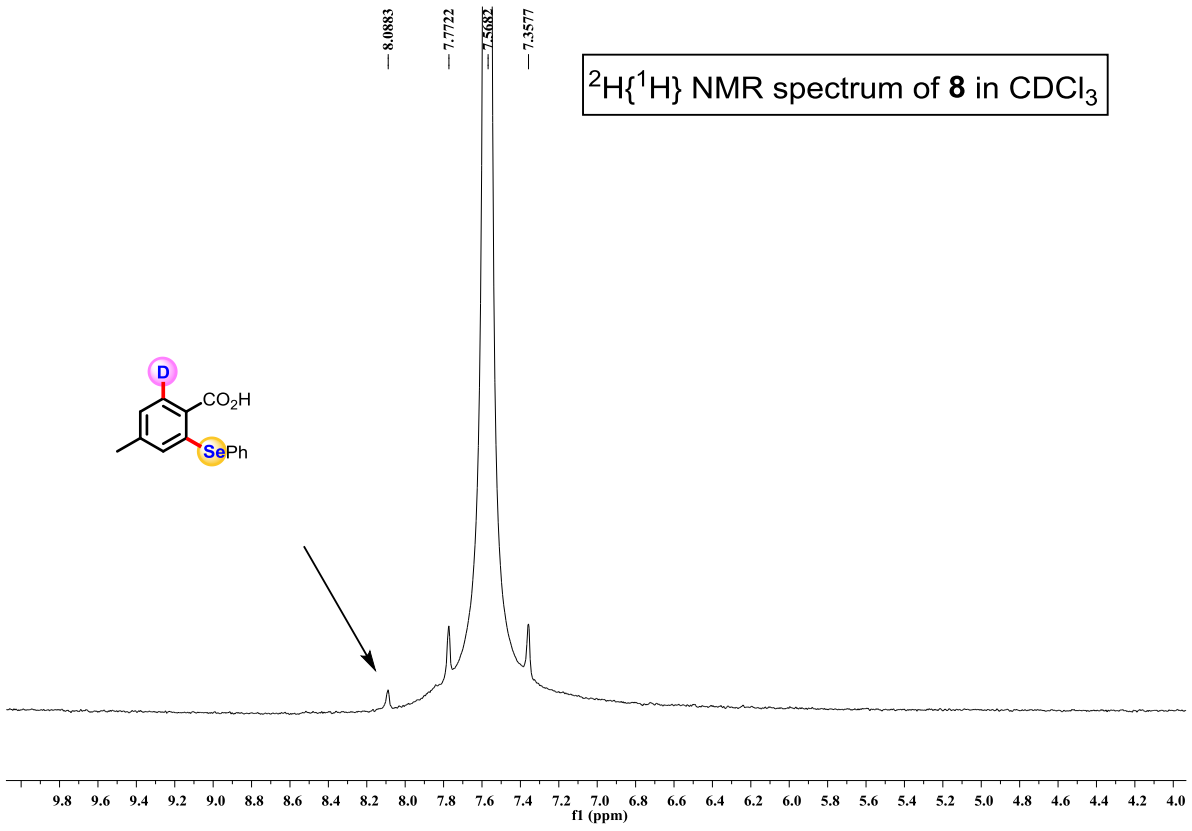
The benzoic acids **1** (0.2 mmol), diphenyl diselenide (**2a**) or disulfide (**5a**) (2 equiv), and $[Ru(p\text{-cymene})Cl_2]_2$ (4 mol%), PCy_3 (8 mol%), and sodium bicarbonate (1 equiv), were taken in a dried screw cap reaction tube with a magnetic stir bar under open air. Then, DMF (1.5mL) was added with a syringe, the tube was capped, and the resulting mixture was heated at 100 °C for 48 h (at 130 °C for **5a**). After completion of the reaction, it was cooled to room temperature, quenched with AcOH and diluted with brine solution and ethyl acetate. The mixture was extracted with ethyl acetate (10 mL, three times). The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was treated with triflic acid at 100 °C for 3 h. After that, it was allowed to cool to room temperature and quenched with water. The mixture was extracted with dichloromethane (DCM) and the organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography (hexane : ethyl acetate = 95 : 5) to provide pure chalcogenoxanthones **7**.

Control experiments:

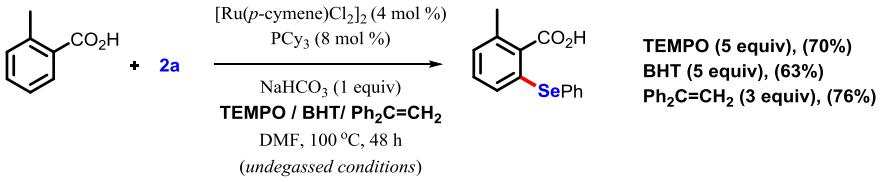
1) Deuterium exchange experiments




7.7339
7.7272
7.7237
7.7204
7.7129
7.7078
7.7037
7.4922
7.4885
7.4837
7.4737
7.4667
7.4606
7.4567
7.4483
7.4342
7.4299
7.4179
7.4136
7.4083
7.2596
7.0116
7.0009
6.9988
6.7081
2.1662
1H NMR spectrum of 8 in CDCl3
D
CO2H
SePh
1.99
3.00
1.02
1.00
3.03
f1 (ppm)


8.0883
7.7722
7.5682
7.3577
2H{1H} NMR spectrum of 8 in CDCl3
D
CO2H
SePh
f1 (ppm)

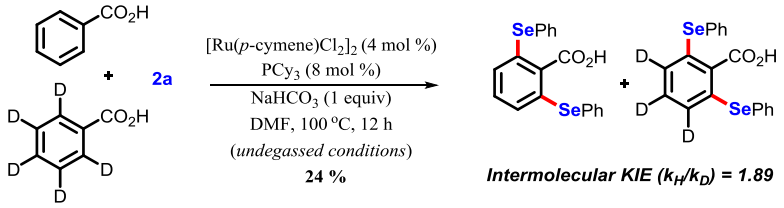
2) Radical scavenging experiment:



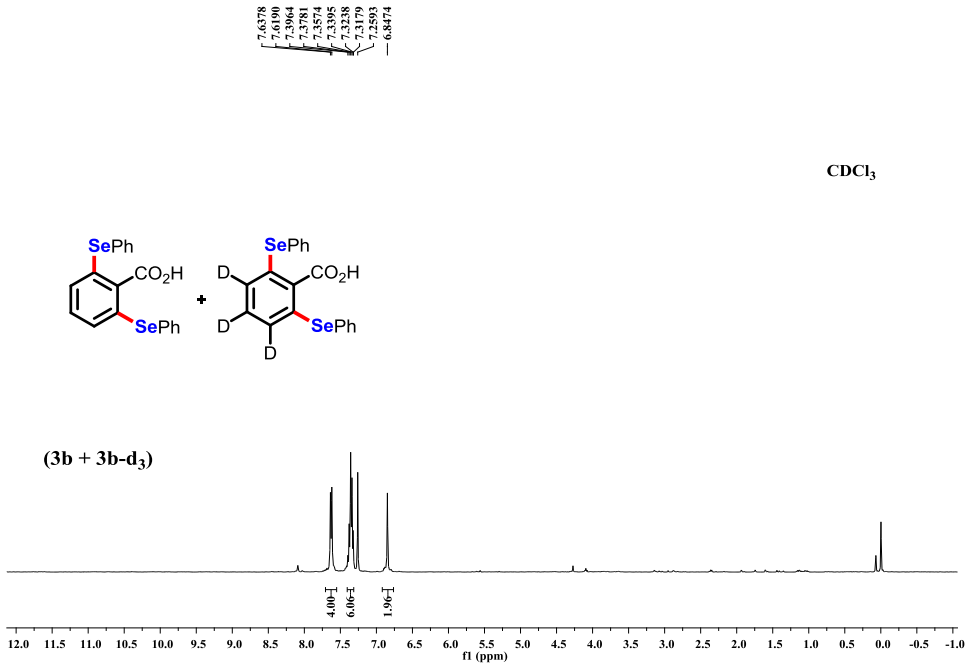
3) Kinetic Isotope Effect:

a) Intermolecular Kinetic Isotopic Experiment:

To demonstrate the intermolecular kinetic isotope effect (KIE), a 1:1 mixture of benzoic acid (**1b**) and the d_5-benzoic acid (**1b-d$_5$**) was subjected to the standard reaction condition for 12 h and the products were isolated by column chromatography. From the ^{1}H NMR, analysis of the H/D ratio of the benzene ring revealed an intermolecular KIE of k_H/k_D = 1.89. This result indicates that *ortho* C–H bond breaking may be involved in the rate determining step.

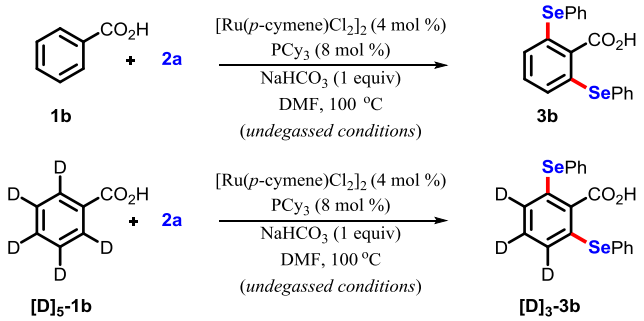


^{1}H NMR spectrum of products of the intermolecular KIE experiment:



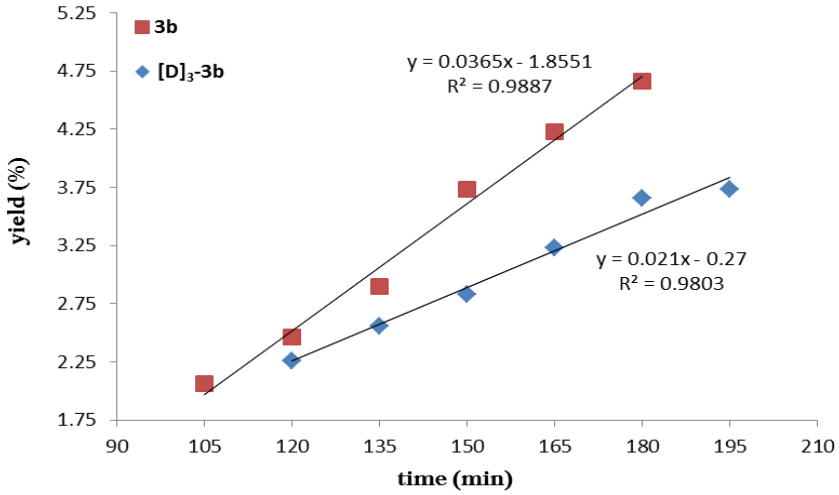
b) Kinetic Isotope Effect by independent experiments:

Two independent reactions with **1b** and **[D]$_5$-1b** under the standard conditions were performed: Following the general procedure of selenylation, **1b** (0.3 mmol) or **[D]$_5$-1b** (0.3 mmol), diphenyldiselenide **2a** (2 equiv), [Ru(*p*-cymene)Cl$_2$]$_2$ (4 mol%), PCy$_3$ (8 mol%), and sodium bicarbonate (1 equiv), were stirred at 100 °C in 3 ml DMF solvent under open atmosphere. After the reaction times indicated below, aliquots of 0.3 mL were taken out of the reaction mixture. The aliquots were acidified, worked up with brine/ethyl acetate mixture. The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. Yields of products were determined by ^{1}H NMR spectroscopy using dibromomethane as an internal standard.



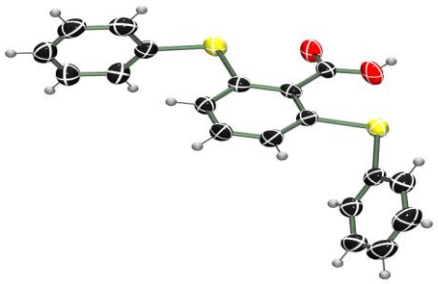
Independent KIE (k_H/k_D) = 1.74

t (min)	105	120	135	150	165	180	195
3b (%)	2.06	2.46	2.90	3.73	4.23	4.66	-
[D]$_5$-3b (%)	-	2.26	2.56	2.83	3.23	3.66	3.73



Crystallographic experimental section:

Crystal structure of compound 3b: CCDC1534856 (Ellipsoid probability 50%)



(*The crystal structure contained two molecules of 3b)*

Table 1. Crystal data and structure refinement for ***3*b** (**CCDC 1534856**).

Identification code	993
Empirical formula	C38 H28 O4 Se4
Formula weight	864.44
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.1260(3) A α = 77.9530(10)^o
	b = 12.9083(3) A β = 80.0760(10)^o
	c = 13.2893(4) A γ = 82.4580(10)^o
Volume	1665.16(8) A^3
Z, Calculated density	2, 1.724 Mg/m^3
Absorption coefficient	4.447 mm^-1
F(000)	848
Crystal size	0.250 x 0.220 x 0.100 mm
Theta range for data collection	1.585 to 24.998^o
Limiting indices	-12<=h<=11, -15<=k<=11, -15<=l<=15

Reflections collected / unique	21799 / 5855 [R(int) = 0.0260]
Completeness to theta = 24.998	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5855 / 0 / 424
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0270, wR2 = 0.0550
R indices (all data)	R1 = 0.0425, wR2 = 0.0592
Extinction coefficient	0.00130(14)
Largest diff. peak and hole	0.391 and -0.466 e.A^-3

Crystal structure of compound 3k: CCDC1534855 (Ellipsoid probability 25%)

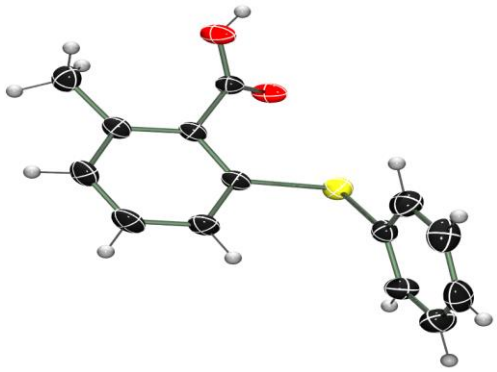
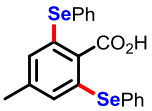


Table 2. Crystal data and structure refinement for **3k** (**CCDC 1534855**).

Identification code	914
Empirical formula	C14 H12 O2 Se
Formula weight	291.20
Temperature	296(2) K
Wavelength	0.71073 Å

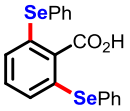
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 7.4743(6) Å α = 90°
	b = 17.3909(14) Å β = 107.933(3)°
	c = 10.0665(6) Å γ = 90°
Volume	1244.92(16) A^3
Z, Calculated density	4, 1.554 Mg/m^3
Absorption coefficient	3.002 mm^-1
F(000)	584
Crystal size	0.220 x 0.120 x 0.100 mm
Theta range for data collection	2.342 to 24.750 deg.
Limiting indices	-8<=h<=8, -20<=k<=20, -11<=l<=11
Reflections collected / unique	14211 / 2126 [R(int) = 0.0470]
Completeness to theta = 24.750	99.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2126 / 0 / 159
Goodness-of-fit on F^2	1.101
Final R indices [I>2sigma(I)]	R1 = 0.0339, wR2 = 0.0798
R indices (all data)	R1 = 0.0608, wR2 = 0.0891
Extinction coefficient	n/a
Largest diff. peak and hole	0.253 and -0.293 e.A^-3

Spectroscopic data:



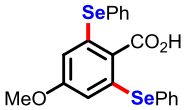
3a

3a: White solid, **Yield**: 96% (86 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.79 –7.52 (m, 4H), 7.50 – 7.31 (m, 6H), 6.70 (s, 2H), 1.96 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.68, 142.37, 138.79, 136.42, 130.25, 129.76, 129.69, 128.90, 126.82, 21.50; **HRMS** (TOF MS ES$^+$) $C_{20}H_{16}O_2Se_2Na^+$ m/z (%) = 470.9361 ([M+Na]$^+$, 100%).



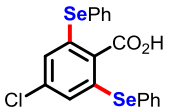
3b

3b: White solid, **Yield**: 82% (71 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 –7.61 (m, 4H), 7.46 –7.31 (m, 6H), 6.90 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.41, 138.73, 136.49, 131.68, 130.11, 129.83, 128.98, 128.93; **HRMS** (TOF MS ES$^+$) $C_{19}H_{14}O_2Se_2Na^+$ m/z (%) = 456.9248 ([M+Na]$^+$, 100%).



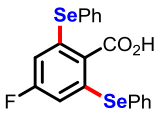
3c

3c: White solid, **Yield**: 86% (79 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.72 – 7.65 (m, 4H), 7.49 – 7.34 (m, 6H), 6.23 (s, 2H), 3.26 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.57, 161.39, 142.73, 137.11, 130.07, 129.76, 129.14, 119.99, 113.68, 54.84; **HRMS** (TOF MS ES$^+$) $C_{20}H_{16}O_3Se_2H^+$ m/z (%) = 464.9539 ([M+H]$^+$, 100%).



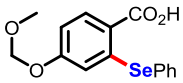
3d

3d: White solid, **Yield**: 61% (57 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 – 7.56 (m, 4H), 7.50 – 7.31 (m, 6H), 6.74 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.82, 142.08, 138.91, 136.92, 130.14, 129.63, 129.25, 127.62, 126.02; **HRMS** (TOF MS ES$^+$) $C_{19}H_{13}O_2ClSe_2Na^+$ m/z (%) = 490.8818 ([M+Na]$^+$, 100%).



3e

3e: White solid, **Yield**: 55% (50 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 – 7.64 (m, 4H), 7.55 – 7.34 (m, 6H), 6.42 (d, *J* = 9.2 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.61, 164.21 (d, *J* = 257.9 Hz), 144.80 (d, *J* = 8.1 Hz), 137.33, 130.18, 129.76, 129.29, 114.52 (d, *J* = 25.2 Hz); **HRMS** (TOF MS ES$^+$) $C_{19}H_{13}O_2FSe_2Na^+$ m/z (%) = 474.9154 ([M+Na]$^+$, 100%).

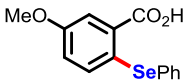


3f

3f: White solid, **Yield**: 70% (47 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.8 Hz, 1H), 7.75 – 7.70 (m, 2H), 7.57 – 7.33 (m, 3H), 6.85 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.53 (d, *J* = 2.4 Hz, 1H), 4.97 (s, 2H), 3.33 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.52, 161.32, 144.07, 137.82, 134.38, 129.96, 129.50, 128.85, 119.87, 116.60, 112.60, 94.16, 56.27; **HRMS** (TOF MS ES$^+$) $C_{15}H_{14}O_4SeNa^+$ m/z (%) = 360.9936 ([M+Na]$^+$, 100%).

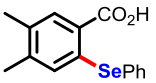
3g

3g: White solid, **Yield**: 93% (54 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 1.4 Hz, 1H), 7.76 – 7.66 (m, 2H), 7.50 – 7.37 (m, 3H), 7.08 (dd, *J* = 8.3, 1.6 Hz, 1H), 6.83 (d, *J* = 8.2 Hz, 1H), 2.32 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.46, 137.80, 137.65, 134.88, 134.68, 132.94, 129.87, 129.25, 129.05, 126.18, 20.63; **HRMS** (TOF MS ES$^+$) $C_{14}H_{12}O_2SeNa^+$ m/z (%) = 314.9929 ([M+Na]$^+$, 100%).



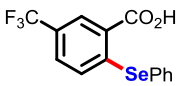
3h

3h: White solid, **Yield**: 75% (46 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 9.0, 2.5 Hz, 3H), 7.49 – 7.35 (m, 3H), 6.93 – 6.77 (m, 2H), 3.81 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.72, 157.47, 137.50, 131.39, 130.52, 129.86, 129.22, 129.19, 127.28, 121.19, 116.19, 55.69; **HRMS** (TOF MS ES$^+$) $C_{14}H_{12}O_3SeNa^+$ m/z (%) = 330.9820 ([M+Na]$^+$, 100%).



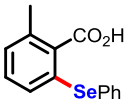
3i

3i: White solid, **Yield**: 82% (50 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.77 – 7.67 (m, 2H), 7.52 – 7.37 (m, 3H), 6.67 (s, 1H), 2.23 (s, 3H), 2.08 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.38, 143.49, 138.05, 137.62, 133.79, 133.38, 130.24, 129.81, 129.19, 129.15, 123.93, 20.30, 19.13; **HRMS** (TOF MS ES$^+$) $C_{15}H_{14}O_2SeNa^+$ m/z (%) = 329.0065 ([M+Na]$^+$, 100%).



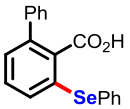
3j

3j: White solid, **Yield**: 74% (51 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.43 (d, *J* = 1.4 Hz, 1H), 7.77 – 7.67 (m, 2H), 7.58 – 7.40 (m, 4H), 7.05 (d, *J* = 8.5 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 170.81, 147.40, 137.69, 130.31, 129.98, 129.85, 129.51 (q, *J* = 3.4 Hz), 129.33 (q, *J* = 3.7 Hz), 128.04, 127.61 (q, *J* = 33.5 Hz), 126.36, 123.81 (q, *J* = 271.8 Hz); **HRMS** (TOF MS ES$^+$) $C_{14}H_9O_2F_3SeK^+$ m/z (%) = 384.9346 ([M+K]$^+$, 100%).



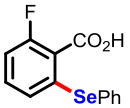
3k

3k: White solid, **Yield**: 90% (52 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.84 (s, 1H), 7.73 – 7.50 (m, 2H), 7.44 – 7.23 (m, 3H), 7.21 – 6.97 (m, 3H), 2.55 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 174.27, 138.45, 135.30, 133.95, 132.90, 131.04, 130.75, 130.21, 129.62, 129.32, 128.37, 21.35; **HRMS** (TOF MS ES$^+$) $C_{14}H_{12}O_2SeNa^+$ m/z (%) = 314.9900 ($[M+Na]^+$, 100%).



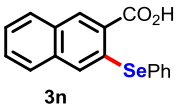
3l

3l: White solid, **Yield**: 83% (59 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.65 – 7.54 (m, 2H), 7.47 – 7.29 (m, 8H), 7.26 – 7.18 (m, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.62, 141.87, 140.38, 135.31, 133.25, 132.80, 131.41, 130.65, 130.27, 129.68, 128.77, 128.57, 128.48, 128.43, 127.89; **HRMS** (TOF MS ES$^+$) $C_{19}H_{14}O_2SeK^+$ m/z (%) = 392.9771 ($[M+K]^+$, 100%).



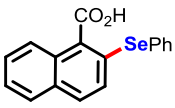
3m

3m: White solid, **Yield**: 75% (44 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 – 7.62 (m, 2H), 7.49 – 7.32 (m, 3H), 7.18 (td, *J* = 8.2, 5.4 Hz, 1H), 6.94 (m, 1H), 6.83 – 6.75 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.82, 162.77 (d, *J* = 260.9 Hz), 141.61, 137.03, 133.37 (d, *J* = 9.6 Hz), 129.99, 129.39, 129.23, 126.01 (d, *J* = 3.3 Hz), 117.69, 113.58 (d, *J* = 23.1 Hz); **HRMS** (TOF MS ES$^+$) $C_{13}H_9O_2FSeNa^+$ m/z (%) = 318.9657 ($[M+Na]^+$, 100%).



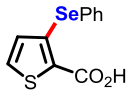
3n

3n: White solid, **Yield**: 66% (43 mg); **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.67 (s, 1H), 8.06 – 8.00 (m, 1H), 7.75 – 7.69 (m, 2H), 7.58 – 7.41 (m, 6H), 7.21 (s, 1H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 168.18, 137.06, 134.72, 133.83, 132.30, 130.21, 130.11, 129.44, 129.15, 129.08, 129.03, 127.04, 126.70, 126.40, 126.24; **HRMS** (TOF MS ES$^+$) $C_{17}H_{12}O_2SeNa^+$ m/z (%) = 350.9906 ($[M+Na]^+$, 100%).



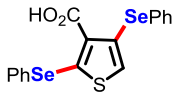
3o

3o: White solid, **Yield**: 78% (51 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.5 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.69 – 7.59 (m, 3H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.20 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.42, 135.35, 133.06, 132.08, 131.10, 130.65, 129.64, 129.02, 128.44, 128.32, 127.83, 126.30, 125.42; **HRMS** (TOF MS ES$^+$) $C_{17}H_{12}O_2SeNa^+$ m/z (%) = 350.9912 ($[M+Na]^+$, 100%).



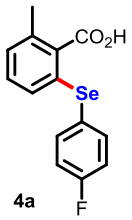
3p

3p: White solid, **Yield**: 88% (50 mg); **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.95 – 7.60 (m, 3H), 7.60 – 7.19 (m, 3H), 6.24 (d, *J* = 5.2 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.34, 138.57, 136.43, 132.37, 129.88, 129.40, 128.58, 127.93, 123.27**; HRMS** (TOF MS ES$^+$) $C_{11}H_8O_2SSeNa^+$ m/z (%) = 306.9330 ([M+Na]$^+$, 100%).



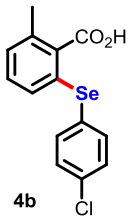
3q

3q: White solid, **Yield**: 69% (61 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.1 Hz, 2H), 7.69 (d, *J* = 6.2 Hz, 2H), 7.53 – 7.31 (m, 6H), 6.14 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 168.21, 150.70, 137.35, 136.73, 131.52, 130.28, 130.00, 129.84, 129.14, 128.57, 127.92, 125.55, 120.08; **HRMS** (TOF MS ES$^+$) $C_{17}H_{12}O_2SSe_2Na^+$ m/z (%) = 462.8777 ([M+Na]$^+$, 100%).



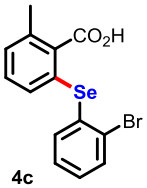
4a

4a: White solid, **Yield**: 72% (45 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 – 7.55 (m, 2H), 7.18 – 7.08 (m, 2H), 7.07 – 6.97 (m, 3H), 2.54 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.42, 163.22 (d, *J* = 7.7 Hz), 138.84, 137.86, 137.80, 134.67, 132.19, 131.20, 129.49 (d, *J* = 29.2 Hz), 125.25 (d, *J* = 3.5 Hz), 116.93 (d, *J* = 21.5 Hz), 21.51; **HRMS** (TOF MS ES$^+$) $C_{14}H_{11}O_2FSeNa^+$ m/z (%) = 332.9819 ([M+Na]$^+$, 100%).



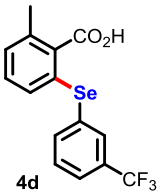
4b

4b: White solid, **Yield**: 70% (46 mg); **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.45 (dd, *J* = 6.6, 1.6 Hz, 2H), 7.34 (d, *J* = 6.7 Hz, 2H), 7.14 (s, 2H), 7.05 (s, 1H), 2.36 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 169.49, 136.83, 135.96, 135.44, 133.17, 130.25, 129.98, 129.48, 129.40, 129.30, 20.03; **HRMS** (TOF MS ES$^+$) $C_{14}H_{11}O_2ClSeNa^+$ m/z (%) = 348.9501 ([M+Na]$^+$, 100%).



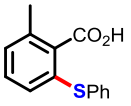
4c

4c: White solid, **Yield**: 64% (47 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.31 – 7.26 (m, 1H), 7.25 – 7.19 (m, 2H), 7.20 – 7.06 (m, 3H), 2.51 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.63, 137.97, 136.09, 135.32, 133.87, 133.04, 132.69, 131.09, 130.64, 129.67, 128.69, 128.19, 126.22, 20.97; **HRMS** (TOF MS ES$^+$) $C_{14}H_{11}O_2BrSeNa^+$ m/z (%) = 392.8985 ([M+Na]$^+$, 100%).



