Supporting Information

Chalcogen bonding enabled photosynthesis of aryl selenides from aryl sulfonium salts

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contents

1. General Information

Chemicals were purchased from HEOWNS or Bidepharm and used without further purification unless otherwise noted. Solvents were purified using a solvent-purification system (VSPS-8, Vigor) that contain activated alumina and molecular sieves. Diselenides[1], dibenzothiophenium salts[2] were prepared according to literature method.

Analytical thin layer chromatography was carried out with silica gel pre-coated glass plates (TLC-Silica gel GF254, coating thickness: 0.25 mm) purchased from Xinnuo Chemical (Yantai, China). Chromatographic purification of the products was performed on silica gel 200-300 mesh. Visualization of the developed TLC plates was performed with ultraviolet irradiation (254 nm) or by staining with basic potassium permanganate solution.

High resolution mass spectra data were determined under conditions of electron spray ionization (ESI) on a ThermoFisher mass spectrometer (Q Exactive Focus) coupled with an ultra-performance liquid chromatography (Vanquish Flex).

IR spectra were taken on a Vertex 70 spectrophotometer and reported as wave numbers (cm^{-1}).

The GC-MS TQ8040 was used in the detection of the reaction mixture.

The SGW X-4 was used to measure the melting point of solids.

UV-vis absorption spectra were acquired on UV-2600 spectrophotometer (Shimadzu, Japan).

^{1}H- and ^{13}C- NMR spectra were recorded at ambient temperature on JEOL JNM-ECZ400S Spectrometer and JEOL JNM-ECZ500R Spectrometer. The chemical shifts are reported in ppm downfield of tetramethylsilane (TMS) and referenced to residual solvent peaks resonance as internal standard. The order of citation in parentheses is a) multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd= doublet of doublet, m = multiplet), b) coupling constants, c) number of protons. Coupling constants (*J*) are reported in Hertz (Hz).

The reaction temperature was monitored by using the IR Thermometer (TA601B).

Photochemical experiments were performed magnetically stirred in 10 mL glass Schlenk tubes, sealed with a rubber septum. The tubes were irradiated with blue light using a LED lamp with a power output of 100 W (see below picture). The distance from the light source to the irradiation vessel is 1 cm to keep the reaction temperature with 60±5 °C. (The purchase

link of LED lamp is https://item.taobao.com/item.htm?spm =a230r.7195193.1997079397.9.212b2e3eGwYjWb&id=520551083325&abbucket=10).

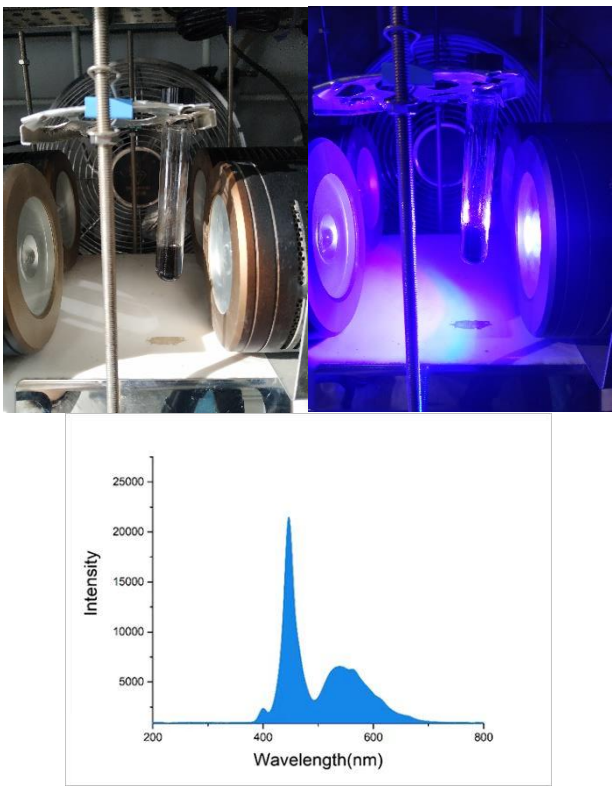
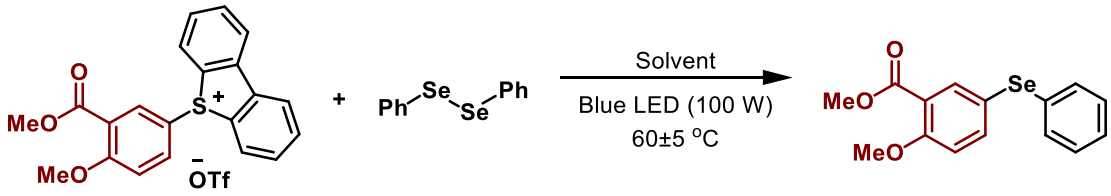


Figure S1. Blue LEDs employed in the reactions.

2. Experimental Procedures

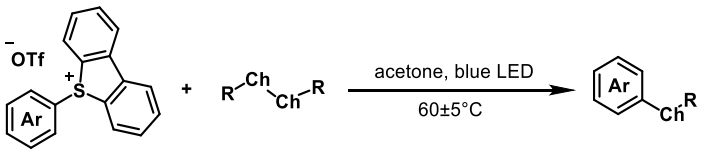
Table S1. Optimization of the reaction conditions



1 2 3

Entry	Solvent	1:2	Yield(%)[a]
1	DCM	2:1	36
2	MeCN	2:1	36
3	THF	2:1	trace
4	Acetone	2:1	82
5	Toluene	2:1	trace
6	DMA	2:1	67
7	DMF	2:1	54
8	DMSO	2:1	28
9	Acetone	1:2	trace
10	Acetone	1.2:1	52
11	Acetone	1.5:1	67
12	Acetone	2.5:1	82
13	Acetone	3:1	83
14	Acetone	4:1	44
15	Acetone	5:1	trace
16[b]	Acetone	2:1	40
17[c]	Acetone	2:1	81
18[d]	Acetone	2:1	41
19[e]	Acetone	2:1	NR

[a]Yield of isolated product; [b]0.2M, [c]0.05M, [d]reaction was carried out at 35 °C, [e]without blue LED.

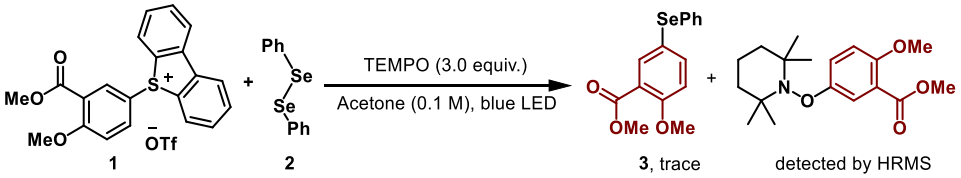


General procedures: In a nitrogen-filled glove box, a 10-mL vial equipped with a magnetic stirring bar was charged sequentially with dichalcogenide (0.1 mmol, 1.0 equiv.), dibenzothiophenium salt (0.2 mmol, 2.0 equiv.), and acetone (1.0 mL). The vial was closed and removed from the glove box. The resulting mixture was allowed to stir at 60±5 °C under blue LED (100 W) irradiation for 12 hours. Upon completion, solvent was removed under vacuum and the residue was subjected to silica gel chromatography using petroleum ether and ethyl

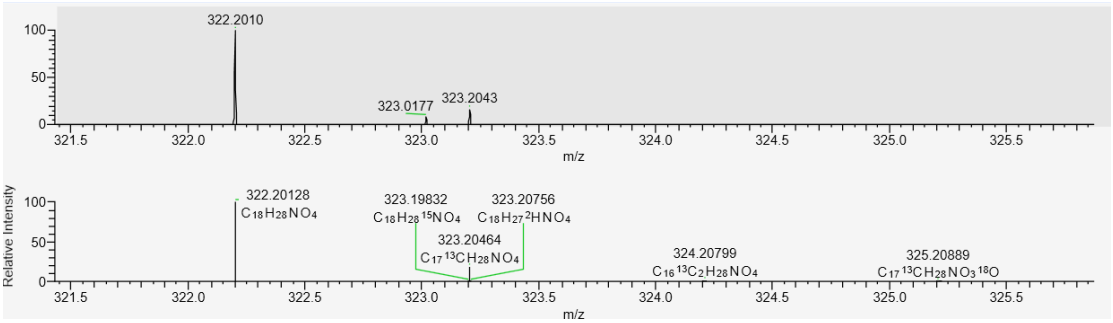
acetate as eluent to afford the desired product.

3. The Mechanism Studies

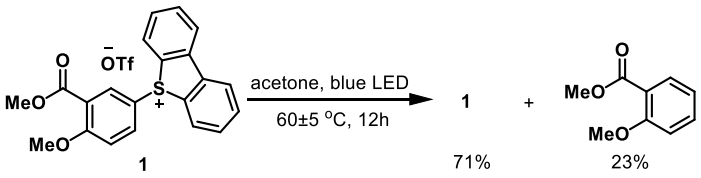
3.1 Radical inhibition experiment



In a nitrogen atmosphere, a dry tube equipped with a stirring bar, 1,2-diphenyldiselane (0.1 mmol, 1.0 equiv.), dibenzothiophenium salt (0.2 mmol, 2.0 equiv.), TEMPO (46.8 mg, 0.30 mmol, 3.0 equiv.) and acetone (1.0 mL) were added. The mixture was stirred under a 100 W blue LED lamp with an interval of 1 cm from the lamp for 12 hours, and a fan was used to keep the reaction temperature at 60±5 ℃. The reaction was absolutely inhibited and the trapped radical species was detected by HRMS. **HRMS (ESI)**: found 314.1017, *m/z* $[M+H]^+$ calcd for $C_{18}H_{28}NO_4^+$: 322.2013; found 322.2010.



3.2 Photolysis experiment



In a nitrogen-filled glove box, a 10-mL vial equipped with a magnetic stirring bar was charged sequentially with dibenzothiophenium salt (0.2 mmol, 2.0 equiv.), and acetone (1.0 mL). The vial was closed and removed from the glove box. The resulting mixture was allowed to stir at 60±5 ℃ under blue LED (100 W) irradiation for 12 hours. The methyl 2-methoxybenzoate was obtained in 23% yield with 71% of **1** remaining (^{1}H NMR spectra analysis using 4-bromoanisole as an internal standard).

3.3 UV-vis absorption spectrometry

UV-vis absorption spectra were recorded using acetone as solvent in 1 cm path quartz cuvettes using a UV-2600 UV-vis spectrometer.

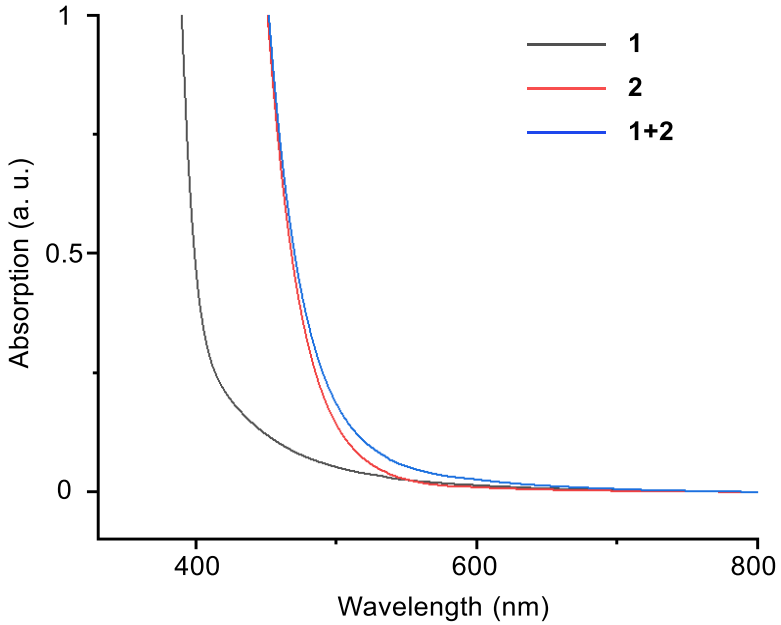


Figure S2. The UV/vis spectra of **1** ($5*10^{-2}$ M), **2** ($2.5*10^{-2}$ M) and the corresponding mixture in acetone.

3.4 Determination of the binding ratio by Job's plot

Job's plot was performed according to the literature method. dibenzothiophenium salt (**1**) and 1,2-diphenyldiselane (**2**) were dissolved in Acetonitrile-D3 (0.5 mL) to provide a mixed solution of 0.1 mol/L. Then, the solution was added to the NMR tube based on the specific ratio in Table S1. The $^{1}H(CH_3)$ chemical shift of free dibenzothiophenium salt solution (0.1 mol/L) is 3.7991 ppm. The Job's plot had a maximum when X (dibenzothiophenium salts) equals to 0.5, suggesting that the binding stoichiometry between 1,2-diphenyldiselane and dibenzothiophenium salt is 1:1.

1 (M)	**2** (M)	X (**1**)	$\delta(^{1}H(CH_3)$, ppm)	Δδ(ppm)	Δδ* X (**1**) $*10^3$
0.10	0	1	3,7991	0	0
0.08	0.02	0.8	3.7981	0.00100	0.08
0.07	0.03	0.7	3.7977	0.001400	0.098
0.05	0.05	0.5	3.7968	0.002300	0.115
0.03	0.07	0.3	3.7957	0.0034000	0.102
0.01	0.09	0.1	3.7939	0.005200	0.052

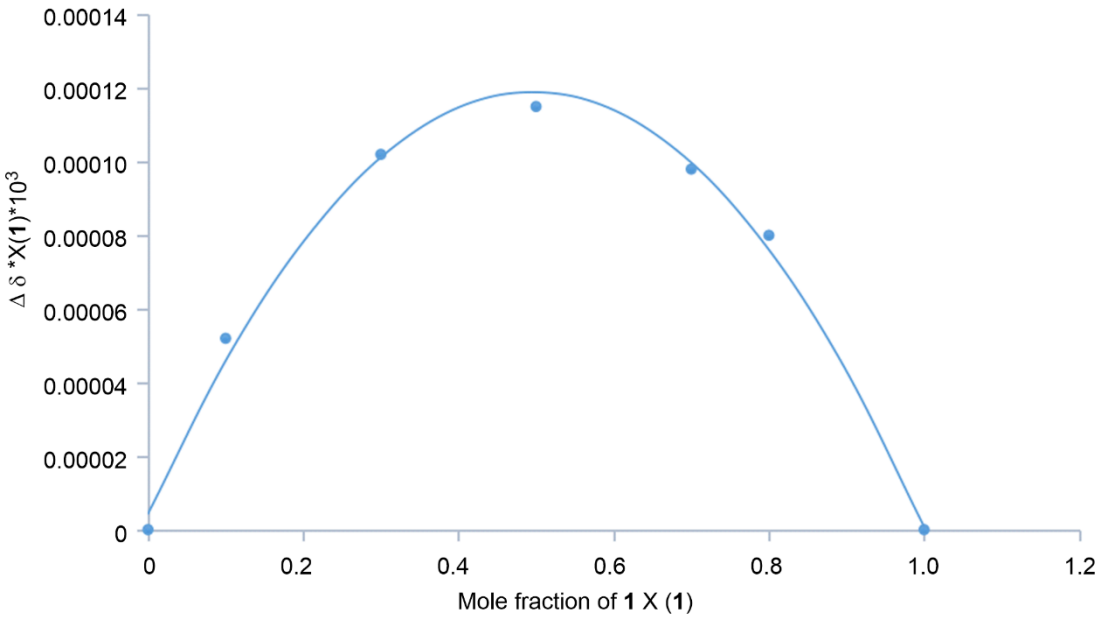


Figure S3. Job's plot for the determination of binding stoichiometry between dibenzothiophenium salt (**1**) and 1,2-diphenyldiselane (**2**).

3.5 ^{1}H NMR titrations of 1,2-diphenyldiselane(2) with dibenzothiophenium salt (1)

Dibenzothiophenium salt (**1**) ($1.00*10^{-2}$ mmol) and 1,2-diphenyldiselane (**2**) were thoroughly mixed in Acetonitrile-D3 (1.0 mL), then the resulted mixture was injected into an NMR tube. The ^{1}H NMR (500 MHz, Acetonitrile-D3, 25 ^{o}C) spectra of the $2.0*10^{-2}$ M Acetonitrile-D3 solution of 1,2-diphenyldiselane (**2**) with increasing concentration of dibenzothiophenium salt (**1**) (corresponding concentration from bottom to top is $2.0*10^{-2}$, $4.0*10^{-2}$, $6.0*10^{-2}$, $8.0*10^{-2}$, $1.0*10^{-1}$, $1.2*10^{-1}$, $1.4*10^{-1}$, $1.6*10^{-1}$ M, $1.8*10^{-1}$ M, $2.0*10^{-1}$ M) were recorded and shown in Figure S2. The titration curve was obtained with the Bindfit program based on the ^{1}H titration experiment (Figure S3), and the association constant Ka between 1,2-diphenyldiselane (**2**) and dibenzothiophenium salt (**1**) was calculated to be 9.60 ± 0.02 M^{-1}.

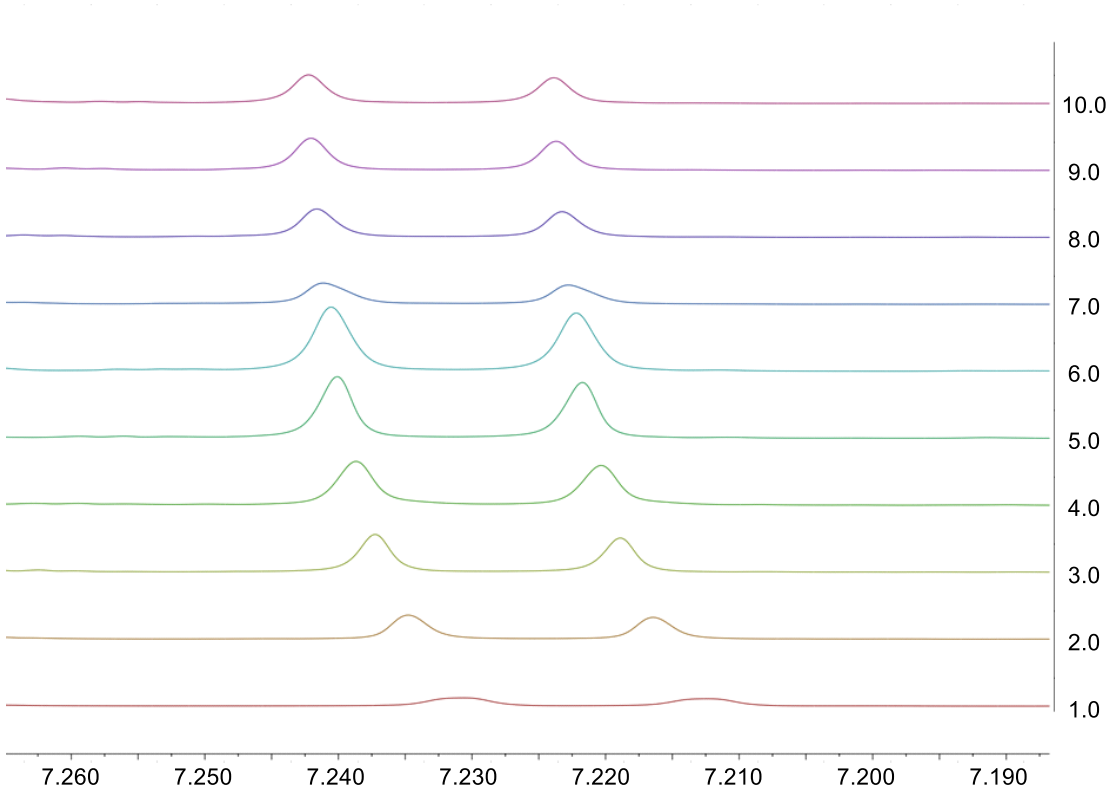
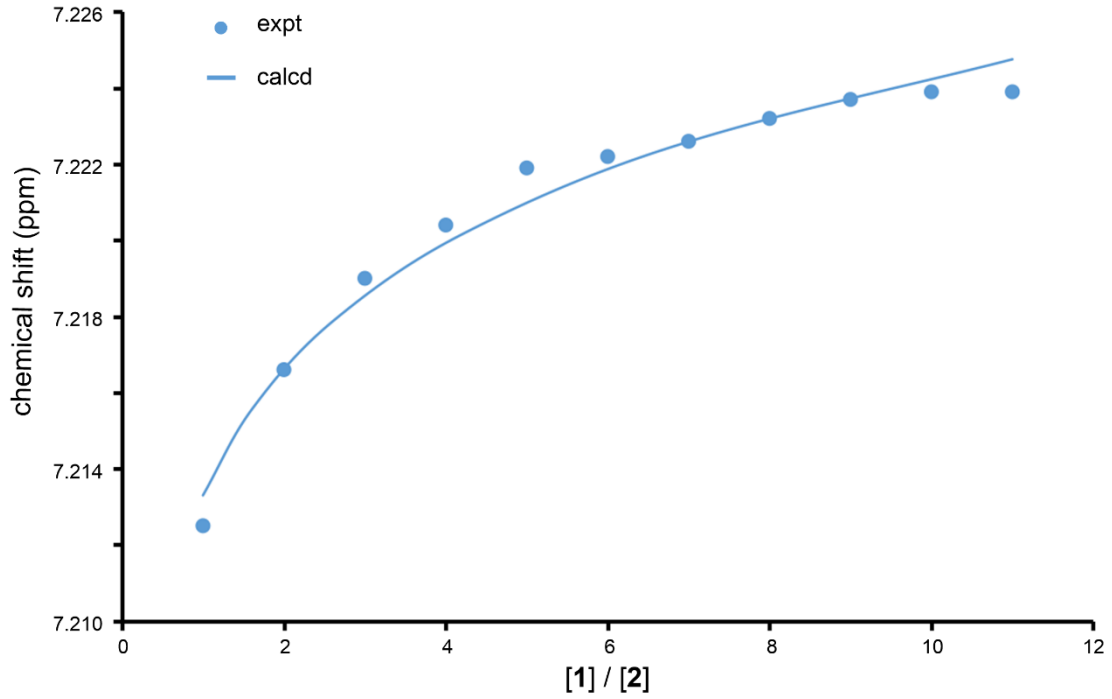


Figure S4. ^{1}H NMR spectra recorded during the titration of 1,2-diphenyldiselane (**2**) (2.0×10^{-2} M) with variable concentrations (1.0-10.0 equiv.) of dibenzothiophenium salt (**1**) in Acetonitrile-D3.



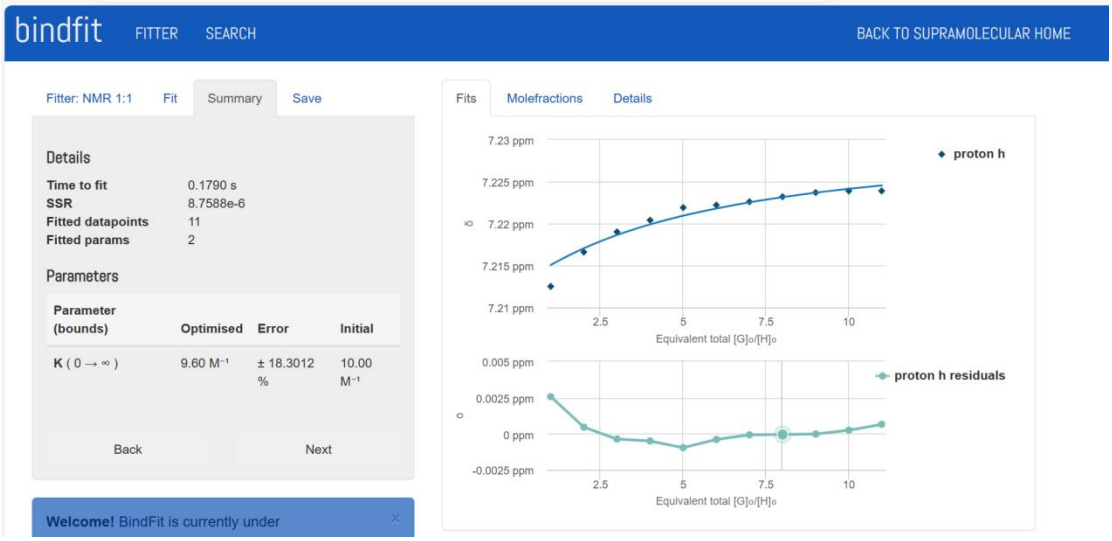
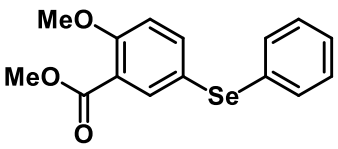
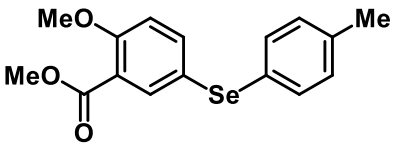


Figure S5. The curve fitting of the ^{1}H NMR titration data by Bindfit program, available online (http://supramolecular.org/); fitting output from Bindfit.

4. Compound Characterization Data

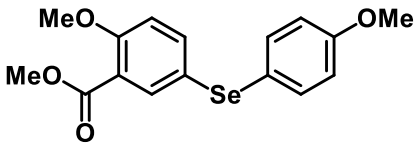


Methyl 2-methoxy-5-(phenylselanyl)benzoate (3): Prepared according to the general procedure, the chromatographic purification using PE and EA (50 : 1) as the eluent afforded **3** as a yellow oil (0.082 mmol, 26.3 mg, 82% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.01 (d, *J* = 2.3 Hz, 1H), 7.66 – 7.64 (m, 1H), 7.40 – 7.29 (m, 2H), 7.24 – 7.19 (m, 3H), 6.91 (d, *J* = 8.7 Hz, 1H), 3.90 (s, 3H), 3.86 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.0, 159.3, 140.2, 138.2, 132.5, 131.5, 129.4, 127.0, 121.2, 120.1, 113.3, 56.3, 52.3. **IR (ATR)**: 2948, 2840, 1728, 1435, 1238, 1081, 1022, 737 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{15}H_{14}O_3SeNa^+$: 345.0000; found 344.9993.

