Electrochemical vicinal amidoselenation of unactivated olefins via tandem Ritter reaction

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Table of Contents

1. General information

General.

Unless otherwise noted, all reagents and solvents were purchased from commercial sources (Adamas-beta, Energy Chemical) and used without further purification.

NMR spectrum

^{1}H and ^{13}C NMR spectra were collected on 400 or 600 MHz NMR spectrometers (Varian Inova-400 or Bruker Avance NEO 600). Chemical shifts for protons were reported in parts per million (ppm) downfield from tetramethylsilane and were referenced to residual protium in the NMR solvents ($CDCl_3$ = δ 7.26). The following abbreviations are used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd=doublet of doublets, dt=doublet of triplet, td= triplet of doublet, qd= quartet of doublets, coupling constants *J* were reported in hertz unit (Hz).

HRMS

High-resolution mass spectra (HRMS) were recorded on Thermo Fisher Scientific QExactive.

Melting point

Melting point (M.P.) was recorded on BÜCHI (M-560).

UV light

Visualization of TLC was achieved by the use of UV light (254 nm).

Materials.

All the chemical reagents were purchased from commercial sources and used as received unless otherwise indicated. Diselenides[1] are known compounds and are synthesized according to the reported method.

The Electrochemical Reaction Instrument.

Electrochemical reactions were performed on IKA ElectraSyn 2.0 pro.

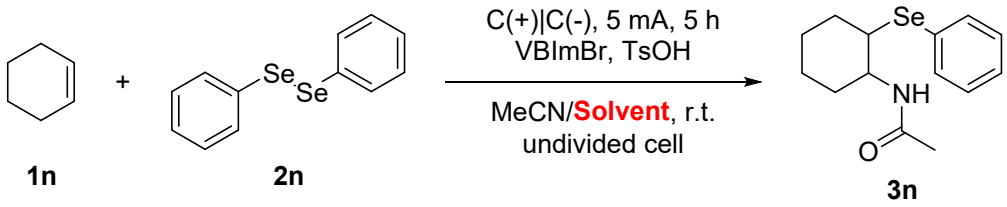
Cyclic voltammetry (CV) was carried out on a CHI660E electrochemical workstation (CH Instruments, Ins).

	
Fig. S1 Instrument for electrolysis	**Fig. S2** Electrode materials

2. Experimental procedures

2.1 Optimization of the amidoselenation reaction for the inactivation of alkenes

2.1.1 Table S1 screening of solvents[a]

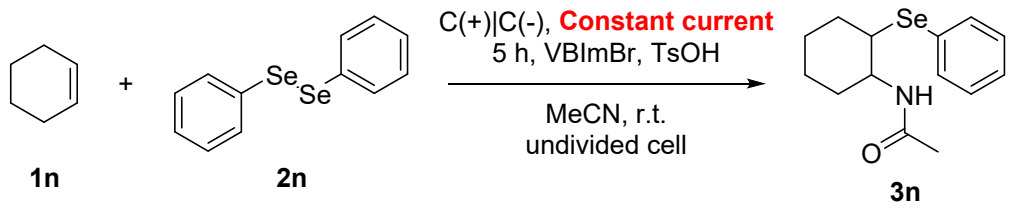


1n **2n** **3n**

Entry	Solvent	Yield (%)[b]
1	-	5
2	CH_2Cl_2	n.r.
3	DMF	n.r.
4	DMAc	n.r.
5	NMP	n.r.
6	DMSO	n.r.
7	CH_3OH	n.r.
8	1.4-Dioxane	n.r.
9	TFE	n.r.

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), VBImBr (0.2 mmol), MeCN/Solvent (4 mL v:v = 1:1), TsOH (0.2mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), constant current = 5 mA, 5 h, room temperature, under air, undivided cell. [b]Isolated yields. n.r. = no reaction. NMP = 1-methyl-2-pyrrolidinone.

2.1.2 Table S2 screening of constant currents[a]

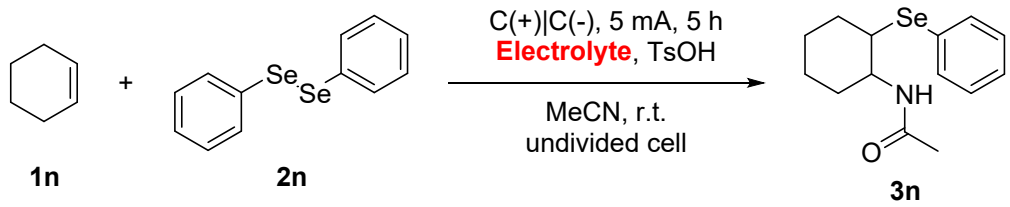


1n 2n 3n

Entry	Constant current (mA)	Yield (%)[b]
1	3	trace
2	5	7
3	7	5
4	10	trace

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), VBImBr (0.2 mmol), MeCN (4 mL), TsOH (0.2 mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), Constant current = x mA, 5 h, room temperature, under air, undivided cell. [b]Isolated yields.

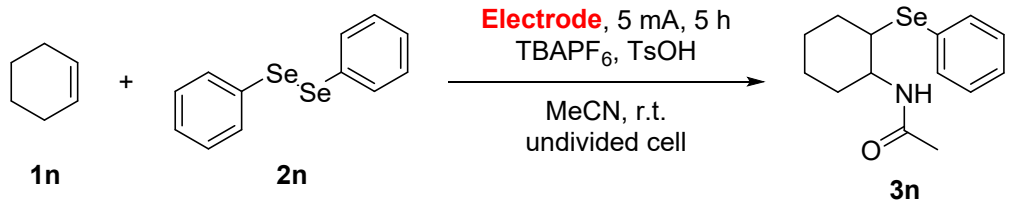
2.1.3 Table S3 screening of electrolytes[a]



Entry	Electrolyte	Yield (%)[b]
1	TBAB	n.r.
2	TBAI	n.r.
3	TBAC	n.r.
4	$TBABF_4$	28
5	$EMIMPF_6$	46
6	Bu_4NOH	trace
7	Me_4NF	11
8	TBAOAc	n.r.
9	$TBAHSO_4$	21
10	$TBAClO_4$	39
11	$TBANO_2$	n.r.
12	KPF_6	39
13	$TBAPF_6$	82

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), Electrolyte (0.2 mmol), MeCN (4 mL), TsOH (0.2 mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), constant current = 5 mA, 5 h, room temperature, under air, undivided cell. [b]Isolated yields. n.r. = no reaction.

2.1.4 Table S4 screening of electrodes[a]

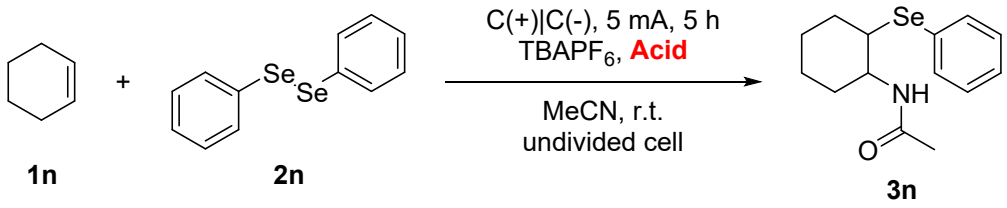


1n 2n 3n

Entry	Electrode	Yield (%)[b]
1	C-C	82
2	C-Ni	80
3	C-Cu	63

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), $TBAPF_6$ (0.2 mmol), MeCN (4 mL), TsOH (0.2 mmol), C anode (immersed surface area 8×5 mm^2), cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), constant current = 5 mA, 5 h, room temperature, under air, undivided cell. [b]Isolated yields.

2.1.5 Table S5 screening of acids[a]

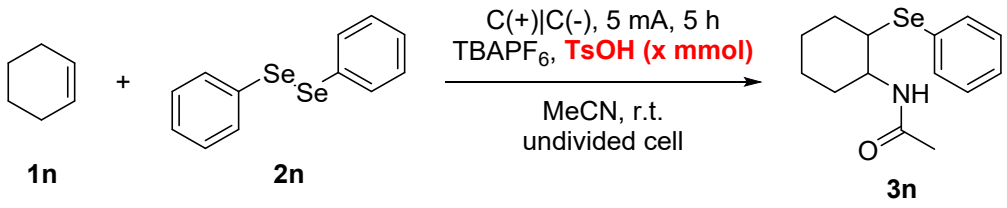


1n **2n** **3n**

Entry	Acid	Yield (%)[b]
1	TsOH	82
2	*p*-Toluic acid	n.d.
3	AcOH	n.d.

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), $TBAPF_6$ (0.2 mmol), MeCN (4 mL), Acid (0.2 mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), constant current = 5 mA, 5 h, room temperature, under air, undivided cell. [b]Isolated yields. n.d. = not detected.

2.1.6 Table S6 screening of TsOH dosages[a]

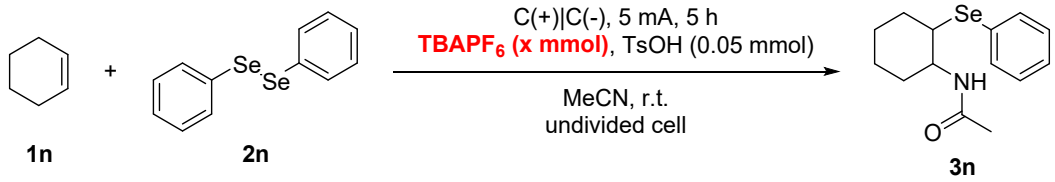


1n 2n 3n

Entry	TsOH (x mmol)	Yield (%)[b]
1	-	17
2	0.025	77
3	0.05	92
4	0.1	56
5	0.15	51
6	0.2	82

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), $TBAPF_6$ (0.2 mmol), MeCN (4 mL), TsOH (x mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), constant current = 5 mA, 5 h, room temperature, under air, undivided cell. [b]Isolated yields.

2.1.7 Table S7 screening of $TBAPF_6$ dosages[a]

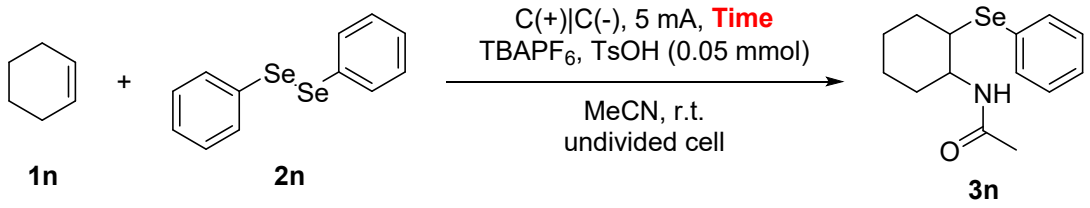


1n **2n** **3n**

Entry	$TBAPF_6$ (x mmol)	Yield (%)[b]
1	0.2	92
2	0.15	66
3	0.1	52
4	0.05	38
5	0.03	30

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), $TBAPF_6$ (x mmol), MeCN (4 mL), TsOH (0.05 mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), constant current = 5 mA, 5 h, room temperature, under air, undivided cell. [b]Isolated yields.

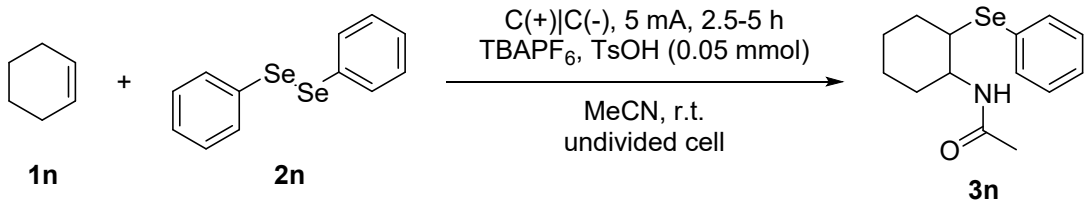
2.1.8 Table S8 screening of times[a]



Entry	Time (h)	Yield (%)[b]
1	3	90
2	5	92
3	8	68
4	10	trace

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), $TBAPF_6$ (0.2 mmol), MeCN (4 mL), TsOH (0.05 mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), constant current = 5 mA, time, room temperature, under air, undivided cell. [b]Isolated yields.

2.1.9 Table S9 screening of 2n dosages[a]

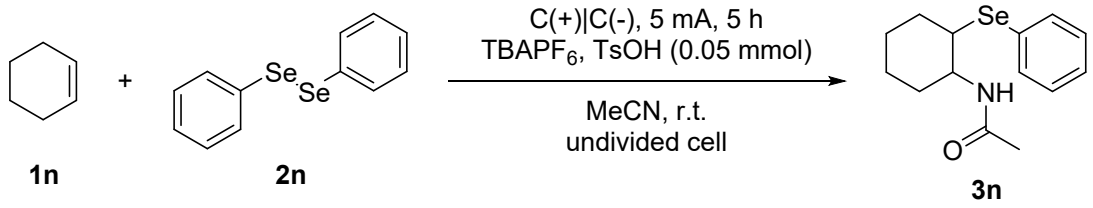


1n **2n** **3n**

Entry	2n (x mmol)	Yield (%)[b]
1[c]	0.075	76
2[d]	0.12	81
3	0.15	84
4	0.2	92
5	0.3	75

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (x mmol), $TBAPF_6$ (0.2 mmol), MeCN (4 mL), TsOH (0.05 mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), the distance between the electrodes (5 mm), constant current = 5 mA, 5 h, room temperature, under air, undivided cell. [b]Isolated yields. [c]2.5 h. [d]3 h.

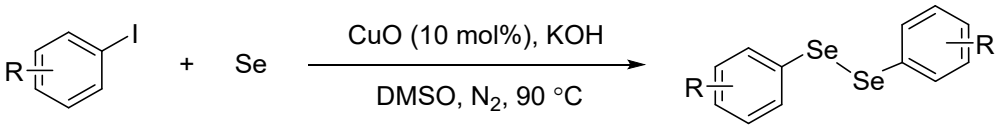
2.1.10 The general procedure for the amidoselenation reaction of cyclohexene



Under air, a mixture of cyclohexene **1n** (30 μL, 0.3 mmol), diphenyl diselenide **2n** (62.4 mg, 0.2 mmol), $TBAPF_6$ (77.5 mg, 0.2 mmol), TsOH (8.6 mg, 0.05 mmol) and MeCN (4 mL) were added in an oven dried undivided bottle (10 mL). The bottle was equipped with graphite rod as the anode and the cathode. The resulting mixture was stirred and electrolyzed at a constant current mode with a constant current of 5 mA at ambient temperature for 5 h. When the reaction was finished, the resulting mixture and all the volatiles were evaporated under reduced pressure. The resultant residue was purified by silica gel column chromatography (eluent: petroleum ether (60-90 ^{o}C)/EtOAc = 1:1, v:v) to afford the desired product **3n** as a white solid (82.5 mg, 92% yield).

2.2 Substrate synthesis method

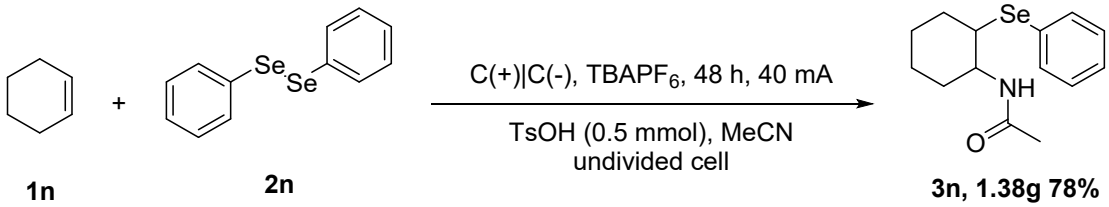
2.2.1 General procedure for the synthesis of diselenides[1]



Under nitrogen atmosphere, a stirred solution of Se (6.0 mmol) powder and aryl iodides (3.0 mmol) in dry DMSO (6.0 mL) was added CuO nanoparticles (10 mol%) followed by KOH (2.0 equiv) at 90 °C. The progress of the reaction was monitored by TLC. After the reaction was complete, the reaction mixture was allowed to cool, which was subjected to column chromatographic separation to give pure diselenides.

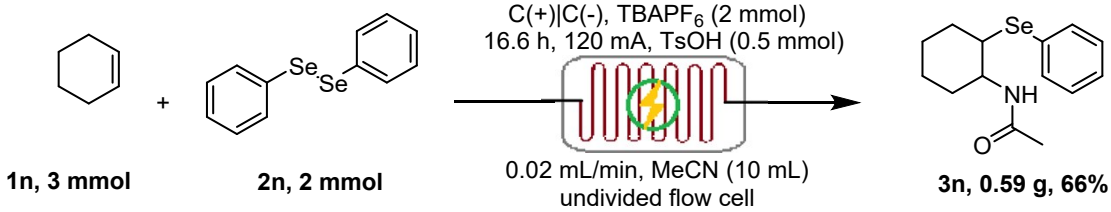
2.3 Scale-up reaction

2.3.1 Gram-scale of amidoselenation synthesis reactions



In the air, cyclohexene **1n** (607 μL, 6 mmol), diphenyldiselenide **2n** (1.25 g, 4 mmol), $TBAPF_6$ (1.55 g, 4 mmol), TsOH (86.1 mg, 0.5 mmol), and MeCN (40 mL) were added to a dry 150 mL beaker. The beaker is equipped with a graphite (27 mm×15.0 mm×1 mm) anode and a graphite (27 mm×15.0 mm×1 mm) cathode. The mixture was subjected to electrolysis at room temperature, with the current set to 40 mA, and the reaction was allowed to proceed for 48 hours. After the reaction, the mixture and all volatile substances were removed by rotary evaporation under reduced pressure. The resulting residue was purified by silica gel column chromatography, using a petroleum ether (60-90 °C)/ethyl acetate = 1:1 (v:v) eluent. The target product **3n** was obtained as a white solid (1.38 g, 78% yield).

2.3.2 Flow electrochemical synthesis of amidoselenation



In air, **1n** (304 μL, 3 mmol), **2n** (0.625 g, 2 mmol), $TBAPF_6$ (0.775 g, 2 mmol), TsOH (86.1 mg, 0.5 mmol), and MeCN (10 mL) were mixed and then aspirated into a syringe. A flow electrochemical reactor, equipped with graphite plates as both the anode and cathode, was used, with the surface area of the graphite plates measuring 8 cm×6 cm. The mixture underwent flow

electrolysis at room temperature under a constant current mode, with a current of 120 mA and a flow rate of 0.2 mL/min for 16.6 hours. Upon completion of the reaction, the mixture and all volatile substances were evaporated under reduced pressure. The resultant residue was purified by silica gel column chromatography (eluent: petroleum ether (60-90 ℃)/ethyl acetate = 1:1, v:v), yielding the target product **3n** as a white solid (0.59 g, 66% yield).

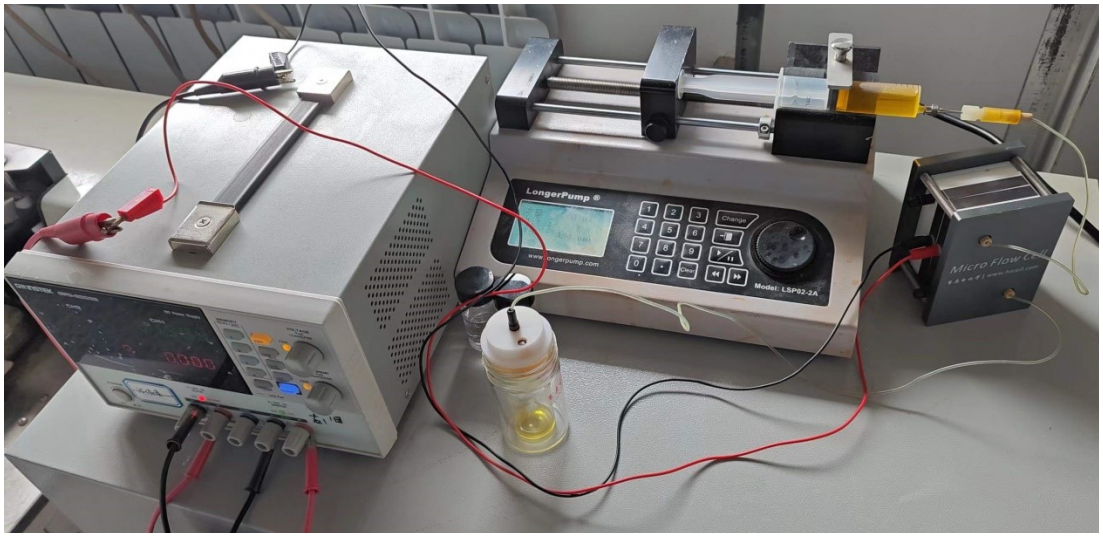


Fig. S3 Flow electrochemical reactor for scale-up experiment

3. Calculation of Green Chemistry Metrics

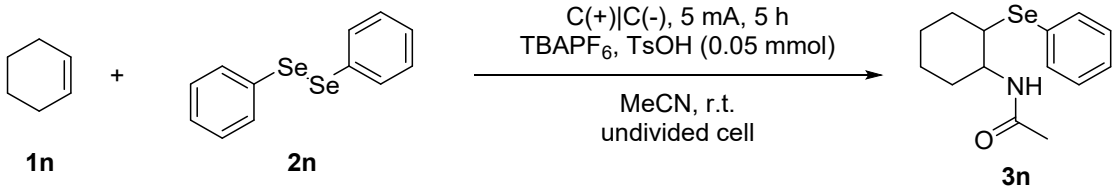
To evaluate the green chemistry aspects of the developed reaction, we calculated the green chemistry metrics, including Atom Economy (AE), Atom Efficiency (AEf) and Reaction Mass Efficiency (RME).[2] Additionally, we compared these metrics with two other efficient synthetic methods for sulfoxides. The chemistry metrics were calculated using the formulas provided below.

$$Atom\ Economy\ (AE)\ (\%) = \frac{Molecular\ Weight\ of\ Desired\ Product}{Sum\ of\ Molecular\ Weights\ of\ All\ Reactants} \times 100$$

$$Atom\ Efficiency\ (AEf)\ (\%) = Atom\ Economy\ (AE)(\%) \times yeild$$

$$Reaction\ Mass\ Efficiency\ (RME)\ (\%) = \frac{Mass\ of\ Desired\ Product}{Mass\ of\ Reactants\ Used} \times 100$$

This work



1n **2n** **3n**

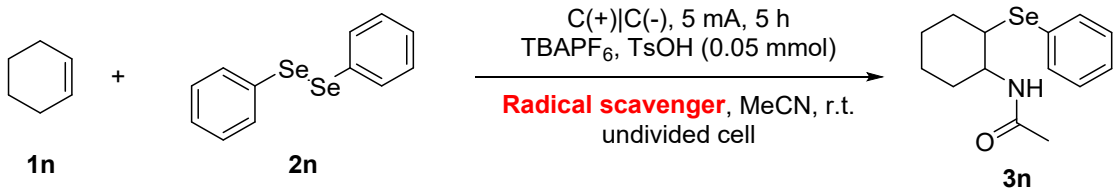
	mmol	mg	MW	Green Chemistry Metrics	
1n	0.3	24.6	82.15	Atom Economy (AE) (%)	84.90%
2n	0.2	62.4	312.13	Atom Efficiency (AEf) (%)	78.11%
TsOH	0.05	9.5	190.22	Reaction Mass Efficiency (RME) (%)	94.01%
MeCN	-	3107	41.05	-	-
$TBAPF_6$	0.2	77.5	387.43	-	-
3n	0.276	81.8	296.283	-	-

Table S10 The green chemistry metrics

4. Mechanistic studies

4.1 Radical trapping experiments

4.1.1 Table S11 the radical capture experiment in the amidoselenation reaction of cyclohexene[a]

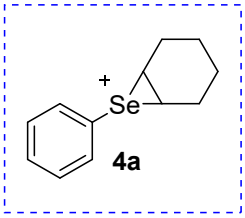


1n **2n** **3n**

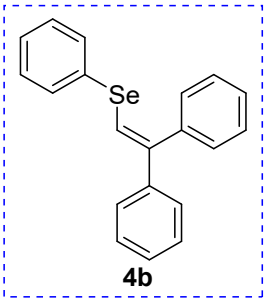
[a]Entry	Radical scavenger (mmol)	Yield (%)[b]
1	none	92
2	BHT (0.2)	55
3	BHT (0.4)	20
4	1,1-diphenythylene (0.2)	trace

[a]Reaction conditions: **1n** (0.3 mmol), **2n** (0.2 mmol), $TBAPF_6$ (0.2 mmol), radical scavenger, MeCN (4.0 mL), TsOH (0.05 mmol), C anode (immersed surface area 8×5 mm^2), C cathode (immersed surface area 8×5 mm^2), 5 mA, 5 h, room temperature, undivided cell. [b]Isolated yields

4.1.2 The HRMS spectra of compound 4a and 4b



Detected by HRMS of **4a** calcd for $C_{12}H_{15}Se^+$ $[M]^+$: 239.0334; Found: 239.0332.