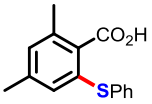
4d

4d: White solid, **Yield**: 68% (49 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.67 (d, *J* = 7.0 Hz, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.20 – 7.05 (m, 3H), 2.51 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.54, 138.43(m), 137.79, 132.49, 131.92, 131.59, 131.12, 130.96 (q, *J* = 3.61 Hz), 130.88, 130.02, 129.84, 124.8 (q, *J* = 3.56 Hz), 123.77 (q, *J* = 271.27 Hz), 21.19; **HRMS** (TOF MS ES$^+$) $C_{15}H_{11}O_2F_3SeNa^+$ m/z (%) = 382.9787([M+Na]$^+$, 100%).



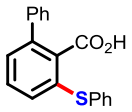
6a

6a: White solid, **Yield**: 72% (35 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 – 7.35 (m, 2H), 7.32 – 7.24 (m, 3H), 7.18 (d, *J* = 7.7 Hz, 1H), 7.13 – 7.08 (m, 2H), 2.44 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.49, 136.34, 135.82, 133.81, 131.72, 130.16, 130.12, 129.36, 129.31, 127.42, 20.16; **HRMS** (TOF MS ES$^+$) $C_{14}H_{12}O_2SNa^+$ m/z (%) = 267.0479 ([M+Na]$^+$, 100%).



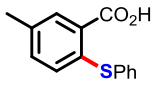
6b

6b: White solid, **Yield**: 75% (39 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 (dt, *J* = 3.3, 2.0 Hz, 2H), 7.32 – 7.20 (m, 3H), 6.94 (s, 2H), 2.42 (s, 3H), 2.22 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.19, 140.50, 136.56, 136.01, 133.88, 132.72, 131.60, 130.70, 130.46, 129.27, 127.31, 21.27, 20.26; **HRMS** (TOF MS ES$^+$) $C_{15}H_{14}O_2SK^+$ m/z (%) = 297.0320 ([M+K]$^+$, 100%).



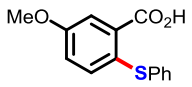
6c

6c: White solid, **Yield**: 64% (39 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 – 7.39 (m, 4H), 7.38 – 7.27 (m, 6H), 7.25 – 7.18 (m, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.41, 141.02, 139.86, 135.05, 134.91, 132.42, 130.88, 130.32, 129.46, 128.82, 128.62, 128.49, 128.19, 127.99, 127.87; **HRMS** (TOF MS ES$^+$) $C_{19}H_{14}O_2SNa^+$ m/z (%) = 329.0613 ($[M+Na]^+$, 100%).



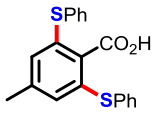
6d

6d: White solid, **Yield**: 68% (33 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 1.5 Hz, 1H), 7.58 – 7.53 (m, 2H), 7.47 – 7.37 (m, 3H), 7.11 (dd, *J* = 8.3, 1.8 Hz, 1H), 6.75 (d, *J* = 8.3 Hz, 1H), 2.32 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.16, 140.58, 135.49, 134.60, 134.30, 132.88, 132.60, 129.86, 129.14, 128.00, 125.72, 20.68; **HRMS** (TOF MS ES$^+$) $C_{14}H_{12}O_2SNa^+$ m/z (%) = 267.0465 ($[M+Na]^+$, 100%).



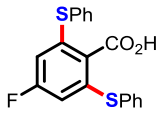
6e

6e: White solid, **Yield**: 66% (34 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 1.9 Hz, 1H), 7.55 – 7.46 (m, 2H), 7.43 – 7.33 (m, 3H), 6.96 – 6.77 (m, 2H), 3.81 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 171.08, 157.30, 134.53, 133.71, 130.50, 129.75, 129.16, 128.84, 128.72, 120.62, 115.96, 55.72; **HRMS** (TOF MS ES$^+$) $C_{14}H_{12}O_3SNa^+$ m/z (%) = 283.0430 ($[M+Na]^+$, 100%).



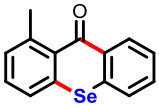
6f

6f: White solid, **Yield**: 60% (42 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42 – 7.36 (m, 4H), 7.33 – 7.23 (m, 6H), 6.94 (s, 2H), 2.12 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 171.53, 141.00, 135.82, 135.15, 132.14, 131.79, 129.42, 129.32, 127.74, 21.32; **HRMS** (TOF MS ES$^+$) $C_{20}H_{16}O_2S_2Na^+$ m/z (%) = 375.0500 ($[M+Na]^+$, 100%).



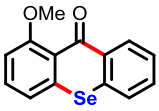
6g

6g: White solid, **Yield**: 54% (39 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 (m, 4H), 7.39 – 7.33 (m, 6H), 6.49 (d, *J* = 9.0 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.30 (d, *J* = 254.7 Hz), 141.90 (d, *J* = 7.5 Hz), 134.36, 132.69, 129.91, 129.63, 129.19, 114.35 (d, *J* = 24.8 Hz); **HRMS** (TOF MS ES$^+$) $C_{19}H_{13}O_2FS_2Na^+$ m/z (%) = 379.0231 ($[M+Na]^+$, 100%).



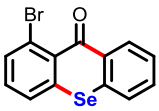
7a

7a: Yellow solid, **Yield**: 86% (47 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.43 – 8.32 (m, 1H), 7.57 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.51 – 7.45 (m, *J* = 7.4, 1.7 Hz, 2H), 7.44 – 7.39 (m, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.23 (dd, *J* = 7.4, 0.5 Hz, 1H), 2.80 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 185.83, 144.21, 135.53, 134.32, 133.25, 131.66, 131.04, 130.99, 130.92, 130.49, 127.71, 126.77, 126.58, 24.44; **HRMS** (TOF MS ES$^+$) $C_{14}H_{10}OSeNa^+$ m/z (%) = 296.9764 ([M+Na]$^+$, 100%).



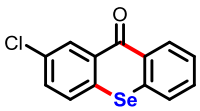
7b

7b: Yellow solid, **Yield**: 60% (35 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.41 – 8.30 (m, 1H), 7.59 – 7.51 (m, 1H), 7.49 – 7.40 (m, 2H), 7.40 – 7.36 (m, 1H), 7.19 (dd, *J* = 7.9, 0.9 Hz, 1H), 6.94 (d, *J* = 8.3 Hz, 1H), 3.98 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 184.06, 162.26, 136.72, 134.90, 132.61, 132.52, 131.52, 130.88, 127.49, 126.90, 121.64, 120.55, 110.11, 56.45; **HRMS** (TOF MS ES$^+$) $C_{14}H_{10}O_2SeH^+$ m/z (%) = 290.9926 ([M+H]$^+$, 100%).



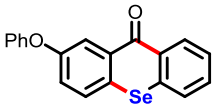
7c

7c: Yellow solid, **Yield**: 65% (44 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.71 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.49 (td, *J* = 7.5, 1.6 Hz, 1H), 7.46 – 7.40 (m, 1H), 7.23 (dd, *J* = 14.9, 7.1 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 183.86, 136.45, 134.37, 133.68, 132.23, 132.00, 131.46, 130.95, 129.78, 127.96, 127.63, 127.21, 124.45; **HRMS** (TOF MS ES$^+$) $C_{13}H_7OBrSeNa^+$ m/z (%) = 360.8763 ([M+Na]$^+$, 100%).



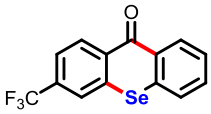
7d

7d: Yellow solid, **Yield**: 67% (39 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.71 – 8.55 (m, 2H), 7.67 – 7.58 (m, 1H), 7.58 – 7.51 (m, 2H), 7.50 – 7.41 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 181.04, 134.89, 133.24, 133.17, 132.61, 132.47, 132.06, 131.67, 131.03, 130.52, 129.74, 128.42, 127.16; **HRMS** (TOF MS ES$^+$) $C_{13}H_7OClSeNa^+$ m/z (%) = 316.9222 ([M+Na]$^+$, 100%).



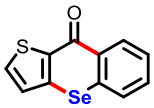
7e

7e: Yellow solid, **Yield**: 62% (44 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 8.1, 1.6 Hz, 1H), 8.26 (d, *J* = 2.8 Hz, 1H), 7.70 – 7.59 (m, 2H), 7.57 – 7.51 (m, 1H), 7.49 – 7.43 (m, 1H), 7.41 – 7.34 (m, 2H), 7.31 (dd, *J* = 8.6, 2.9 Hz, 1H), 7.19 – 7.13 (m, 1H), 7.09 – 7.03 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 181.63, 156.83, 156.64, 135.23, 132.33, 132.26, 131.64, 130.50, 130.16, 129.89, 128.65, 128.46, 126.94, 124.29, 124.15, 119.89, 119.39; **HRMS** (TOF MS ES$^+$) $C_{19}H_{12}O_2SeH^+$ m/z (%) = 353.0100 ([M+H]$^+$, 100%).



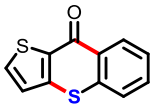
7f

7f: Yellow solid, **Yield**: 58% (38 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.91 (d, *J* = 1.8 Hz, 1H), 8.65 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.80 – 7.70 (m, 2H), 7.64 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.61 – 7.55 (m, 1H), 7.54 – 7.46 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 181.19, 139.51, 134.56, 132.92, 131.74, 131.11, 130.64, 129.40 (q, *J* = 33.8 Hz), 129.30, 128.65 (q, *J* = 3.9 Hz), 128.42, 128.08 (q, *J* = 3.3 Hz), 127.52, 123.82 (q, *J* = 272.0 Hz); **HRMS** (TOF MS ES$^+$) $C_{14}H_7OF_3SeH^+$ m/z (%) = 328.9662 ([M+H]$^+$, 100%).



7g

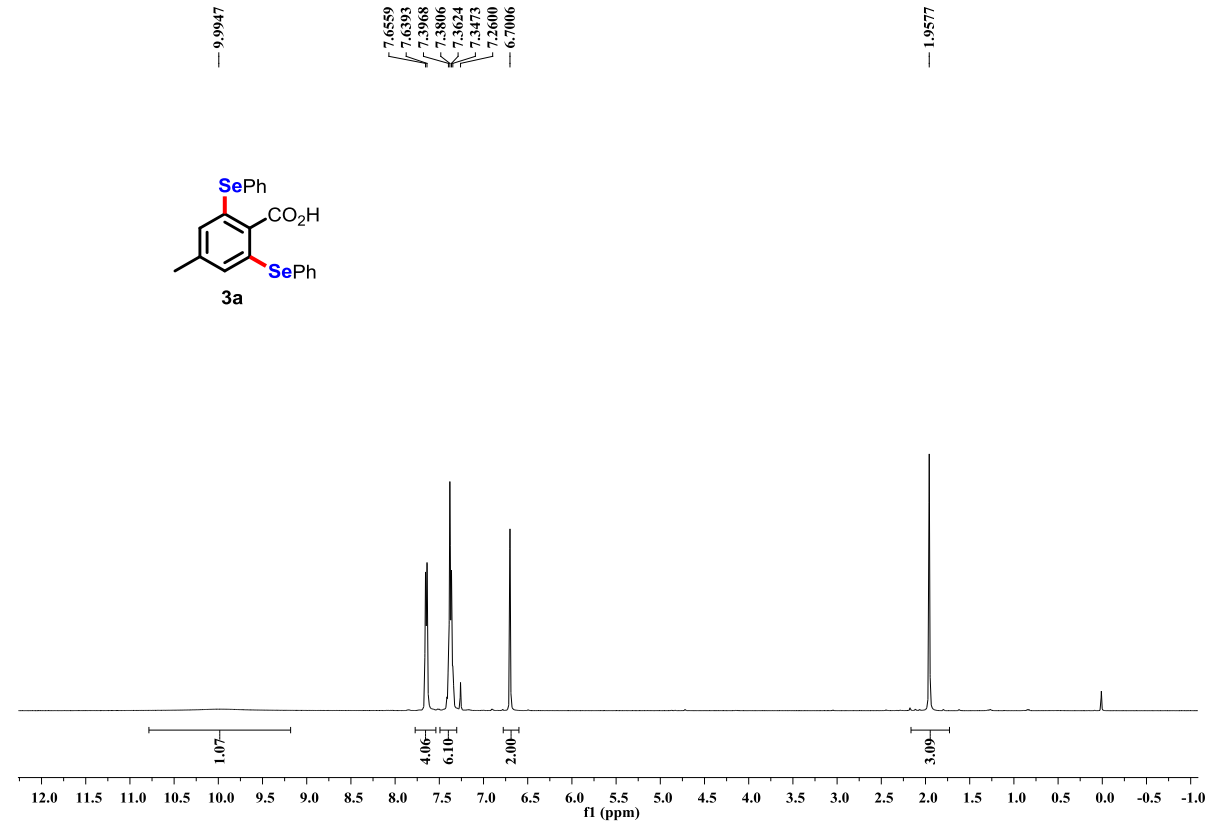
7g: Yellowish solid, **Yield**: 81% (43 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.80 – 8.69 (m, 1H), 7.90 (d, *J* = 5.2 Hz, 1H), 7.73 (dd, *J* = 7.1, 2.0 Hz, 1H), 7.64 – 7.52 (m, 2H), 7.33 (d, *J* = 5.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 176.58, 135.51, 134.91, 134.47, 134.31, 131.78, 130.72, 130.59, 128.91, 127.38, 127.34; **HRMS** (TOF MS ES$^+$) $C_{11}H_6OSSeNa^+$ m/z (%) = 288.9219 ([M+Na]$^+$, 100%).

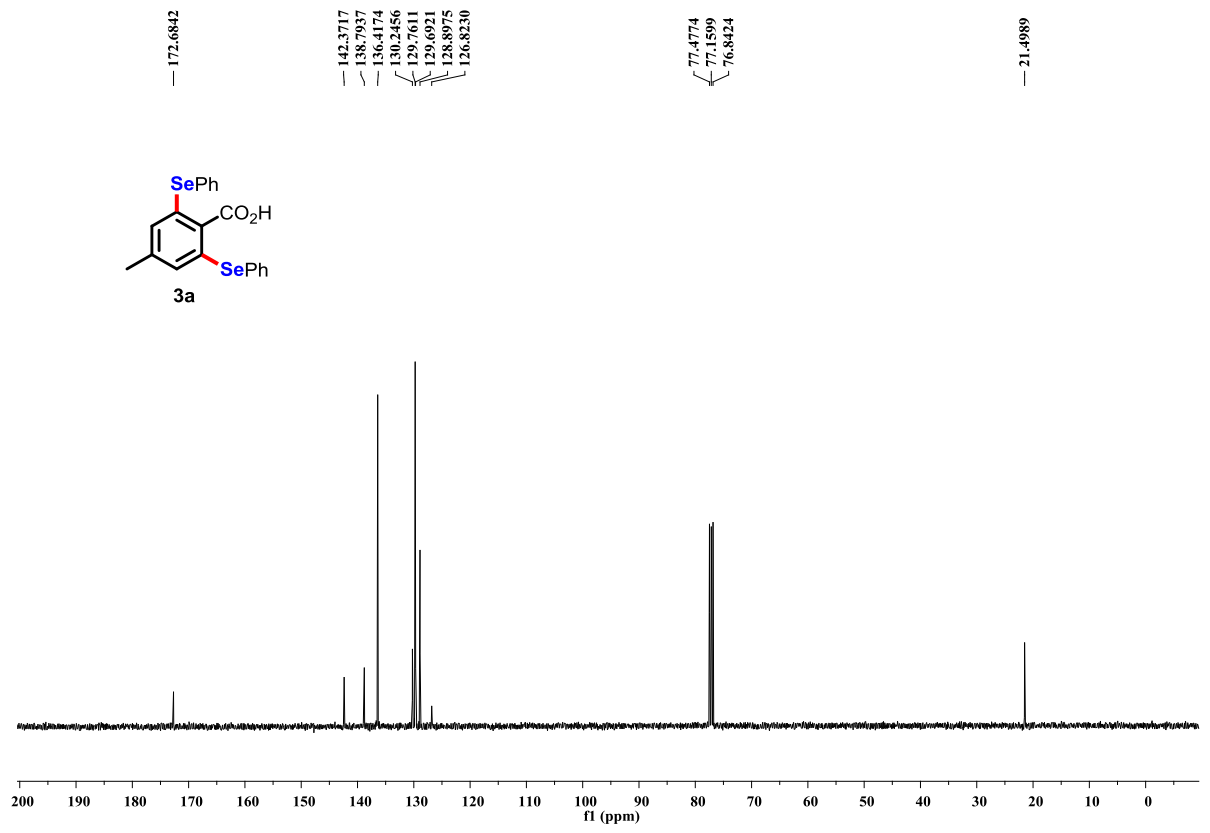


7h

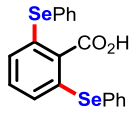
7h: White solid, **Yield**: 70% (31 mg); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.68 (dd, *J* = 8.4, 1.5 Hz, 1H), 7.89 (d, *J* = 5.3 Hz, 1H), 7.72 – 7.62 (m, 2H), 7.61 – 7.54 (m, 1H), 7.29 (d, *J* = 5.3 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 175.25, 138.73, 137.29, 134.77, 133.62, 131.80, 129.14, 127.08, 126.77, 125.53; **HRMS** (TOF MS ES$^+$) $C_{11}H_6OS_2Na^+$ m/z (%) = 240.9774 ([M+Na]$^+$, 100%).

NMR Spectra

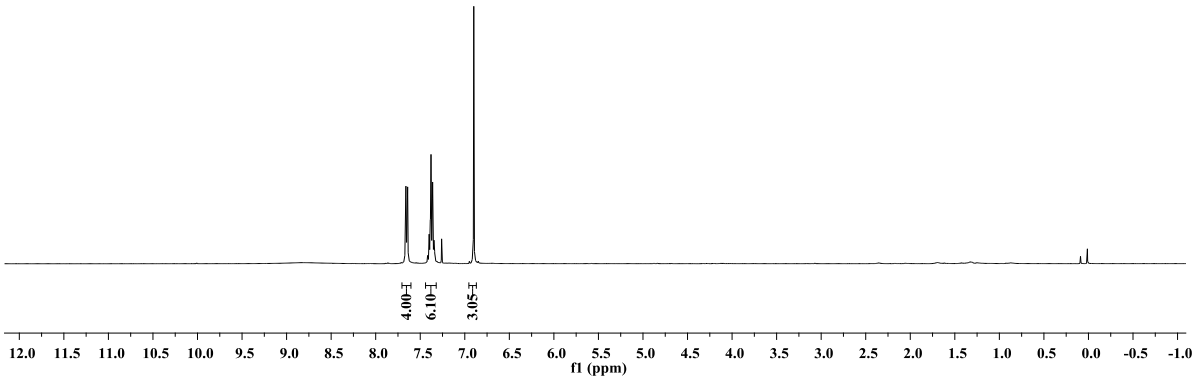

9.9947
7.6559
7.6393
7.3968
7.3806
7.3624
7.3473
7.2600
6.7006
1.9577
SePh
CO2H
SePh
3a
1.07
4.06
6.10
2.00
3.09
f1 (ppm)

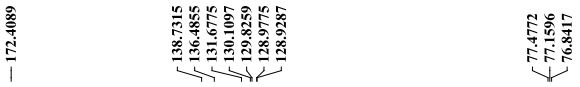

172.6842
142.3717
138.7937
136.4174
130.2456
129.7611
129.6921
128.8975
126.8230
77.4774
77.1599
76.8424
21.4989
SePh
CO2H
SePh
3a
f1 (ppm)

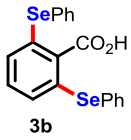

7.6649
7.6610
7.6509
7.6460
7.6414
7.3994
7.3979
7.3912
7.3869
7.3792
7.3612
7.3502
7.3459
7.3394
7.2601
6.8992


SePh
CO2H
SePh

3b

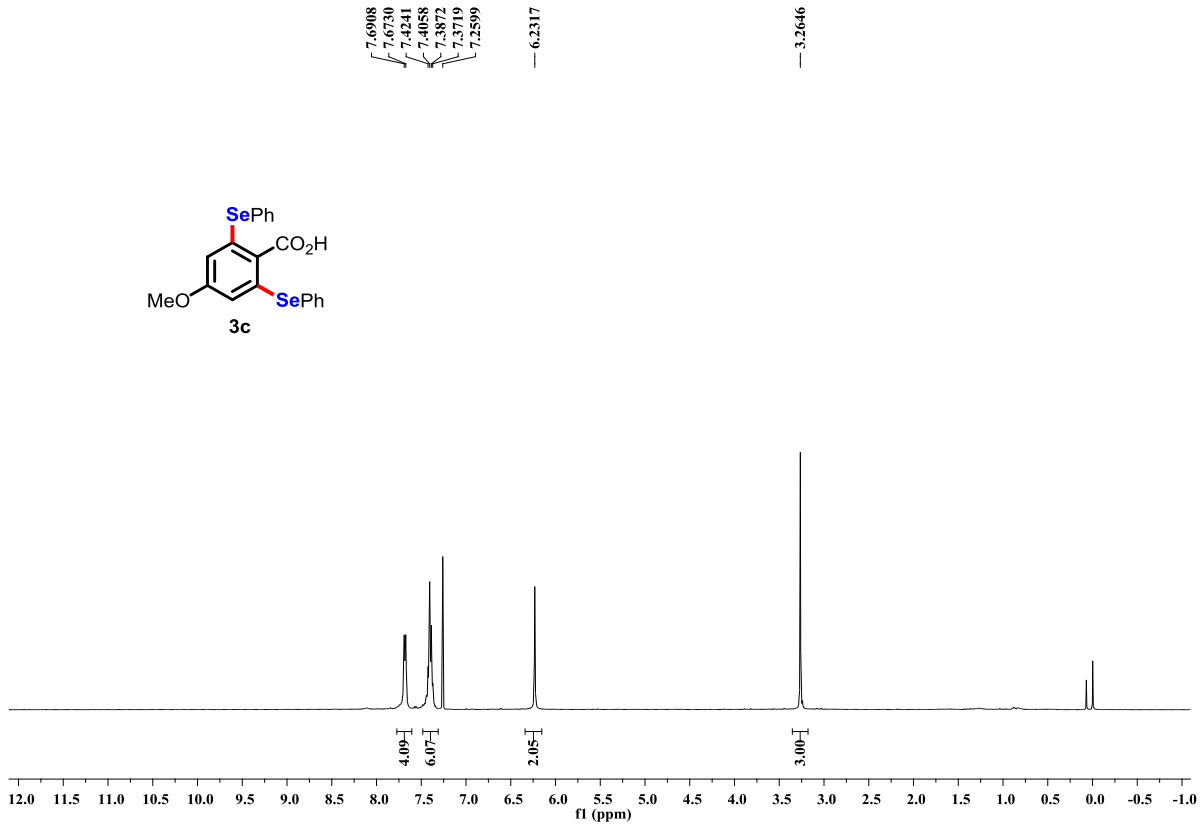

4.00
6.10
3.05
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

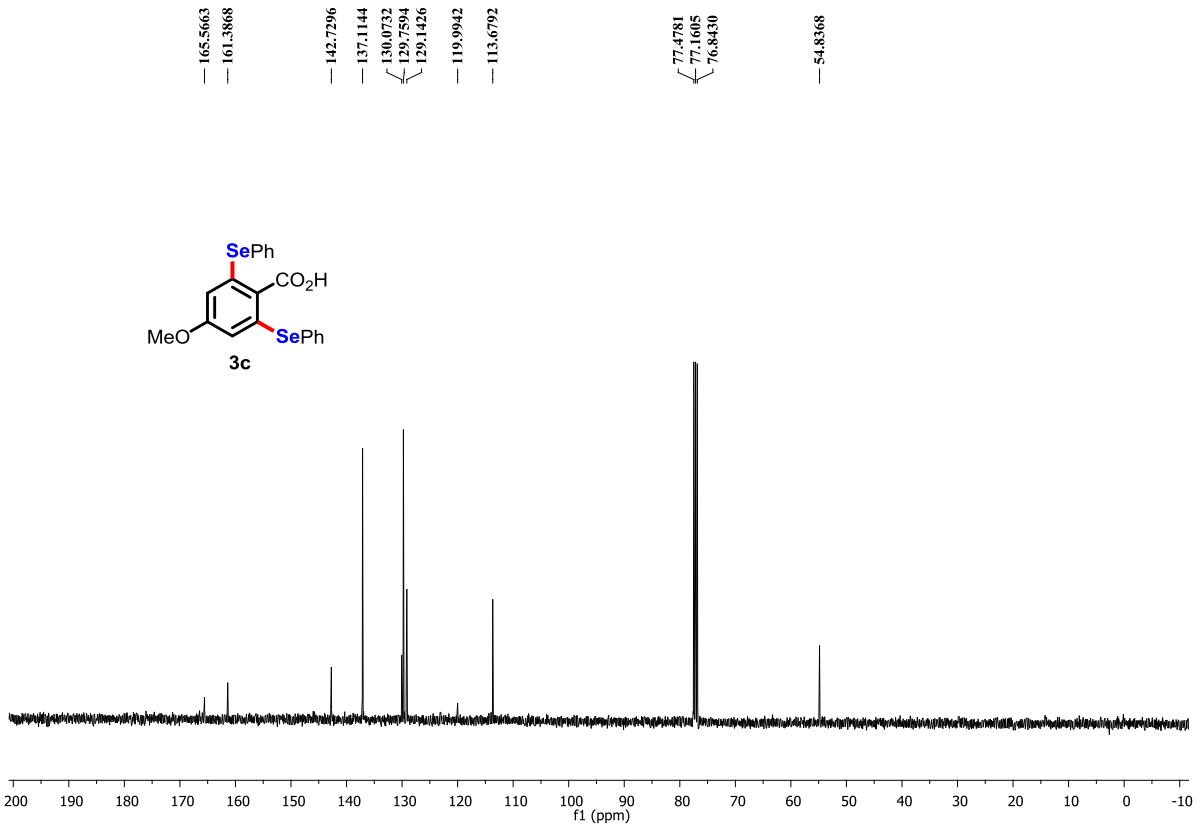

172.4089
138.7315
136.4855
131.6775
130.1097
129.8259
128.9775
128.9287
77.4772
77.1596
76.8417

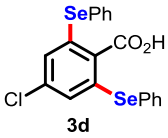

SePh
CO2H
SePh

3b

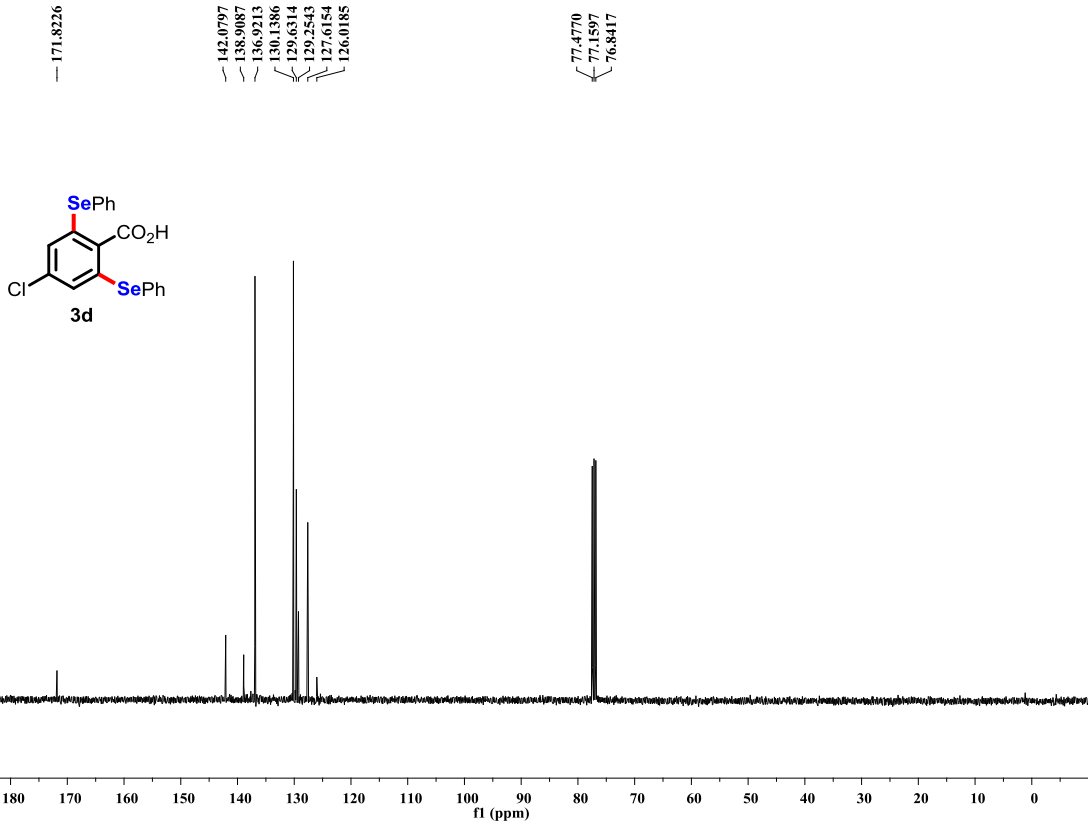
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.6908
7.6730
7.4241
7.4058
7.3872
7.3719
7.2599
6.2317
3.2646
SePh
CO2H
MeO
SePh
3c
4.09
6.07
2.05
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