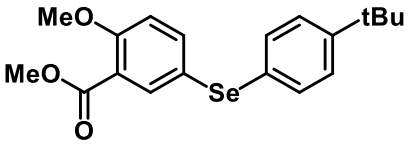


Methyl 2-methoxy-5-(p-tolylselanyl)benzoate (4): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **4** as a yellow oil (0.060 mmol, 20.2 mg, 60% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.00 (d, *J* = 2.2 Hz, 1H), 7.65 – 7.63 (m, 1H), 7.23 – 7.07 (m, 3H), 7.01 (d, *J* = 6.6 Hz, 1H), 6.91 (d, *J* = 8.7 Hz, 1H), 3.90 (s, 3H), 3.86 (s, 3H), 2.27 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.1, 159.2, 140.1, 138.1, 132.1, 129.2, 128.6, 127.9, 121.1, 120.2, 113.3, 56.3, 52.3, 21.4. **IR**

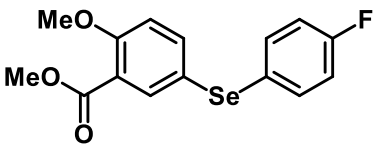
(ATR): 2946, 2840, 1729, 1485, 1233, 1079, 1021, 771 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{16}H_{16}O_3SeNa^+$: 359.0157; found 359.0150.



Methyl 2-methoxy-5-((4-methoxyphenyl)selanyl)benzoate (5): Prepared according to the general procedure, the chromatographic purification using PE and EA (500 : 1) as the eluent afforded **5** as a yellow oil (0.075 mmol, 26.5 mg, 75% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.92 (d, *J* = 2.3 Hz, 1H), 7.53 – 7.51 (m, 1H), 7.46 – 7.38 (m, 2H), 6.87 (d, *J* = 8.7 Hz, 1H), 6.85 – 6.80 (m, 2H), 3.87 (s, 3H), 3.86 (s, 3H), 3.79 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.1, 159.6, 158.7, 138.3, 136.2, 135.1, 122.2, 121.3, 120.9, 115.2, 113.2, 56.2, 55.4, 52.3. **IR (ATR)**: 2947, 2838, 1728, 1487, 1241, 1153, 1024, 816 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{16}H_{16}O_4SeNa^+$: 375.0106; found 375.0102.

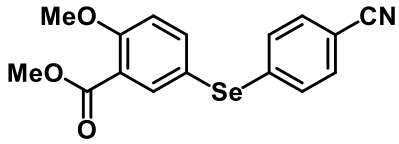


Methyl 5-((4-(tert-butyl)phenyl)selanyl)-2-methoxybenzoate (6): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **6** as a yellow oil (0.072 mmol, 27.1 mg, 72% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.01 (d, *J* = 2.3 Hz, 1H), 7.64 – 7.62 (m, 1H), 7.31 – 7.23 (m, 4H), 6.91 (d, *J* = 8.7 Hz, 1H), 3.90 (s, 3H), 3.87 (s, 3H), 1.29 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.1, 159.2, 150.4, 139.9, 137.9, 131.6, 128.6, 126.6, 121.1, 120.6, 113.3, 56.3, 52.3, 34.7, 31.4. **IR (ATR)**: 2951, 2844, 1732, 1476, 1242, 1182, 1083, 815, 755 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{19}H_{22}O_3SeNa^+$: 401.0626; found 401.0619.

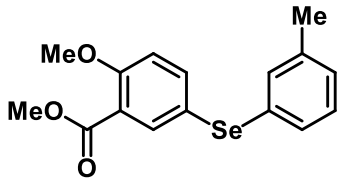


Methyl 5-((4-fluorophenyl)selanyl)-2-methoxybenzoate (7): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **7** as a yellow oil (0.088 mmol, 30.0 mg, 88% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.97 (d, *J* = 2.3 Hz, 1H), 7.61 – 7.59 (m, 1H), 7.41 – 7.35 (m, 2H), 6.98 –

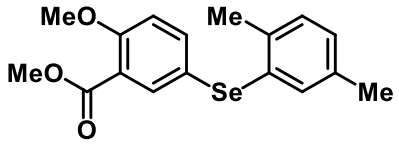
6.94 (m, 2H), 6.91 (d, *J* = 8.6 Hz, 1H), 3.90 (s, 3H), 3.88 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.0, 162.4 (d, *J* = 247.1 Hz), 159.2, 139.5, 137.5, 134.3, 134.2, 126.6, 121.0 (d, *J* = 65.5 Hz), 116.6 (d, *J* = 21.7 Hz), 113.4, 56.3, 52.3. **IR (ATR)**: 2948, 2841, 1727, 1585, 1483, 1249, 1080, 812 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{15}H_{13}FO_3SeNa^+$: 362.9906; found 362.9901.



Methyl 5-((4-cyanophenyl)selanyl)-2-methoxybenzoate (8): Prepared according to the general procedure, the chromatographic purification using PE and EA (10 : 1) as the eluent afforded **8** as a yellow solid (0.067 mmol, 23.2 mg, 67% yield). **Melting Point:** 147 – 148 °C. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.07 (d, *J* = 2.3 Hz, 1H), 7.74 – 7.72 (m, 1H), 7.50 – 7.37 (m, 2H), 7.27 (d, *J* = 1.8 Hz, 2H), 7.01 (d, *J* = 8.6 Hz, 1H), 3.96 (s, 3H), 3.89 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 165.7, 160.2, 141.9, 141.6, 140.0, 132.6, 129.5, 121.8, 118.9, 116.9, 113.7, 109.6, 56.3, 52.5. **IR (ATR)**: 2949, 2846, 1730, 1484, 1243, 1082, 1015, 818 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{16}H_{13}NO_3SeNa^+$: 369.9953; found 369.9948.

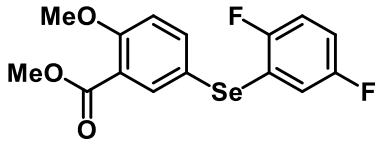


Methyl 2-methoxy-5-(m-tolylselanyl)benzoate (9): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **9** as a yellow oil (0.057 mmol, 19.2 mg, 57% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.01 (d, *J* = 2.3 Hz, 1H), 7.65 – 7.63 (m, 1H), 7.19 (s, 1H), 7.15 – 7.11 (m, 2H), 7.03 (d, *J* = 6.4 Hz, 1H), 6.92 (d, *J* = 8.6 Hz, 1H), 3.91 (s, 3H), 3.87 (s, 3H), 2.29 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.1, 159.2, 140.1, 139.3, 138.1, 132.2, 132.1, 129.2, 128.6, 127.9, 121.2, 120.3, 113.3, 56.3, 52.3, 21.4. **IR (ATR)**: 2948, 2841, 1731, 1590, 1486, 1241, 1082, 774 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{16}H_{16}O_3SeNa^+$: 359.0157; found 359.0151.

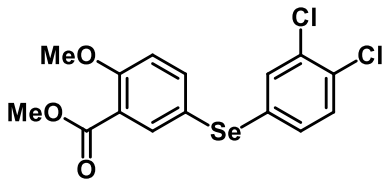


Methyl 5-((2,5-dimethylphenyl)selanyl)-2-methoxybenzoate (10): Prepared according to the

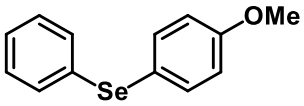
general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **10** as a yellow oil (0.044 mmol, 15.4 mg, 44% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.96 (d, *J* = 2.3 Hz, 1H), 7.57 – 7.55 (m, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 6.99 – 6.90 (m, 3H), 3.92 (s, 3H), 3.87 (s, 3H), 2.34 (s, 3H), 2.21 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.1, 159.1, 139.8, 137.8, 136.5, 135.7, 132.5, 130.2, 128.2, 121.2, 119.9, 113.4, 56.3, 52.3, 21.7, 21.0. **IR (ATR)**: 2948, 2850, 1732, 1486, 1242, 1082, 812 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{17}H_{18}O_3SeNa^+$: 373.0307; found 373.0313.



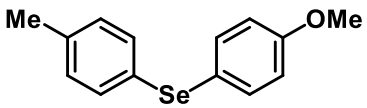
Methyl 5-((2,5-difluorophenyl)selanyl)-2-methoxybenzoate (11): Prepared according to the general procedure I, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **11** as a yellow oil (0.050 mmol, 17.9 mg, 50% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.08 (d, *J* = 2.3 Hz, 1H), 7.74 – 7.72 (m, 1H), 7.03 – 6.91 (m, 2H), 6.86 – 6.83 (m, 1H), 6.63 – 6.60 (m, 1H), 3.95 (s, 3H), 3.89 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 165.7, 160.2, 141.9, 139.9, 121.7, 117.72 (d, *J* = 25.9 Hz), 117.70 (d, *J* = 24.7 Hz), 116.3, 116.13 (d, *J* = 25.4 Hz), 116.06 (d, *J* = 25.4 Hz), 114.63 (d, *J* = 24.3 Hz), 114.56 (d, *J* = 24.3 Hz), 113.7, 56.3, 52.4. **IR (ATR)**: 2947, 2839, 1727, 1487, 1231, 1079, 1022, 812 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{15}H_{12}F_2O_3SeNa^+$: 380.9812; found 380.9808.



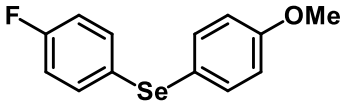
Methyl 5-((3,4-dichlorophenyl)selanyl)-2-methoxybenzoate (12): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **12** as a yellow solid (0.057 mmol, 22.3 mg, 57% yield). **Melting Point:** 85 – 86 °C. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.03 (d, *J* = 1.8 Hz, 1H), 7.68 – 7.66 (m, 1H), 7.37 (d, *J* = 2.1 Hz, 1H), 7.26 (d, *J* = 1.1 Hz, 1H), 7.11 (m, 1H), 6.97 (d, *J* = 8.6 Hz, 1H), 3.93 (s, 3H), 3.89 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 165.8, 159.8, 140.8, 138.9, 133.4, 132.7, 132.2, 131.0, 130.1, 121.5, 118.7, 113.6, 56.3, 52.4. **IR (ATR)**: 2948, 2844, 1732, 1456, 1244, 1082, 1027, 814 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{15}H_{12}Cl_2O_3SeNa^+$: 390.9406; found 390.9496.



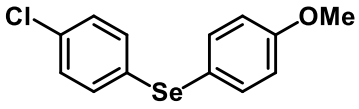
(4-methoxyphenyl)(phenyl)selane (13): Prepared according to the general procedure, the chromatographic purification using PE and EA (50 : 1) as the eluent afforded **13** as a yellow oil (0.072 mmol, 18.9 mg, 72% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.51 (d, *J* = 8.7 Hz, 2H), 7.35 – 7.29 (m, 2H), 7.24 – 7.17 (m, 3H), 6.86 (d, *J* = 8.7 Hz, 2H), 3.81 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 159.9, 136.7, 133.3, 131.0, 129.3, 126.6, 120.0, 115.3, 55.4. Analytical data for compound **13** was consistent with the reported literature.[3]



(4-methoxyphenyl)(p-tolyl)selane (14): Prepared according to the general procedure, the chromatographic purification using PE and EA (50 : 1) as the eluent afforded **14** as a colorless oil (0.054 mmol, 15.0 mg, 54% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.46 (d, *J* = 6.6 Hz, 8H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.83 (d, *J* = 6.7 Hz, 2H), 3.79 (s, 3H), 2.30 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 159.6, 136.9, 135.9, 131.9, 130.1, 129.0, 120.9, 115.1, 55.4, 21.2. Analytical data for compound **14** was consistent with the reported literature.[3]

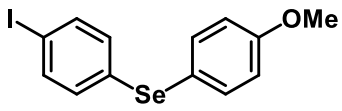


(4-fluorophenyl)(4-methoxyphenyl)selane (15): Prepared according to the general procedure, the chromatographic purification using PE and EA (150 : 1) as the eluent afforded **15** as a yellow oil (0.053 mmol, 15.0mg, 53% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.51 – 7.43 (m, 2H), 7.36 – 7.33 (m, 2H), 6.96 – 6.92 (m, 2H), 6.86 – 6.83 (m, 2H), 3.81 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 162.2 (d, *J* = 246.5 Hz), 159.8, 136.0, 133.6 (d, *J* = 7.7 Hz), 127.4, 120.7, 116.5 (d, *J* = 21.6 Hz), 115.3, 55.5. Analytical data for compound **15** was consistent with the reported literature.[3]

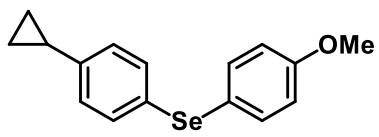


(4-chlorophenyl)(4-methoxyphenyl)selane (16): Prepared according to the general procedure, the chromatographic purification using PE and EA (250 : 1) as

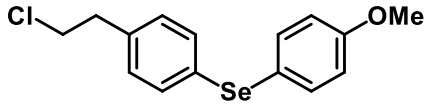
the eluent afforded **16** as a white solid (0.071 mmol, 21.0mg, 71% yield). **Melting Point:** 54 – 55 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.49 (d, *J* = 8.6 Hz, 2H), 7.23 (d, *J* = 8.6 Hz, 2H), 7.17 (d, *J* = 8.6 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 3.81 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 160.1, 136.8, 132.6, 132.2, 131.7, 129.4, 119.6, 115.4, 55.5. Analytical data for compound **16** was consistent with the reported literature.[3]



(4-iodophenyl)(4-methoxyphenyl)selane (17): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **17** as a white solid (0.060 mmol, 23.3mg, 60% yield). **Melting Point:** 96 – 97 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.50 (d, *J* = 8.4 Hz, 4H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 3.82 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 160.2, 138.2, 137.0, 133.7, 132.5, 119.3, 115.4, 91.6, 55.5. **IR (ATR)**: 2987, 2922, 1654, 1593, 1456, 1407, 1272, 737 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{13}H_{11}IOSeNa^+$: 412.8912; found 412.8913.

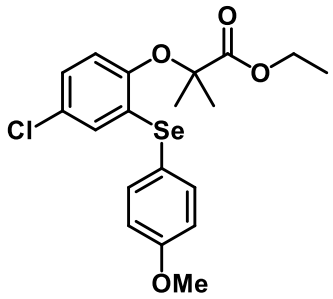


(4-cyclopropylphenyl)(4-methoxyphenyl)selane (18): Prepared according to the general procedure, the chromatographic purification using PE and EA (50 : 1) as the eluent afforded **18** as a yellow oil (0.053 mmol, 16.0 mg, 53% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.46 (d, *J* = 8.7 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 6.94 (d, *J* = 8.2 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 3.80 (s, 3H), 1.87 – 1.82 (m, 1H), 0.96 – 0.93 (m, 2H), 0.67 – 0.64 (m, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 159.6, 143.1, 135.8, 132.0, 128.9, 126.7, 121.0, 115.2, 55.4, 15.2, 9.5. **IR (ATR)**: 3001, 2835, 1591, 1489, 1246, 1173, 1030, 814 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+K]^+$ calcd for $C_{16}H_{16}OSeK^+$: 342.9998; found 343.0001.

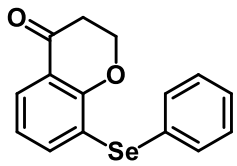


(4-(2-chloroethyl)phenyl)(4-methoxyphenyl)selane (19): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **19** as a yellow oil (0.051 mmol,

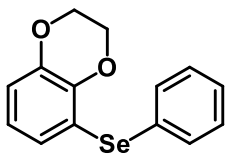
16.5 mg, 51% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.50 (d, *J* = 6.9 Hz, 2H), 7.28 (d, *J* = 7.2 Hz, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 6.86 (d, *J* = 6.9 Hz, 2H), 3.81 (s, 3H), 3.67 (t, *J* = 6.0 Hz, 2H), 3.00 (t, *J* = 6.0 Hz, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 159.9, 136.7, 133.3, 131.7, 131.3, 129.8, 120.0, 115.3, 55.4, 44.9, 38.8. **IR (ATR)**: 2957, 2925, 2359, 1591, 1489, 1288, 1247, 1030, 814, 507 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{15}H_{15}ClOSeNa^+$: 348.9869; found 348.9864.



Ethyl 2-(4-chloro-2-((4-methoxyphenyl)selanyl)phenoxy)-2-methylpropanoate (20): Prepared according to the general procedure, the chromatographic purification using PE and EA (20 : 1) as the eluent afforded **20** as a yellow oil (0.057 mmol, 24.4 mg, 57% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.56 (d, *J* = 8.8 Hz, 2H), 6.99 – 6.90 (m, 3H), 6.65 – 6.59 (m, 2H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.86 (s, 3H), 1.64 (s, 6H), 1.28 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 174.2, 160.7, 150.6, 138.9, 130.3, 128.3, 128.0, 125.8, 117.7, 116.6, 115.7, 80.7, 61.8, 55.5, 25.2, 14.2. **IR (ATR)**: 2987, 2359, 1734, 1591, 1461, 1248, 1136, 827 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{19}H_{21}ClO_4SeNa^+$: 451.0186; found 451.0176.

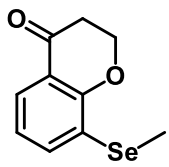


8-(phenylselanyl)chroman-4-one (21): Prepared according to the general procedure, the chromatographic purification using PE and EA (50 : 1) as the eluent afforded **21** as a yellow oil (0.082 mmol, 24.8 mg, 82% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.09 (d, *J* = 2.3 Hz, 1H), 7.60 – 7.57 (m, 1H), 7.40 – 7.36 (m, 2H), 7.24 – 7.22 (m, 3H), 6.89 (d, *J* = 8.6 Hz, 1H), 4.53 (t, *J* = 6.5 Hz, 2H), 2.80 (t, *J* = 6.5 Hz, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 191.1, 161.7, 141.9, 133.0, 132.3, 131.8, 129.5, 127.4, 122.5, 122.1, 119.4, 67.2, 37.7. **IR (ATR)**: 2987, 2922, 1654, 1593, 1456, 1407, 1272, 737 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{15}H_{12}O_2SeNa^+$: 326.9895; found 326.9889.

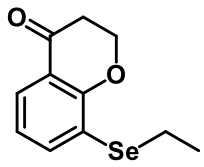


5-(phenylselanyl)-2,3-dihydrobenzo[b][1,4]dioxine (22): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **22** as a yellow oil (0.093

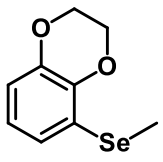
mmol, 27.0 mg, 93% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.40 – 7.37 (m, 2H), 7.25 – 7.19 (m, 3H), 7.08 (d, *J* = 2.0 Hz, 1H), 7.03 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.80 (d, *J* = 8.3 Hz, 1H), 4.26 – 4.24 (m, 4H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 144.1, 143.9, 132.6, 131.7, 129.3, 127.9, 126.9, 123.5, 121.1, 118.3, 64.5, 64.4. **IR (ATR)**: 2923, 1578, 1489, 1281, 1249, 1062, 894, 737 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{14}H_{12}O_2SeNa^+$: 314.9895; found 314.9894.



8-(methylselanyl)chroman-4-one (23): Prepared according to the general procedure, the chromatographic purification using PE and EA (50 : 1) as the eluent afforded **23** as a yellow oil (0.067 mmol, 16.1 mg, 67% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.96 (s, 1H), 7.56 (d, *J* = 8.6, 1H), 6.89 (d, *J* = 8.6, 1H), 4.67 – 4.37 (t, *J* = 6.5 Hz, 2H), 2.80 (t, *J* = 6.5 Hz, 2H), 2.34 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 191.4, 160.9, 139.3, 129.5, 123.6, 122.0, 118.9, 67.2, 37.8, 8.4. **IR (ATR)**: 2972, 2926, 1690, 1596, 1477, 1409, 1273, 1031 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{10}H_{10}O_2SeNa^+$: 264.9738; found 264.9734.

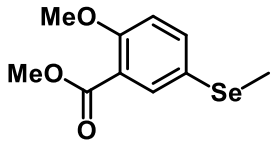


8-(ethylselanyl)chroman-4-one (24): Prepared according to the general procedure, the chromatographic purification using PE and EA (50 : 1) as the eluent afforded **24** as a yellow oil (0.070 mmol, 17.8 mg, 70% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.03 (d, *J* = 2.3 Hz, 1H), 7.61 (dd, *J* = 8.6, 2.3 Hz, 1H), 6.89 (d, *J* = 8.6 Hz, 1H), 4.53 (t, *J* = 6.5 Hz, 2H), 2.88 (q, *J* = 7.5 Hz, 2H), 2.81 (t, *J* = 6.5 Hz, 2H), 1.40 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 191.4, 161.3, 141.4, 132.0, 121.9, 121.8, 118.9, 67.2, 37.8, 22.3, 15.6. **IR (ATR)**: 2963, 2922, 1692, 1595, 1477, 1408, 1276, 1031 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{11}H_{12}O_2SeNa^+$: 278.9895; found 278.9882.

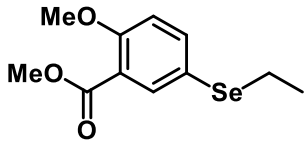


5-(methylselanyl)-2,3-dihydrobenzo[b][1,4]dioxine (25): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **25** as a yellow oil (0.079 mmol, 18.0 mg, 79% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 6.99 – 6.97 (m, 1H), 6.95 – 6.91 (m, 1H), 6.77 – 6.74 (m, 1H), 4.23 (d, *J* = 2.4 Hz, 4H), 2.29 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 144.0, 142.8, 124.9, 122.6, 120.5, 118.0, 64.5, 64.4, 8.5. **IR (ATR)**: 2976, 2927, 1579, 1489, 1281, 1249, 1063,

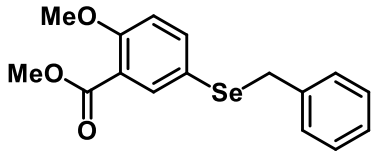
894 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+H]^+$ calcd for $C_9H_{10}O_2SeH^+$: 230.9919; found 230.9922.



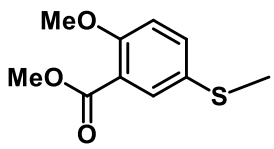
Methyl 2-methoxy-5-(methylselanyl)benzoate (26): Prepared according to the general procedure, the chromatographic purification using PE and EA (50 : 1) as the eluent afforded **26** as a yellow oil (0.082 mmol, 21.2mg, 82% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.90 (s, 1H), 7.58 (d, *J* = 8.7 Hz, 1H), 6.90 (d, *J* = 8.7 Hz, 1H), 3.89 (s, 6H), 2.33 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.2, 158.3, 137.2, 135.2, 121.5, 120.9, 113.1, 56.3, 52.3, 8.8. **IR (ATR)**: 2956, 2839, 1717, 1488, 1259, 1082, 1011, 818, 738 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{10}H_{12}O_3SeNa^+$: 282.9844; found 282.9841.



Methyl 5-(ethylselanyl)-2-methoxybenzoate (27): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **27** as a yellow oil (0.081 mmol, 22.1mg, 81% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.97 (d, *J* = 2.3 Hz, 1H), 7.65 – 7.62 (m, 1H), 6.90 (d, *J* = 8.6 Hz, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 2.86 (q, *J* = 7.5 Hz, 2H), 1.39 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.2, 158.8, 139.5, 137.4, 120.9, 119.8, 112.9, 56.3, 52.3, 22.6, 15.7. **IR (ATR)**: 2951, 1730, 1486, 1434, 1231, 1080, 1032, 814 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{11}H_{14}O_3SeNa^+$: 297.0000; found 296.9994.



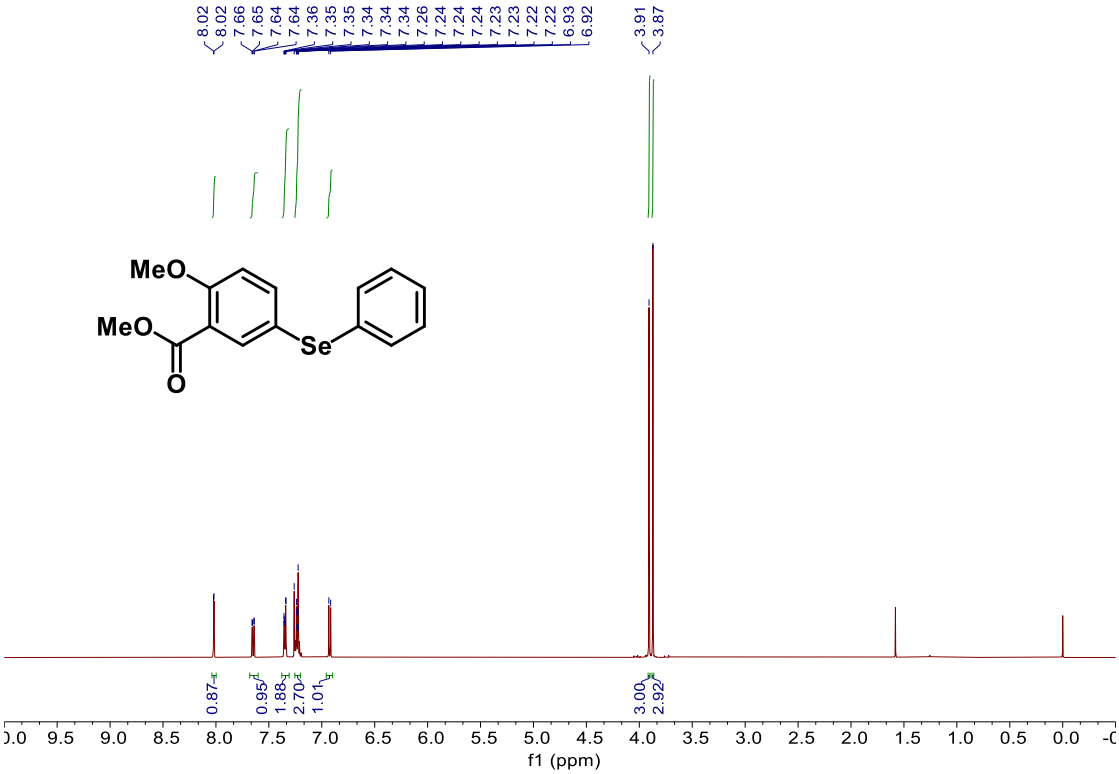
Methyl 5-(benzylselanyl)-2-methoxybenzoate (28): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **28** as a yellow oil (0.051 mmol, 17.0 mg, 51% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.87 (d, *J* = 2.2 Hz, 1H), 7.47 – 7.45 (m, 1H), 7.24 – 7.17 (m, 3H), 7.14 – 7.08 (m, 2H), 6.82 (d, *J* = 8.6 Hz, 1H), 4.02 (s, 2H), 3.89 (s, 3H), 3.87 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.1, 159.2, 140.5, 138.8, 138.5, 129.0, 128.5, 127.0, 120.6, 119.6, 112.7, 56.2, 52.2, 33.2. **IR (ATR)**: 2970, 1732, 1489, 1435, 1243, 1081, 758, 678 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{16}H_{16}O_3SeNa^+$: 359.0157; found 359.0150.