Detected by HRMS of 4**b** calcd for $C_{20}H_{17}Se^+$ $[M+H]^+$: 337.0490; Found: 337.0483.

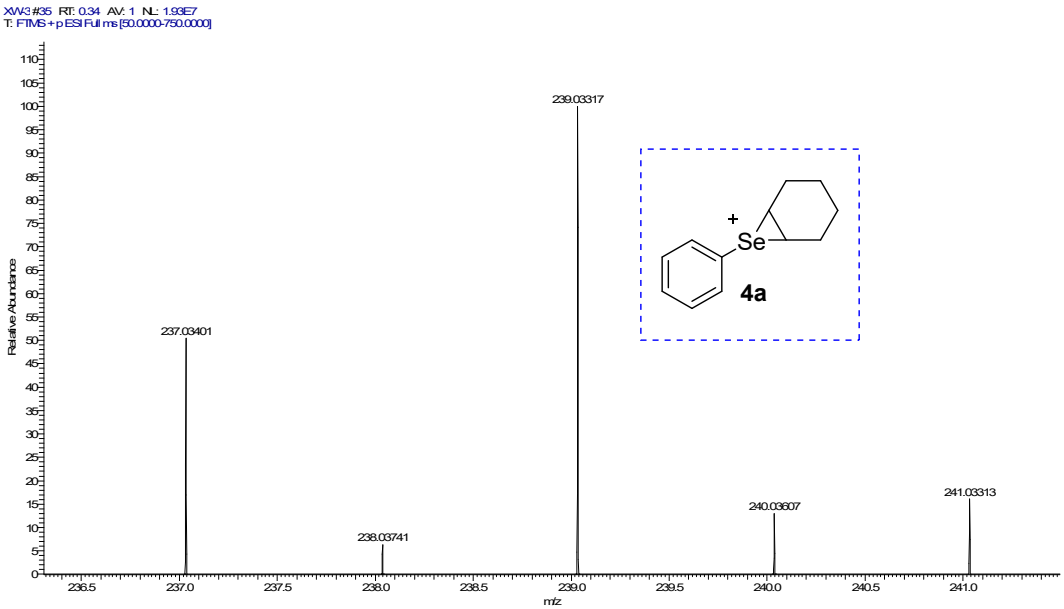


Fig. S4 The HRMS spectra of compound **4a**

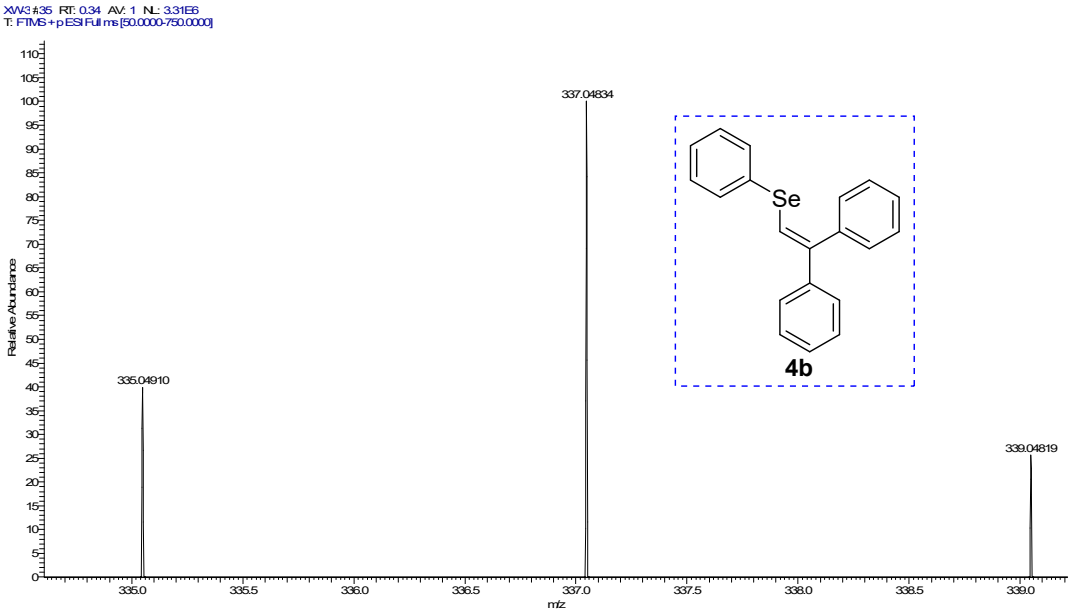
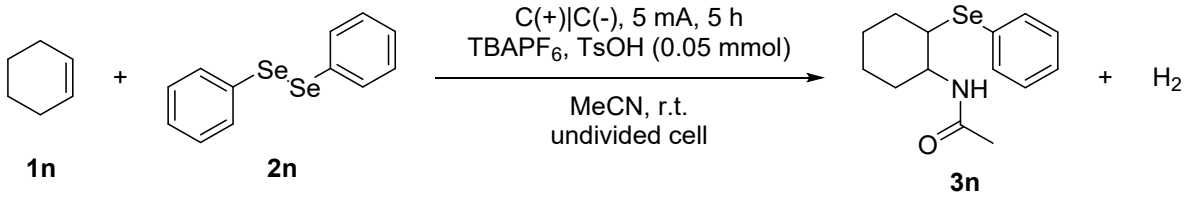


Fig. S5 The HRMS spectra of compound **4b**

4.2 The hydrogen detection experiment[a]



0 min 0 ppm | 3 min 478 ppm | 5 min 658 ppm | 10 min 948 ppm | 12 min 1000 ppm

Fig. S6 The hydrogen detection experiment

In order to demonstrate the release of H_2 during electrochemical aminoselenation of cyclohexene, the model reaction of cyclohexene **1n** and diphenyl diselenide **2n** was monitored by a H_2 detector under standard conditions. Just as shown in Fig. S6, as the reaction proceeded, the H_2 was observed clearly, and the concentration increased gradually.

4.3 DFT calculations on the plausible mechanism

4.3.1 Computation details:

All calculations have been performed using the DFT method implemented in the commercial Gaussian 16[3] program package. Molecular geometries of the model complexes were optimized at the PBE0(D3BJ)/Def2SVP[4-6] level with the SMD[7] solvation model and acetonitrile as the solvent. As soon as the convergences of optimizations were obtained, the frequency calculations ate the same level have been performed to identify all the stationary points as minima or transition states, which has the unique imaginary frequencies. And the intrinsic reaction coordinate (IRC)[8] calculations have confirmed that all stationary points were smoothly connected to each other. All of the optimized geometries mentioned were built by GaussView 6.0.[9]

4.3.2 The DFT calculation process for the Markovnikov and anti-Markovnikov additions of allylbenzene

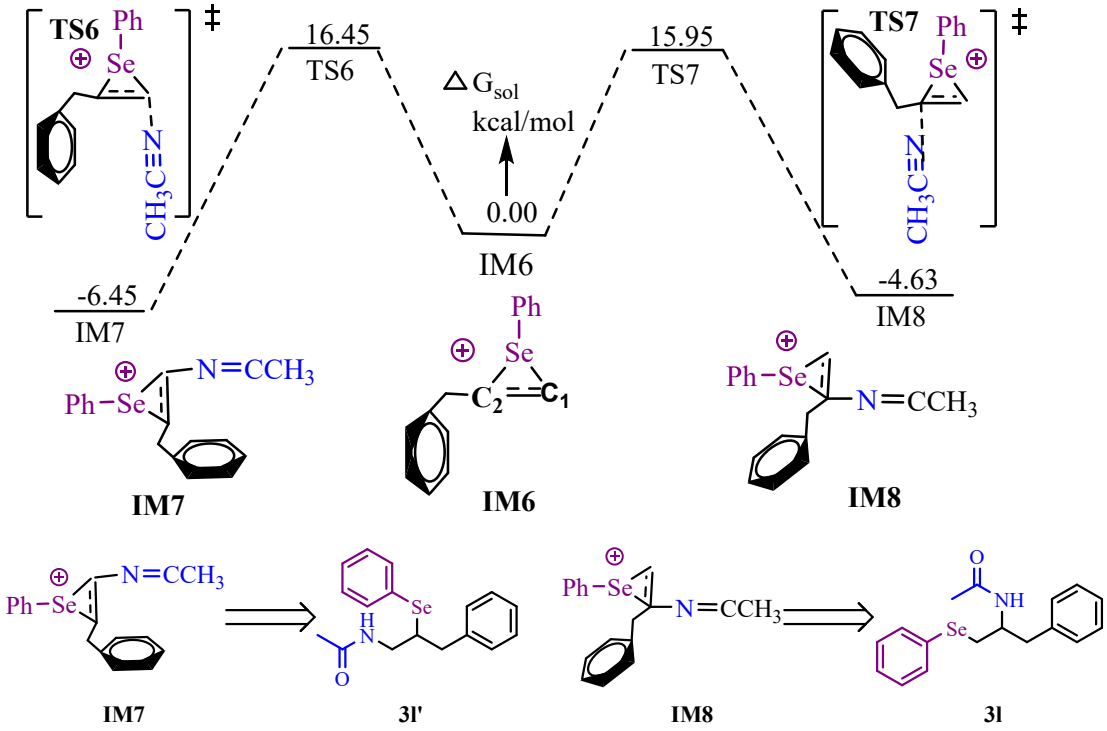


Fig. S7 Computed reaction free energy diagram for the formation of **3l`** and **3l**

4.3.3 Optimized corresponding structures of intermediates and transition states

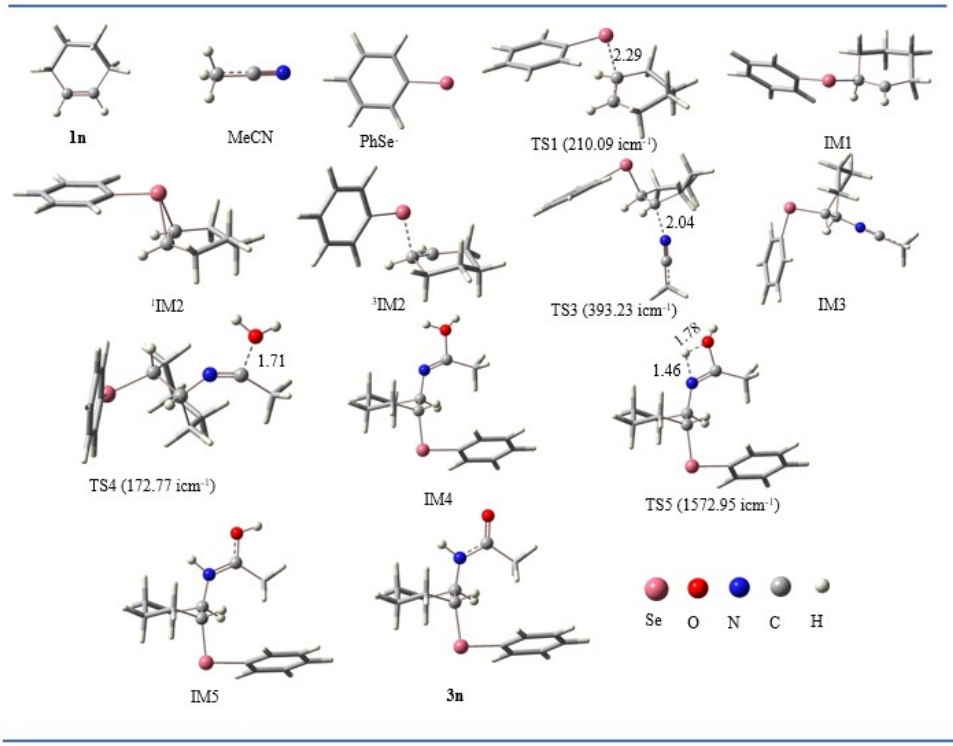


Fig. S8 Optimized corresponding structures of intermediates and transition states along pathway of Fig. 3 (the manuscript) at the PBE0(D3BJ)/Def2svp level (distances in Å, in parentheses are the unique imaginary frequencies of the transition state) with SMD solvation model and acetonitrile as the solvent

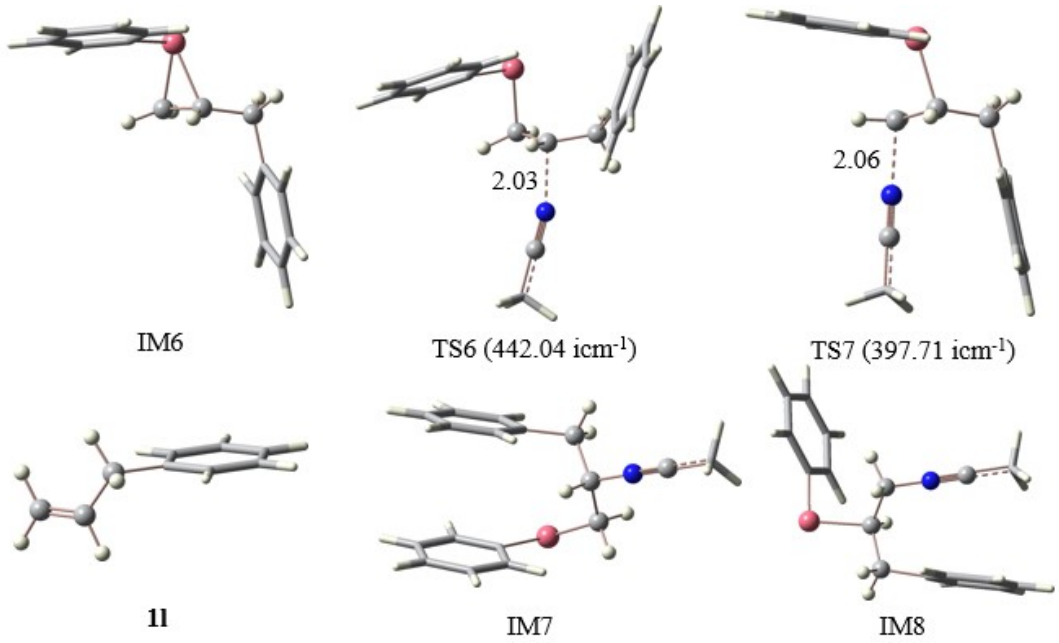


Fig. S9 Optimized corresponding structures of intermediates and transition states along pathway of Fig. S7 at the PBE0(D3BJ)/Def2svp level (distances in Å, in parentheses are the unique imaginary frequencies of the transition state) with SMD solvation model and acetonitrile as the solvent

4.3.4 Cartesian coordinates and energies of DFT-computed structures

Standard orientation, imaginary frequencies, thermodynamic energies of All Stationary Points

1n (Charge = 0 Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.693260	1.183891	0.317315
2	6	0	1.490495	-0.045308	-0.108455
3	6	0	0.667179	-1.298850	-0.057177
4	6	0	-0.668017	-1.298489	0.057100
5	6	0	-1.490494	-0.044437	0.108594
6	6	0	-0.692547	1.184257	-0.317396
7	1	0	1.883349	0.089304	-1.134682
8	1	0	2.384891	-0.165303	0.526975
9	1	0	0.584058	1.182689	1.416710
10	1	0	1.242518	2.102778	0.057287
11	1	0	-1.202627	-2.254041	0.114390
12	1	0	-2.385157	-0.163728	-0.526571
13	1	0	-1.882918	0.090402	1.134971
14	1	0	-0.583314	1.182694	-1.416795
15	1	0	-1.241285	2.103523	-0.057609
16	1	0	1.201226	-2.254701	-0.114568

0 imaginary frequencies

Sum of electronic and zero-point Energies= -234.066747

Sum of electronic and thermal Energies= -234.061250

Sum of electronic and thermal Enthalpies= -234.060306

Sum of electronic and thermal Free Energies= -234.095347

MeCN (Charge = 0 Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	-0.000000	-1.172687
2	1	0	-0.000000	1.034048	-1.547238
3	1	0	0.895512	-0.517024	-1.547238
4	1	0	-0.895512	-0.517024	-1.547238
5	6	0	0.000000	0.000000	0.274715
6	7	0	0.000000	0.000000	1.432792

0 imaginary frequencies

Sum of electronic and zero-point Energies= -132.458538
Sum of electronic and thermal Energies= -132.454957
Sum of electronic and thermal Enthalpies= -132.454013
Sum of electronic and thermal Free Energies= -132.481493

PhSe• (Charge = 0 Multiplicity = 2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	1.836246	-0.000008	-0.000003
2	6	0	-0.062994	-0.000191	0.000020
3	6	0	-0.764711	-1.213572	-0.000017
4	6	0	-0.764446	1.213445	0.000029
5	6	0	-2.159109	-1.205151	0.000029
6	1	0	-0.223256	-2.162957	-0.000079
7	6	0	-2.158786	1.205323	-0.000029
8	1	0	-0.222666	2.162664	0.000060
9	6	0	-2.862193	0.000147	-0.000008
10	1	0	-2.699269	-2.155721	0.000044
11	1	0	-2.698878	2.155949	-0.000055
12	1	0	-3.954854	0.000323	-0.000021

0 imaginary frequencies
Sum of electronic and zero-point Energies= -2632.077723
Sum of electronic and thermal Energies= -2632.071986
Sum of electronic and thermal Enthalpies= -2632.071042
Sum of electronic and thermal Free Energies= -2632.109351

TS1 (Charge = 0, Multiplicity = 2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.769530	-0.103191	0.428441
2	6	0	-2.691346	0.887740	0.865040
3	6	0	-1.322540	0.239352	1.032953
4	6	0	-1.200189	-1.153005	0.863063
5	6	0	-2.132457	-1.942229	0.013266
6	6	0	-3.232156	-1.085130	-0.603876
7	1	0	-2.637778	1.723492	0.147986
8	1	0	-2.965352	1.345877	1.829440
9	1	0	-4.126195	-0.672519	1.305174
10	1	0	-4.639495	0.446462	0.036665

11	1	0	-0.316433	-1.657729	1.266239
12	1	0	-1.558490	-2.476854	-0.766826
13	1	0	-2.576849	-2.746876	0.632239
14	1	0	-2.825268	-0.523792	-1.463320
15	1	0	-4.036566	-1.726943	-0.995147
16	1	0	-0.692747	0.675613	1.814953
17	34	0	-0.106468	1.109267	-0.703897
18	6	0	1.558641	0.307313	-0.252369
19	6	0	2.390763	0.896809	0.710776
20	6	0	1.958000	-0.889232	-0.865231
21	6	0	3.600519	0.295705	1.055661
22	1	0	2.085329	1.830172	1.190744
23	6	0	3.170351	-1.485095	-0.518402
24	1	0	1.313202	-1.353306	-1.615735
25	6	0	3.993287	-0.895456	0.442334
26	1	0	4.241394	0.762381	1.808495
27	1	0	3.472599	-2.417883	-1.001959
28	1	0	4.942499	-1.364669	0.713600

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1 imaginary frequencies (210.09 icm^{-1})
Sum of electronic and zero-point Energies= -2866.154559
Sum of electronic and thermal Energies= -2866.142112
Sum of electronic and thermal Enthalpies= -2866.141168
Sum of electronic and thermal Free Energies= -2866.197249

IM1 (Charge = 0, Multiplicity = 2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.663496	1.857167	0.545852
2	6	0	1.415016	1.000649	0.730709
3	6	0	1.306055	-0.051760	-0.370201
4	6	0	2.573046	-0.804040	-0.582924
5	6	0	3.870254	-0.072201	-0.531364
6	6	0	3.917117	0.992251	0.564005
7	1	0	1.467563	0.487937	1.706573
8	1	0	0.507502	1.623899	0.741609
9	1	0	2.601229	2.403328	-0.413090
10	1	0	2.709281	2.620030	1.339833
11	1	0	2.528433	-1.761261	-1.114337
12	1	0	4.705225	-0.784684	-0.427557
13	1	0	4.031864	0.428252	-1.511956
14	1	0	3.996648	0.498757	1.548680

15	1	0	4.821008	1.610739	0.445074
16	1	0	1.015679	0.442058	-1.319764
17	34	0	-0.113134	-1.371629	-0.004480
18	6	0	-1.667184	-0.259605	-0.050240
19	6	0	-2.745743	-0.614515	0.770613
20	6	0	-1.781047	0.851439	-0.894873
21	6	0	-3.924583	0.129692	0.739988
22	1	0	-2.660010	-1.473494	1.441777
23	6	0	-2.956111	1.602723	-0.903790
24	1	0	-0.957023	1.135999	-1.552982
25	6	0	-4.033149	1.244394	-0.092116
26	1	0	-4.760035	-0.159522	1.383153
27	1	0	-3.030364	2.472694	-1.561804
28	1	0	-4.953454	1.833506	-0.106830

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0 imaginary frequencies
Sum of electronic and zero-point Energies= -2866.154451
Sum of electronic and thermal Energies= -2866.141903
Sum of electronic and thermal Enthalpies= -2866.140959
Sum of electronic and thermal Free Energies= -2866.195918