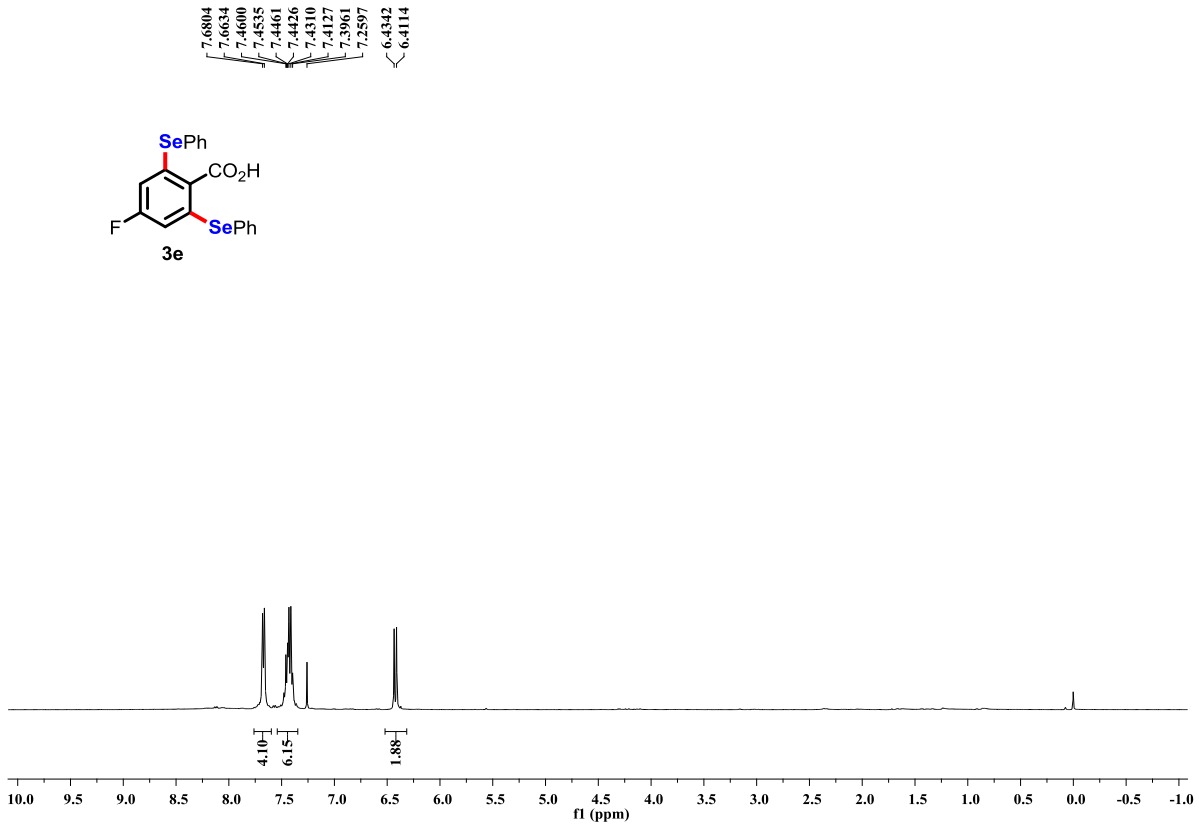

165.5663
161.3868
142.7296
137.1144
130.0732
129.7594
129.1426
119.9942
113.6792
77.4781
77.1605
76.8430
54.8368
SePh
CO2H
MeO
SePh
3c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



3d



SePh
CO2H
Cl
SePh
3d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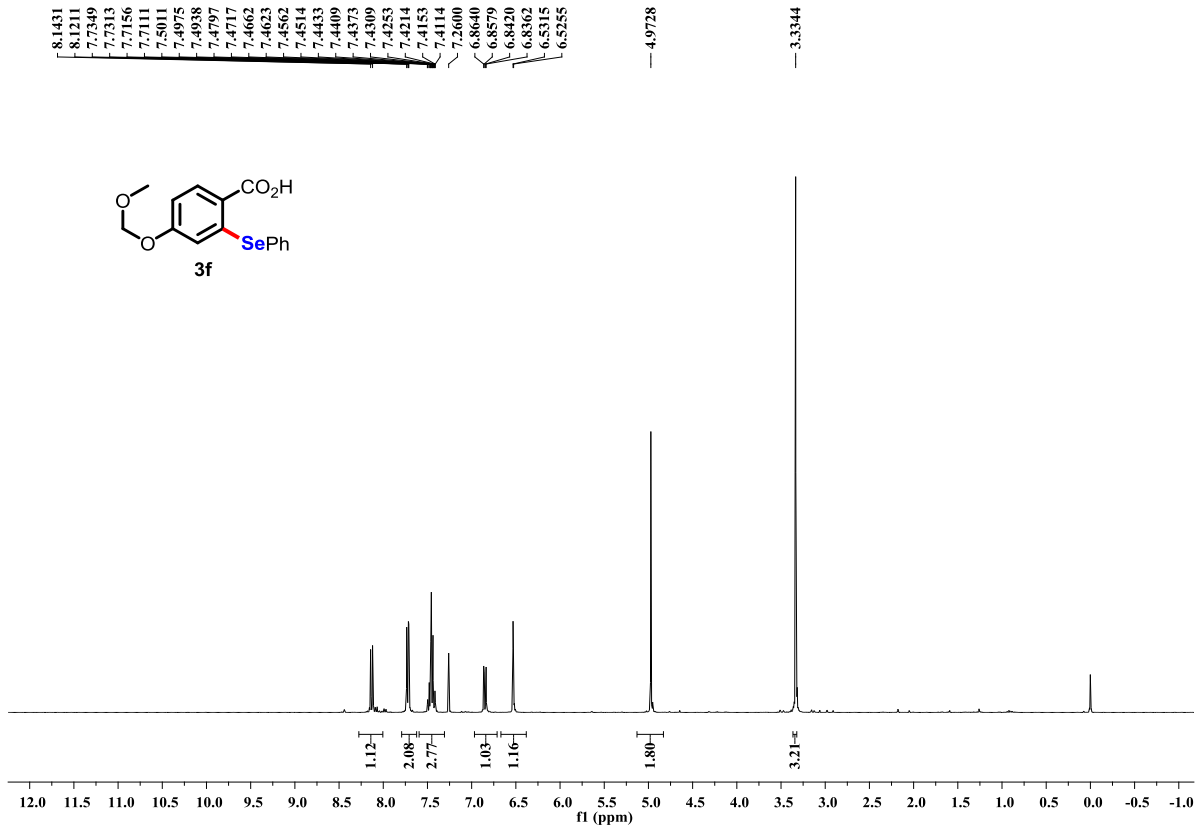
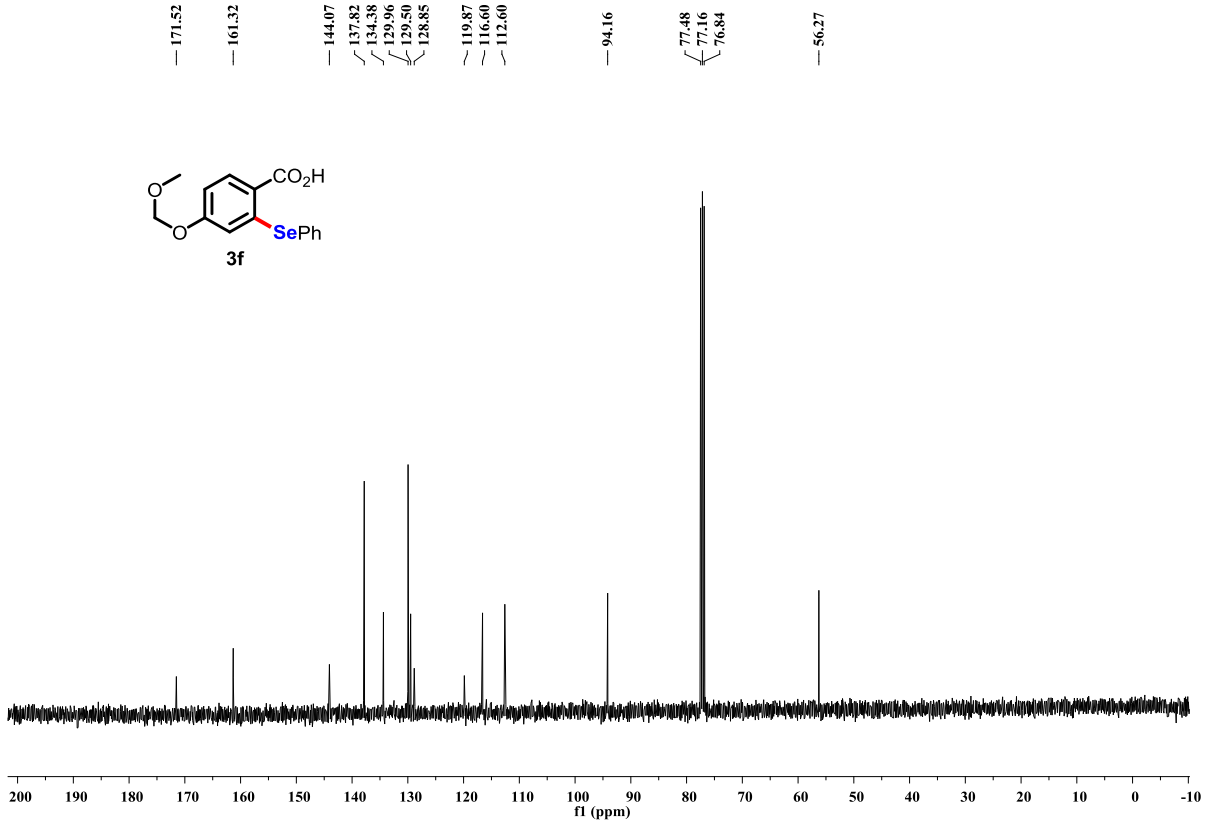
7.4600
7.4535
7.4461
7.4426
7.4310
7.4127
7.3961
7.2597
6.4342
6.4114
SePh
CO2H
F
SePh
3e
4.10
6.15
1.88
f1 (ppm)
171.6111
165.4879
162.9268
144.8445
144.7634
137.3346
130.1761
129.7624
129.2890
114.6581
114.4061
77.4778
77.1661
76.8427
SePh
CO2H
F
SePh
3e
f1 (ppm)


8.1431
8.1211
7.7349
7.7313
7.7156
7.7111
7.5011
7.4975
7.4938
7.4797
7.4717
7.4662
7.4623
7.4562
7.4514
7.4433
7.4409
7.4373
7.4309
7.4253
7.4214
7.4153
7.4114
7.2600
6.8640
6.8579
6.8420
6.8362
6.5315
6.5255
4.9728
3.3344
CO2H
O
O
SePh
3f
1.12
2.08
2.77
1.03
1.16
1.80
3.21
f1 (ppm)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161.32
144.07
137.82
134.38
129.96
129.50
128.85
119.87
116.60
112.60
94.16
77.48
77.16
76.84
56.27
CO2H
O
O
SePh
3f
f1 (ppm)


8.0283
8.0249
7.7338
7.7303
7.7267
7.7194
7.7145
7.7103
7.4705
7.4633
7.4572
7.4533
7.4449
7.4300
7.4267
7.4143
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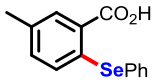
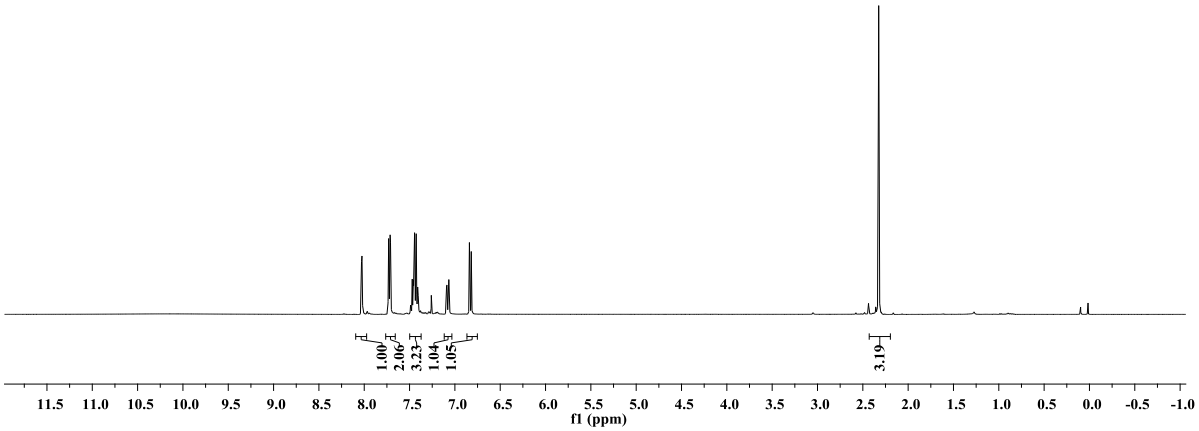
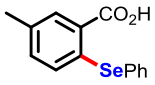
7.0707
7.0668
6.8398
6.8192
2.3248


CO2H
SePh

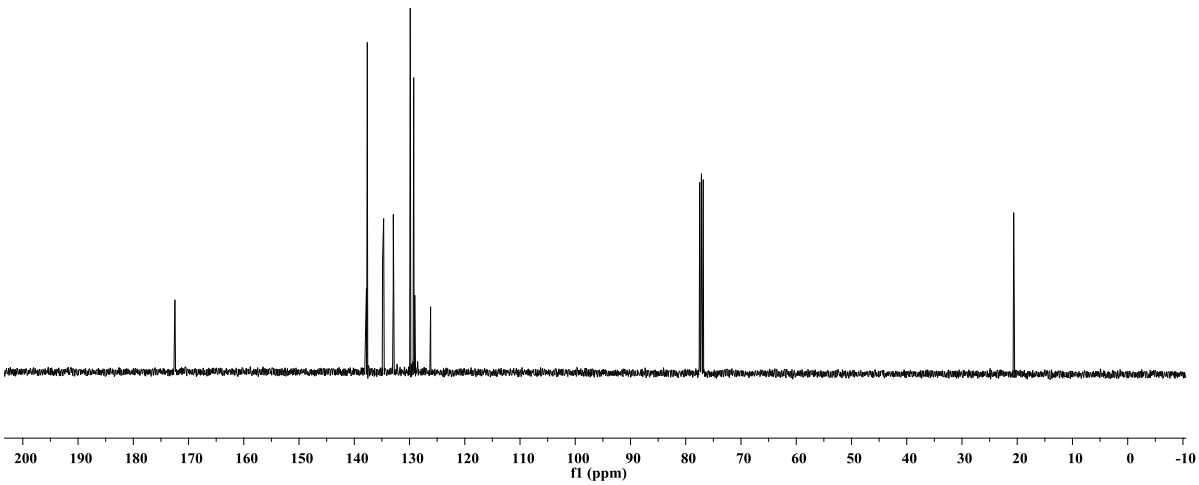
3g


1.00
2.06
3.23
1.04
1.05
3.19
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


172.4587
137.7998
137.6471
134.8834
134.6842
132.9358
129.8730
129.2454
129.0467
126.1845
77.4777
77.1602
76.8422
20.6349


CO2H
SePh

3g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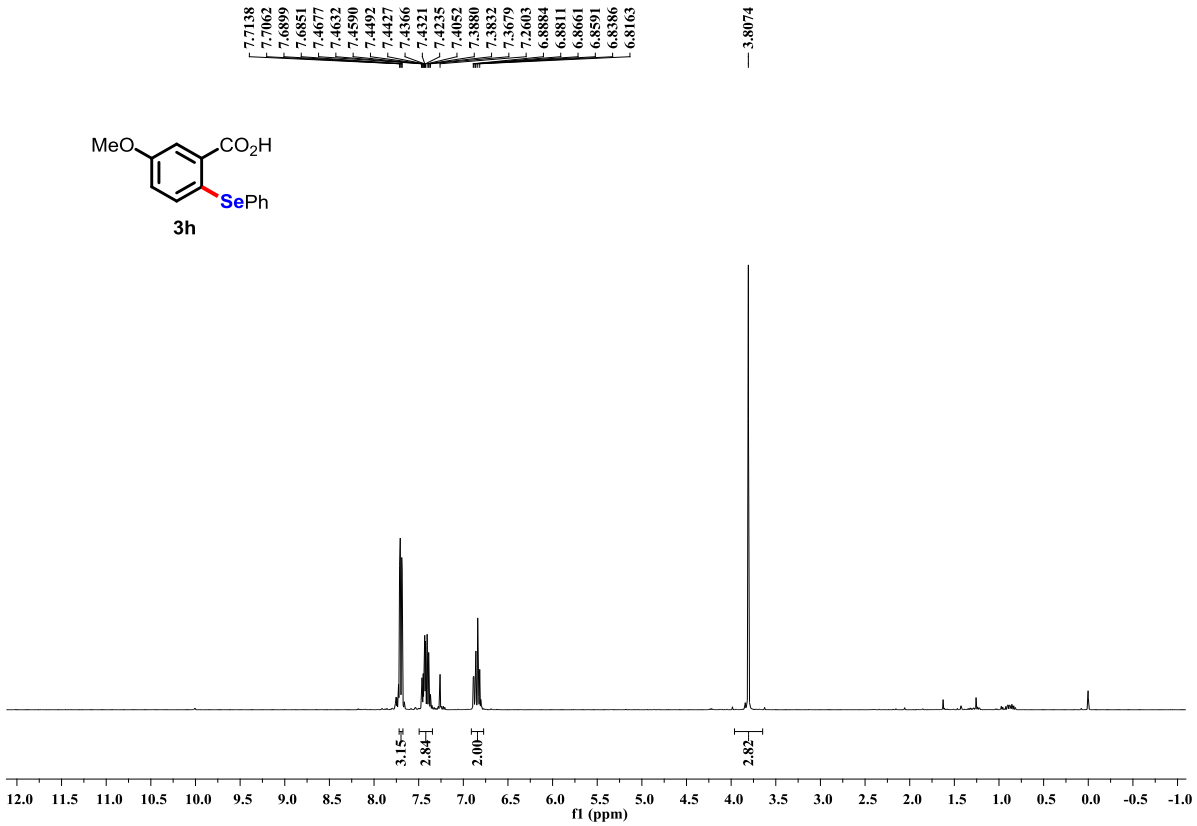
f1 (ppm)


7.7138
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7.6899
7.6851
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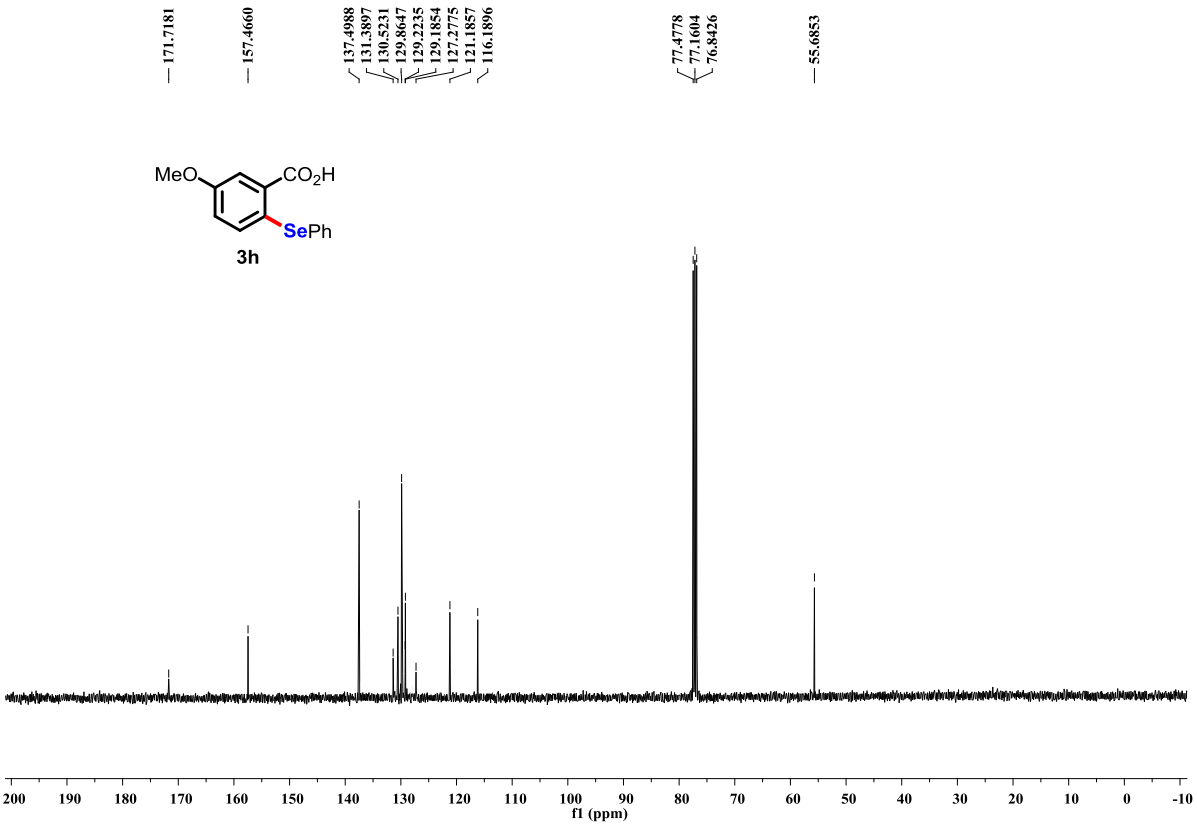
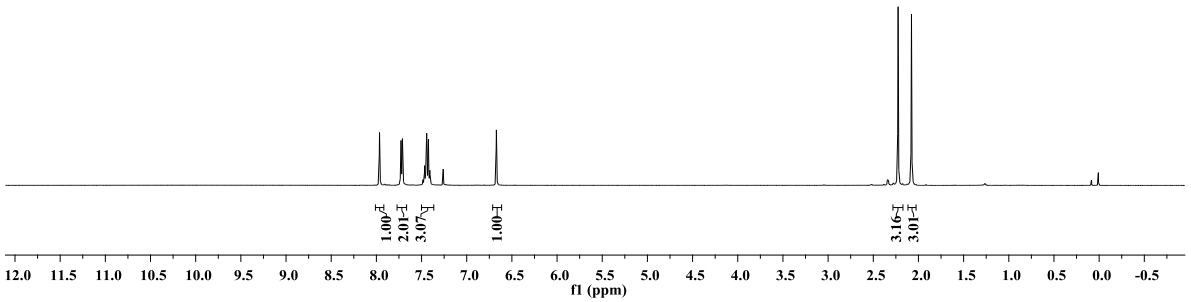
7.4632
7.4590
7.4492
7.4427
7.4366
7.4321
7.4235
7.4052
7.3880
7.3832
7.3679
7.2603
6.8884
6.8811
6.8661
6.8591
6.8386
6.8163
3.8074
MeO
CO2H
SePh
3h
3.15
2.84
2.00
2.82
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


171.7181
157.4660
137.4988
131.3897
130.5231
129.8647
129.2235
129.1854
127.2775
121.1857
116.1896
77.4778
77.1604
76.8426
55.6853
MeO
CO2H
SePh
3h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

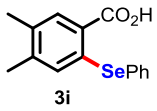

7.9651
7.7309
7.7274
7.7235
7.7166
7.7117
7.7074
7.4876
7.4841
7.4804
7.4760
7.4661
7.4650
7.4584
7.4529
7.4488
7.4431
7.4273
7.4241
7.4120
7.4081
7.4021
7.2602
6.6716
2.2252
2.0769


CO2H
SePh

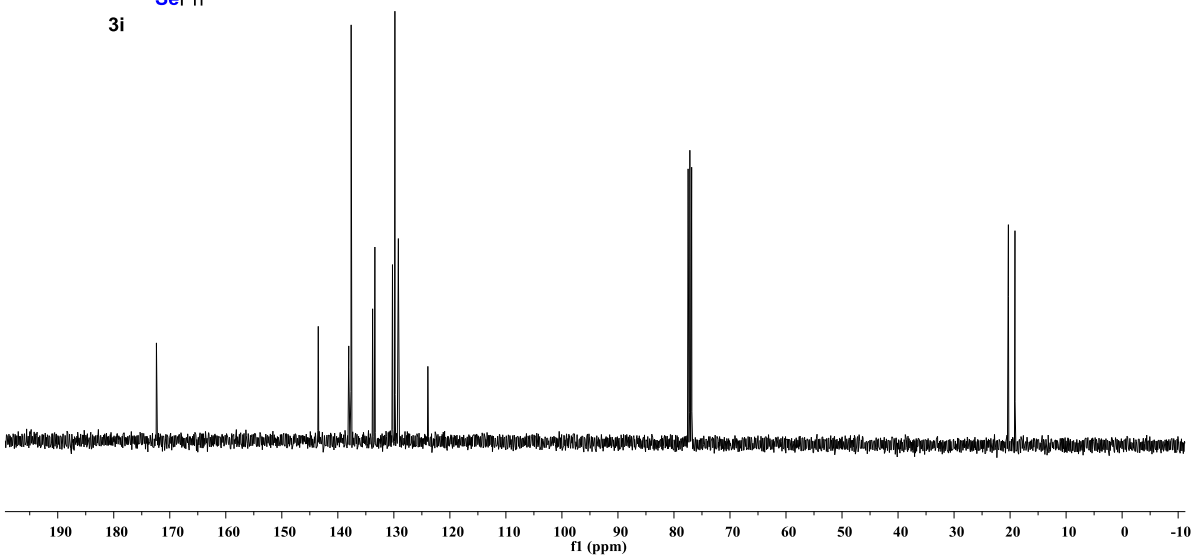
3i


1.00
2.01
3.07
1.00
3.16
3.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

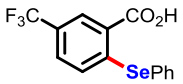

172.3809
143.4908
138.0522
137.6216
133.7928
133.3840
130.2416
129.8104
129.1921
129.1469
123.9283
77.4777
77.1603
76.8426
20.3035
19.1299