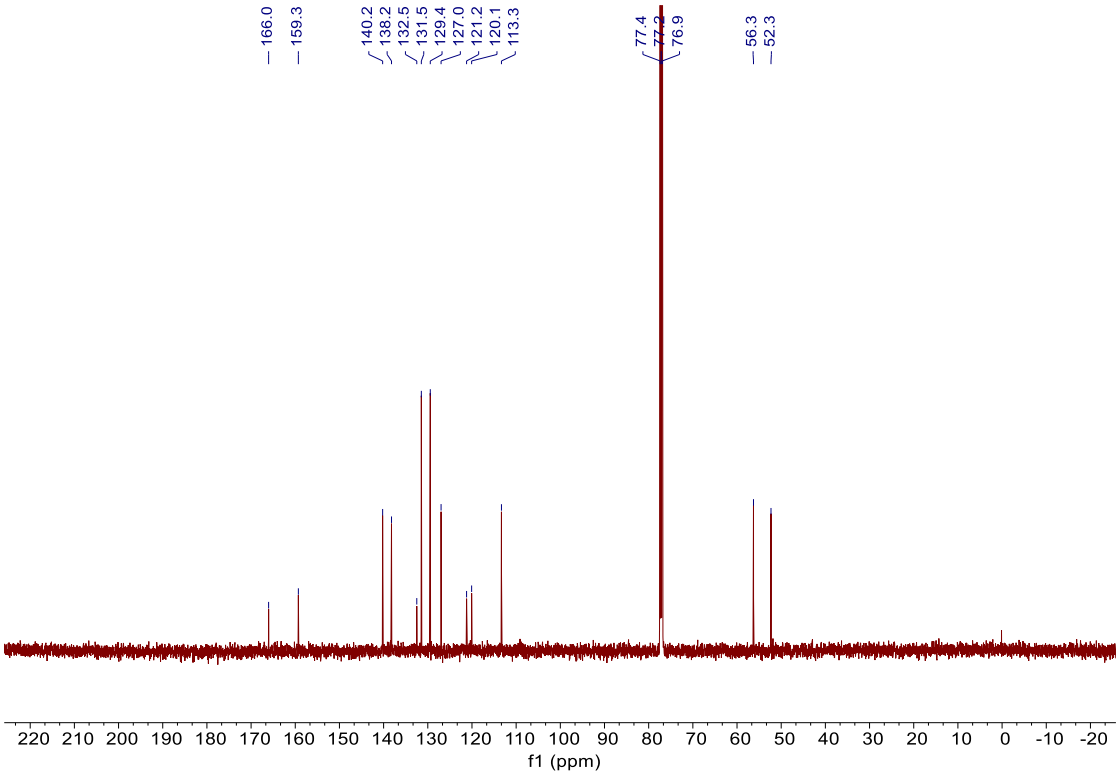
Methyl 2-methoxy-5-(methylthio)benzoate (29): Prepared according to the general procedure, the chromatographic purification using PE and EA (100 : 1) as the eluent afforded **29** as a yellow oil (0.057 mmol, 12.1 mg, 57% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.75 (s, 1H), 7.43 (d, *J* = 8.7 Hz, 1H), 6.93 (d, *J* = 8.6 Hz, 1H), 3.89-3.89 (m, 6H), 2.47 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.4, 157.7, 133.8, 131.8, 129.1, 120.8, 113.0, 56.4, 52.3, 17.8. **IR (ATR)**: 2951, 1731, 1490, 1434, 1299, 1242, 1081, 814 cm^{-1}. **HRMS (ESI)**: *m/z* $[M+Na]^+$ calcd for $C_{10}H_{12}O_3SNa^+$: 235.0399; found 235.0395.

5. NMR Spectra

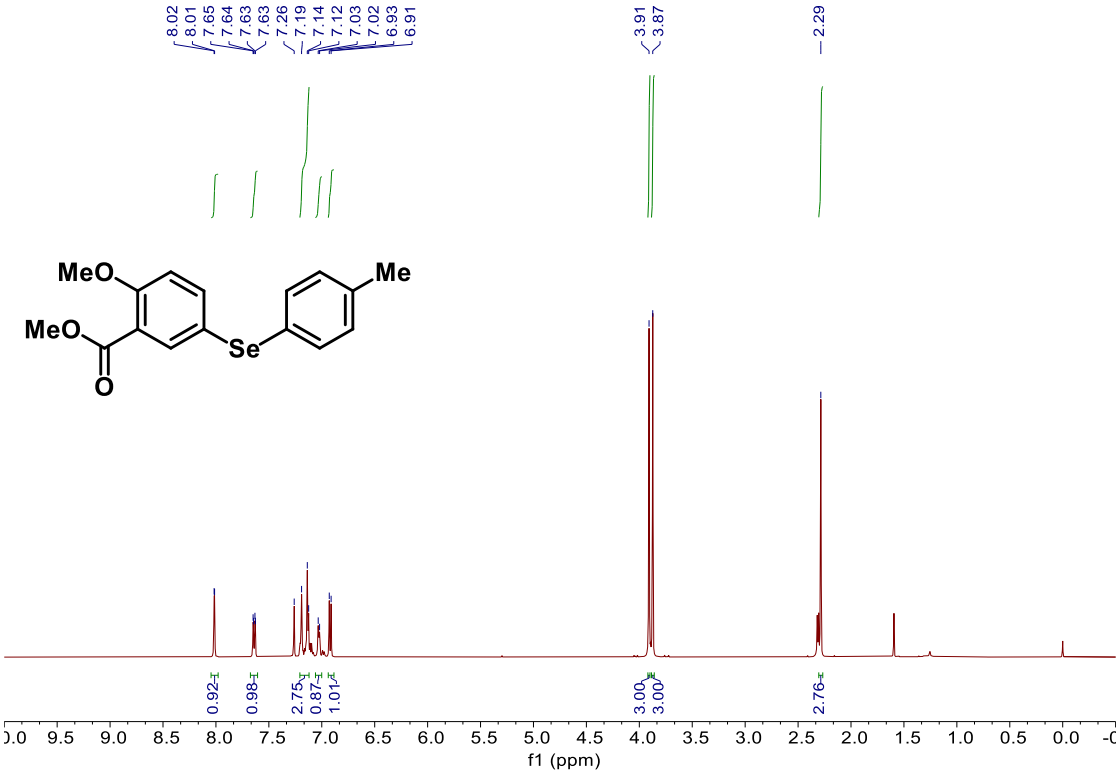
^{1}H NMR of compound 3 (500 MHz in $CDCl_3$)



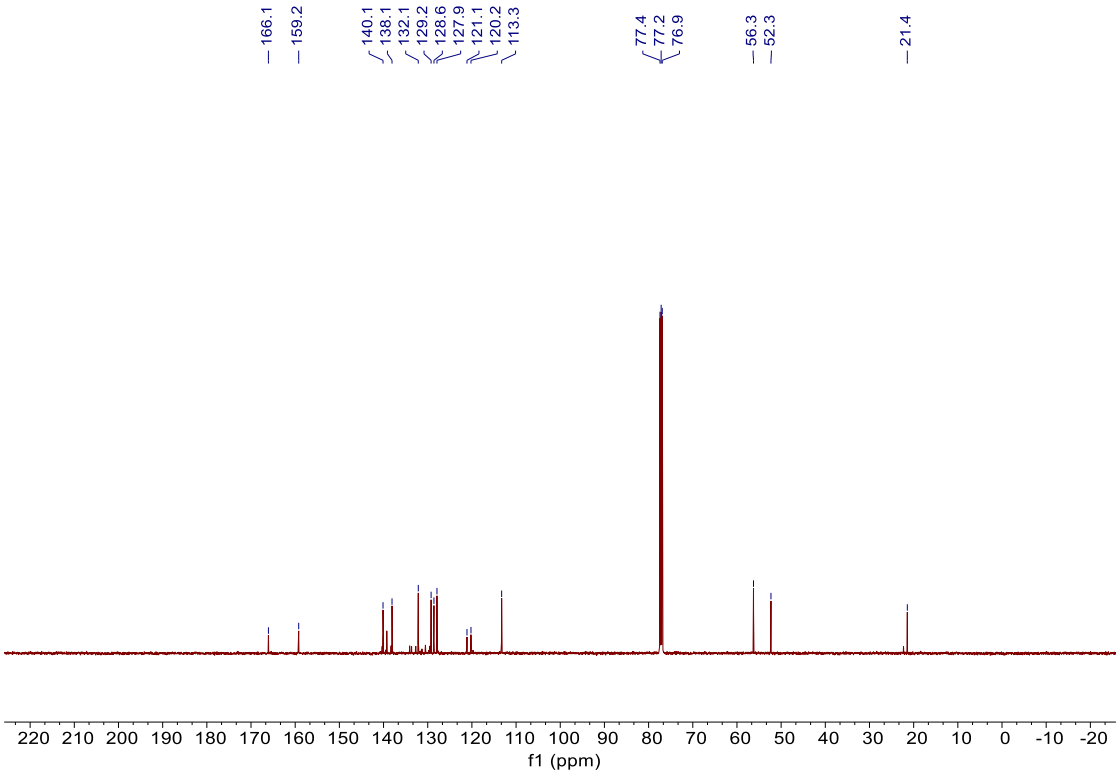
^{13}C NMR of compound 3 (126 MHz in $CDCl_3$)



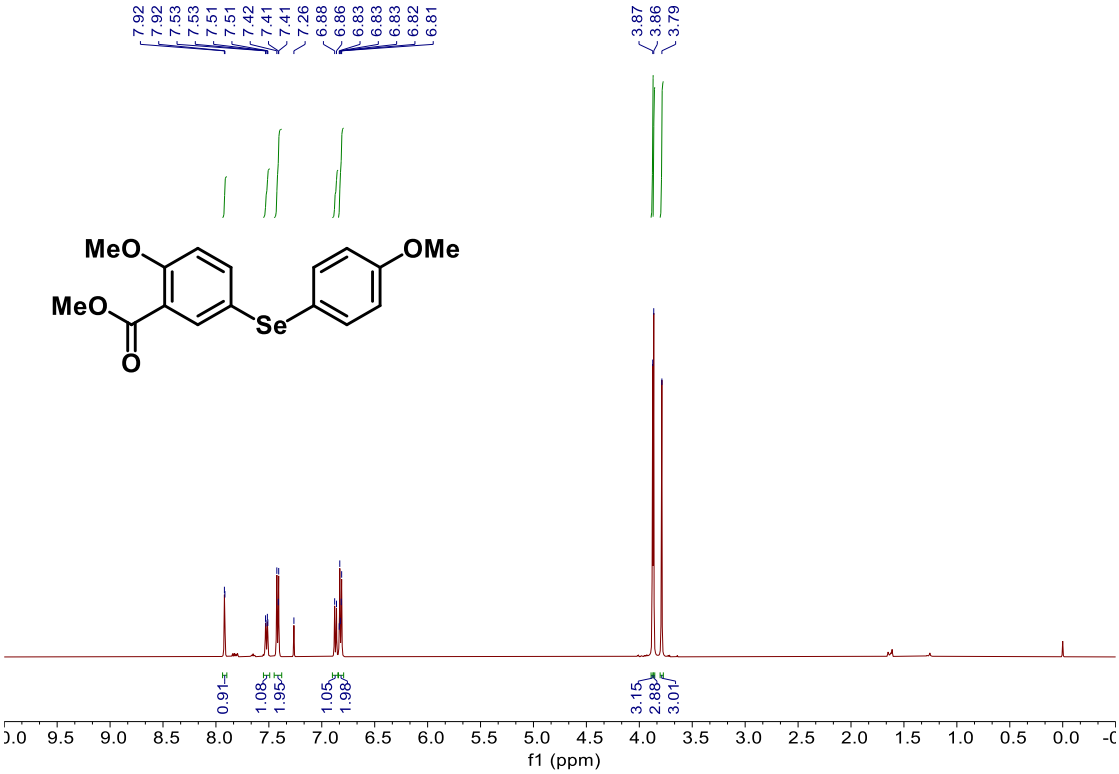
^{1}H NMR of compound 4 (500 MHz in $CDCl_3$)



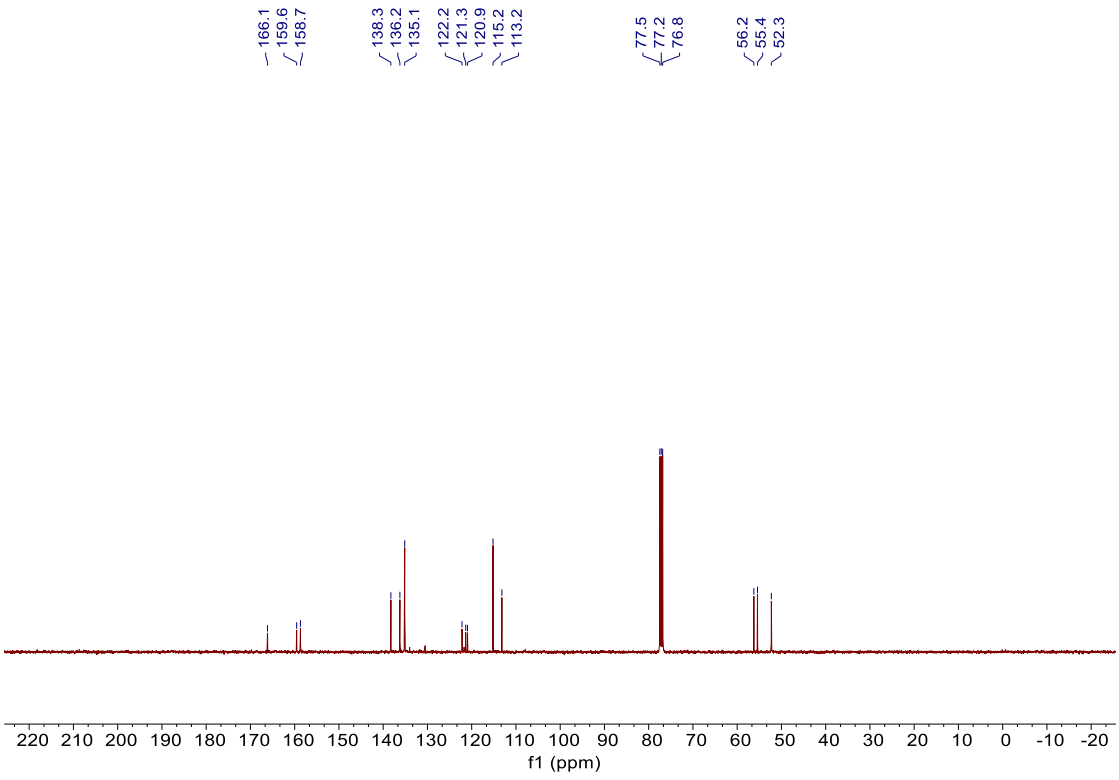
^{13}C NMR of compound 4 (126 MHz in $CDCl_3$)



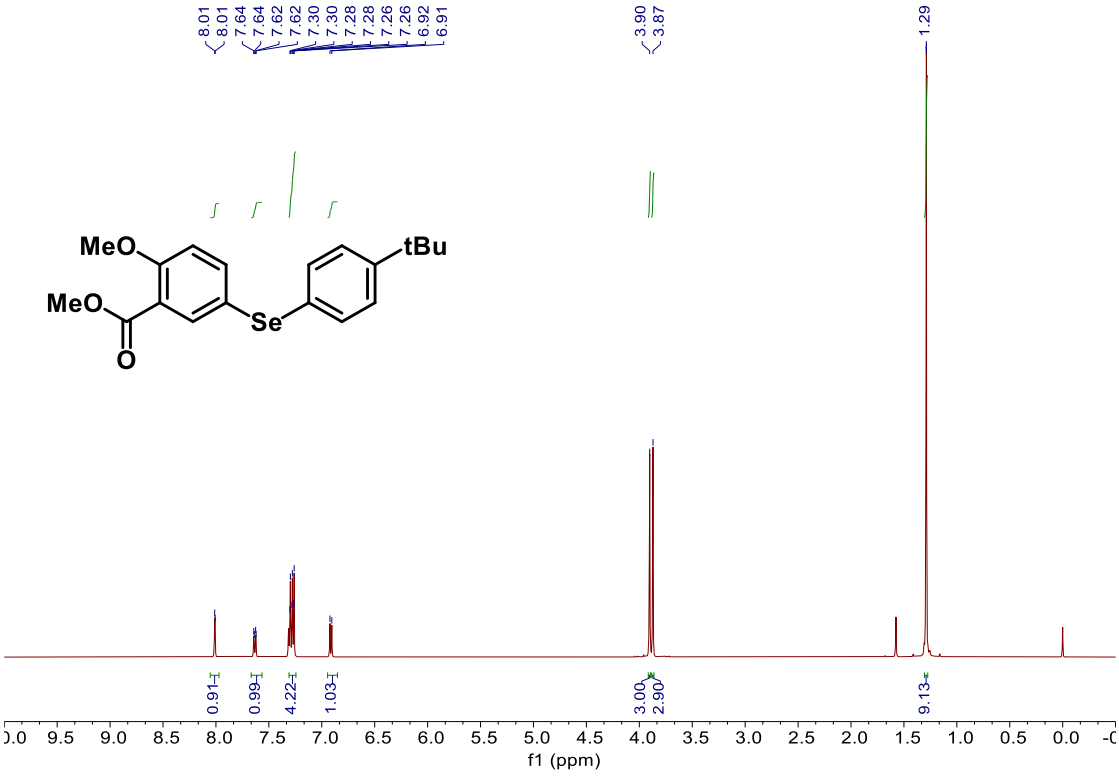
^{1}H NMR of compound 5 (500 MHz in $CDCl_3$)



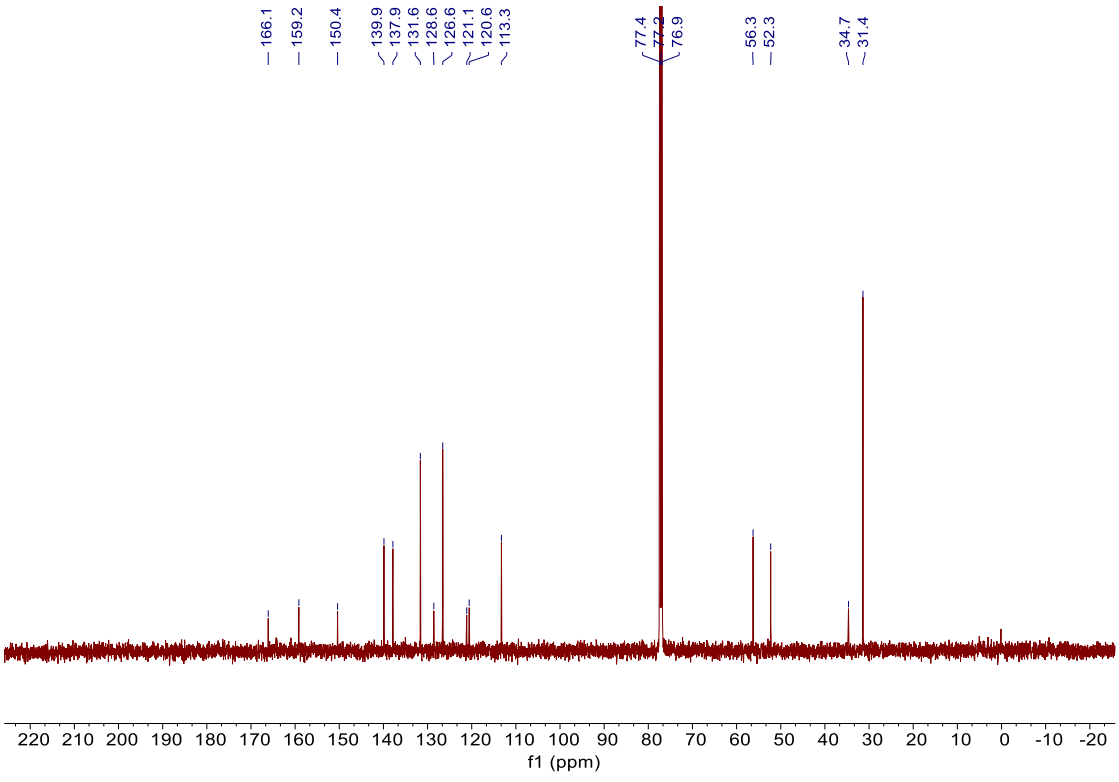
^{13}C NMR of compound 5 (101 MHz in $CDCl_3$)



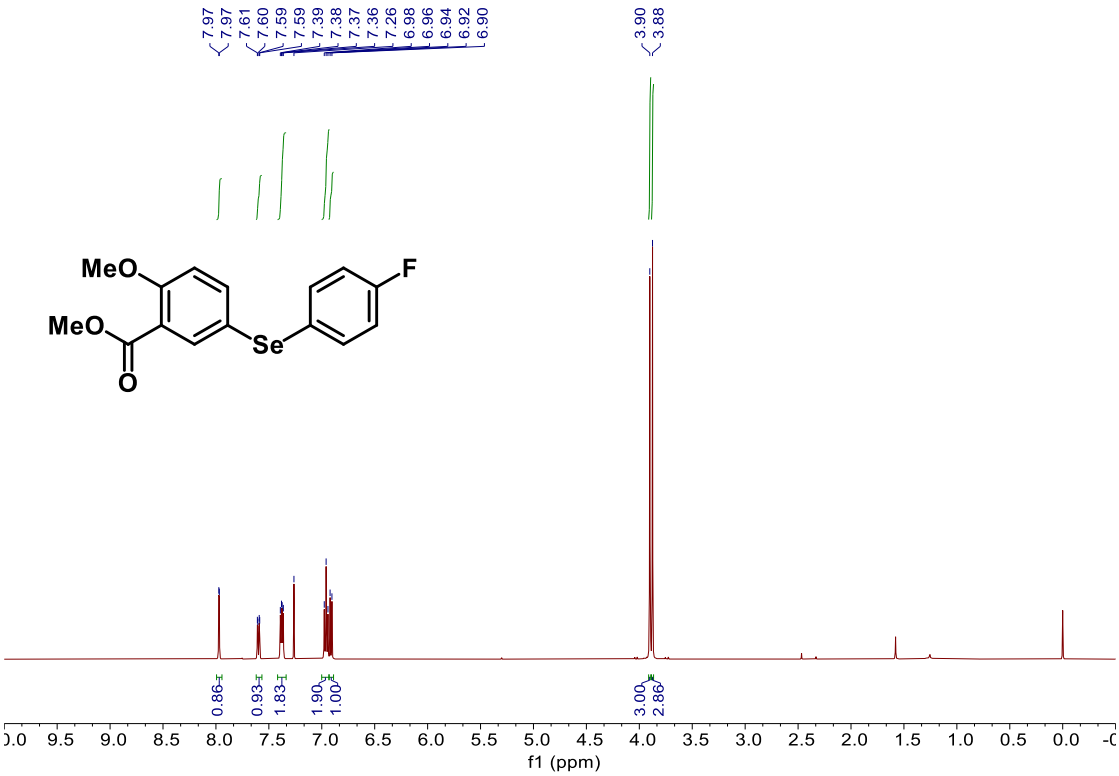
^{1}H NMR of compound 6 (500 MHz in $CDCl_3$)



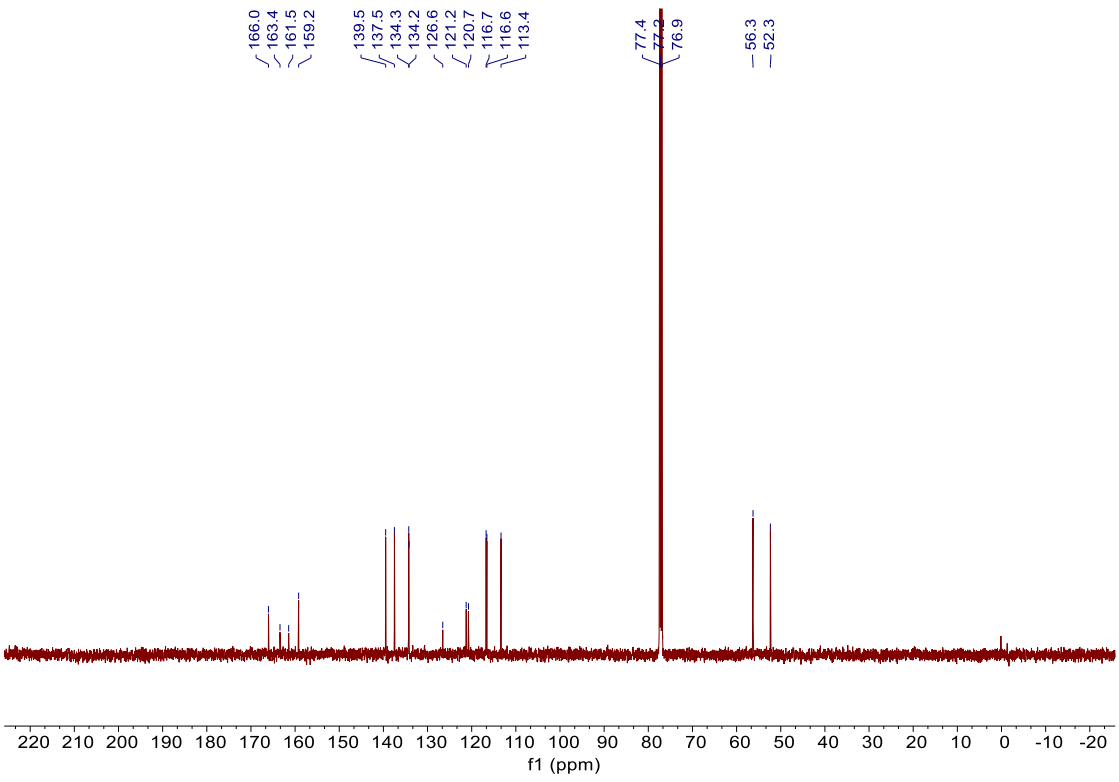
^{13}C NMR of compound 6 (126 MHz in $CDCl_3$)