[1]IM2 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.711810	0.645584	0.475719
2	6	0	-2.466194	1.528315	0.409009
3	6	0	-1.184939	0.783983	0.721352
4	6	0	-1.157168	-0.673183	0.812370
5	6	0	-2.404058	-1.479801	0.603978
6	6	0	-3.482492	-0.721042	-0.155765
7	1	0	-2.383234	2.003290	-0.580704
8	1	0	-2.536642	2.355683	1.131598
9	1	0	-4.002552	0.501457	1.530431
10	1	0	-4.547363	1.167704	-0.013426
11	1	0	-0.381516	-1.119472	1.443329
12	1	0	-2.154024	-2.442656	0.134679
13	1	0	-2.763990	-1.715598	1.622671
14	1	0	-3.187359	-0.604539	-1.215193
15	1	0	-4.411004	-1.310806	-0.154490
16	1	0	-0.419407	1.326186	1.285186
17	34	0	-0.229272	-0.030917	-0.875933
18	6	0	1.571995	-0.006398	-0.233376

19	6	0	2.224604	-1.216732	0.009404
20	6	0	2.228405	1.218216	-0.096397
21	6	0	3.557444	-1.192893	0.416786
22	1	0	1.697214	-2.165726	-0.113147
23	6	0	3.560694	1.225964	0.313247
24	1	0	1.704359	2.154774	-0.301250
25	6	0	4.222326	0.024436	0.569647
26	1	0	4.077782	-2.132952	0.615149
27	1	0	4.083217	2.178266	0.430947
28	1	0	5.266918	0.036884	0.890113

0 imaginary frequencies
Sum of electronic and zero-point Energies= -2866.022471
Sum of electronic and thermal Energies= -2866.010506
Sum of electronic and thermal Enthalpies= -2866.009562
Sum of electronic and thermal Free Energies= -2866.061928

^{3}IM2 (Charge = 1, Multiplicity = 3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.827595	-0.610075	-0.726441
2	6	0	-3.635115	0.537348	0.264828
3	6	0	-2.548030	0.282024	1.245175
4	6	0	-1.338975	-0.429078	0.854307
5	6	0	-1.540530	-1.508752	-0.204786
6	6	0	-2.497521	-1.073021	-1.305237
7	1	0	-3.380131	1.460569	-0.300637
8	1	0	-4.572256	0.771486	0.793816
9	1	0	-4.309193	-1.457807	-0.208886
10	1	0	-4.512573	-0.297371	-1.529581
11	1	0	-0.749419	-0.765702	1.717936
12	1	0	-0.575080	-1.838317	-0.616497
13	1	0	-1.961977	-2.376329	0.333464
14	1	0	-2.040284	-0.252573	-1.888956
15	1	0	-2.651046	-1.908125	-2.006094
16	1	0	-2.557860	0.795991	2.210854
17	34	0	-0.066333	1.015475	0.056209
18	6	0	1.616029	0.229285	0.031099
19	6	0	1.916307	-1.010407	0.633666
20	6	0	2.624761	0.969936	-0.627902
21	6	0	3.212883	-1.495536	0.569940
22	1	0	1.147555	-1.584452	1.152170

23	6	0	3.915573	0.467115	-0.681684
24	1	0	2.381203	1.929546	-1.091005
25	6	0	4.211235	-0.763424	-0.085477
26	1	0	3.454155	-2.452876	1.036950
27	1	0	4.698382	1.033890	-1.190209
28	1	0	5.229710	-1.156557	-0.129343

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0 imaginary frequencies

Sum of electronic and zero-point Energies= -2865.962099

Sum of electronic and thermal Energies= -2865.949495

Sum of electronic and thermal Enthalpies= -2865.948550

Sum of electronic and thermal Free Energies= -2866.003307

TS3 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.068707	-1.435271	-0.592872
2	6	0	-1.936433	-0.884284	-1.463166
3	6	0	-0.809176	-0.236138	-0.666820
4	6	0	-1.055953	0.020980	0.749903
5	6	0	-1.901094	-0.910222	1.560524
6	6	0	-2.550380	-2.004651	0.720850
7	1	0	-1.511464	-1.677681	-2.096765
8	1	0	-2.327207	-0.119517	-2.152058
9	1	0	-3.788689	-0.630537	-0.368310
10	1	0	-3.621684	-2.200864	-1.156854
11	1	0	-0.348401	0.666821	1.275660
12	1	0	-1.275234	-1.320172	2.367916
13	1	0	-2.662240	-0.296956	2.067176
14	1	0	-1.817807	-2.806175	0.517249
15	1	0	-3.364617	-2.467400	1.297489
16	1	0	-0.322713	0.596834	-1.185009
17	34	0	0.684967	-1.489818	-0.204568
18	6	0	2.082434	-0.191735	-0.062991
19	6	0	2.525921	0.485300	-1.204012
20	6	0	2.686668	0.033836	1.177176
21	6	0	3.567441	1.404736	-1.095022
22	1	0	2.057290	0.294209	-2.172795
23	6	0	3.736627	0.947273	1.273791
24	1	0	2.334513	-0.499703	2.063226
25	6	0	4.174034	1.634214	0.141360
26	1	0	3.912416	1.938640	-1.984030

27	1	0	4.210633	1.125482	2.242271
28	1	0	4.994181	2.352129	0.221410
29	6	0	-2.804813	2.613102	0.204910
30	7	0	-2.289159	1.638071	0.546978
31	6	0	-3.457386	3.827145	-0.216513
32	1	0	-3.824597	3.705371	-1.246047
33	1	0	-4.303871	4.040800	0.452140
34	1	0	-2.740362	4.660335	-0.178908

1 imaginary frequencies （393.23 icm^{-1}）

Sum of electronic and zero-point Energies= -2998.465931

Sum of electronic and thermal Energies= -2998.449103

Sum of electronic and thermal Enthalpies= -2998.448158

Sum of electronic and thermal Free Energies= -2998.514511

IM3 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.008971	-1.108208	1.130841
2	6	0	1.791281	-0.359070	1.654643
3	6	0	1.101646	0.459498	0.562088
4	6	0	0.802851	-0.351746	-0.710581
5	6	0	2.022573	-1.132272	-1.186303
6	6	0	2.662604	-1.965734	-0.081188
7	1	0	1.033440	-1.068163	2.022183
8	1	0	2.048619	0.304480	2.493574
9	1	0	3.799176	-0.386190	0.857232
10	1	0	3.425359	-1.729878	1.938358
11	1	0	0.449902	0.330674	-1.496520
12	1	0	1.739482	-1.759824	-2.045282
13	1	0	2.758953	-0.401926	-1.566655
14	1	0	1.973325	-2.772678	0.223671
15	1	0	3.566980	-2.458636	-0.470333
16	1	0	0.175625	0.916429	0.945293
17	34	0	-0.702718	-1.579834	-0.370973
18	6	0	-2.045528	-0.242256	-0.092177
19	6	0	-2.629065	-0.103624	1.171530
20	6	0	-2.459376	0.578457	-1.147937
21	6	0	-3.622905	0.854808	1.376561
22	1	0	-2.302080	-0.742898	1.995227
23	6	0	-3.441232	1.544126	-0.932107
24	1	0	-2.014174	0.459403	-2.139174

25	6	0	-4.026333	1.681311	0.328207
26	1	0	-4.077918	0.958938	2.364935
27	1	0	-3.758912	2.186220	-1.757740
28	1	0	-4.801204	2.434512	0.491918
29	6	0	3.451673	3.540079	-0.466984
30	1	0	3.736332	3.433988	-1.524864
31	1	0	2.900505	4.480921	-0.317434
32	1	0	4.350152	3.525037	0.168598
33	6	0	2.608419	2.444665	-0.100479
34	7	0	1.933628	1.566249	0.199061

0 imaginary frequencies
Sum of electronic and zero-point Energies= -2998.505617
Sum of electronic and thermal Energies= -2998.489509
Sum of electronic and thermal Enthalpies= -2998.488565
Sum of electronic and thermal Free Energies= -2998.552139

TS4 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.508405	-1.633769	1.104809
2	6	0	1.455709	-0.617378	1.533510
3	6	0	0.928393	0.203269	0.360492
4	6	0	0.443497	-0.673999	-0.803094
5	6	0	1.493053	-1.706582	-1.200480
6	6	0	1.994149	-2.529276	-0.017655
7	1	0	0.589752	-1.141056	1.969266
8	1	0	1.838218	0.058759	2.313434
9	1	0	3.420226	-1.111262	0.764785
10	1	0	2.809054	-2.239844	1.973816
11	1	0	0.209005	-0.025044	-1.658289
12	1	0	1.094631	-2.356130	-1.995611
13	1	0	2.340494	-1.154191	-1.645318
14	1	0	1.176427	-3.164830	0.365218
15	1	0	2.788358	-3.213720	-0.355192
16	1	0	0.094262	0.844772	0.690417
17	34	0	-1.246262	-1.584798	-0.349671
18	6	0	-2.310208	-0.019793	-0.059531
19	6	0	-2.947212	0.153992	1.173745
20	6	0	-2.474775	0.935665	-1.069672
21	6	0	-3.745435	1.277577	1.393576
22	1	0	-2.812131	-0.587812	1.964827

23	6	0	-3.256787	2.065787	-0.836143
24	1	0	-1.992492	0.795513	-2.040617
25	6	0	-3.896525	2.237295	0.393087
26	1	0	-4.242506	1.406670	2.358562
27	1	0	-3.376295	2.812361	-1.625712
28	1	0	-4.514473	3.121184	0.570281
29	6	0	4.019635	1.839697	1.044552
30	1	0	4.967662	1.474735	0.620111
31	1	0	4.130797	2.902925	1.302612
32	1	0	3.779178	1.263327	1.946873
33	6	0	2.933308	1.664739	0.080201
34	7	0	1.896224	1.131508	-0.183247
35	8	0	3.353214	2.736991	-1.188297
36	1	0	2.807265	2.501990	-1.967476
37	1	0	4.294974	2.694953	-1.458435

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1 imaginary frequencies （172.77 icm^{-1}）

Sum of electronic and zero-point Energies= -3074.751828

Sum of electronic and thermal Energies= -3074.734486

Sum of electronic and thermal Enthalpies= -3074.733542

Sum of electronic and thermal Free Energies= -3074.798532

IM4 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.267086	-0.952946	1.054610
2	6	0	1.975476	-0.381499	1.624481
3	6	0	1.136347	0.341686	0.574319
4	6	0	0.913898	-0.509303	-0.687898
5	6	0	2.203993	-1.123937	-1.216416
6	6	0	2.991985	-1.860083	-0.138940
7	1	0	1.353632	-1.195164	2.032422
8	1	0	2.178064	0.311807	2.455934
9	1	0	3.927018	-0.125809	0.740138
10	1	0	3.806845	-1.503230	1.841574
11	1	0	0.450495	0.118676	-1.462578
12	1	0	1.977421	-1.785468	-2.067240
13	1	0	2.819470	-0.298357	-1.614472
14	1	0	2.424247	-2.746910	0.195492
15	1	0	3.936438	-2.236203	-0.563207
16	1	0	0.153558	0.595671	1.003992
17	34	0	-0.430159	-1.912845	-0.329827

18	6	0	-1.908797	-0.719889	-0.079112
19	6	0	-2.530233	-0.637002	1.171173
20	6	0	-2.366370	0.071891	-1.139044
21	6	0	-3.600705	0.238807	1.360024
22	1	0	-2.169032	-1.251111	1.999742
23	6	0	-3.425548	0.956379	-0.939822
24	1	0	-1.892483	-0.003287	-2.121301
25	6	0	-4.045199	1.040370	0.308627
26	1	0	-4.082673	0.300002	2.339216
27	1	0	-3.774975	1.577070	-1.769057
28	1	0	-4.878549	1.730998	0.460585
29	6	0	-0.123157	3.165158	0.052362
30	1	0	-0.151780	4.059297	0.694870
31	1	0	-0.473970	3.445772	-0.952947
32	1	0	-0.791537	2.401775	0.469224
33	6	0	1.241745	2.622092	-0.029404
34	7	0	1.825602	1.552766	0.155997
35	8	0	2.180540	3.669501	-0.553333
36	1	0	2.094117	4.559988	-0.134702
37	1	0	3.112427	3.345493	-0.488636

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0 imaginary frequencies

Sum of electronic and zero-point Energies= -3074.757468

Sum of electronic and thermal Energies= -3074.740032

Sum of electronic and thermal Enthalpies= -3074.739087

Sum of electronic and thermal Free Energies= -3074.804609

TS5 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.279800	-0.908915	1.045925
2	6	0	1.981832	-0.374478	1.637784
3	6	0	1.122690	0.354382	0.609208
4	6	0	0.910173	-0.465192	-0.676484
5	6	0	2.210098	-1.041151	-1.223385
6	6	0	3.013595	-1.791609	-0.167672
7	1	0	1.377759	-1.209295	2.028124
8	1	0	2.175753	0.302795	2.484055
9	1	0	3.927030	-0.065050	0.748276
10	1	0	3.832839	-1.467945	1.817119
11	1	0	0.433815	0.176259	-1.432131
12	1	0	1.993126	-1.682716	-2.091647

13	1	0	2.810731	-0.194730	-1.601396
14	1	0	2.460735	-2.694645	0.147371
15	1	0	3.961919	-2.142300	-0.604490
16	1	0	0.138844	0.589280	1.045885
17	34	0	-0.409350	-1.898551	-0.350959
18	6	0	-1.902863	-0.730499	-0.071231
19	6	0	-2.504450	-0.660321	1.189530
20	6	0	-2.388567	0.058342	-1.120811
21	6	0	-3.582640	0.201124	1.399386
22	1	0	-2.121810	-1.272882	2.009548
23	6	0	-3.456157	0.927720	-0.900991
24	1	0	-1.929488	-0.006689	-2.110780
25	6	0	-4.055202	0.999895	0.358211
26	1	0	-4.048595	0.253172	2.386807
27	1	0	-3.827549	1.546561	-1.721989
28	1	0	-4.894612	1.679272	0.526666
29	6	0	-0.196880	3.189547	-0.160399
30	1	0	-0.284388	4.141881	0.385082
31	1	0	-0.441895	3.378798	-1.217766
32	1	0	-0.896303	2.453566	0.254895
33	6	0	1.171206	2.683354	-0.069871
34	7	0	1.753397	1.609065	0.241460
35	8	0	2.269078	3.498684	-0.476728
36	1	0	2.380755	4.336616	0.032485
37	1	0	2.826992	2.522676	-0.125103

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1 imaginary frequencies （1572.95 icm^{-1}）

Sum of electronic and zero-point Energies= -3074.742089

Sum of electronic and thermal Energies= -3074.725207

Sum of electronic and thermal Enthalpies= -3074.724263

Sum of electronic and thermal Free Energies= -3074.788518

IM5 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.464219	-0.531604	0.915907
2	6	0	2.155892	-0.078307	1.554991
3	6	0	1.162624	0.500527	0.551132
4	6	0	0.964583	-0.400923	-0.677758
5	6	0	2.284668	-0.870839	-1.275526
6	6	0	3.213135	-1.493127	-0.239396
7	1	0	1.659931	-0.943537	2.022397

8	1	0	2.330355	0.659155	2.353798
9	1	0	4.037008	0.339385	0.547617
10	1	0	4.096984	-1.003476	1.683690
11	1	0	0.382073	0.147745	-1.431997
12	1	0	2.086371	-1.567502	-2.104542
13	1	0	2.778036	0.011028	-1.723011
14	1	0	2.764347	-2.425264	0.148063
15	1	0	4.163983	-1.778356	-0.716035
16	1	0	0.197016	0.651620	1.051203
17	34	0	-0.184547	-1.939565	-0.205521
18	6	0	-1.788505	-0.908877	-0.005071
19	6	0	-2.269664	-0.602184	1.271999
20	6	0	-2.463267	-0.437522	-1.137402
21	6	0	-3.413240	0.185544	1.413979
22	1	0	-1.743350	-0.972246	2.155211
23	6	0	-3.601430	0.354641	-0.989067
24	1	0	-2.092751	-0.686946	-2.134986
25	6	0	-4.076042	0.668682	0.285702
26	1	0	-3.783633	0.426017	2.413862
27	1	0	-4.122298	0.725317	-1.875687
28	1	0	-4.968628	1.289124	0.399224
29	6	0	-0.627005	2.791041	-0.051173
30	1	0	-1.075444	3.679207	-0.514152
31	1	0	-1.034280	1.884867	-0.520950
32	1	0	-0.897421	2.768423	1.016853
33	6	0	0.845522	2.831880	-0.172965
34	7	0	1.613786	1.822579	0.108672
35	8	0	1.456796	3.917022	-0.555038
36	1	0	2.617340	1.966074	-0.021685
37	1	0	0.819146	4.626763	-0.753662

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0 imaginary frequencies

Sum of electronic and zero-point Energies= -3074.831018

Sum of electronic and thermal Energies= -3074.814422

Sum of electronic and thermal Enthalpies= -3074.813477

Sum of electronic and thermal Free Energies= -3074.876301

3n (Charge = 0, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.467447	-0.542703	0.913069
2	6	0	2.163863	-0.081485	1.557105

3	6	0	1.195699	0.551247	0.556925
4	6	0	0.967708	-0.355980	-0.665567
5	6	0	2.276045	-0.838543	-1.279130
6	6	0	3.202760	-1.484970	-0.255684
7	1	0	1.658562	-0.950732	2.008450
8	1	0	2.354393	0.637678	2.369282
9	1	0	4.045460	0.328697	0.554166
10	1	0	4.099898	-1.033569	1.669950
11	1	0	0.382681	0.197048	-1.414749
12	1	0	2.069264	-1.521326	-2.118090
13	1	0	2.777534	0.045567	-1.712642
14	1	0	2.745318	-2.417891	0.120900
15	1	0	4.148804	-1.775445	-0.739755
16	1	0	0.231702	0.706773	1.060452
17	34	0	-0.188696	-1.896952	-0.201256
18	6	0	-1.798719	-0.874702	-0.009029
19	6	0	-2.295967	-0.578772	1.264455
20	6	0	-2.467573	-0.402631	-1.144546
21	6	0	-3.448591	0.196917	1.399616
22	1	0	-1.774185	-0.947262	2.151026
23	6	0	-3.614788	0.377586	-1.003640
24	1	0	-2.084734	-0.642199	-2.139950
25	6	0	-4.105606	0.679669	0.267788
26	1	0	-3.830365	0.429126	2.397233
27	1	0	-4.129624	0.748910	-1.893578
28	1	0	-5.005062	1.291147	0.375880
29	6	0	-0.559686	2.831979	-0.001515
30	1	0	-1.022386	3.757455	-0.364419
31	1	0	-0.991429	1.972937	-0.536847
32	1	0	-0.798111	2.705476	1.066202
33	6	0	0.930625	2.933588	-0.211338
34	7	0	1.676729	1.851359	0.131483
35	8	0	1.456490	3.948028	-0.650363
36	1	0	2.669635	1.953046	-0.059318

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0 imaginary frequencies

Sum of electronic and zero-point Energies= -3074.401543

Sum of electronic and thermal Energies= -3074.384805

Sum of electronic and thermal Enthalpies= -3074.383861

Sum of electronic and thermal Free Energies= -3074.448103

1l (Charge = 0 Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.325512	-0.864607	0.216956
2	6	0	-1.011607	-1.281588	-0.004401
3	6	0	0.004121	-0.352304	-0.255103
4	6	0	-1.637102	1.430133	-0.053444
5	6	0	-2.642941	0.492885	0.192511
6	1	0	-3.104985	-1.606644	0.410131
7	1	0	-0.768336	-2.348066	0.015285
8	1	0	-1.876194	2.496907	-0.074154
9	1	0	-3.671086	0.821413	0.365696
10	6	0	-0.326615	1.009899	-0.272596
11	1	0	0.457942	1.749308	-0.459585
12	6	0	1.428550	-0.794870	-0.500422
13	1	0	1.466517	-1.896009	-0.453752
14	1	0	1.738037	-0.503853	-1.518466
15	6	0	2.392421	-0.220616	0.493670
16	1	0	2.204367	-0.480715	1.543739
17	6	0	3.422819	0.572384	0.191230
18	1	0	3.637893	0.857975	-0.844968
19	1	0	4.091034	0.961785	0.965662

0 imaginary frequencies
Sum of electronic and zero-point Energies= -348.149946
Sum of electronic and thermal Energies= -348.141841
Sum of electronic and thermal Enthalpies= -348.140897
Sum of electronic and thermal Free Energies= -348.183869

IM6 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.437070	1.838509	-0.271145
2	6	0	3.312841	1.239560	-0.838256
3	6	0	2.907657	-0.038702	-0.435724
4	6	0	4.768732	-0.105298	1.120242
5	6	0	5.167540	1.167608	0.710292
6	1	0	4.745919	2.834208	-0.600030
7	1	0	2.743279	1.766390	-1.609354
8	1	0	5.338741	-0.638208	1.885761
9	1	0	6.050065	1.635757	1.153829
10	6	0	3.644732	-0.703567	0.552006

11	1	0	3.338295	-1.703537	0.872111
12	6	0	1.666512	-0.667063	-1.023925
13	1	0	1.501764	-0.298618	-2.045849
14	1	0	1.770427	-1.761698	-1.060824
15	6	0	0.487633	-0.291648	-0.167364
16	1	0	0.205606	0.767389	-0.171057
17	6	0	0.105685	-1.062268	1.007954
18	1	0	0.641506	-1.992376	1.223963
19	1	0	-0.361549	-0.561707	1.860722
20	34	0	-1.195138	-1.372325	-0.456846
21	6	0	-2.495066	-0.035184	-0.031157
22	6	0	-2.752054	0.968516	-0.966820
23	6	0	-3.214082	-0.128978	1.161177
24	6	0	-3.742227	1.908856	-0.687292
25	1	0	-2.182746	1.018996	-1.897968
26	6	0	-4.199542	0.820429	1.426628
27	1	0	-3.004514	-0.928197	1.875973
28	6	0	-4.462133	1.835496	0.505801
29	1	0	-3.949418	2.703683	-1.407676
30	1	0	-4.765785	0.763280	2.359244
31	1	0	-5.236663	2.576085	0.719412

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0 imaginary frequencies
Sum of electronic and zero-point Energies= -2980.106315
Sum of electronic and thermal Energies= -2980.091967
Sum of electronic and thermal Enthalpies= -2980.091023
Sum of electronic and thermal Free Energies= -2980.150638

TS6 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.868559	0.328467	-1.870107
2	6	0	2.634293	-0.284195	-1.662626
3	6	0	2.409644	-1.070537	-0.525197
4	6	0	4.689827	-0.633766	0.184581
5	6	0	4.900226	0.157915	-0.944308
6	1	0	4.028301	0.941637	-2.760981
7	1	0	1.829701	-0.146029	-2.391000
8	1	0	5.493540	-0.776141	0.911813
9	1	0	5.868070	0.639620	-1.105777
10	6	0	3.451302	-1.241561	0.392051
11	1	0	3.285224	-1.851690	1.284349

