Metal-free synthesis of selenoesters directly from carboxylic acids using bifunctional selenoureas under batch, continuous-flow conditions

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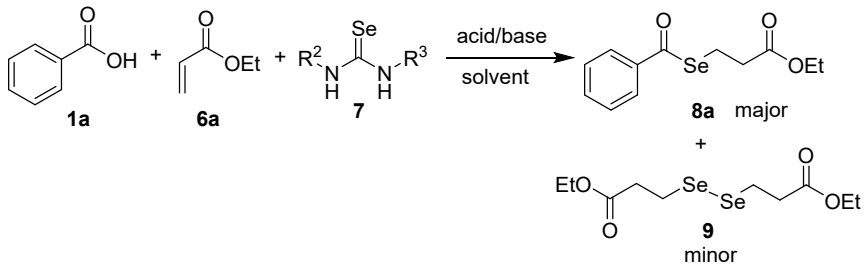
Unless otherwise mentioned, all the solvents, reactants and reagents were purchased from commercial suppliers and used without further purification. Acrylates, carboxylic acids and amines were purchased from TCI, Chennai, India**.** Ethyl acetate, *n*-hexane and toluene were procured from Signa/Merck, India. TLC plates were visualized by exposure to ultra violet light (UV) or staining with iodine vapor. ^{1}H NMR and ^{13}C NMR spectra were obtained by using a JEOL 400 MHz NMR spectrometer. Chemical shifts for protons are reported in parts per million (δ scale) and are referenced to residual protium in the NMR solvents [$CDCl_3$: δ 7.26]. Chemical shifts for carbon resonances are reported in parts per million (δ scale) and are referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.0). Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), integration, and coupling constant in Hertz (Hz).

Flow reactor: VAPOURTEC R series, Instrument serial no. P1720, Software: VI.222, pump: VAPOURTEC R2C. Reactor volume: 10 mL FEP coil (1.3 mm ID and 1.6 mm OD).

Table 1. Optimization of reaction for synthesis of selenoesters[a]



entries	equiv of **1a**	equiv of **6a**	**7** (equiv)	Acid/Base (equiv)	Solvent	Temp.	Time (h)	Yield (%)[b]

						(°C)		
1	1.0	1.0	**7a** (1.0)	Et_3N (1.0)	CH_2Cl_2	40	12	0
2	1.0	1.0	**1.0**	Et_3N (1.0)	toluene	60	12	10
3	1.0	1.0	**7a** (1.0)	Et_3N (1.0)	THF	80	24	trace
4	1.0	1.0	**7a** (1.0)	Et_3N (1.0)	toluene	90	24	22
5	1.0	1.0	**7a** (1.0)	DIPEA (1.0)	toluene	90	24	30
6	1.0	1.0	**7a** (1.0)	DABCO (1.0)	toluene	90	24	30
7	1.0	1.0	**7a** (1.0)	BF_3 (1.0)	toluene	90	24	trace
8	1.0	2.0	**7a** (1.0)	DIPEA (1.0)	toluene	90	24	34
9	1.0	2.0	**7b** (1.0)	DIPEA (1.0)	toluene	90	24	38
10	1.0	2.0	**7b** (2.0)	DIPEA (1.0)	toluene	90	24	42
11	1.0	2.0	**7b** (2.0)	DIPEA (2.0)	toluene	90	24	51(72)[c]
12	1.0	2.0	**7b** (2.0)	DIPEA (2.0)	toluene	100	24	50
13	1.0	3.0	**7b** (2.0)	DIPEA (2.0)	toluene	90	24	50
14	1.0	2.0	**7b** (3.0)	DIPEA (2.0)	toluene	90	24	51
15	2.0	2.0	**7b** (1.0)	DIPEA (2.0)	toluene	90	24	39

[a]The selenourea **7a**/**7b**, Michael acceptor **6a**, DIPEA, in toluene (0.3M) were taken in a sealed tubed, the solvent was degassed and heated at 90°C for 6h, then acid **1a** was added and heated at 90°C for 12-24h. [b]Isolated yield. [c]Yield written in parentheses was determined by ^{1}H NMR spectroscopic analysis of the crude reaction mass. DIPEA: Di isopropyl ethylamine.

Our initial study started with the synthesis of selenourea **7a** and **7b** using reported methods.[7] We attempted first reaction using selenourea **7a** in dichloromethane (table 1, entry 1), considering its good solubility. However, the desired selenoester was not formed. Though it is partially soluble in toluene, we used toluene and raised the reaction temperature to 60°C,

and the desired selenoesters **8a** was isolated in 12% yield (table 1, entry 2). But, the reaction in THF provided trace amount of desired compound (table 1, entry 3). When we increased the reaction time to 24h (table 1, entry 4), and changed the base to DIPEA (table 1, entry 5), the yield was improved to 30%. Use of stronger base like 1,4-diazabicyclo[2.2. 2]octane (DABCO) could not improve yield (table 1, entry 6). The attempt to activate the carbonyl group of **6a** with Lewis acid for better yield, did not provide the desired selenoester (table 1, entry 7). Increasing the mole ratio of **6a** (table 1, entry 8) and changing the selenourea to **7b** (table 1, entry 9) gave higher yield (38%). The yield was improved when **7b** mole ratio was increased (table 1, entry 10), and base was increased to 2.0 equiv. (table 1, entry 11). There was no enhancement of yield, when the reaction temperature (table 1, entry 12), mole ratio of Michael acceptor **6a** (table 1, entry 13), selenourea **7b** (table 1, entry 14) and acid **1a** (table 1, entry 15) were increased. When we tried to understand the reasons for low yield, we could find the formation diselenide **9** as a side product. The ^{1}H NMR spectrum of crude reaction mass was recorded utilizing mesitylene as an internal standard and found the yield of 72%, whereas isolated yield was 51% (table 1, entry 11). The optimized condition was found to be (table 1, entry 11) reaction of the selenourea **7b** (2.0mmol), Michael acceptor **6a** (2.0mmol), DIPEA (2.0mmol), in toluene (3.0mL) at 90°C for 6h, followed by addition of the acid **1a** (1.0mmol), and heating at 90°C for 24h.

Standard procedure A for synthesis of selenoesters:

The selenourea **7b** (2.0mmol), Michael acceptor **6** (2.0mmol), DIPEA (2.0mmol), in toluene (3.0mL) were taken in a sealed tubed, the solvent was degassed and heated at 90°C for 6-8h, then acid **1** (1.0mmol) was added and heated at 90°C for 24h. The crude reaction mass was washed with water, evaporated under vacuum and column purified using silica gel column chromatography.

Standard Procedure B: using a flow reactor:

The selenourea **7b** (2.0mmol), Michael acceptor **6** (2.0mmol), DIPEA (2.0mmol), in toluene (3.0mL) were taken in a flask, the solvent was degassed and heated at 90°C until the selenourea **7b** gets dissolved. The benzoic acid (1.0 mmol) in toluene (3.0mL) was heated at 90°C in another flask until it gets dissolved. The both solutions were pumped from two separate pumps, under N_2 atmosphere. The reaction was run at 120 °C with residence time 30min., in a 10mL reactor. Flow rate: 333µL/min. residence time: 30.0min.

Computational Method

All the calculation for this article were carried out using Gaussion16 software package[3] at B3lyp/6-31++(d,p) level[4] of density functional theory. Geometries of all the structures and transition states were optimized in the toluene solvent as all the experimental reaction were performed in this solvent using CPCM[5] solvation model. All reactants and intermediates have zero imaginary frequencies in their harmonic vibrational frequencies, whereas all transition states have a single imaginary frequency. Electronic and zero-point energies were scaled using 0.961 scaling factor.[6]

In order to understand the reaction mechanism, we have carried out quantum chemical calculations (Figure 1) in the absence and presence of selenourea, 1-cyclohexyl-3-phenylselenourea (**S1**). This selenourea may exist in two tautomeric forms based on the migration of hydrogens atoms from amino groups to Se atom (via 1,3-H shift). Tautomer **T1** which is formed by the migration of hydrogen from the nitrogen (Np) which is attached to phenyl ring is more stable by 3.38 kcal/mol compared to tautomer **T2** which is formed by the migration of hydrogen atom from nitrogen (Nc) attached to cyclohexyl group. This higher stability of **T1** may be correlated with its deprotonation energy. Deprotonation energies associated are 310.61 and 312.98 kcal/mol respectively, for removal of the hydrogen from Np and Nc nitrogen atoms. Suggesting that the migration of hydrogen is slightly easier for tautomer **T1**. On the same line formation of nucleophile **Nu1** is easier compared to nucleophile **Nu2** in the presence of base as indicated by deprotonation energies of Nc and Np atoms, respectively. This nucleophile **Nu1** is more stable than nucleophile **Nu2** by 2.39 kcal/mol.

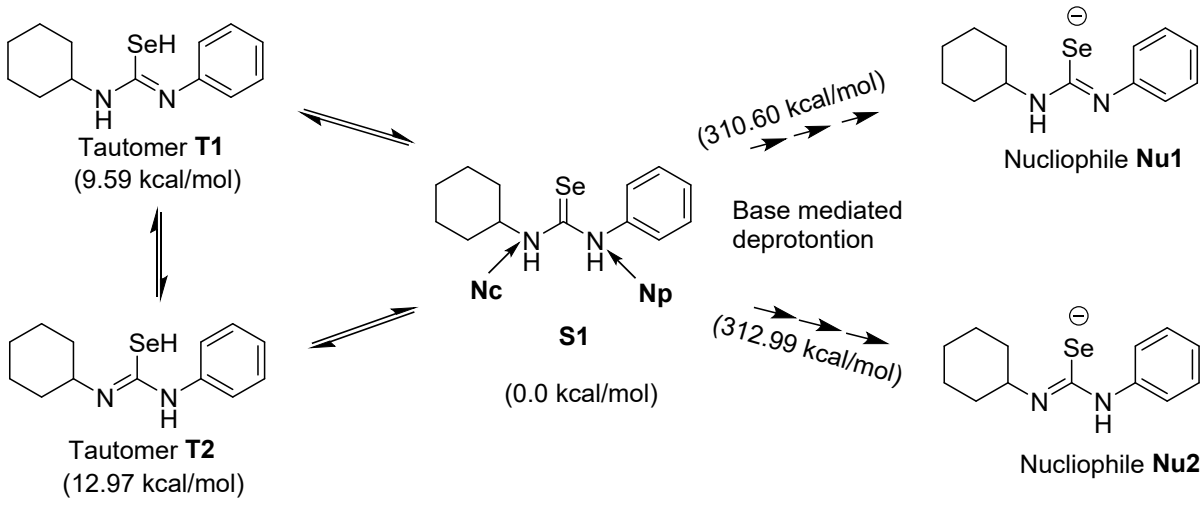


Fig. 1 Two possible tautomeric forms and nucleophiles of selenourea and relative energies of tautomers computed at B3lyp/6-31++(d,p) level in the toluene solvent.

Reaction starts with attack of nucleophilic Se atom of selenourea at beta carbon of Michael acceptor (Figure 2). Here, we have two nucleophiles based on which hydrogen is abstracted by base, and attack of them lead to formation of a bond between nucleophlic Se and beta carbon of acceptor. In both transition states (**TS1** and **TS2**) free amino groups of nucleophiles involve in hydrogen bonding with carbonyl oxygen atom of Michael acceptor. Barrier associated with these are 59.42 and 62.93 kcal/mol, respectively, suggesting that attack

of **Nu1** is preferred over **Nu2** by 3.51 kcal/mol. In addition, formation of **INT1** is preferred over **INT2** by around 5.6 kcal/mol.

In other possibility, one molecule of selenourea may assist carbonyl oxygen of Michael acceptor by hydrogen bonding interactions during the attack of nucleophiles **Nu1** and **Nu2**. In the both observed transition states (**TS1'** and **TS2'**) hydrogen atoms of amino groups (selenourea) make stabilizing hydrogen bonds with oxygen atom of acceptor (Figure 3). The computed energy barriers for the attack of **Nu1** and **Nu2** are found to be 40.44 and 46.49 kcal/mol, respectively. This revealed that attack of **Nu1** is preferred by about 6.05 kcal/mol over **Nu2** attack. The barriers of selenourea assisted pathways are lower, around 16-19 kcal/mol, compared to pathways which do not involve selenourea as a hydrogen bond donor. Additionally, **INT1'** formation is favored by about 4.17 kcal/mol over **INT2'** formation.

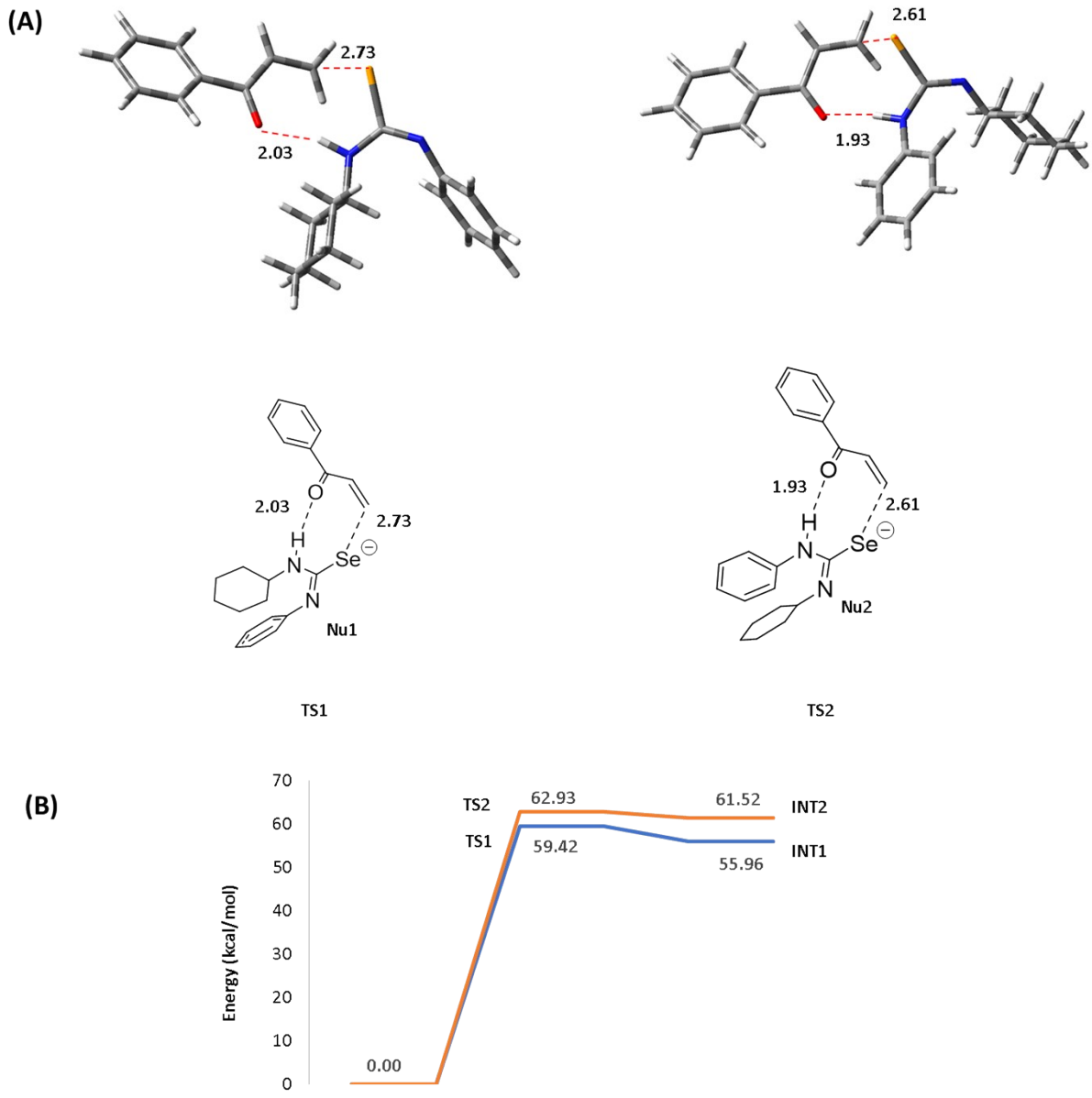


Fig. 2 Energy profiles for the addition of nucleophiles to Michael acceptor without hydrogen bonding support of selenourea to carbonyl oxygen. (A) 3D geometries of transition states (TS1 and TS2) at B3lyp/6-31++(d,p) level in toluene and their 2D presentation. (B) Potential energy surface for the addition of nucleophiles. The energy of the Michael acceptor, nucleophile Nu1 and a proton is taken as a reference (0.00 kcal/mol) for generating this potential energy surface.

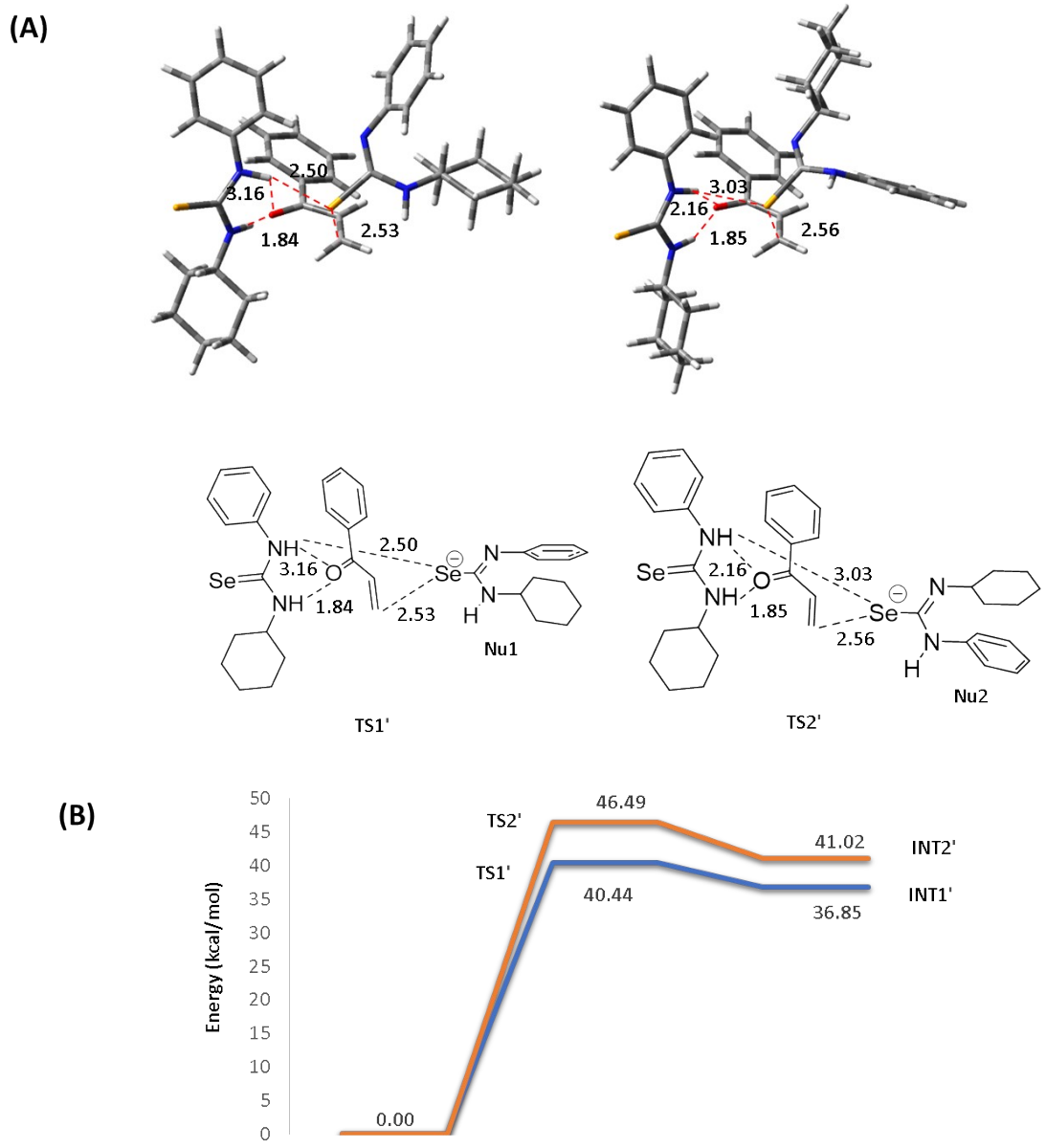


Fig. 3 Energy profiles for the addition of nucleophiles to Michael acceptor with hydrogen bonding support of selenourea to carbonyl oxygen. (A) 3D geometries of transition states (TS1' and TS2') at B3lyp/6-31++(d,p) level in the toluene and their 2D presentation. (B) Potential energy surface for the addition of nucleophiles. The energy of the Michael acceptor, nucleophile Nu1, selenourea (S1) and a proton is taken as a reference (0.00 kcal/mol) for generating this potential energy surface.

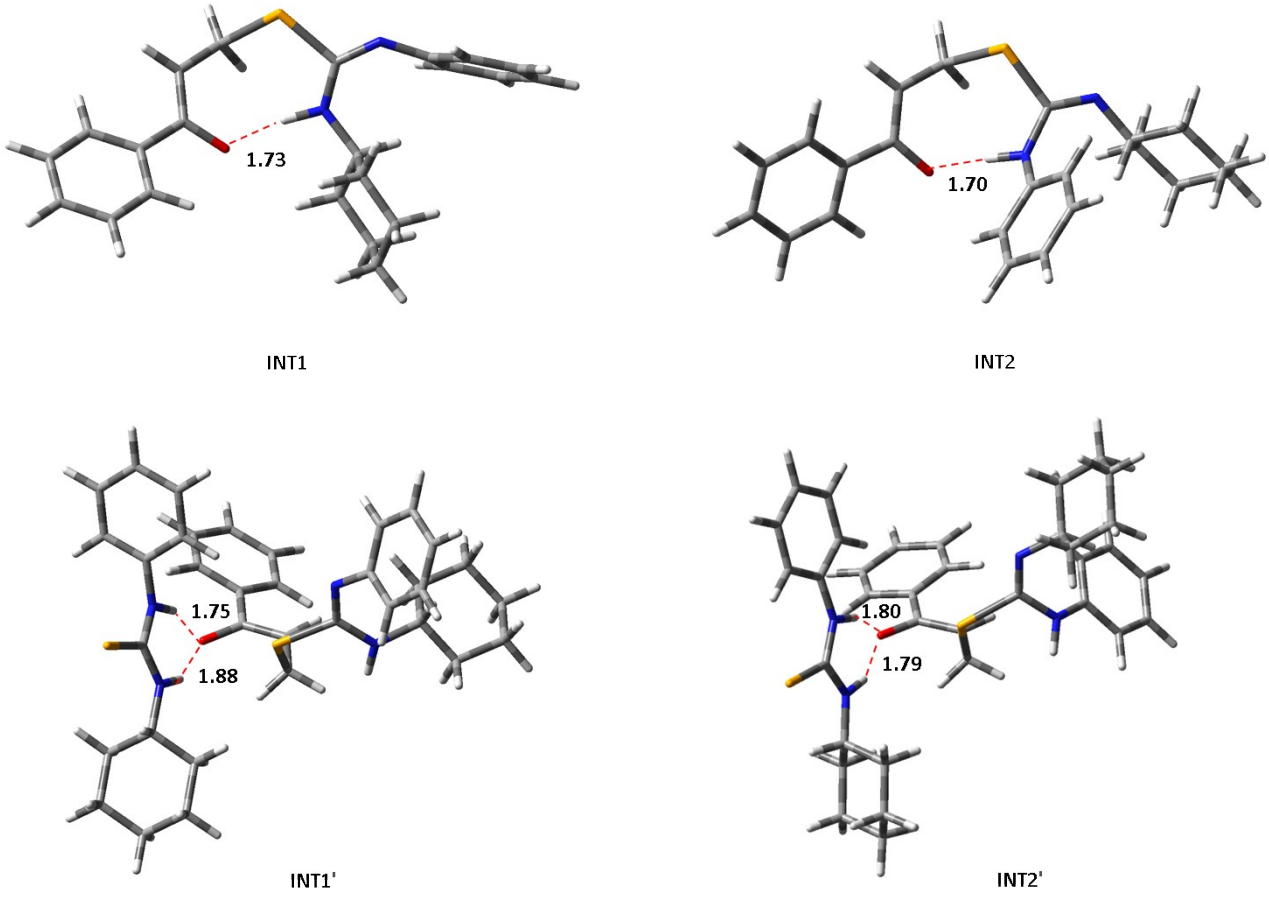
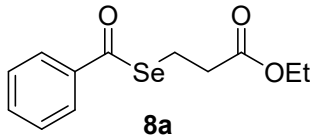


Fig. 4 3D geometries of post-transition state anion intermediates for each potential energy surface given in Figure 2 and Figure 3.