CO2H
SePh

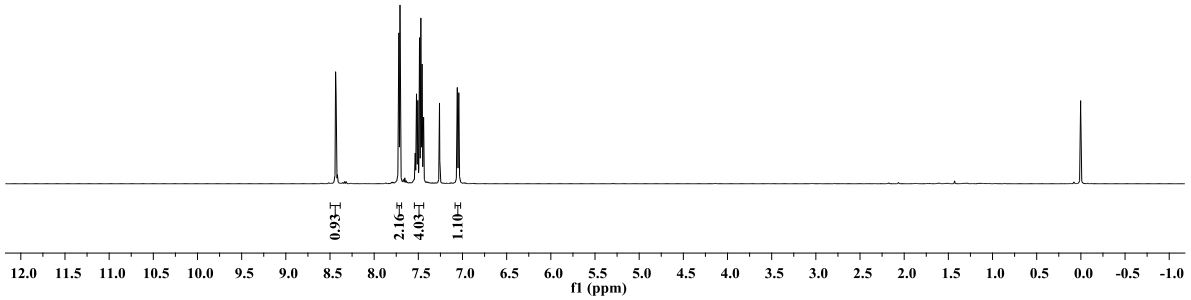
3i

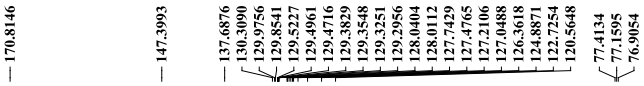

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

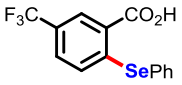

8.4365
8.4318
7.7238
7.7202
7.7115
7.7074
7.7039
7.5353
7.5329
7.5254
7.5207
7.5161
7.5088
7.5061
7.5025
7.4865
7.4832
7.4748
7.4713
7.4614
7.4573
7.4450
7.4402
7.2602
7.0588
7.0417


F3C
CO2H
SePh

3j

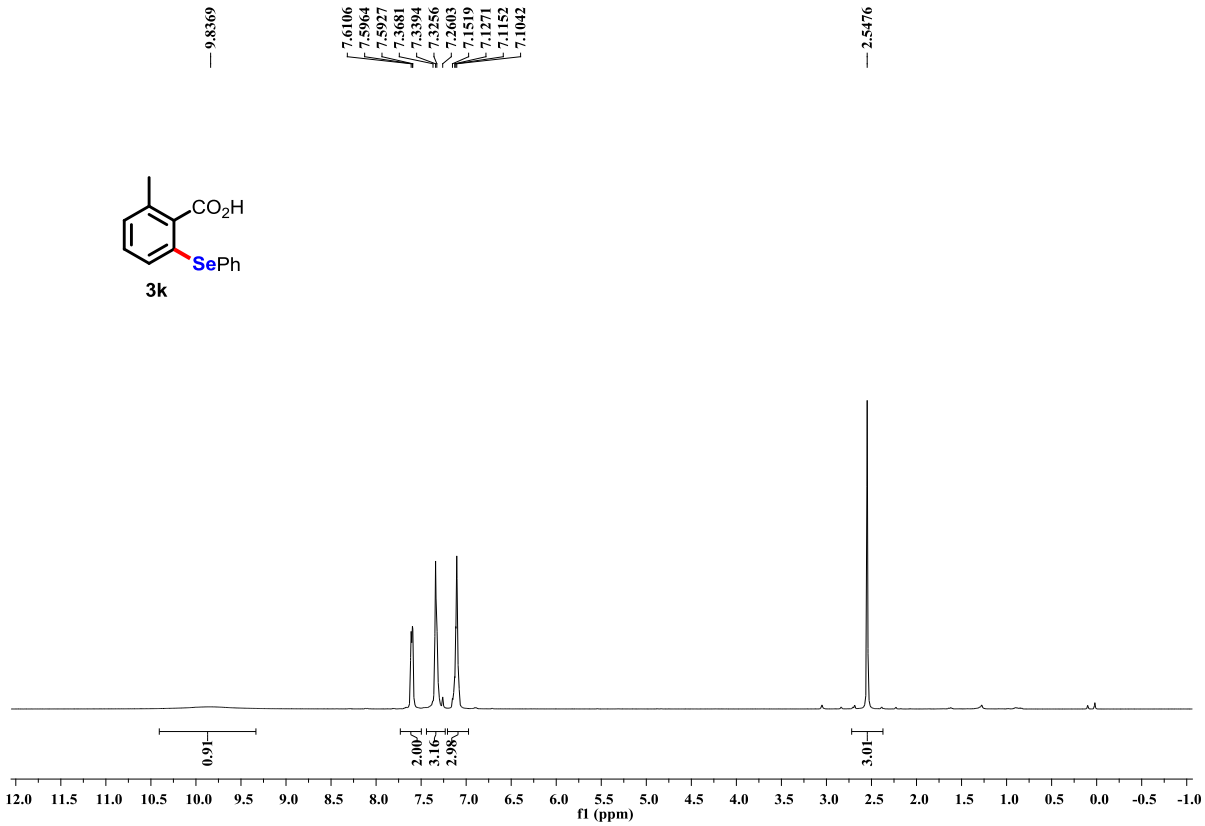

0.93
2.16
4.03
1.10
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

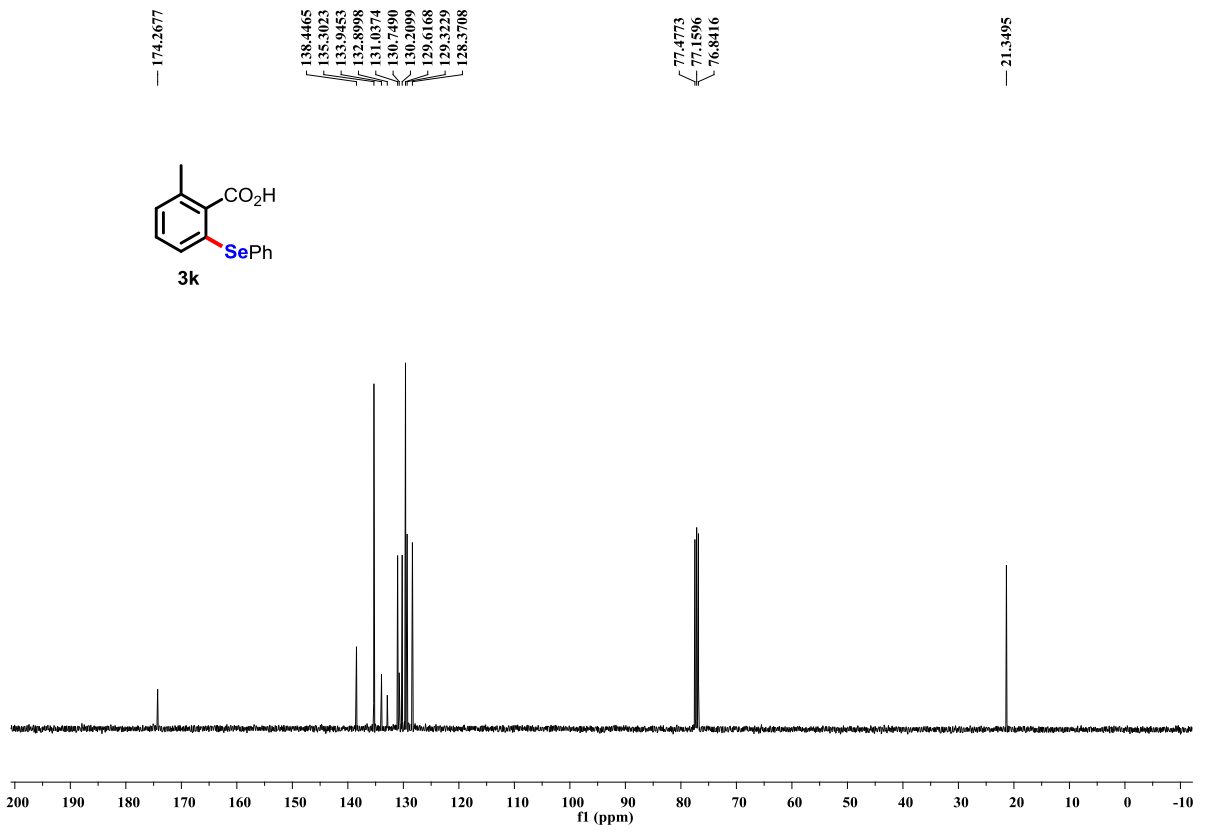

170.8146
147.3993
137.6876
130.3090
129.9756
129.8541
129.5227
129.4961
129.4716
129.3829
129.3548
129.3251
129.2956
128.0404
128.0112
127.7429
127.4765
127.2106
127.0488
126.3618
124.8871
122.7254
120.5648
77.4134
77.1595
76.9054

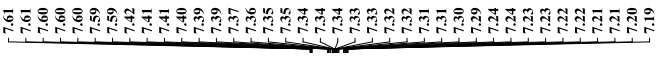

F3C
CO2H
SePh

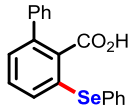
3j

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

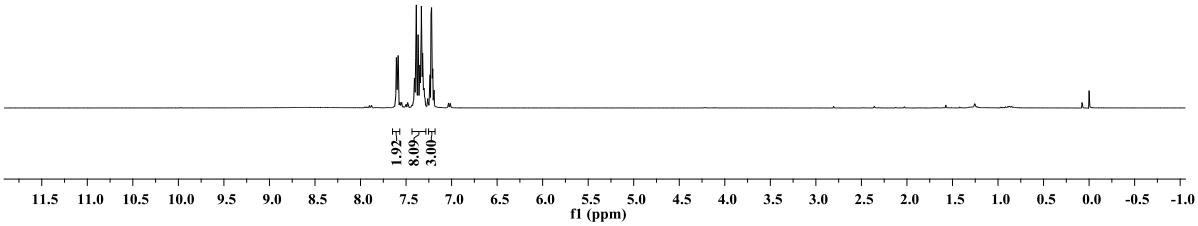

9.8369
7.6106
7.5964
7.5927
7.3681
7.3394
7.3256
7.2603
7.1519
7.1271
7.1152
7.1042
2.5476
CO2H
SePh
3k
0.91
2.00
3.16
2.98
3.01
f1 (ppm)


174.2677
138.4465
135.3023
133.9453
132.8998
131.0374
130.7490
130.2099
129.6168
129.3229
128.3708
77.4773
77.1596
76.8416
21.3495
CO2H
SePh
3k
f1 (ppm)

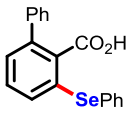

7.61
7.61
7.60
7.60
7.60
7.59
7.59
7.42
7.41
7.41
7.40
7.39
7.39
7.37
7.36
7.35
7.35
7.34
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.29
7.24
7.24
7.23
7.23
7.22
7.22
7.21
7.21
7.20
7.19


Ph
CO2H
SePh

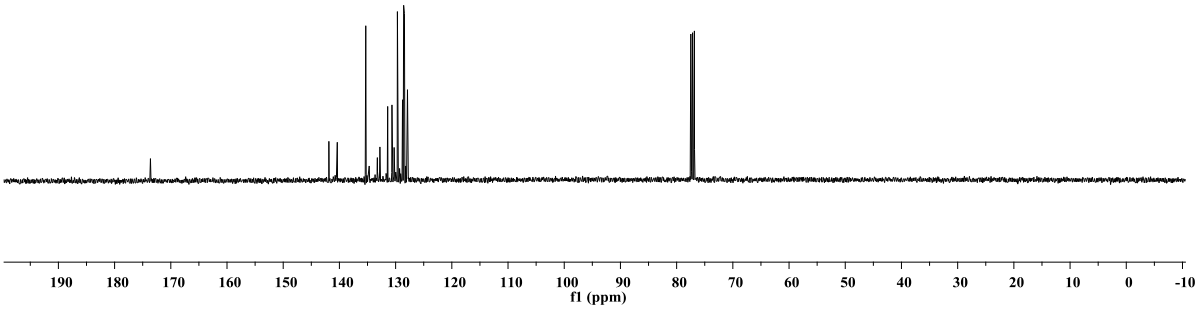
3l


1.92
8.09
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

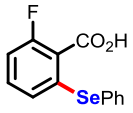

173.6235
141.8720
140.3790
135.3124
133.2490
132.7957
131.4140
130.6511
130.2654
129.6826
128.7745
128.5745
128.4789
128.4299
127.8876
77.4775
77.1600
76.8422


Ph
CO2H
SePh

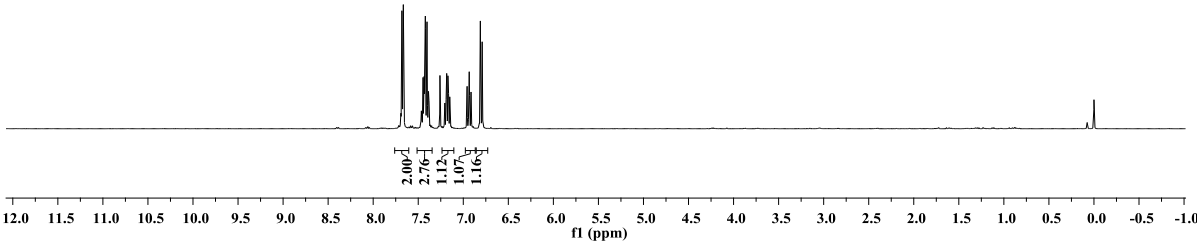
3l


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

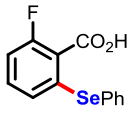

7.6917
7.6850
7.6811
7.6772
7.6710
7.6655
7.6610
7.4690
7.4651
7.4615
7.4565
7.4464
7.4397
7.4339
7.4296
7.4256
7.4211
7.4166
7.4072
7.4025
7.3964
7.3905
7.3863
7.3808
7.2588
7.2530
7.2044
7.1909
7.1840
7.1705
7.1635
7.1500
6.9605
6.9576
6.9396
6.9374
6.9339
6.9318
6.9137
6.9109
6.8104
6.7904
6.7888


F
CO2H
SePh

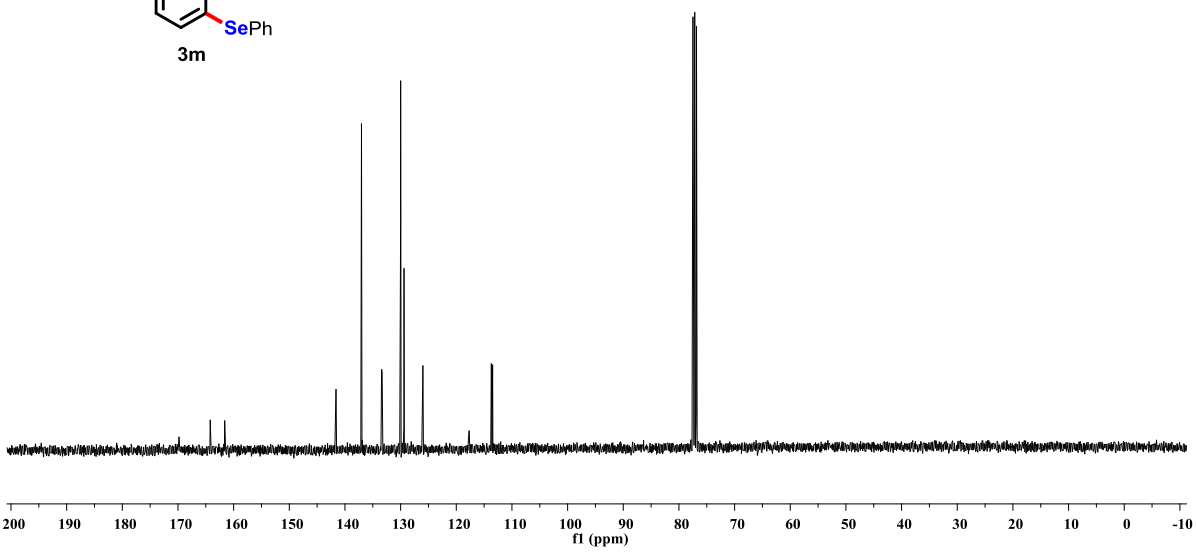
3m

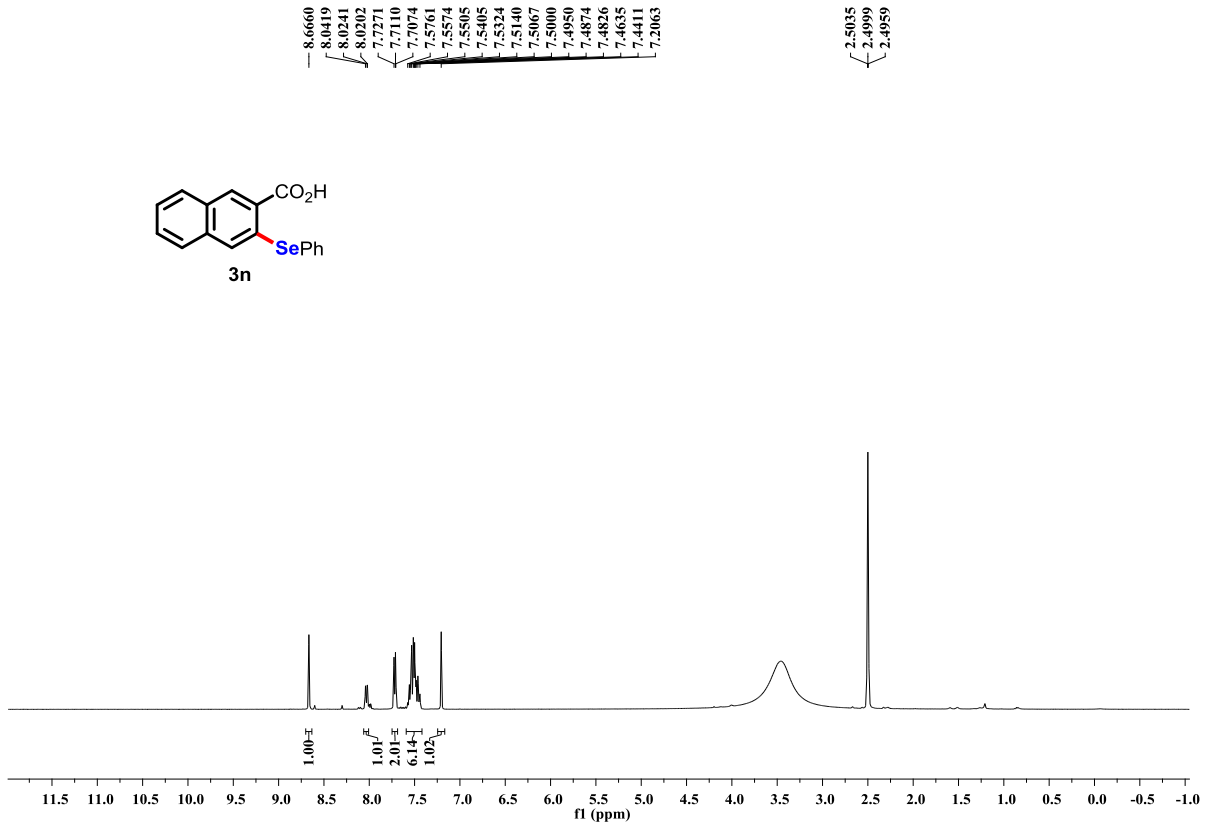

2.00
2.76
1.12
1.07
1.16
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

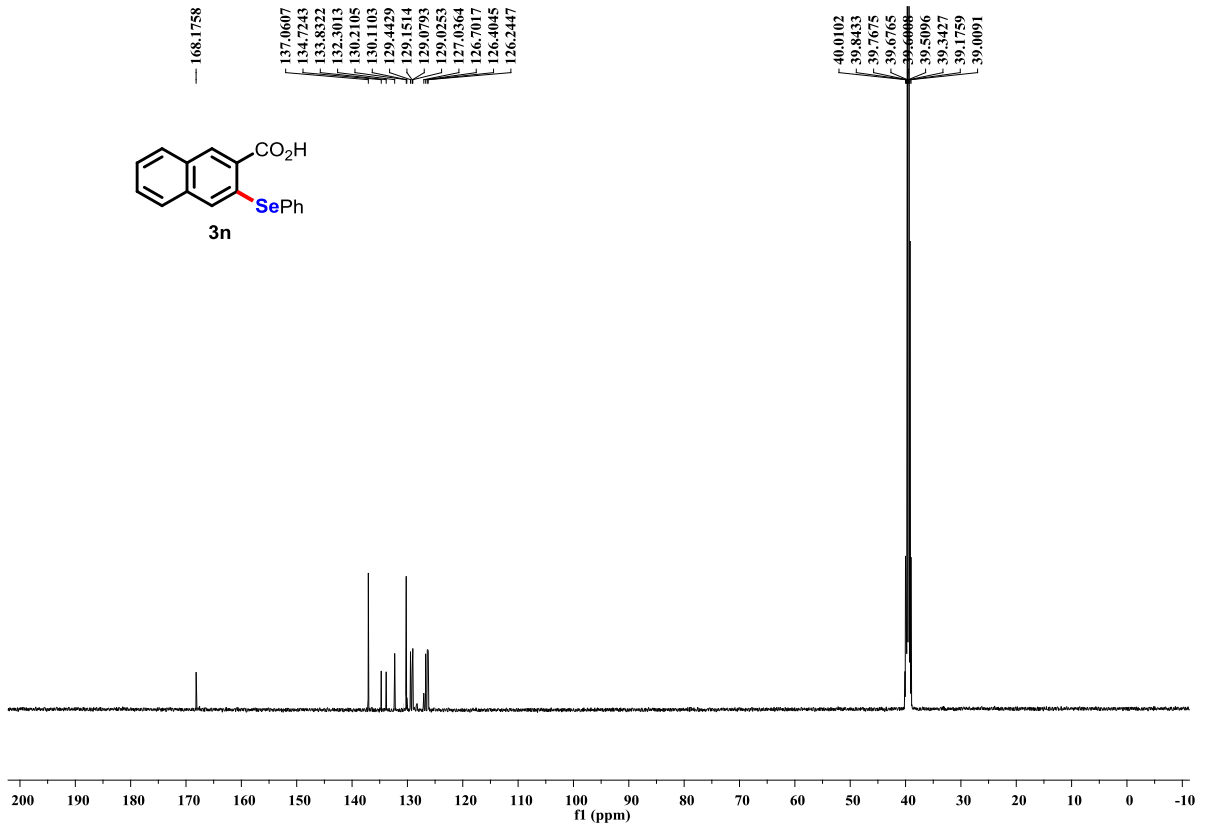

169.8159
164.2022
161.6100
141.6072
137.0261
133.4187
133.3227
129.9903
129.3889
129.2306
126.0321
125.9995
117.8126
117.6908
113.7026
113.4729
77.4781
77.1601
76.8427


F
CO2H
SePh

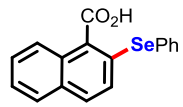
3m


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

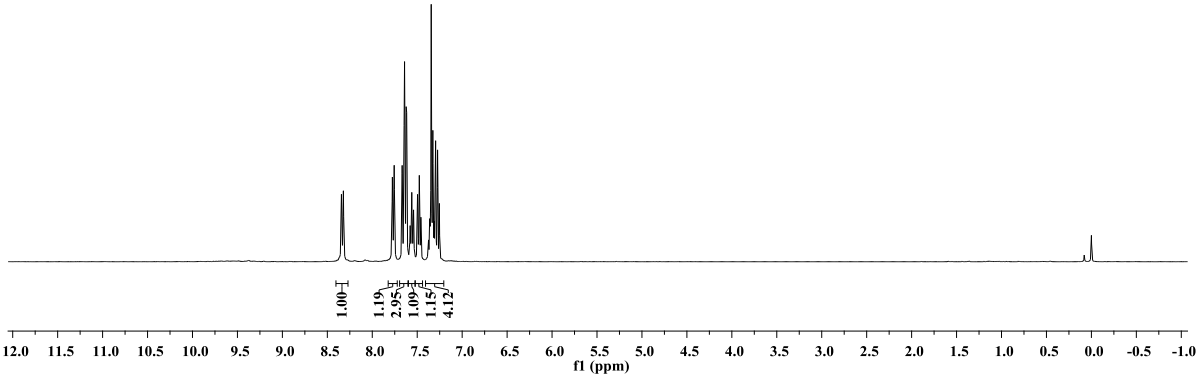

8.6660
8.0419
8.0241
8.0202
7.7271
7.7110
7.7074
7.5761
7.5574
7.5505
7.5405
7.5324
7.5140
7.5067
7.5000
7.4950
7.4874
7.4826
7.4635
7.4411
7.2063
2.5035
2.4999
2.4959
CO2H
SePh
3n
1.00
1.01
2.01
6.14
1.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

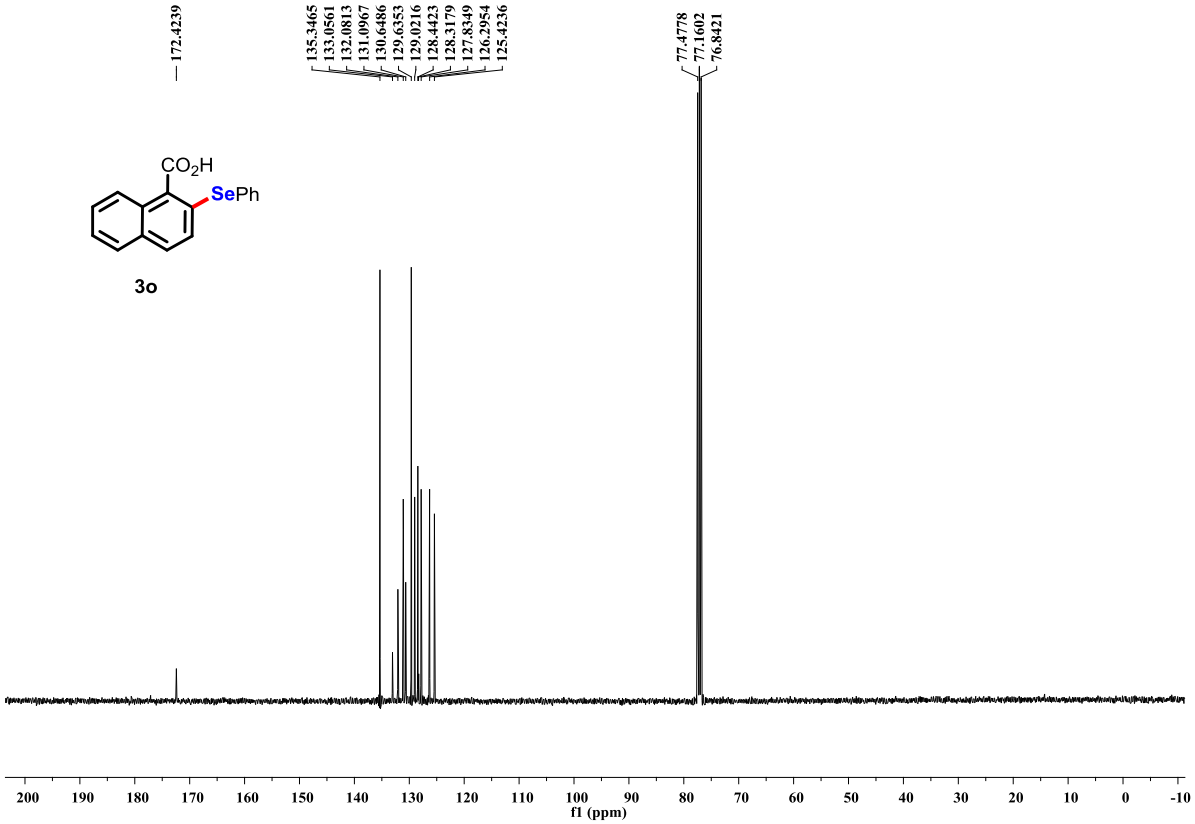

168.1758
137.0607
134.7243
133.8322
132.3013
130.2105
130.1103
129.4429
129.1514
129.0793
129.0253
127.0364
126.7017
126.4045
126.2447
40.0102
39.8433
39.7675
39.6765
39.6000
39.5096
39.3427
39.1759
39.0091
CO2H
SePh
3n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.3428
8.3215
7.7763
7.7562
7.6675
7.6461
7.6409
7.6367
7.6231
7.6176
7.5785
7.5606
7.5408
7.4961
7.4768
7.4592
7.3594
7.3442
7.3262
7.3119
7.3041
7.2953
7.2736
7.2538