12	6	0	1.054878	-1.681823	-0.275123
13	1	0	0.726198	-2.253617	-1.156455
14	1	0	1.110125	-2.381357	0.572972
15	6	0	0.003263	-0.625704	0.005156
16	1	0	-0.228173	0.019888	-0.850329
17	6	0	-0.022752	0.048262	1.292535
18	1	0	0.343974	-0.473451	2.179043
19	1	0	-0.680103	0.905934	1.439274
20	34	0	-1.708264	-1.453652	0.610327
21	6	0	-2.916880	-0.125400	-0.047841
22	6	0	-3.084344	0.042565	-1.425898
23	6	0	-3.665596	0.626842	0.861229
24	6	0	-3.997249	0.986479	-1.892505
25	1	0	-2.502992	-0.559321	-2.128782
26	6	0	-4.583185	1.562047	0.382849
27	1	0	-3.528452	0.485009	1.935831
28	6	0	-4.746656	1.743838	-0.990400
29	1	0	-4.128026	1.125775	-2.968485
30	1	0	-5.169688	2.153735	1.090039
31	1	0	-5.464206	2.479852	-1.361510
32	6	0	3.443212	3.063162	0.891479
33	1	0	3.209301	3.994678	1.427254
34	1	0	4.397547	2.657635	1.256852
35	1	0	3.522535	3.268376	-0.185940
36	6	0	2.395764	2.098691	1.117815
37	7	0	1.566038	1.317420	1.299794

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1 imaginary frequencies （442.04 icm^{-1}）

Sum of electronic and zero-point Energies= -3112.554223

Sum of electronic and thermal Energies= -3112.535148

Sum of electronic and thermal Enthalpies= -3112.534204

Sum of electronic and thermal Free Energies= -3112.605914

IM7 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.158321	2.592288	-1.119511
2	6	0	-0.833271	2.209742	-1.328365
3	6	0	-0.004262	1.879920	-0.250832
4	6	0	-1.859551	2.319653	1.256548
5	6	0	-2.677061	2.646428	0.174184
6	1	0	-2.790142	2.844908	-1.975107

7	1	0	-0.434201	2.159962	-2.345038
8	1	0	-2.255047	2.358556	2.274787
9	1	0	-3.717158	2.939285	0.338762
10	6	0	-0.533994	1.943660	1.044676
11	1	0	0.097147	1.701678	1.905160
12	6	0	1.442077	1.515521	-0.477064
13	1	0	1.672464	1.497209	-1.552370
14	1	0	2.070286	2.300065	-0.025967
15	6	0	1.853722	0.172864	0.150481
16	1	0	1.280320	0.004299	1.075668
17	6	0	1.756086	-1.064207	-0.746083
18	1	0	2.443528	-0.961277	-1.599701
19	1	0	2.047113	-1.959408	-0.179064
20	34	0	0.037326	-1.349396	-1.594258
21	6	0	-1.115150	-1.414940	-0.073312
22	6	0	-2.438979	-0.999008	-0.257752
23	6	0	-0.697524	-1.871274	1.181789
24	6	0	-3.334305	-1.032187	0.809736
25	1	0	-2.765681	-0.632149	-1.234271
26	6	0	-1.595544	-1.880480	2.249299
27	1	0	0.325233	-2.222847	1.336664
28	6	0	-2.914293	-1.462588	2.068915
29	1	0	-4.364744	-0.700715	0.657544
30	1	0	-1.258564	-2.226711	3.229934
31	1	0	-3.613837	-1.473234	2.908329
32	6	0	5.690600	0.367326	1.287458
33	1	0	6.064894	1.385521	1.100990
34	1	0	5.766575	0.128162	2.359131
35	1	0	6.267416	-0.360402	0.696490
36	6	0	4.317947	0.300535	0.892406
37	7	0	3.215181	0.251008	0.579626

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0 imaginary frequencies

Sum of electronic and zero-point Energies= -3112.590208

Sum of electronic and thermal Energies= -3112.571722

Sum of electronic and thermal Enthalpies= -3112.570778

Sum of electronic and thermal Free Energies= -3112.639514

TS7 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.569424	-2.131126	-0.153147

2	6	0	-2.912555	-1.118929	-0.853622
3	6	0	-2.472166	0.032067	-0.193461
4	6	0	-3.349366	-0.859632	1.885627
5	6	0	-3.786350	-2.005663	1.219050
6	1	0	-3.909779	-3.024598	-0.683070
7	1	0	-2.733417	-1.223769	-1.927303
8	1	0	-3.519671	-0.752007	2.960056
9	1	0	-4.297505	-2.799770	1.769349
10	6	0	-2.698760	0.153389	1.182953
11	1	0	-2.361069	1.051238	1.709296
12	6	0	-1.732999	1.110731	-0.943803
13	1	0	-1.794480	0.955094	-2.030162
14	1	0	-2.199921	2.087623	-0.742637
15	6	0	-0.292850	1.218281	-0.537128
16	1	0	-0.025151	0.869094	0.464469
17	6	0	0.791687	1.297398	-1.502467
18	1	0	0.526704	1.728852	-2.475216
19	1	0	1.757855	1.645211	-1.122659
20	34	0	0.804042	-0.666723	-1.698821
21	6	0	1.849696	-1.097167	-0.155593
22	6	0	1.271768	-1.875802	0.851507
23	6	0	3.181169	-0.681495	-0.061413
24	6	0	2.034428	-2.233716	1.963144
25	1	0	0.229605	-2.194084	0.770283
26	6	0	3.930196	-1.033915	1.059896
27	1	0	3.629816	-0.084281	-0.859145
28	6	0	3.359297	-1.810493	2.069816
29	1	0	1.585122	-2.840516	2.753191
30	1	0	4.969497	-0.705670	1.140102
31	1	0	3.951916	-2.087729	2.945220
32	6	0	0.447429	5.400778	1.297651
33	1	0	-0.459828	5.985758	1.507861
34	1	0	0.995462	5.224420	2.234764
35	1	0	1.088009	5.955669	0.596695
36	6	0	0.079756	4.135812	0.712508
37	7	0	-0.222335	3.124988	0.242815

---

1 imaginary frequencies （393.71 icm^{-1}）

Sum of electronic and zero-point Energies= -3112.552409

Sum of electronic and thermal Energies= -3112.533131

Sum of electronic and thermal Enthalpies= -3112.532187

Sum of electronic and thermal Free Energies= -3112.606714

IM8 (Charge = 1, Multiplicity = 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.083260	0.307788	1.587874
2	6	0	-2.863709	-0.356998	1.477918
3	6	0	-2.520499	-1.032039	0.298356
4	6	0	-4.655462	-0.372196	-0.655331
5	6	0	-4.982053	0.306024	0.518551
6	1	0	-4.335842	0.831007	2.513973
7	1	0	-2.161888	-0.349030	2.317191
8	1	0	-5.355618	-0.384201	-1.494822
9	1	0	-5.937562	0.829958	0.603521
10	6	0	-3.432819	-1.036657	-0.762627
11	1	0	-3.176968	-1.562596	-1.686981
12	6	0	-1.169355	-1.681726	0.158144
13	1	0	-0.960262	-2.308466	1.039336
14	1	0	-1.165652	-2.342306	-0.723461
15	6	0	-0.032689	-0.666958	0.030288
16	1	0	0.052898	-0.068036	0.949272
17	6	0	-0.145284	0.269111	-1.172520
18	1	0	-0.418503	-0.278759	-2.087441
19	1	0	0.801905	0.800097	-1.351946
20	34	0	1.649566	-1.675531	-0.136545
21	6	0	2.856133	-0.208780	0.112565
22	6	0	2.898839	0.475515	1.333090
23	6	0	3.715437	0.160543	-0.927379
24	6	0	3.786508	1.536746	1.501942
25	1	0	2.238171	0.176666	2.151118
26	6	0	4.614576	1.212480	-0.744587
27	1	0	3.676901	-0.371957	-1.880759
28	6	0	4.647473	1.904184	0.465808
29	1	0	3.812922	2.073269	2.453916
30	1	0	5.286237	1.496771	-1.558696
31	1	0	5.347574	2.731951	0.604282
32	6	0	-2.851514	3.149971	-0.567382
33	1	0	-2.416259	4.114037	-0.871758
34	1	0	-3.754185	2.936560	-1.159126
35	1	0	-3.101788	3.169731	0.504027
36	6	0	-1.890864	2.115465	-0.795107
37	7	0	-1.123724	1.282647	-0.976676

0 imaginary frequencies

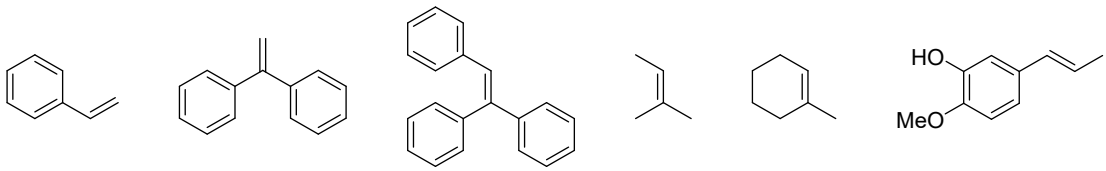
Sum of electronic and zero-point Energies= -3112.591435

Sum of electronic and thermal Energies= -3112.572683
Sum of electronic and thermal Enthalpies= -3112.571739
Sum of electronic and thermal Free Energies= -3112.642413

4.4 The cyclic voltammetry of olefins within the reaction system

4.4.1 The cyclic voltammetry of unreacted olefins within the reaction system

Unreacted olefins:



The cyclic voltammogram:

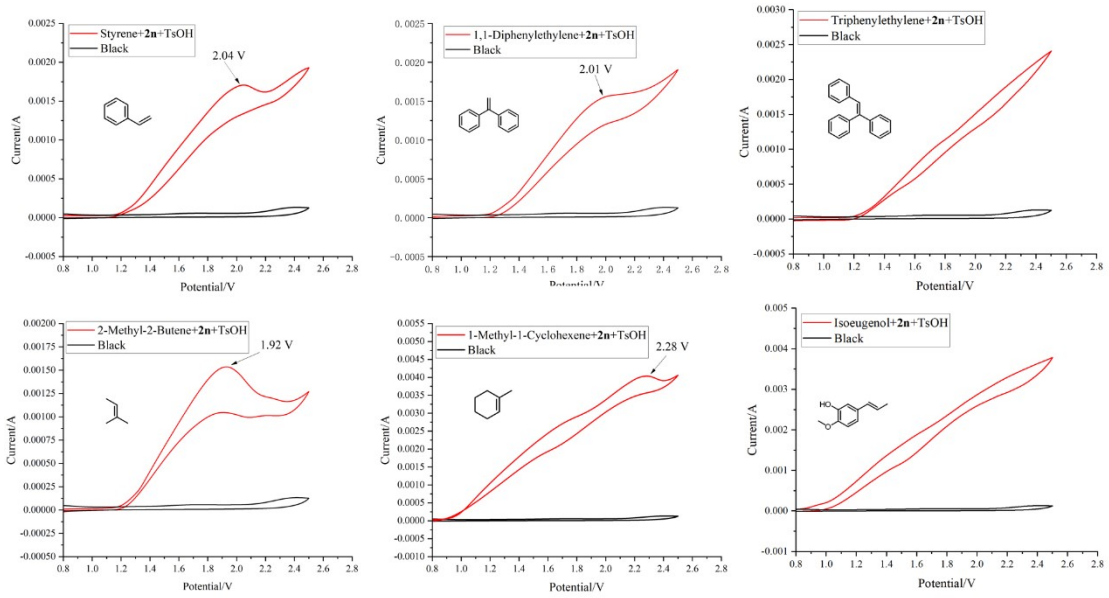
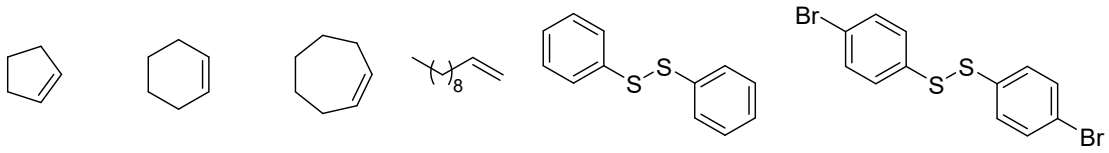


Fig. S10 CV experiments. Red Line: cyclic voltammetry of **1** (0.3 mmol), **2n** (0.2 mmol), $TBAPF_6$ (0.2 mmol) and TsOH (0.05 mmol) in MeCN (4.0 mL) under air. Black Line: cyclic voltammetry of $TBAPF_6$ (0.2 mmol) in MeCN (4.0 mL) under air. A glassy carbon disk (R = 5.5 mm, h = 10 mm) was used as the working electrode. A Pt disk (R = 5.5 mm, h = 10 mm) and Ag/AgCl (R = 5.0 mm, h = 10 mm) were used as the counter and reference electrodes, respectively. The scan rate was 150 mV/s.

4.4.2 The cyclic voltammograms of cyclopentene, cyclohexene, cycloheptene, 1-dodecene, phenyl disulfide and 1,2-bis(4-bromophenyl) disulfane within the reaction system



The cyclic voltammogram:

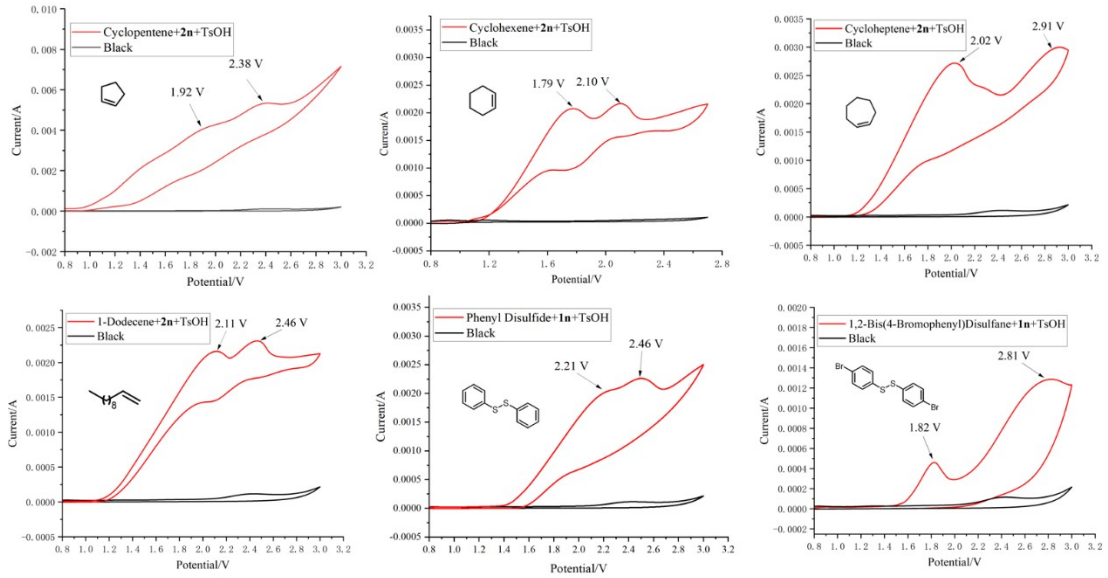


Fig. S11 CV experiments. Red Line: cyclic voltammetry of **1** (0.3 mmol), **2** (0.2 mmol), $TBAPF_6$ (0.2 mmol) and TsOH (0.05 mmol) in MeCN (4.0 mL) under air. Black Line: cyclic voltammetry of $TBAPF_6$ (0.2 mmol) in MeCN (4.0 mL) under air. A glassy carbon disk (R = 5.5 mm, h = 10 mm) was used as the working electrode. A Pt disk (R = 5.5 mm, h = 10 mm) and Ag/AgCl (R = 5.0 mm, h = 10 mm) were used as the counter and reference electrodes, respectively. The scan rate was 150 mV/s.

4.5 The atomic dipole corrected Hirshfeld (ADCH)[10]

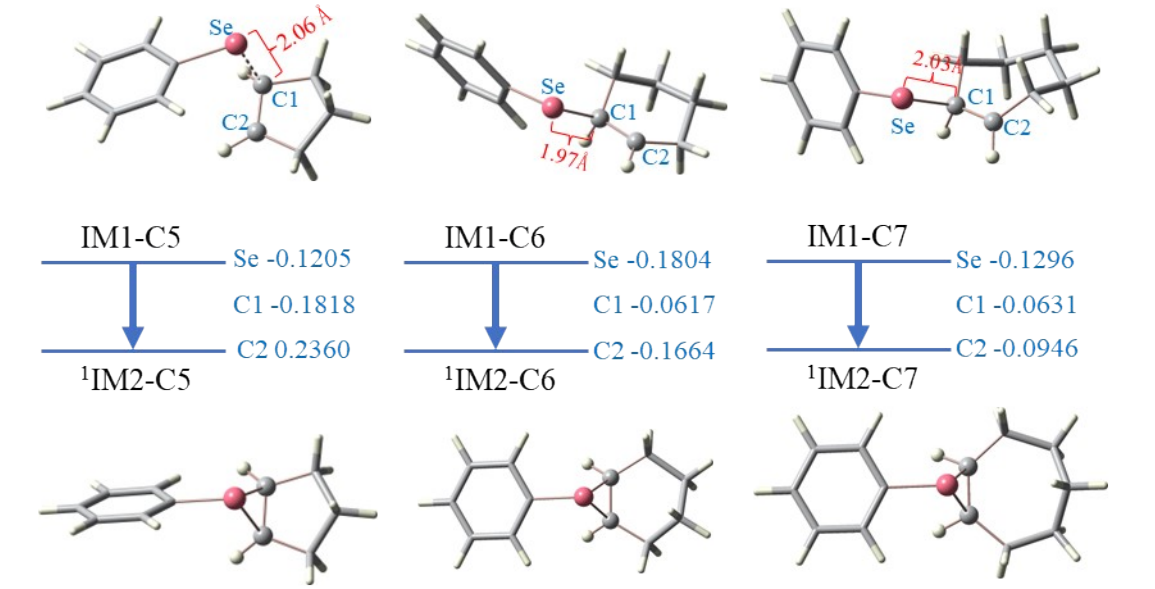


Fig. S12 ADCH atomic charge analysis of the **IM1→^{1}IM2** transformation process for cyclopentene, cyclohexene, and cycloheptene.

Computational analysis confirmed that the structural transition from **IM1** to **^{1}IM2** is the rate-determining step regulating product yield. The **IM1** structural variations of cyclopentene, cyclohexene and cycloheptene show Se-C1 bond lengths of 2.06 Å, 1.97 Å and 2.03 Å, respectively, indicating more stable Se-C1 bonding in cyclohexene.

ADCH atomic charge analysis (Multiwfn 3.8)[11] shows:

• Se charge: -0.1804 (cyclohexene) < -0.1296 (cycloheptene) <-0.1205 (cyclopentene)

• C1 charge: -0.0617 (cyclohexene) > -0.0631 (cycloheptene) < +0.01818 (cyclopentene)

• C2 charge: -0.1664 (cyclohexene) < -0.0946 (cycloheptene) < +0.236 (cyclopentene)

These charge distributions, shaped by structural differences, critically govern the **IM1→^{1}IM2** transition:

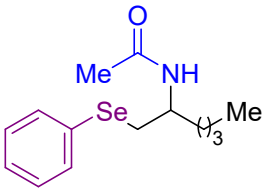
Cyclopentene: The positive C2 charge (+0.236) hinders electron loss needed for cationic-intermediate formation, blocking **IM1→^{1}IM2** conversion.

Cyclohexene: The negative C2 charge (-0.1664) promotes single-electron oxidation, enabling efficient **IM1→^{1}IM2** progression.

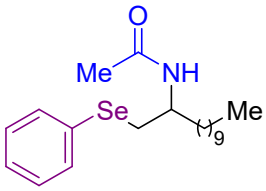
Cycloheptene: The near-neutral C2 charge (-0.0946) allows slight electron loss, permitting partial **IM1→^{1}IM2** progression.

This explains the significant yield differences: **3m** has nearly zero yield (unactivated), **3o** has a lower yield (limited electron transfer), and **3n** has a high yield (optimal radical stabilization and **IM1→^{1}IM2** conversion).

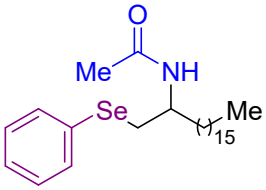
5. Analytical data



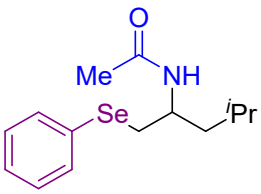
***N*-(1-(phenylselanyl)hexan-2-yl)acetamide (3a):** Known compound.[12] (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 85.2 mg, yield: 95%. white solid. m.p.: 64.3-65.1 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.53 (dt, *J* = 6.5, 1.7 Hz, 2H), 7.27-7.23 (m, 3H), 5.41 (d, *J* = 8.8 Hz, 1H), 4.20-4.14 (m, 1H), 3.17 (dd, *J* = 12.8, 5.0 Hz, 1H), 3.09 (dd, *J* = 12.8, 4.8 Hz, 1H), 1.81 (s, 3H), 1.60-1.54 (m, 1H), 1.52-1.45 (m, 1H), 1.28-1.24 (m, 4H), 0.86 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.7, 132.7, 130.4, 129.4, 127.2, 49.3, 34.1, 33.8, 28.3, 23.4, 22.6, 14.1.



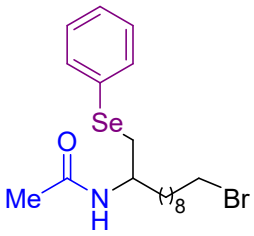
***N*-(1-(phenylselanyl)dodecan-2-yl)acetamide (3b):** Known compound.[12] (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 73.6 mg, yield: 64%. white solid. m.p.: 66.4-67.2 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.53 (dt, *J* = 6.5, 1.7 Hz, 2H), 7.27 (t, *J* = 1.9 Hz, 1H), 7.26-7.21 (m, 2H), 5.40 (d, *J* = 8.7 Hz, 1H), 4.20-4.14 (m, 1H), 3.17 (dd, *J* = 12.8, 5.0 Hz, 1H), 3.09 (dd, *J* = 12.8, 4.8 Hz, 1H), 1.81 (s, 3H), 1.60-1.57 (m, 1H), 1.49-1.44 (m, 1H), 1.26-1.22 (m, 16H), 0.88 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.5, 132.5, 130.2, 129.2, 126.9, 49.1, 34.2, 33.6, 31.8, 29.5, 29.5, 29.4, 29.3, 29.3, 25.9, 23.2, 22.6, 14.1.