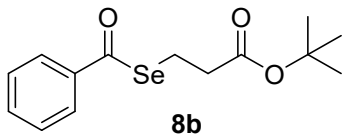
Ethyl 3-(benzoylselanyl)propanoate(8a):



8a

The standard procedure was followed. **8a** was isolated as a colourless liquid after column purification (EtOAc/n-hexane, 1:20). ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 7.88 (2H, *J* = 8.44, 1.26 Hz, dd), 7.57 (1H, *J* = 7.41 Hz, d), 7.44 (2H, *J* = 7.91, 7.45 Hz, dd), 4.16 (2H, *J* = 7.13 Hz, q), 3.28 (2H, *J* = 6.99 Hz, t), 2.83 (2H, *J* = 6.99 Hz, t), 1.28-1.24 (3H, m); ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 194.6, 172.3, 139.0, 133.8, 128.9, 127.3, 60.9, 35.4, 19.6, 14.3; HRMS calculated for $[M+Na]^{+}$($C_{12}H_{14}O_3SeNa$) 309.0006, found 309.0026.

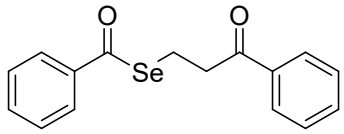
***tert*-Butyl 3-(benzoylselanyl)propanoate(8b):**



8b

The standard procedure was followed. **8b** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20). ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 7.89-7.87 (2H, m), 7.60-7.55 (1H, m), 7.46-7.42 (2H, m), 3.24 (2H, *J* = 6.95 Hz, t), 2.75 (2H, *J* = 6.95 Hz, t), 1.45 (9H, s); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 194.8, 171.6, 139.0, 133.7, 128.9, 127.2, 81.1, 36.5, 28.2, 19.9; HRMS calculated for $[M+Na]^+$($C_{14}H_{18}O_3SeNa$) 337.0319, found 337.0303.

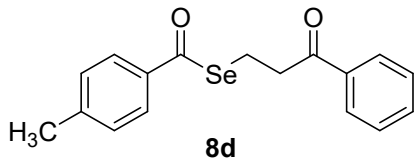
Se-3-oxo-3-phenylpropyl benzoselenoate(8c):



8c

The standard procedure was followed. **8c** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.98-7.96 (2H, m), 7.90-7.87 (2H, m), 7.59-7.54 (2H, m), 7.48-7.42 (4H, m), 3.54 (2H, *J*=8.0Hz, t), 3.42 (2H, *J*= 8.0Hz, t); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 198.8, 195.6,139.0, 136.5, 133.8, 133.5,128.9, 128.7, 128.2, 127.2, 39.7, 18.9; HRMS calculated for $[M+H]^+$($C_{16}H_{15}O_2Se$) 319.0237, found 319.0225.

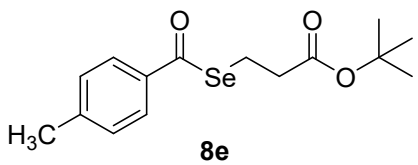
Se-3-oxo-3-phenylpropyl 4-methylbenzoselenoate(8d)



8d

The standard procedure was followed. **8d** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20). ^{1}H-NMR (400 MHz, $CDCL_3$) δ 7.98-7.96 (2H, m), 7.78 (2H, *J* = 8.23 Hz, d), 7.54 (1H, *J* = 7.38 Hz, d), 7.47-7.43 (2H, m), 7.25-7.22 (2H, m), 3.53 (2H, *J*=8.0Hz, t), 3.40 (2H, *J*=8.0Hz,t), 2.38 (3H, s); ^{13}C-NMR (101 MHz, $CDCL_3$) δ 198.8, 194.7, 144.7, 136.6, 133.4, 130.7, 129.6, 129.5, 128.7, 128.2, 127.3, 39.8, 21.8, 18.8; HRMS calculated for $[M+Na]^+$($C_{17}H_{16}O_2SeNa$) 355.0213, found 355.0236.

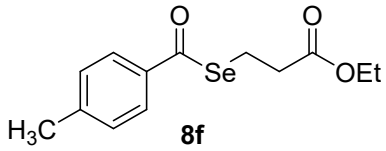
***tert*-Butyl 3-(4-methylbenzoylselanyl)propanoate(8e):**



8e

The standard procedure was followed. **8e** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.78 (2H, *J* = 6.49, 1.74 Hz, dd), 7.25-7.22 (2H, m), 3.23 (2H, *J* = 6.98 Hz, t), 2.74 (2H, *J* = 6.98 Hz, t), 2.38 (3H, s), 1.45 (9H, s); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 194.5, 171.9, 144.8, 136.7, 129.5, 127.3, 81.0, 36.9, 28.2, 21.8, 19.7; HRMS calculated for $[M+Na]^+$($C_{15}H_{20}O_3SeNa$) 351.0475, found 351.0544.

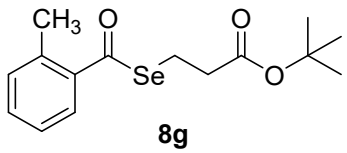
Ethyl 3-(4-methylbenzoylselanyl)propanoate(8f):



8f

The standard procedure was followed. **8f** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.78-7.76 (2H, m), 7.25-7.22 (2H, m), 4.15 (2H, *J* = 7.16 Hz, q), 3.26 (2H, *J* = 6.95 Hz, t), 2.82 (2H, *J* = 6.99 Hz, t), 2.38 (3H, s), 1.27-1.23 (3H, m); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 194.0, 172.5, 144.8, 136.4, 129.6, 127.4, 60.8, 35.5, 21.8, 19.4, 14.3; HRMS calculated for $[M+Na]^+$($C_{13}H_{16}O_3SeNa$) 323.0162, found 323.0151.

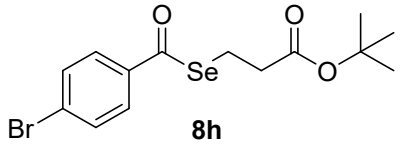
***tert*-Butyl 3-(2-methylbenzoylselanyl)propanoate(8g):**



8g

The standard procedure was followed. **8g** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.77 (1H, *J* = 7.76, 1.26 Hz, dd), 7.37 (1H, *J* = 7.53, 1.34 Hz, dd), 7.27-7.25 (1H, m), 7.23-7.21 (1H, m), 3.20 (2H, *J* = 7.03 Hz, t), 2.75 (2H, *J* = 6.99 Hz, t), 2.46 (3H, s), 1.45 (9H, *J* = 2.75 Hz, s); ^{13}C-NMR (101 MHz, CDC_3) δ 197.0, 171.7, 139.3, 136.1, 132.0, 131.8, 128.9, 126.0, 81.1, 36.6, 28.2, 20.8, 20.7; HRMS calculated for $[M+Na]^+$($C_{15}H_{20}O_3SeNa$) 351.0475, found 351.0453.

***tert*-Butyl 3-(4-bromobenzoylselanyl)propanoate(8h):**

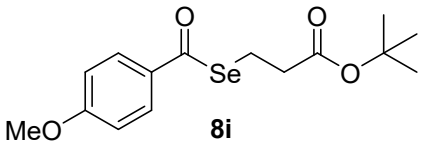


8h

The standard procedure was followed. **8h** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.74 (2H, *J*=8.0Hz, d), 7.58 (2H, *J* = 8.0 Hz, d), 3.25 (2H, *J* = 6.92 Hz, t), 2.74 (2H, *J* = 6.92 Hz, t), 1.45 (9H, s); ^{13}C-

NMR (101 MHz, $CDCl_3$) δ 194.0, 171.4, 137.6, 132.2, 128.8, 128.6, 81.4, 36.4, 28.2, 20.2; HRMS calculated for $[M+Na]^+(C_{14}H_{17}BrO_3SeNa)$ 414.9424, found 414.9403.

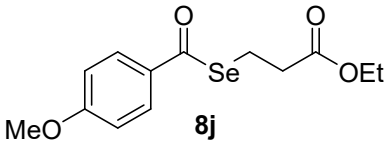
***tert*-Butyl 3-(4-methoxybenzoylselanyl)propanoate(8i):**



8i

The standard procedure was followed. **8i** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.85 (2H, *J* = 9.02 Hz, d), 6.91 (2H, *J* = 8.94 Hz, d), 3.85 (3H, s), 3.22 (2H, *J* = 6.95 Hz, t), 2.73 (2H, *J* = 6.99 Hz, t), 1.44 (9H, s); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 192.8, 171.7, 164.1, 131.9, 129.5, 114.0, 81.0, 55.7, 36.6, 28.2, 19.7; HRMS calculated for $[M+Na]^+(C_{15}H_{20}O_4SeNa)$ 367.0425, found 367.0478.

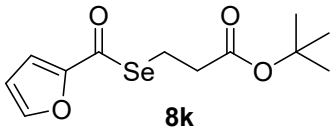
Ethyl 3-(4-methoxybenzoylselanyl)propanoate(8j):



8j

The standard procedure was followed. **8j** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.85 (2H, *J* = 9.02 Hz, d), 6.91 (2H, *J* = 8.94 Hz, d), 4.15 (2H, *J* = 7.18 Hz, q), 3.85 (3H, s), 3.25 (2H, *J* = 6.99 Hz, t), 2.81 (2H, *J* = 6.95 Hz, t), 1.24 (3H, *J*= 4.0Hz,t); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 192.7, 172.8, 164.3, 131.6, 129.6, 114.0, 60.8, 55.7, 35.6, 19.4, 14.3; HRMS calculated for $[M+Na]^+(C_{13}H_{16}O_4SeNa)$ 339.0112, found 339.0102.

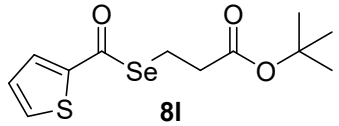
***tert*-Butyl 3-(furan-2-carbonylselanyl)propanoate(8k):**



8k

The standard procedure was followed. **8k** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.52 (1H, *J* = 8.60, 0.57 Hz, dd), 7.34 (1H, *J* = 2.18 Hz, t), 7.11 (1H, *J* = 8.64, 2.52 Hz, dd), 3.06 (2H, *J* = 7.22 Hz, t), 2.71 (2H, *J* = 7.22 Hz, t), 1.44 (9H, s); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 171.5, 147.9, 147.1, 138.4, 124.6, 119.2, 81.1, 37.1, 28.2, 24.0; HRMS calculated for $[M]^+(C_{12}H_{17}O_4Se)$ 305.0292, found 305.0256.

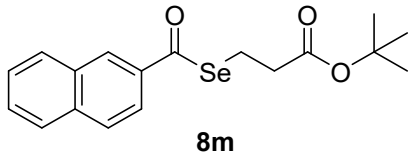
***tert*-Butyl 3-(thiophene-2-carbonylselanyl)propanoate(8l):**



8l

The standard procedure was followed. **8l** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.78 (1H, *J* = 3.86, 1.17 Hz, dd), 7.65 (1H, *J* = 4.95, 1.17 Hz, dd), 7.11 (1H, *J* = 4.95, 3.86 Hz, dd), 3.24 (2H, *J* = 6.89 Hz, t), 2.76 (2H, *J* = 6.89 Hz, t), 1.44 (9H, s); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 185.1, 171.9, 133.4, 131.5, 127.8, 81.5, 36.6, 28.2, 22.8; HRMS calculated for $[M+Na]^+$($C_{12}H_{16}O_3SSeNa$) 342.9883, found 342.9868.

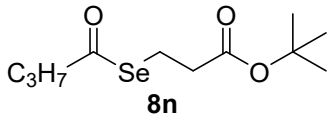
***tert*-Butyl 3-(2-naphthoylselanyl)propanoate(8m):**



8m

The standard procedure was followed. **8m** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.44 (1H, s), 7.97 (1H, *J* = 8.03, 0.60 Hz, dd), 7.90-7.85 (3H, m), 7.62-7.53 (2H, m), 3.30 (2H, *J* = 6.95 Hz, t), 2.79 (2H, *J* = 6.95 Hz, t), 1.46 (9H, s); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 194.6, 171.7, 136.3, 136.0, 132.6, 129.7, 128.9, 128.8, 128.7, 127.9, 127.1, 123.0, 81.1, 36.5, 28.2, 20.1; HRMS calculated for $[M+Na]^+$($C_{18}H_{20}O_3SeNa$) 387.0475, found 387.0462.

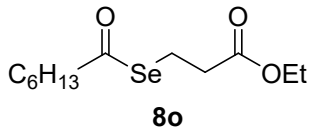
***tert*-Butyl 3-(butyrylselanyl)propanoate(8n):**



8n

The standard procedure was followed. **8n** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.04 (2H, *J* = 6.99 Hz, t), 2.65 (2H, *J* = 7.03 Hz, t), 2.60 (2H, *J*= 8.0Hz, t), 1.65-1.60 (2H, m), 1.43 (9H, s), 0.90 (3H, *J* = 7.34 Hz, t); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 202.1, 171.7, 81.0, 47.9, 36.9, 28.2, 22.1, 19.7, 13.8; HRMS calculated for $[M+Na]^+$($C_{11}H_{20}O_3SeNa$) 303.0475, found 303.0621.

Ethyl 3-(heptanoylselanyl)propanoate(8o):

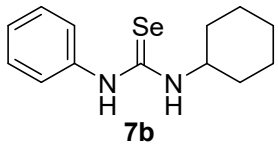


8o

The standard procedure was followed. **8o** was isolated as colourless liquid after column purification(EtOAc/n-hexane, 1:20); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.13 (2H, *J* = 7.13 Hz, q),

3.08 (2H, *J* = 7.03 Hz, t), 2.73 (2H, *J* = 6.99 Hz, t), 2.59 (2H, *J* = 7.57 Hz, t), 1.64-1.58 (2H, m), 1.24 (9H, *J* = 1.76 Hz, d), 0.88-0.81 (3H, m); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 201.8, 172.3, 60.8, 48.2, 35.5, 31.5, 29.8, 28.6, 25.4, 22.8, 22.5, 19.4, 14.3, 14.1.

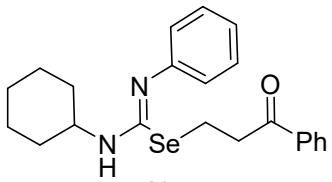
Synthesis of 1-cyclohexyl-3-phenylselenourea(7b):[1]



7b

^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.43 (1H, s), 7.43 (2H, *J* = 7.72 Hz, t), 7.33-7.28 (1H, m), 7.18 (2H, *J* = 7.64 Hz, d), 6.11 (1H, s), 4.32 (1H, s), 2.08-2.05 (2H, m), 1.64-1.57 (3H, m), 1.45-1.23 (2H, m), 1.15-1.10 (3H, m); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 176.7, 135.8, 130.5, 127.7, 125.1, 56.9, 32.6, 25.4, 24.7; HRMS calculated for $[M+H]^+$($C_{13}H_{19}N_2Se$) 283.0713, found 283.0728.

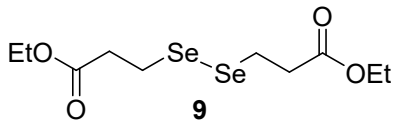
***N*-cyclohexyl-5-oxo-*N′*,5-diphenylpentanamidine(10):**



10

1-phenylprop-2-en-1-one **6c** (100.1mg, 0.757mmol), 1-cyclohexyl-3-phenylselenourea **7b** (320.2mg, 1.134mmol) and Di isopropyl ethyl amine (261.3mg, 2.268mmol) were dissolved in toluene (3.0mL), heated at 90C for 12h. The N-cyclohexyl-5-oxo-N',5-diphenylpentanamidine (**10**) was isolated as a yellowish solid, after column purification(EtOAc/n-hexane, 1:5; *Rf* 0.65); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.01-7.98 (2H, m), 7.56-7.38 (6H, m), 7.19-7.16 (2H, m), 5.42 (1H, *J* = 7.89 Hz, d), 4.66-4.62 (2H, m), 4.40 (1H, *J* = 4.12 Hz, t), 3.54-3.50 (2H, m), 1.98-1.94 (2H, m), 1.53-1.51 (3H, m), 1.37-1.33 (2H, m), 1.04-0.96 (3H, m); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 198.6, 179.8, 141.1, 136.8, 133.3, 130.9, 129.1, 128.7, 128.3, 127.8, 56.5, 53.5, 37.3, 32.6, 25.4, 24.6. HRMS calculated for $[M+H]^+$($C_{22}H_{26}N_2OSe$) 414.121 found 415.1273; HRMS calculated for $[M+H]^+$($C_{22}H_{27}N_2OSe$) 415.1289, found 415.1273.

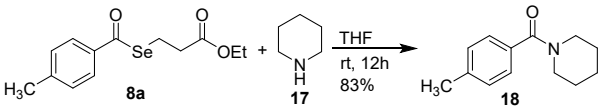
Diethyl 3,3'-diselanediyldipropionate(9):[2]



9

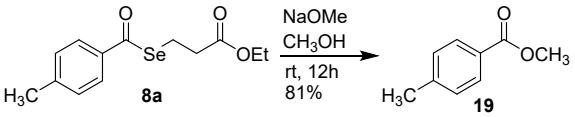
^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.17-4.11 (4H, m), 3.08 (4H, *J* = 7.23 Hz, t), 2.79 (4H, *J* = 7.18 Hz, t), 1.25 (6H, *J* = 7.15, t); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 172.1, 60.8, 36.0, 23.4, 14.3.

Piperidin-1-yl(*p*-tolyl)methanone (18).[8]



To a solution of thioester **8a** (29.9 mg, 0.1 mmol) in THF (0.5 mL) was added piperidine (17.1 mg, 0.2 mmol). The reaction was stirred at rt for 12h, and then excess solvent was evaporated under vacuum. The crude product was purified by silica gel column chromatography (eluted with 30% ethyl acetate in *n*-hexane) to give compound **18** (16.2 mg, 83%) as off white solid. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.28 (2H, *J* = 8.0 Hz, d), 7.18 (2H, *J* = 8.0 Hz, d), 3.67 (2H, bs), 3.35 (2H, bs), 2.35 (3H, s), 1.65-1.55 (6H, m); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 170.6, 139.5, 133.7, 129.1, 127.0, 48.9, 43.2, 26.7, 25.9, 24.7, 21.4.

Methyl 4-methylbenzoate (19).[9]



To a solution of thioester **8a** (29.8 mg, 0.1 mmol) in Methanol (0.5 mL) was added sodium methoxide (16.3 mg, 0.3 mmol). The reaction was stirred at rt for 12h, quenched with water (0.5 mL), and then excess solvent was evaporated under vacuum. The crude product was dissolved in ethyl acetate (2.0 mL) and washed with water (2.0 mL). The organic layer was evaporated under vacumm, purified by silica gel column chromatography (eluted with 5% ethyl acetate in *n*-hexane) to give compound **19** (12.5 mg, 81%) as a colourless liquid. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.93 (2H, *J* = 8.0 Hz, d), 7.23 (2H, *J* = 8.0 Hz, d), 3.89 (3H, s), 2.40 (3H, s); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 167.3, 143.6, 129.7, 129.2, 127.5, 52.0, 21.7.

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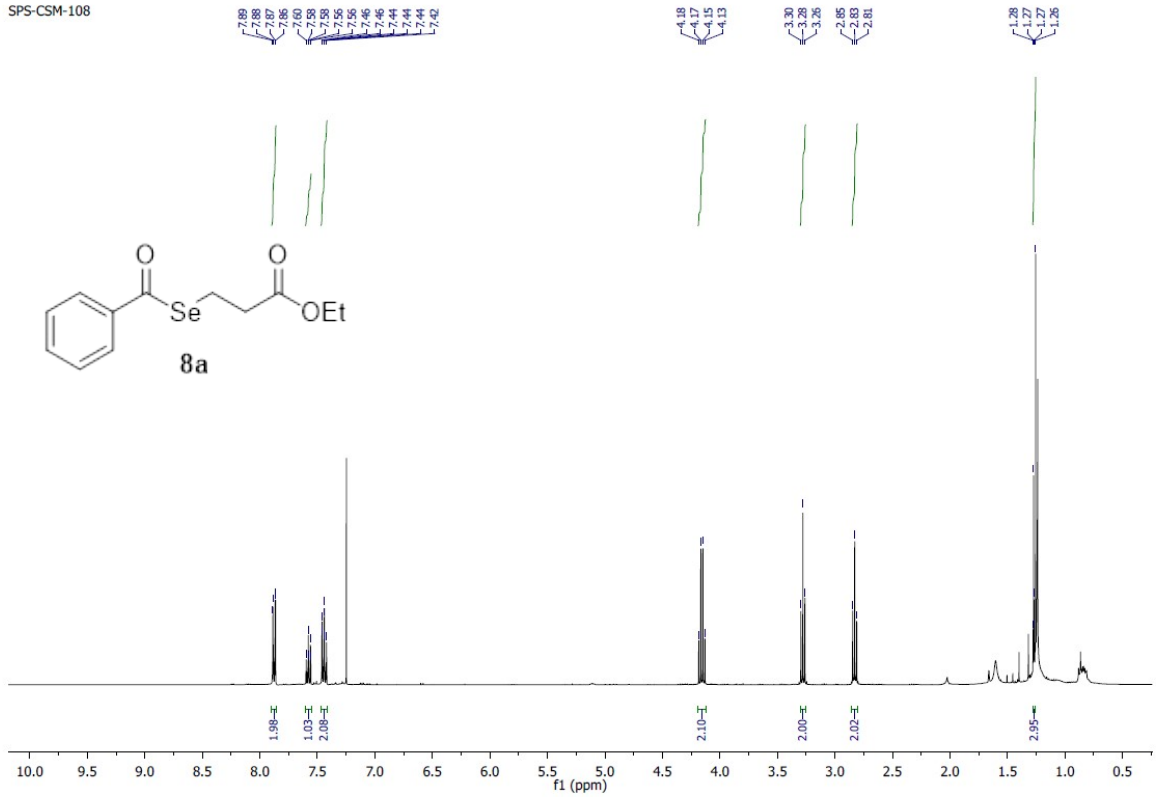
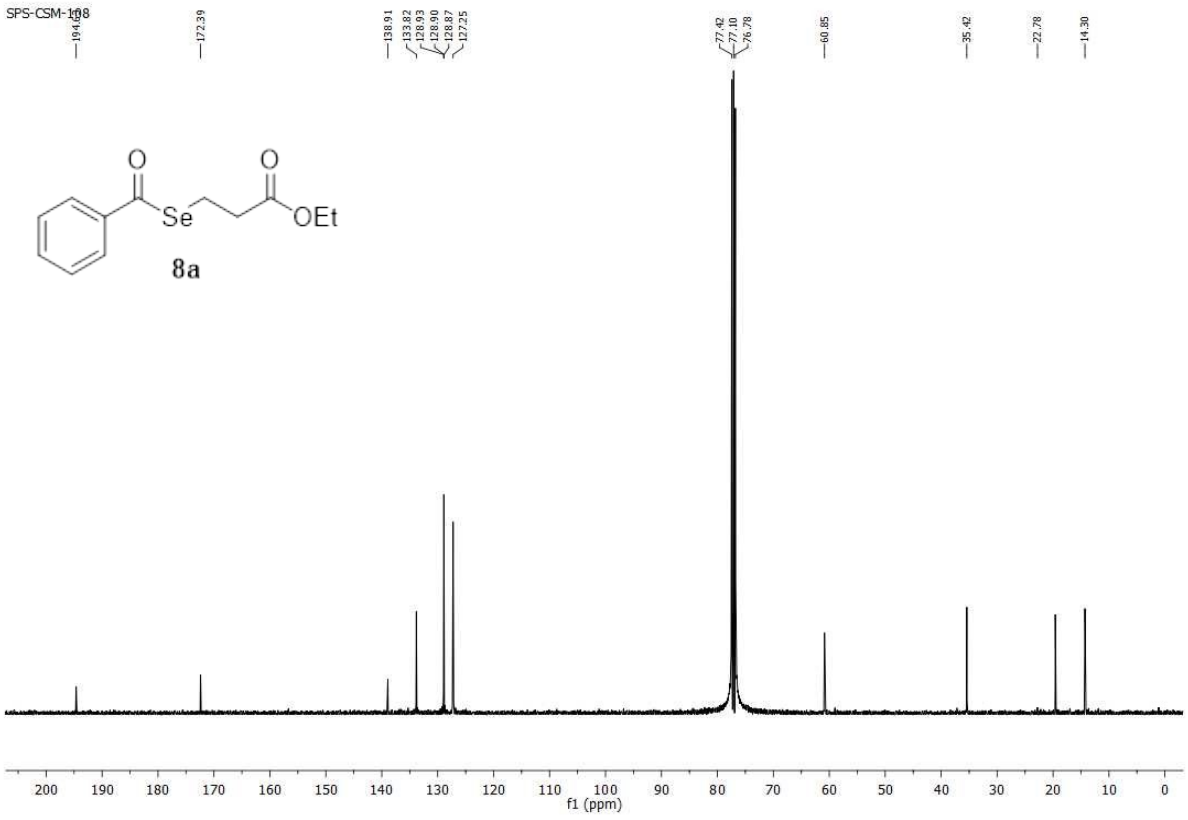
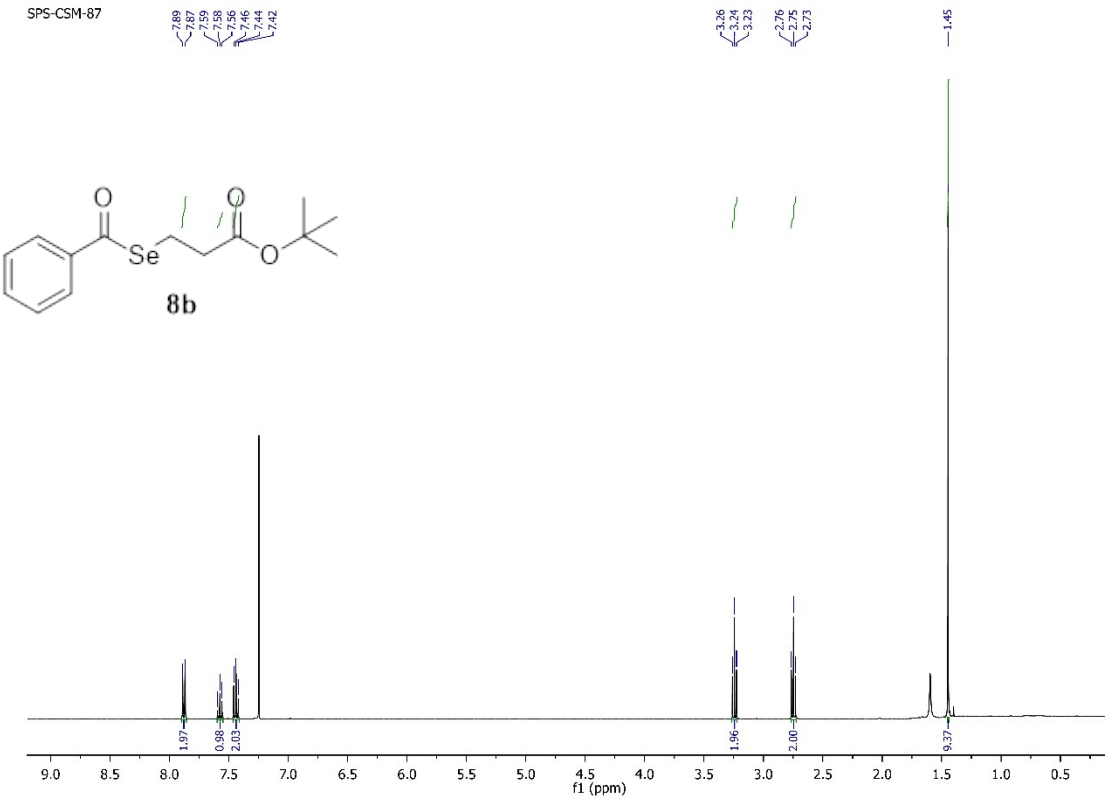