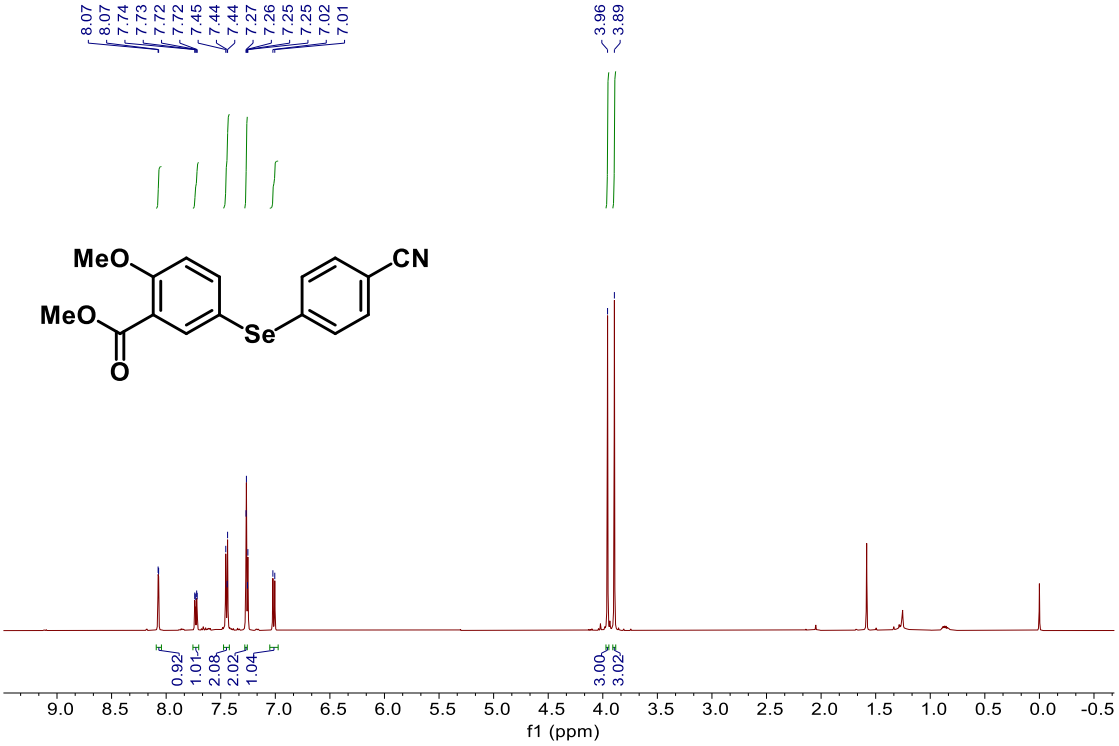
^{1}H NMR of compound 7 (500 MHz in $CDCl_3$)



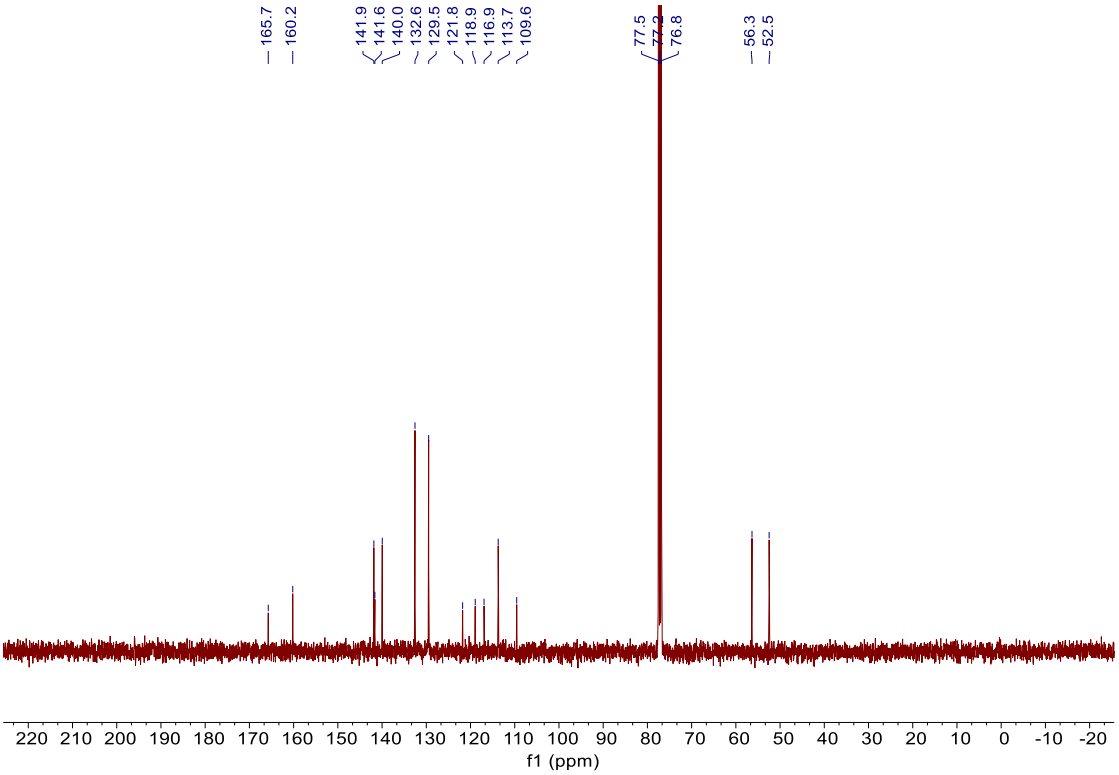
^{13}C NMR of compound 7 (126 MHz in $CDCl_3$)



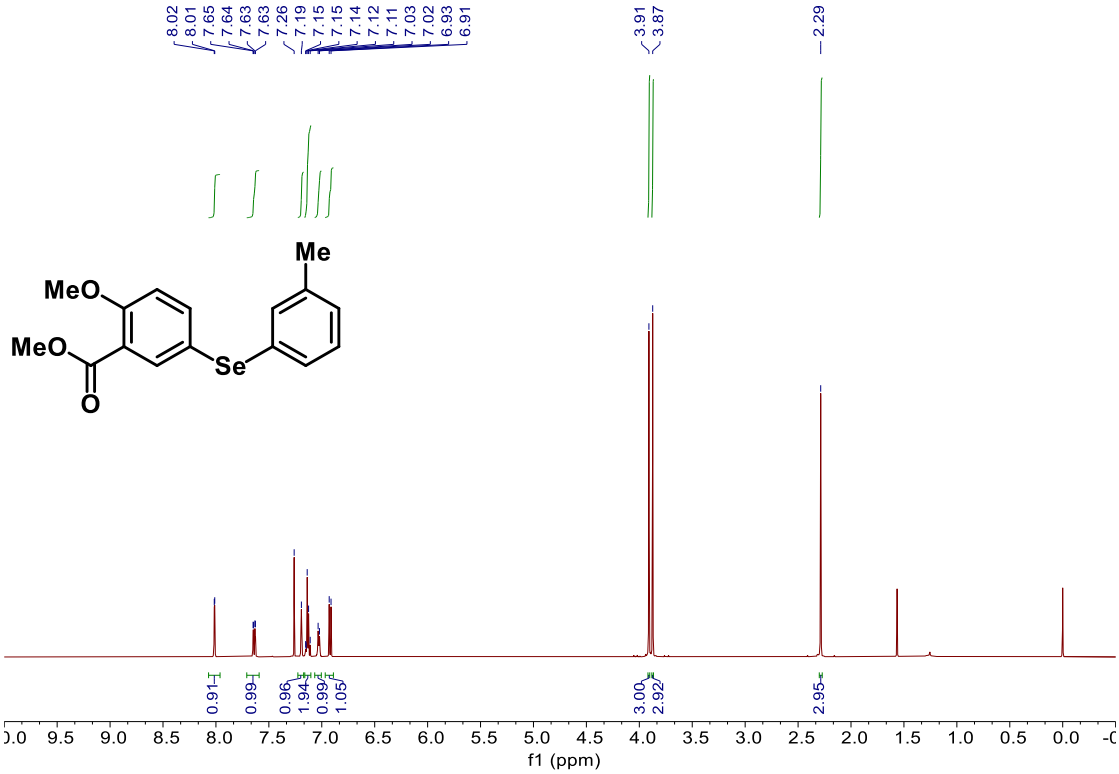
^{1}H NMR of compound 8 (500 MHz in $CDCl_3$)



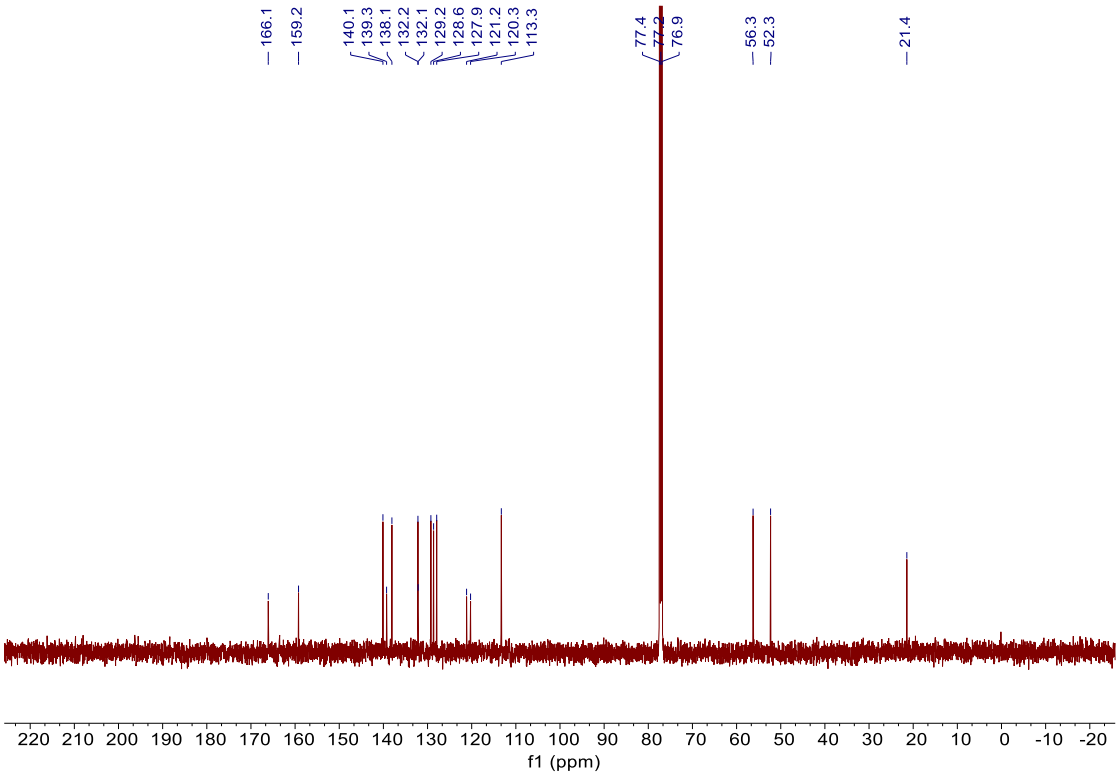
^{13}C NMR of compound 8 (101 MHz in $CDCl_3$)



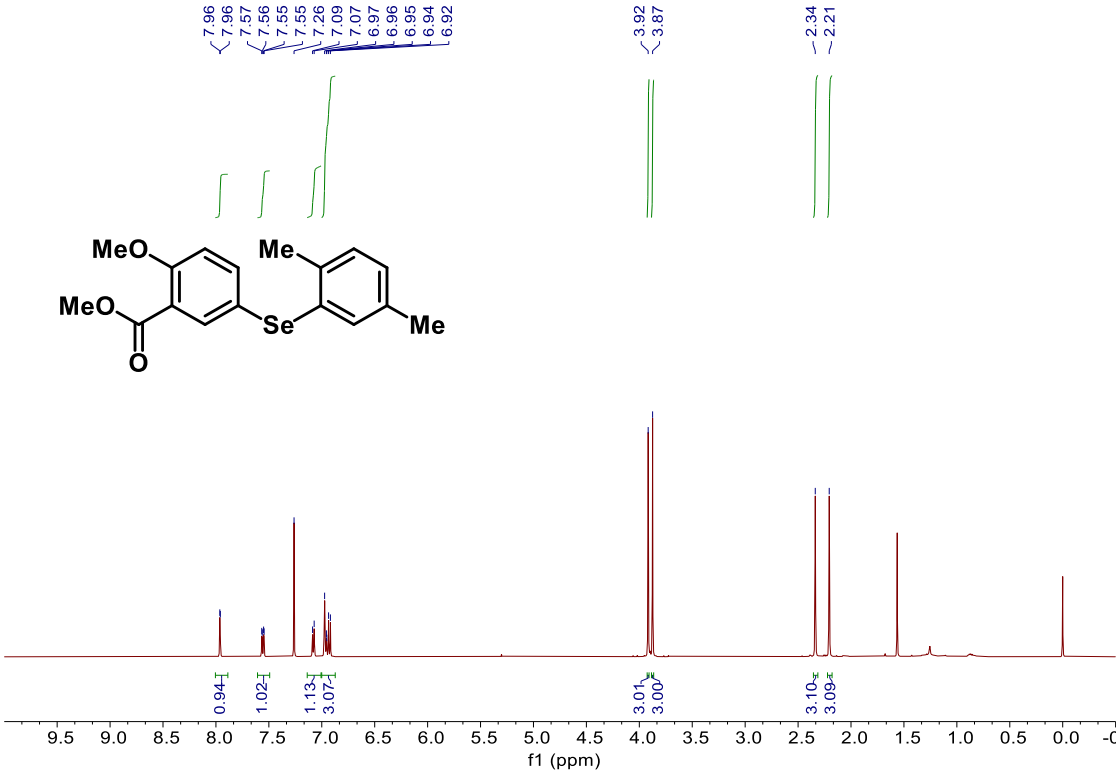
^{1}H NMR of compound 9 (500 MHz in $CDCl_3$)



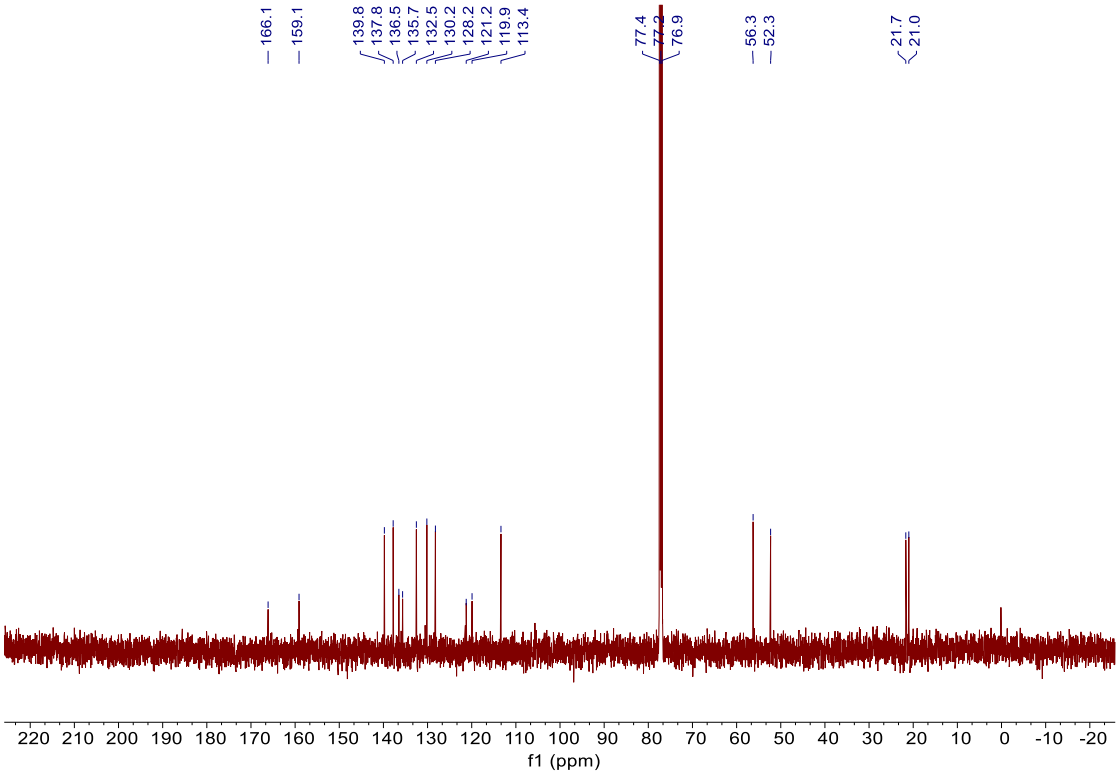
^{13}C NMR of compound 9 (126 MHz in $CDCl_3$)



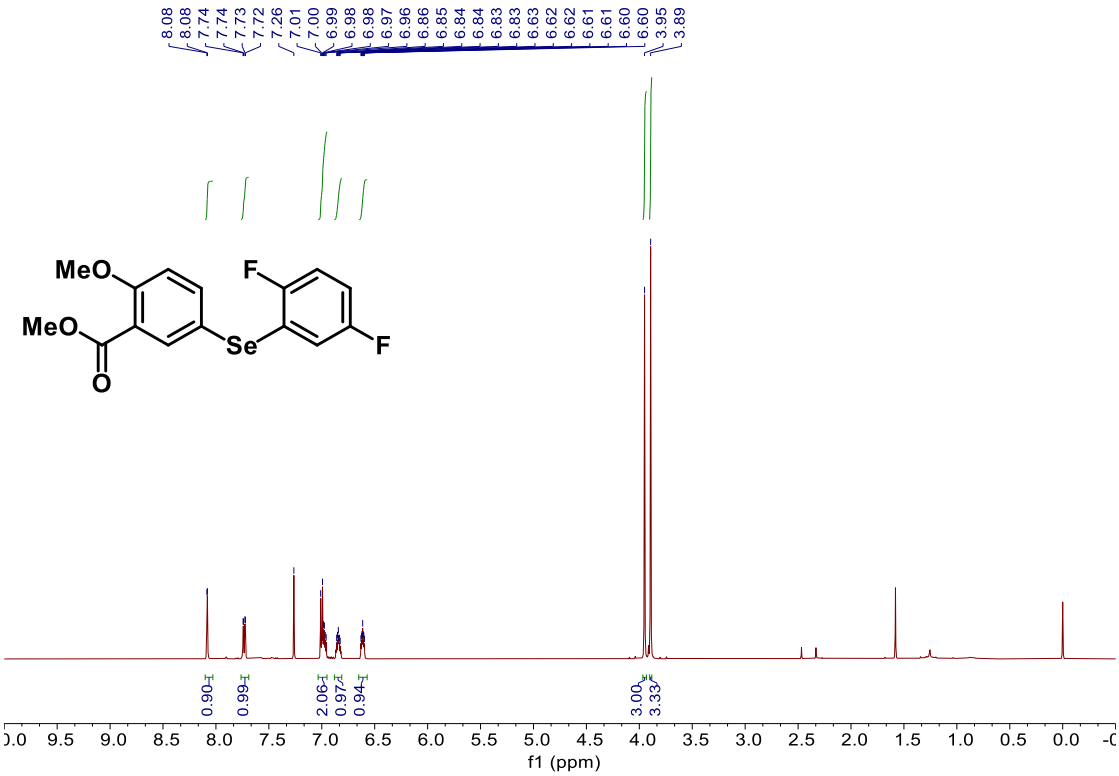
^{1}H NMR of compound 10 (500 MHz in $CDCl_3$)



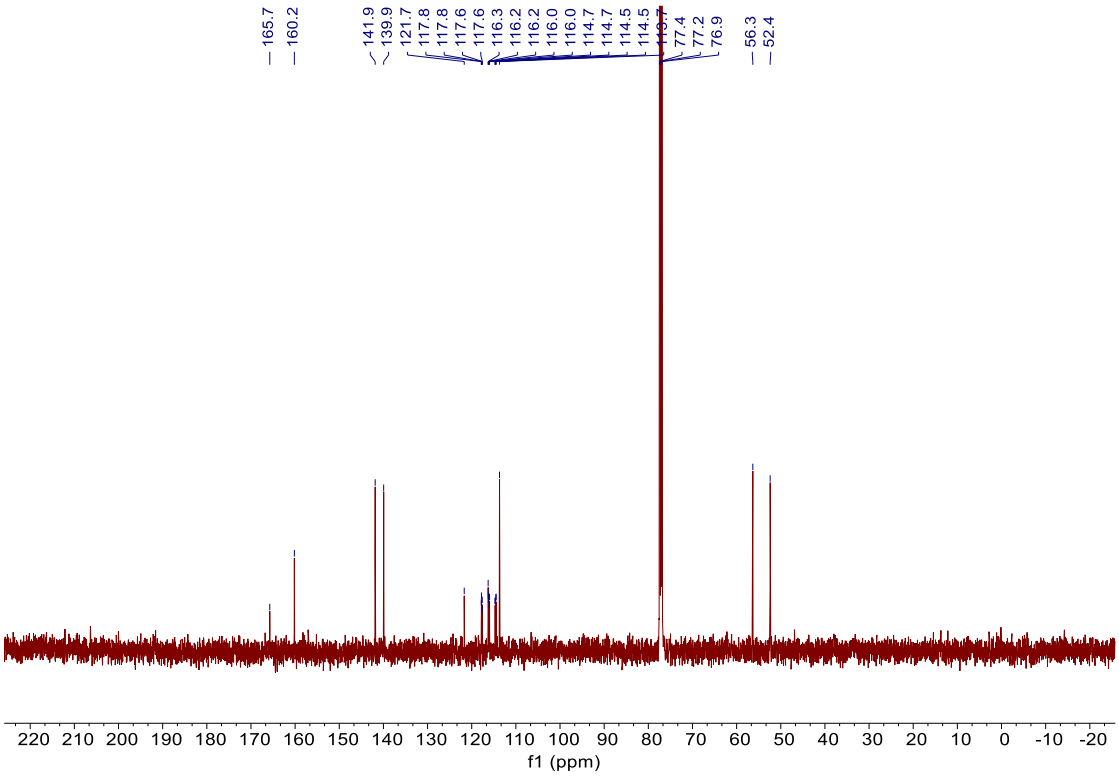
^{13}C NMR of compound 10 (126 MHz in $CDCl_3$)



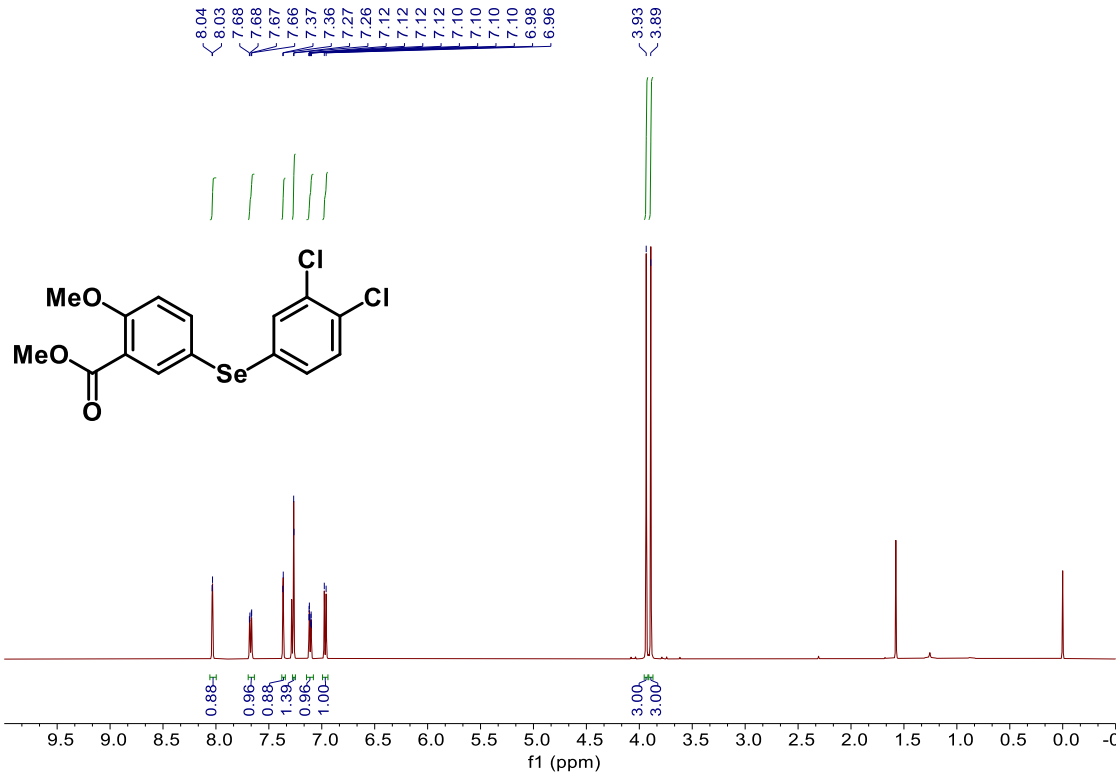
^{1}H NMR of compound 11 (500 MHz in $CDCl_3$)