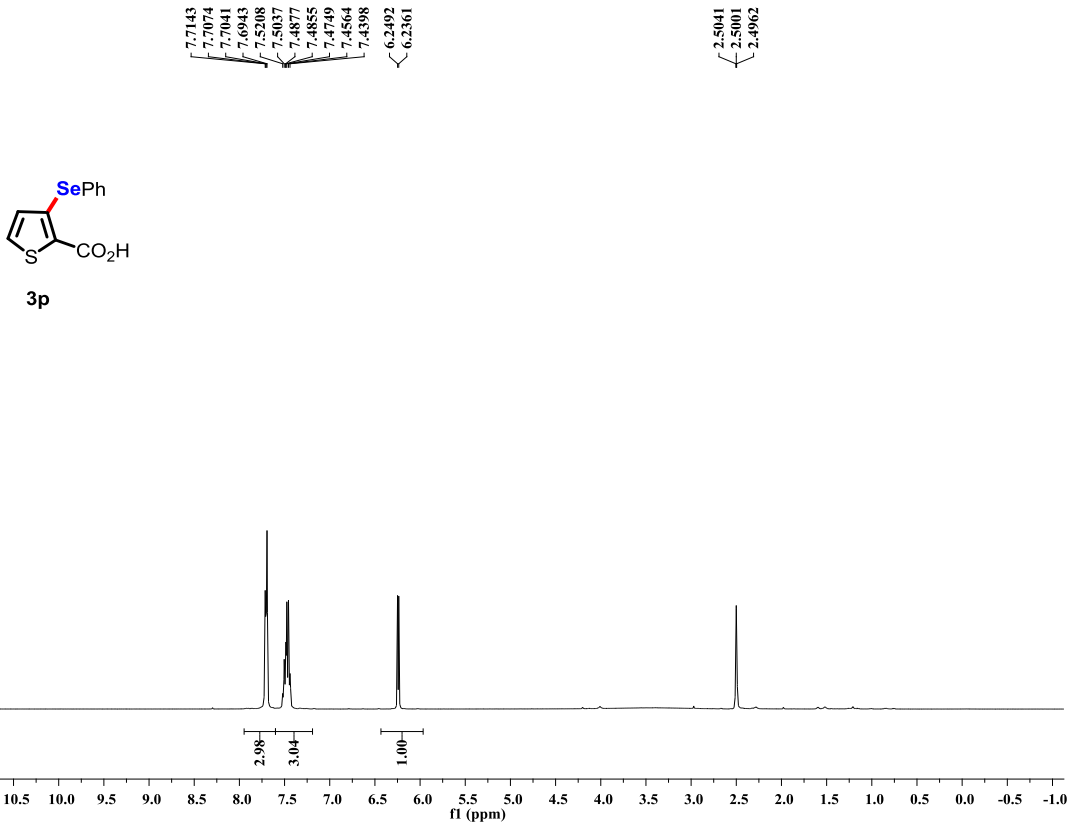

CO2H
SePh

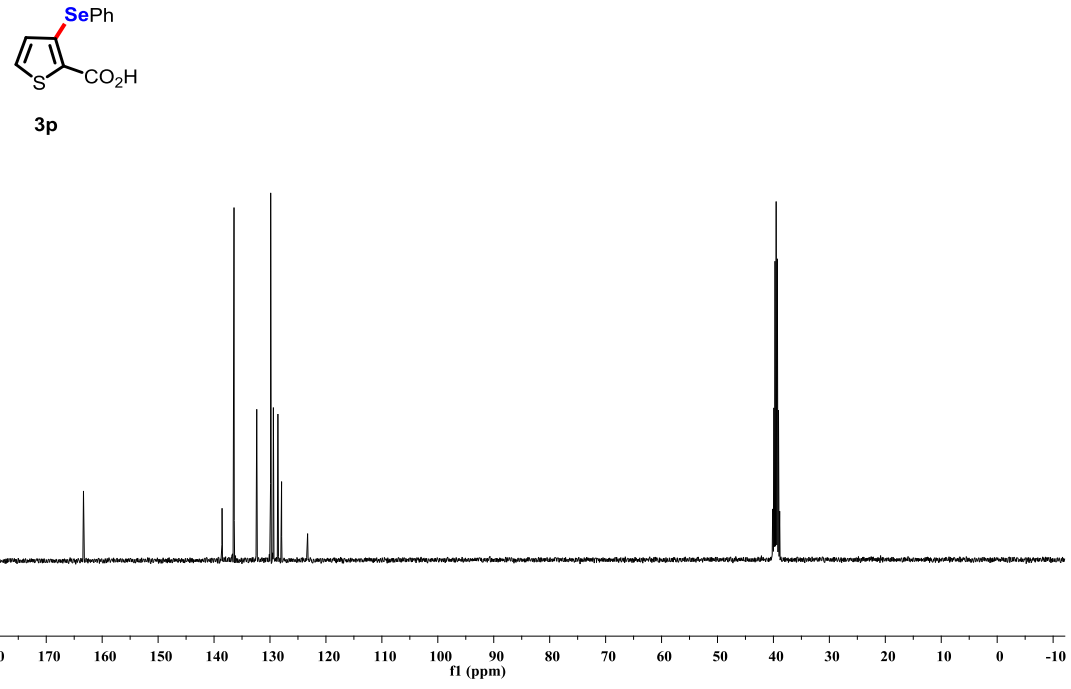
3o

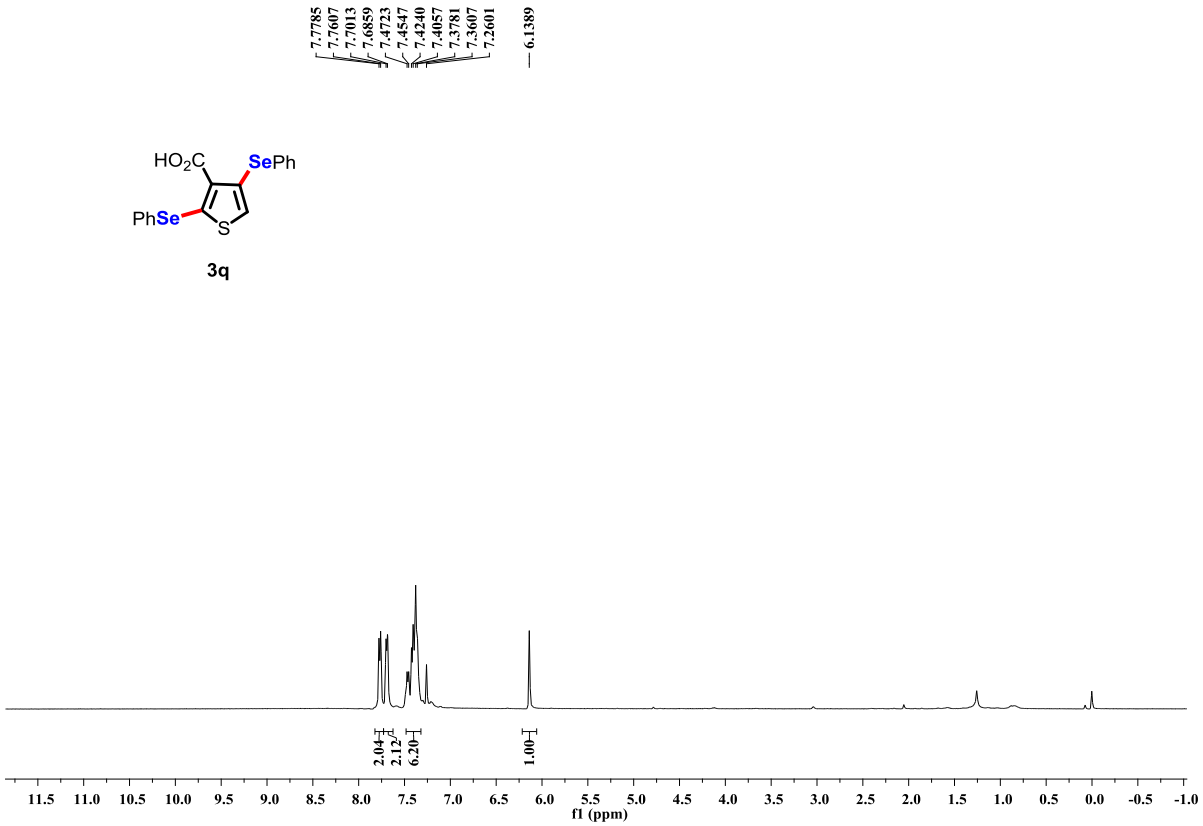

1.00
1.19
2.95
1.09
1.15
4.12
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

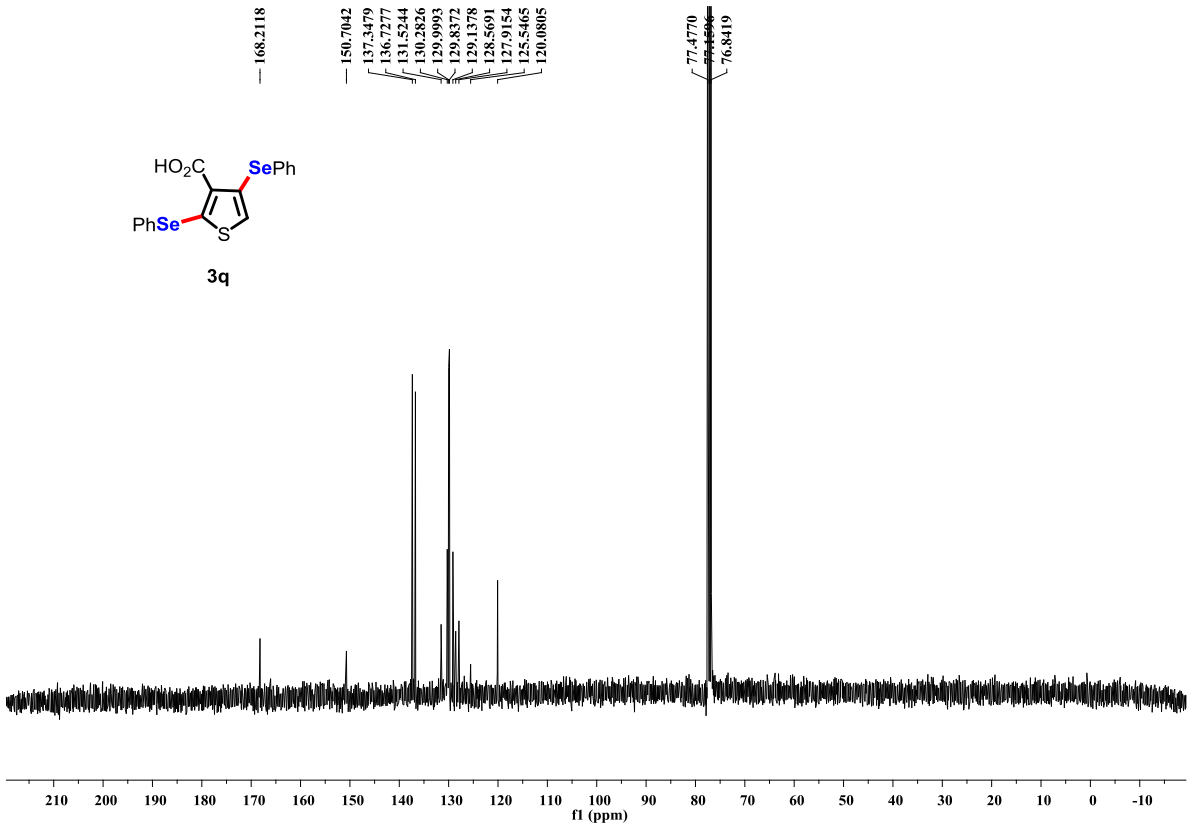

172.4239
135.3465
133.0561
132.0813
131.0967
130.6486
129.6353
129.0216
128.4423
128.3179
127.8349
126.2954
125.4236
77.4778
77.1602
76.8421
CO2H
SePh
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3o


7.7143
7.7074
7.7041
7.6943
7.5208
7.5037
7.4877
7.4855
7.4749
7.4564
7.4398
6.2492
6.2361
2.5041
2.5001
2.4962
SePh
CO2H
S
3p
2.98
3.04
1.00
f1 (ppm)


163.3431
138.5669
136.4318
132.3675
129.8771
129.3954
128.5821
127.9278
123.2738
40.1365
39.9278
39.7191
39.5104
39.3014
39.0929
38.8836
SePh
CO2H
S
3p
f1 (ppm)


7.7785
7.7607
7.7013
7.6859
7.4723
7.4547
7.4240
7.4057
7.3781
7.3607
7.2601
6.1389
HO2C
SePh
PhSe
S
3q
2.04
2.12
6.20
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


168.2118
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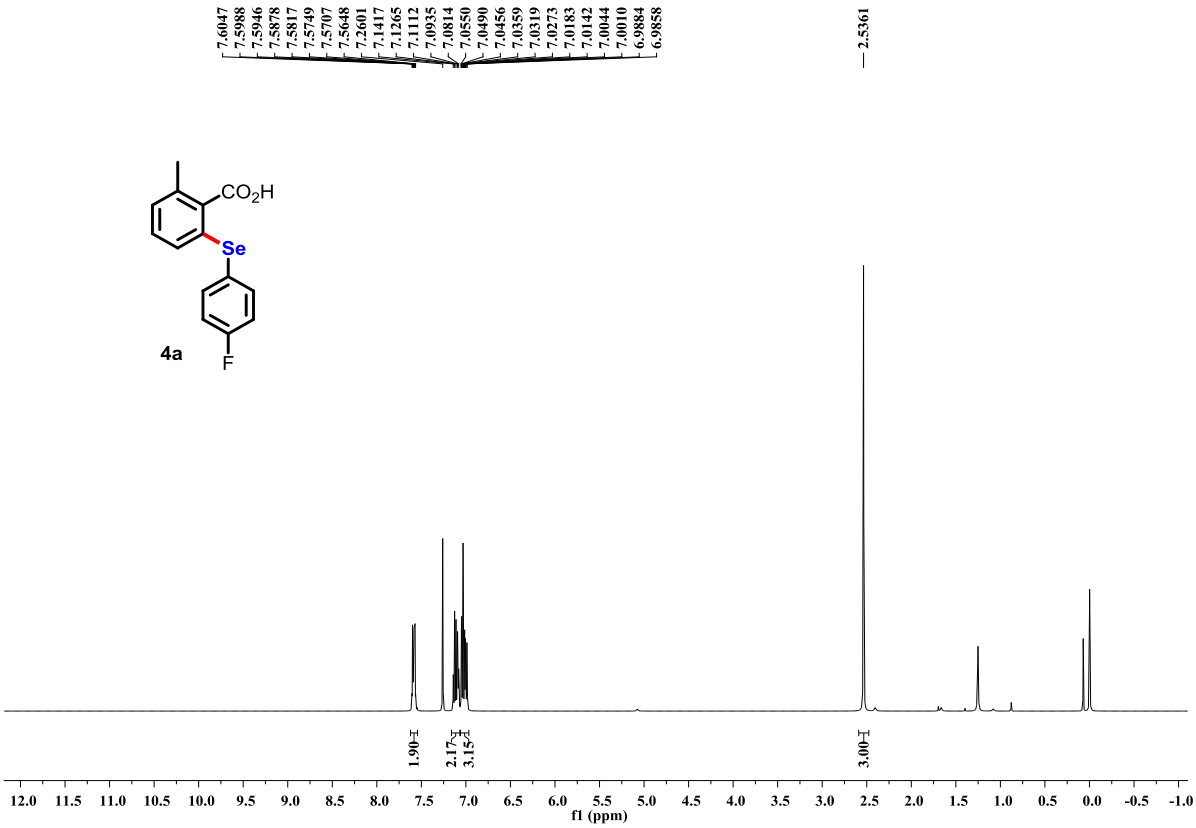
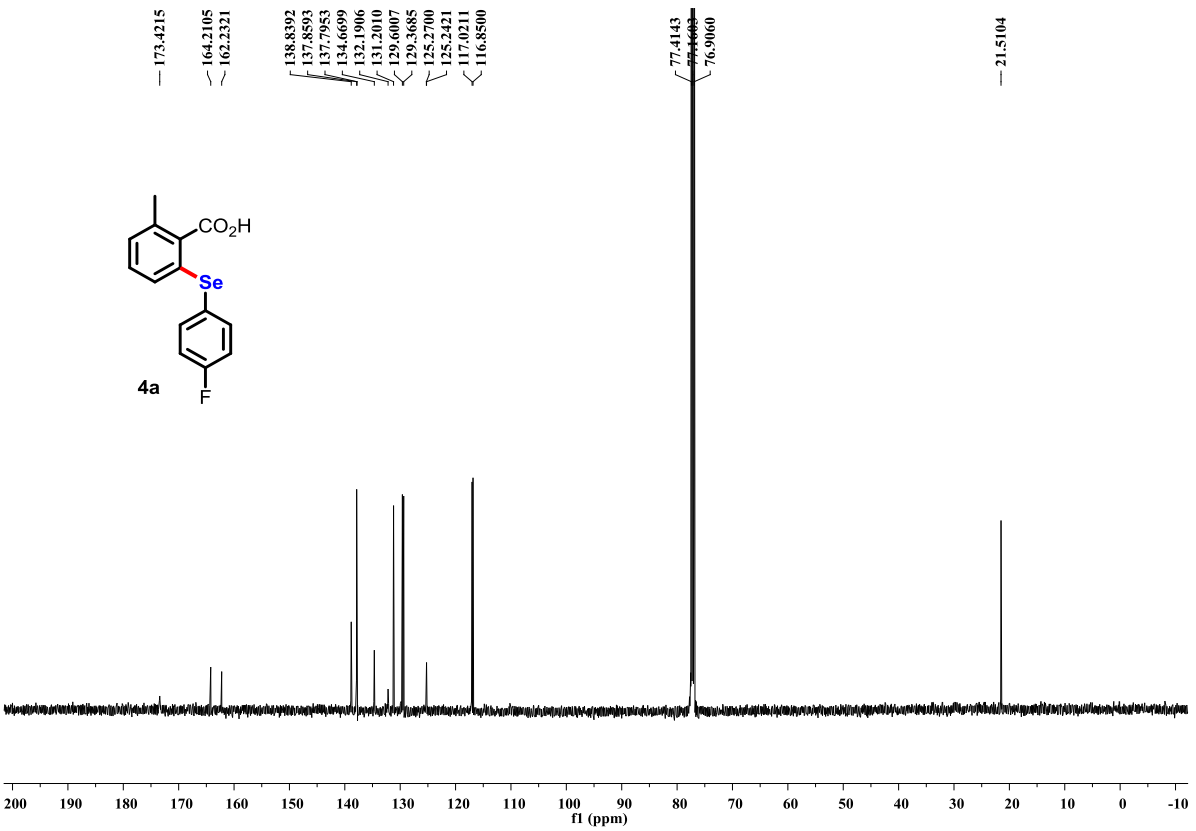
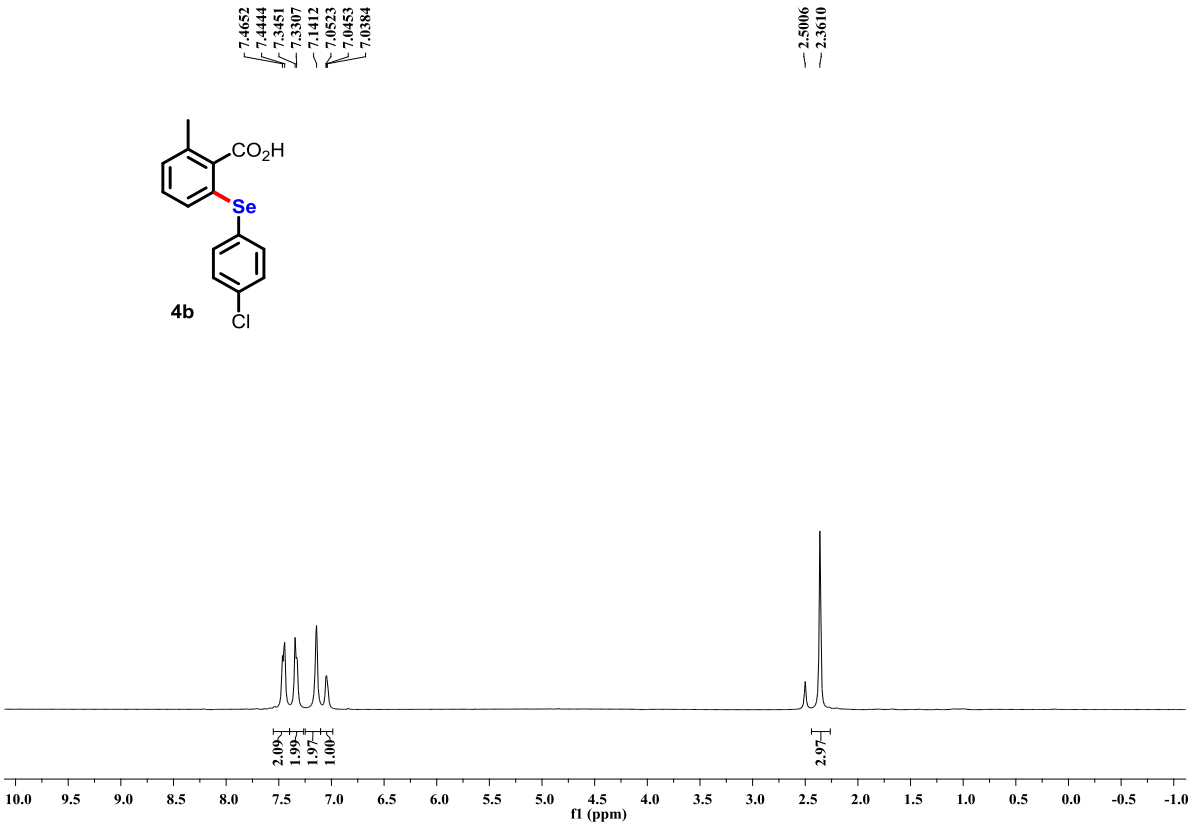
137.3479
136.7277
131.5244
130.2826
129.9993
129.8372
129.1378
128.5691
127.9154
125.5465
120.0805
77.4770
76.8419
HO2C
SePh
PhSe
S
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.6047
7.5988
7.5946
7.5878
7.5817
7.5749
7.5707
7.5648
7.2601
7.1417
7.1265
7.1112
7.0935
7.0814
7.0550
7.0490
7.0456
7.0359
7.0319
7.0273
7.0183
7.0142
7.0044
7.0010
6.9884
6.9858
2.5361
CO2H
Se
F
4a
1.90
2.17
3.15
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