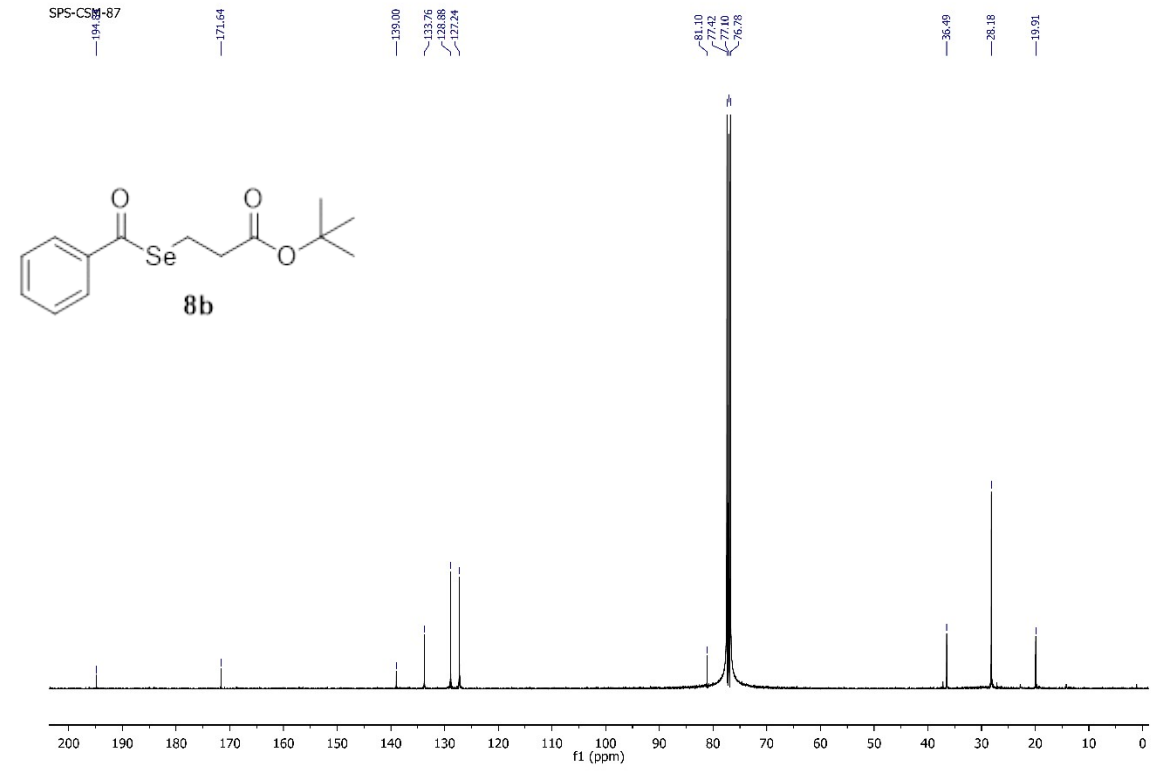
^{1}H NMR spectrum of **8a**.



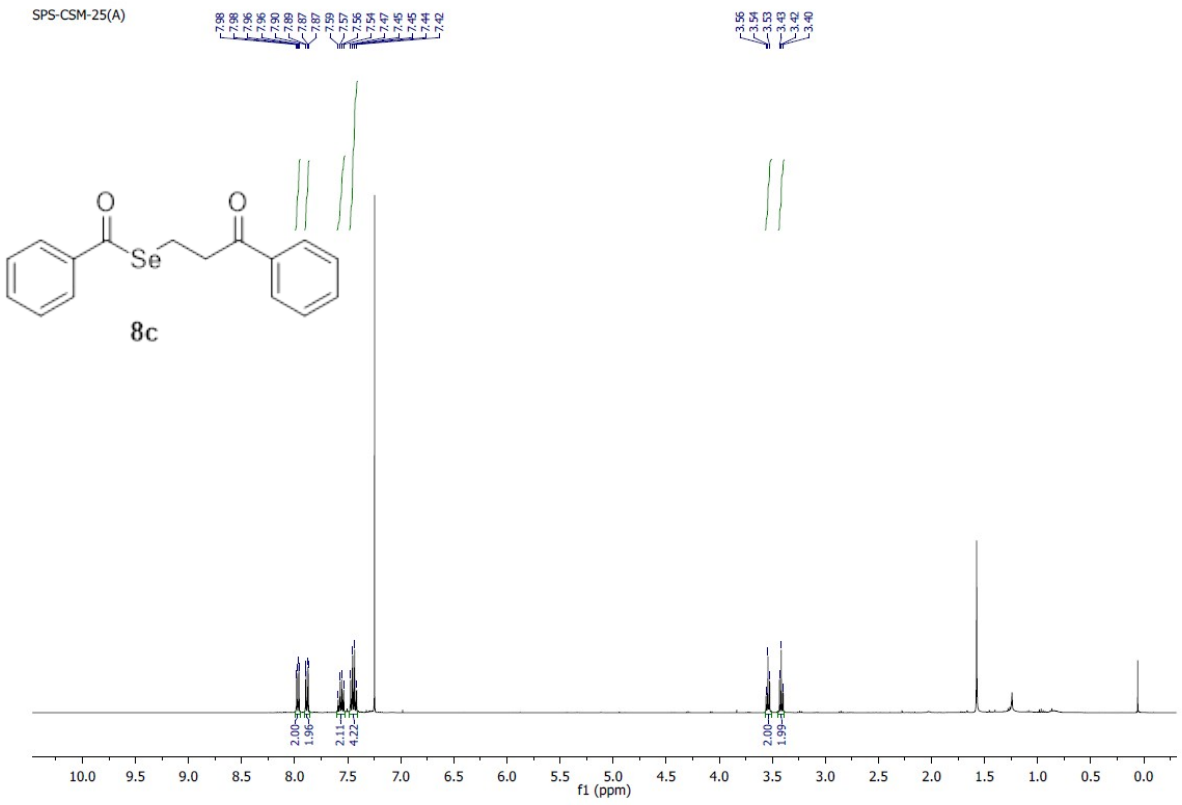
^{13}C NMR spectrum of **8a**.



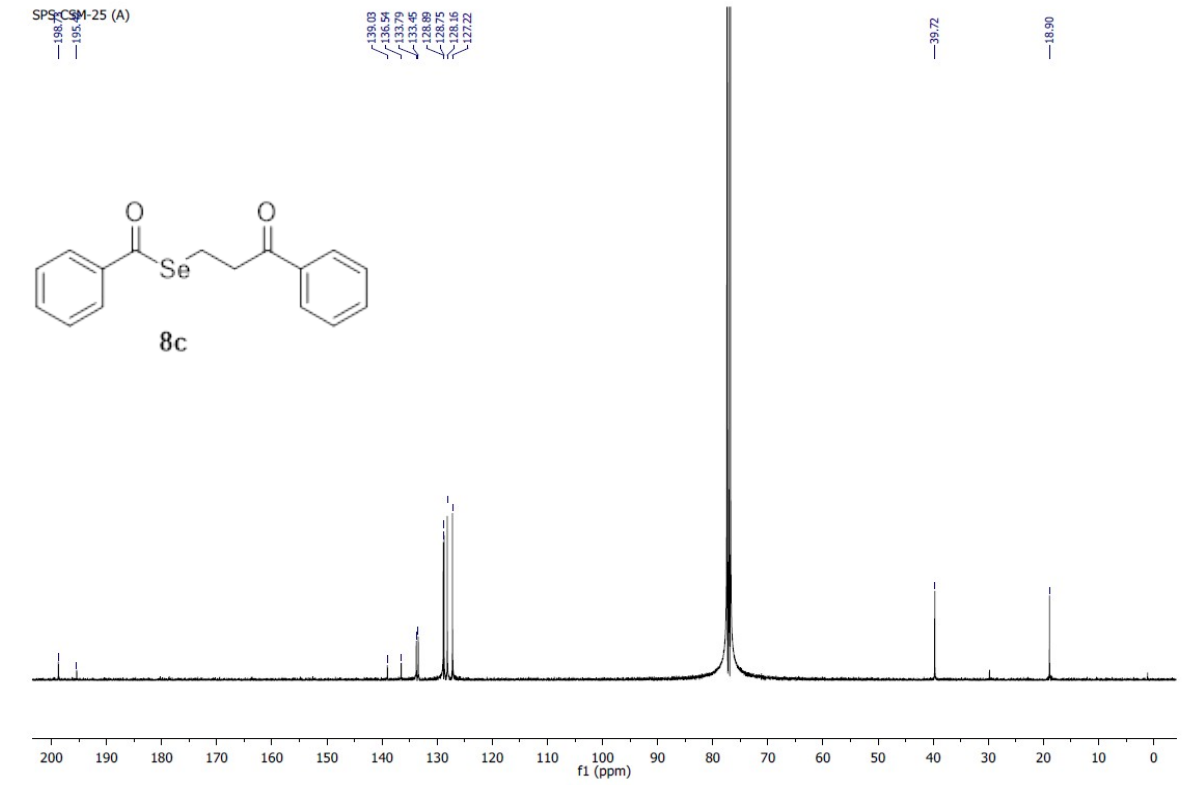
^{1}H NMR spectrum of **8b**.



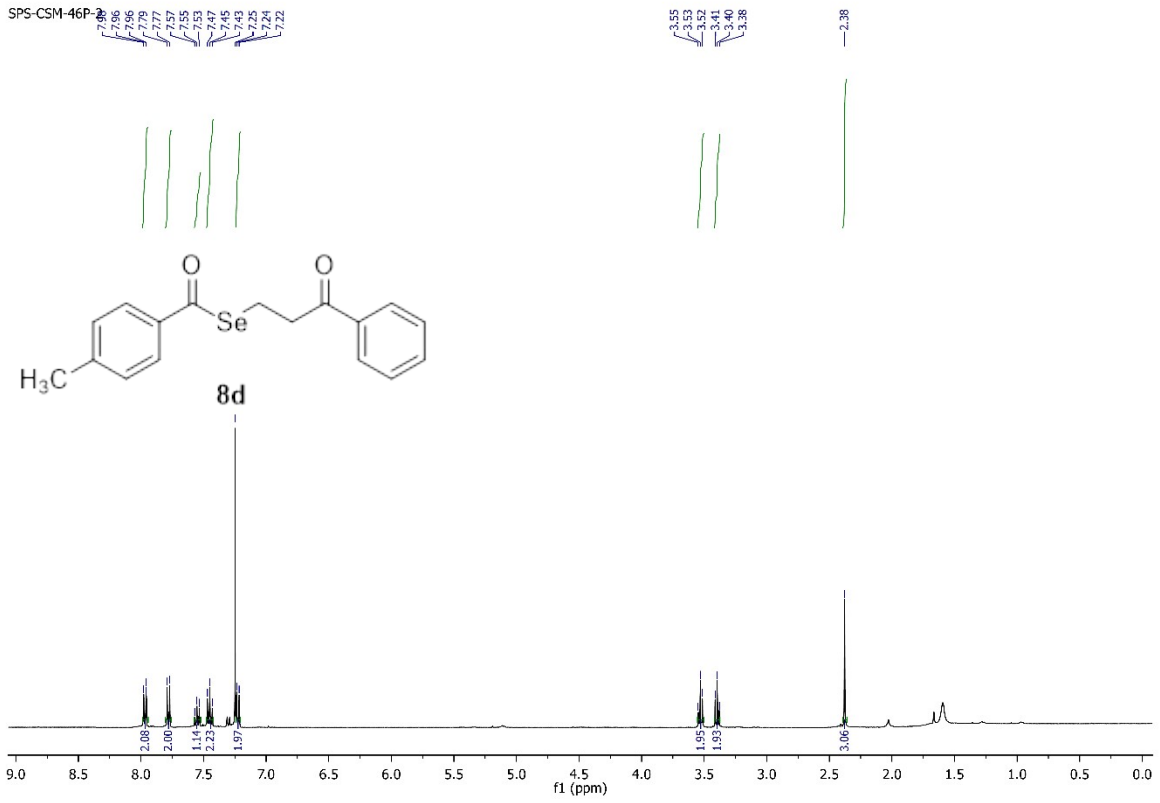
^{13}C NMR spectrum of **8b**.



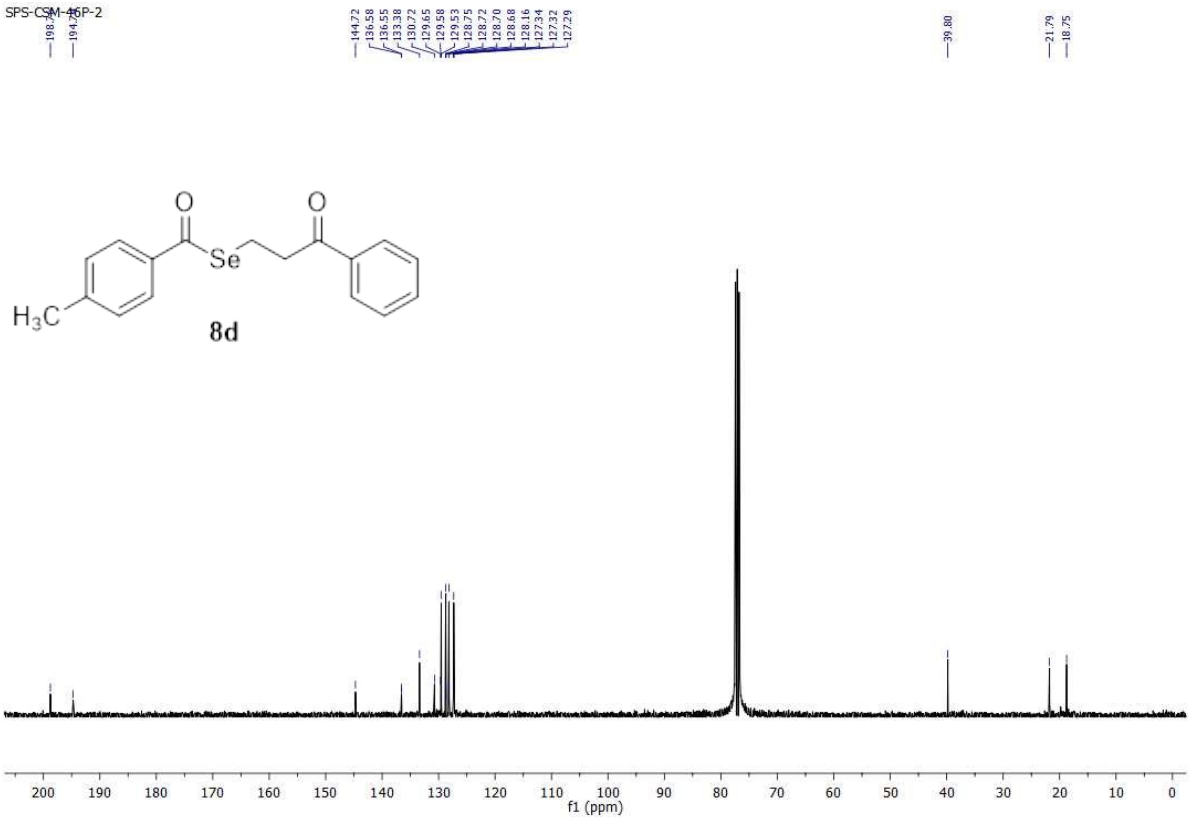
^{1}H NMR spectrum of **8c**.



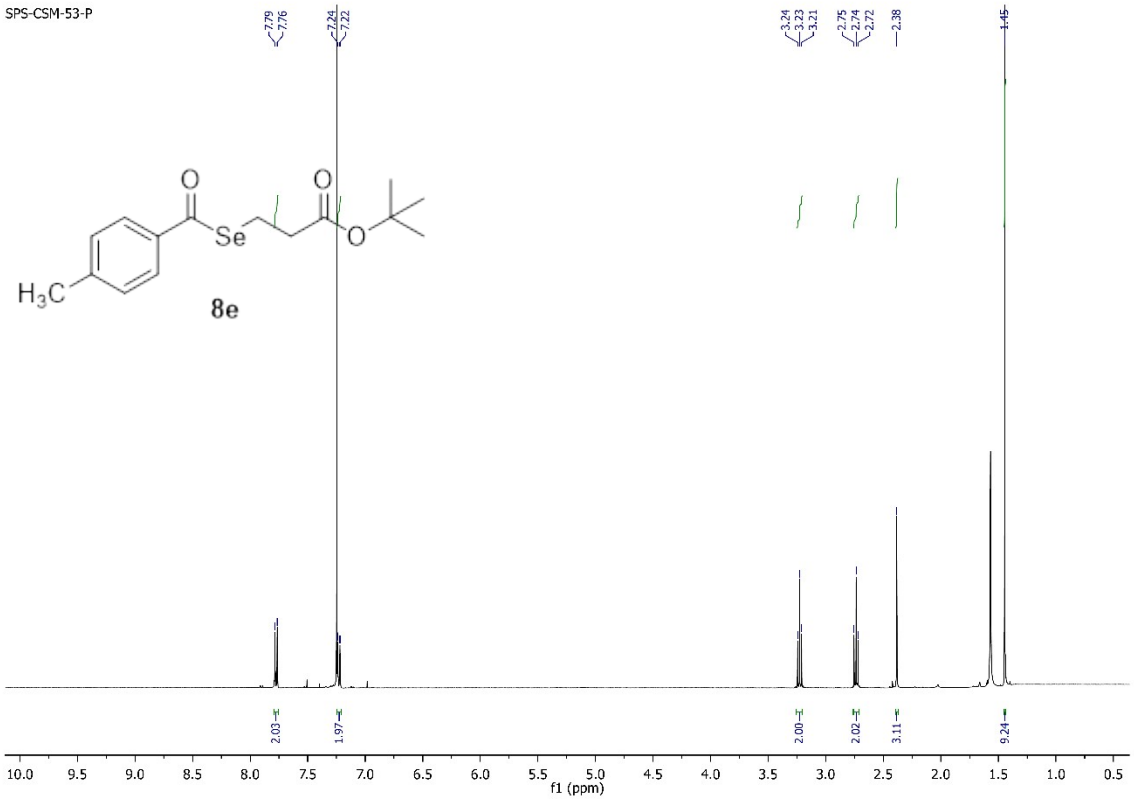
^{13}C NMR spectrum of **8c**.



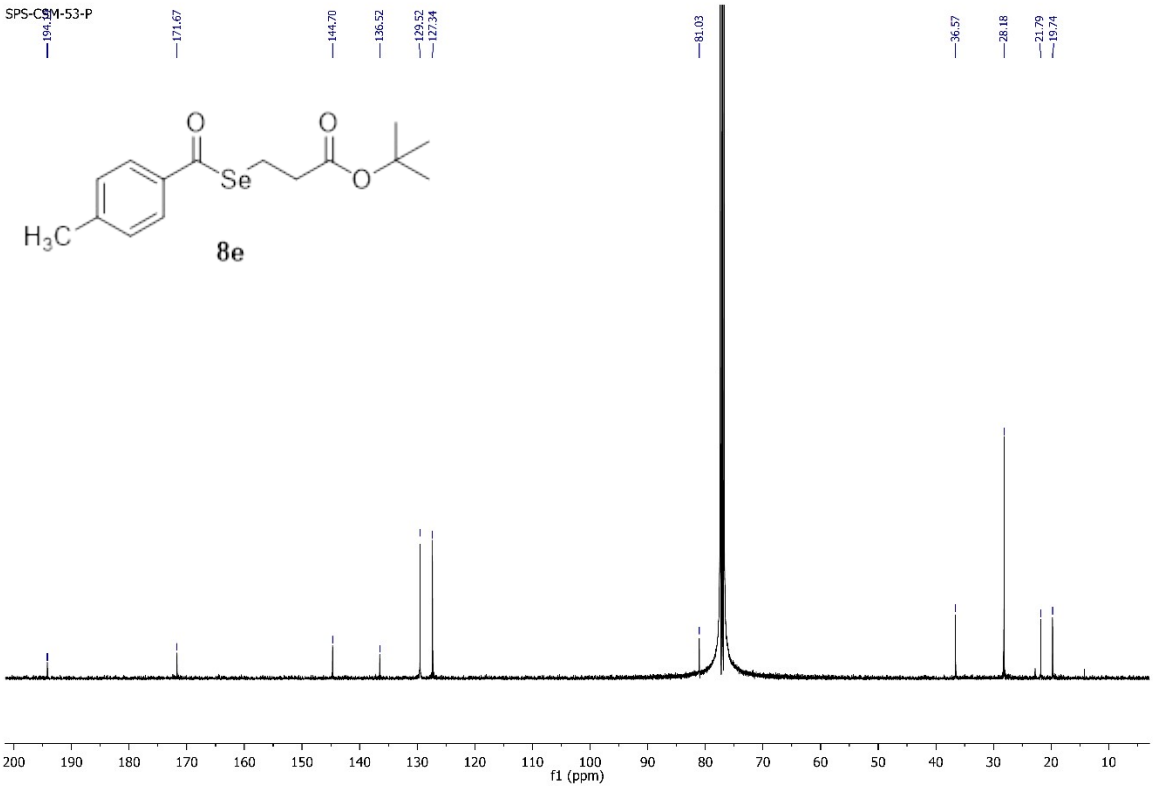
^{1}H NMR spectrum of **8d**.