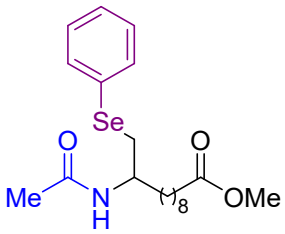
***N*-(1-(phenylselanyl)octadecan-2-yl)acetamide (3c):** Known compound.[12]. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 92.5 mg, yield: 66%, white solid. m.p.: 80.1-81.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.53 (dt, *J* = 6.5, 1.7 Hz, 2H), 7.27 (t, *J* = 2.1 Hz, 1H), 7.25-7.21 (m, 2H), 5.40 (d, *J* = 8.7 Hz, 1H), 4.20-4.14 (m, 1H), 3.17 (dd, *J* = 12.8, 5.0 Hz, 1H), 3.09 (dd, *J* = 12.8, 4.8 Hz, 1H), 1.80 (s, 3H), 1.57-1.54 (m, 1H), 1.50-1.45 (m, 1H), 1.29-1.23 (m, 28H), 0.88 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.5, 132.5, 130.2, 129.2, 127.0, 49.1, 34.2, 33.6, 31.9, 29.6, 29.6, 29.6, 29.6, 29.6, 29.5, 29.4, 29.3, 29.3, 25.9, 23.2, 22.6, 14.1.



***N*-(4-methyl-1-(phenylselanyl)pentan-2-yl)acetamide (3d):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 48.1 mg, yield: 54%, yellow oil. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.52 (dt, *J* = 6.6 Hz, *J* = 1.6 Hz, 2H), 7.28-7.26 (m, 1H), 7.26-7.21 (m, 2H), 5.38 (d, *J* = 8.8 Hz, 1H), 4.31-4.25 (m, 1H), 3.18 (dd, *J* = 12.8, 5.0 Hz, 1H), 3.07 (dd, *J* = 12.8, 4.5 Hz, 1H), 1.79 (s, 3H), 1.58-1.53 (m, 1H), 1.42-1.39 (m, 2H), 0.89 (d, *J* = 6.6 Hz, 3H), 0.86 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 132.7, 130.5, 129.4, 127.2, 47.3, 43.6, 34.4, 25.1, 23.4, 23.0, 22.4. **HRMS (ESI)** m/z Calcd for $C_{14}H_{21}NOSeNa$ $[M+Na]^+$: 322.0681; Found: 322.0673.

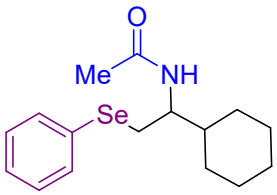


***N*-(11-bromo-1-(phenylselanyl)undecan-2-yl)acetamide (3e):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 99.5 mg, yield: 74%, brown solid. m.p.: 163.7-164.8 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.52 (dt, *J* = 6.6, 1.9 Hz, 2H), 7.28-7.26 (m, 1H), 7.25-7.21 (m, 2H), 5.43 (d, *J* = 8.7 Hz, 1H), 4.20-4.14 (m, 1H), 3.40 (t, *J* = 6.8 Hz, 2H), 3.16 (dd, *J* = 12.8, 5.0 Hz, 1H), 3.09 (dd, *J* = 12.8, 4.8 Hz, 1H), 1.86-1.82 (m, 2H), 1.80 (s, 3H), 1.59-1.54 (m, 1H), 1.41-1.39 (m, 1H), 1.30-1.22 (m, 12H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.7, 132.7, 130.4, 129.4, 127.2, 49.2, 34.4, 34.2, 33.8, 32.9, 29.4, 29.4, 28.8, 28.3, 26.1, 23.4. **HRMS (ESI)** m/z Calcd for $C_{19}H_{30}BrNOSeNa$ $[M+Na]^+$: 470.0568; Found: 470.0556.

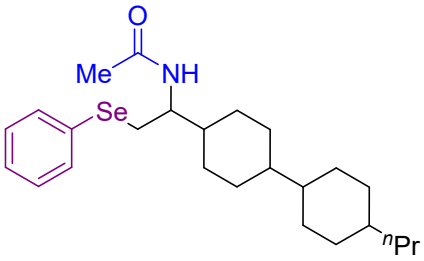


Methyl 10-acetamido-11-(phenylselanyl)undecanoate (3f): New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 93.8 mg, yield: 76%, white solid. m.p.: 70.8-71.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.53 (dt, *J* = 6.6, 1.6 Hz, 2H), 7.30-7.26 (m, 1H), 7.26-7.22 (m, 2H), 5.41 (d, *J* = 8.7 Hz, 1H), 4.19-4.13 (m, 1H), 3.66 (s, 3H), 3.16 (dd, *J* = 12.8, 5.0 Hz, 1H), 3.09 (dd, *J* = 12.8, 4.8 Hz, 1H), 2.29 (td, *J* = 7.6, 3.3 Hz, 2H), 1.81 (s, 3H), 1.62-1.58 (m, 3H), 1.49-1.43 (m, 1H), 1.31-1.26 (m, 5H), 1.24-1.22 (m, 5H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 174.3, 169.5, 134.9, 132.5, 130.2, 129.2, 127.0, 51.4, 49.0, 34.2, 34.0, 33.6, 29.2, 29.1, 29.0, 29.0,

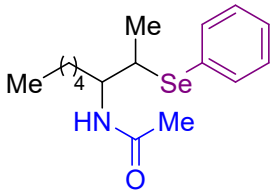
29.0, 25.9, 24.8, 23.2. **HRMS (ESI)** m/z Calcd for $C_{20}H_{31}NO_3SeNa$ $[M+Na]^+$: 436.1361; Found: 436.1357.



***N*-(1-cyclohexyl-3-(phenylselanyl)propyl)acetamide (3g):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 91.4 mg, yield: 90%, white solid. m.p.: 123.9-124.8 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ7.54-7.51 (m, 2H), 7.27-7.23 (m, 3H), 5.51 (d, *J* = 9.3 Hz, 1H), 4.05-4.00 (m, 1H), 3.14 (d, *J* = 5.2 Hz, 2H), 1.84 (s, 3H), 1.76-1.69 (m, 3H), 1.67-1.61 (m, 2H), 1.54-1.48 (m, 1H), 1.20-1.10 (m, 3H), 1.01-0.92 (m, 2H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 132.7, 130.2, 129.1, 127.0, 53.5, 40.8, 31.6, 29.6, 28.8, 26.1, 25.8, 25.8, 23.2. **HRMS (ESI)** m/z Calcd for $C_{17}H_{25}NOSeNa$ $[M+Na]^+$: 348.0837; Found: 348.0829.

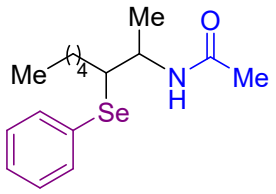


***N*-(2-(phenylselanyl)-1-(4'-propyl-[1,1'-bi(cyclohexan)]-4-yl)ethyl)acetamide (3h):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 63.6 mg, yield: 47%, white solid. m.p.: 172.8-173.5 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.53 (dt, *J* = 6.1, 2.1 Hz, 2H), 7.28-7.26 (m, 1H), 7.26-7.23 (m, 2H), 5.39 (d, *J* = 9.3 Hz, 1H), 4.02-3.98 (m, 1H), 3.14 (d, *J* = 5.1 Hz, 2H), 1.82 (s, 3H), 1.79-1.64 (m, 9H), 1.45-1.42 (m, 1H), 1.31-1.27 (m, 3H), 1.14-1.11 (m, 3H), 0.99-0.89 (m, 8H), 0.86 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 132.7, 130.2, 129.2, 127.1, 53.6, 43.2, 42.9, 41.0, 39.7, 37.5, 33.5, 31.8, 29.9, 29.9, 29.9, 29.4, 29.4, 29.1, 23.2, 19.9, 14.4. **HRMS (ESI)** m/z Calcd for $C_{25}H_{39}NOSeNa$ $[M+Na]^+$: 472.2089; Found: 472.2083.

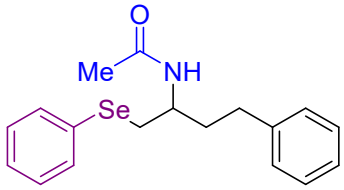


***N*-(2-(phenylselanyl)octan-3-yl)acetamide (3j):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 23.7 mg, yield: 24%, brown solid. m.p.: 68.7-69.1 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.60-7.58 (m, 2H), 7.28-7.26 (m, 3H), 5.57 (d, *J* = 9.0 Hz, 1H), 4.34-4.28 (m, 1H), 3.24-3.22 (m, 1H), 1.93 (s, 3H), 1.69-1.64 (m, 1H), 1.62-1.57 (m, 2H), 1.51-1.47 (m, 1H), 1.29-1.24 (m, 4H), 1.17 (d, *J* = 6.7 Hz, 3H), 0.87 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.5, 134.3, 131.7, 130.1, 129.3, 127.6, 53.9, 48.9, 33.3, 31.7, 27.9, 23.6, 22.7, 20.3, 14.2. **HRMS (ESI)** m/z

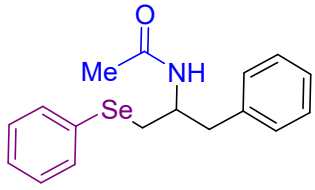
Calcd for $C_{16}H_{25}NOSeNa$ $[M+Na]^+$: 350.0994; Found: 350.0986.



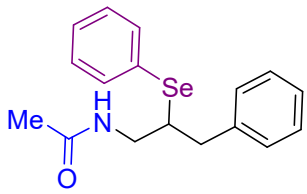
***N*-(3-(phenylselanyl)octan-2-yl)acetamide (3j`):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 21.6 mg, yield: 22%, yellow solid. m.p.: 74.3-75.6 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.61-7.58 (m, 2H), 7.29-7.26 (m, 3H), 5.47 (d, *J* = 9.4 Hz, 1H), 4.11-4.06 (m, 1H), 3.51 (qd, *J* = 7.1, 3.3 Hz, 1H), 1.96 (s, 3H), 1.58-1.52 (m, 1H), 1.47-1.42 (m, 1H), 1.41 (d, *J* = 7.1 Hz, 3H), 1.26-1.16 (m, 6H), 0.84 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.9, 135.0, 129.3, 129.1, 127.9, 54.3, 45.3, 34.1, 31.7, 26.0, 23.6, 22.6, 20.0, 14.1. **HRMS (ESI)** m/z Calcd for $C_{16}H_{25}NOSeNa$ $[M+Na]^+$: 350.0994; Found: 350.0989.



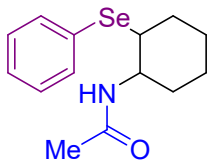
***N*-(4-phenyl-1-(phenylselanyl)butan-2-yl)acetamide (3k):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 51.8 mg, yield: 50%, white solid. m.p.: 103.2-104.5 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.53 (dt, *J* = 6.1, 1.9 Hz, 2H), 7.31-7.26 (m, 3H), 7.26-7.23 (m, 2H), 7.20-7.16 (m, 1H), 7.14-7.11 (m, 2H), 5.46 (d, *J* = 8.8 Hz, 1H), 4.28-4.22 (m, 1H), 3.18 (dd, *J* = 12.9, 5.1 Hz, 1H), 3.11 (dd, *J* = 12.9, 4.9 Hz, 1H), 2.63-2.60 (m, 2H), 1.96-1.91 (m, 1H), 1.88-1.81 (m, 1H), 1.78 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.7, 141.4, 132.8, 130.2, 129.4, 128.6, 128.6, 128.4, 127.3, 126.2, 49.2, 36.1, 33.8, 32.5, 23.4. **HRMS (ESI)** m/z Calcd for $C_{18}H_{21}NOSeNa$ $[M+Na]^+$: 370.0681; Found: 370.0673.



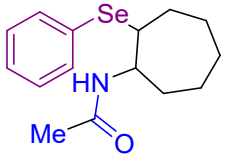
***N*-(1-phenyl-3-(phenylselanyl)propan-2-yl)acetamide (3l):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 31 mg, yield: 31%, white solid. m.p.: 107.6-108.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.52-7.49 (m, 2H), 7.29-7.26 (m, 2H), 7.26-7.20 (m, 4H), 7.15-7.12 (m, 2H), 5.50 (d, *J* = 8.3 Hz, 1H), 4.45-4.39 (m, 1H), 3.11 (dd, *J* = 12.9, 5.2 Hz, 1H), 2.99 (dd, *J* = 12.9, 5.2 Hz, 1H), 2.94-2.86 (m, 2H), 1.76 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.7, 137.4, 132.8, 130.1, 129.4, 128.7, 127.3, 126.8, 50.4, 39.9, 32.2, 23.3. **HRMS (ESI)** m/z Calcd for $C_{17}H_{19}NOSeNa$ $[M+Na]^+$: 356.0524; Found: 356.0516.



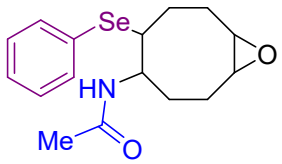
***N*-(3-phenyl-2-(phenylselanyl)propyl)acetamide (3l`):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 20.8 mg, yield: 21%, yellow oil. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.52-7.49 (m, 2H), 7.32-7.28 (m, 4H), 7.28-7.27 (m, 1H), 7.25-7.21 (m, 1H), 7.20-7.18 (m, 2H), 5.77 (s, 1H), 3.58-3.51 (m, 2H), 3.38-3.32 (m, 1H), 2.99 (dd, *J* = 14.3, 6.8 Hz, 1H), 2.93 (dd, *J* = 14.3, 7.4 Hz, 1H), 1.87 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 170.1, 138.9, 135.1, 129.4, 129.2, 128.7, 128.2, 128.1, 126.9, 46.7, 43.4, 40.0, 23.3. **HRMS (ESI)** m/z Calcd for $C_{17}H_{19}NOSeNa$ $[M+Na]^+$: 356.0524; Found: 356.0517.



***N*-(2-(phenylselanyl)cyclohexyl)acetamide (3n):** Known compound.[13] (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 81.9 mg, yield: 92%. white solid. m.p.: 118.2-119.5 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.57 (d, *J* = 5.3 Hz, 2H), 7.29-7.26 (m, 3H), 5.50 (d, *J* = 3.4 Hz 1H), 3.83-3.79 (m, 1H), 3.02 (t, *J* = 11.0 Hz, 1H), 2.16 (t, *J* = 16.0 Hz, 2H), 1.90 (s, 3H), 1.68 (s, 2H), 1.53 (q, *J* = 12.5 Hz, 1H), 1.39-1.31 (m, 1H), 1.26-1.15 (m, 2H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.4, 135.5, 129.2, 128.4, 127.9, 53.4, 48.1, 34.2, 33.9, 26.8, 24.7, 23.6.

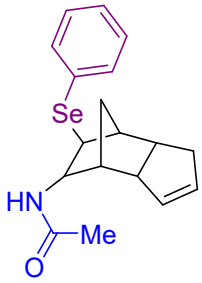


***N*-(2-(phenylselanyl)cycloheptyl)acetamide (3o):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 11.3 mg, yield: 12%, white solid. m.p.: 103.4-103.8 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.57-7.54 (m, 2H), 7.28 (t, *J* = 3.2 Hz, 3H), 5.52 (d, *J* = 8.0 Hz, 1H), 4.07-4.03 (m, 1H), 3.23 (td, *J* = 9.0, 3.3 Hz, 1H), 2.11-2.06 (m, 1H), 1.97-1.92 (m, 1H), 1.89 (s, 3H), 1.84-1.77 (m, 2H), 1.77-1.70 (m, 2H), 1.68-1.63 (m, 1H), 1.60-1.57 (m, 2H), 1.48-1.42 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.2, 134.8, 129.7, 129.3, 127.7, 55.8, 50.6, 33.8, 32.8, 28.1, 26.6, 23.7, 23.6. **HRMS (ESI)** m/z Calcd for $C_{15}H_{21}NOSeNa$ $[M+Na]^+$: 334.0671; Found: 334.0681.

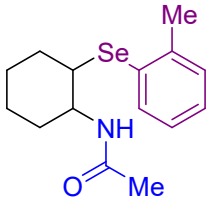


***N*-(5-(phenylselanyl)-9-oxabicyclo[6.1.0]nonan-4-yl)acetamide (3p):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 66.2 mg, yield:

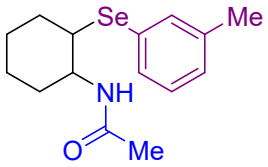
65%, yellow solid. m.p.: 118.7-119.1 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.52 (dt, *J* = 7.5, 1.7 Hz, 2H), 7.28-7.23 (m, 3H), 5.81 (d, *J* = 8.1 Hz, 1H), 4.32-4.25 (m, 1H), 4.02 (t, *J* = 5.6 Hz, 1H), 3.88 (t, *J* = 5.6 Hz, 1H), 3.76-3.71 (m, 1H), 3.16-3.12 (m, 1H), 2.33 (dd, *J* = 14.5, 5.7 Hz, 1H), 2.06-2.03 (m, 2H), 1.97 (s, 3H), 1.85-1.83 (m, 1H), 1.78-1.70 (m, 1H), 1.64-1.57 (m, 1H), 1.45-1.38 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.7, 134.1, 129.1, 128.3, 127.5, 68.8, 67.2, 48.4, 44.4, 27.7, 26.1, 24.9, 24.8, 23.2. **HRMS (ESI)** m/z Calcd for $C_{16}H_{21}NO_2SeNa$ $[M+Na]^+$: 362.0630; Found: 362.0617.



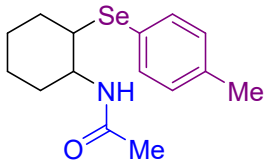
***N*-((3*aS*,4*R*,6*S*,7*S*,7*aR*)-6-(phenylselanyl)-3a,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoinden-5-yl)acetamide (3q):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 76.5 mg, yield: 74%, yellow solid. m.p.: 148.8-149.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.48-7.41 (m, 2H), 7.29-7.23 (m, 3H), 6.35 (d, *J* = 8.8 Hz, 1H), 5.74 (dd, *J* = 5.6, 2.3 Hz, 1H), 5.48 (dd, *J* = 5.6, 2.6 Hz, 1H), 4.05-4.00 (m, 1H), 3.52 (s, 1H), 2.83 (dd, *J* = 8.5, 2.5 Hz, 1H), 2.64-2.59 (m, 1H), 2.28-2.23 (m, 2H), 2.13 (d, *J* = 4.1 Hz, 1H), 2.00-1.96 (m, 1H), 1.95 (s, 3H), 1.93-1.91 (m, 1H), 1.73-1.68 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.2, 133.5, 132.3, 131.2, 130.4, 129.4, 127.2, 54.3, 52.9, 50.5, 48.1, 46.2, 42.4, 39.5, 38.2, 23.8. **HRMS (ESI)** m/z Calcd for $C_{18}H_{21}NOSe$ $[M+H]^+$: 348.0861; Found: 348.0854.



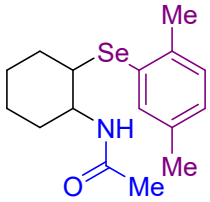
***N*-(2-(*o*-tolylselanyl)cyclohexyl)acetamide (3r):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 61.8 mg, yield: 66%, white solid. m.p.: 123.2-124.9 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.55 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.22-7.15 (m, 2H), 7.10 (td, *J* = 7.5, 1.7 Hz, 1H), 5.48 (d, *J* = 8.3 Hz, 1H), 3.92-3.87 (m, 1H), 3.08 (td, *J* = 11.1, 3.9 Hz, 1H), 2.43 (s, 3H), 2.18-2.14 (m, 1H), 2.14-2.09 (m, 1H), 1.85 (s, 3H), 1.71-1.66 (m, 2H), 1.60-1.53 (m, 1H), 1.42-1.34 (m, 1H), 1.25-1.23 (m, 1H), 1.20-1.16 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.4, 141.3, 134.9, 130.4, 130.2, 127.8, 126.6, 53.9, 47.7, 34.1, 33.6, 26.7, 24.7, 23.5, 23.2. **HRMS (ESI)** m/z Calcd for $C_{15}H_{21}NOSeNa$ $[M+Na]^+$: 334.0681; Found: 334.0672.



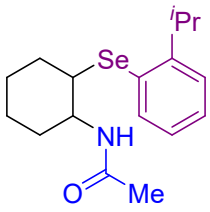
***N*-(2-(*m*-tolylselanyl)cyclohexyl)acetamide (3s):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 64.8 mg, yield: 70%, white solid. m.p.: 110.8-111.5 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.40 (t, *J* = 1.7 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.12-7.08 (m, 1H), 5.42 (d, *J* = 8.1 Hz, 1H), 3.82-3.76 (m, 1H), 3.00 (td, *J* = 11.2, 4.0 Hz, 1H), 2.33 (s, 3H), 2.21-2.13 (m, 2H), 1.89 (s, 3H), 1.71-1.66 (m, 2H), 1.58-1.50 (m, 1H), 1.38-1.34 (m, 1H), 1.26-1.22 (m, 1H), 1.18-1.15 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.4, 139.0, 136.1, 132.4, 129.0, 128.8, 128.3, 53.6, 48.1, 34.3, 34.0, 26.8, 24.7, 23.6, 21.4. **HRMS (ESI)** m/z Calcd for $C_{15}H_{21}NOSeNa$ $[M+Na]^+$: 334.0681; Found: 334.0674.



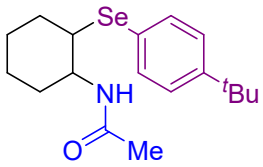
***N*-(2-(*p*-tolylselanyl)cyclohexyl)acetamide (3t):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 59.8 mg, yield: 64%, yellow solid. m.p.: 116.6-117.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.45 (dt, *J* = 8.4, 2.2 Hz, 2H), 7.09 (d, *J* = 7.7 2H), 5.44 (d, *J* = 8.0 Hz, 1H), 3.78-3.71 (m, 1H), 2.92 (td, *J* = 11.3, 3.9 Hz, 1H), 2.33 (s, 3H), 2.20-2.16 (m, 1H), 2.14-2.09 (m, 1H), 1.92 (s, 3H), 1.69-1.65 (m, 2H), 1.54-1.46 (m, 1H), 1.35-1.31 (m, 1H), 1.24-1.20 (m, 1H), 1.18-1.11 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 138.4, 136.2, 130.2, 124.5, 53.6, 48.3, 34.5, 34.2, 27.1, 25.0, 23.8, 21.5. **HRMS (ESI)** m/z Calcd for $C_{15}H_{21}NOSeNa$ $[M+Na]^+$: 334.0681; Found: 334.0675.