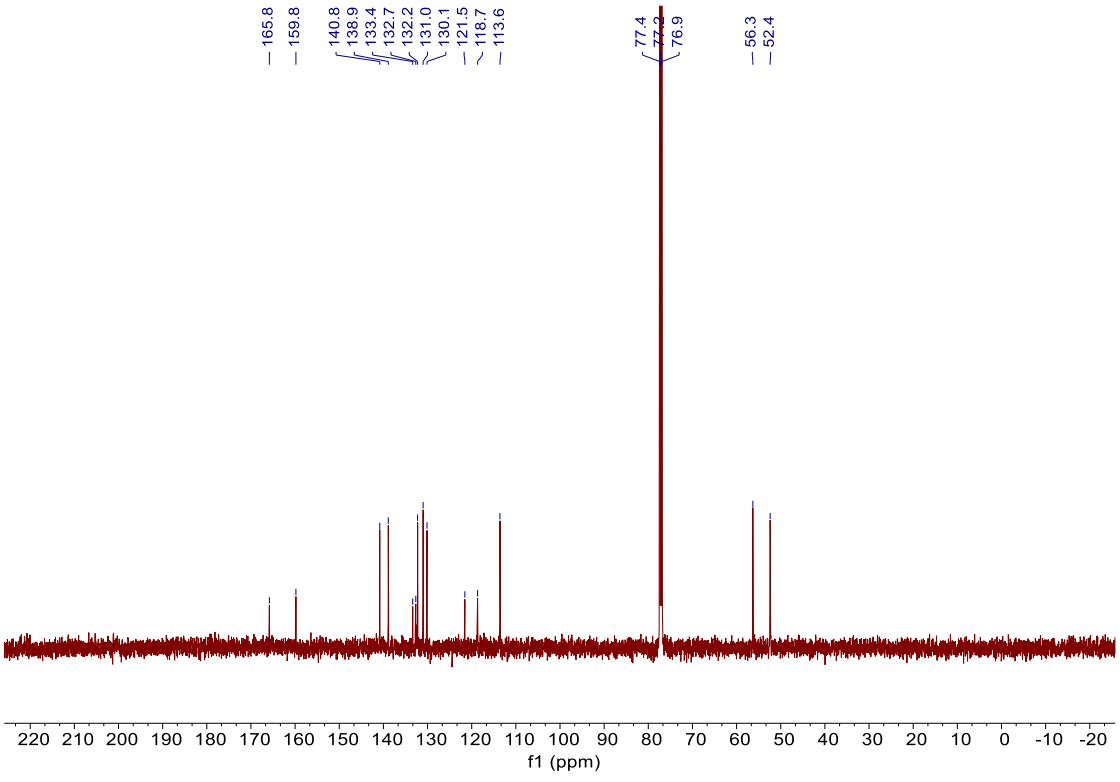
^{13}C NMR of compound 11 (126 MHz in $CDCl_3$)



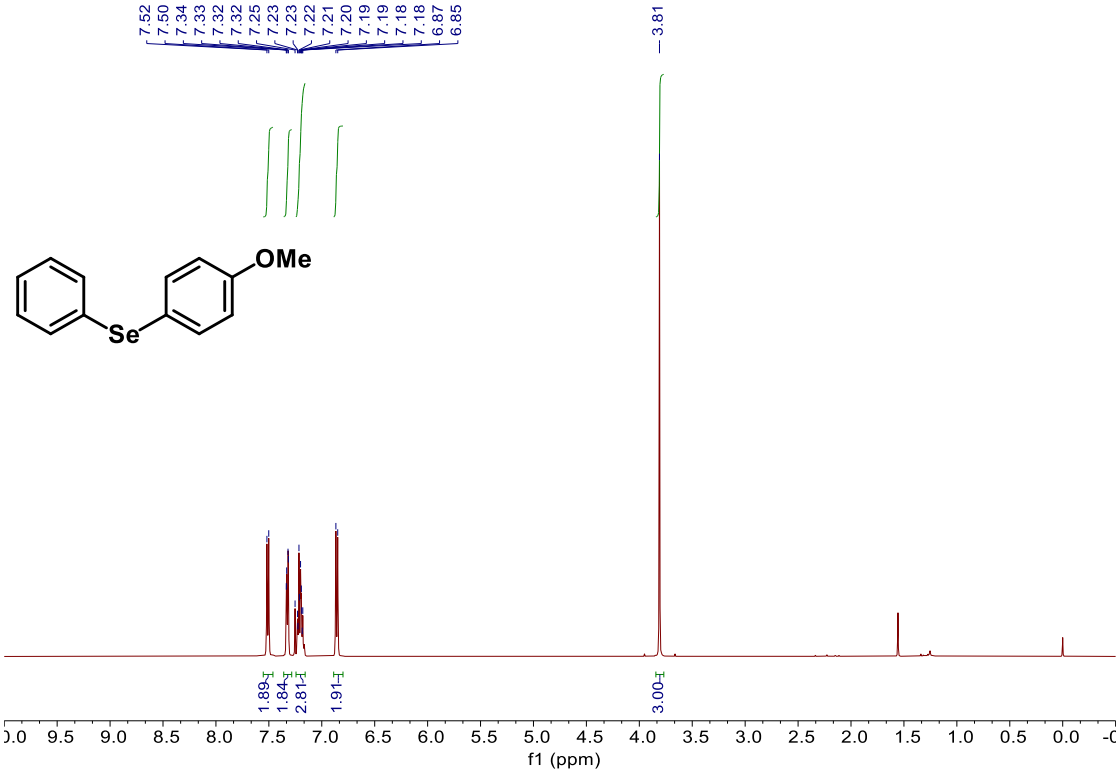
^{1}H NMR of compound 12 (500 MHz in $CDCl_3$)



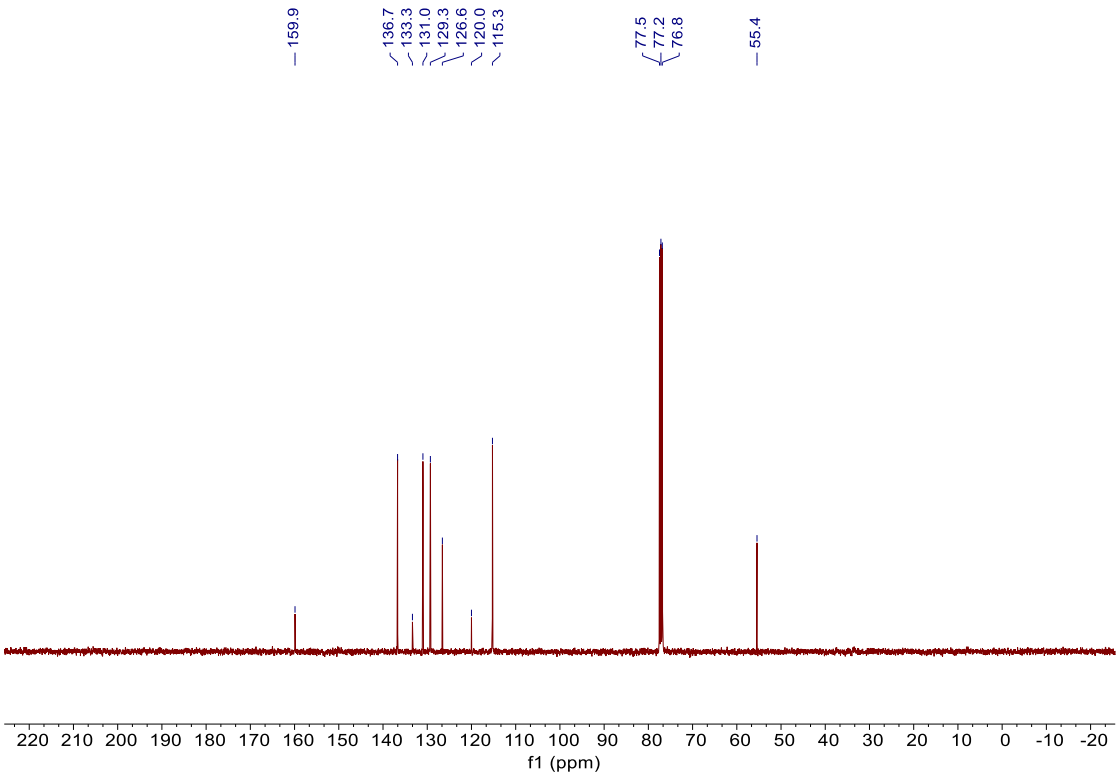
^{13}C NMR of compound 12 (126 MHz in $CDCl_3$)



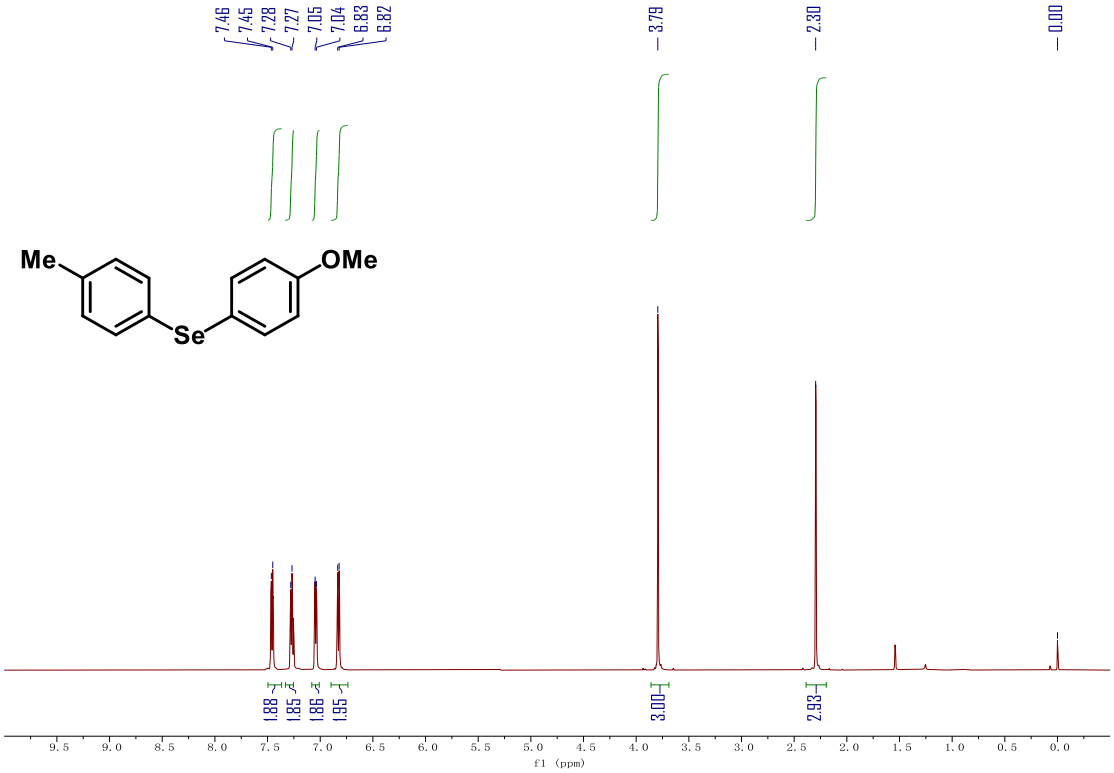
^{1}H NMR of compound 13 (500 MHz in $CDCl_3$)



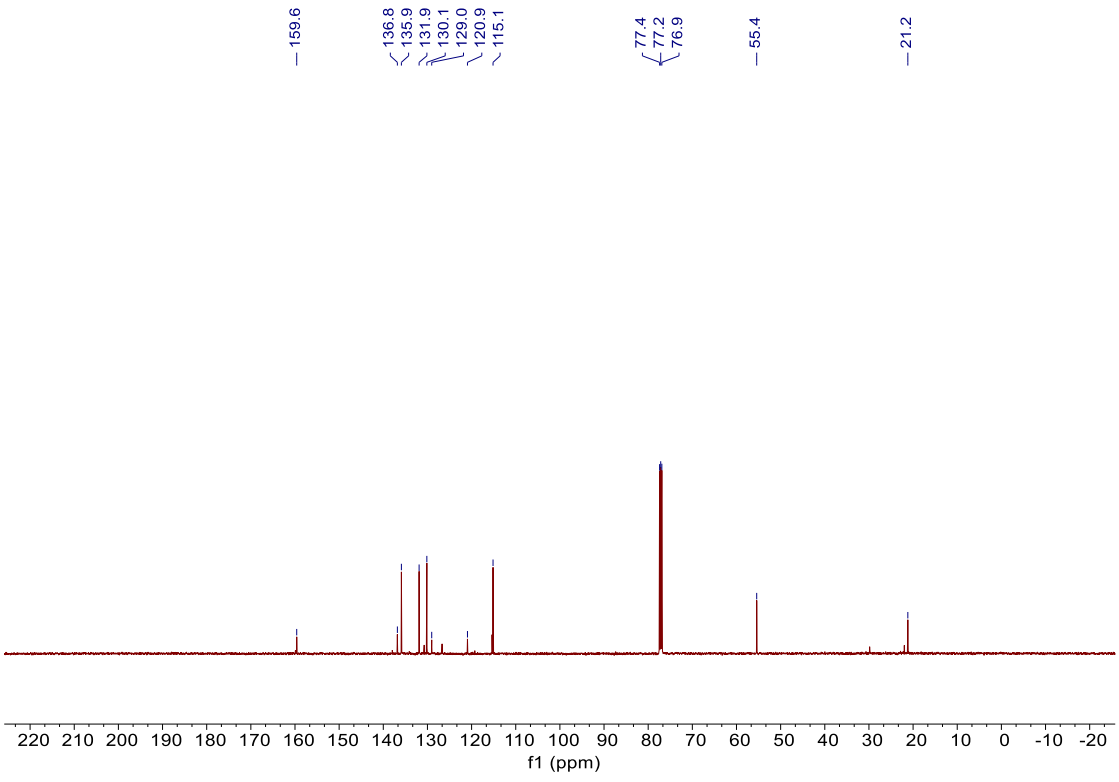
^{13}C NMR of compound 13 (126 MHz in $CDCl_3$)



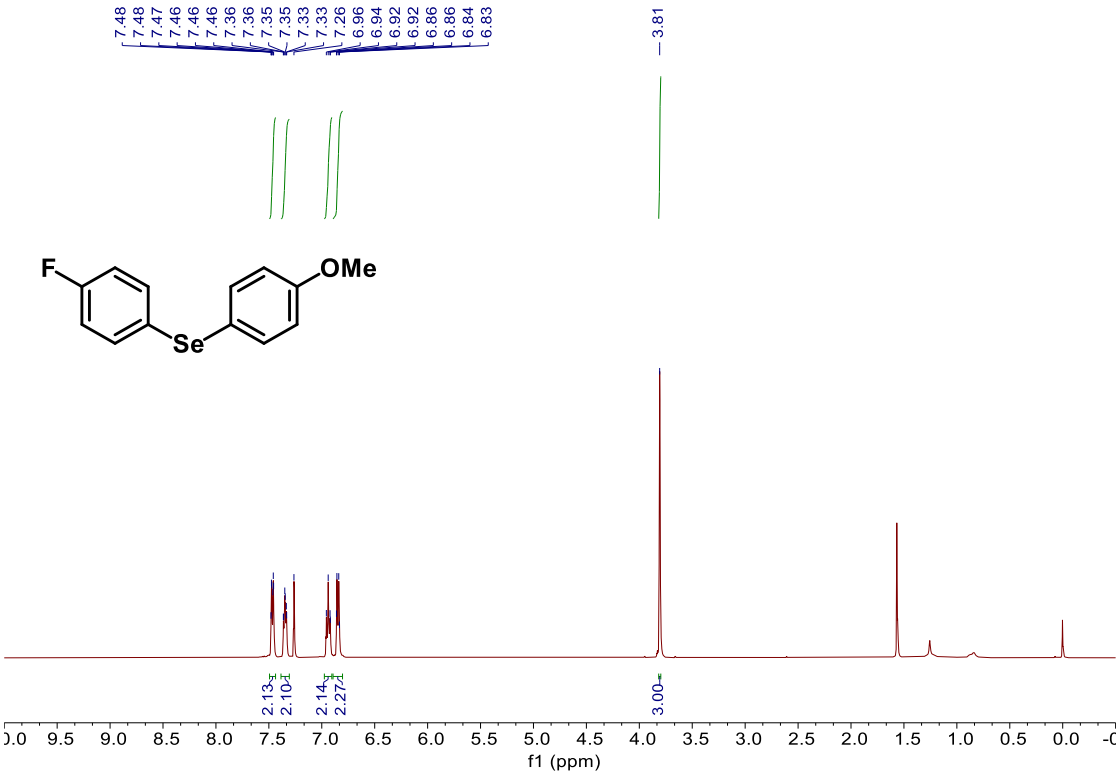
^{1}H NMR of compound 14 (500 MHz in $CDCl_3$)



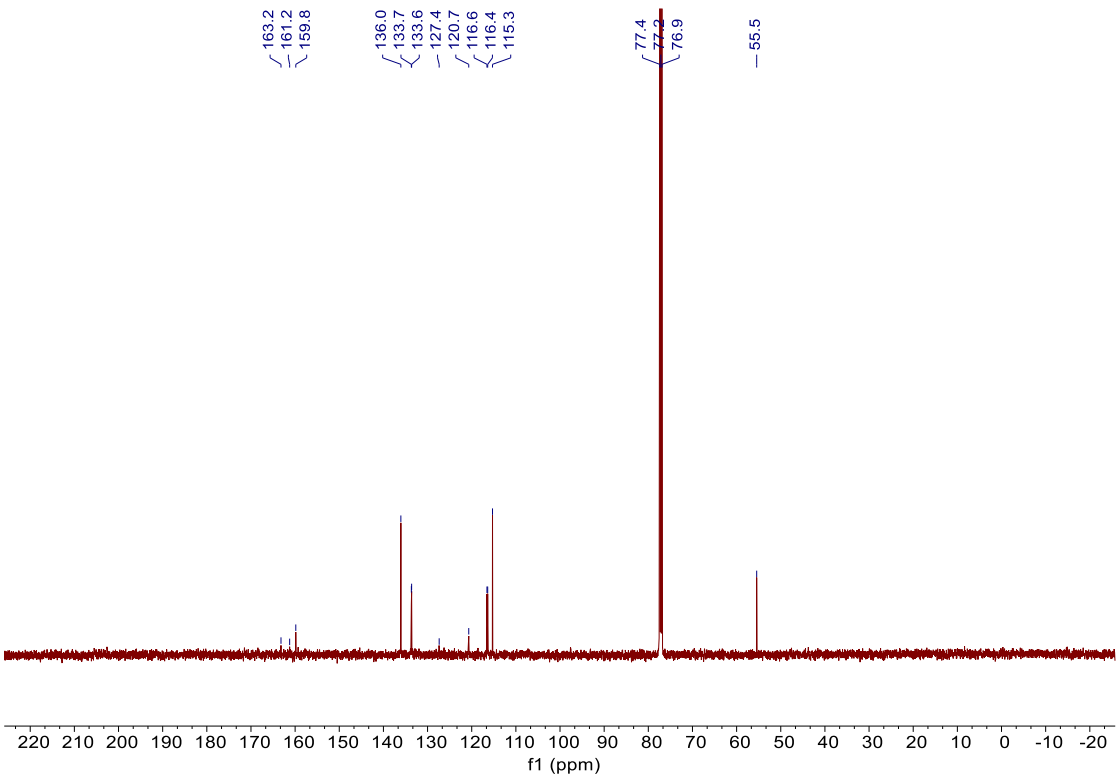
^{13}C NMR of compound 14 (126 MHz in $CDCl_3$)



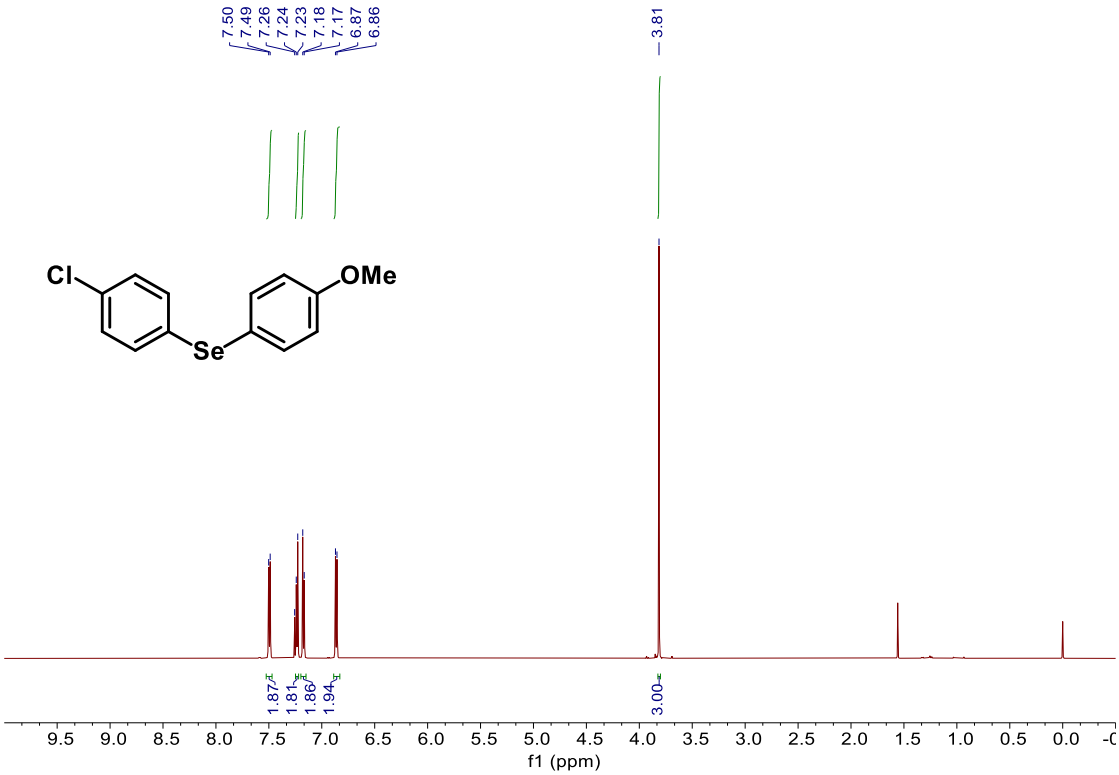
^{1}H NMR of compound 15 (500 MHz in $CDCl_3$)



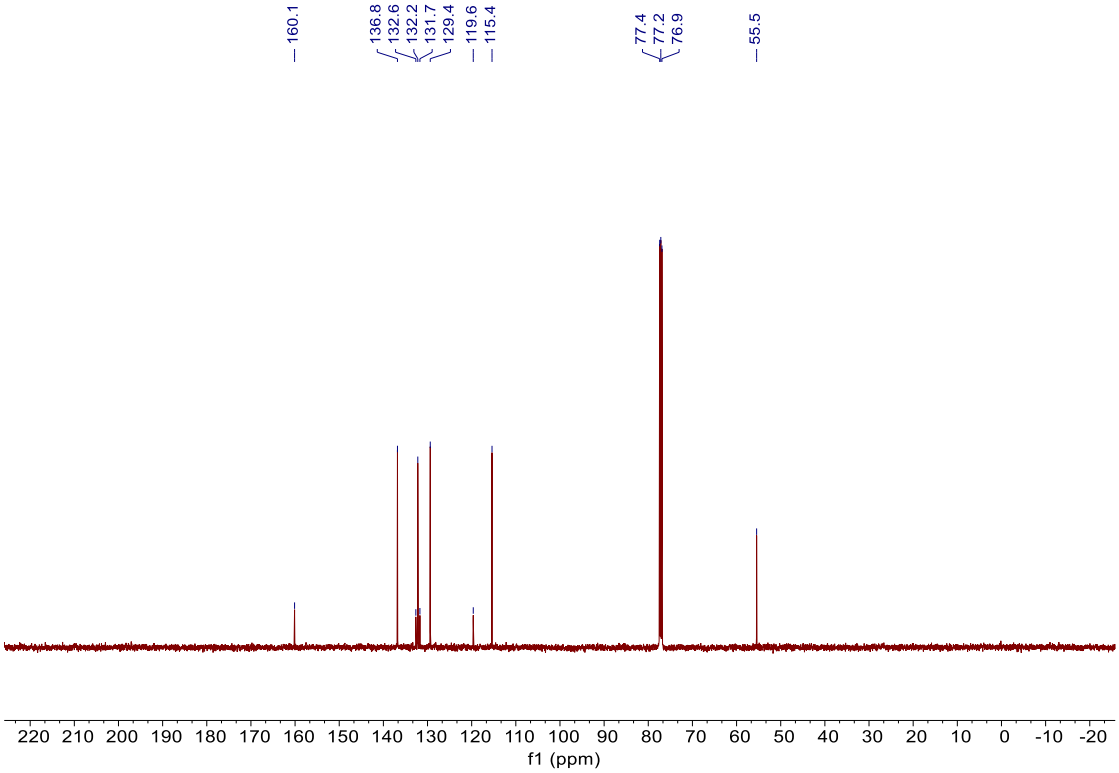
^{13}C NMR of compound 15 (126 MHz in $CDCl_3$)