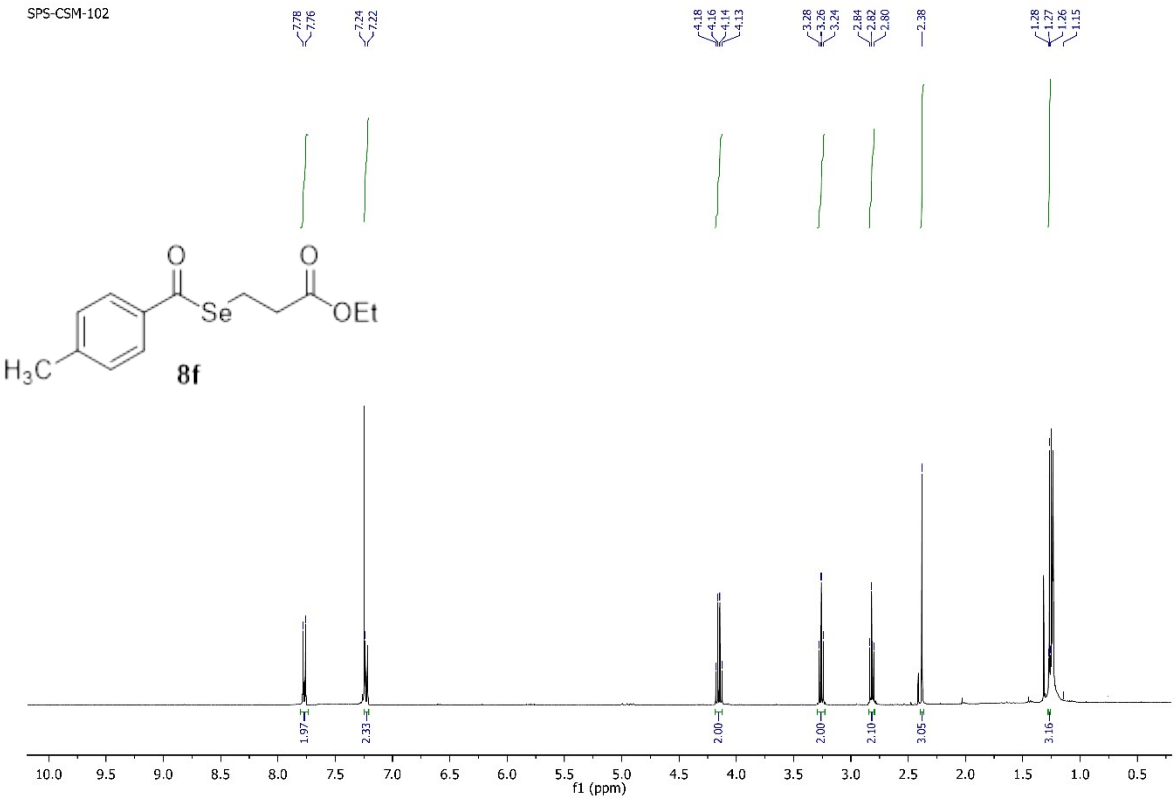
^{13}C NMR spectrum of **8d**.



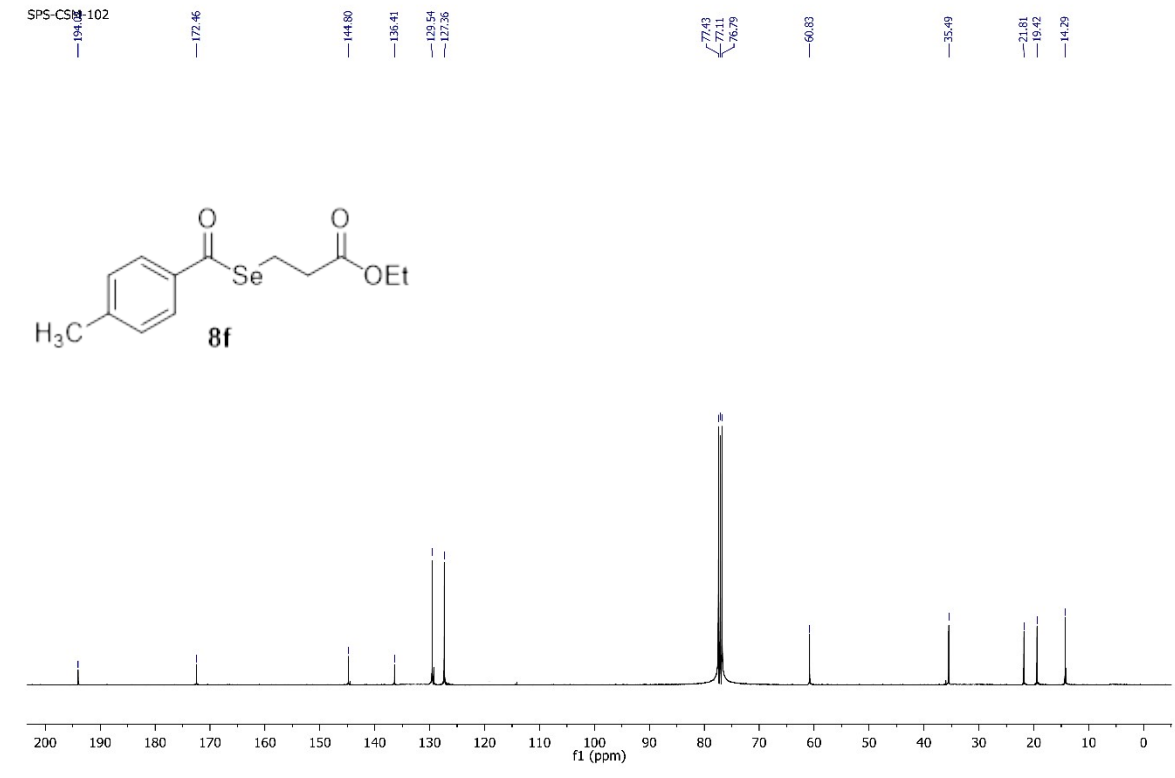
^{1}H NMR spectrum of **8e**.



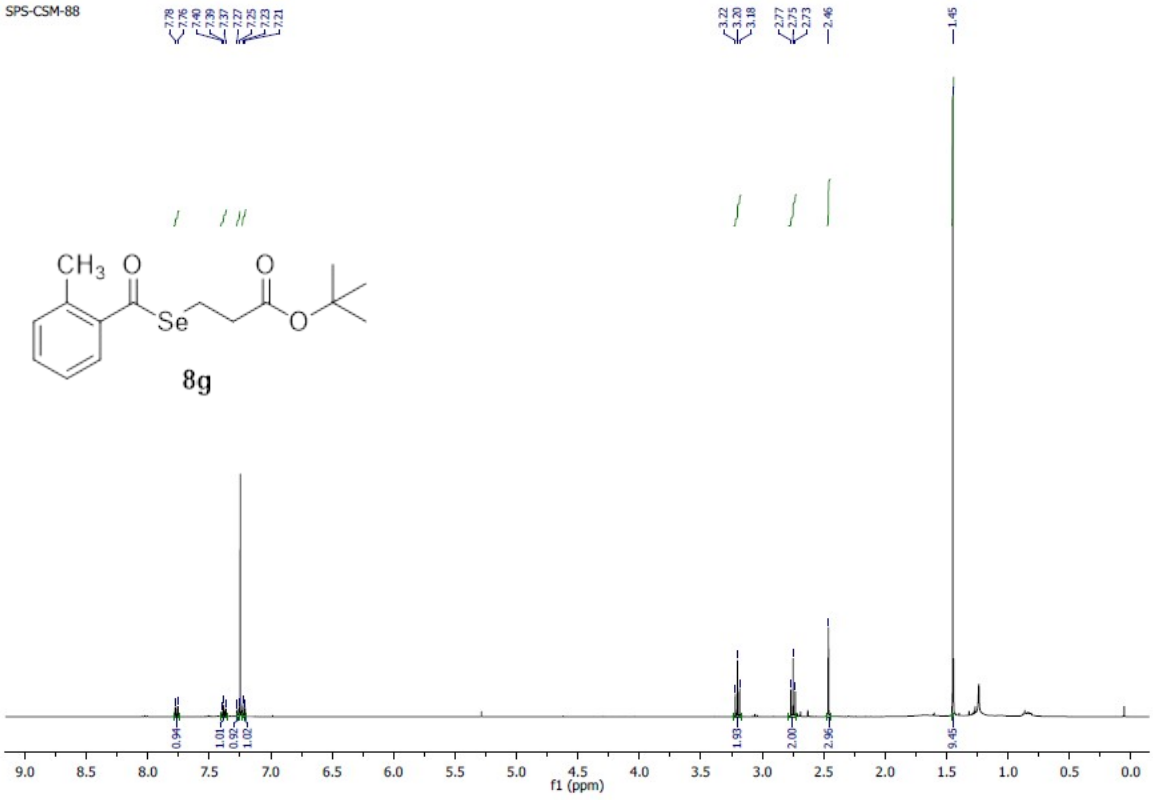
^{13}C NMR spectrum of **8e**.



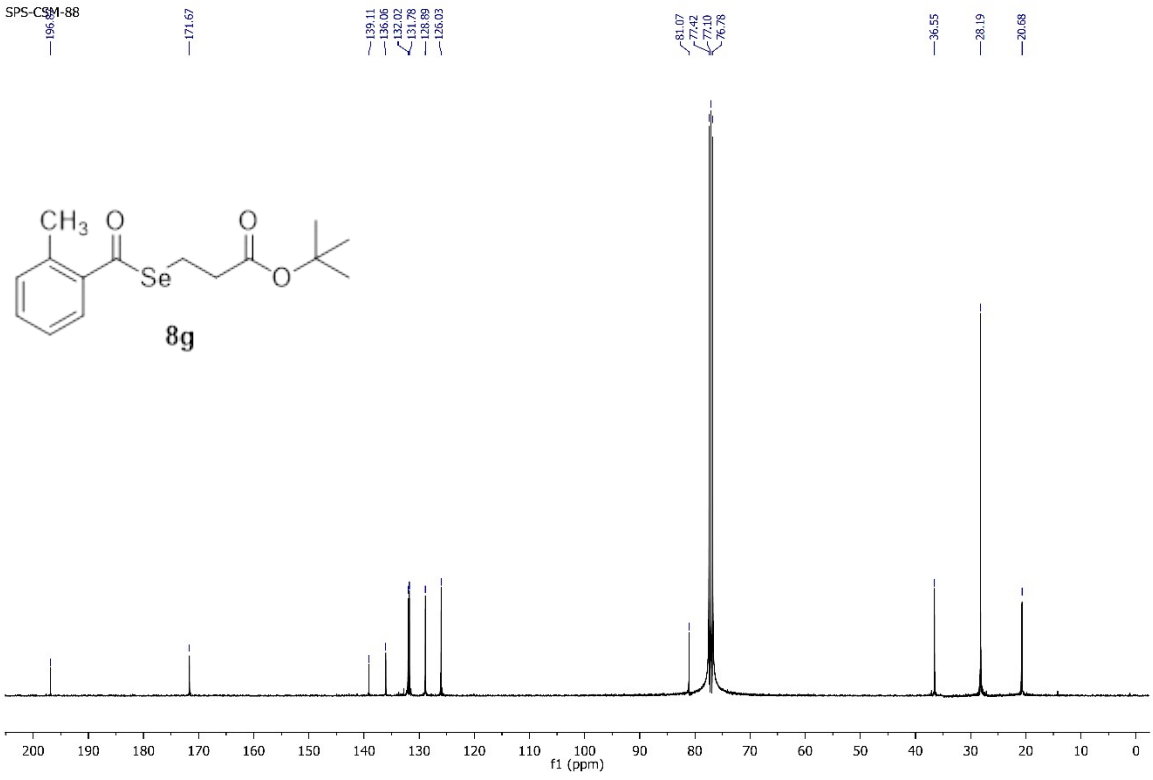
^{1}H NMR spectrum of **8f**.



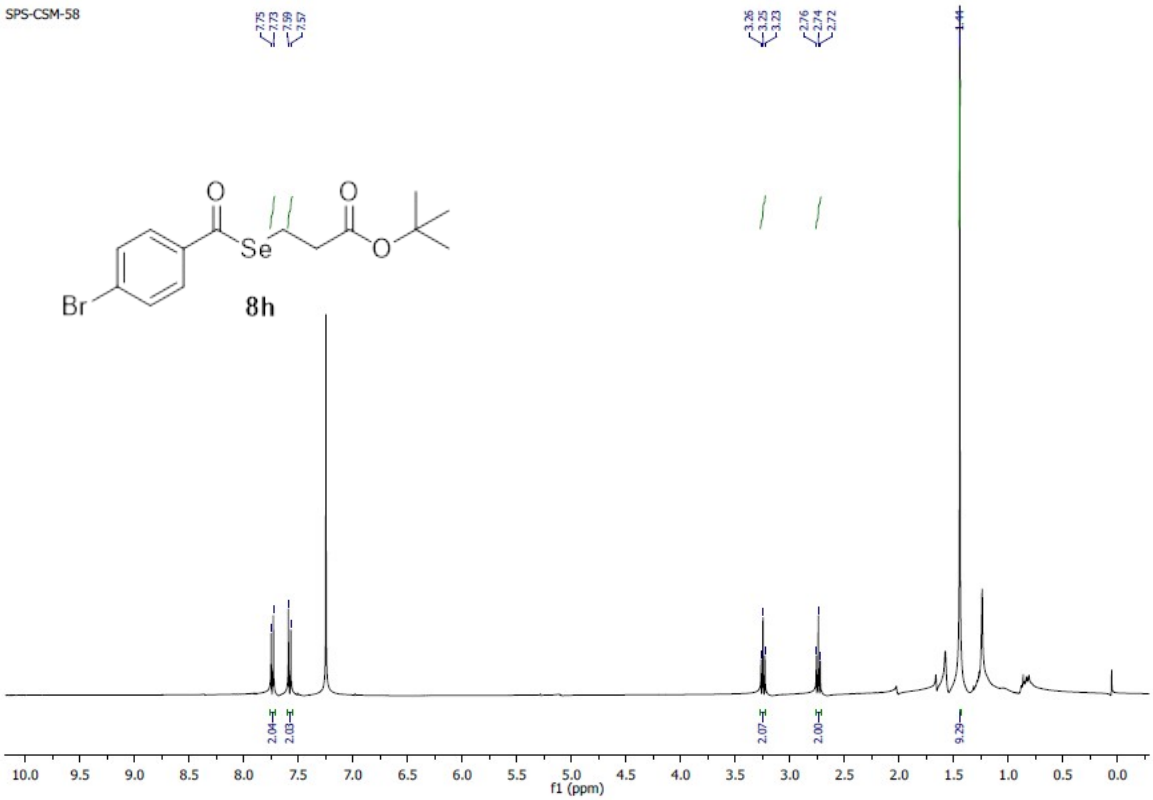
^{13}C NMR spectrum of **8f**.



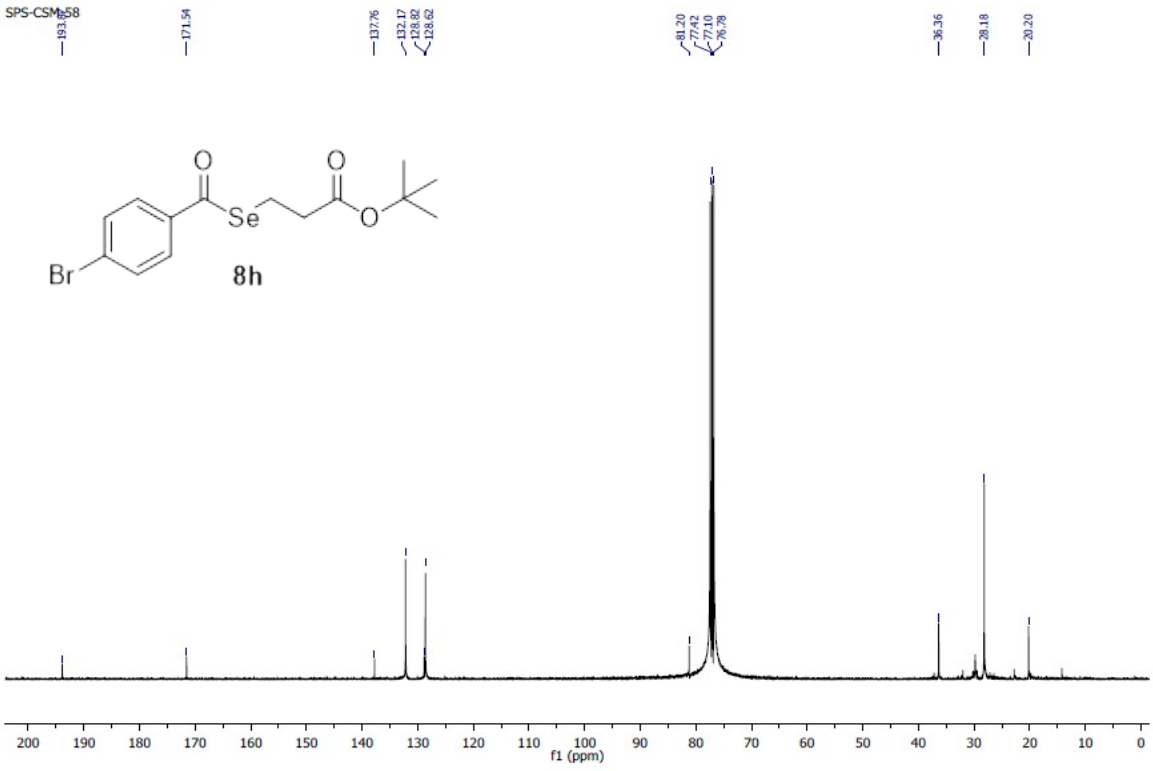
^{1}H NMR spectrum of **8g**.



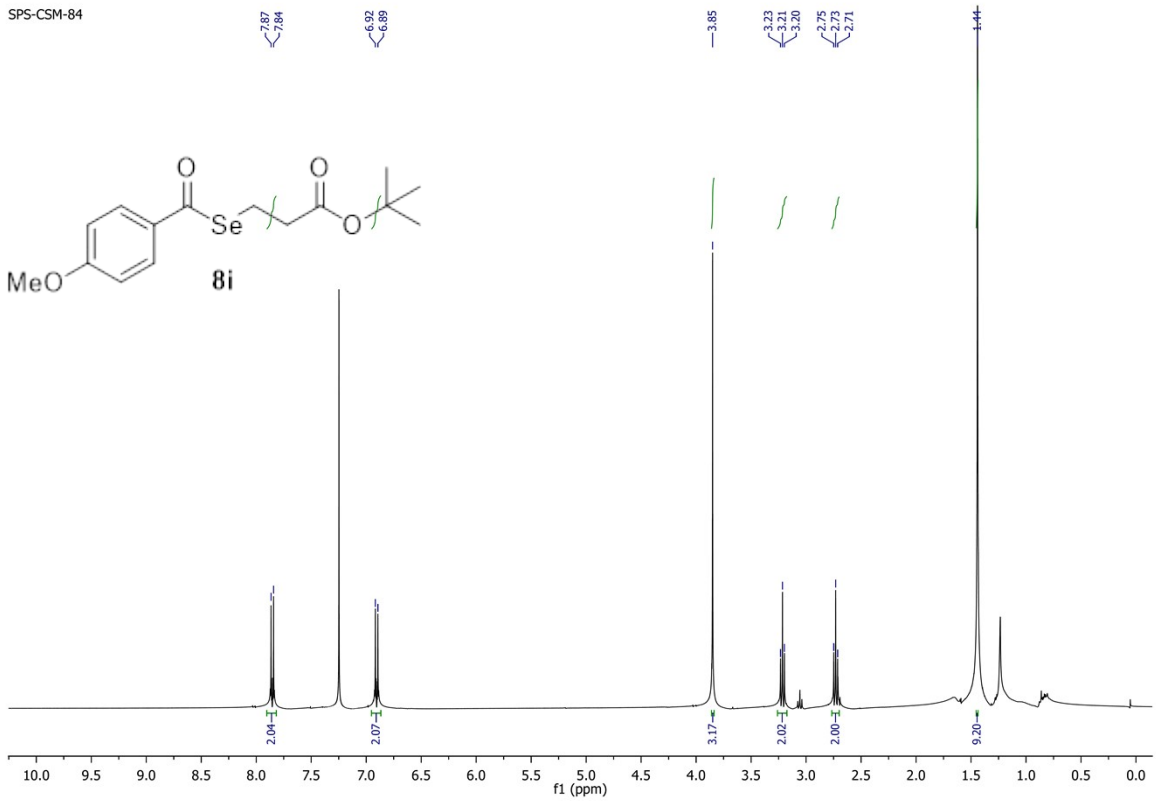
^{13}C NMR spectrum of **8g**.



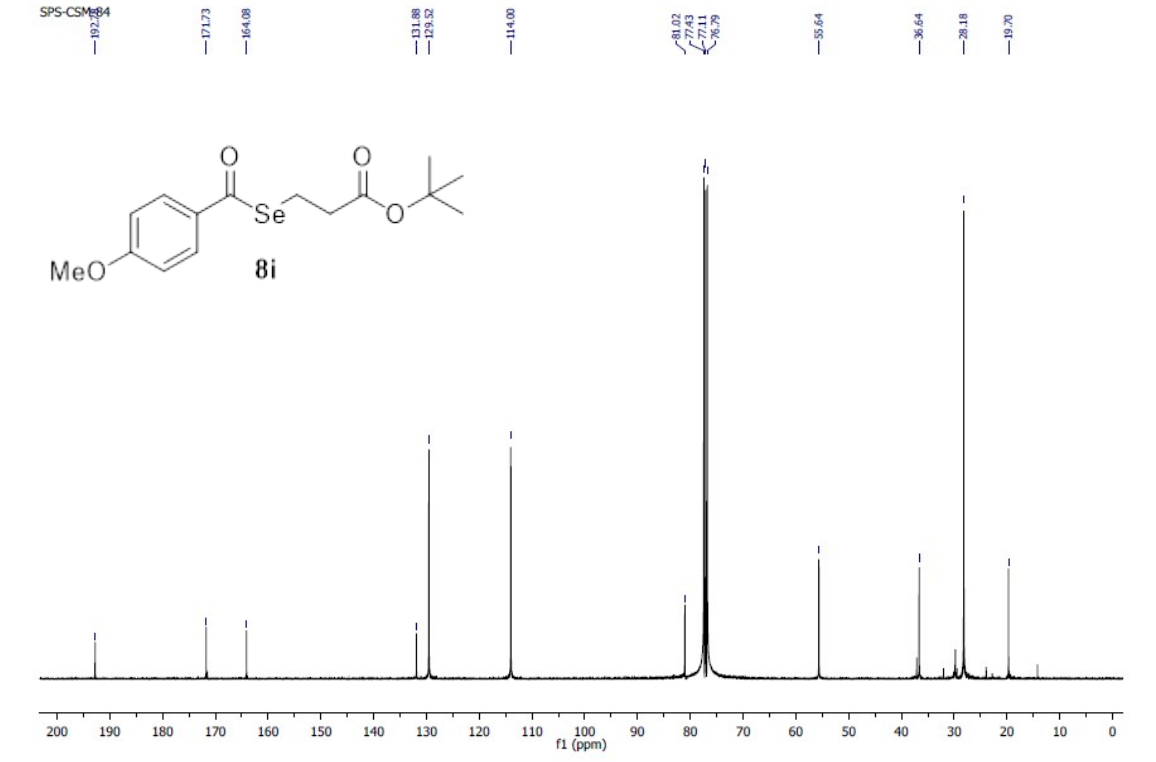
^{1}H NMR spectrum of **8h**.



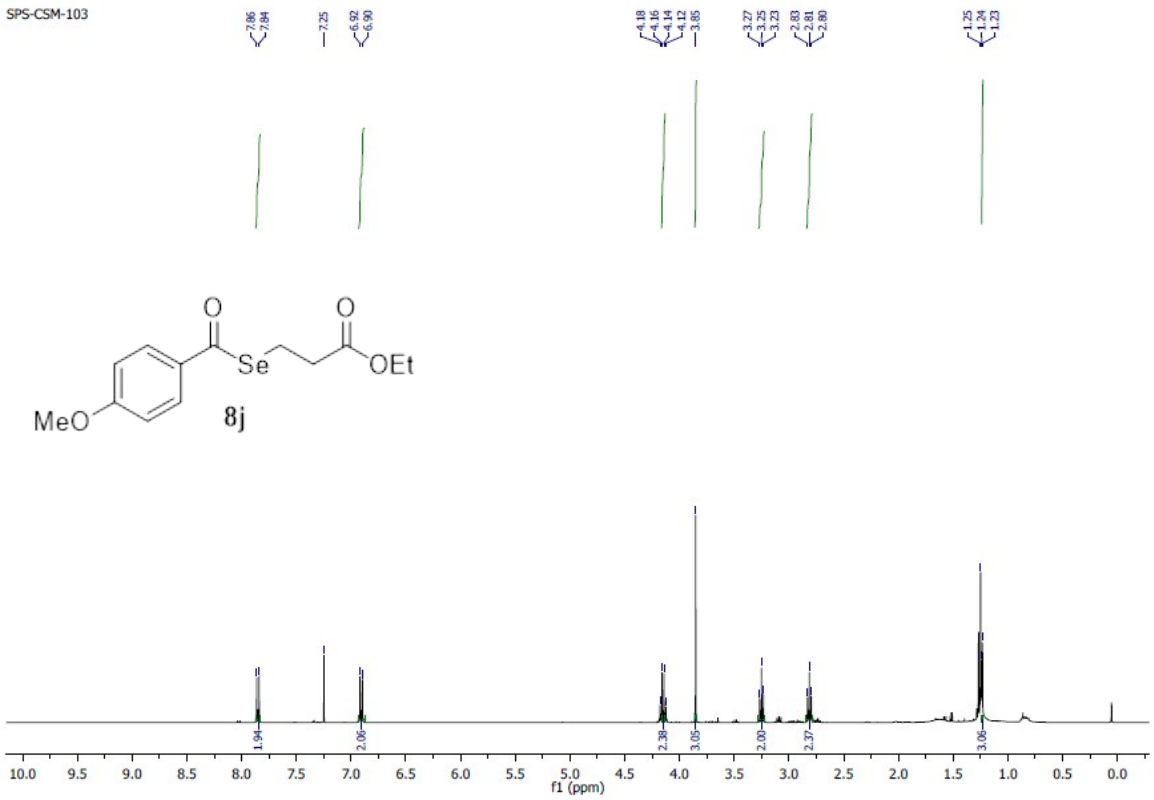
^{13}C NMR spectrum of **8h**.