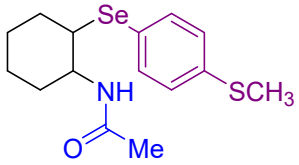
***N*-(2-((2,5-dimethylphenyl)selanyl)cyclohexyl)acetamide (3u):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 62.5 mg, yield: 64%, white solid. m.p.: 126.3-127.4 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.39 (s, 1H), 7.10 (d, *J* = 7.7 Hz, 1H), 7.01-6.98 (m, 1H), 5.39 (d, *J* = 8.0 Hz, 1H), 3.91-3.85 (m, 1H), 3.04 (td, *J* = 11.1, 3.9 Hz, 1H), 2.40 (s, 3H), 2.30 (s, 3H), 2.21-2.16 (m, 1H), 2.14-2.10 (m, 1H), 1.85 (s, 3H), 1.75-1.66 (m, 3H), 1.60-1.53 (m, 1H), 1.43-1.36 (m, 1H), 1.25-1.24 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.2, 138.1, 135.9, 135.7, 129.8, 129.8, 128.6, 53.9, 47.5, 34.0, 33.5, 26.7, 24.5, 23.3, 22.5, 20.7. **HRMS (ESI)** m/z Calcd for $C_{16}H_{23}NOSeNa$ $[M+Na]^+$: 348.0837; Found: 348.0828.



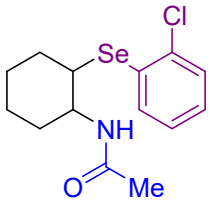
***N*-(2-((2-isopropylphenyl)selanyl)cyclohexyl)acetamide (3v):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 60 mg, yield: 59%, yellow solid. m.p.: 99.3-100.7 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.57 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.30-7.27 (m, 2H), 7.10 (td, *J* = 7.2, 1.8 Hz, 1H), 5.41 (d, *J* = 8.2 Hz, 1H), 3.92-3.87 (m, 1H), 3.55-3.50 (m, 1H), 3.07 (td, *J* = 11.1, 3.9 Hz, 1H), 2.21-2.16 (m, 1H), 2.09-2.06 (m, 1H), 1.86 (s, 3H), 1.72-1.65 (m, 2H), 1.60-1.53 (m, 1H), 1.43-1.35 (m, 1H), 1.26-1.23 (m, 1H), 1.21 (dd, *J* = 6.9, 2.8 Hz, 6H). 1.19-1.15 (m, 1H), **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.3, 151.4, 135.1, 129.6, 128.1, 126.4, 125.8, 53.8, 48.1, 34.2, 33.6, 32.9, 26.7, 24.6, 23.9, 23.8, 23.4. **HRMS (ESI)** m/z Calcd for $C_{17}H_{25}NOSeNa$ $[M+Na]^+$: 362.0994; Found: 362.0984.



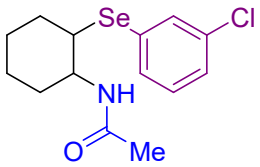
***N*-(2-((4-(*tert*-butyl)phenyl)selanyl)cyclohexyl)acetamide (3w):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 50.9 mg, yield: 48%, yellow solid. m.p.: 120.3-121.4 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.48 (dt, *J* = 8.3, 2.4 Hz, 2H), 7.29 (dt, *J* = 8.9, 2.5 Hz, 2H), 5.51 (d, *J* = 8.1 Hz, 1H), 3.81-3.75 (m, 1H), 2.97 (td, *J* = 11.2, 3.9 Hz, 1H), 2.20-2.12 (m, 2H), 1.88 (s, 3H), 1.69-1.65 (m, 2H), 1.56-1.49 (m, 1H), 1.36-1.32 (m, 1H), 1.30 (s, 9H), 1.26-1.21 (m, 1H), 1.19-1.14 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.4, 151.2, 135.4, 126.3, 124.7, 53.6, 47.9, 34.7, 34.2, 33.9, 31.4, 26.8, 24.7, 23.6. **HRMS (ESI)** m/z Calcd for $C_{18}H_{27}NOSeNa$ $[M+Na]^+$: 376.1150; Found: 376.1144.



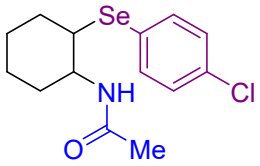
***N*-(2-((4-(methylthio)phenyl)selanyl)cyclohexyl)acetamide (3x):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 53.4 mg, yield: 52%, white solid. m.p.: 149.3-150.1 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.48 (d, *J* = 8.3 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 5.43 (d, *J* = 8.2 Hz, 1H), 3.79-3.73 (m, 1H), 2.92 (td, *J* = 11.2, 3.9 Hz, 1H), 2.47 (s, 3H), 2.20-2.15 (m, 1H), 2.14-2.08 (m, 1H), 1.94 (s, 3H), 1.70-1.65 (m, 2H), 1.52-1.45 (m, 1H), 1.36-1.31 (m, 1H), 1.24-1.19 (m, 1H), 1.18-1.13 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.3, 139.0, 136.3, 126.7, 123.6, 53.0, 48.1, 34.1, 33.8, 26.7, 24.6, 23.5, 15.5. **HRMS (ESI)** m/z Calcd for $C_{14}H_{18}NOSSe$ $[M+Na]^+$: 366.0401; Found: 366.0393.



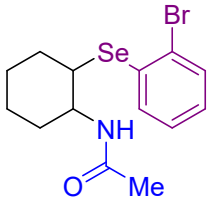
***N*-(2-((2-chlorophenyl)selanyl)cyclohexyl)acetamide (3y):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 70.6 mg, yield: 71%, yellow solid. m.p.: 102.4-103.2 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.64 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.41 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.23-7.17 (m, 2H), 5.50 (d, *J* = 8.0 Hz, 1H), 3.95-3.90 (m, 1H), 3.29 (td, *J* = 10.7, 4.0 Hz, 1H), 2.22-2.17 (m, 1H), 2.13-2.10 (m, 1H), 1.90 (s, 3H), 1.72-1.61 (m, 4H), 1.47-1.38 (m, 1H), 1.30-1.25 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.4, 137.7, 135.5, 129.7, 129.6, 128.7, 127.1, 52.9, 47.2, 33.7, 33.3, 26.3, 24.4, 23.4. **HRMS (ESI)** m/z Calcd for $C_{14}H_{18}ClNOSeNa$ $[M+Na]^+$: 354.0134; Found: 354.0124.



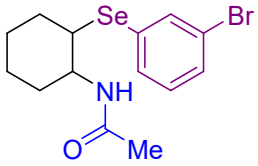
***N*-(2-((3-chlorophenyl)selanyl)cyclohexyl)acetamide (3z):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 65.7 mg, yield: 66%, white solid. m.p.: 124.7-125.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.56 (t, *J* = 1.8 Hz, 1H), 7.44 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.25-7.24 (m, 1H), 7.20 (t, *J* = 7.8 Hz, 1H), 5.41 (d, *J* = 8.4 Hz, 1H), 3.86-3.80 (m, 1H), 3.04 (td, *J* = 11.1, 4.0 Hz, 1H), 2.16-2.09 (m, 2H), 1.91 (s, 3H), 1.71-1.66 (m, 2H), 1.57-1.50 (m, 1H), 1.37-1.34 (m, 1H), 1.26-1.22 (m, 2H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.2, 134.6, 134.4, 133.1, 130.0, 129.9, 127.8, 52.9, 48.5, 34.0, 33.7, 26.5, 24.5, 23.4. **HRMS (ESI)** m/z Calcd for $C_{14}H_{18}ClNOSeNa$ $[M+Na]^+$: 354.0134; Found: 354.0126.



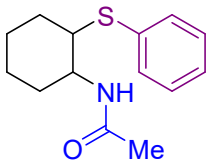
***N*-(2-((4-chlorophenyl)selanyl)cyclohexyl)acetamide (3aa):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 85.5 mg, yield: 86%, white solid. m.p.: 133.5-134.2 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.3 Hz, 2H), 5.45 (d, *J* = 8.4 Hz, 1H), 3.83-3.77 (m, 1H), 2.97 (td, *J* = 11.1, 3.9 Hz, 1H), 2.18-2.06 (m, 2H), 1.94 (s, 3H), 1.70-1.64 (m, 2H), 1.52-1.45 (m, 1H), 1.38-1.30 (m, 1H), 1.27-1.23 (m, 1H), 1.21-1.18 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.3, 137.0, 134.3, 129.2, 126.0, 52.8, 48.3, 34.0, 33.7, 26.6, 24.6, 23.5. **HRMS (ESI)** m/z Calcd for $C_{14}H_{18}ClNOSe$ $[M+Na]^+$: 354.0134; Found: 354.0122.



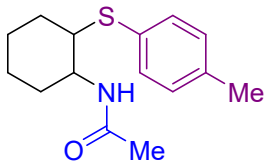
***N*-(2-((2-bromophenyl)selanyl)cyclohexyl)acetamide (3ab):** New compound.(Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 76.5 mg, yield: 68%, yellow solid. m.p.: 99.1-101.2 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.64 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.59 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.23 (td, *J* = 7.6, 1.4 Hz, 1H), 7.12 (td, *J* = 7.6, 1.6 Hz, 1H), 5.47 (d, *J* = 8.1 Hz, 1H), 3.97-3.91 (m, 1H), 3.30 (td, *J* = 10.5, 3.8 Hz, 1H), 2.24-2.19 (m, 1H), 2.15-2.11 (m, 1H), 1.91 (s, 3H), 1.71-1.63 (m, 4H), 1.46-1.42 (m, 1H), 1.29-1.27 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 135.2, 133.2, 132.4, 128.8, 127.9, 52.9, 47.8, 33.7, 33.3, 26.5, 24.5, 23.6. **HRMS (ESI)** m/z Calcd for $C_{14}H_{18}BrNOSe$ $[M+Na]^+$: 397.9629; Found: 397.9624.



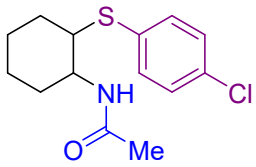
***N*-(2-((3-bromophenyl)selanyl)cyclohexyl)acetamide (3ac):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 94.6 mg, yield: 84%, yellow solid. m.p.: 124.7-125.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.73 (t, *J* = 1.8 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.41 (dt, *J* = 6.8, 1.0 Hz, 1H), 7.15 (t, *J* = 7.8 Hz, 1H), 5.45 (d, *J* = 8.5 Hz, 1H), 3.89-3.81 (m, 1H), 3.05 (td, *J* = 11.1, 4.0 Hz, 1H), 2.17-2.10 (m, 2H), 1.92 (s, 3H), 1.73-1.65 (m, 3H), 1.58-1.50 (m, 1H), 1.38-1.35 (m, 1H), 1.25-1.24 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.3, 137.5, 133.7, 130.8, 130.5, 130.4, 122.7, 53.0, 48.6, 34.0, 33.8, 26.6, 24.6, 23.5. **HRMS (ESI)** m/z Calcd for $C_{14}H_{18}BrNOSeNa$ $[M+Na]^+$: 397.9629; Found: 397.9617.



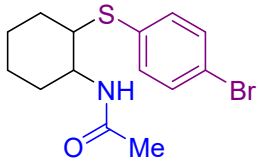
***N*-(2-(phenylthio)cyclohexyl)acetamide (3ad):** Known compound.[14] (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 45.1 mg, yield: 60%. white solid. m.p.: 96.2-97.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.45-7.42 (m, 2H), 7.31-7.28 (m, 2H), 7.26-7.23 (m, 1H), 5.47 (d, *J* = 7.9 Hz, 1H), 3.78-3.72 (m, 1H), 2.91 (td, *J* = 10.8, 3.8 Hz, 1H), 2.20-2.16 (m, 1H), 2.10-2.06 (m, 1H), 1.90 (s, 3H), 1.74-1.64 (m, 3H), 1.44-1.40 (m, 1H), 1.37-1.33 (m, 1H), 1.21-1.17 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 134.0, 133.1, 129.1, 127.5, 53.0, 51.8, 33.7, 33.1, 25.9, 24.7, 23.6.



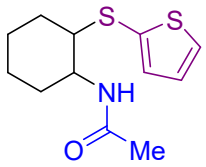
***N*-(2-(*p*-tolylthio)cyclohexyl)acetamide (3ae):** Known compound.[15] (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 32.9 mg, yield: 42%. white solid. m.p.: 103.2-101.4 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.33 (dt, *J* = 8.6, 2.3 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 5.55 (d, *J* = 7.0 Hz, 1H), 3.71-3.65 (m, 1H), 2.80 (td, *J* = 10.9, 3.8 Hz, 1H), 2.32 (s, 3H), 2.20-2.16 (m, 1H), 2.07-2.03 (m, 1H), 1.93 (s, 3H), 1.72-1.70 (m, 1H), 1.66-1.63 (m, 1H), 1.41-1.35 (m, 1H), 1.33-1.28 (m, 1H), 1.26-1.21 (m, 1H), 1.19-1.13 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 137.8, 134.0, 129.8, 129.7, 52.9, 52.0, 33.7, 33.1, 26.0, 24.6, 23.6, 21.2.



***N*-(2-((4-chlorophenyl)thio)cyclohexyl)acetamide (3af):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 55.2 mg, yield: 65%, white solid. m.p.: 106.2-107.3 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.38 (dt, *J* = 9.2, 2.7 Hz, 2H), 7.26 (dt, *J* = 9.2, 2.7 Hz, 2H), 5.45 (d, *J* = 8.3 Hz, 1H), 3.77-3.72 (m, 1H), 2.87 (td, *J* = 10.6, 3.8 Hz, 1H), 2.18-2.14 (m, 1H), 2.06-2.02 (m, 1H), 1.95 (s, 3H), 1.73-1.65 (m, 2H), 1.40-1.32 (m, 2H),1.29-1.23 (m, 2H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 134.7, 133.8, 132.2, 129.8, 129.2, 127.0, 52.5, 51.9, 33.5, 32.9, 25.8, 24.5, 23.7. **HRMS (ESI)** m/z Calcd for $C_{14}H_{18}ClNOSNa$ $[M+Na]^+$: 306.0690; Found: 306.0688.



***N*-(2-((4-bromophenyl)thio)cyclohexyl)acetamide (3ag):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 55.2 mg, yield: 65%, white solid. m.p.: 113.1-114.7 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.42 (dt, *J* = 9.2, 2.7 Hz, 2H), 7.31 (dt, *J* = 9.2, 2.7 Hz, 2H), 5.44 (d, *J* = 8.2 Hz, 1H), 3.78-3.72 (m, 1H), 2.89 (td, *J* = 10.6, 3.8 Hz, 1H), 2.18-2.14 (m, 1H), 2.06-2.02 (m, 1H), 1.94 (s, 3H), 1.73-1.69 (m, 1H), 1.68-1.65 (m, 1H), 1.41-1.33 (m, 2H), 1.29-1.24 (m, 2H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 134.8, 132.9, 132.2, 121.8, 52.5, 51.8, 33.5, 32.8, 25.8, 24.5, 23.7. **HRMS (ESI)** m/z Calcd for $C_{14}H_{19}BrNOS$ $[M+H]^+$: 328.0365; Found: 328.0361.



***N*-(2-(thiophen-2-ylthio)cyclohexyl)acetamide (3ah):** New compound. (Eluent: petroleum ether (60-90 °C)/EtOAc = 1:1, v:v). 55.2 mg, yield: 65%, white solid. m.p.: 125.9-126.4 °C. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.38 (dd, *J* = 5.3, 1.3 Hz, 1H), 7.15 (dd, *J* = 3.5, 1.3 Hz, 1H), 6.99 (dd, *J* = 5.4, 3.5 Hz, 1H), 5.57 (d, *J* = 6.9 Hz, 1H), 3.68-3.62 (m, 1H), 2.60 (td, *J* = 11.2, 3.8 Hz, 1H), 2.22-2.18 (m, 1H), 2.11-2.07 (m, 1H), 2.01 (s, 3H), 1.74-1.71 (m, 1H), 1.67-1.64 (m, 1H), 1.44-1.41 (m, 1H), 1.31-1.28 (m, 1H), 1.24-1.21 (m, 1H), 1.18-1.11 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 169.6, 136.3, 130.6, 127.9, 54.0, 52.3, 34.0, 33.2, 26.2, 24.6, 23.7. **HRMS (ESI)** m/z Calcd for $C_{12}H_{17}NOS_2Na$ $[M+Na]^+$: 278.0644; Found: 278.0634.

6. References

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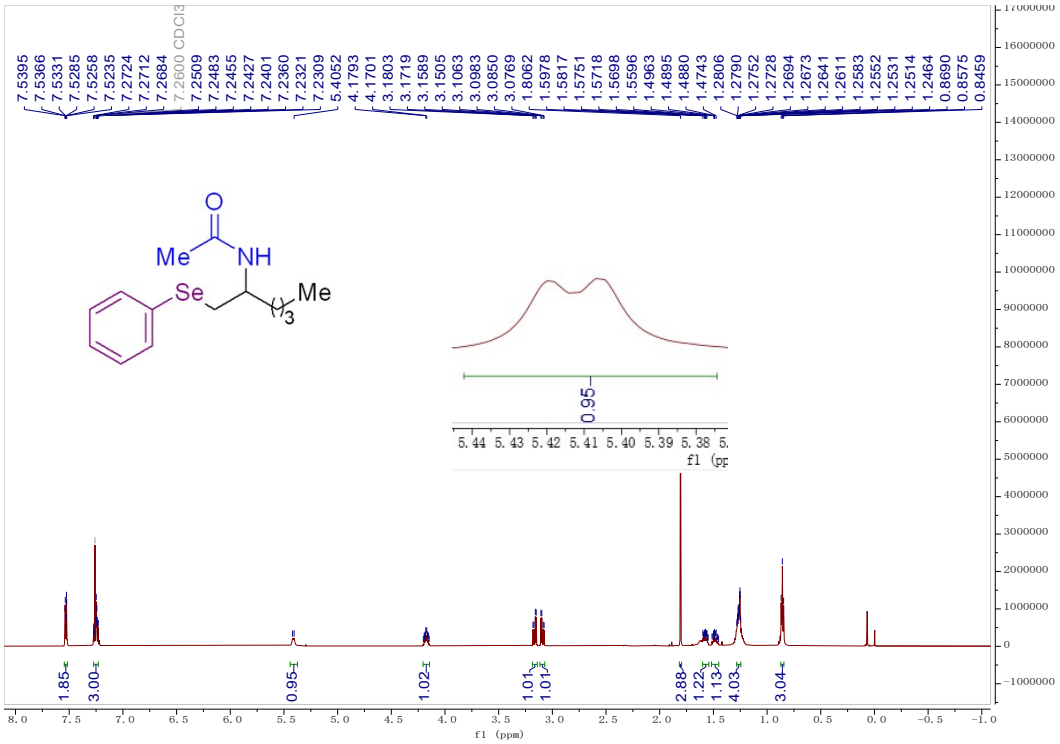
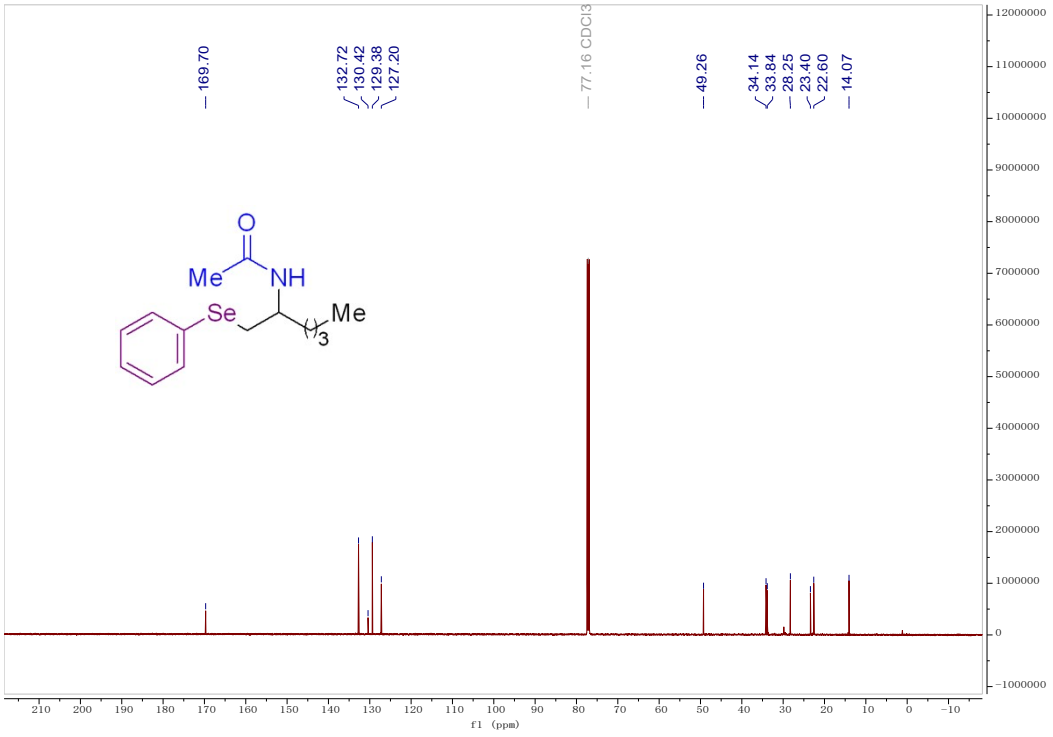
7. NMR spectra of the products

^{1}H NMR of product 3a in $CDCl_3$ (600 MHz)

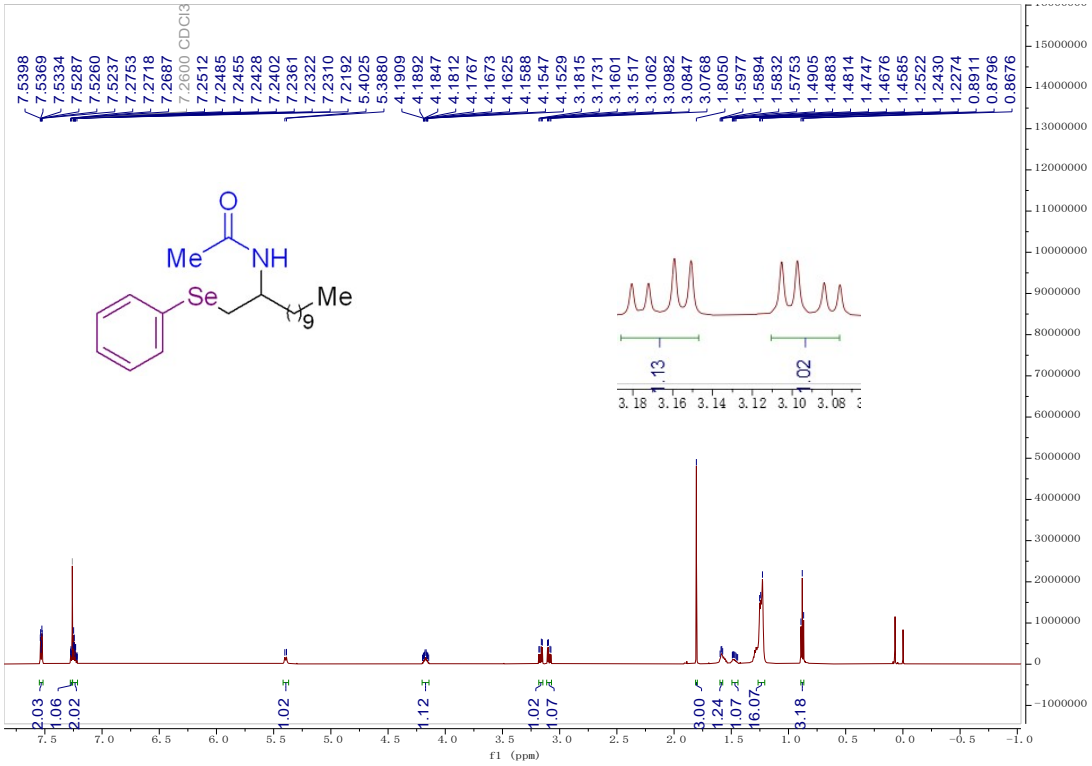


13

C NMR of product 3a in $CDCl_3$ (151 MHz)