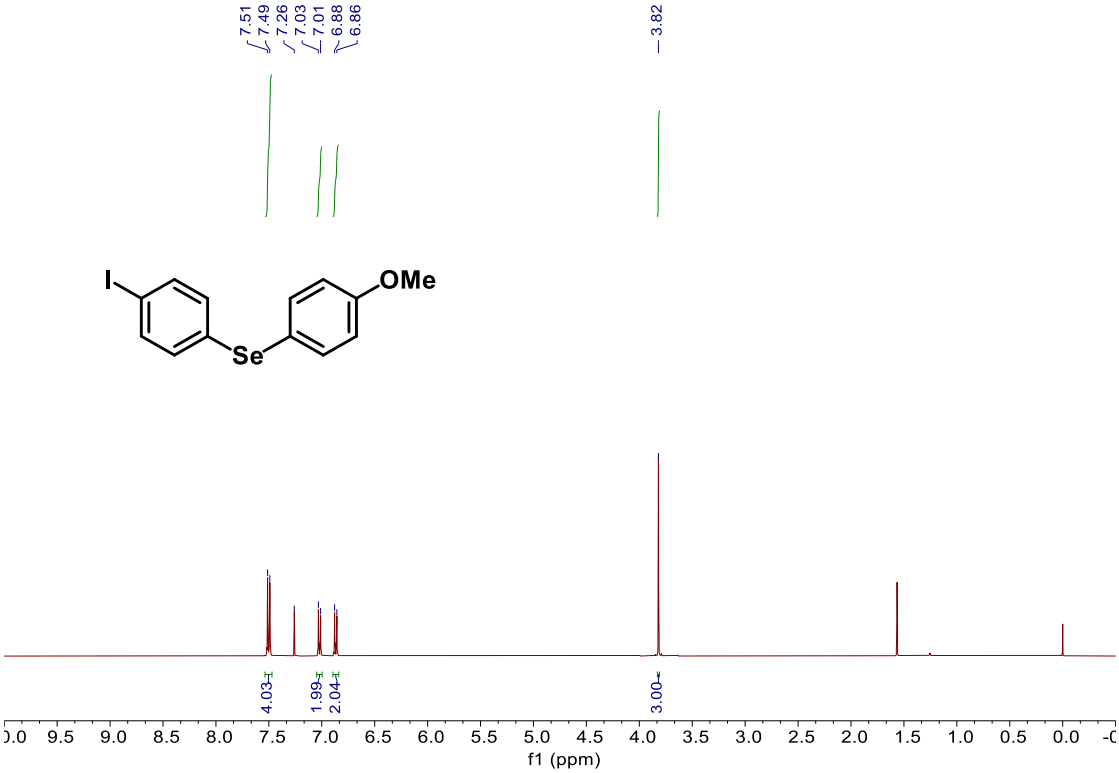
^{1}H NMR of compound 16 (600 MHz in $CDCl_3$)



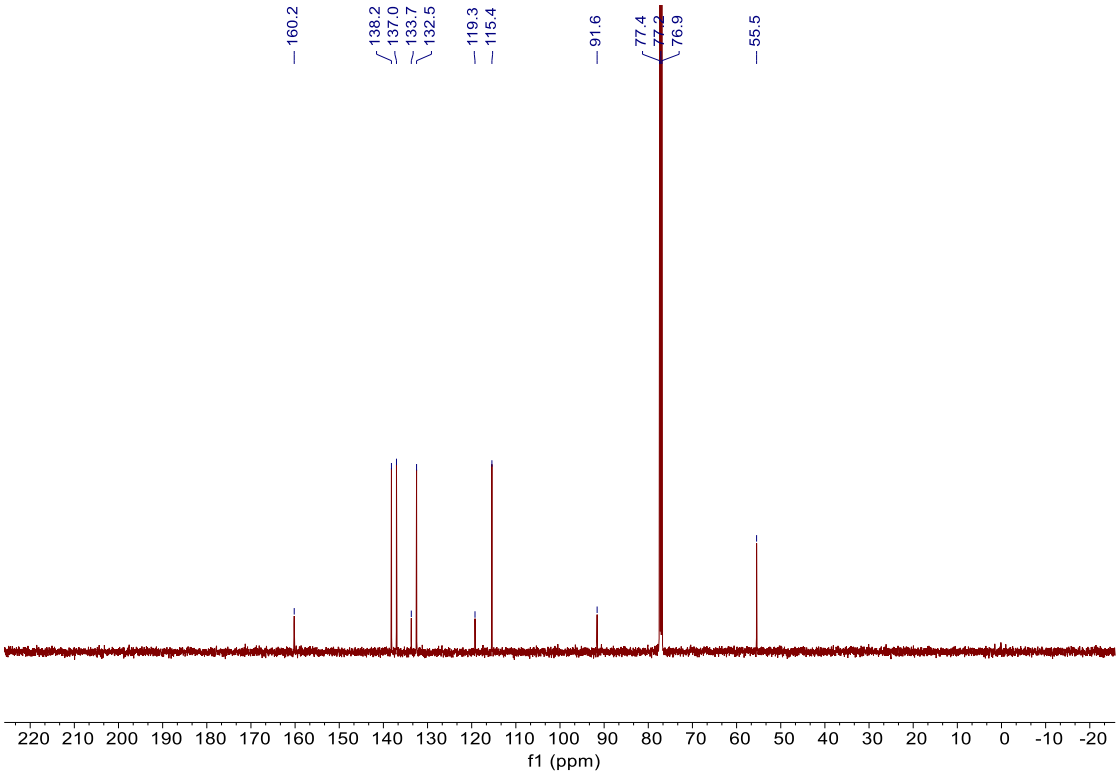
^{13}C NMR of compound 16 (126 MHz in $CDCl_3$)



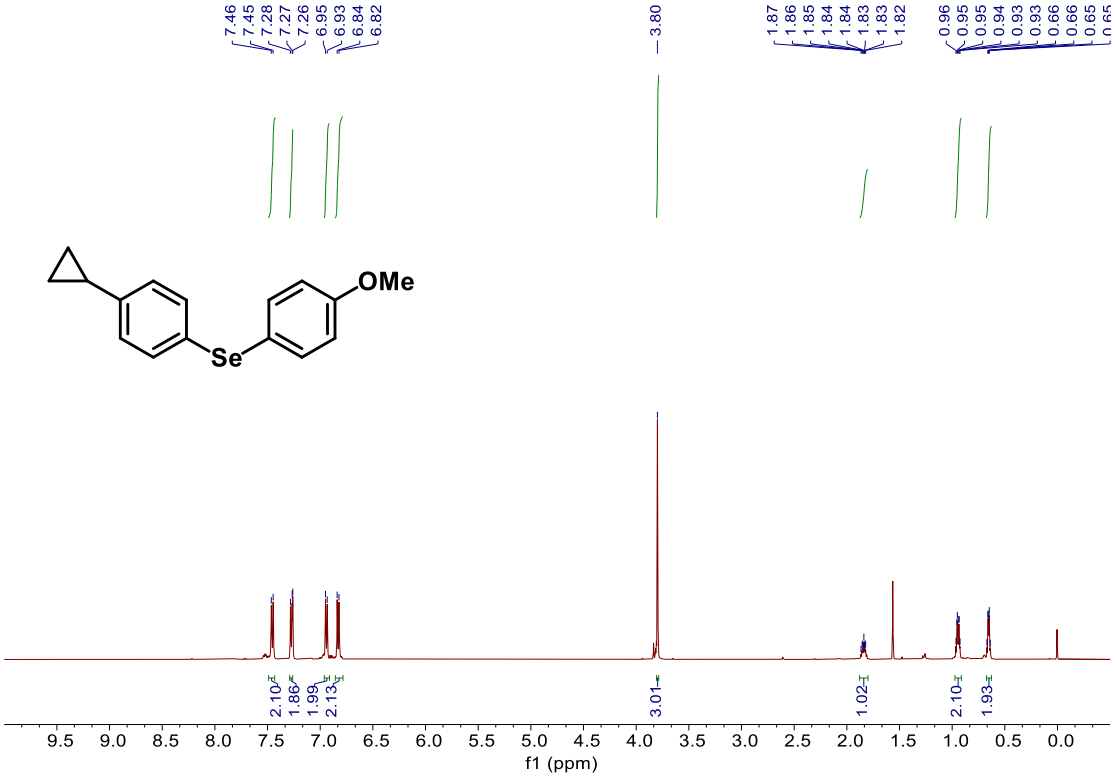
^{1}H NMR of compound 17 (400 MHz in $CDCl_3$)



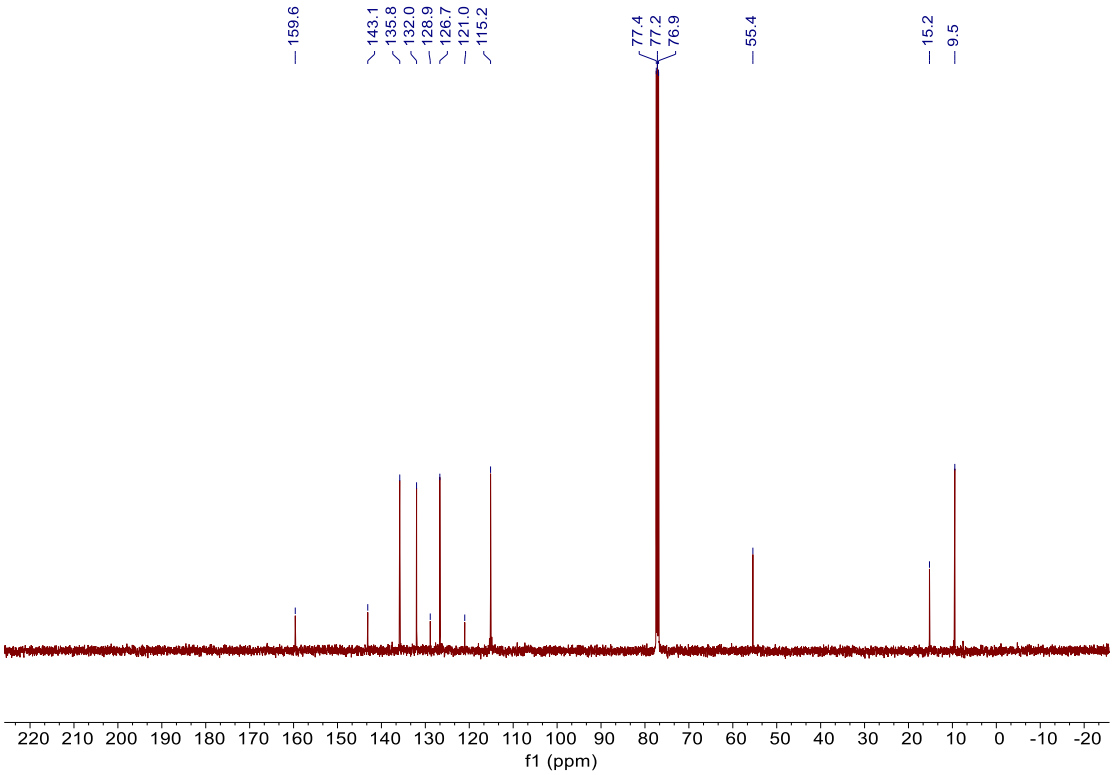
^{13}C NMR of compound 17 (126 MHz in $CDCl_3$)



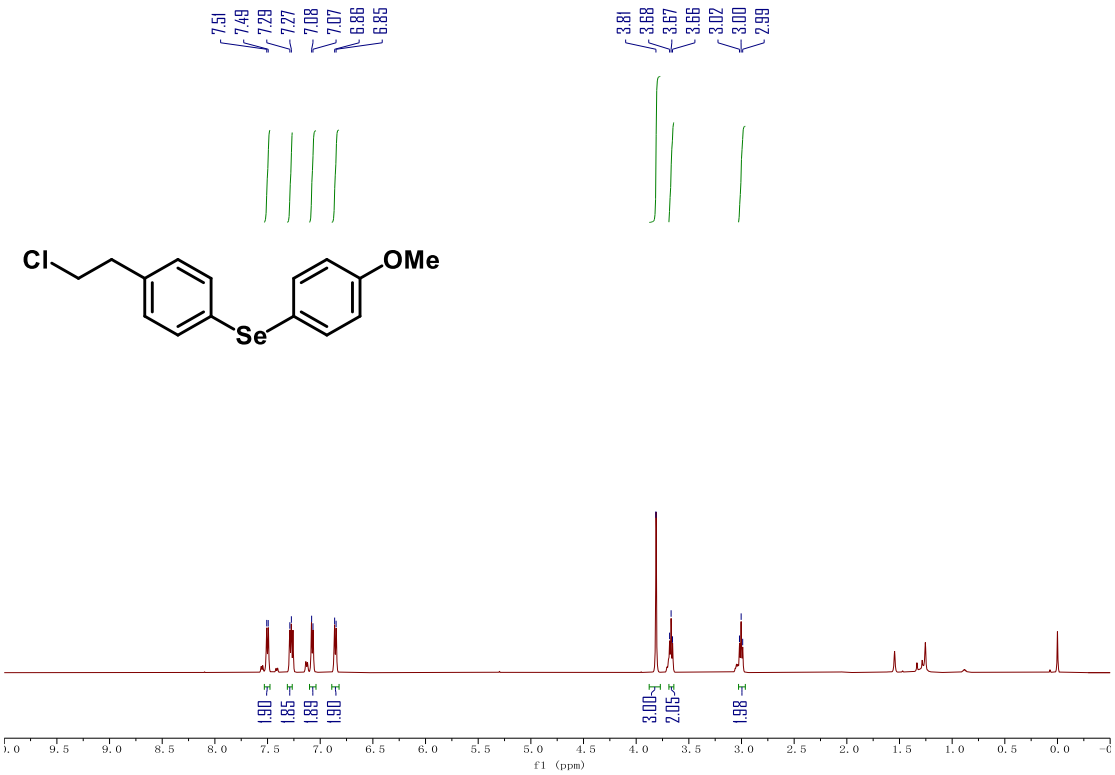
^{1}H NMR of compound 18 (500 MHz in $CDCl_3$)



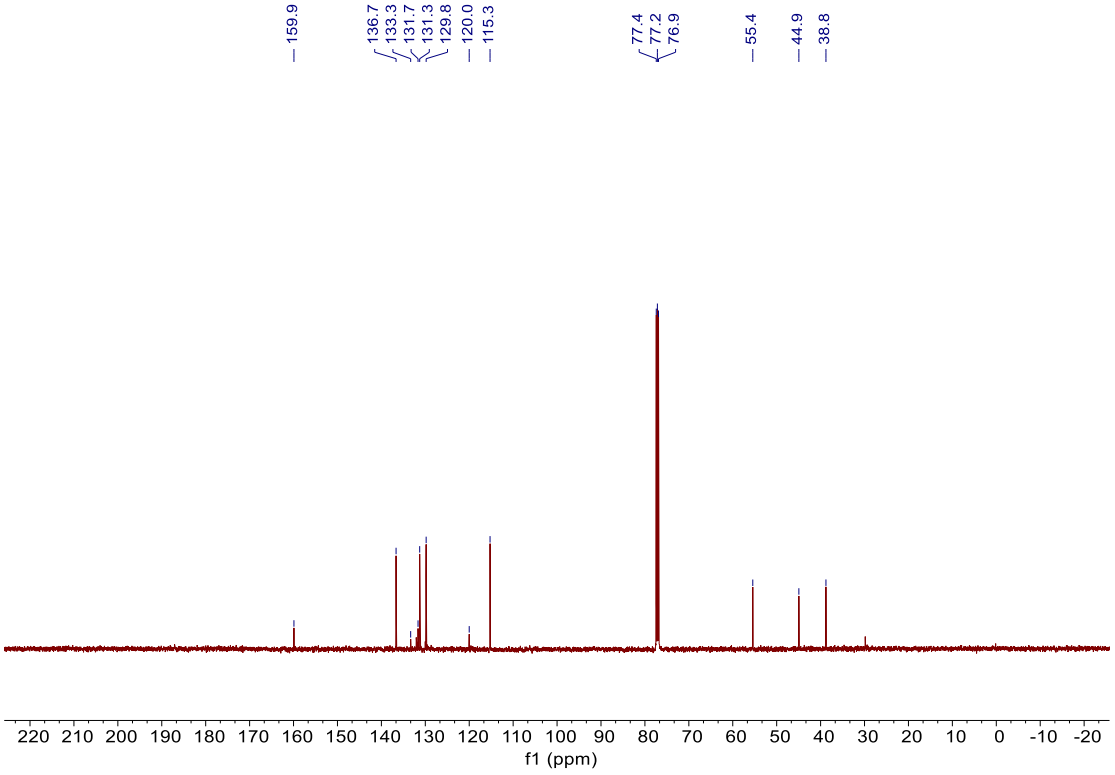
^{13}C NMR of compound 18 (126 MHz in $CDCl_3$)



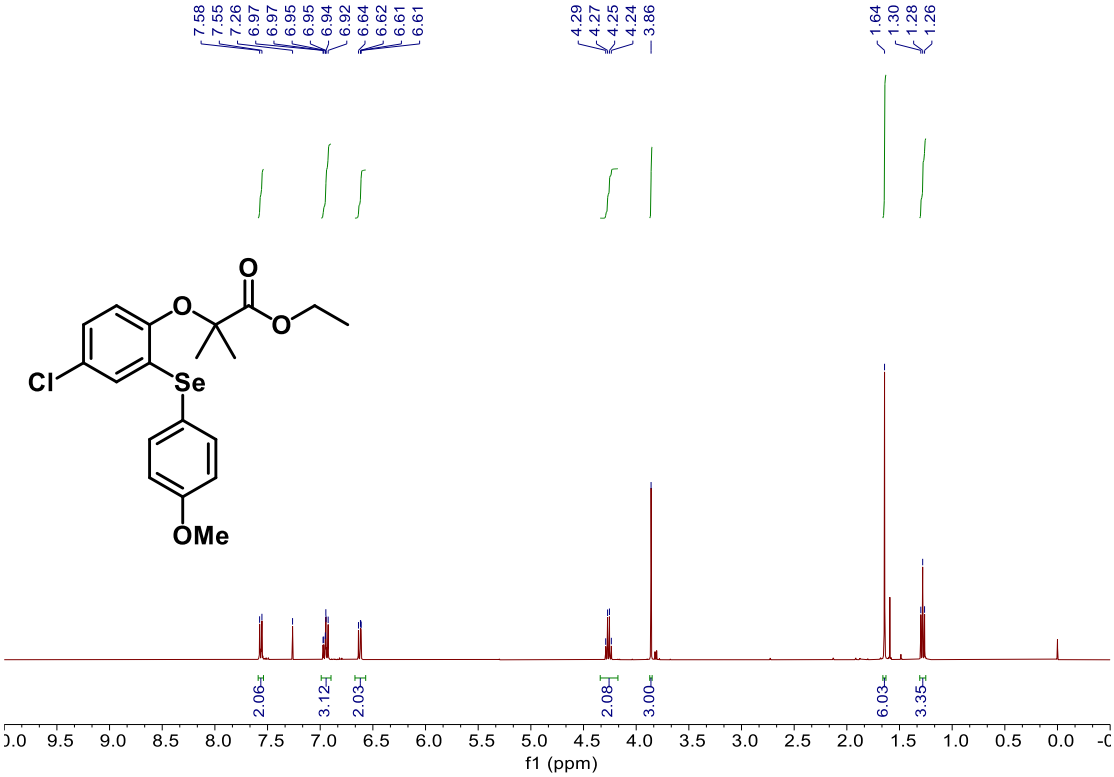
^{1}H NMR of compound 19 (500 MHz in $CDCl_3$)



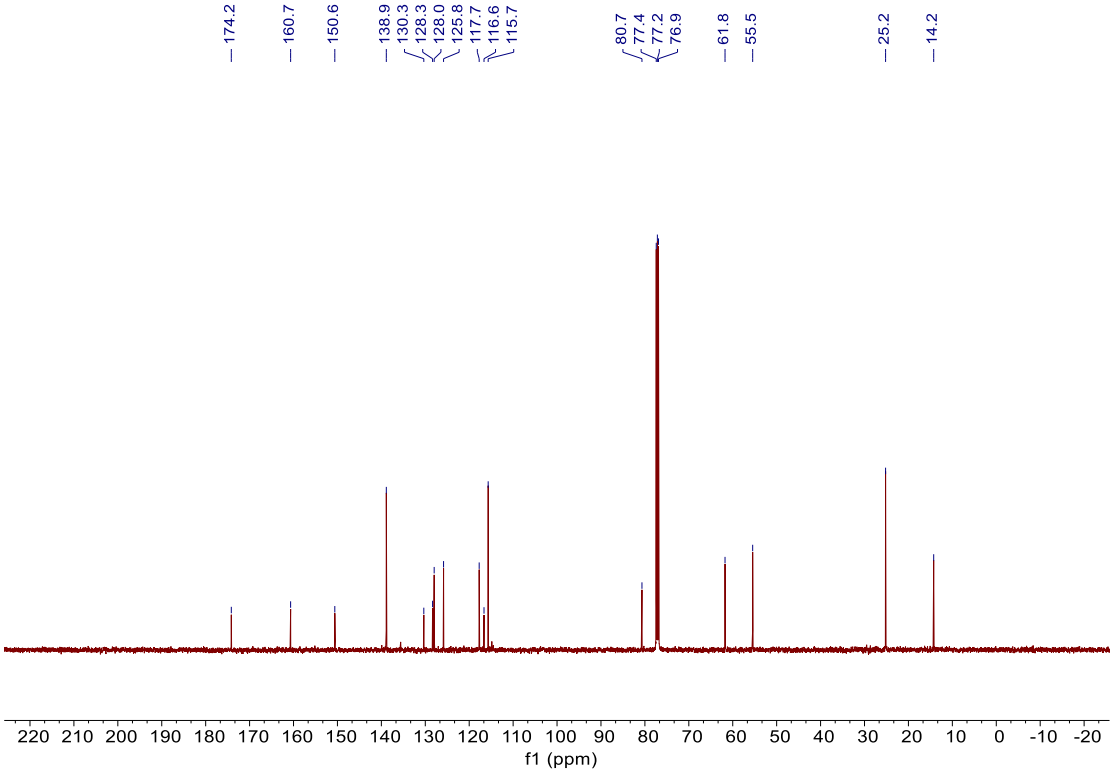
^{13}C NMR of compound 19 (126 MHz in $CDCl_3$)



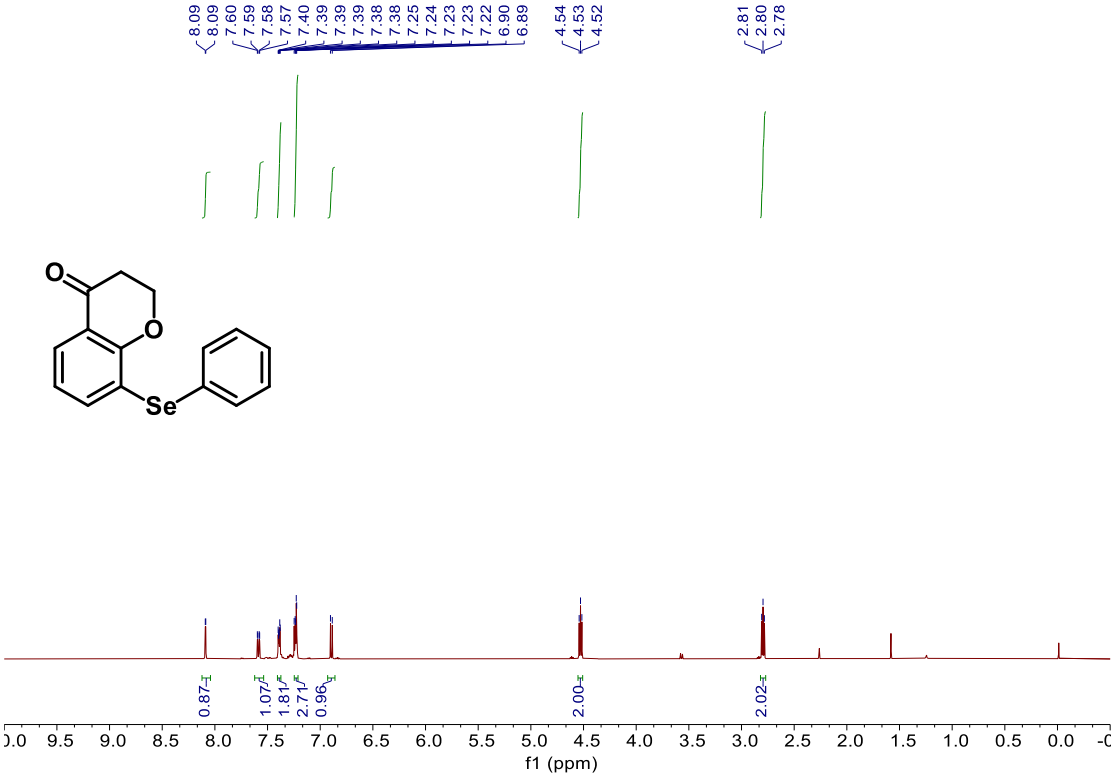
^{1}H NMR of compound 20 (400 MHz in $CDCl_3$)



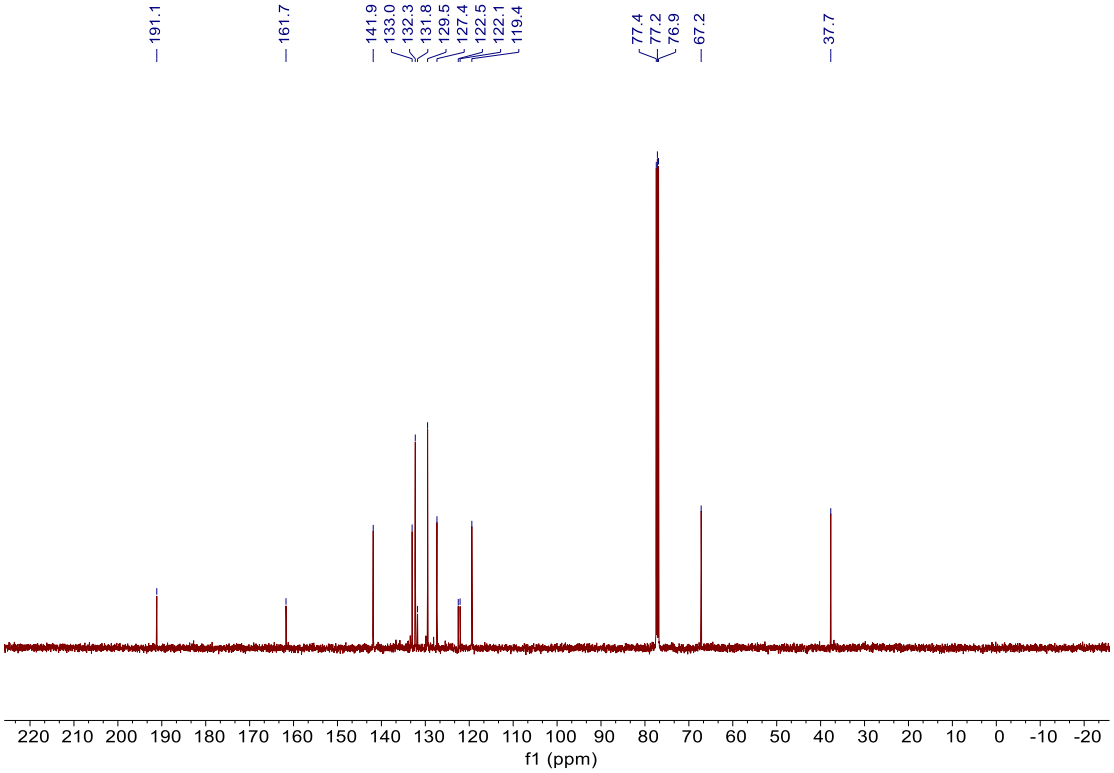
^{13}C NMR of compound 20 (126 MHz in $CDCl_3$)