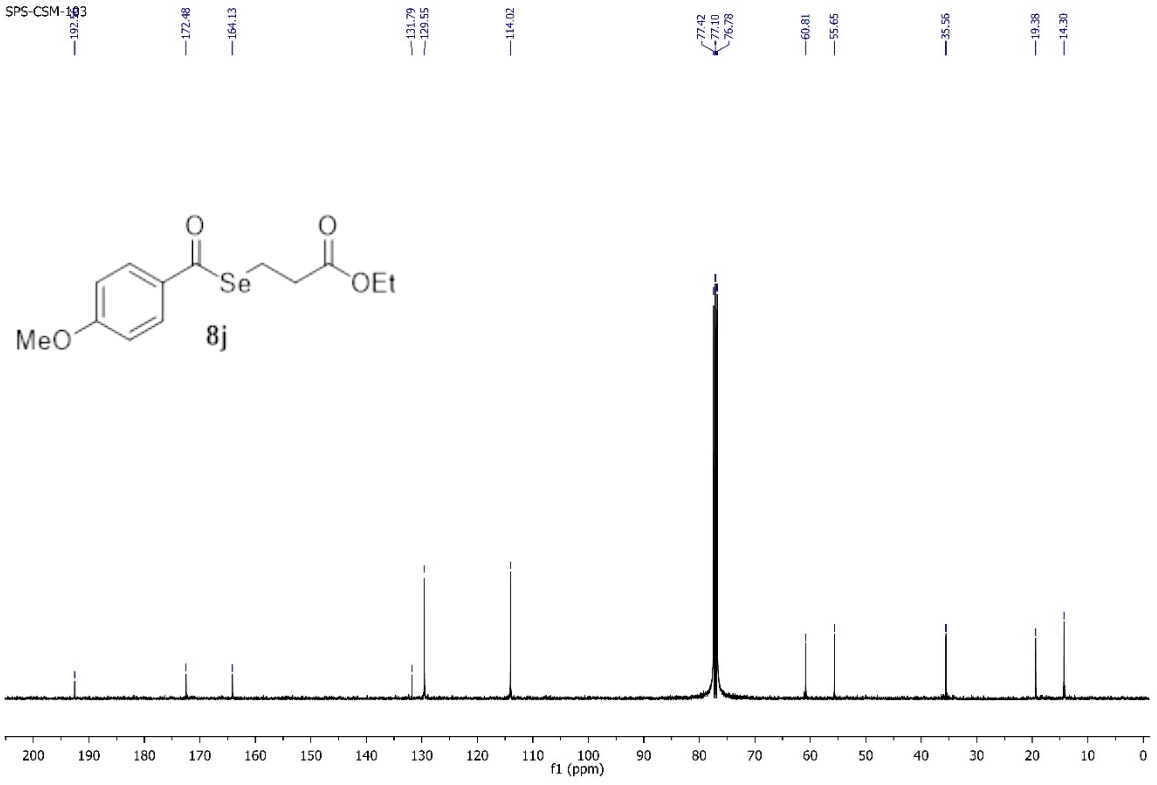
^{1}H NMR spectrum of **8i**.



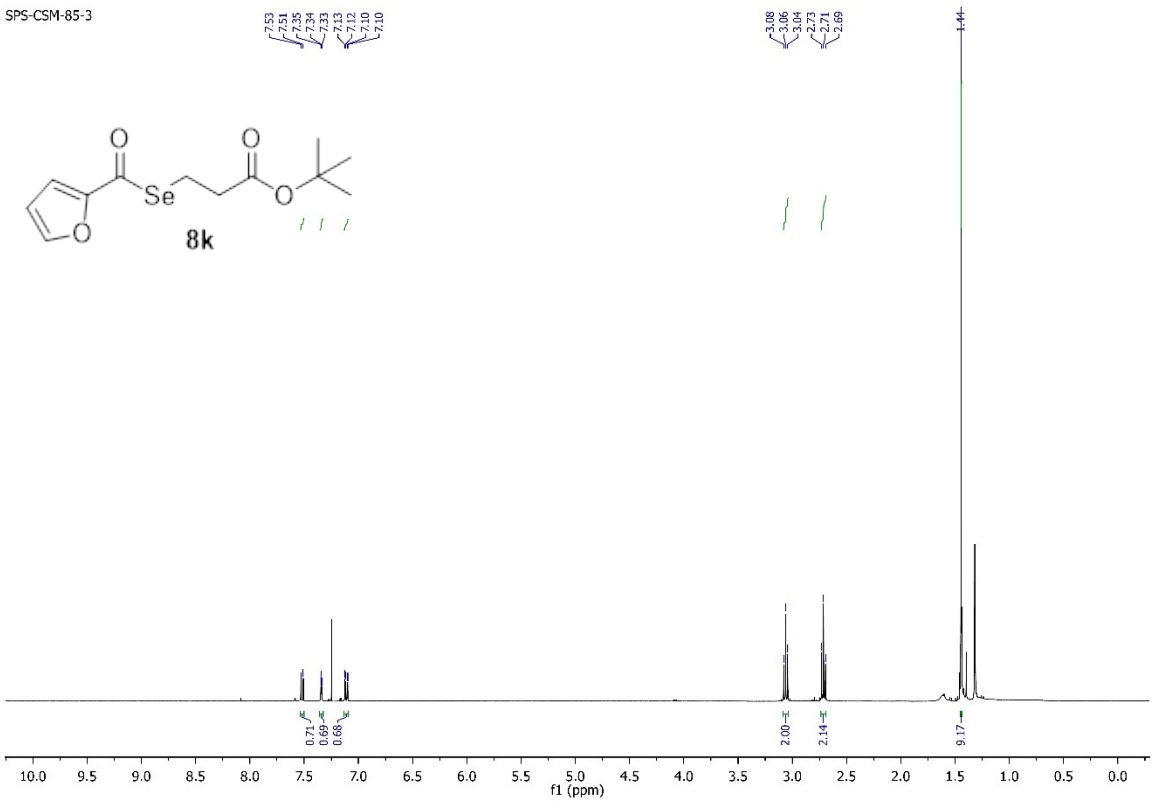
^{13}C NMR spectrum of **8i**.



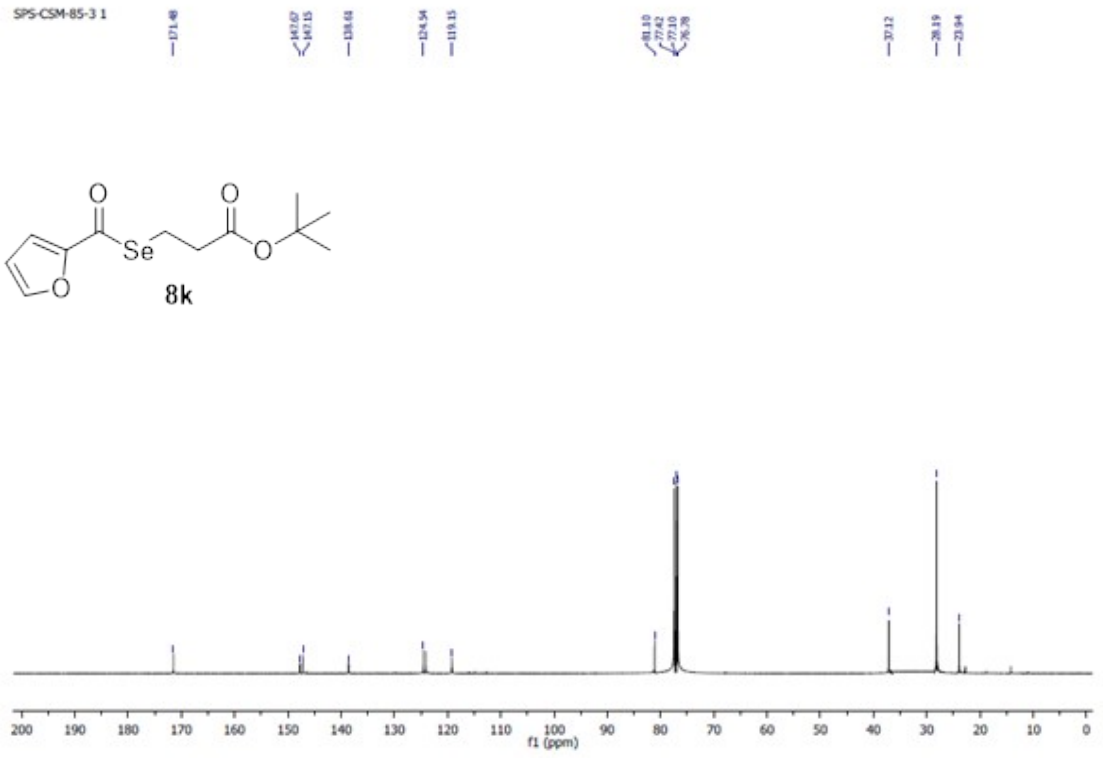
^{1}H NMR spectrum of **8j**.



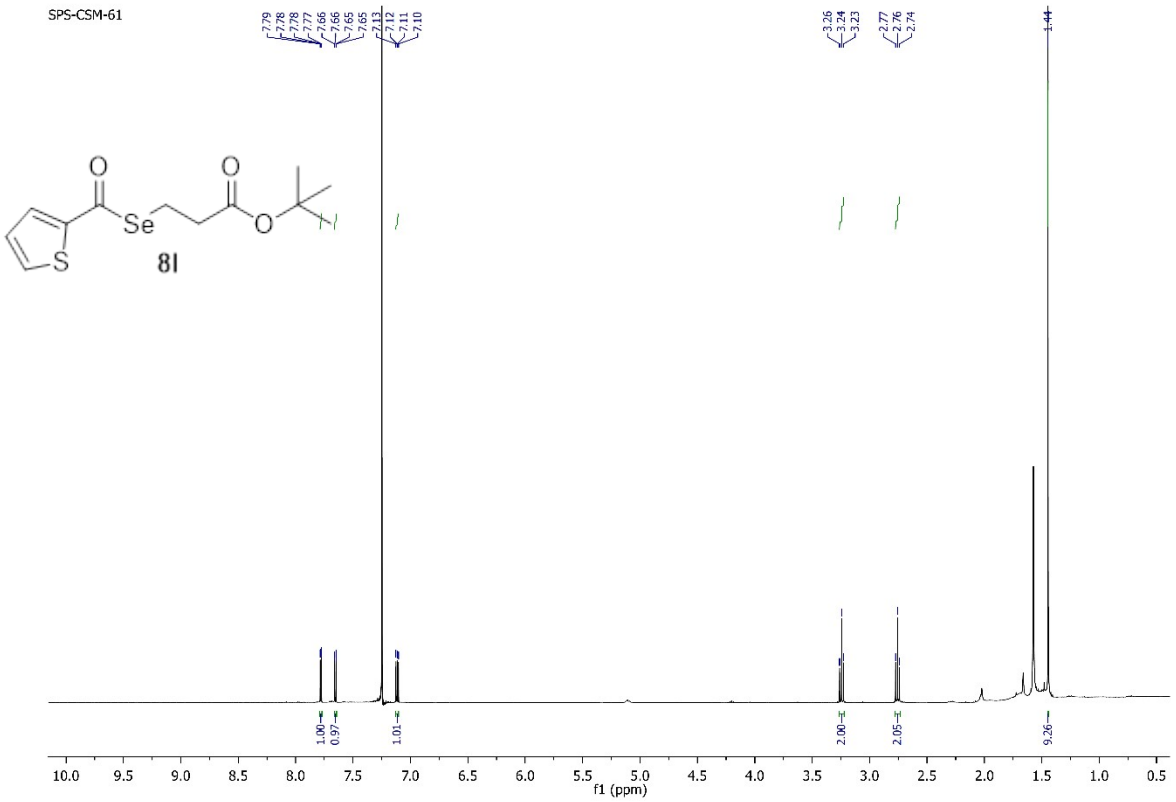
^{13}C NMR spectrum of **8j**.



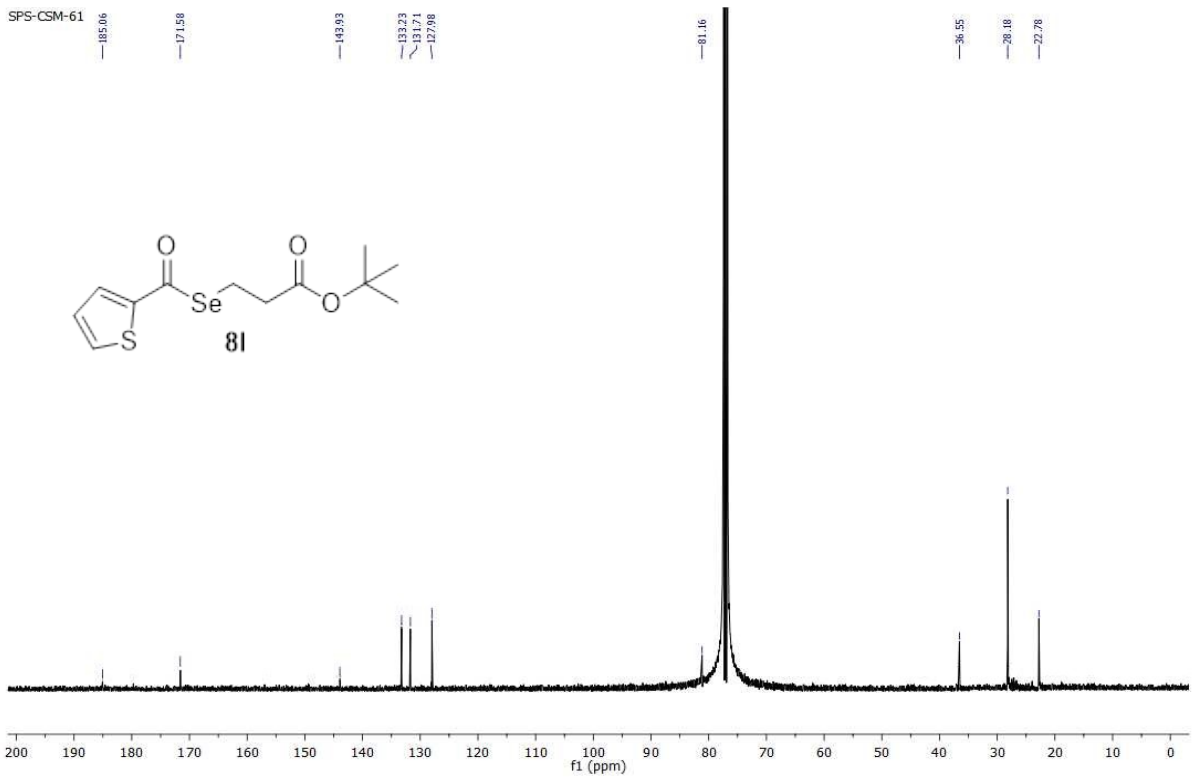
^{1}H NMR spectrum of **8k**.



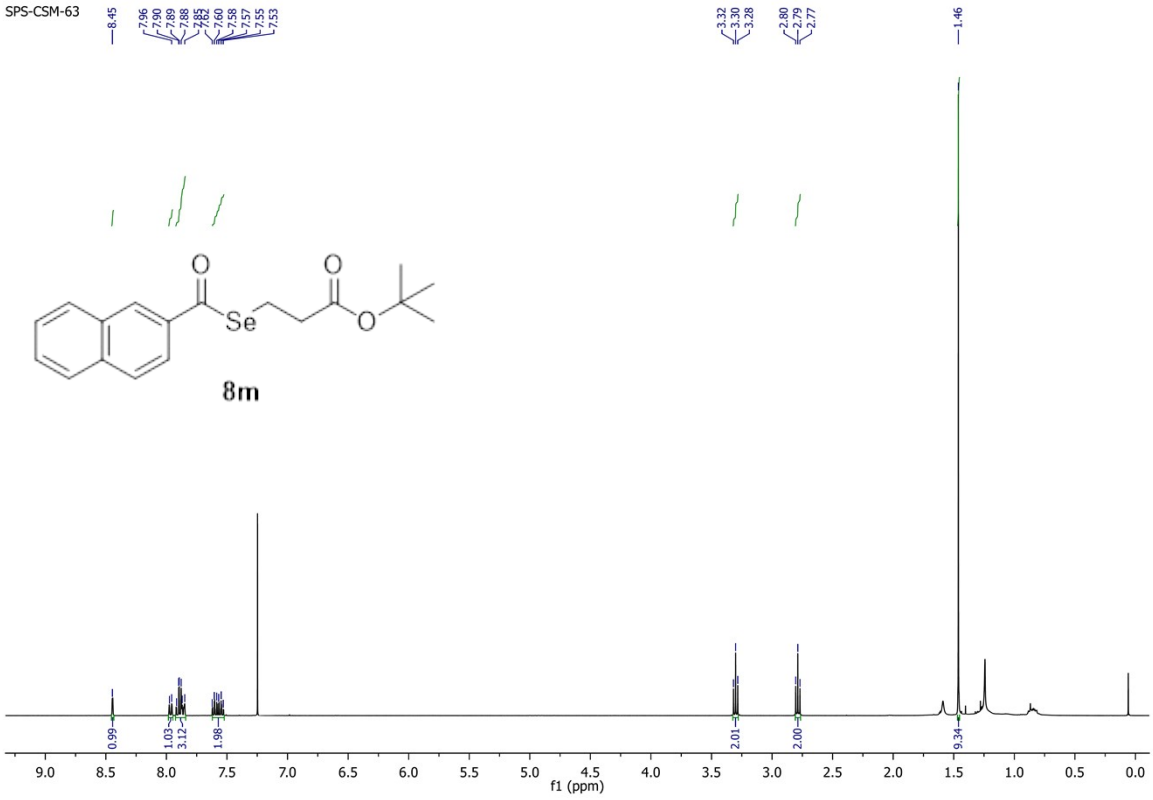
^{13}C NMR spectrum of **8k**.



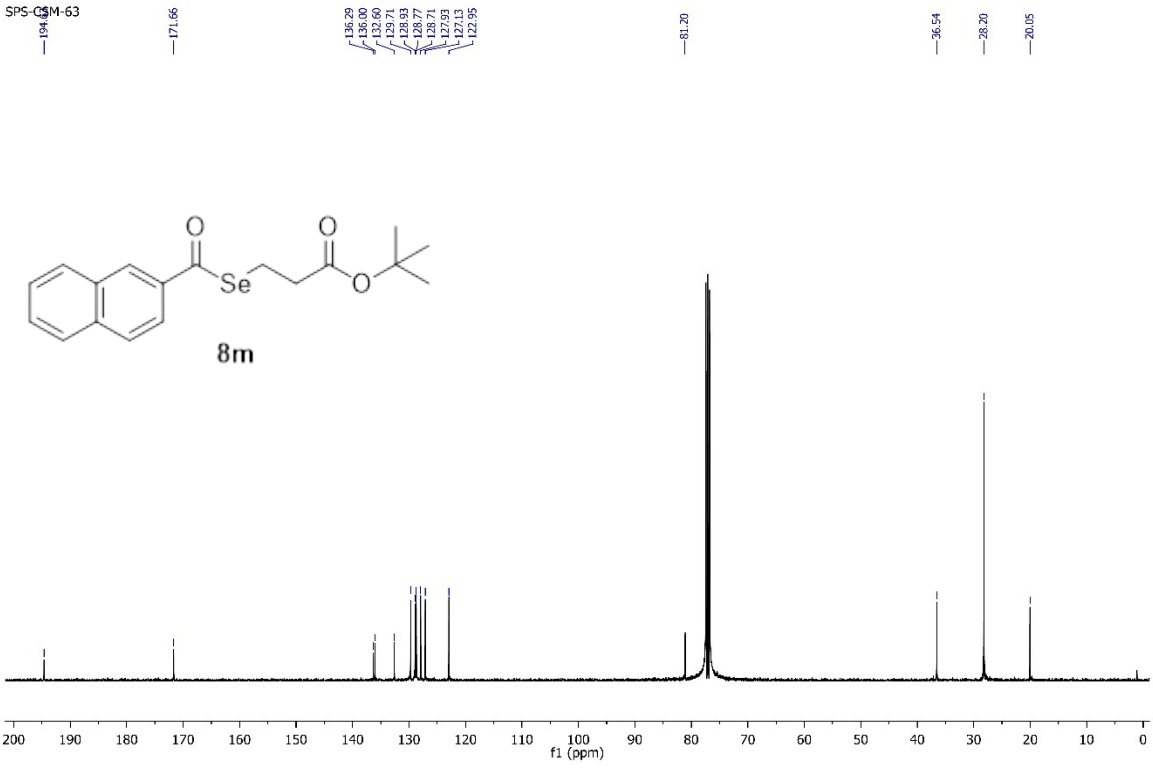
^{1}H NMR spectrum of **8l**.



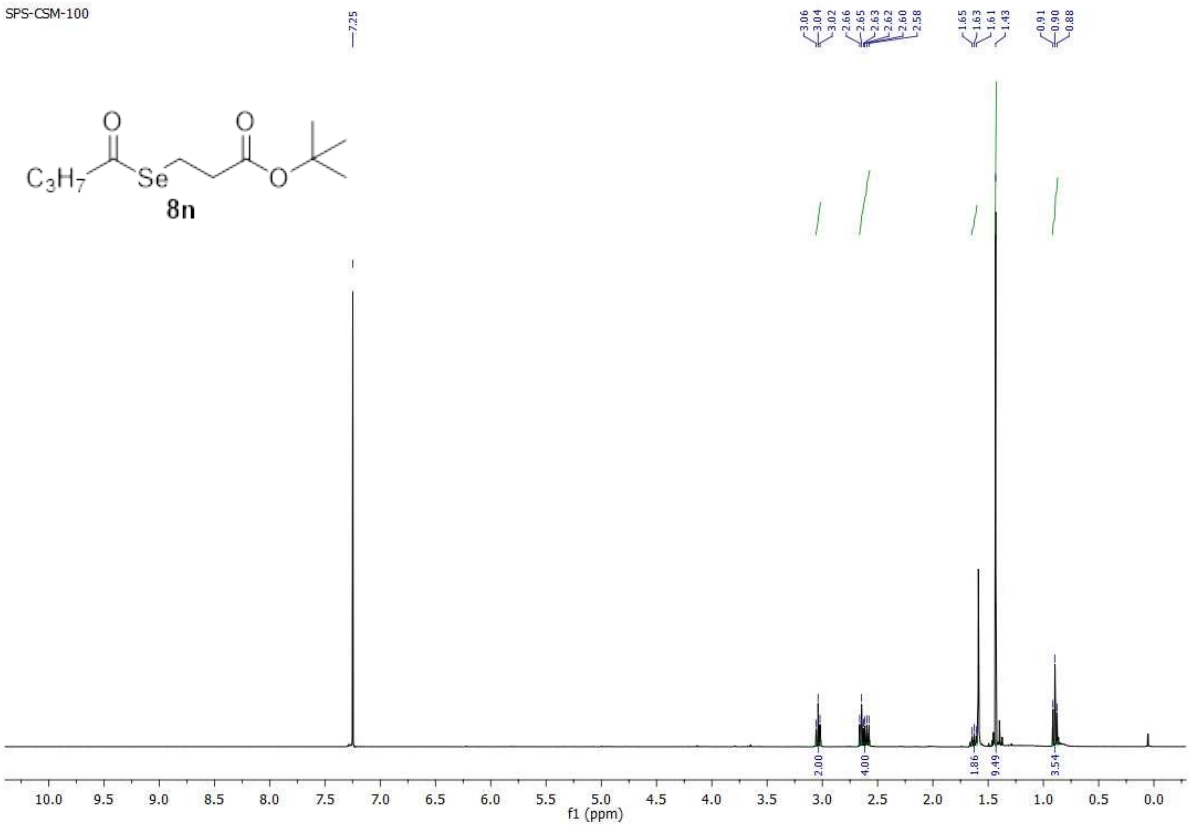
^{13}C NMR spectrum of **8l**.