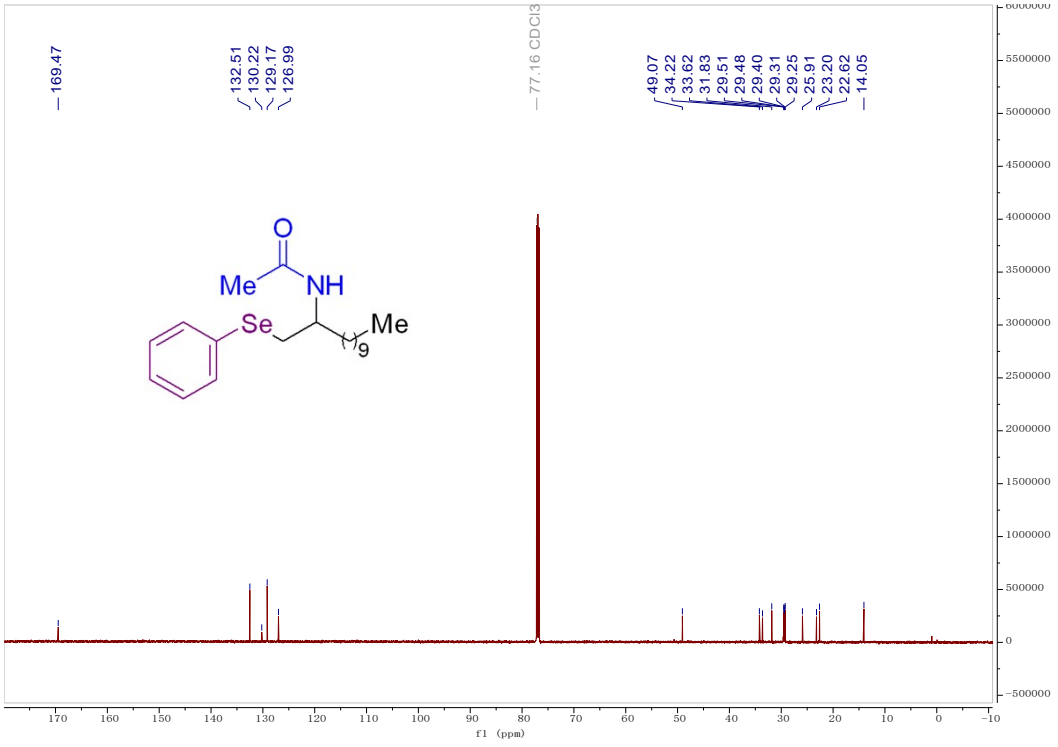


^{1}H NMR of product 3b in $CDCl_3$ (600 MHz)

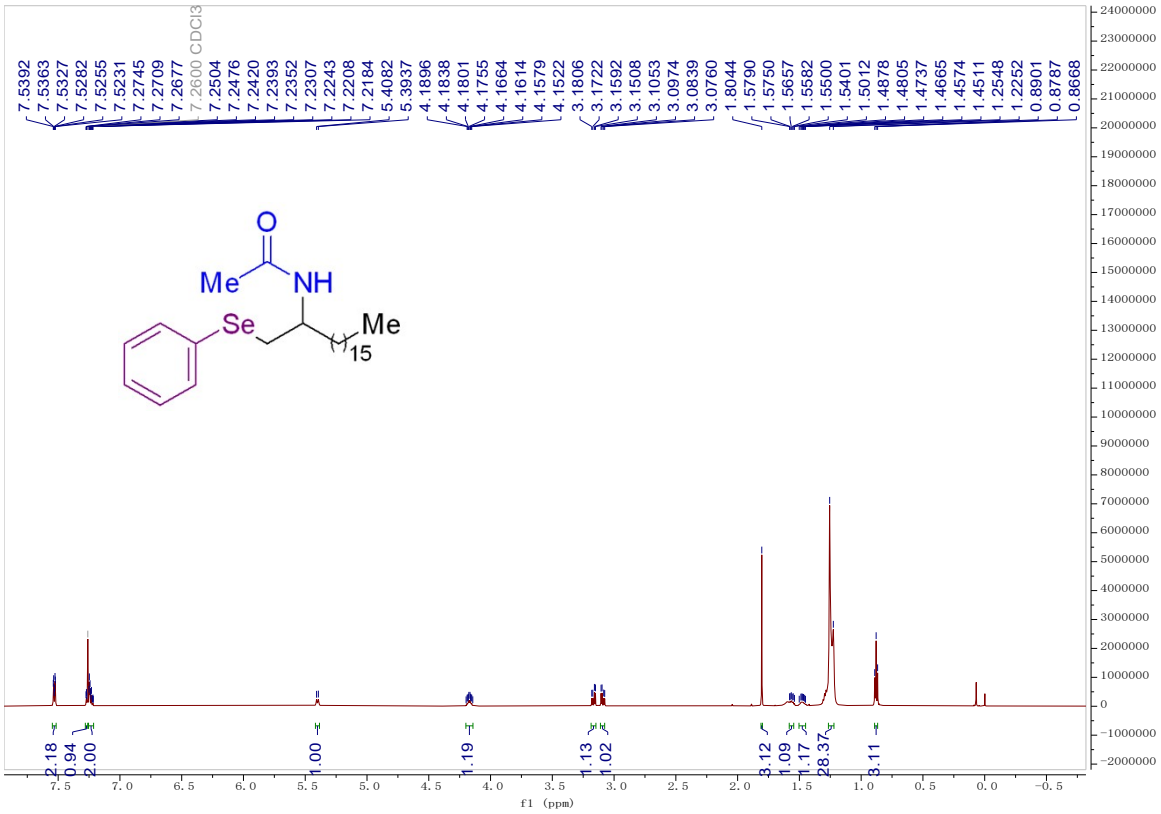


1

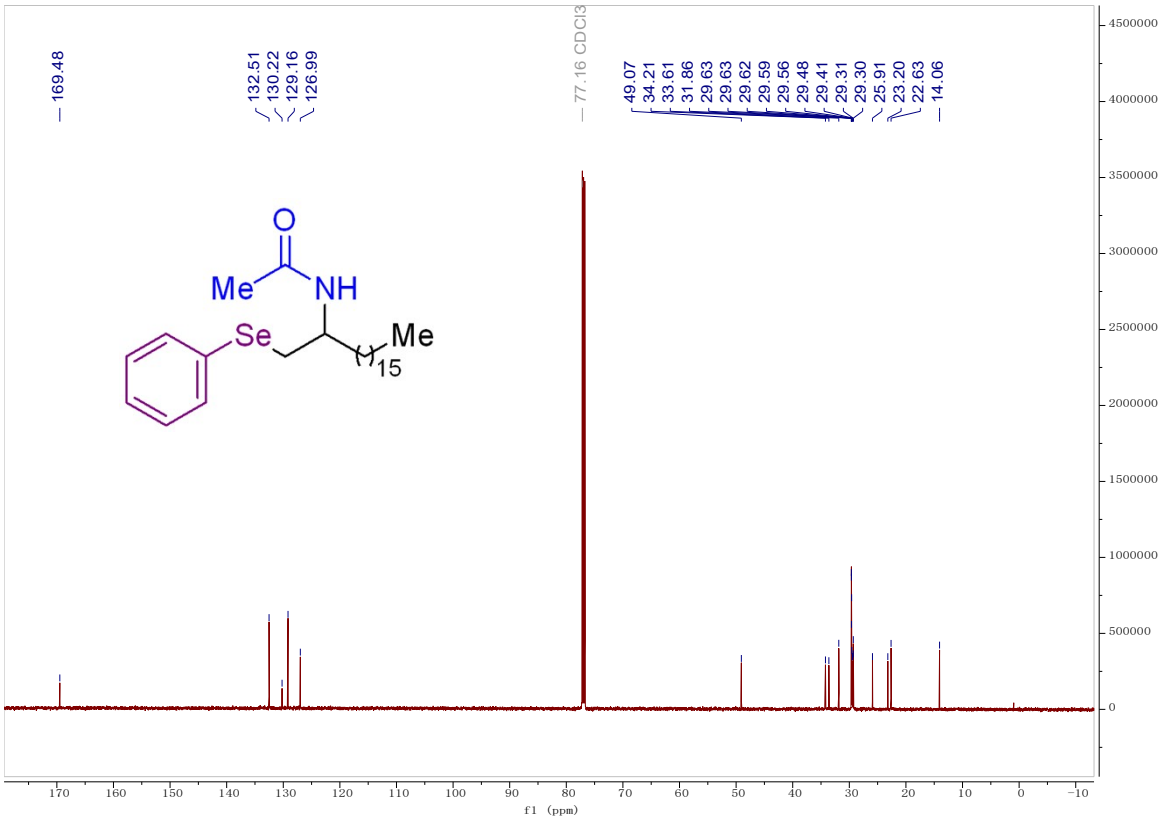
^{3}C NMR of product 3b in $CDCl_3$ (151 MHz)



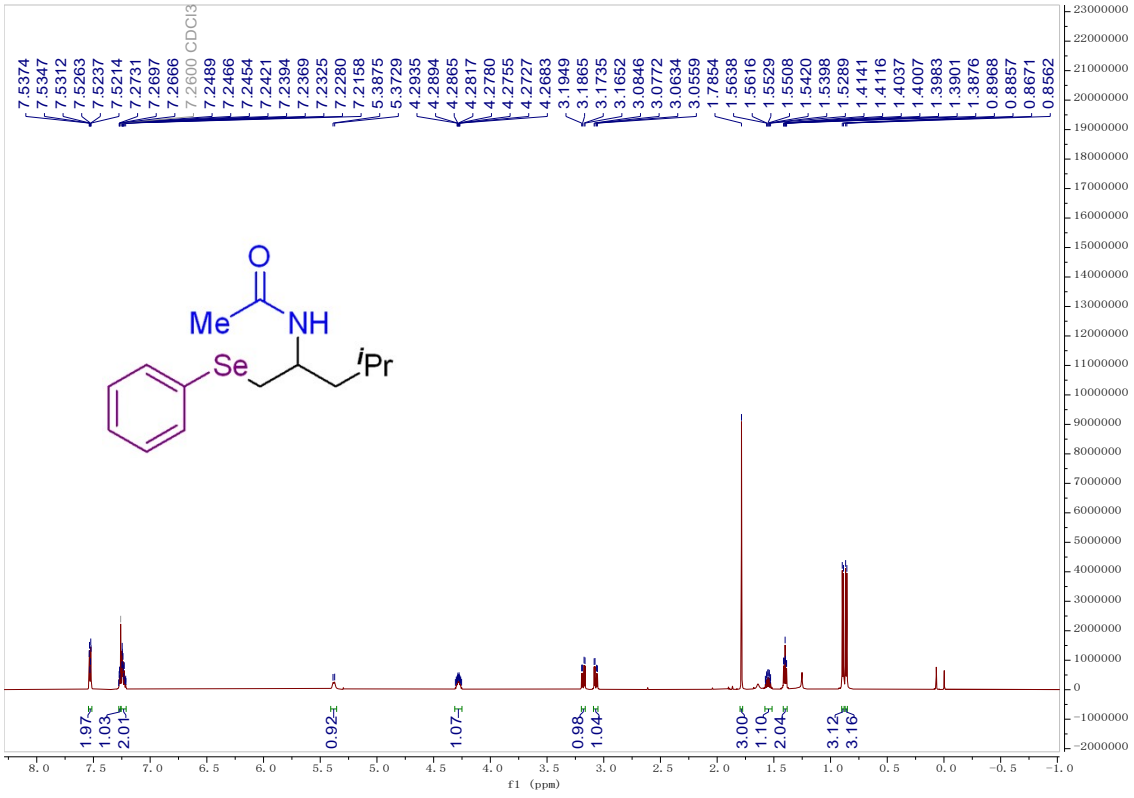
^{1}H NMR of product 3c in $CDCl_3$ (600 MHz)



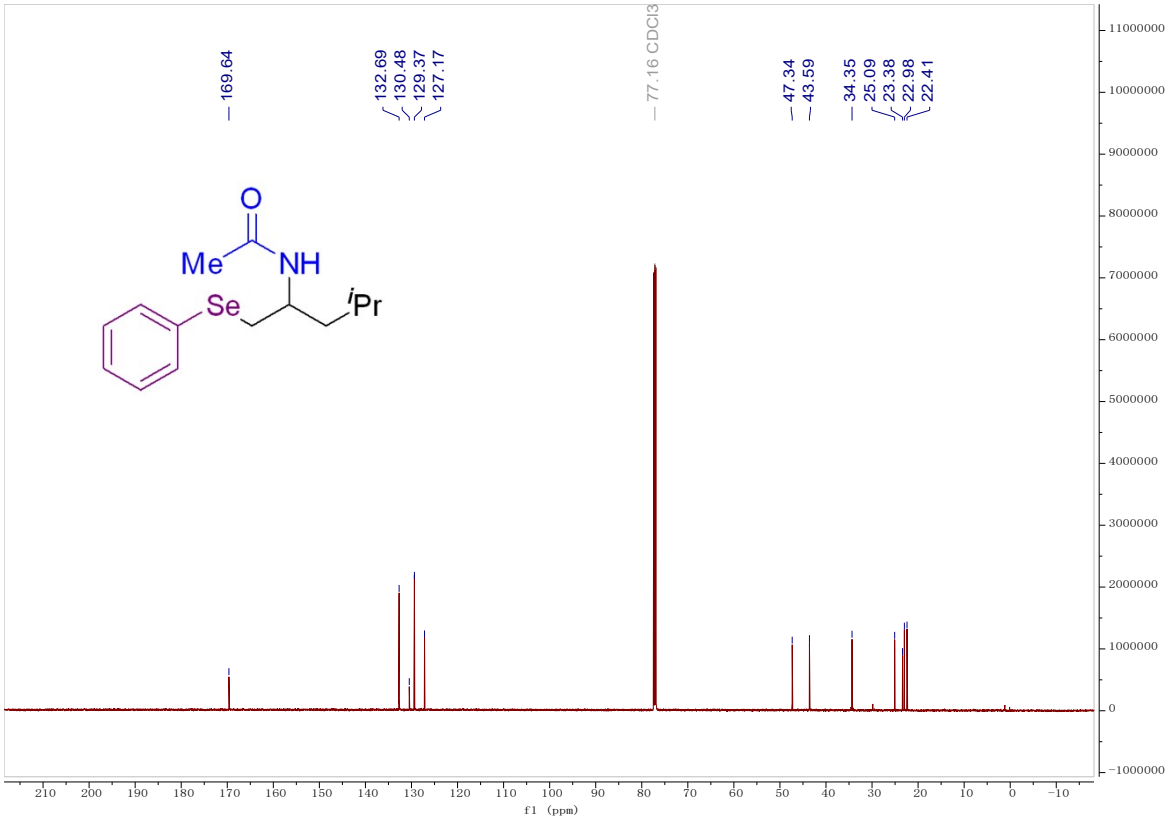
^{13}C NMR of product 3c in $CDCl_3$ (151 MHz)



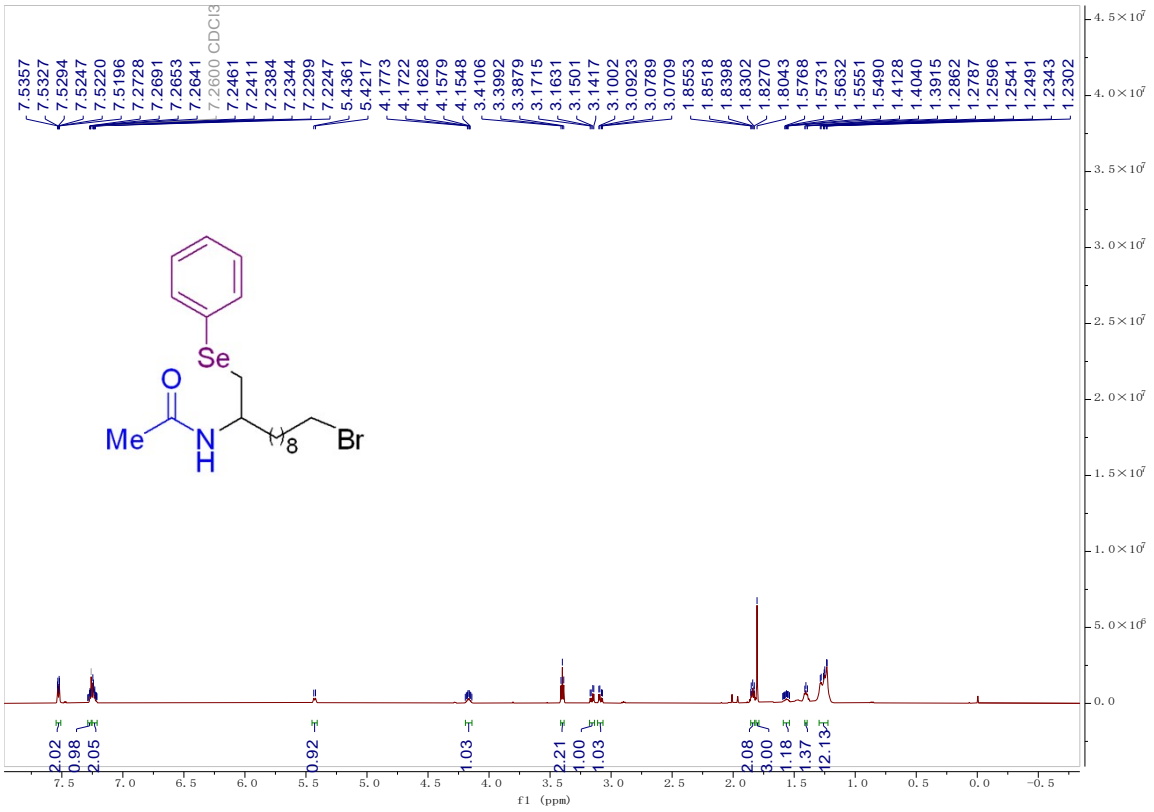
^{1}H NMR of product 3d in $CDCl_3$ (600 MHz)



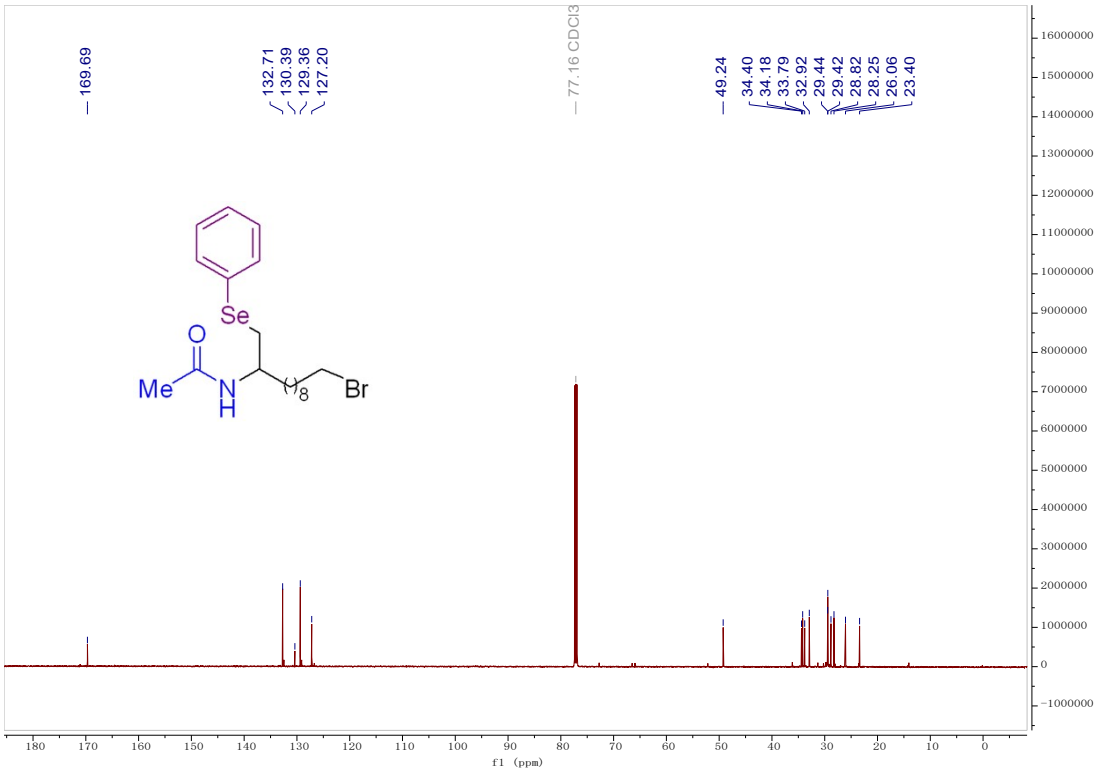
^{13}C NMR of product 3d in $CDCl_3$ (151 MHz)