173.4215
164.2105
162.2321
138.8392
137.8593
137.7953
134.6699
132.1906
131.2010
129.6007
129.3685
125.2700
125.2421
117.0211
116.8500
77.4143
77.1603
76.9060
21.5104
CO2H
Se
F
4a
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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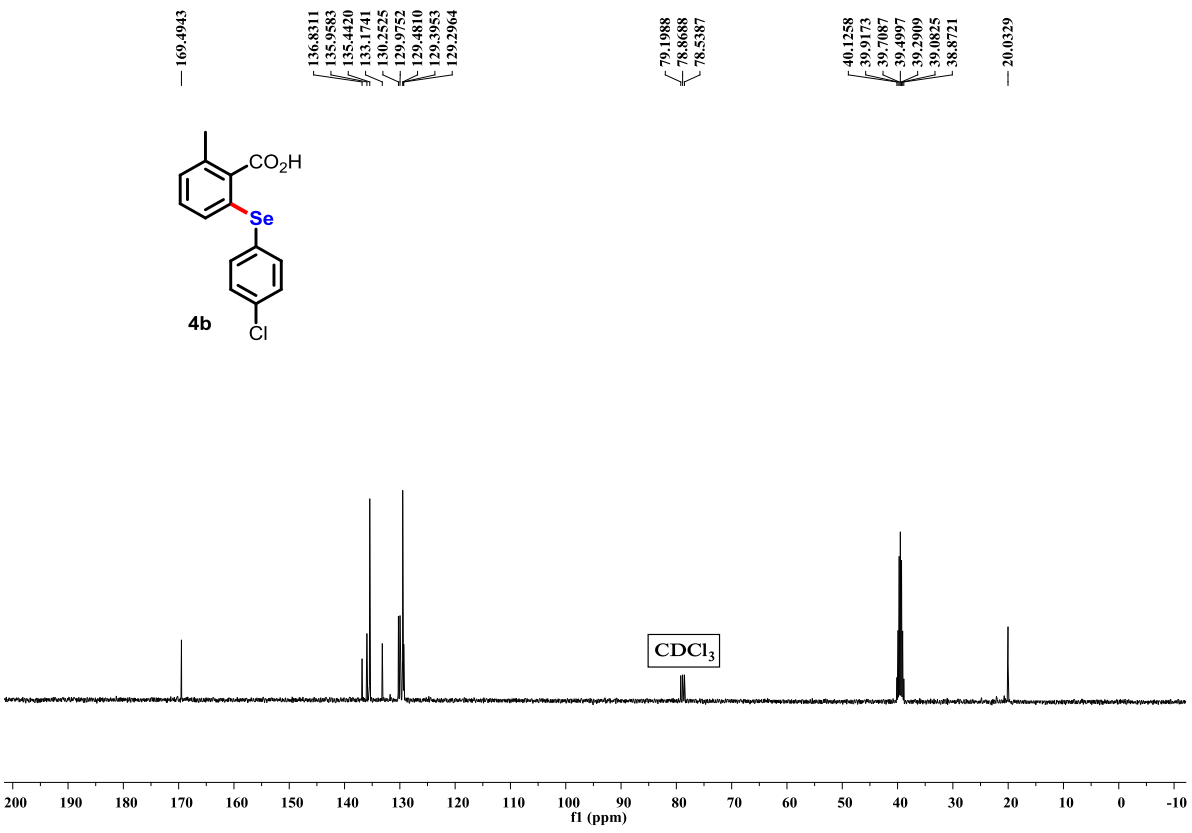
7.0523
7.0453
7.0384
2.5006
2.3610
CO2H
Se
Cl
4b
2.09
1.99
1.97
1.00
2.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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135.4420
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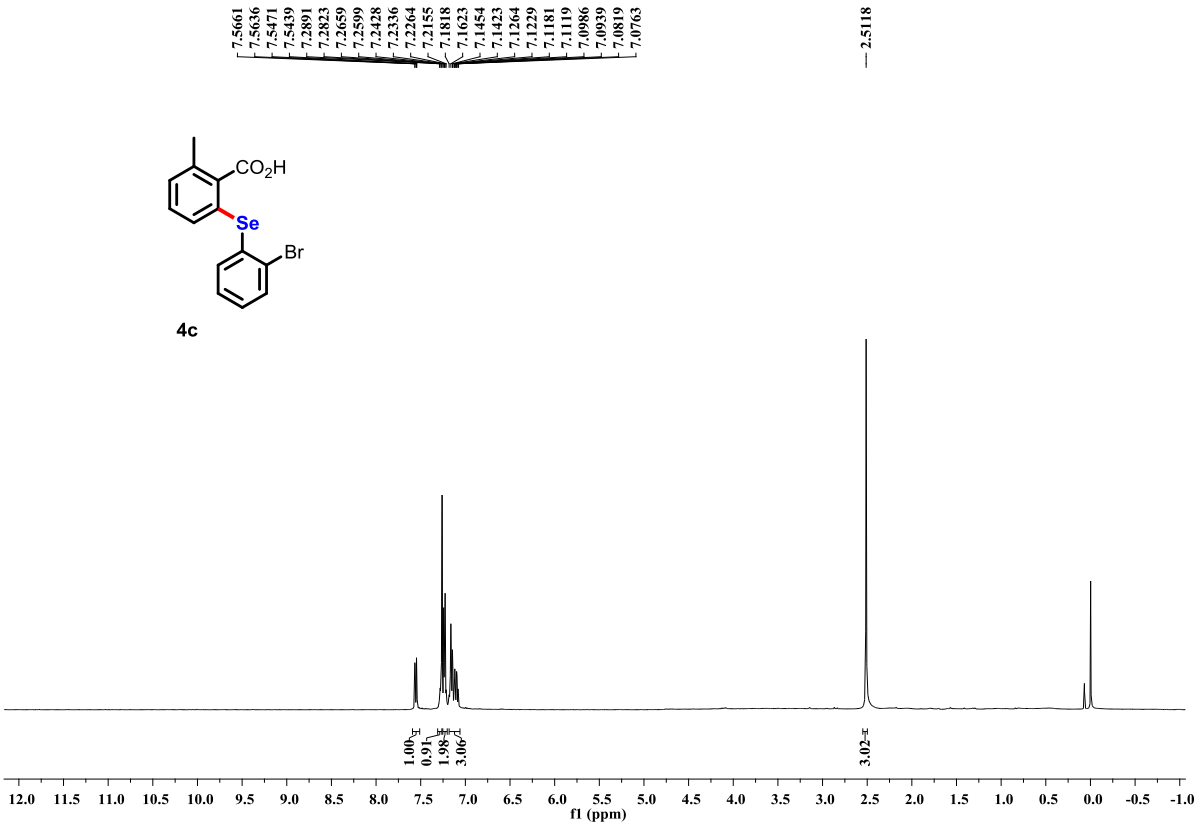
130.2525
129.9752
129.4810
129.3953
129.2964
79.1988
78.8688
78.5387
40.1258
39.9173
39.7087
39.4997
39.2909
39.0825
38.8721
20.0329
CO2H
Se
Cl
4b
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.5636
7.5471
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7.2891
7.2823
7.2659
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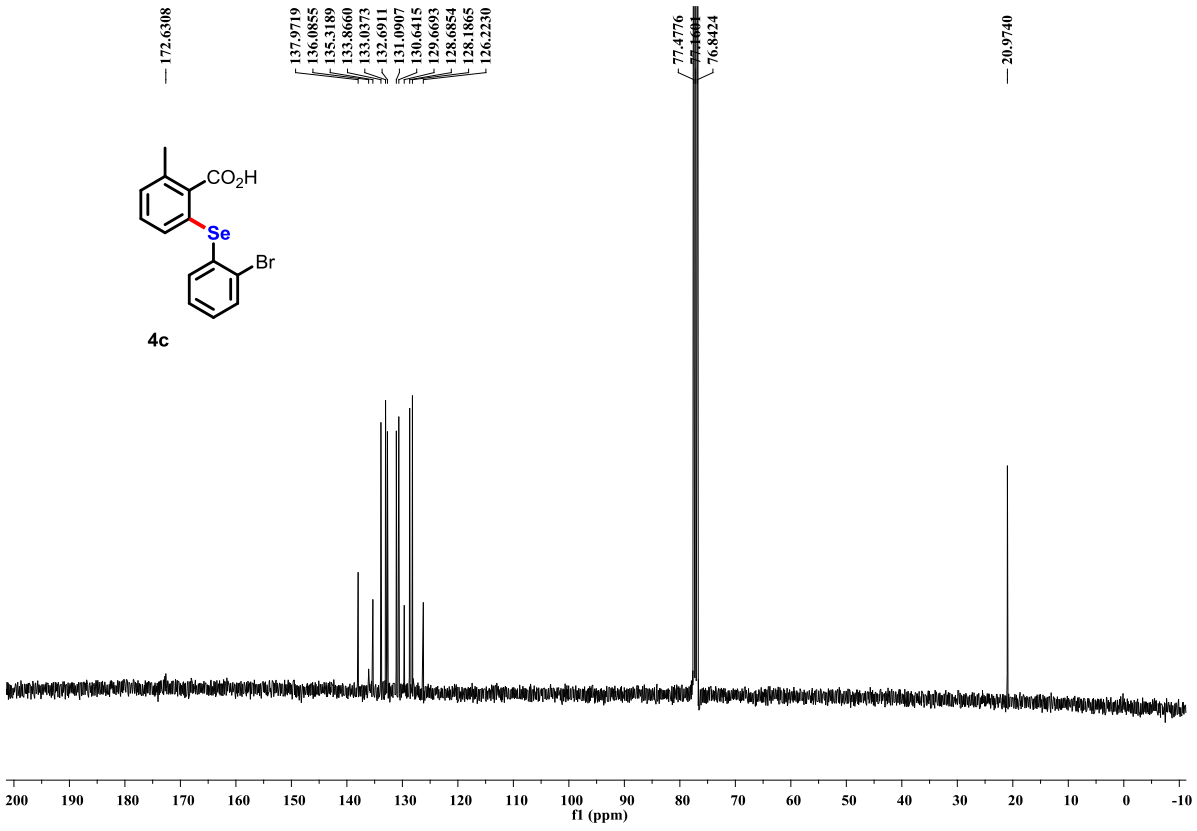
7.2428
7.2336
7.2264
7.2155
7.1818
7.1623
7.1454
7.1423
7.1264
7.1229
7.1181
7.1119
7.0986
7.0939
7.0819
7.0763
2.5118
CO2H
Se
Br
4c
1.00
0.91
1.98
3.06
3.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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132.6911
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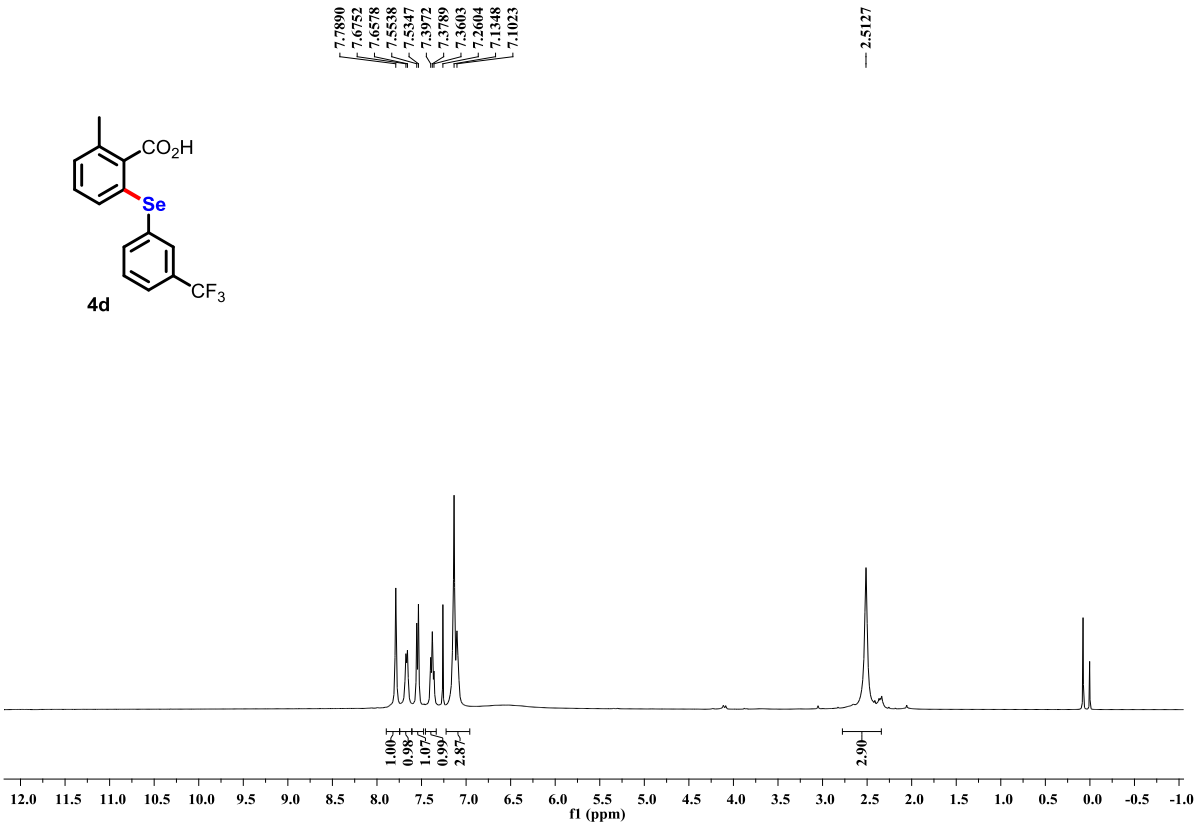
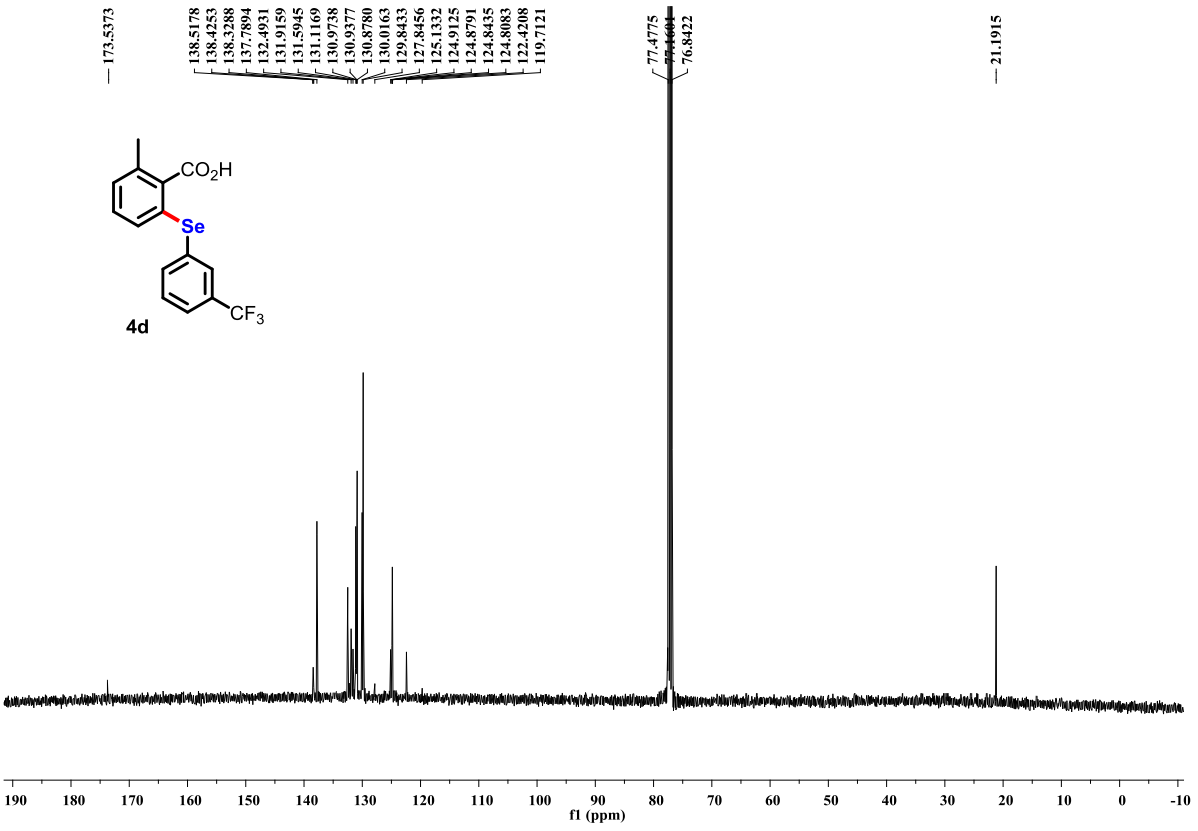
128.6854
128.1865
126.2230
77.4776
77.1661
76.8424
20.9740
CO2H
Se
Br
4c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.7890
7.6752
7.6578
7.5538
7.5347
7.3972
7.3789
7.3603
7.2604
7.1348
7.1023
2.5127
CO2H
Se
CF3
4d
1.00
0.98
1.07
0.99
2.87
2.90
f1 (ppm)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131.9159
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131.1169
130.9738
130.9377
130.8780
130.0163
129.8433
127.8456
125.1332
124.9125
124.8791
124.8435
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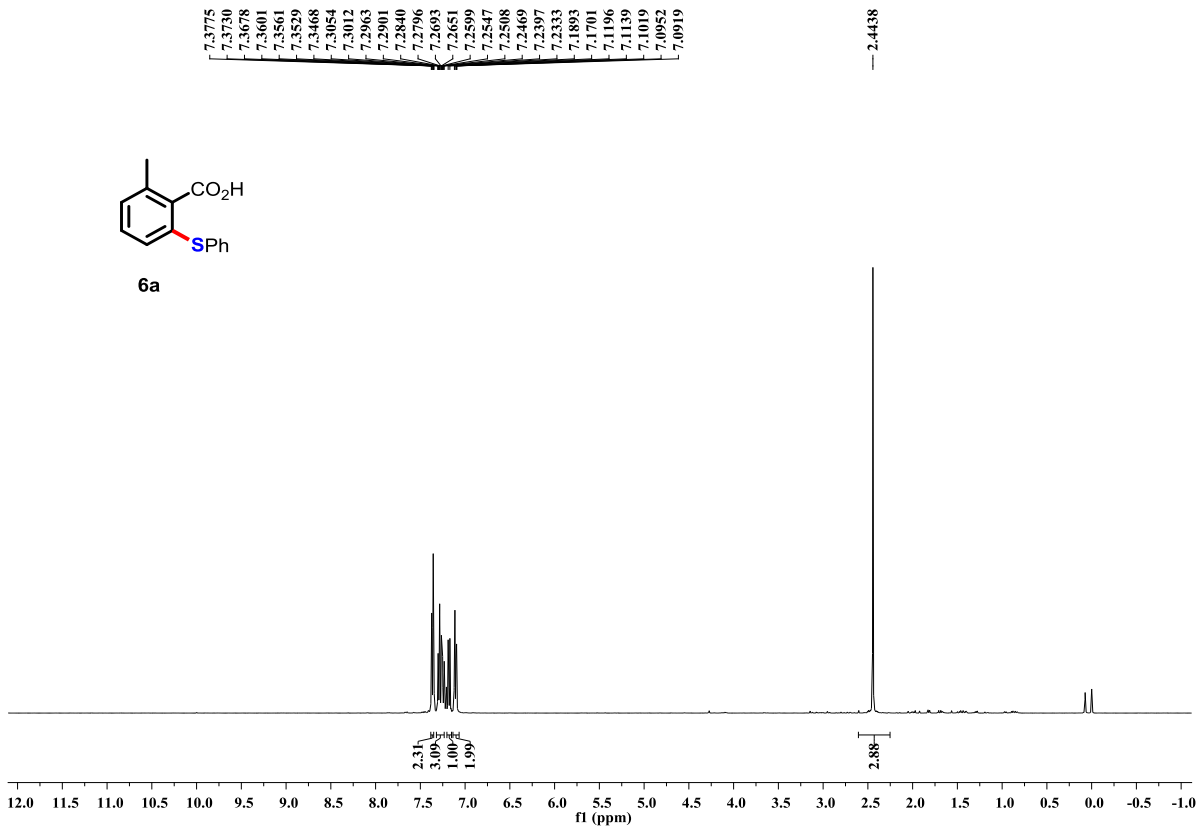
119.7121
77.4775
76.8422
21.1915
CO2H
Se
CF3
4d
f1 (ppm)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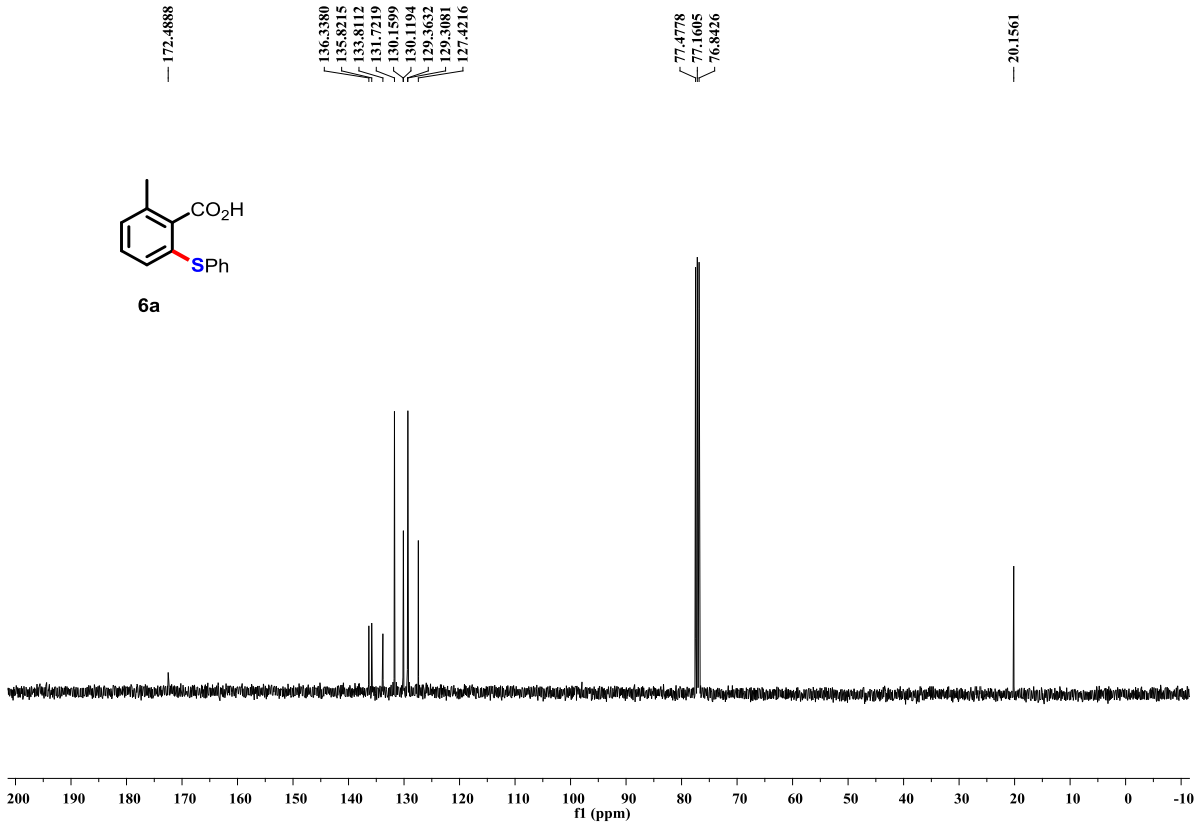
7.3561
7.3529
7.3468
7.3054
7.3012
7.2963
7.2901
7.2840
7.2796
7.2693
7.2651
7.2599
7.2547
7.2508
7.2469
7.2397
7.2333
7.1893
7.1701
7.1196
7.1139
7.1019
7.0952
7.0919
2.4438
CO2H
SPh
6a
2.31
3.09
1.00
1.99
2.88
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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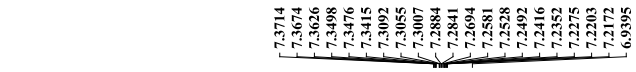
135.8215
133.8112
131.7219
130.1599
130.1194
129.3632
129.3081
127.4216
77.4778
77.1605
76.8426
20.1561
CO2H
SPh
6a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.3674
7.3626
7.3498
7.3476
7.3415
7.3092
7.3055
7.3007
7.2884
7.2841
7.2694
7.2581
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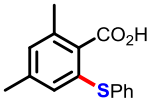
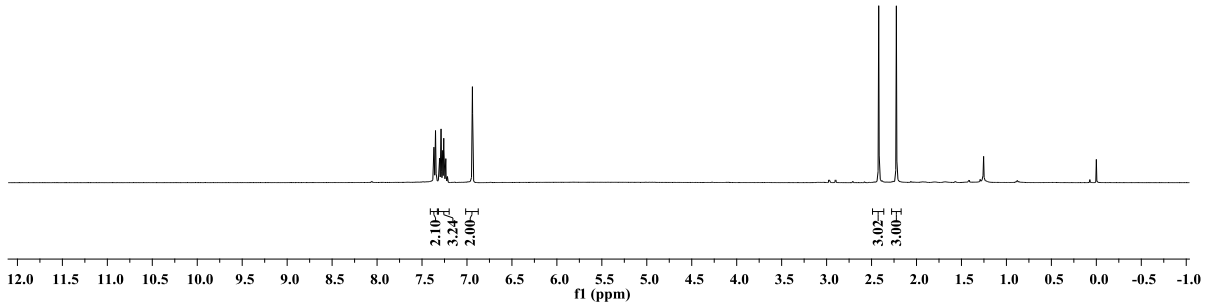
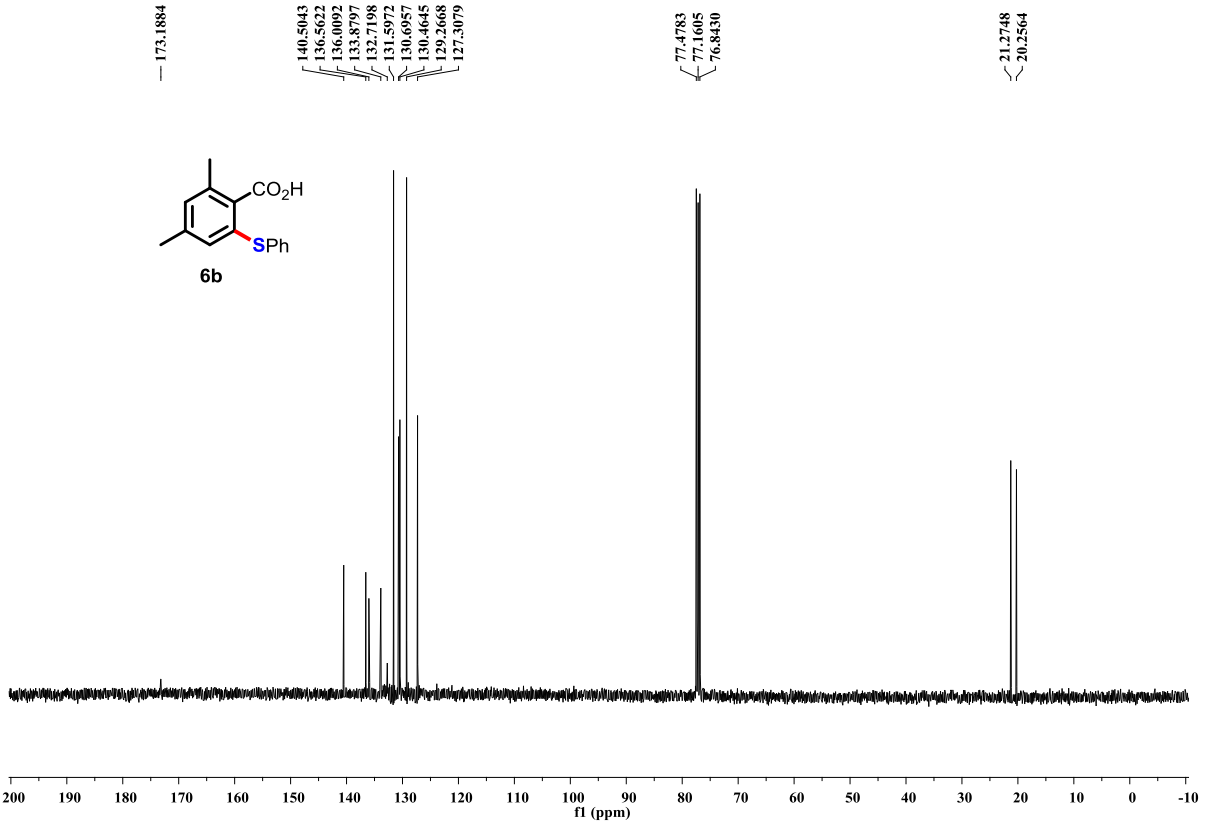
7.2416
7.2352
7.2275
7.2203
7.2172
6.9395
2.4204
2.2243


CO2H
SPh

6b


2.10
3.24
2.00
3.02
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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136.0092
133.8797
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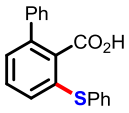
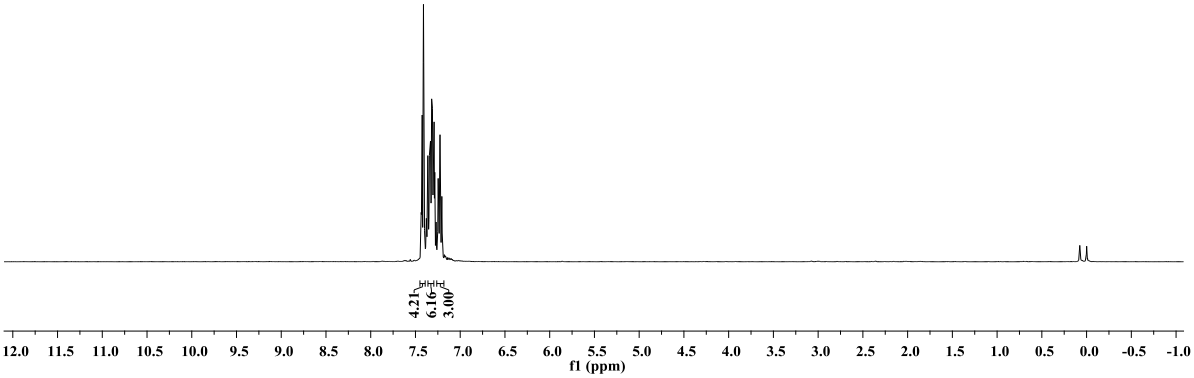
131.5972
130.6957
130.4645
129.2668
127.3079
77.4783
77.1605
76.8430
21.2748
20.2564
CO2H
SPh
6b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

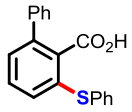

7.4350
7.4298
7.4250
7.4222
7.4132
7.4106
7.4052
7.3781
7.3620
7.3442
7.3320
7.3192
7.3104
7.2993
7.2918
7.2844
7.2697
7.2462
7.2386
7.2257
7.2053


Ph
CO2H
SPh

6c

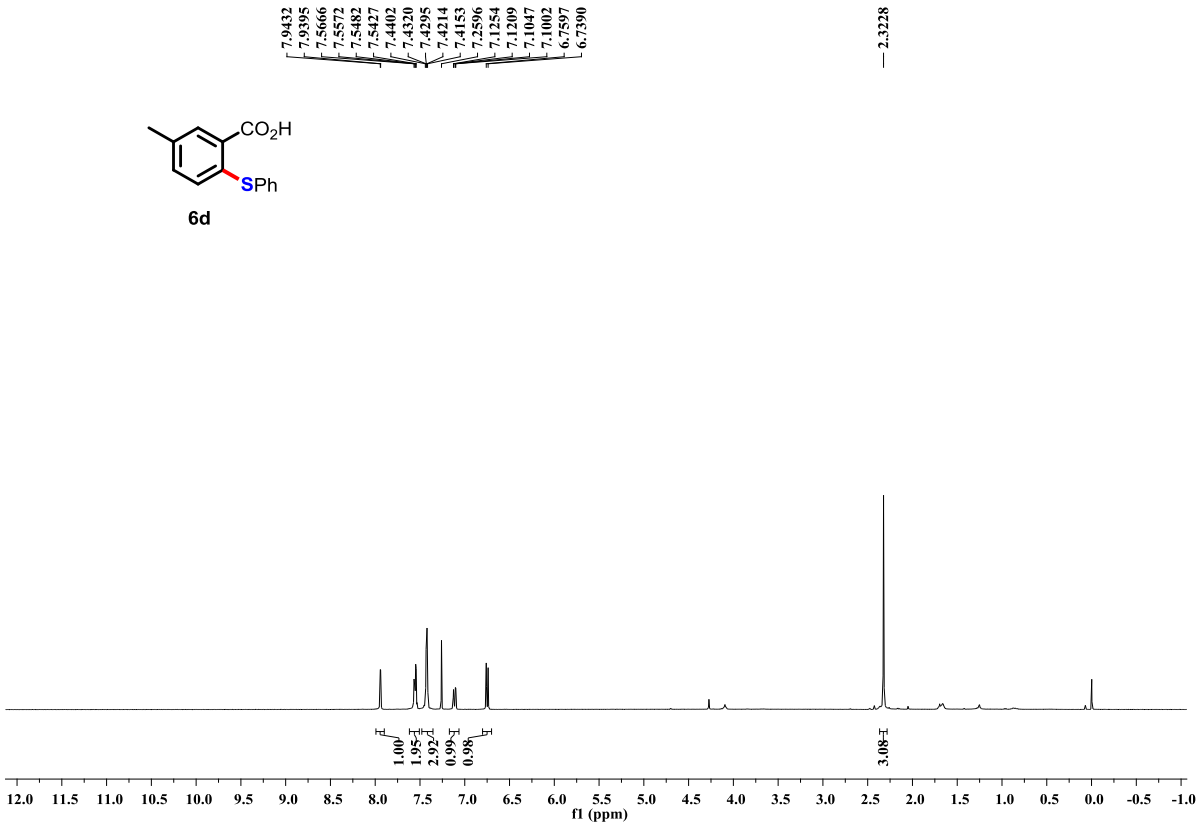

4.21
6.16
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


173.4099
141.0175
139.8597
135.0502
134.9082
132.4238
130.8802
130.3189
129.4608
128.8239
128.6203
128.4911
128.1932
127.9941
127.8691
77.4773
77.1596
76.8418