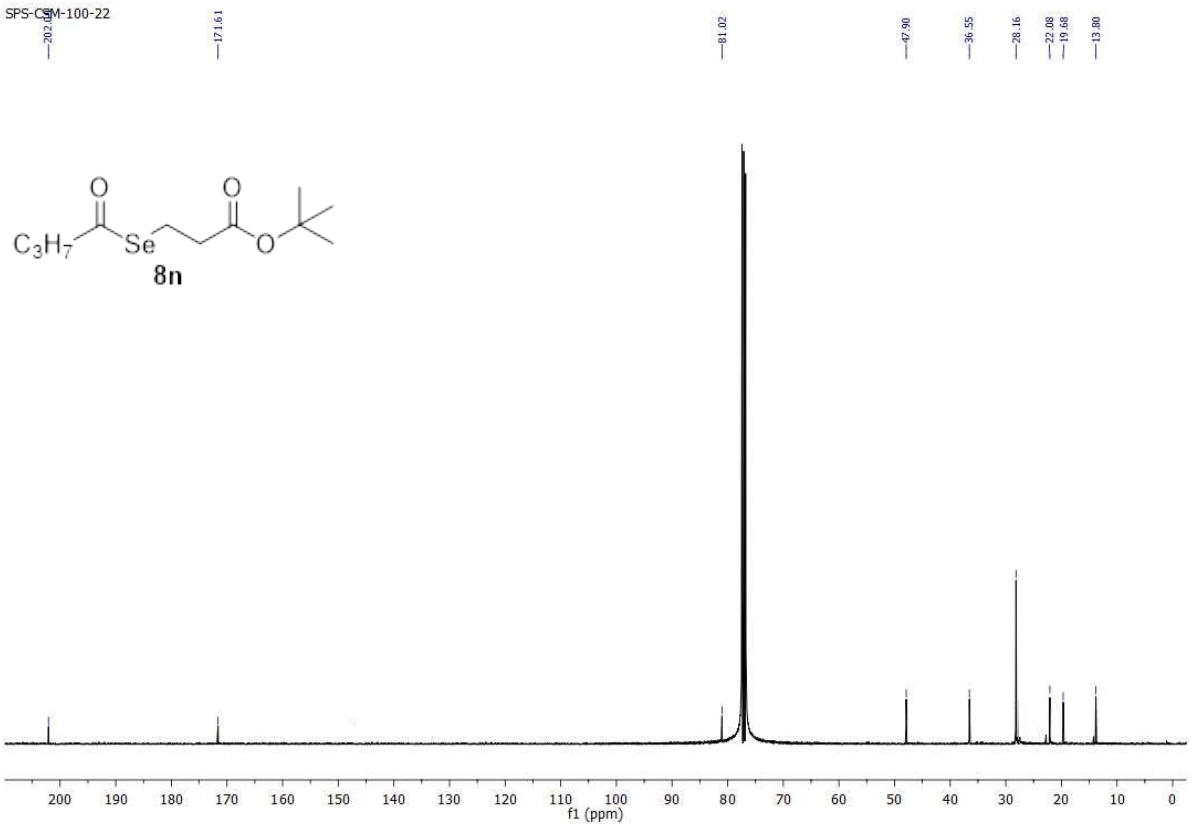
^{1}H NMR spectrum of **8m**.



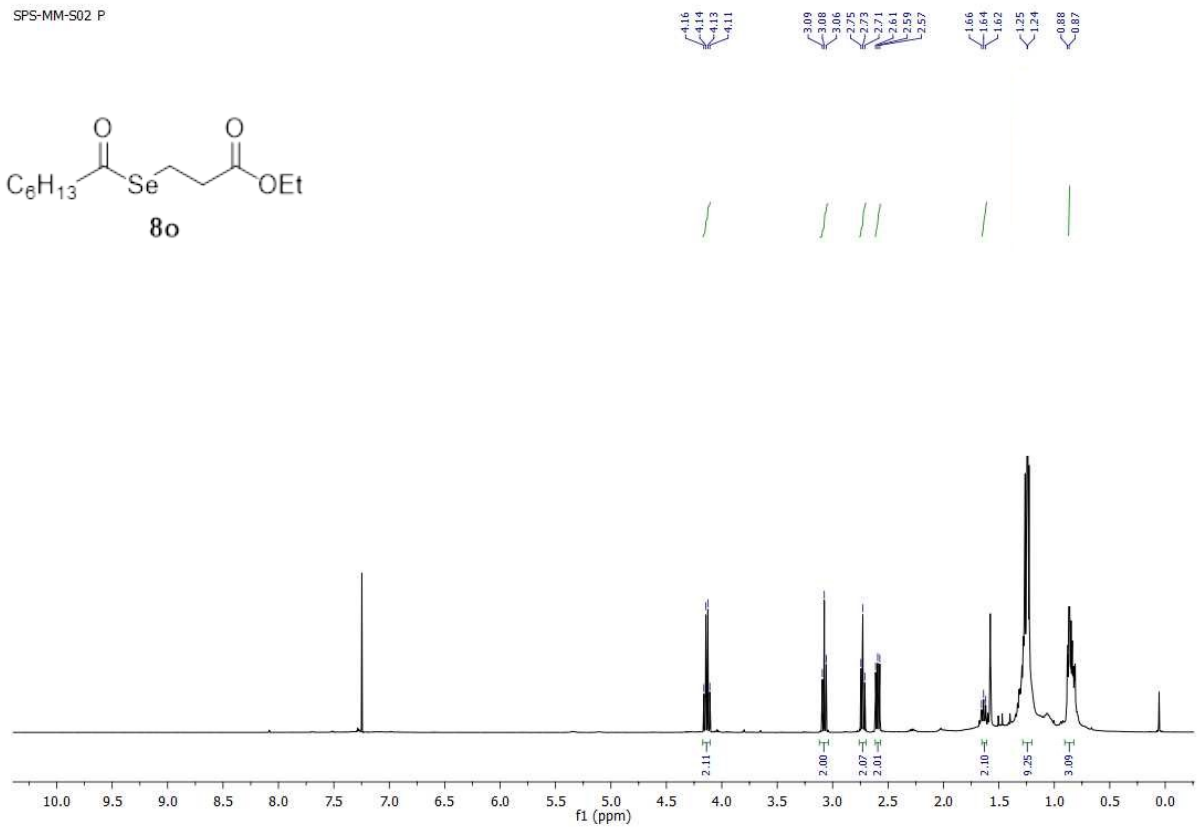
^{13}C NMR spectrum of **8m**.



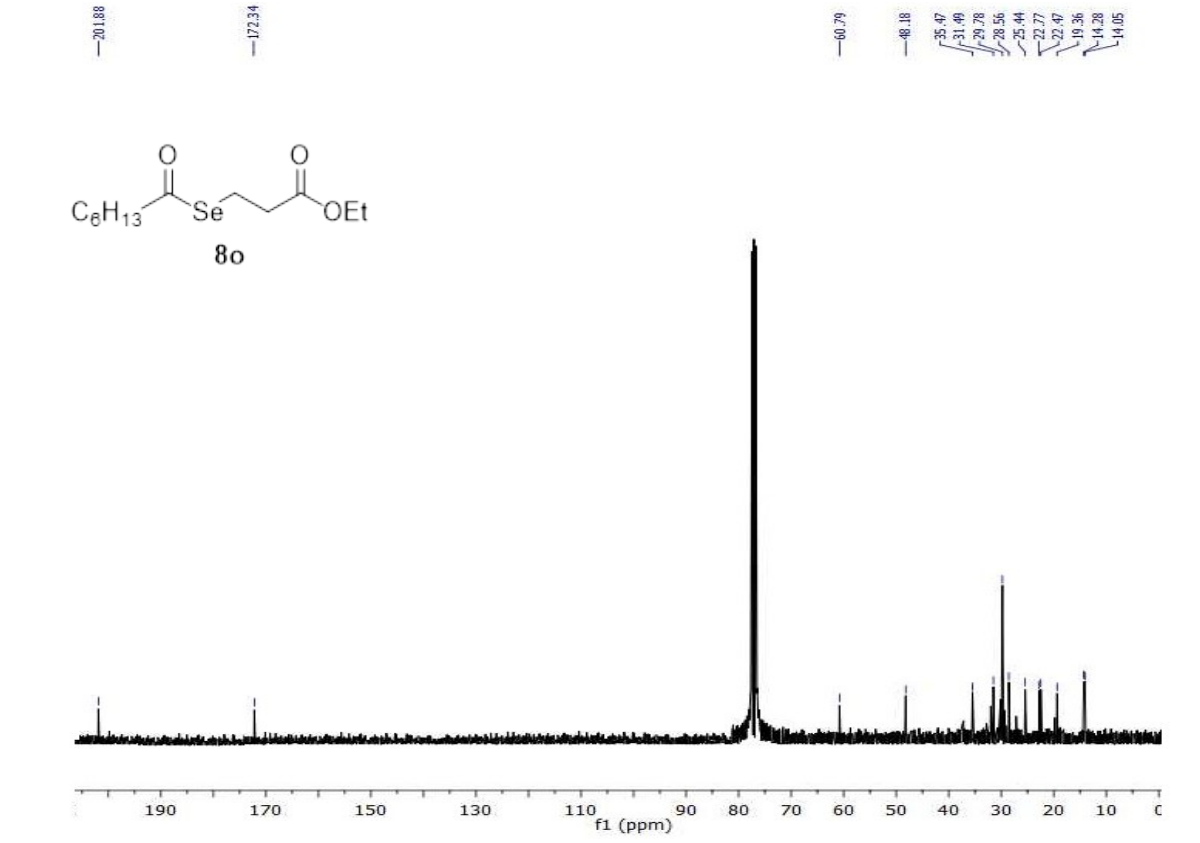
^{1}H NMR spectrum of **8n**.



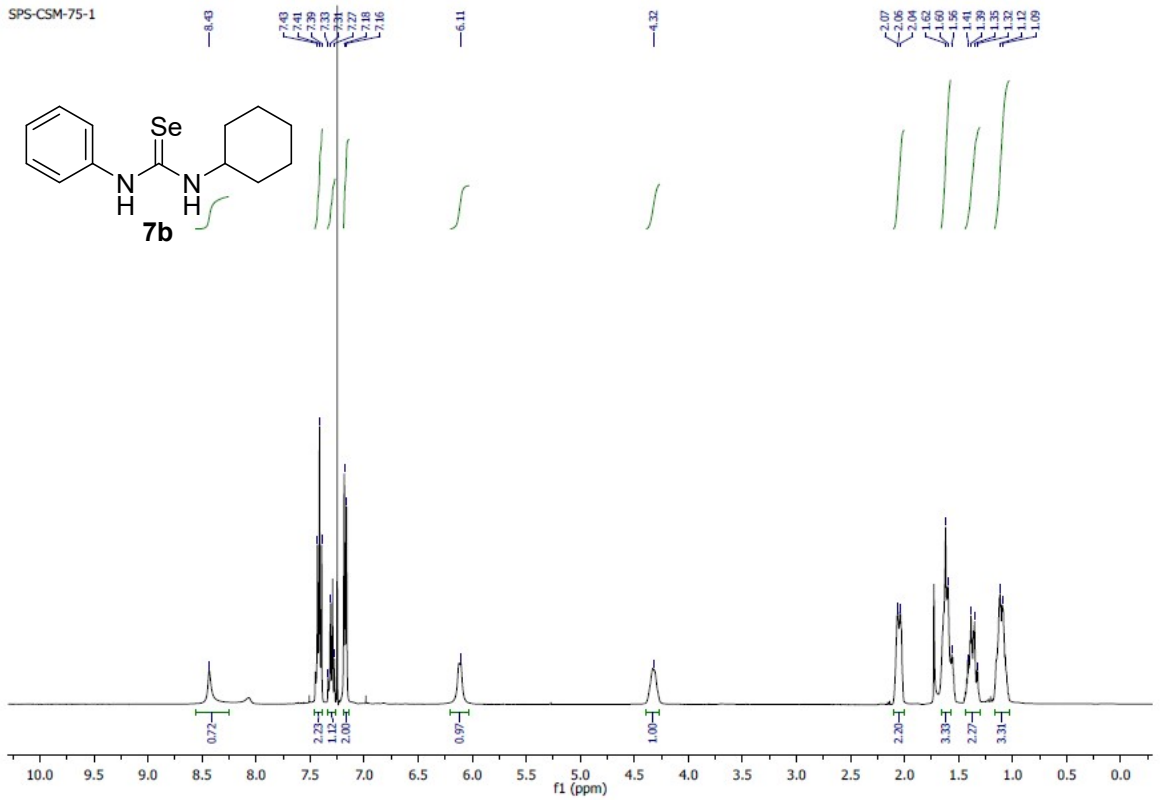
^{13}C NMR spectrum of **8n**.



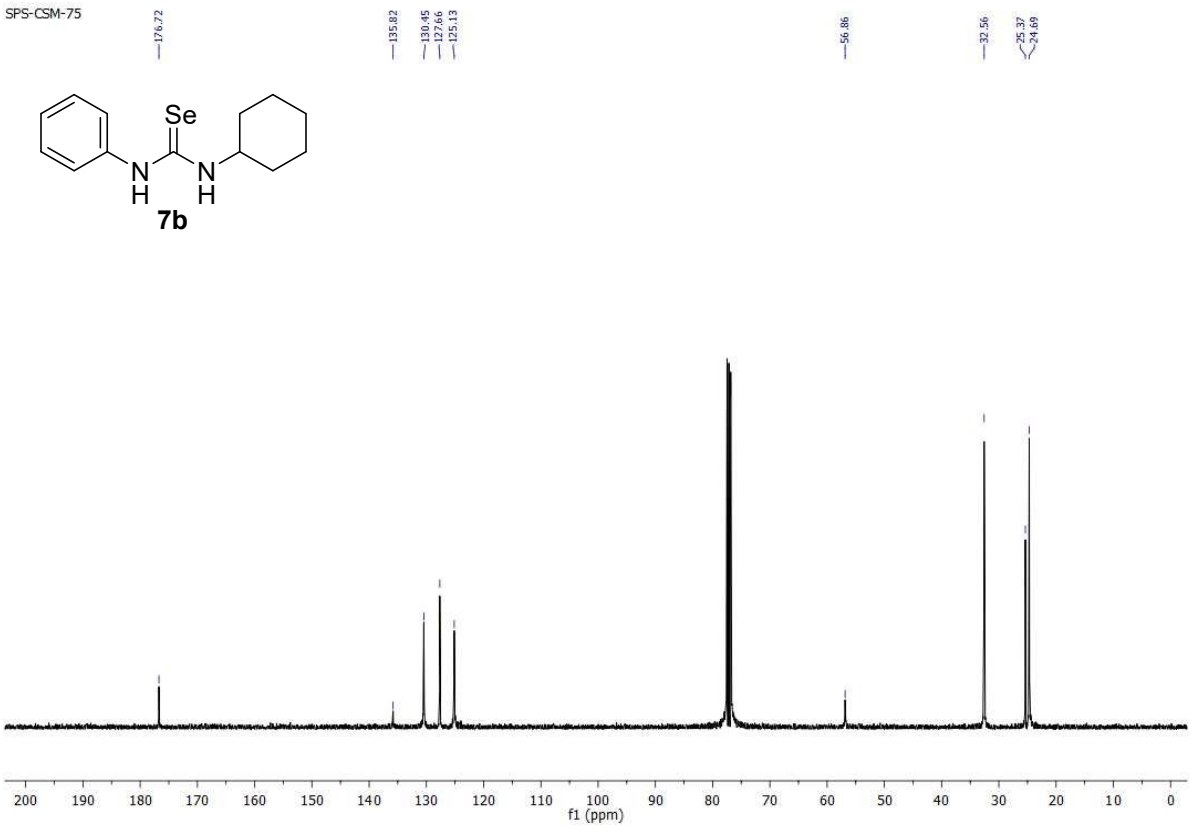
^{1}H NMR spectrum of **8o**.



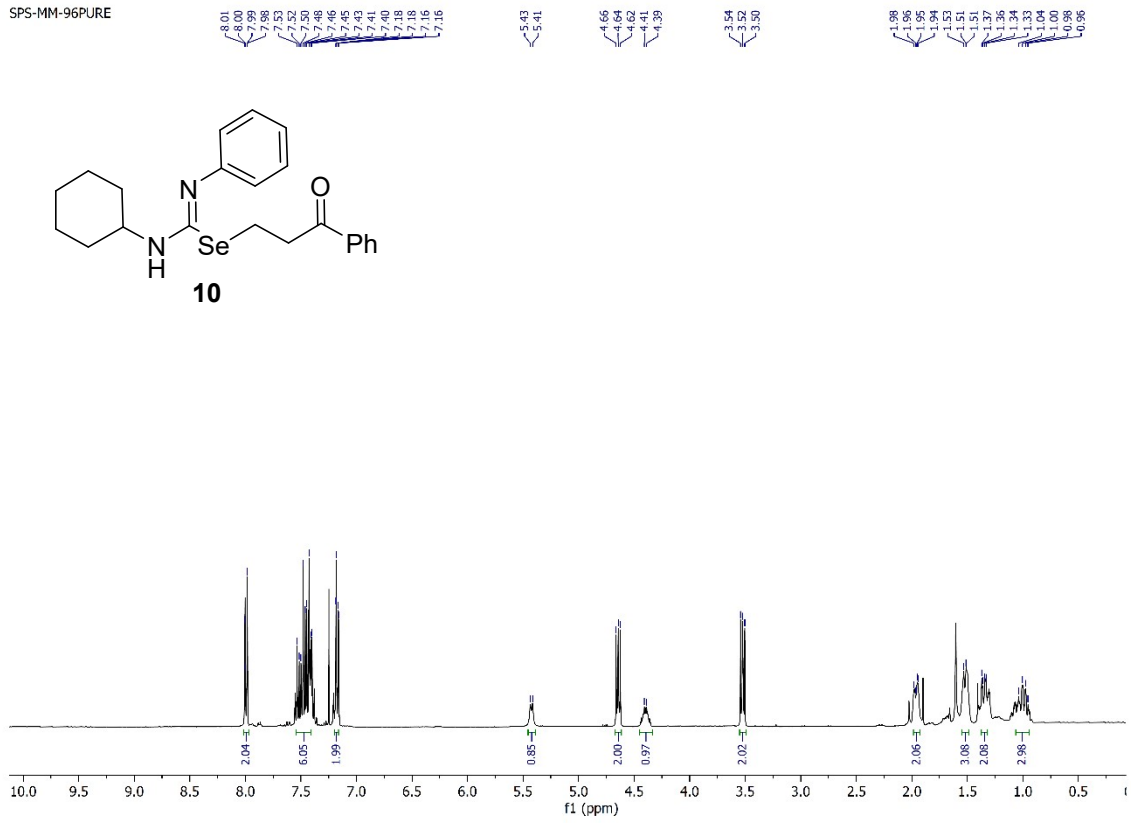
^{13}C NMR spectrum of **8o**.



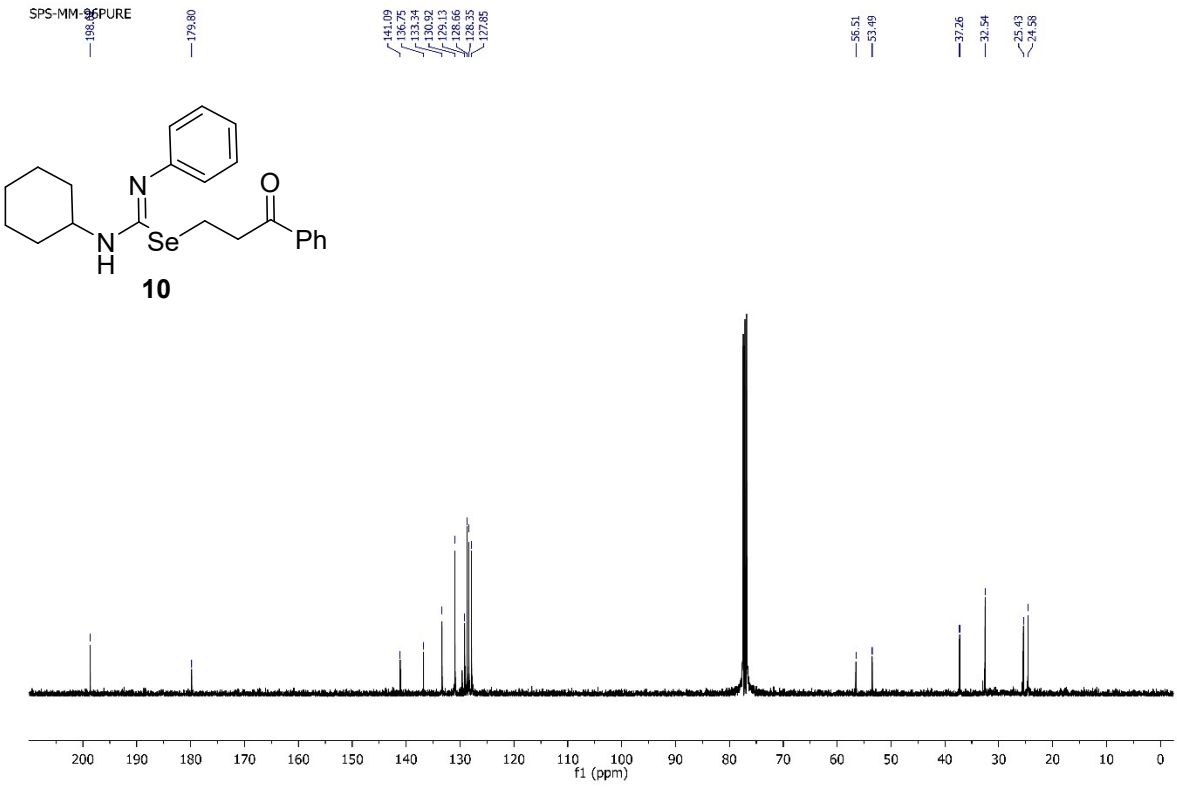
^{1}H NMR spectrum of **7b**.



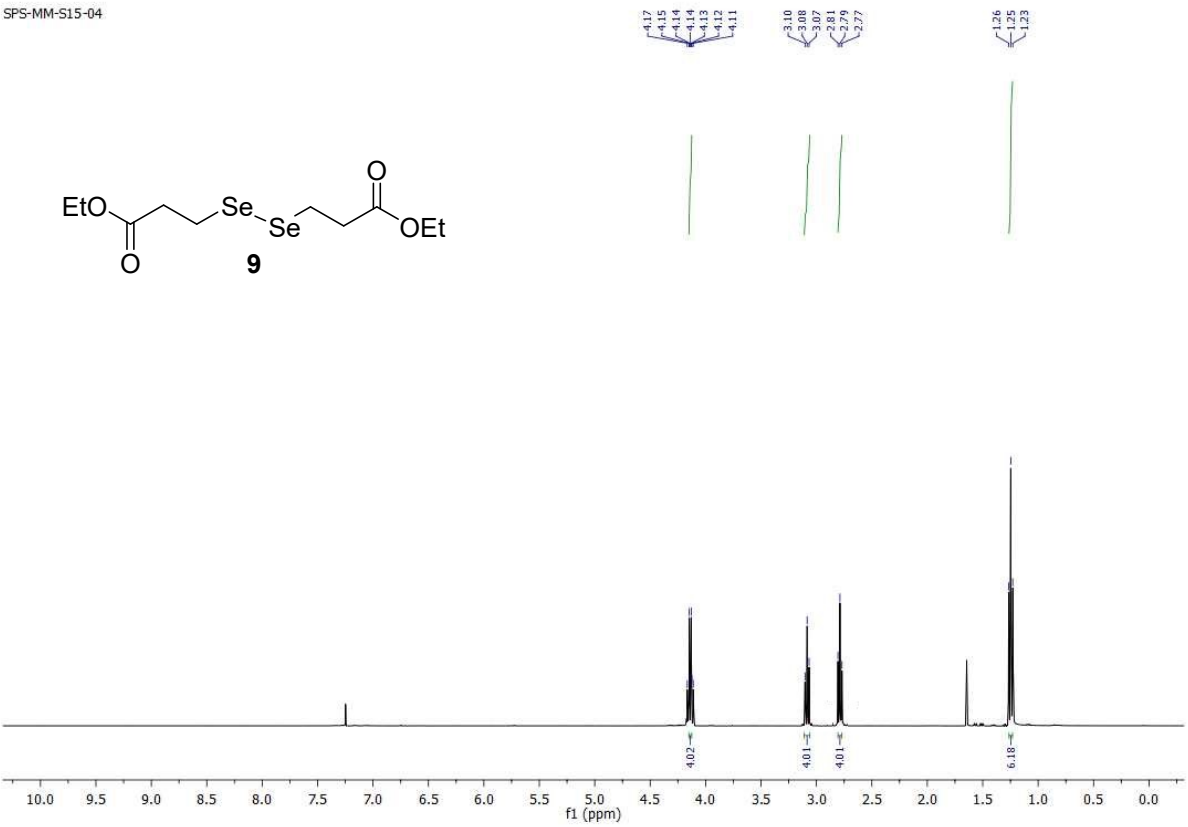
^{13}C NMR spectrum of **7b**.