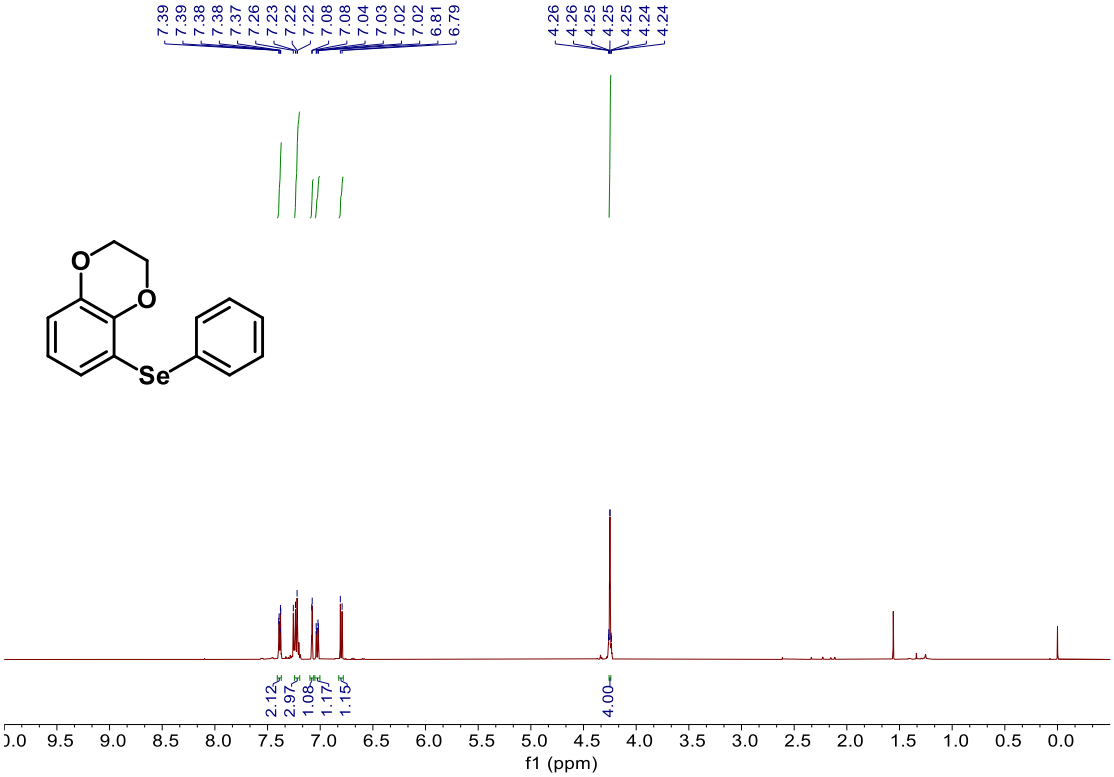
^{1}H NMR of compound 21 (500 MHz in $CDCl_3$)



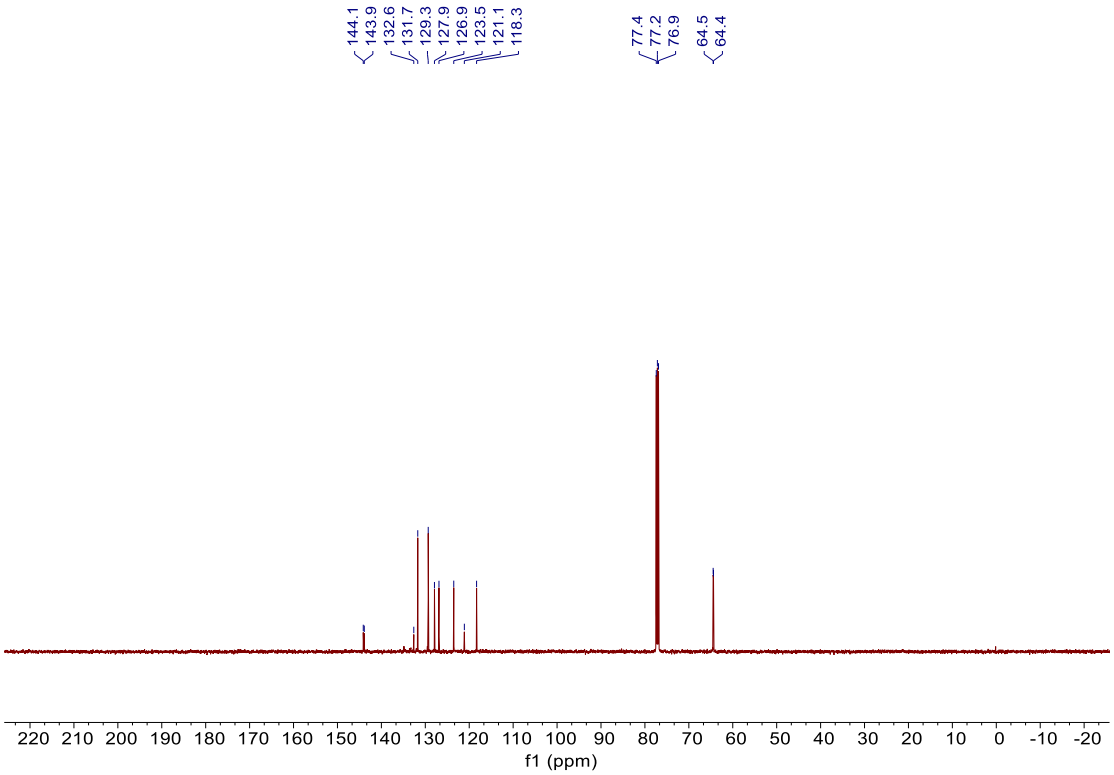
^{13}C NMR of compound 21 (126 MHz in $CDCl_3$)



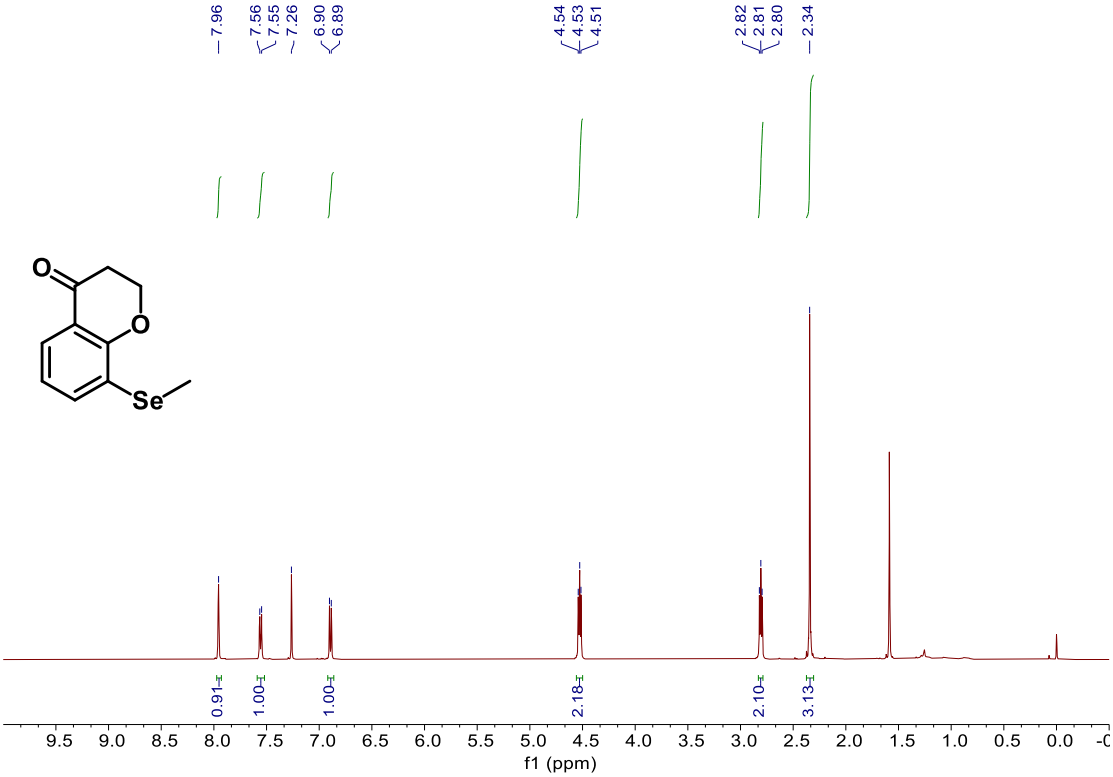
^{1}H NMR of compound 22 (500 MHz in $CDCl_3$)



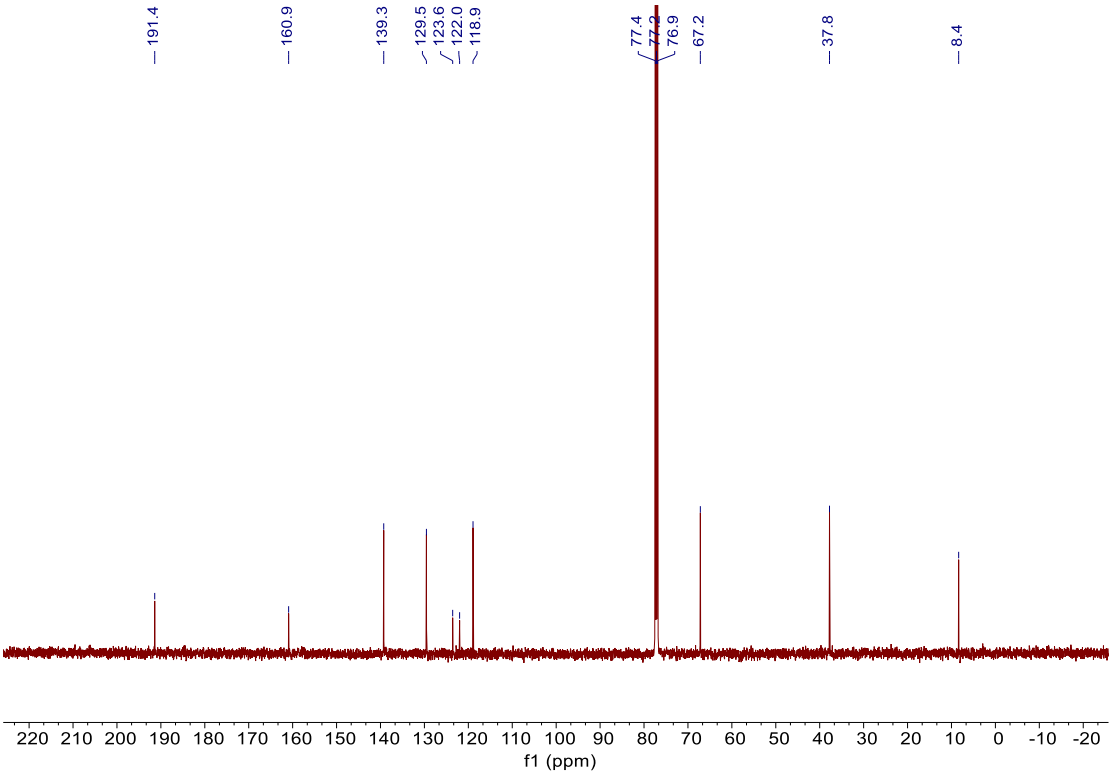
^{13}C NMR of compound 22 (126 MHz in $CDCl_3$)



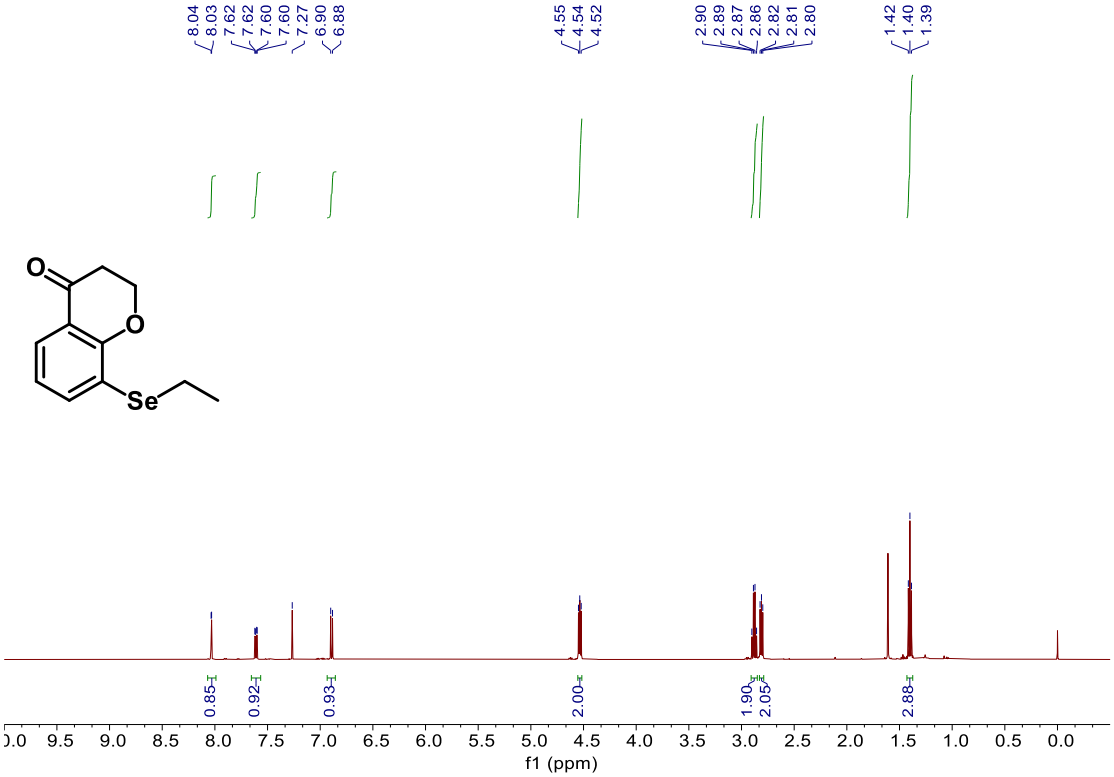
^{1}H NMR of compound 23 (500 MHz in $CDCl_3$)



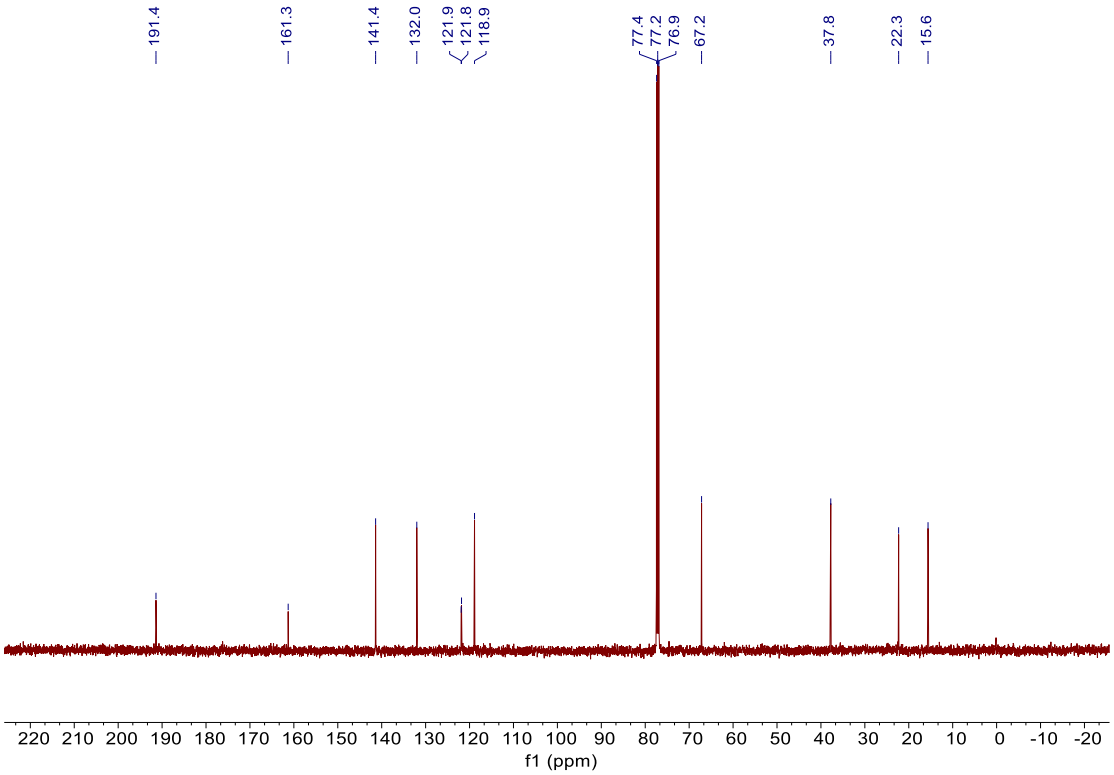
^{13}C NMR of compound 23 (126 MHz in $CDCl_3$)



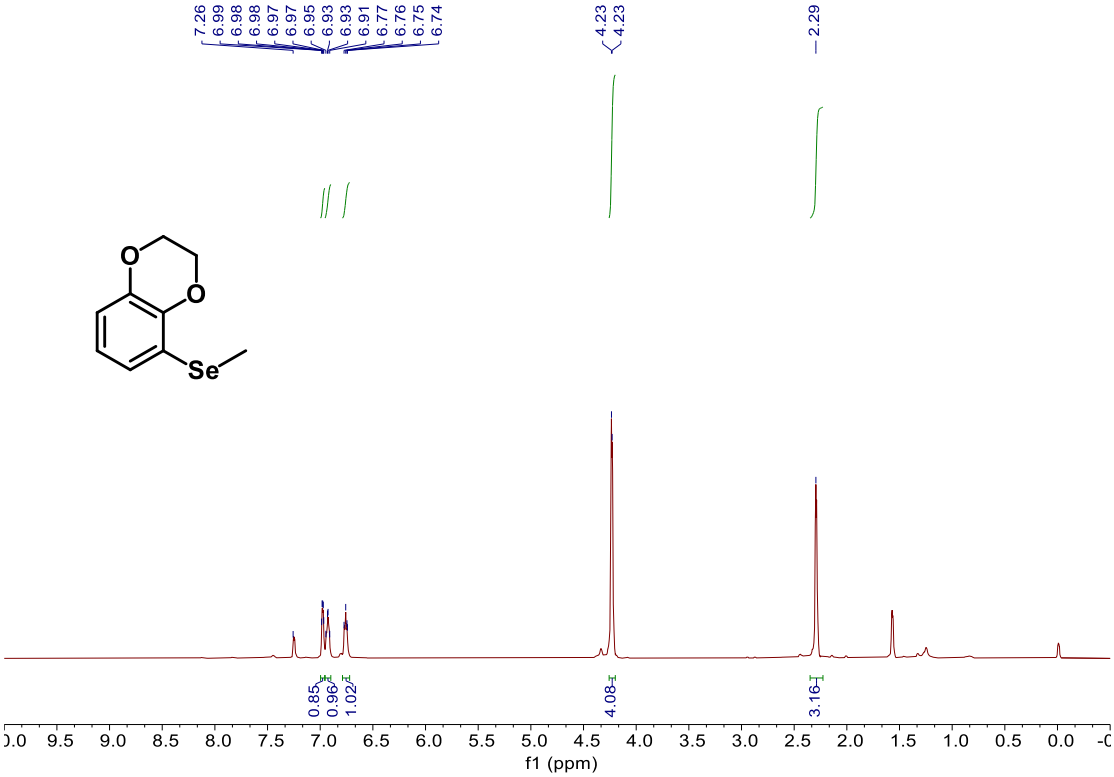
^{1}H NMR of compound 24 (500 MHz in $CDCl_3$)



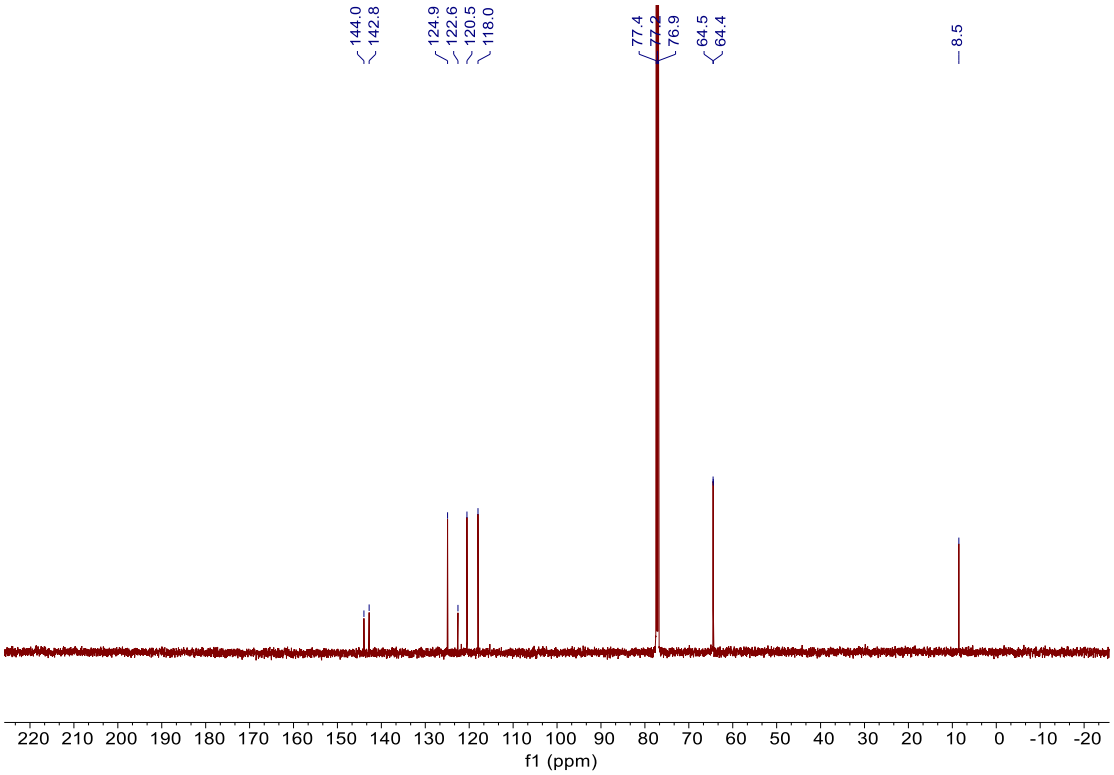
^{13}C NMR of compound 24 (126 MHz in $CDCl_3$)



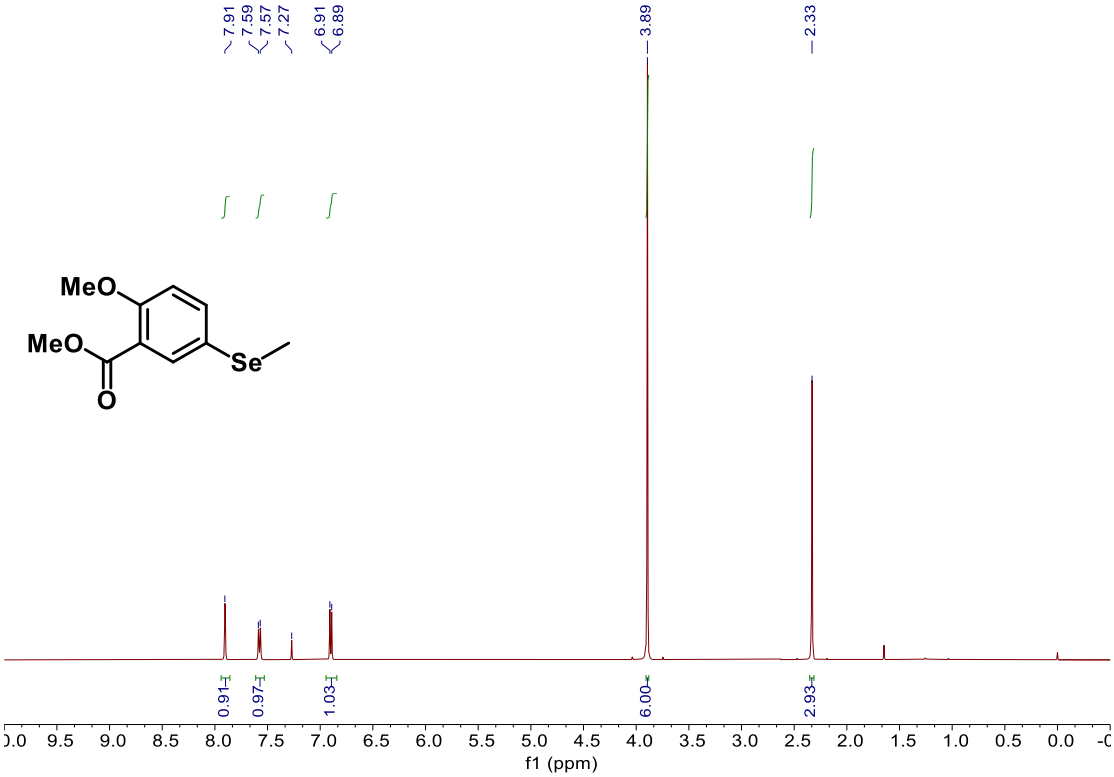
^{1}H NMR of compound 25 (500 MHz in $CDCl_3$)