Ph
CO2H
SPh

6c

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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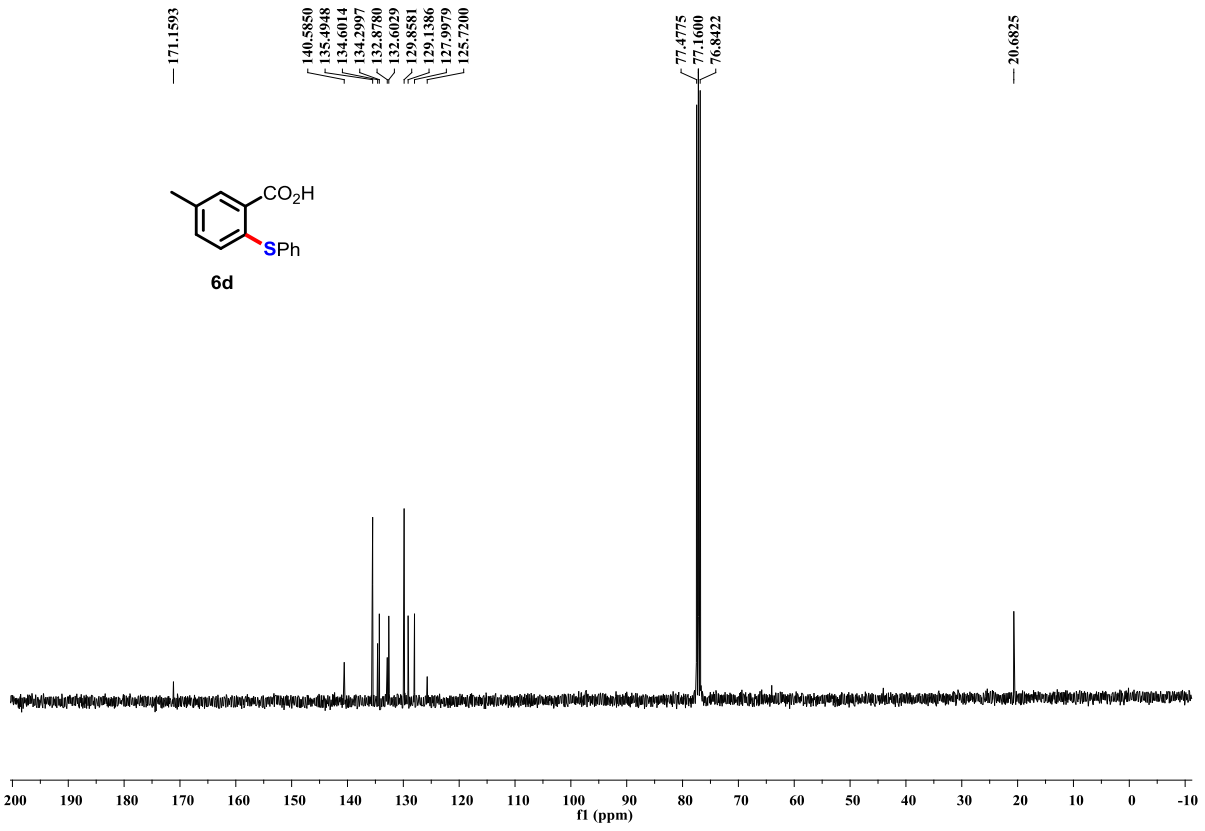
7.9395
7.5666
7.5572
7.5482
7.5427
7.4402
7.4320
7.4295
7.4214
7.4153
7.2596
7.1254
7.1209
7.1047
7.1002
6.7597
6.7390
2.3228
CO2H
SPh
6d
1.00
1.95
2.92
0.99
0.98
3.08
f1 (ppm)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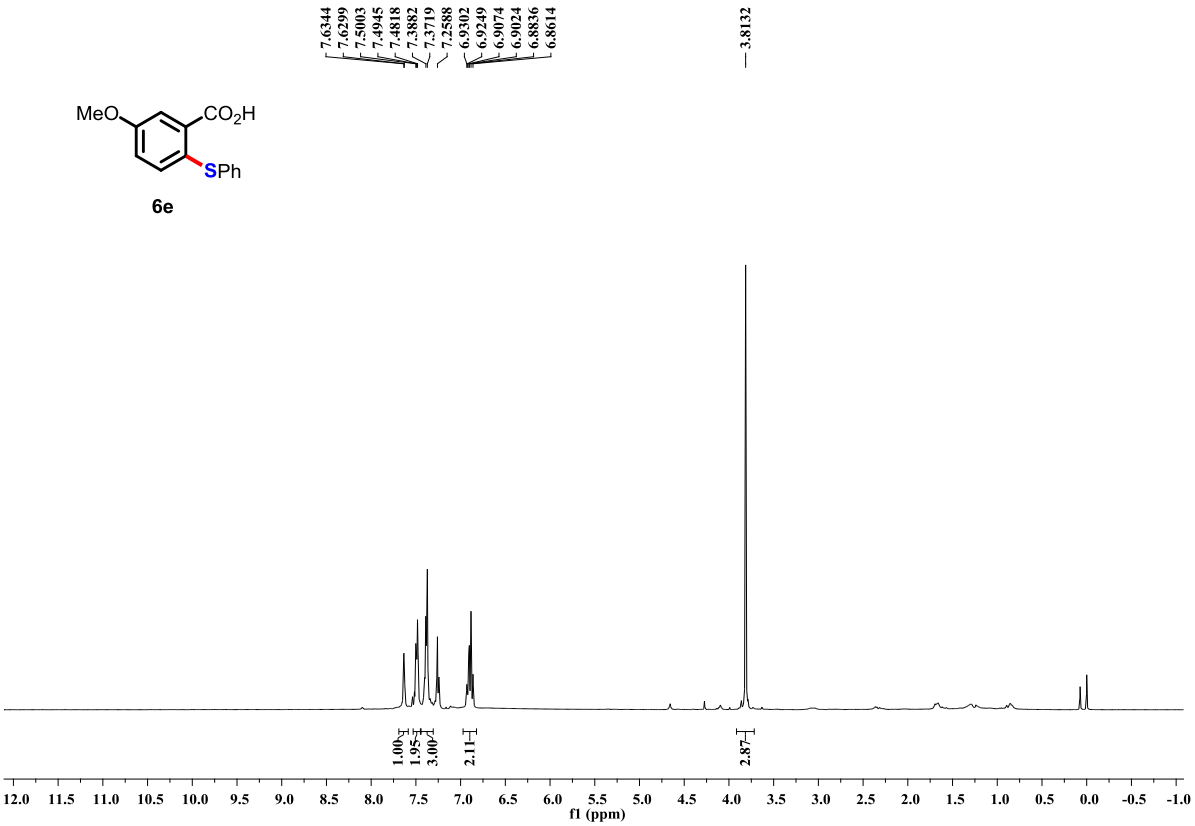
134.6014
134.2997
132.8780
132.6029
129.8581
129.1386
127.9979
125.7200
77.4775
77.1600
76.8422
20.6825
CO2H
SPh
6d
f1 (ppm)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7.5003
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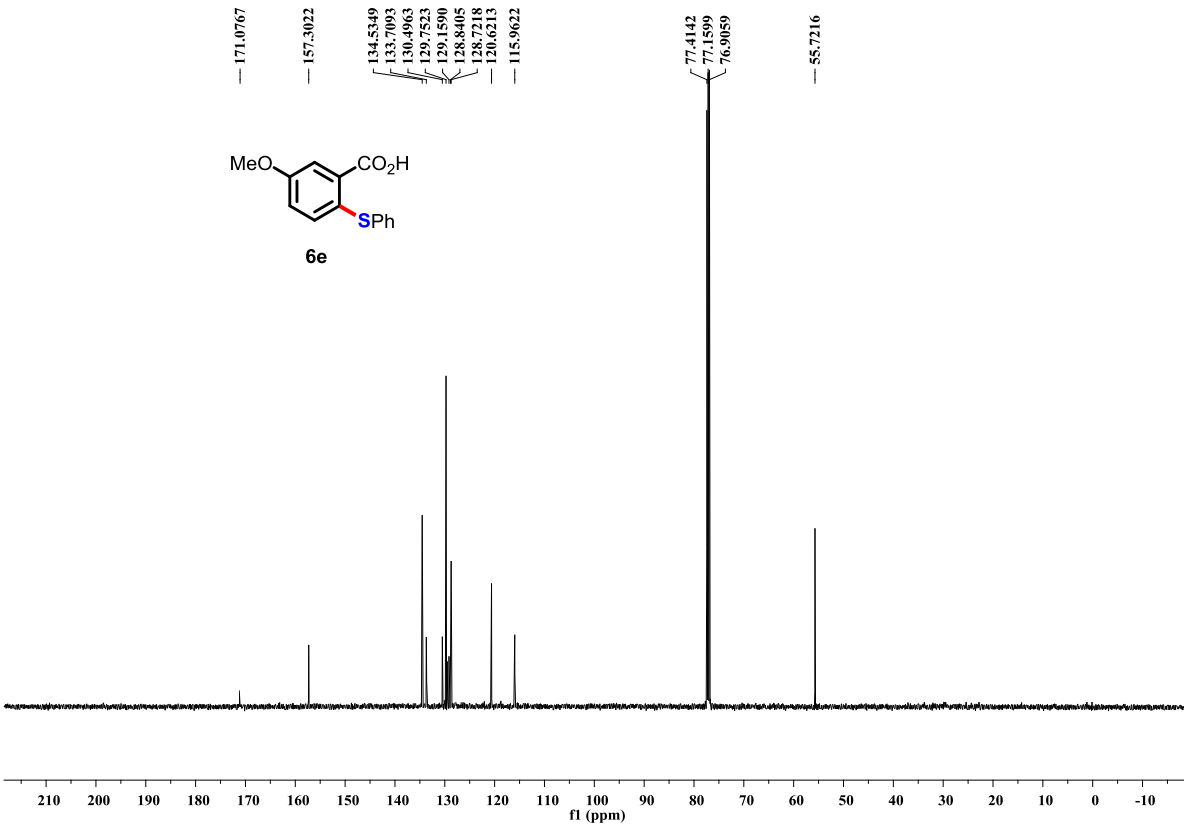
7.4818
7.3882
7.3719
7.2588
6.9302
6.9249
6.9074
6.9024
6.8836
6.8614
3.8132
MeO
CO2H
SPh
6e
1.00
1.95
3.00
2.11
2.87
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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129.1590
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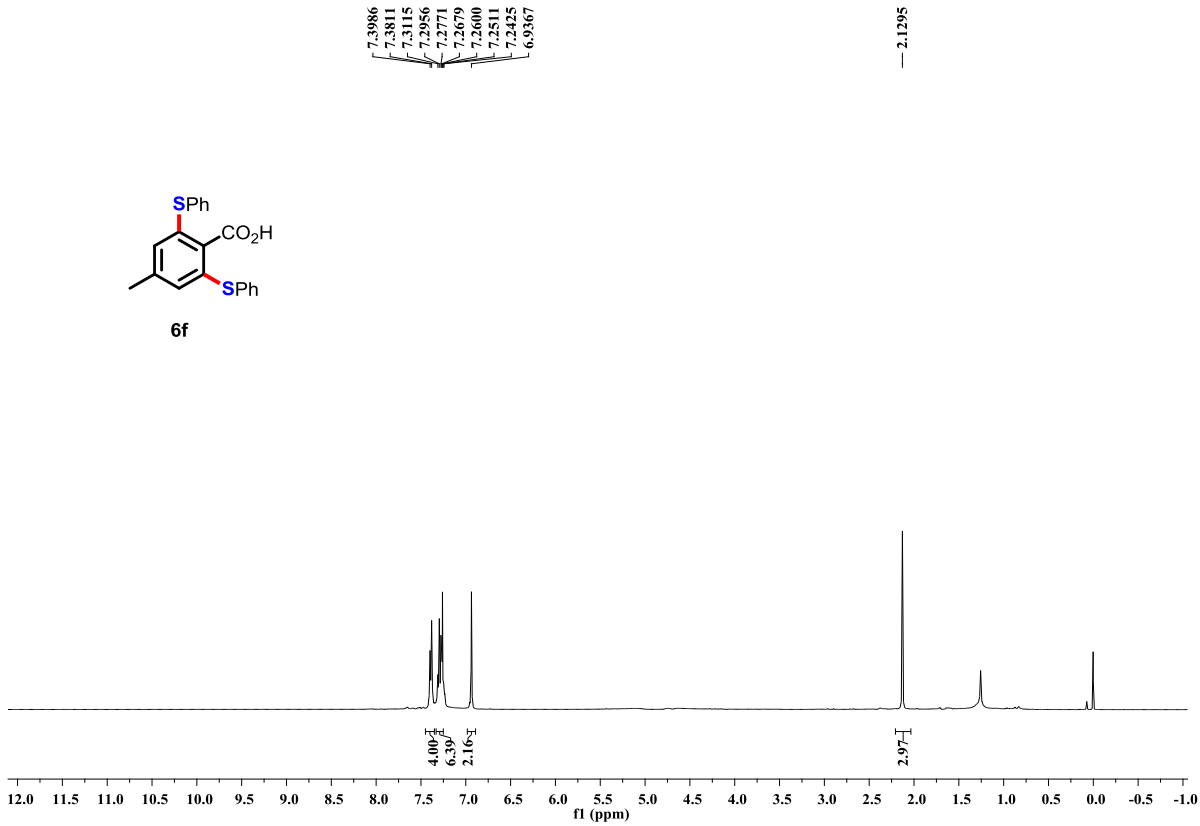
128.7218
120.6213
115.9622
77.4142
77.1599
76.9059
55.7216
MeO
CO2H
SPh
6e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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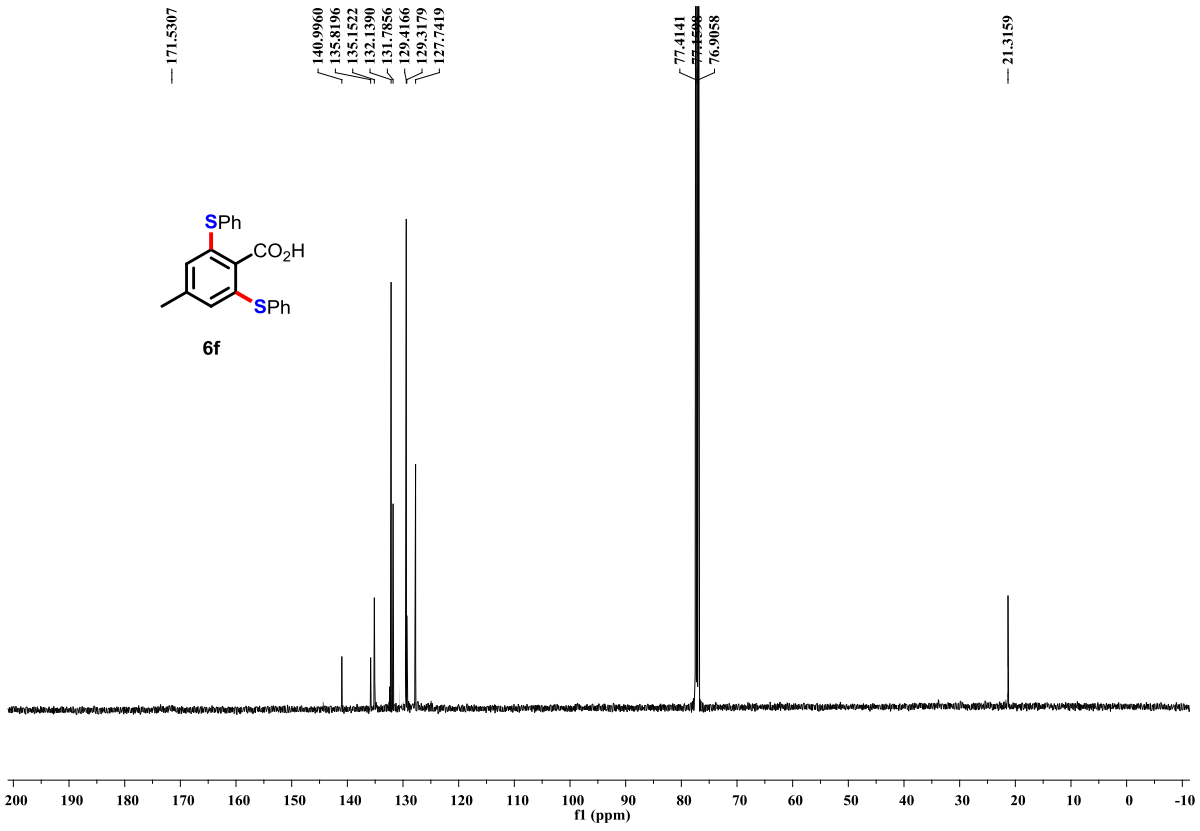
7.2956
7.2771
7.2679
7.2600
7.2511
7.2425
6.9367
2.1295
SPh
CO2H
SPh
6f
4.00
6.39
2.16
2.97
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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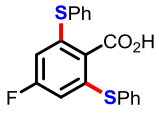
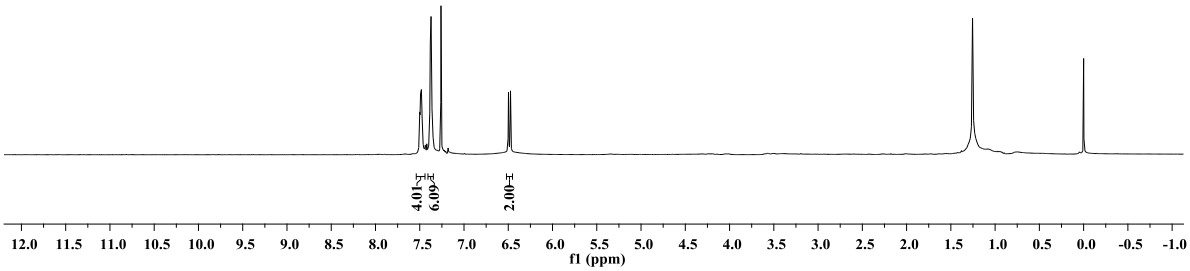
135.1522
132.1390
131.7856
129.4166
129.3179
127.7419
77.4141
76.9058
21.3159
SPh
CO2H
SPh
6f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


SPh
CO2H
F
SPh

6g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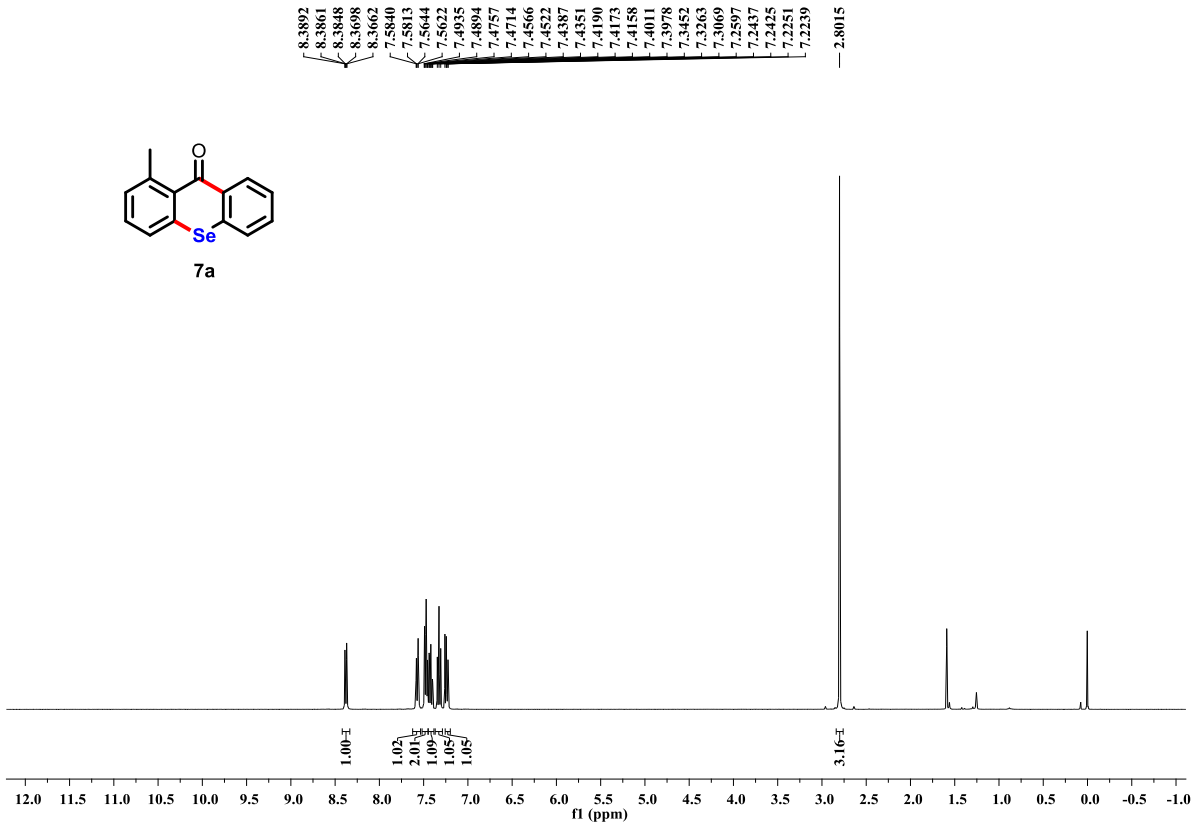
7.4771
7.3809
7.3722
7.3665
7.2602
6.4975
6.4749
4.01
6.09
2.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