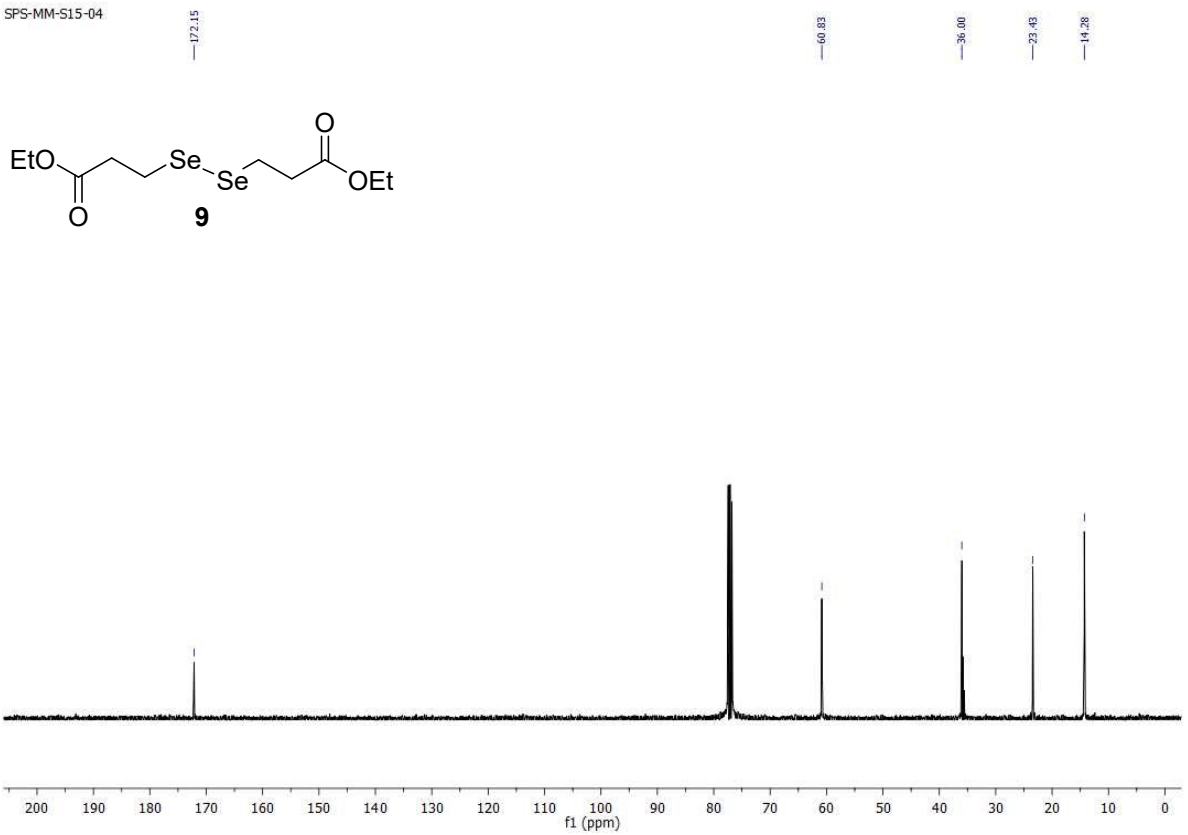
^{1}H NMR spectrum of **10**.



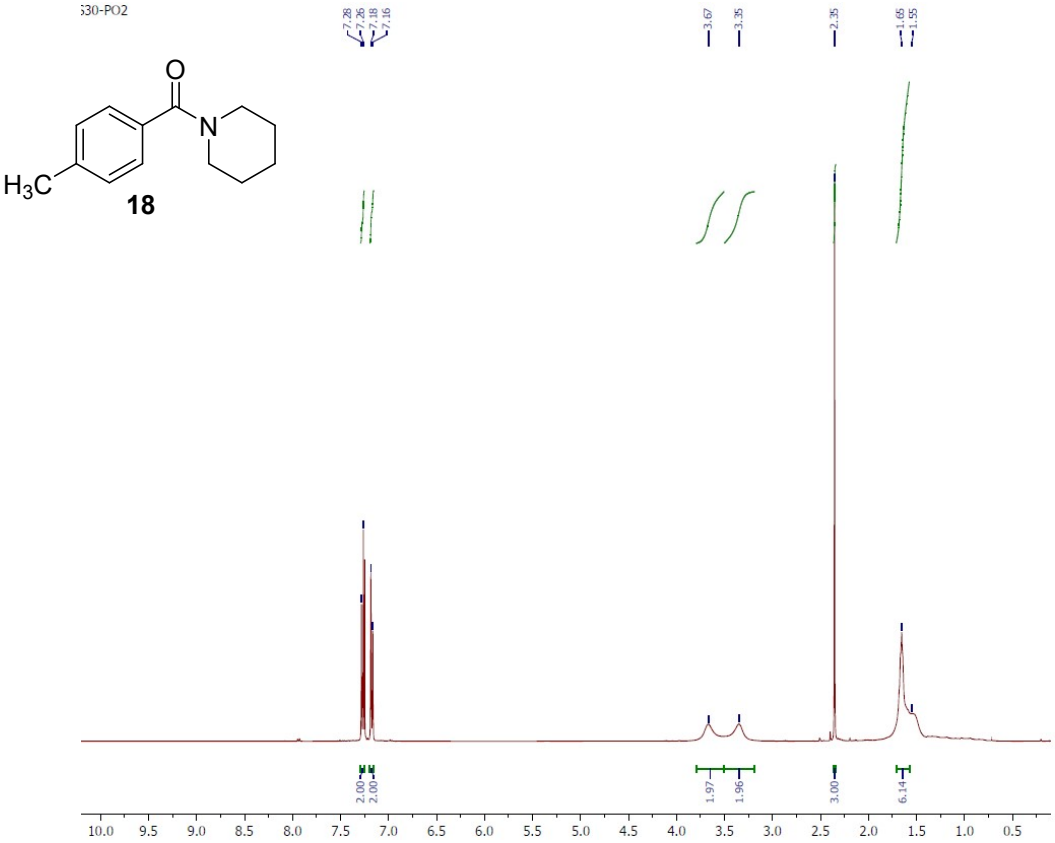
^{13}C NMR spectrum of **10**.



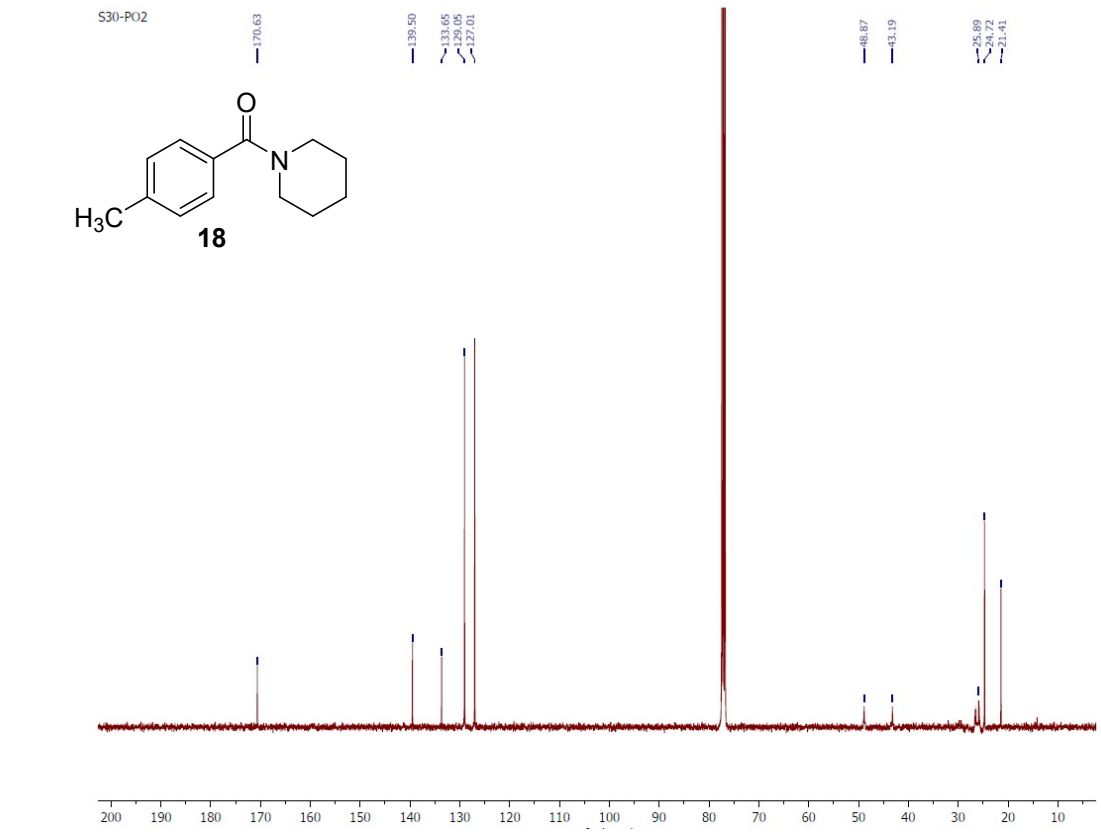
^{1}H NMR spectrum of **9**.



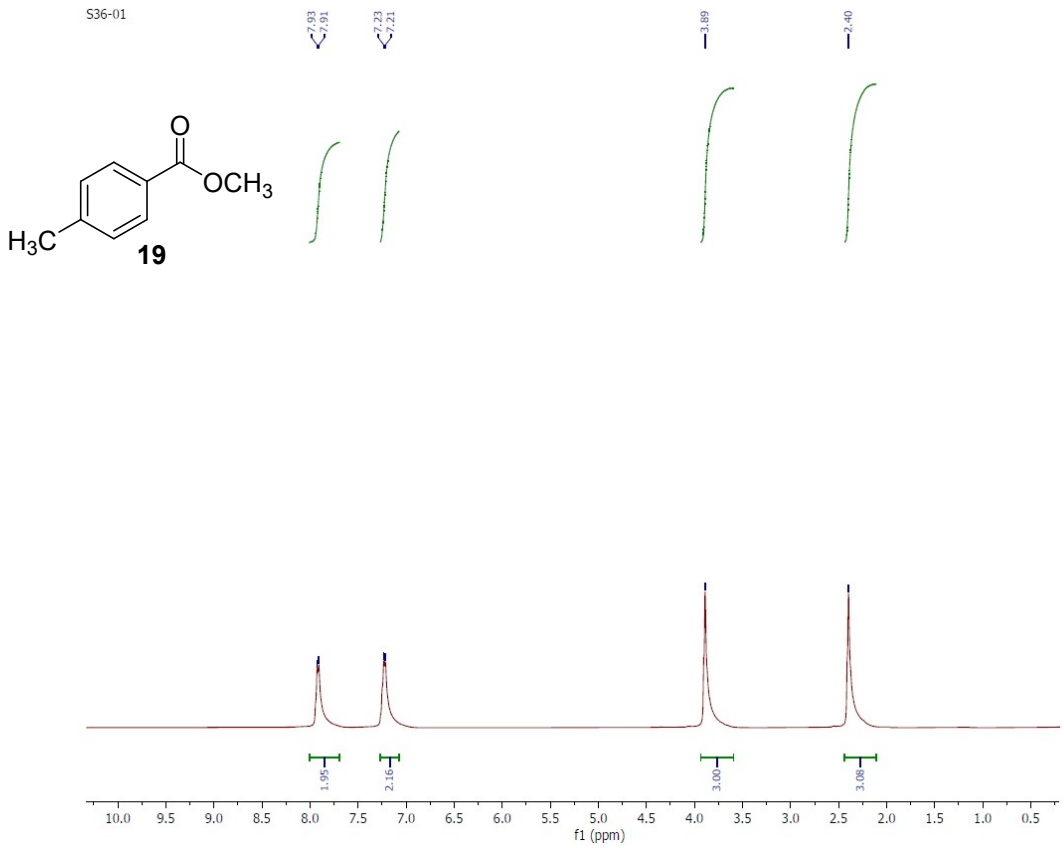
^{13}C NMR spectrum of **9**.



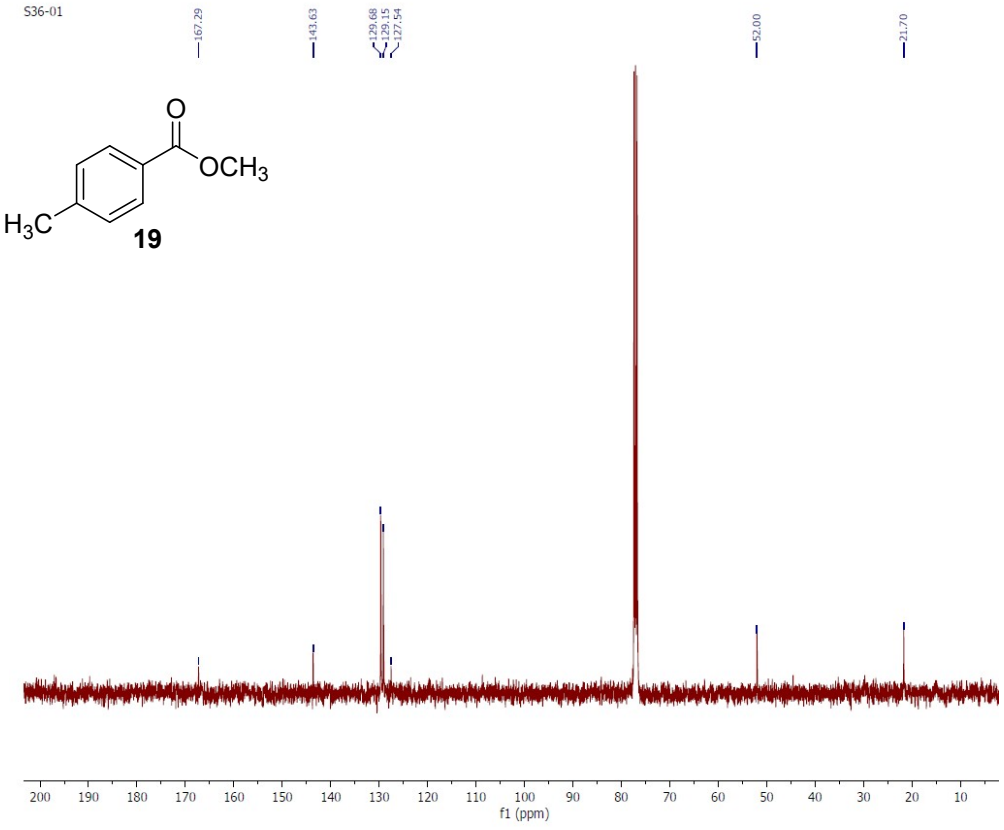
^{1}H NMR spectrum of **18**.



^{13}C NMR spectrum of **18**.



^{1}H NMR spectrum of **19**.



^{13}C NMR spectrum of **19**.

Cartesian coordinates and absolute energies:

S1

Electronic Energy (in Hartree) -3015.2209968

Zero-point Energy Correction (in Hartree) 0.2925487

0 1

C	-0.178775	0.273723	-0.019992
N	-1.272624	1.019150	0.316480
H	-1.118002	2.006639	0.485912
N	0.997501	0.878912	0.247378
H	0.973579	1.752328	0.762860
Se	-0.306868	-1.376020	-0.802981
C	-2.643753	0.635028	0.249759
C	-3.533609	1.470799	-0.434280
C	-3.131312	-0.435492	1.008310
C	-4.905188	1.203964	-0.406379
H	-3.150349	2.319087	-0.994709
C	-4.499858	-0.706298	1.021028
H	-2.440046	-1.050353	1.572984
H	-5.589257	1.850482	-0.947874
H	-4.872435	-1.547434	1.597981
C	2.333505	0.346327	-0.034382
C	3.260591	1.482427	-0.490571
C	2.900557	-0.396359	1.188043
H	2.205825	-0.368645	-0.852721
C	4.684714	0.965190	-0.752111
H	3.296415	2.258578	0.289709
H	2.848121	1.951553	-1.391688
C	4.324564	-0.908612	0.920627
H	2.916019	0.293888	2.044580
H	2.231583	-1.223217	1.448623
C	5.255945	0.226834	0.468819
H	5.334928	1.802518	-1.031798
H	4.666196	0.281775	-1.612646
H	4.719224	-1.391943	1.822163
H	4.289641	-1.682108	0.140446
H	6.252048	-0.168691	0.236294
H	5.386098	0.940394	1.295611
C	-5.389985	0.105922	0.308458
H	-6.454599	-0.107339	0.324656

T1

Electronic Energy (in Hartree) -3015.20147481

Zero-point Energy Correction (in Hartree) 0.2881437

0 1

C	0.224955	-0.479586	-0.284765
N	1.228991	-1.173668	0.096411
N	-1.008612	-1.066104	-0.411792
Se	0.239787	1.377052	-0.871563
C	2.550072	-0.725539	0.217700
C	3.559583	-1.360616	-0.528257
C	2.918061	0.230677	1.184804
C	4.897589	-1.007702	-0.348462
H	3.277154	-2.124008	-1.246741
C	4.262322	0.560811	1.374246
H	2.150325	0.679898	1.807476
H	5.664052	-1.496738	-0.943360
H	4.530274	1.294354	2.129716
C	-2.286797	-0.366817	-0.225770
C	-3.427830	-1.242660	-0.761695
C	-2.523302	0.023697	1.245437
H	-2.258403	0.545258	-0.835456
C	-4.794894	-0.569292	-0.559418
H	-3.415464	-2.206306	-0.230500
H	-3.252557	-1.459522	-1.821550
C	-3.890518	0.694928	1.445977
H	-2.473799	-0.891375	1.853503
H	-1.713990	0.677388	1.589602
C	-5.030543	-0.184712	0.910028
H	-5.589516	-1.237190	-0.911984
H	-4.846946	0.334787	-1.182818
H	-4.043032	0.914902	2.509210
H	-3.900586	1.662008	0.922814
H	-5.991361	0.333556	1.014165
H	-5.098499	-1.099084	1.517045
C	5.257316	-0.040092	0.597159
H	6.300650	0.223147	0.742649
H	-0.996491	-2.026317	-0.080130
H	1.666691	1.535283	-0.594758

T2

Electronic Energy (in Hartree) -3015.19537746

Zero-point Energy Correction (in Hartree) 0.2874048

0 1

C	0.148352	-0.181720	-0.622120
N	1.356737	-0.705451	-1.067172
N	-0.907266	-0.887885	-0.617395
Se	0.165598	1.727591	-0.210639

C	2.586854	-0.599704	-0.355273
C	3.778599	-0.721797	-1.084730
C	2.637269	-0.481237	1.041439
C	5.008941	-0.711090	-0.426152
H	3.730327	-0.830857	-2.164428
C	3.874093	-0.441472	1.690299
H	1.716172	-0.426198	1.612127
H	5.925618	-0.808938	-1.000288
H	3.904909	-0.339505	2.771237
C	-2.208013	-0.316031	-0.293797
C	-3.299506	-0.985782	-1.142881
C	-2.492004	-0.494405	1.211807
H	-2.225862	0.764941	-0.521102
C	-4.701574	-0.483832	-0.764497
H	-3.237429	-2.071781	-0.988350
H	-3.095125	-0.803859	-2.204772
C	-3.895287	0.001279	1.592541
H	-2.400025	-1.563209	1.449063
H	-1.725672	0.028382	1.796316
C	-4.981784	-0.667231	0.735692
H	-5.457146	-1.010113	-1.360204
H	-4.789640	0.582120	-1.020549
H	-4.077410	-0.188421	2.657315
H	-3.946703	1.091203	1.456014
H	-5.968136	-0.260081	0.989927
H	-5.014932	-1.741606	0.967850
H	1.217363	-1.591542	-1.543070
C	5.062878	-0.552993	0.962678
H	6.020576	-0.528528	1.473685
H	1.533572	1.929357	-0.687099

Nu1

Electronic Energy (in Hartree) -3014.71461803

Zero-point Energy Correction (in Hartree) 0.2806728

-1 1

C	0.250849	-0.116658	-0.280461
N	1.270227	-0.940313	-0.185140
N	-0.942285	-0.790103	-0.520325
Se	0.153020	1.778513	-0.216936
C	2.617802	-0.668537	-0.029100
C	3.463836	-1.811102	-0.021895
C	3.254143	0.586349	0.142719
C	4.843168	-1.715286	0.137956
H	2.992314	-2.782094	-0.149513

C	4.639666	0.675518	0.307189
H	2.649814	1.483665	0.145209
H	5.447343	-2.620092	0.133176
H	5.088494	1.658757	0.436299
C	-2.286099	-0.299132	-0.255332
C	-3.296809	-1.019958	-1.161097
C	-2.675981	-0.437243	1.230495
H	-2.279377	0.765916	-0.508877
C	-4.735947	-0.547579	-0.895884
H	-3.233868	-2.105592	-0.984321
H	-3.021783	-0.853975	-2.209604
C	-4.111541	0.044256	1.491743
H	-2.587975	-1.495681	1.521350
H	-1.959334	0.124509	1.839654
C	-5.118714	-0.683284	0.587112
H	-5.437735	-1.112133	-1.523399
H	-4.827693	0.506915	-1.194016
H	-4.373320	-0.100803	2.547918
H	-4.169286	1.125699	1.300698
H	-6.132507	-0.295663	0.753026
H	-5.141427	-1.749771	0.857541
C	5.451651	-0.462706	0.305525
H	6.527989	-0.379936	0.432619
H	-0.816074	-1.794069	-0.437486

Nu2

Electronic Energy (in Hartree) -3014.71149446

Zero-point Energy Correction (in Hartree) 0.2813856

-1 1

C	0.103074	-0.139639	-0.112298
N	1.294150	-0.890128	-0.015518
N	-0.941218	-0.912025	-0.116636
Se	0.136393	1.754840	-0.210905
C	2.659546	-0.645484	0.030592
C	3.494546	-1.789343	0.105938
C	3.284710	0.617578	0.021763
C	4.880357	-1.677408	0.161984
H	3.035794	-2.776071	0.110529
C	4.677078	0.715129	0.080709
H	2.668407	1.504785	-0.029501
H	5.483358	-2.580619	0.216119
H	5.126210	1.705801	0.070724
C	-2.278030	-0.354273	-0.157015
C	-3.179565	-1.208195	-1.065398

C	-2.865763	-0.277216	1.267190
H	-2.253760	0.671328	-0.558528
C	-4.631756	-0.703219	-1.071984
H	-3.150490	-2.250246	-0.713005
H	-2.768371	-1.208442	-2.083008
C	-4.315859	0.230791	1.267301
H	-2.827680	-1.282379	1.713603
H	-2.228365	0.370989	1.879463
C	-5.210066	-0.619545	0.350430
H	-5.256583	-1.354746	-1.697705
H	-4.665329	0.296186	-1.530529
H	-4.716424	0.235242	2.290110
H	-4.333186	1.274309	0.920224
H	-6.229530	-0.211382	0.323870
H	-5.288472	-1.635567	0.766286
H	1.051518	-1.873357	0.036343
C	5.493425	-0.417575	0.151664
H	6.574853	-0.324930	0.195589

TS1

Electronic Energy (in Hartree) -3437.72389438

Zero-point Energy Correction (in Hartree) 0.4226587

-1 1

C	-4.483568	0.066662	0.258758
C	-5.632684	-0.562981	0.767201
C	-4.643722	1.191484	-0.567881
C	-6.906450	-0.077585	0.460532
H	-5.532781	-1.421585	1.423642
C	-3.089346	-0.407338	0.573847
C	-5.915081	1.672758	-0.882019
H	-3.753374	1.676834	-0.953607
C	-7.052724	1.039701	-0.368243
H	-7.784033	-0.569328	0.871496
C	-2.883134	-1.784968	0.934877
O	-2.143760	0.412676	0.467159
H	-6.020325	2.539926	-1.528479
H	-8.043558	1.414999	-0.609234
C	-1.640828	-2.244093	1.305810
H	-1.495292	-3.281924	1.581373
H	-0.875111	-1.553484	1.633011
Se	0.093499	-2.601254	-0.777570
C	1.370329	-1.226662	-0.376219
N	2.612227	-1.450875	-0.692851
N	0.841048	-0.086827	0.179041