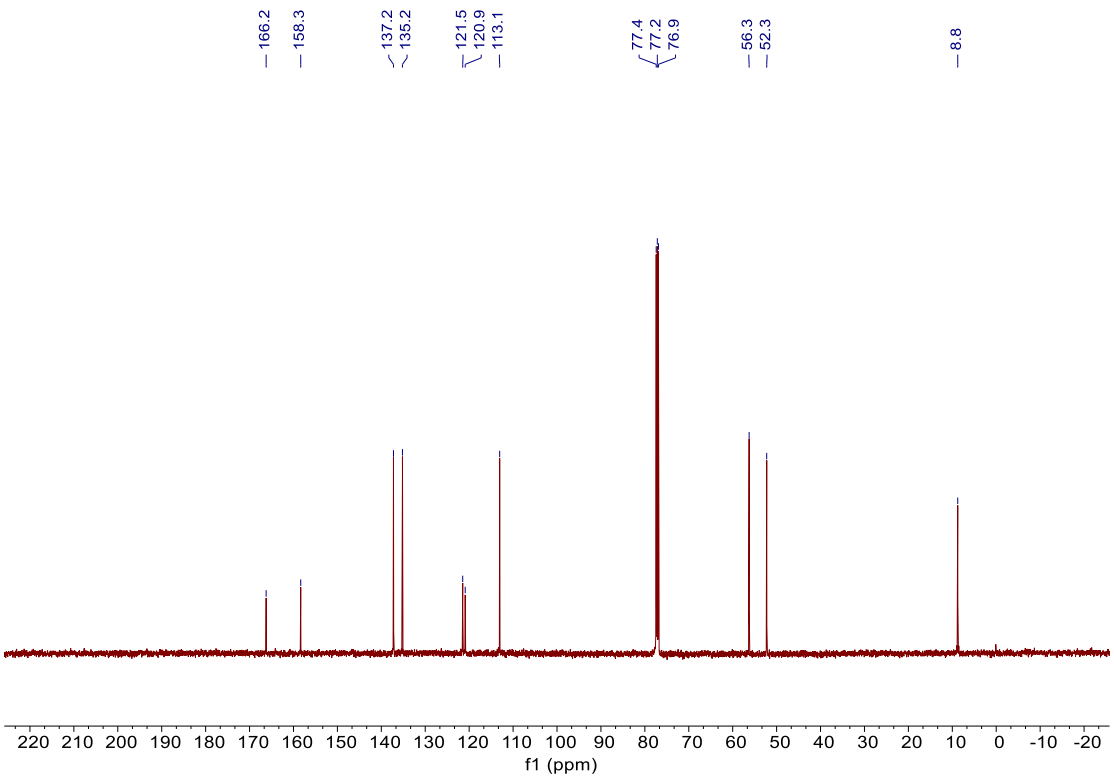
^{13}C NMR of compound 25 (126 MHz in $CDCl_3$)



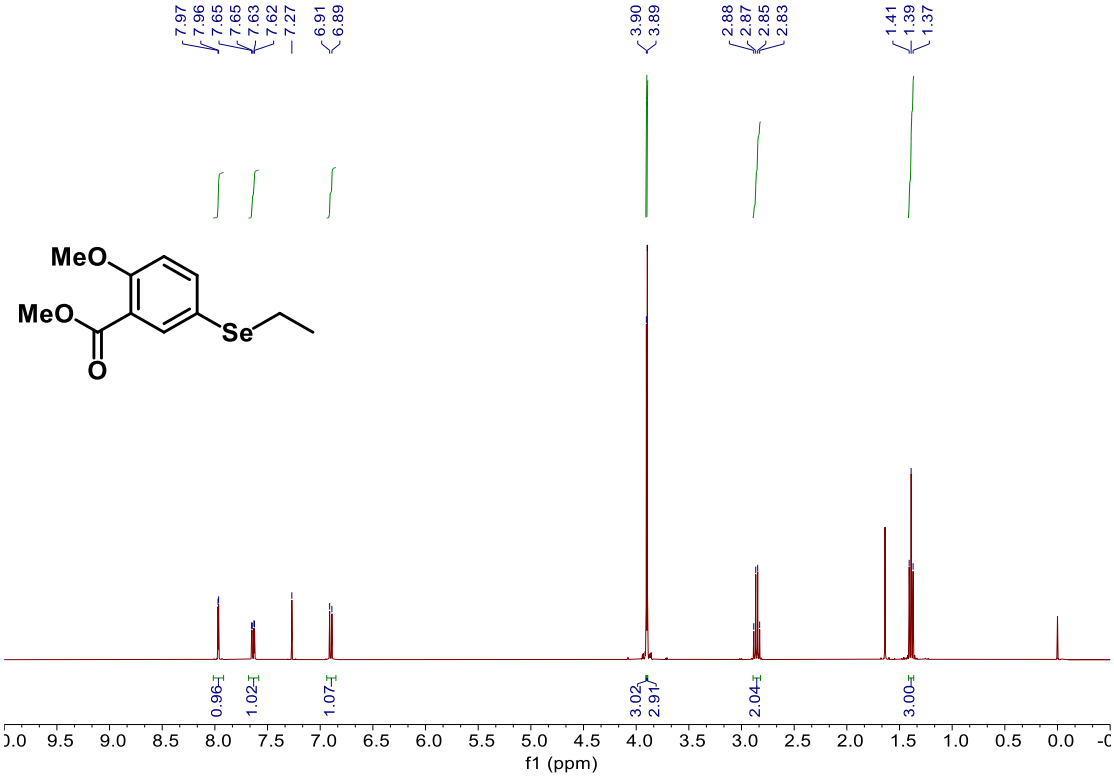
^{1}H NMR of compound 26 (500 MHz in $CDCl_3$)



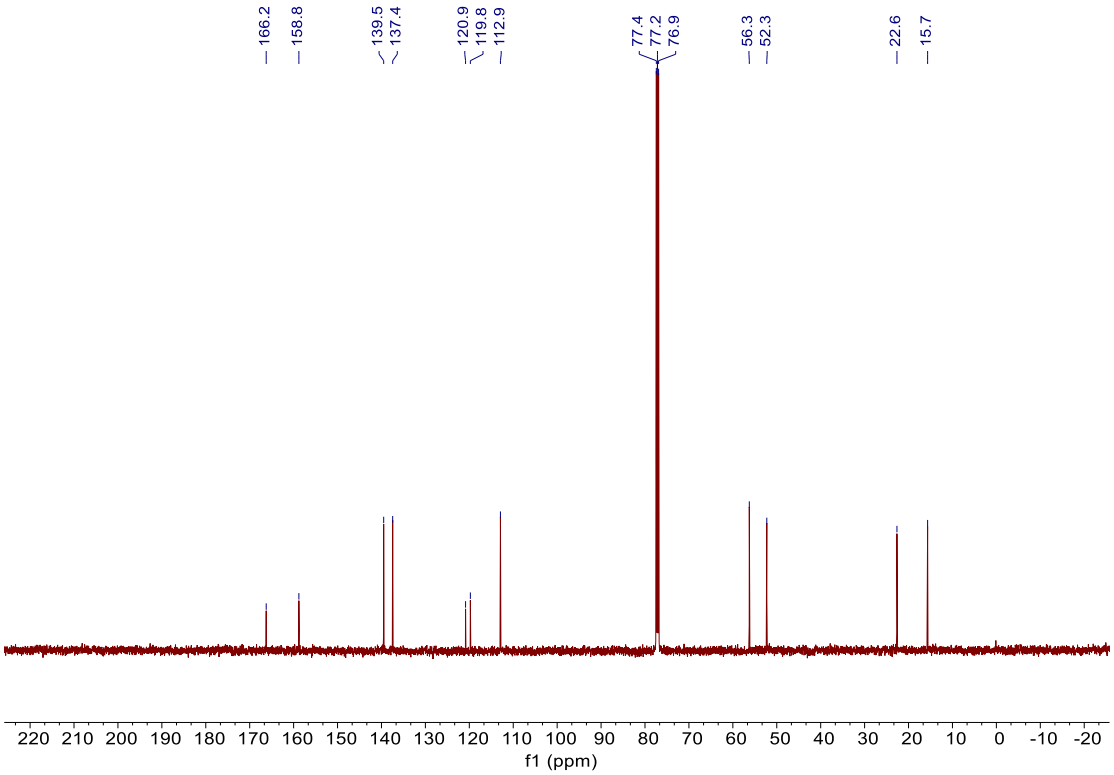
^{13}C NMR of compound 26 (126 MHz in $CDCl_3$)



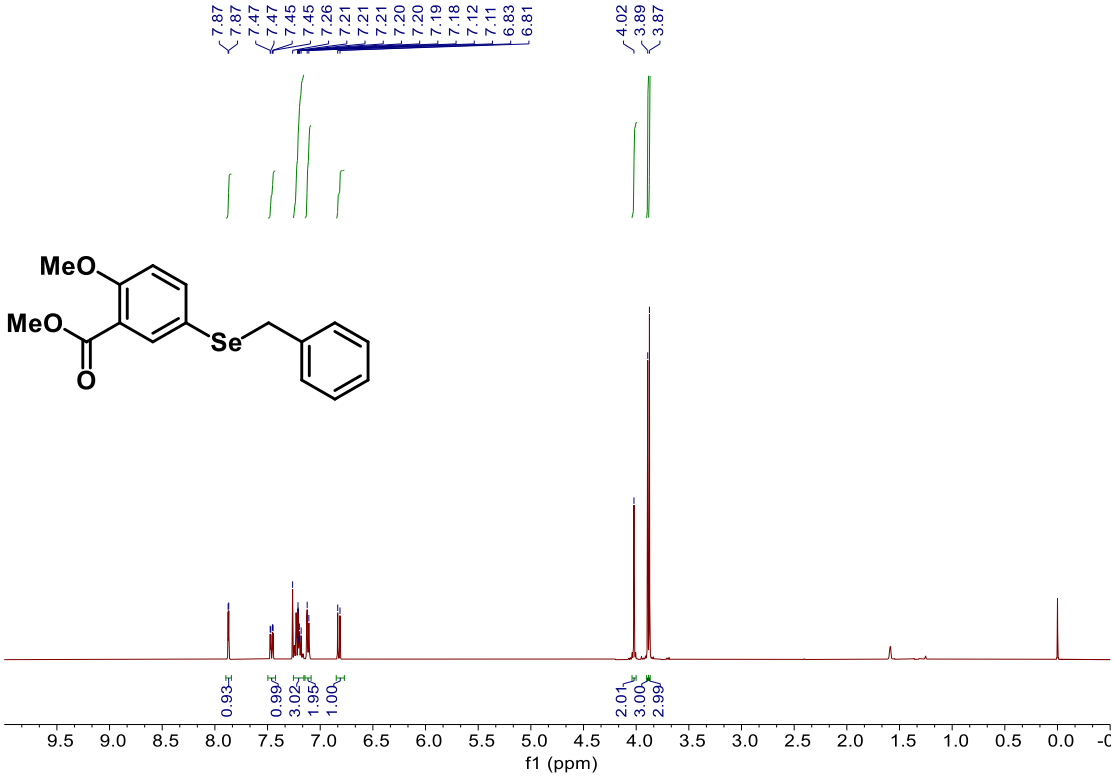
^{1}H NMR of compound 27 (400 MHz in $CDCl_3$)



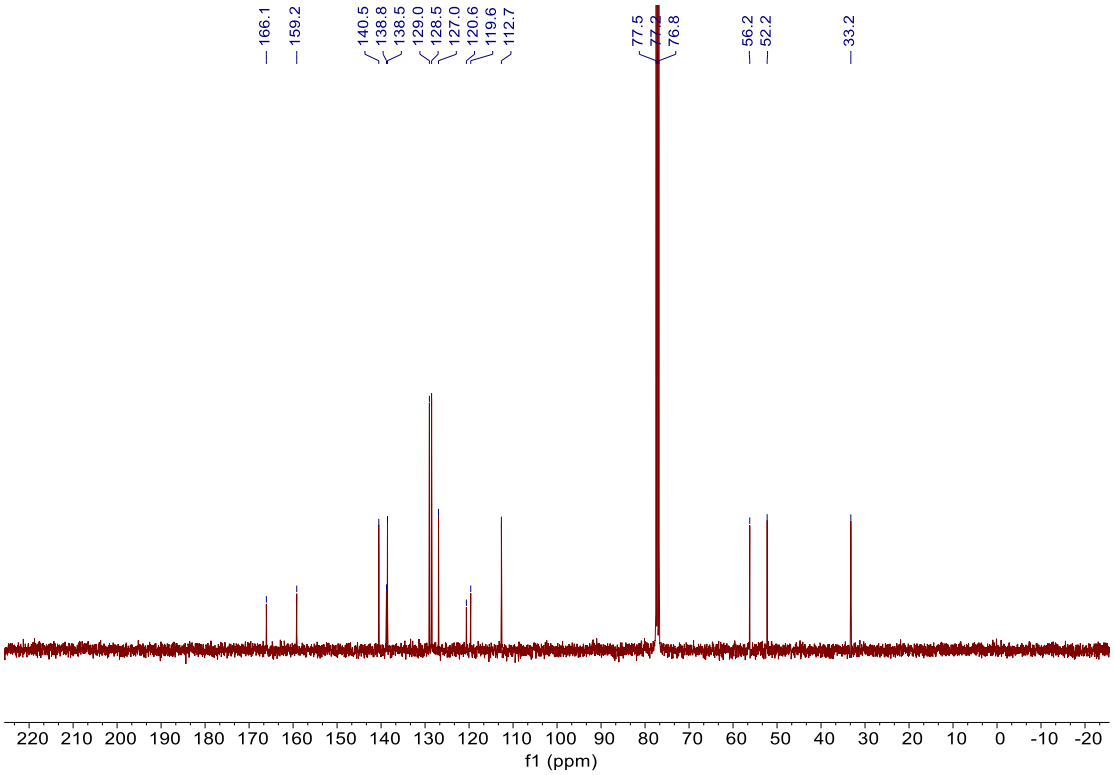
^{13}C NMR of compound 27 (126 MHz in $CDCl_3$)



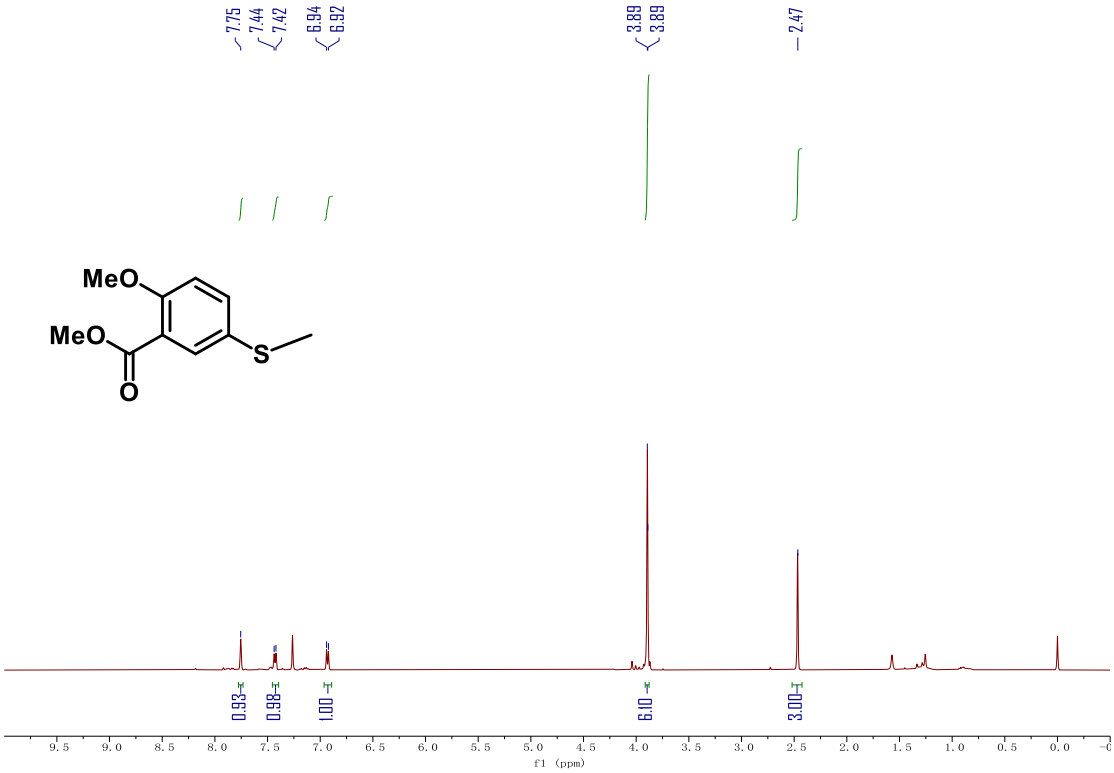
^{1}H NMR of compound 28 (400 MHz in $CDCl_3$)



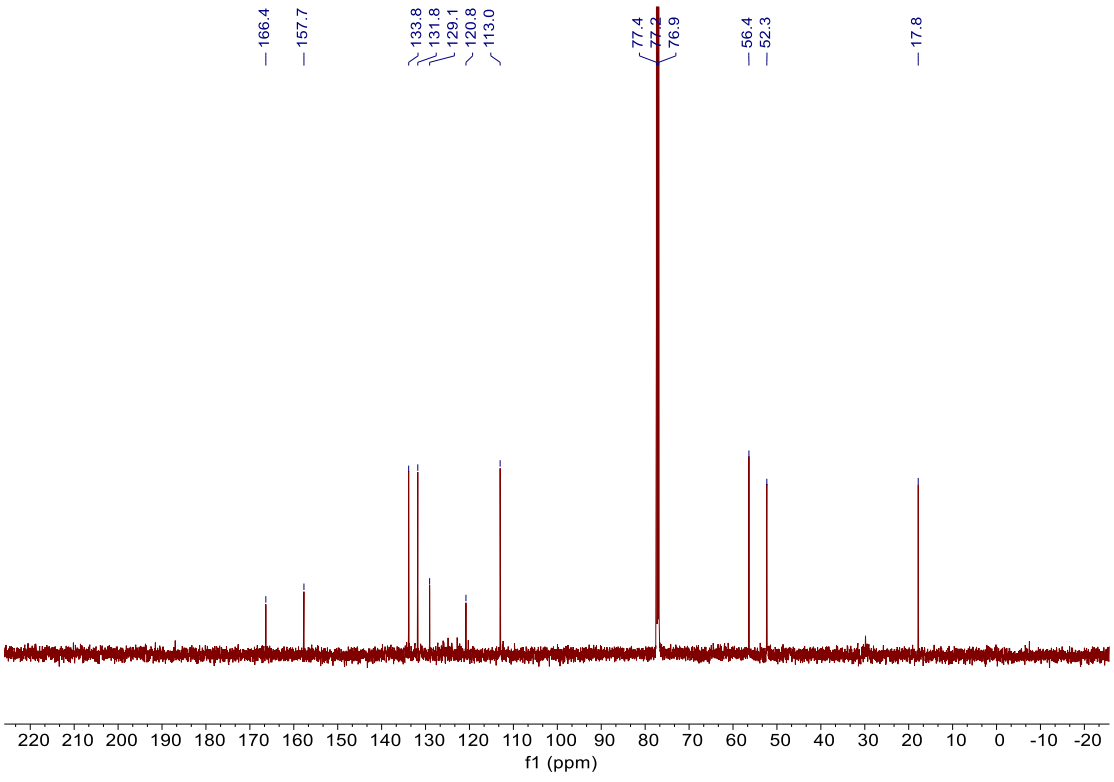
^{13}C NMR of compound 28 (101 MHz in $CDCl_3$)



^{1}H NMR of compound 29 (500 MHz in $CDCl_3$)



^{13}C NMR of compound 29 (126 MHz in $CDCl_3$)



6. Computational Details

All structures were optimized in acetone with the SMD[4] solvent model at B3LYP[5]-D3BJ[6]/6-31G(d,p) level. Harmonic vibrational frequencies were calculated at the same level to verify that the minima have no imaginary frequency. The vertical excitation energies were calculated at TD[7]-B3LYP-D3BJ/6-311++G(d,p) level with the optimized geometries in the ground state. The non-covalent interactions (NCI)[8] and the quantum theory of atoms in molecules (QTAIM)[9] analyses were carried out by Multiwfn[10] program. All the calculations were performed by using Gaussian 16 program.[11] The selected calculated structures were illustrated by using the CYLview[12] or VMD[13] programs.

Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K for the Optimized Structures [BSI= 6-31G(d,p)]

DSe

B3LYP-D3BJ/BSI SCF energy in solution:
-4877.7228649 a.u.

Se	1.140103	-0.298085	-0.323584
Se	-1.140103	0.298085	-0.323584
C	1.140103	-1.621975	1.137976
H	0.848510	-1.140858	2.071305
H	0.463952	-2.440022	0.891283
H	2.167016	-1.989011	1.211415
C	-1.140103	1.621975	1.137976
H	-0.848510	1.140858	2.071305
H	-0.463952	2.440022	0.891283
H	-2.167016	1.989011	1.211415

1^{+}

B3LYP-D3BJ/BSI SCF energy in solution:
-1434.2804558 a.u.

C	3.418433	-2.458117	1.951510
C	2.666975	-3.293337	1.117161
C	2.023354	-2.777566	-0.011641
C	2.157175	-1.417907	-0.245895
C	2.899847	-0.551207	0.573668
C	3.542760	-1.092473	1.688786
H	3.914747	-2.879036	2.819886
H	2.582939	-4.351305	1.341451
H	1.440411	-3.414977	-0.667429
H	4.127685	-0.453377	2.341827
C	2.110449	1.020669	-1.052816
C	1.926055	2.245766	-1.674285
C	2.534500	3.355879	-1.081026
C	3.301366	3.210773	0.080638
C	3.477350	1.963239	0.682564
C	2.871668	0.840645	0.114397
H	1.330415	2.344162	-2.575363
H	2.410688	4.335125	-1.530917
H	3.769240	4.084232	0.523052
H	4.073763	1.861486	1.583087
S	1.435378	-0.539016	-1.638093
C	-0.312366	-0.454336	-1.288231
C	-0.775474	-0.049438	-0.040207
C	-1.193503	-0.805514	-2.312761
C	-2.142800	0.022637	0.212270
H	-0.093334	0.217705	0.758529
C	-2.559074	-0.751430	-2.072132
H	-0.826773	-1.119988	-3.284482
C	-3.056353	-0.342949	-0.819783
H	-3.239527	-1.031723	-2.864604
O	-4.364190	-0.297301	-0.544623

C	-5.307426	-0.675353	-1.557237
H	-6.287524	-0.559690	-1.094633
H	-5.233134	-0.018224	-2.429349
H	-5.164037	-1.717334	-1.860511
C	-2.500968	0.482268	1.591811
O	-1.672603	0.568383	2.483853
O	-3.785670	0.813062	1.747073
C	-4.152110	1.275130	3.063114
H	-5.219277	1.488500	3.007825
H	-3.956076	0.501972	3.809735
H	-3.595707	2.179294	3.321512

IM1

B3LYP-D3BJ/BSI SCF energy in solution:
-6312.019496 a.u.

C	-0.660618	4.055296	-0.441527
C	-0.211518	3.605415	-1.688164
C	0.026225	2.245429	-1.909724
C	-0.191137	1.386790	-0.844318
C	-0.638163	1.805933	0.420405
C	-0.877904	3.167595	0.613980
H	-0.846786	5.113867	-0.291816
H	-0.050171	4.312779	-2.494564
H	0.368981	1.883459	-2.872982
H	-1.232080	3.525374	1.574830
C	-0.487486	-0.552127	0.811741
C	-0.565225	-1.746970	1.509239
C	-0.991719	-1.680331	2.838768
C	-1.321942	-0.450652	3.419143
C	-1.232205	0.739552	2.695456
C	-0.804940	0.699203	1.366905
H	-0.306660	-2.693649	1.048294
H	-1.067516	-2.593133	3.419787
H	-1.656220	-0.420738	4.451011
H	-1.492476	1.687805	3.153949
S	0.007154	-0.398672	-0.909430
C	1.775488	-0.659972	-0.897880
C	2.597608	-0.015642	0.021181
C	2.300364	-1.533826	-1.851795
C	3.974468	-0.225326	0.003612
H	2.193270	0.659572	0.766225
C	3.668875	-1.763594	-1.874442
H	1.657007	-2.034082	-2.568399
C	4.523878	-1.124007	-0.957291
H	4.070686	-2.447500	-2.609534
O	5.844508	-1.336485	-0.936398
C	6.419236	-2.258092	-1.873299
H	7.486079	-2.266907	-1.650271
H	6.006977	-3.263337	-1.740408
H	6.262103	-1.922629	-2.903334
C	4.737501	0.538822	1.040887
O	4.182714	1.124449	1.956719
O	6.061112	0.546041	0.859642
C	6.815722	1.291714	1.836387
H	7.858960	1.180444	1.542030
H	6.526373	2.345275	1.822556
H	6.656534	0.884314	2.837527
Se	-4.308974	-0.919934	0.777532
Se	-3.526833	0.356271	-1.037434
C	-3.721684	-2.712756	0.210626
H	-2.670132	-2.677816	-0.069464
H	-3.858548	-3.364064	1.077336
H	-4.335141	-3.060872	-0.620119
C	-4.898823	-0.073671	-2.386577
H	-4.872488	-1.138908	-2.614619
H	-5.879133	0.222889	-2.014385
H	-4.639347	0.506427	-3.275708

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