SPh
CO2H
F
SPh

6g

164.3063
162.2841
141.9265
141.8700
134.3580
132.6915
129.9148
129.6345
129.1937
114.4529
114.2553
77.4142
77.1601
76.9058
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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8.3662
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7.5622
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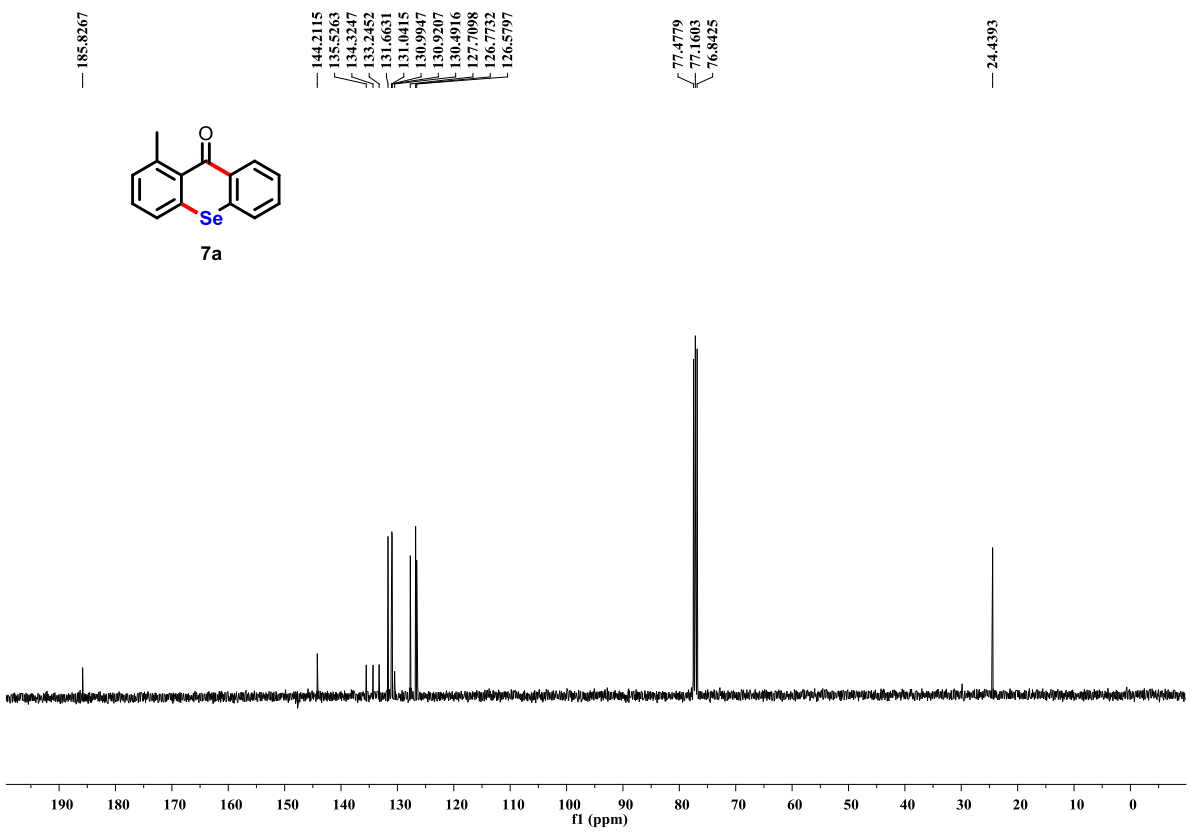
7.4894
7.4757
7.4714
7.4566
7.4522
7.4387
7.4351
7.4190
7.4173
7.4158
7.4011
7.3978
7.3452
7.3263
7.3069
7.2597
7.2437
7.2425
7.2251
7.2239
2.8015
O
Se
7a
1.00
1.02
2.01
1.09
1.05
1.05
3.16
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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130.9207
130.4916
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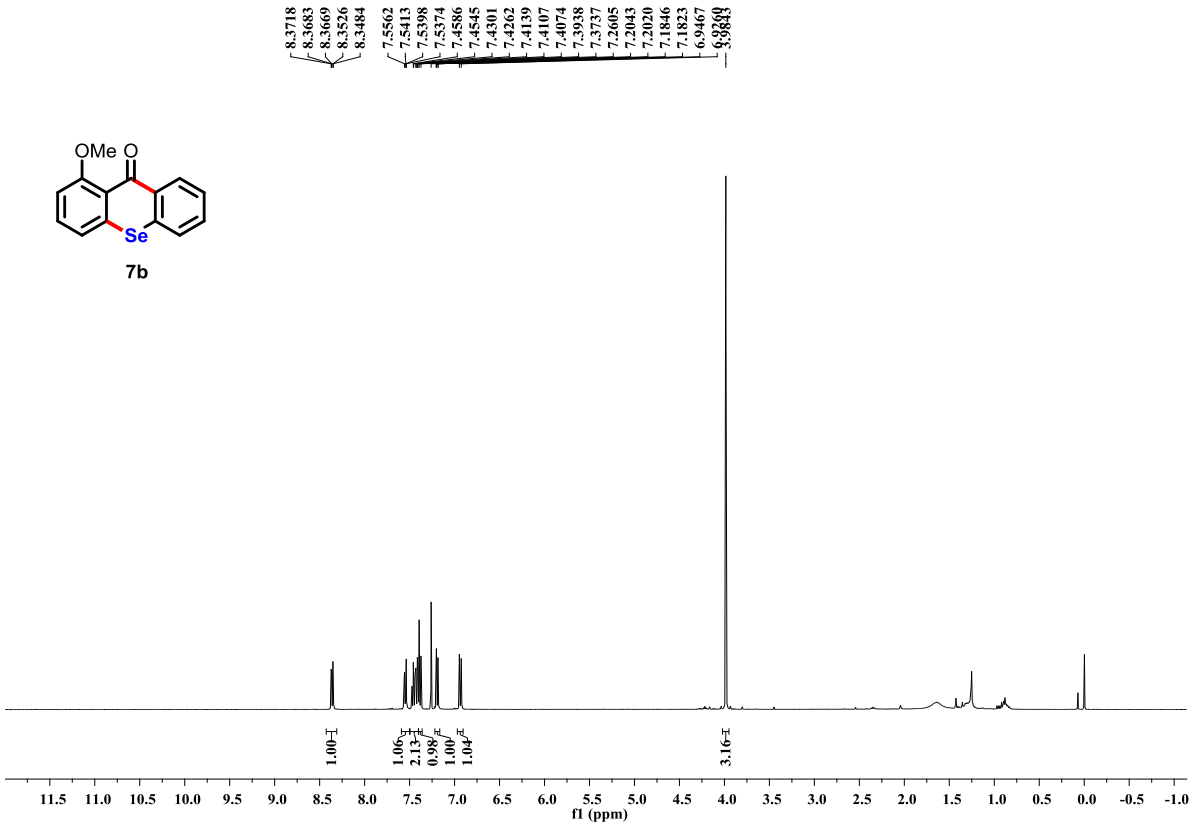
126.7732
126.5797
77.4779
77.1603
76.8425
24.4393
O
Se
7a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.3669
8.3526
8.3484
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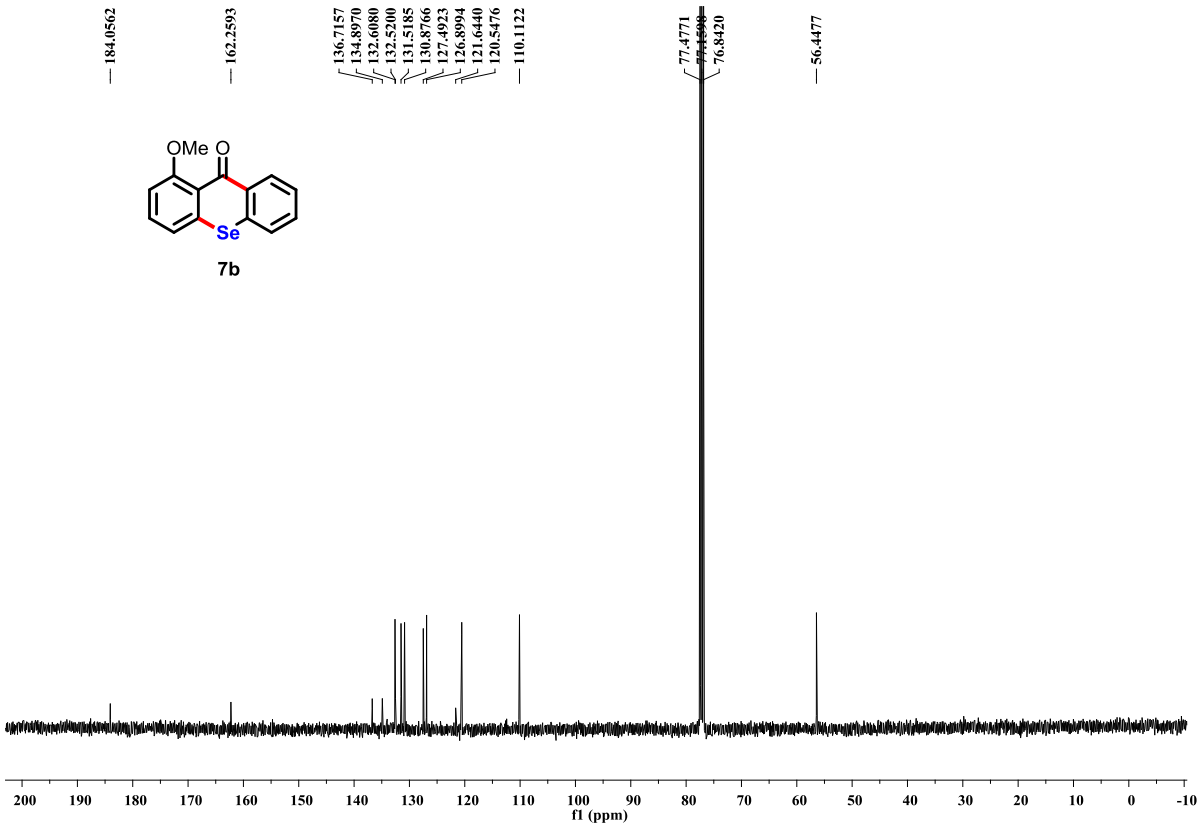
7.4586
7.4545
7.4301
7.4262
7.4139
7.4107
7.4074
7.3938
7.3737
7.2605
7.2043
7.2020
7.1846
7.1823
6.9467
6.8260
3.9843
OMe O
Se
7b
1.00
1.06
2.13
0.98
1.00
1.04
3.16
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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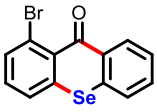
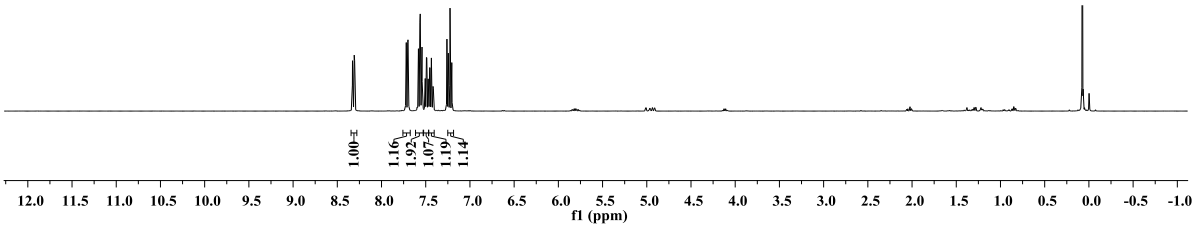
134.8970
132.6080
132.5200
131.5185
130.8766
127.4923
126.8994
121.6440
120.5476
110.1122
77.4771
76.8420
56.4477
OMe O
Se
7b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

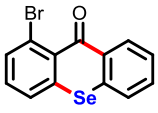

8.3281
8.3239
8.3086
8.3044
7.7231
7.7201
7.7035
7.7006
7.5853
7.5823
7.5774
7.5654
7.5621
7.5458
7.5420
7.5095
7.5056
7.4918
7.4879
7.4725
7.4683
7.4554
7.4515
7.4379
7.4359
7.4323
7.4178
7.4143
7.2602
7.2446
7.2251
7.2052


Br
O
Se

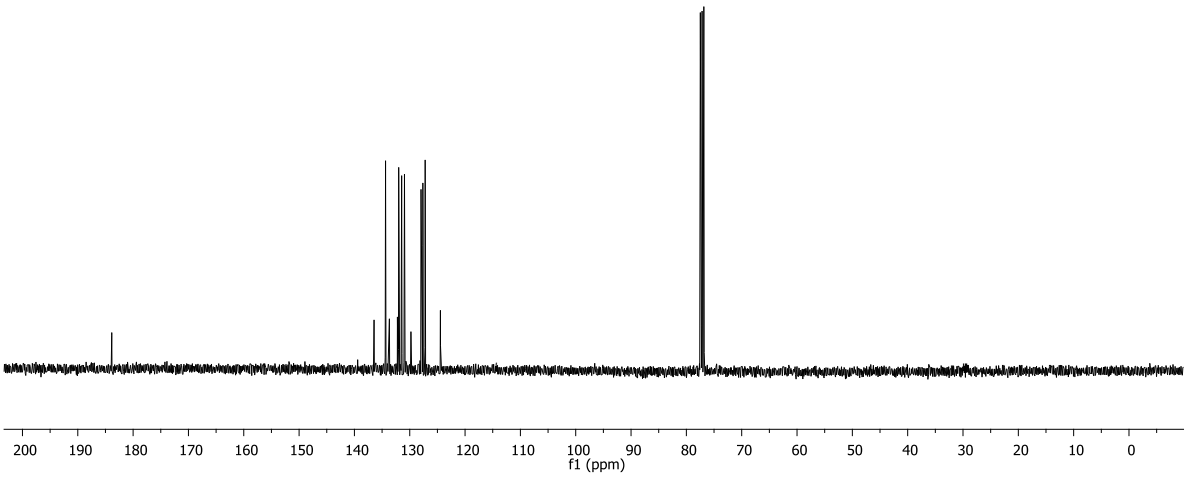
7c

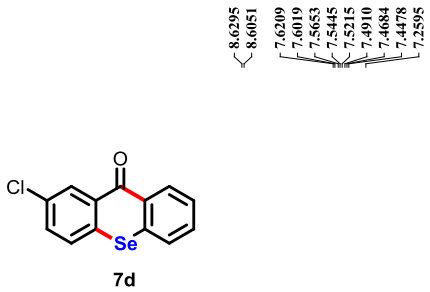

1.00
1.16
1.92
1.07
1.19
1.14
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


183.8616
136.4518
134.3716
133.6783
132.2276
131.9961
131.4610
130.9544
129.7844
127.9647
127.6258
127.2109
124.4537
77.4779
77.1604
76.8425

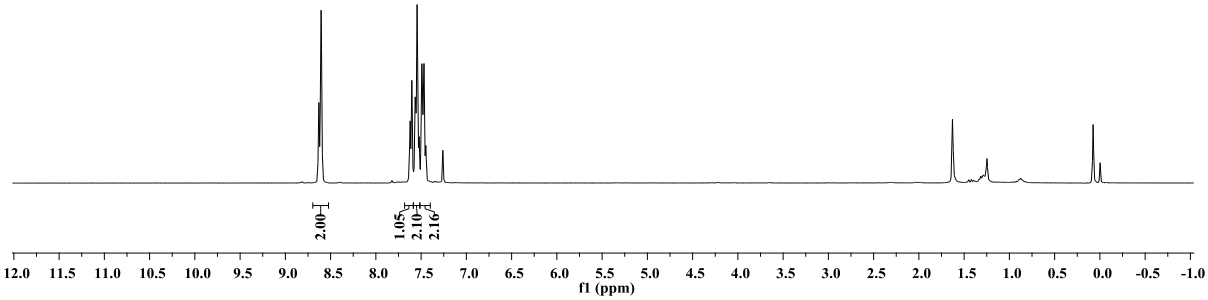

Br
O
Se

7c

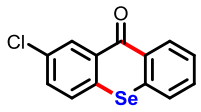

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.6295
8.6051
7.6209
7.6019
7.5653
7.5445
7.5215
7.4910
7.4684
7.4478
7.2595
O
Cl
Se

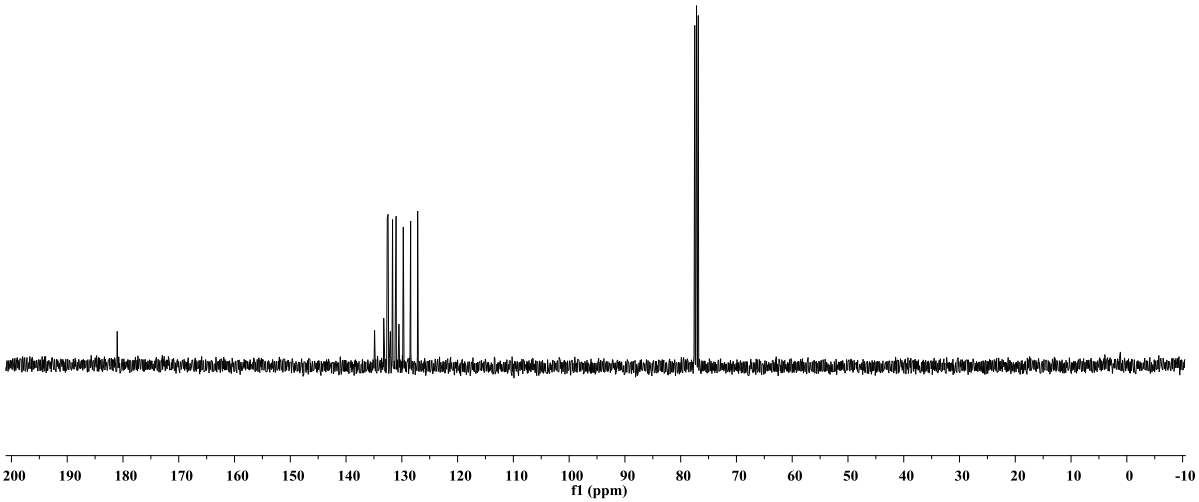
7d

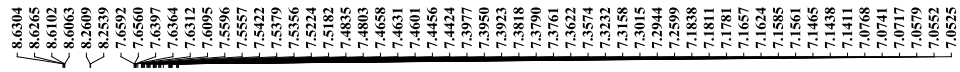

2.00
1.05
2.10
2.16
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

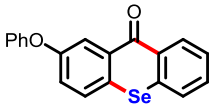

181.0356
134.8858
133.2438
133.1637
132.6134
132.4691
132.0619
131.6652
131.0288
130.5229
129.7419
128.4178
127.1618
77.4778
77.1600
76.8424


O
Cl
Se

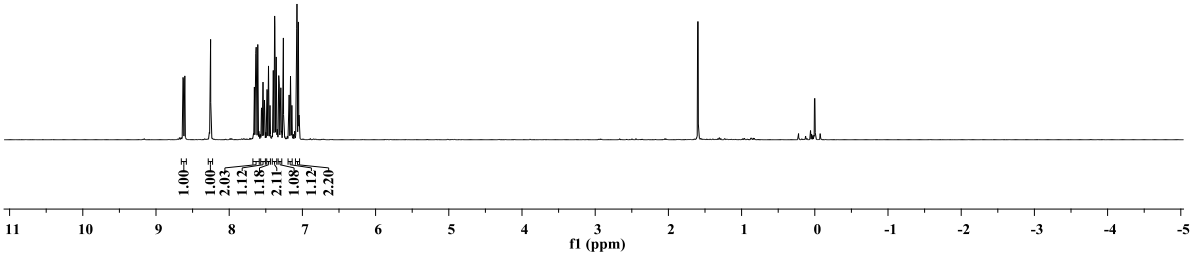
7d

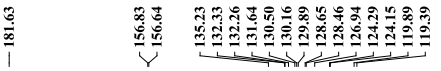

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

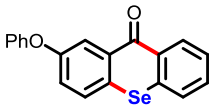

8.6304
8.6265
8.6102
8.6063
8.2609
8.2539
7.6592
7.6560
7.6397
7.6364
7.6312
7.6095
7.5596
7.5557
7.5422
7.5379
7.5356
7.5224
7.5182
7.4835
7.4803
7.4658
7.4631
7.4601
7.4456
7.4424
7.3977
7.3950
7.3923
7.3818
7.3790
7.3761
7.3622
7.3574
7.3232
7.3158
7.3015
7.2944
7.2599
7.1838
7.1811
7.1781
7.1657
7.1624
7.1585
7.1561
7.1465
7.1438
7.1411
7.0768
7.0741
7.0717
7.0579
7.0552
7.0525


O
PhO
Se

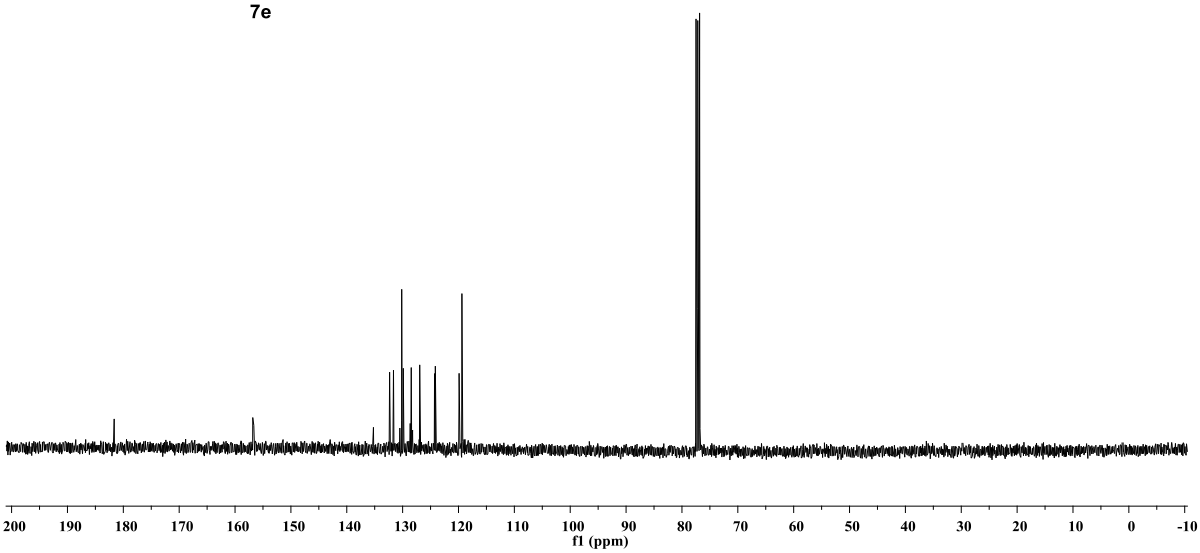
7e


1.00
1.00
2.03
1.12
1.18
2.11
1.08
1.12
2.20
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)

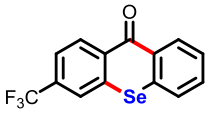

181.63
156.83
156.64
135.23
132.33
132.26
131.64
130.50
130.16
129.89
128.65
128.46
126.94
124.29
124.15
119.89
119.39
77.48
77.16
76.84


O
PhO
Se

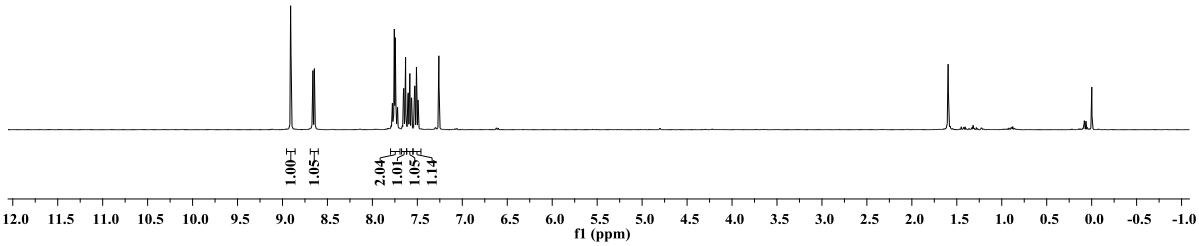
7e

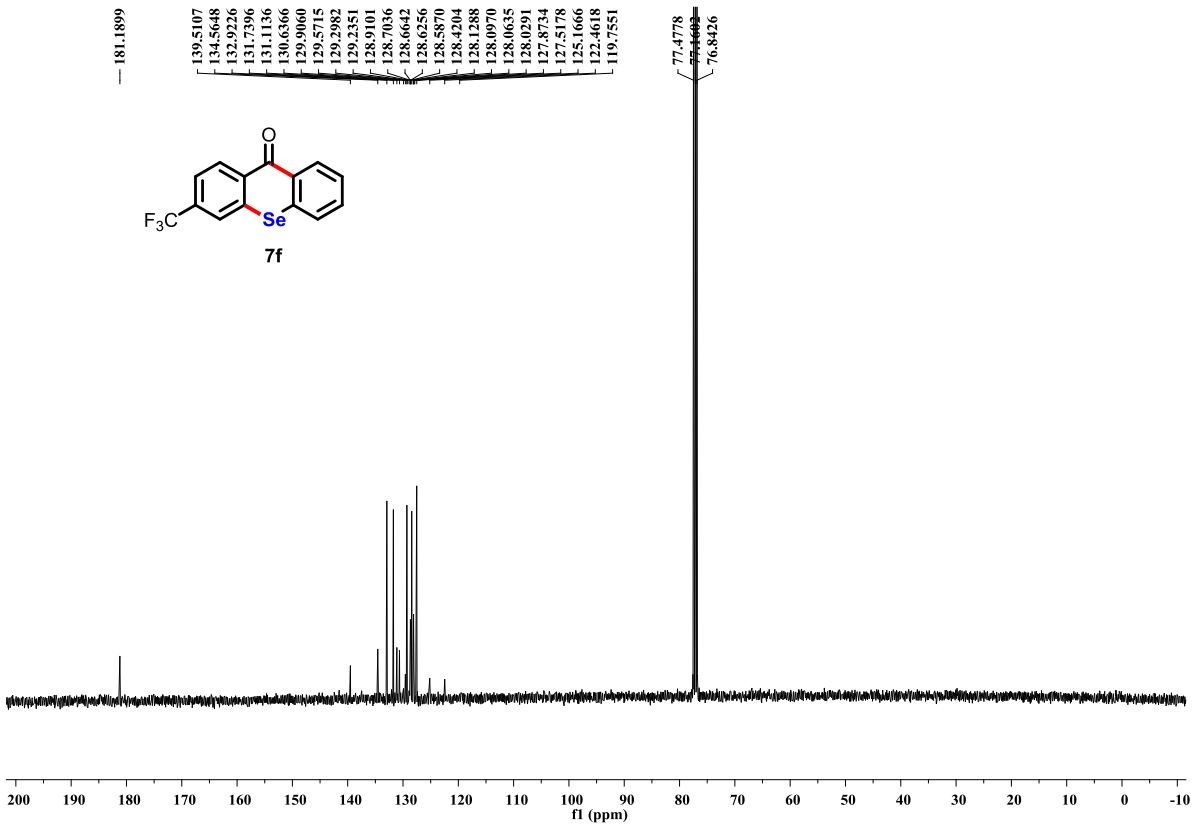

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.9097
8.9051
8.6657
8.6616
8.6456
8.6414
7.7775
7.7564
7.7457
7.7409
7.7249
7.7198
7.6546
7.6507
7.6350
7.6309
7.6048
7.6009
7.5874
7.5835
7.5675
7.5637
7.5305
7.5267
7.5134
7.5100
7.5069
7.4926
7.4894
7.2605


O
F3C
Se

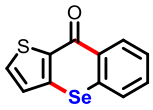
7f


1.00
1.05
2.04
1.01
1.05
1.14
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

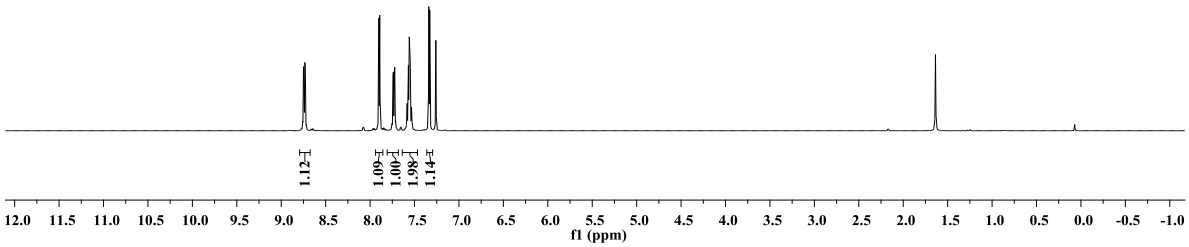

181.1899
139.5107
134.5648
132.9226
131.7396
131.1136
130.6366
129.9060
129.5715
129.2982
129.2351
128.9101
128.7036
128.6642
128.6256
128.5870
128.4204
128.1288
128.0970
128.0635
128.0291
127.8734
127.5178
125.1666
122.4618
119.7551
77.4778
76.8426
O
F3C
Se
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

7f


8.7492
8.7449
8.7346
8.7298
7.9017
7.8914
7.7418
7.7376
7.7289
7.7230
7.5867
7.5833
7.5727
7.5686
7.5630
7.5588
7.5533
7.5477
7.5443
7.5337
7.5303
7.3391
7.3288
7.2598


O
S
Se

7g

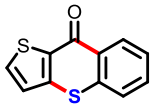

1.12
1.09
1.00
1.98
1.14
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


O
S
Se

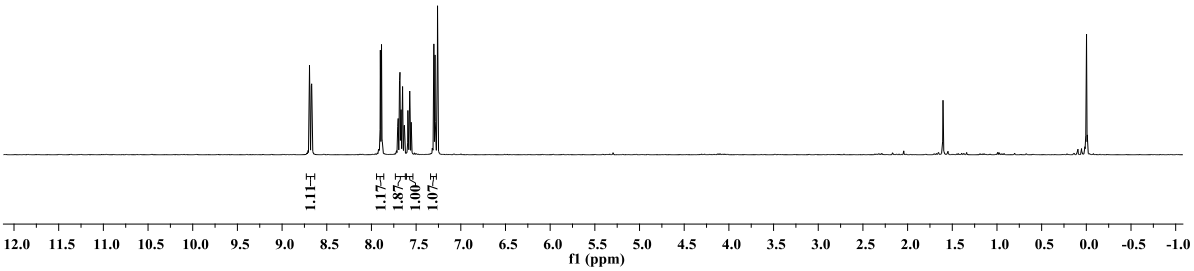
7g

176.5781
135.5149
134.9076
134.4716
134.3120
131.7773
130.7225
130.5899
128.9053
127.3792
127.3353
77.4779
77.1605
76.8425
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.6933
8.6897
8.6726
8.6687
7.9004
7.8873
7.7060
7.7009
7.6859
7.6807
7.6724
7.6685
7.6556
7.6517
7.6478
7.6351
7.6313
7.5924
7.5882
7.5758
7.5716
7.5680
7.5551
7.5512
7.3015
7.2884
7.2606


O
S
S

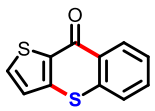
7h


1.11
1.17
1.87
1.00
1.07
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

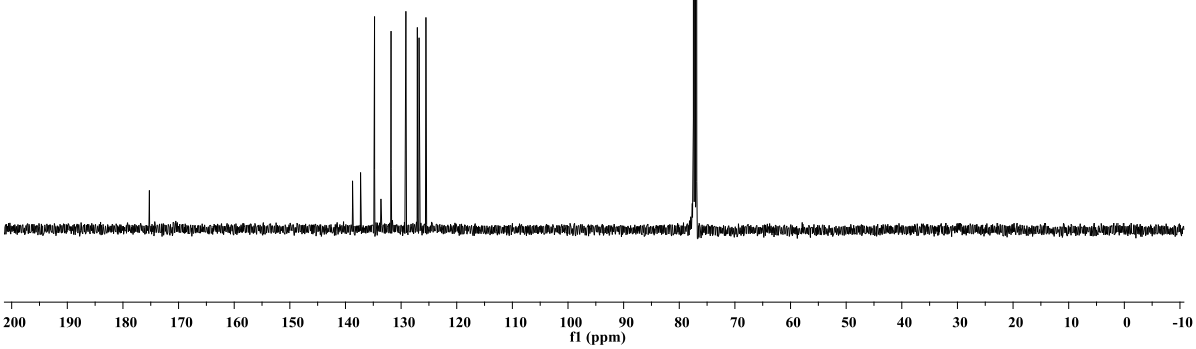

175.2492


138.7279
137.2869
134.7713
133.6239
131.8021
129.1374
127.0838
126.7678
125.5348


77.4139
76.9058


O
S
S

7h


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)