H	-3.690497	-2.492798	0.775154
H	-0.180928	-0.058593	0.187979
C	3.750876	-0.872648	-0.168358
C	4.853248	-0.618244	-1.020901
C	3.952541	-0.681302	1.223379
C	6.069968	-0.161827	-0.515769
H	4.727453	-0.791941	-2.086126
C	5.176563	-0.234387	1.720590
H	3.132247	-0.888632	1.905315
C	6.248473	0.036136	0.860051
H	6.891056	0.032265	-1.202396
H	5.296557	-0.101490	2.793618
H	7.199748	0.385508	1.251383
C	1.453911	1.244981	0.095791
C	1.291299	1.862139	-1.308756
C	0.848918	2.159160	1.172477
H	2.521915	1.147853	0.301375
C	1.896356	3.273533	-1.375209
H	0.219783	1.906617	-1.549884
H	1.758599	1.204171	-2.050760
C	1.443623	3.575327	1.104124
H	-0.239469	2.203196	1.034218
H	1.025519	1.717622	2.160972
C	1.297527	4.191065	-0.297225
H	1.739081	3.703148	-2.372857
H	2.984789	3.208300	-1.230921
H	0.962690	4.217370	1.853125
H	2.510845	3.533040	1.367165
H	1.776194	5.178621	-0.328217
H	0.230518	4.349997	-0.511722

TS2

Electronic Energy (in Hartree) -3437.71821382

Zero-point Energy Correction (in Hartree) 0.4225657

-1 1

C	-4.462693	-0.159549	0.584106
C	-5.550261	-1.029773	0.772790
C	-4.722432	1.212112	0.423489
C	-6.859652	-0.543092	0.793473
H	-5.373620	-2.090107	0.923173
C	-3.031462	-0.629983	0.571755
C	-6.030030	1.699065	0.433106
H	-3.879867	1.881369	0.284257
C	-7.105146	0.823168	0.621119

H	-7.687300	-1.229492	0.951047
C	-2.747149	-1.988753	0.224841
O	-2.131079	0.212261	0.839187
H	-6.211797	2.761925	0.297410
H	-8.123791	1.201453	0.634221
C	-1.455296	-2.485524	0.263832
H	-1.264907	-3.532597	0.062335
H	-0.707480	-1.987109	0.867964
Se	0.005403	-1.811438	-1.802538
C	1.244071	-0.797825	-0.740646
N	2.465303	-1.173841	-0.638471
N	0.664683	0.329759	-0.104772
C	3.397173	-0.554766	0.303441
C	3.480797	-1.444702	1.563134
C	4.783316	-0.439679	-0.355584
H	3.081826	0.446928	0.627020
C	4.550250	-0.950540	2.550512
H	3.709610	-2.471081	1.244142
H	2.496792	-1.474097	2.046083
C	5.853542	0.061495	0.626172
H	5.061035	-1.432145	-0.736901
H	4.722425	0.223930	-1.226768
C	5.926999	-0.825257	1.879334
H	4.606301	-1.630972	3.410246
H	4.253223	0.030875	2.948332
H	6.831173	0.097408	0.127990
H	5.618799	1.092880	0.927860
H	6.662486	-0.423752	2.588775
H	6.279679	-1.826824	1.591578
C	1.020948	1.660782	-0.320303
C	2.064217	2.059184	-1.180340
C	0.292060	2.666262	0.354977
C	2.364143	3.412758	-1.350580
H	2.623276	1.309407	-1.728790
C	0.601170	4.012055	0.174586
H	-0.523318	2.370378	1.008700
H	3.170600	3.690995	-2.024796
H	0.021807	4.762965	0.706221
H	-3.537429	-2.595875	-0.205122
H	-0.321017	0.205512	0.149216
C	1.645401	4.403212	-0.674697
H	1.886727	5.453509	-0.809796

INT1

Electronic Energy (in Hartree) -3437.72959782

Zero-point Energy Correction (in Hartree) 0.4228602

-1 1

C	-4.273398	0.116293	0.038174
C	-5.493462	-0.555303	0.241596
C	-4.308894	1.355181	-0.625333
C	-6.698768	-0.016784	-0.214682
H	-5.502892	-1.496435	0.782604
C	-2.943176	-0.417132	0.510443
C	-5.511359	1.894243	-1.089325
H	-3.370598	1.881363	-0.766120
C	-6.715414	1.211809	-0.885962
H	-7.628425	-0.552045	-0.037046
C	-2.790983	-1.773724	0.751503
O	-1.987420	0.445588	0.644191
H	-5.509740	2.851219	-1.605835
H	-7.653379	1.632128	-1.239392
C	-1.516935	-2.314781	1.228050
H	-1.603767	-3.307163	1.674726
H	-0.978884	-1.659109	1.914860
Se	-0.050657	-2.712472	-0.210594
C	1.198262	-1.225225	-0.077029
N	2.344328	-1.504189	-0.609679
N	0.725328	-0.096861	0.500451
H	-3.577023	-2.472614	0.484691
H	-0.312519	-0.020057	0.594972
C	3.574829	-0.892804	-0.435696
C	4.375258	-0.601862	-1.563983
C	4.150008	-0.697780	0.844007
C	5.673498	-0.112517	-1.418399
H	3.956439	-0.773136	-2.551559
C	5.451320	-0.213483	0.979549
H	3.563465	-0.941447	1.725893
C	6.226310	0.088134	-0.147263
H	6.261096	0.108400	-2.306454
H	5.865873	-0.076038	1.975589
H	7.239198	0.464771	-0.037372
C	1.383481	1.215758	0.430024
C	1.177010	1.883964	-0.944769
C	0.848956	2.106948	1.562761
H	2.456127	1.079242	0.586117
C	1.810105	3.284217	-0.988973
H	0.097906	1.956430	-1.135290

H	1.600410	1.245263	-1.728626
C	1.480613	3.507221	1.517142
H	-0.241720	2.182090	1.469486
H	1.054176	1.625740	2.527074
C	1.284563	4.176380	0.146892
H	1.615132	3.751677	-1.962608
H	2.902581	3.191980	-0.900110
H	1.052770	4.133413	2.310357
H	2.557800	3.428812	1.727071
H	1.786021	5.152811	0.126620
H	0.213105	4.366882	-0.010763

INT2

Electronic Energy (in Hartree) -3437.72053193

Zero-point Energy Correction (in Hartree) 0.4226414

-1 1

C	4.131298	-0.172684	-0.643920
C	5.088002	-0.456051	0.349061
C	4.474551	0.759387	-1.639165
C	6.343985	0.154864	0.334568
H	4.843144	-1.141744	1.154251
C	2.757505	-0.797228	-0.686261
C	5.733862	1.363183	-1.663235
H	3.727940	0.994975	-2.390210
C	6.678287	1.065114	-0.675263
H	7.060500	-0.073887	1.119720
C	2.534781	-2.003770	-0.040922
O	1.857675	-0.170590	-1.375890
H	5.976412	2.072714	-2.450888
H	7.655860	1.539989	-0.685376
C	1.257485	-2.704655	-0.135385
H	1.336936	-3.783687	0.004531
H	0.705208	-2.494092	-1.052879
Se	-0.211162	-2.299606	1.322860
C	-1.273536	-0.963948	0.384195
N	-2.535358	-1.145709	0.364876
N	-0.574625	0.143341	-0.134899
C	-3.413124	-0.203793	-0.338581
C	-3.675357	-0.748792	-1.758269
C	-4.733138	-0.062836	0.437265
H	-2.958164	0.790116	-0.440881
C	-4.695279	0.112822	-2.519429
H	-4.047559	-1.779174	-1.670855
H	-2.726137	-0.796416	-2.304269

C	-5.751697	0.803466	-0.320019
H	-5.145987	-1.068231	0.599390
H	-4.532742	0.359423	1.429608
C	-6.008633	0.262111	-1.735470
H	-4.888100	-0.325906	-3.506812
H	-4.266806	1.109484	-2.698768
H	-6.691359	0.854535	0.244834
H	-5.373424	1.833716	-0.391115
H	-6.701908	0.920049	-2.275370
H	-6.498058	-0.720374	-1.661929
C	-0.587224	1.390791	0.500369
C	-1.403511	1.687753	1.609761
C	0.253834	2.407871	-0.004553
C	-1.405331	2.970843	2.164381
H	-2.036637	0.917264	2.036405
C	0.248311	3.678630	0.564532
H	0.911513	2.170784	-0.835078
H	-2.050018	3.174381	3.016044
H	0.905368	4.442537	0.156038
H	3.323324	-2.466769	0.542618
H	0.330437	-0.068932	-0.616263
C	-0.585392	3.979195	1.651192
H	-0.589852	4.973543	2.088189

TS1'

Electronic Energy (in Hartree) -6452.97592132

Zero-point Energy Correction (Hartree) 0.7160247

-1 1

C	0.310926	-2.623090	2.809919
C	-0.653044	-3.555394	3.230263
C	1.078570	-1.966420	3.786508
C	-0.848220	-3.819682	4.587806
H	-1.242206	-4.093713	2.494699
C	0.583064	-2.333690	1.357982
C	0.878595	-2.221706	5.143802
H	1.828122	-1.253457	3.459967
C	-0.086112	-3.150145	5.550760
H	-1.591685	-4.551054	4.893206
C	-0.442741	-2.583108	0.396441
O	1.719829	-1.875733	1.057345
H	1.474348	-1.696195	5.885275
H	-0.239446	-3.352693	6.607254
C	-0.223978	-2.400072	-0.961412
H	-1.444692	-2.806618	0.744415

H	-0.975293	-2.711704	-1.677607
H	0.789698	-2.376626	-1.341465
C	3.233945	1.149910	-0.388677
N	2.071356	1.571263	0.206746
H	1.245704	1.033685	-0.081270
N	3.228890	-0.169468	-0.641232
H	2.531476	-0.738179	-0.140105
C	1.777414	2.775710	0.871804
C	0.460431	3.261289	0.791211
C	2.713920	3.453917	1.667896
C	0.102850	4.429657	1.465451
C	2.342126	4.618619	2.340932
H	3.722794	3.071138	1.754203
H	-0.918602	4.792451	1.390273
H	3.078881	5.134151	2.951390
Se	4.607830	2.270123	-0.894556
C	4.275733	-0.915405	-1.334811
C	5.227274	-1.584186	-0.324889
C	3.652335	-1.953115	-2.282220
H	4.842753	-0.186436	-1.921994
C	6.308386	-2.413807	-1.035396
H	4.636474	-2.231403	0.337382
H	5.684243	-0.809980	0.301712
C	4.738047	-2.774687	-2.995847
H	3.009959	-2.629527	-1.701377
H	3.012059	-1.441577	-3.010696
C	5.690618	-3.445443	-1.992963
H	6.942128	-2.914497	-0.292585
H	6.965895	-1.740832	-1.604851
H	4.269682	-3.528675	-3.640782
H	5.316440	-2.112560	-3.656446
H	6.480135	-3.989460	-2.527329
H	5.132218	-4.191540	-1.408931
H	-0.279480	2.715951	0.210804
Se	-0.378773	0.021595	-1.695058
C	-2.197951	0.353854	-1.181279
N	-3.114167	-0.360606	-1.928575
N	-2.440306	1.199892	-0.232038
H	-2.673967	-0.971517	-2.605084
C	-4.442597	-0.802103	-1.481686
C	-5.217875	-1.338531	-2.694496
C	-4.365982	-1.863558	-0.366590
H	-4.979489	0.068283	-1.093730
C	-6.615772	-1.838548	-2.295590

H	-4.648582	-2.167920	-3.142197
H	-5.291610	-0.553734	-3.456657
C	-5.766419	-2.347902	0.041731
H	-3.773328	-2.714374	-0.732465
H	-3.831987	-1.450135	0.496132
C	-6.549944	-2.881500	-1.168012
H	-7.124611	-2.256556	-3.172956
H	-7.220447	-0.983567	-1.961116
H	-5.683300	-3.121995	0.814502
H	-6.320977	-1.513275	0.494167
H	-7.563308	-3.175190	-0.866585
H	-6.057454	-3.790296	-1.544177
C	-3.639863	1.883082	-0.039909
C	-4.136252	2.059326	1.269736
C	-4.289458	2.571524	-1.092008
C	-5.261643	2.848995	1.509944
H	-3.621411	1.565865	2.089112
C	-5.405355	3.369946	-0.840696
H	-3.903778	2.471210	-2.102486
C	-5.908266	3.510674	0.458884
H	-5.628601	2.957974	2.527617
H	-5.883097	3.891308	-1.666903
H	-6.778175	4.132496	0.649548
C	1.041401	5.123431	2.236013
H	0.760521	6.033614	2.758332

TS2'

Electronic Energy (in Hartree) -6452.96678604

Zero-point Energy Correction (in Hartree) 0.7165508

-1 1

C	-0.528412	-0.415346	3.460490
C	-1.459537	-1.180000	4.183894
C	-0.131265	0.828019	3.980091
C	-1.990977	-0.706287	5.385860
H	-1.761761	-2.155772	3.817569
C	0.085356	-0.887809	2.172682
C	-0.664989	1.305608	5.177282
H	0.599858	1.407941	3.427414
C	-1.598401	0.540062	5.885213
H	-2.705816	-1.312792	5.935373
C	-0.583192	-1.880072	1.394376
O	1.176200	-0.357345	1.815775
H	-0.353654	2.274188	5.558970
H	-2.013148	0.909653	6.819097

C	-0.023054	-2.378559	0.230325
H	-1.601542	-2.147646	1.650325
H	-0.521343	-3.162712	-0.326360
H	1.044457	-2.300936	0.070547
C	3.483174	0.835592	-0.449091
N	2.302330	1.501319	-0.305389
H	1.568903	0.932622	0.121148
N	3.464419	-0.376645	0.140807
H	2.626544	-0.605444	0.688043
C	1.859855	2.805664	-0.593232
C	0.489816	3.040587	-0.352708
C	2.664601	3.866282	-1.040744
C	-0.057680	4.303220	-0.562047
C	2.099511	5.129830	-1.236837
H	3.713808	3.696398	-1.233505
H	-1.117033	4.457051	-0.376193
H	2.739216	5.938983	-1.580163
Se	4.986519	1.454139	-1.332141
C	4.532508	-1.370387	0.122464
C	4.625120	-2.057435	1.494618
C	4.325399	-2.396944	-1.007034
H	5.464785	-0.829448	-0.069744
C	5.722027	-3.134598	1.503581
H	3.657751	-2.520571	1.737292
H	4.817546	-1.303490	2.267100
C	5.425118	-3.470134	-0.994944
H	3.342784	-2.873487	-0.881353
H	4.306096	-1.869794	-1.967255
C	5.522234	-4.159535	0.375384
H	5.739283	-3.638003	2.478175
H	6.702298	-2.651199	1.382472
H	5.233493	-4.210076	-1.781958
H	6.390666	-3.001137	-1.233793
H	6.342735	-4.888491	0.378095
H	4.597273	-4.725004	0.561034
H	-0.141545	2.219363	-0.023189
Se	-0.225709	-0.698402	-1.703473
C	-2.078333	-0.317577	-1.403133
N	-2.963074	-0.953018	-2.342572
N	-2.464662	0.477716	-0.477954
H	-2.488959	-1.108410	-3.224431
C	-5.426317	2.782248	-1.189049
C	-4.008849	2.196775	-1.279666
C	-3.859402	0.926280	-0.416069

C	-4.251631	1.219881	1.040231
C	-5.668330	1.808297	1.141768
C	-5.825874	3.063713	0.268148
H	-6.142541	2.073027	-1.629209
H	-5.489268	3.701143	-1.786061
H	-3.276647	2.939353	-0.934431
H	-3.753213	1.956133	-2.317797
H	-4.559606	0.177938	-0.812071
H	-4.175330	0.301006	1.634702
H	-3.521443	1.924868	1.460312
H	-6.400287	1.052496	0.820469
H	-5.901427	2.041844	2.188407
H	-5.185666	3.863404	0.668706
H	-6.858409	3.433443	0.316032
C	-5.627841	-4.122041	-1.463296
C	-5.346252	-3.751590	-2.784532
C	-4.460654	-2.711550	-3.058289
C	-3.828510	-2.007487	-2.011914
C	-4.105564	-2.388612	-0.685978
C	-4.998207	-3.431050	-0.424390
H	-6.320612	-4.930641	-1.250895
H	-5.819637	-4.275886	-3.610568
H	-4.251468	-2.430954	-4.087860
H	-3.619919	-1.872424	0.133774
H	-5.194792	-3.706333	0.608596
C	0.742376	5.363172	-1.005223
H	0.314365	6.348598	-1.165750

INT1'

Electronic Energy (in Hartree) -6452.98272357

Zero-point Energy Correction (in Hartree) 0.7171594

-1 1

C	0.916798	-3.982929	-0.734790
C	0.015690	-4.935037	-1.244209
C	1.920588	-4.426371	0.144493
C	0.113796	-6.282710	-0.890527
H	-0.750188	-4.624349	-1.948407
C	0.877959	-2.528591	-1.118572
C	2.016665	-5.771940	0.505830
H	2.627285	-3.700075	0.531804
C	1.116926	-6.709184	-0.012742
H	-0.585723	-7.002017	-1.308854
C	-0.297277	-1.946828	-1.553156
O	1.999894	-1.876372	-1.003341

H	2.798942	-6.091050	1.189918
H	1.197283	-7.757903	0.261339
C	-0.312989	-0.536583	-1.959569
H	-1.100943	-0.273172	-2.667776
H	0.639203	-0.219886	-2.386389
C	3.228560	0.766560	0.522820
N	2.798336	-0.357451	1.144254
H	2.410309	-1.082668	0.511372
N	3.105723	0.731273	-0.819552
H	2.688544	-0.129373	-1.199855
C	2.573399	-0.502211	2.546354
C	1.299023	-0.252412	3.067854
C	3.592525	-0.973031	3.381177
C	1.051730	-0.456777	4.427910
C	3.340456	-1.181109	4.739352
H	4.573748	-1.167606	2.960032
H	0.062691	-0.255370	4.829802
H	4.134853	-1.544815	5.385393
Se	3.943473	2.201733	1.443431
C	3.618617	1.726891	-1.754343
C	5.050620	1.388463	-2.210204
C	2.670358	1.859852	-2.956293
H	3.645100	2.679137	-1.213613
C	5.574655	2.421194	-3.220689
H	5.047409	0.389185	-2.669271
H	5.701755	1.339374	-1.330400
C	3.195224	2.889949	-3.969115
H	2.575304	0.882564	-3.453184
H	1.670822	2.140529	-2.605117
C	4.627372	2.564698	-4.422798
H	6.579664	2.138987	-3.559033
H	5.675188	3.395744	-2.721197
H	2.522016	2.937072	-4.834205
H	3.181213	3.887198	-3.506141
H	4.993307	3.341972	-5.106024
H	4.620486	1.623035	-4.991415
H	0.521430	0.108103	2.401508
Se	-0.475539	0.845425	-0.434530
C	-2.379292	0.952911	-0.123092
N	-3.199703	0.783732	-1.211011
N	-2.709023	1.234023	1.092164
H	-2.713226	0.601196	-2.078155
C	-4.554377	0.206121	-1.155950
C	-5.195582	0.326206	-2.546067

C	-4.545257	-1.257979	-0.675807
H	-5.147112	0.800222	-0.453165
C	-6.606163	-0.284897	-2.571226
H	-4.559492	-0.196399	-3.277042
H	-5.227668	1.380689	-2.845208
C	-5.960584	-1.856943	-0.686718
H	-3.891460	-1.841670	-1.339050
H	-4.109994	-1.313351	0.327973
C	-6.607888	-1.739893	-2.075561
H	-7.014884	-0.226080	-3.587355
H	-7.268717	0.315805	-1.932013
H	-5.921983	-2.906270	-0.370270
H	-6.583716	-1.330590	0.050571
H	-7.633678	-2.128474	-2.052383
H	-6.049725	-2.365397	-2.787411
C	-3.903472	1.843570	1.483635
C	-4.555320	1.395676	2.650874
C	-4.382641	3.019216	0.864526
C	-5.683344	2.056690	3.139074
H	-4.164119	0.519209	3.159248
C	-5.505368	3.680365	1.363741
H	-3.866547	3.401539	-0.011222
C	-6.169412	3.203701	2.500529
H	-6.176385	1.682124	4.032609
H	-5.855390	4.582873	0.868582
H	-7.042244	3.721961	2.886863
C	2.070456	-0.920862	5.266144
H	1.876232	-1.081097	6.323144
H	-1.230537	-2.498966	-1.540180

INT2'

Electronic Energy (in Hartree) -6452.97591925

Zero-point Energy Correction (in Hartree) 0.7169947

-1 1

C	-0.487048	3.324963	1.985269
C	0.747519	3.914537	2.316990
C	-1.616167	3.696529	2.735652
C	0.833797	4.884593	3.317364
H	1.647944	3.628094	1.783518
C	-0.666918	2.331150	0.868300
C	-1.531479	4.662076	3.741229
H	-2.560426	3.218232	2.498783
C	-0.304739	5.263107	4.039620

H	1.797224	5.332038	3.549185
C	0.305922	2.178204	-0.095841
O	-1.794543	1.674986	0.860442
H	-2.423540	4.940453	4.296982
H	-0.234423	6.014092	4.822062
C	0.107580	1.268195	-1.231649
H	0.691676	1.530970	-2.113870
H	-0.939438	1.173239	-1.522137
C	-3.468042	-1.068999	0.132052
N	-2.619433	-0.970827	1.195970
H	-2.114722	-0.067382	1.214311
N	-3.439749	0.034545	-0.643872
H	-2.833269	0.802085	-0.308761
C	-2.311952	-1.795935	2.290845
C	-1.294364	-1.311042	3.141270
C	-2.929934	-3.017518	2.609430
C	-0.913486	-2.021421	4.275872
C	-2.531863	-3.722333	3.749337
H	-3.705022	-3.405013	1.964341
H	-0.126946	-1.623284	4.911132
H	-3.023012	-4.665427	3.975612
Se	-4.587250	-2.490127	-0.261289
C	-4.209119	0.256957	-1.862968
C	-4.633689	1.732254	-1.940403
C	-3.422014	-0.167051	-3.118745
H	-5.105370	-0.369102	-1.795081
C	-5.421589	2.021204	-3.228168
H	-3.740357	2.372648	-1.908732
H	-5.233342	1.983503	-1.057380
C	-4.215484	0.123564	-4.402262
H	-2.468719	0.379189	-3.143662
H	-3.179927	-1.232763	-3.044086
C	-4.636548	1.599598	-4.480696
H	-5.674508	3.087680	-3.276547
H	-6.374825	1.473629	-3.198971
H	-3.618519	-0.150682	-5.281105
H	-5.113704	-0.510554	-4.424043
H	-5.237731	1.777608	-5.381629
H	-3.737549	2.226931	-4.571648
H	-0.806107	-0.371662	2.899075
Se	0.535113	-0.699258	-0.841475
C	2.468326	-0.694744	-0.899810
N	3.046328	0.173269	-1.854537
N	3.076409	-1.533144	-0.157382

H	2.455903	0.332248	-2.660390
C	6.030651	-3.608541	-1.384520
C	4.577294	-3.139253	-1.214583
C	4.489768	-1.855857	-0.361780
C	5.173782	-2.069244	0.998318
C	6.628932	-2.536530	0.837062
C	6.724155	-3.804497	-0.026996
H	6.587935	-2.863280	-1.970761
H	6.054053	-4.541036	-1.962535
H	3.985325	-3.922767	-0.722306
H	4.113330	-2.956415	-2.191104
H	5.026995	-1.061917	-0.899372
H	5.132671	-1.142191	1.582940
H	4.598262	-2.819172	1.557767
H	7.219106	-1.735210	0.368524
H	7.074166	-2.714500	1.823969
H	6.244444	-4.639216	0.504655
H	7.774563	-4.086722	-0.173833
C	5.658579	3.416922	-1.130372
C	5.153835	3.162349	-2.410942
C	4.294618	2.087884	-2.634455
C	3.918824	1.240086	-1.574870
C	4.416290	1.502061	-0.287281
C	5.277539	2.581399	-0.076671
H	6.328228	4.253644	-0.957324
H	5.429379	3.803277	-3.243983
H	3.907646	1.898373	-3.632702
H	4.113309	0.879645	0.546775
H	5.646124	2.770334	0.927902
C	-1.529509	-3.238190	4.592509
H	-1.231033	-3.795215	5.475977
H	1.237503	2.729038	-0.041009