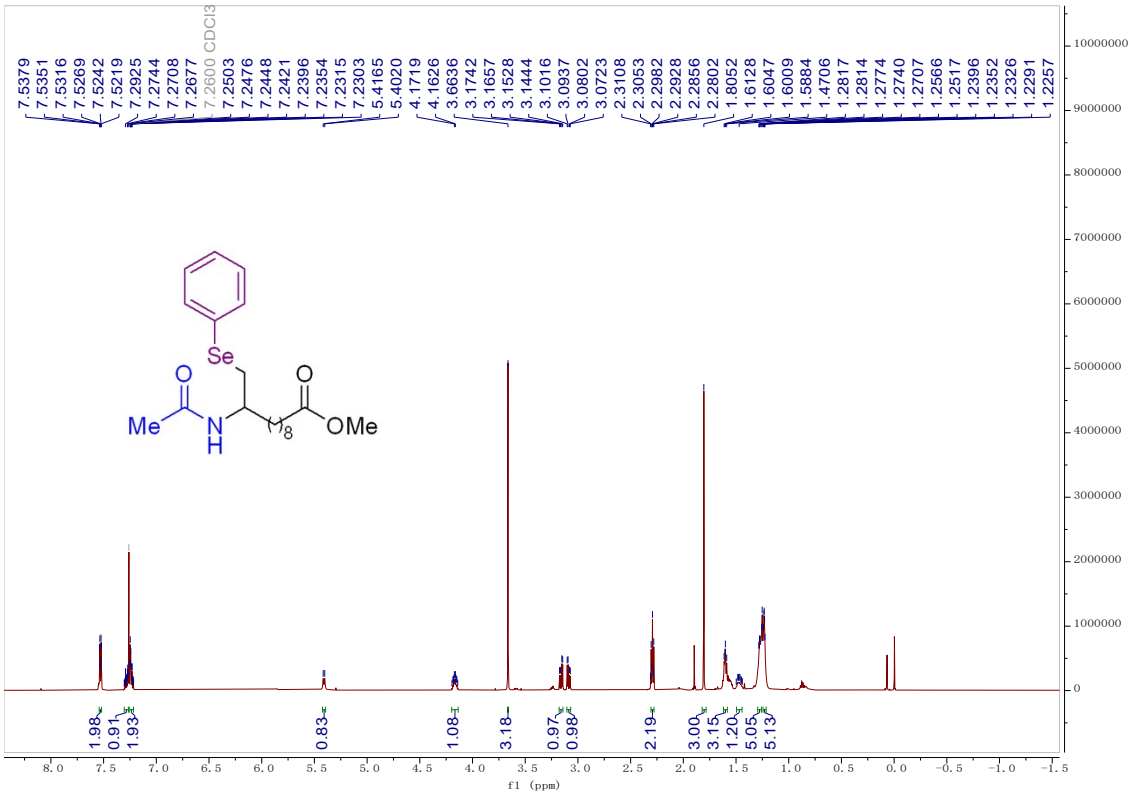
^{1}H NMR of product 3e in $CDCl_3$ (600 MHz)



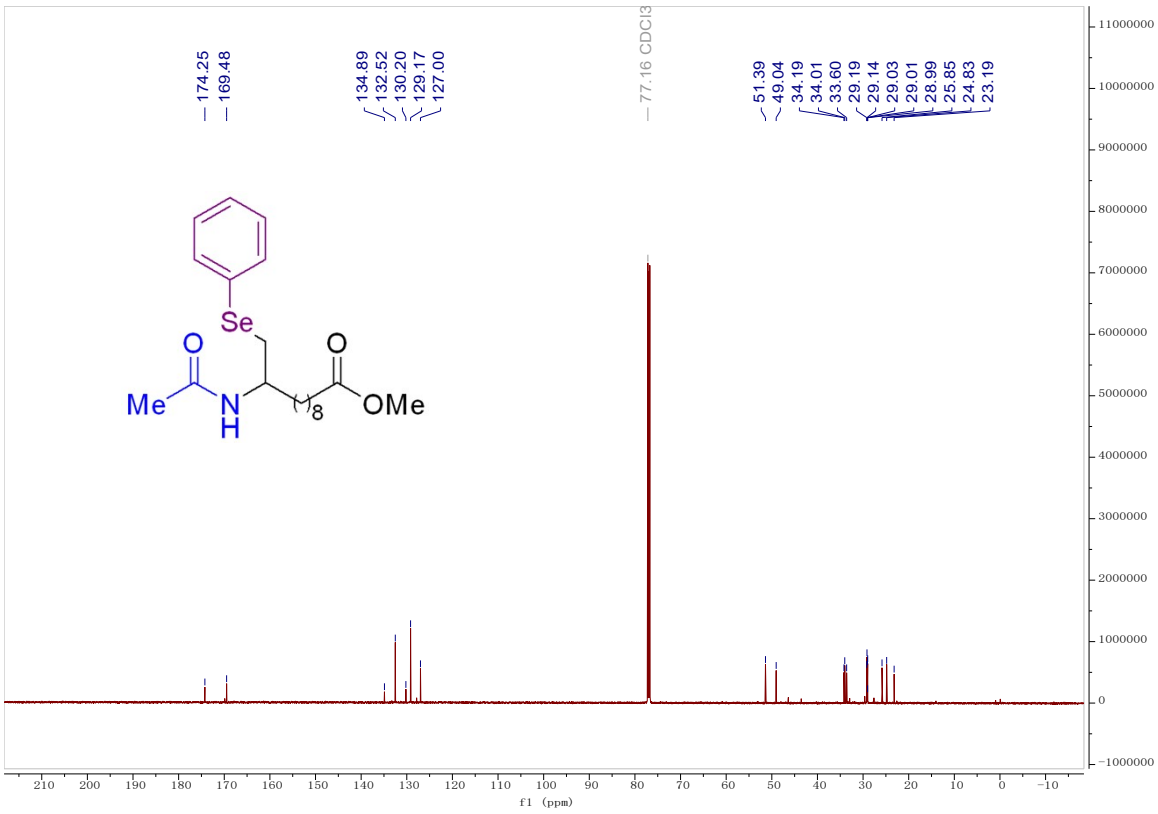
^{13}C NMR of product 3e in $CDCl_3$ (151 MHz)



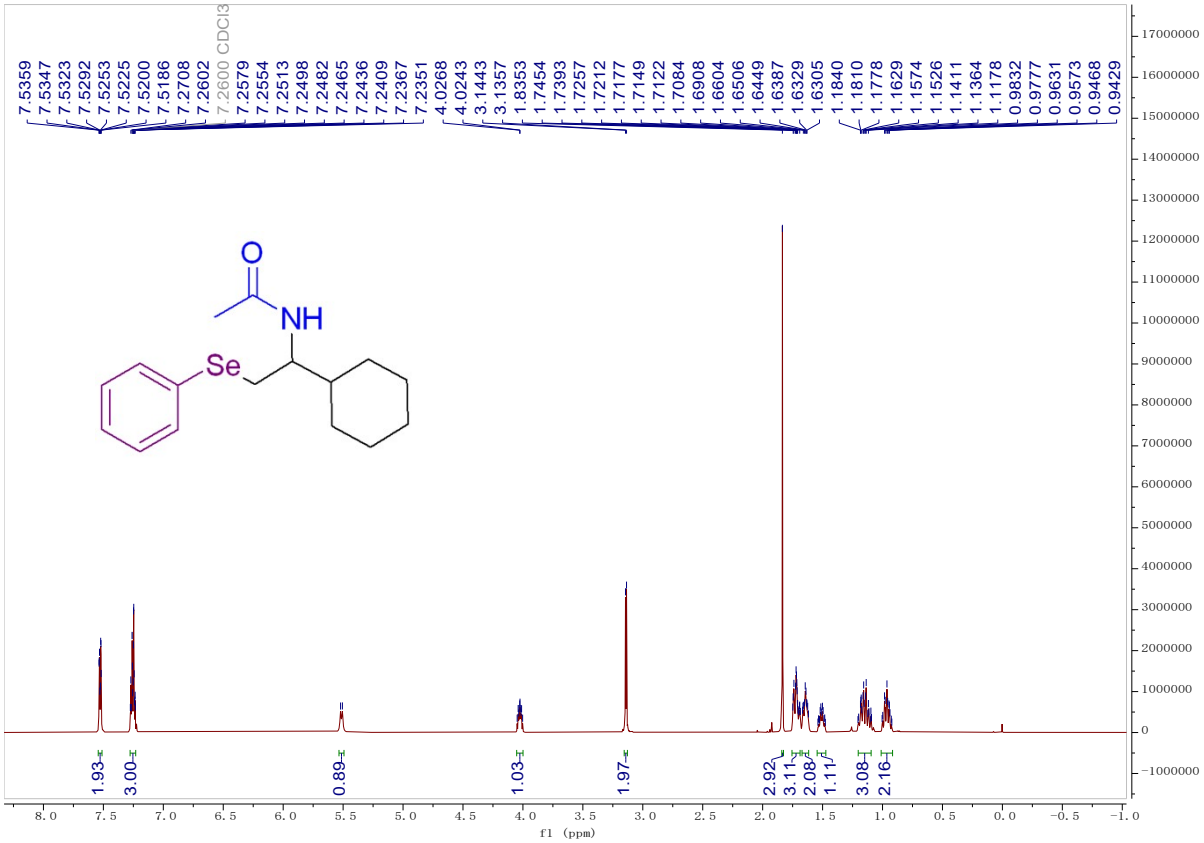
^{1}H NMR of product 3f in $CDCl_3$ (600 MHz)



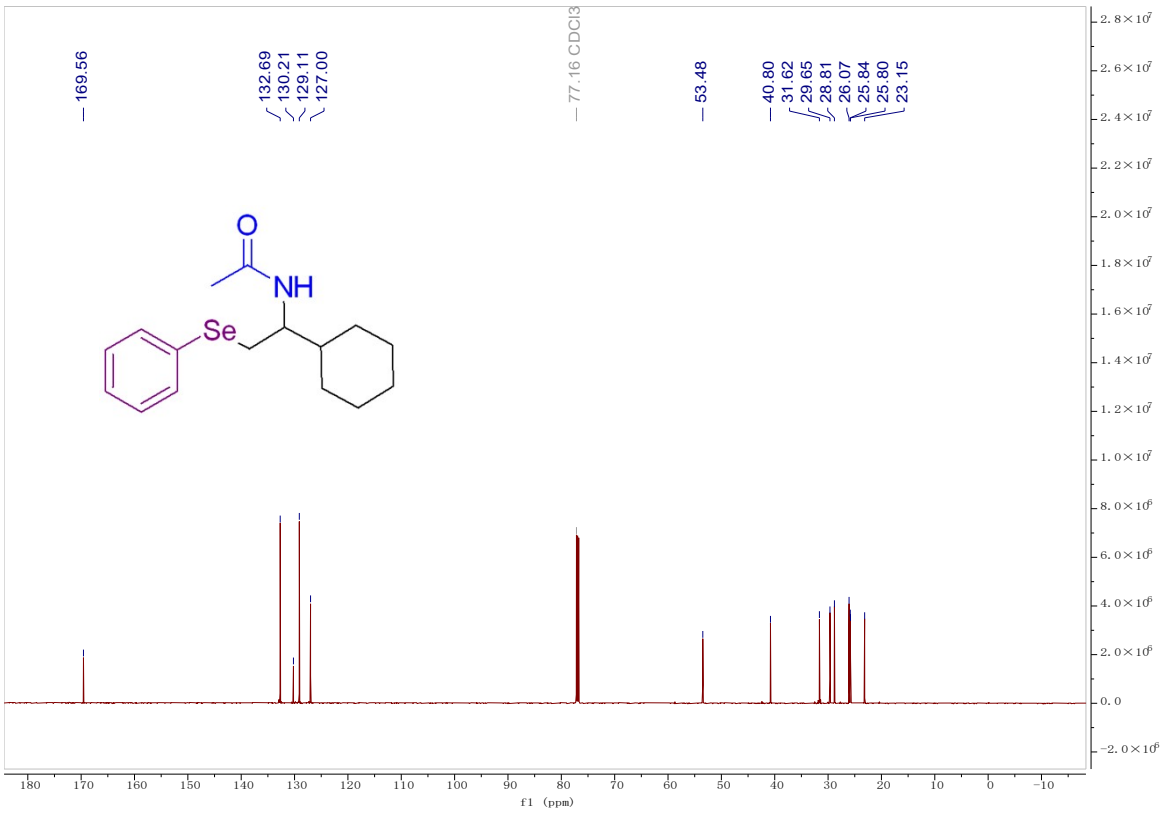
^{13}C NMR of product 3f in $CDCl_3$ (151 MHz)



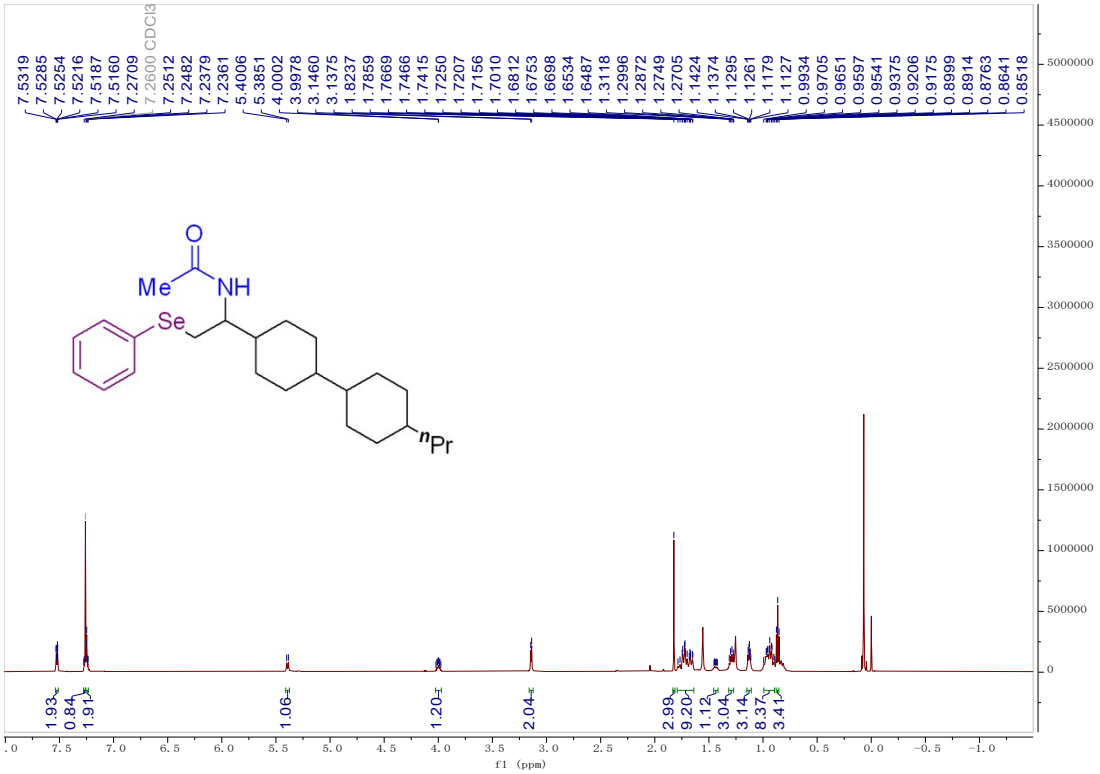
^{1}H NMR of product 3g in $CDCl_3$ (600 MHz)



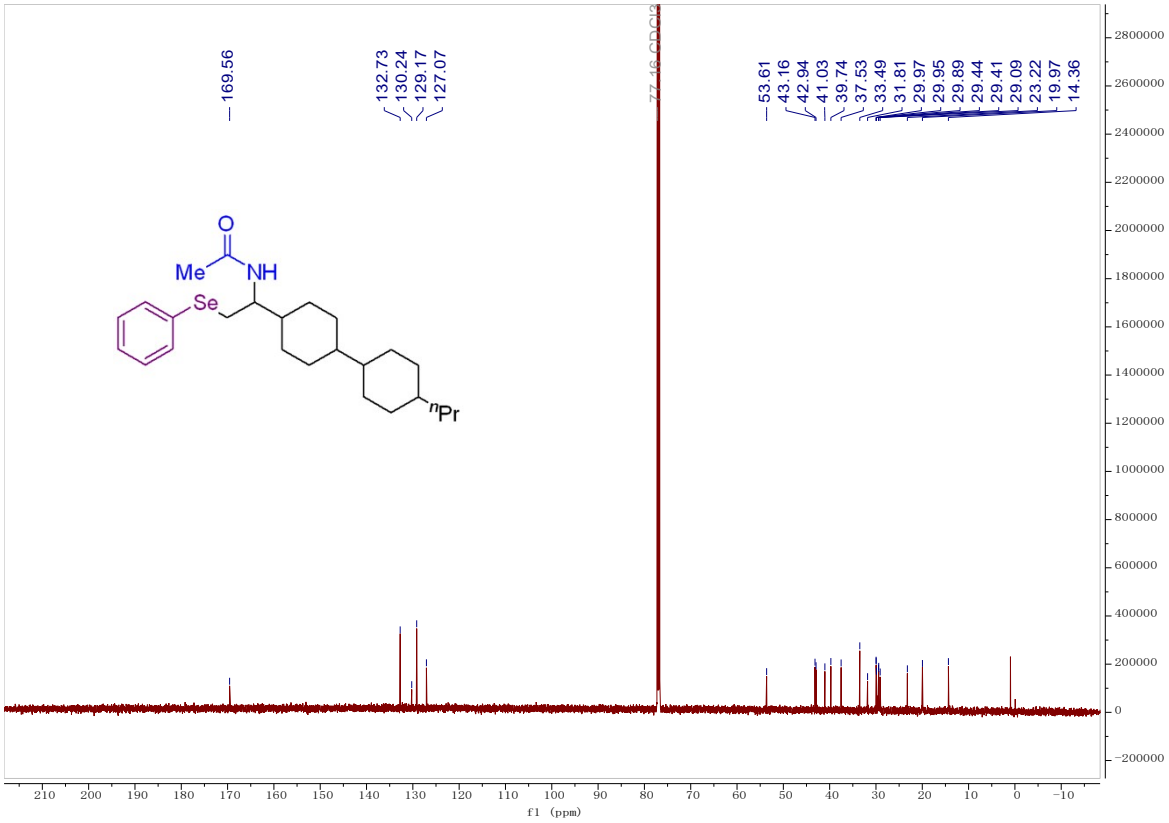
^{13}C NMR of product 3g in $CDCl_3$ (151 MHz)



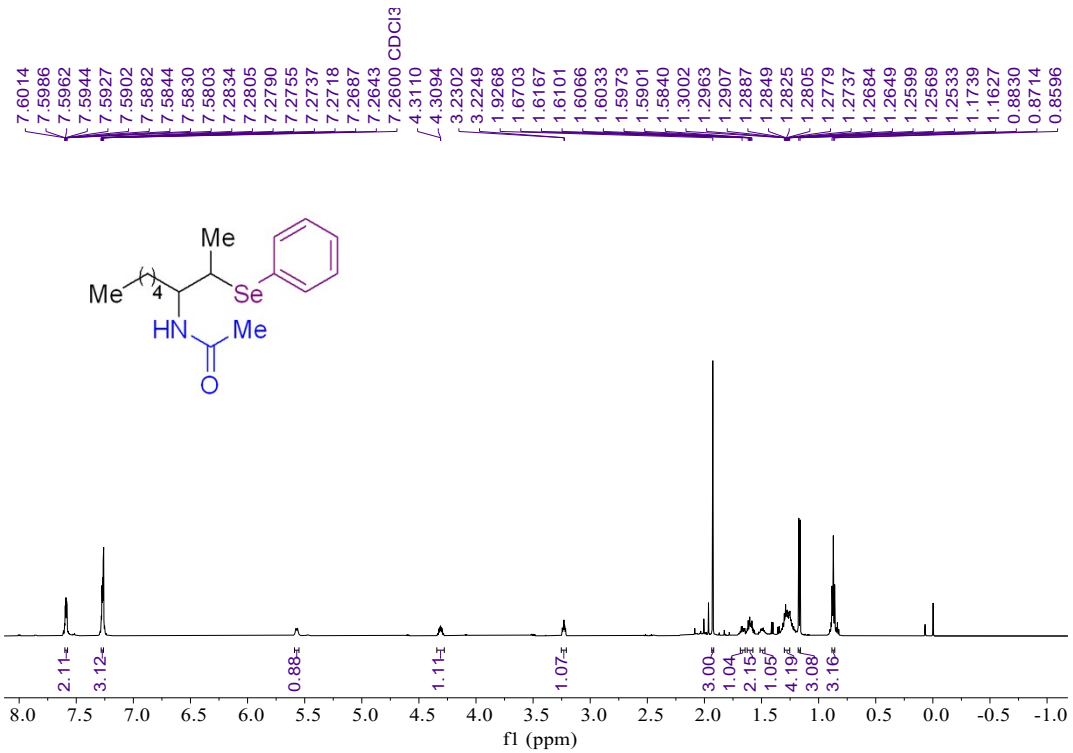
^{1}H NMR of product 3h in $CDCl_3$ (600 MHz)



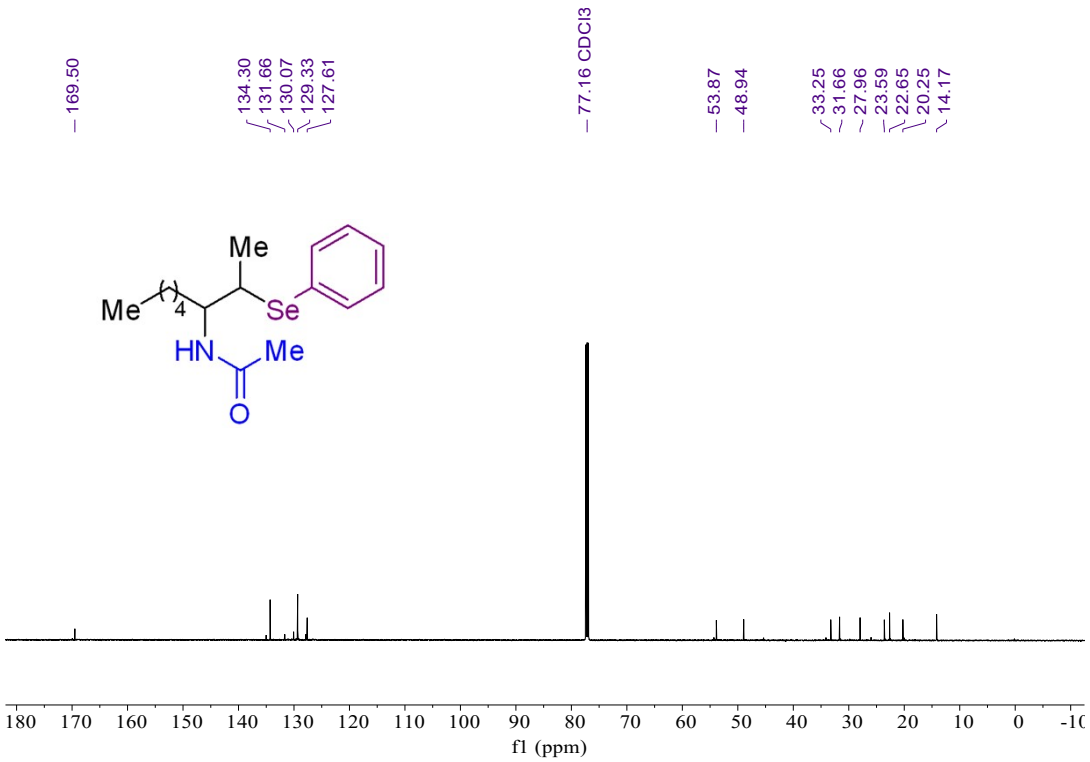
^{13}C NMR of product 3h in $CDCl_3$ (151 MHz)



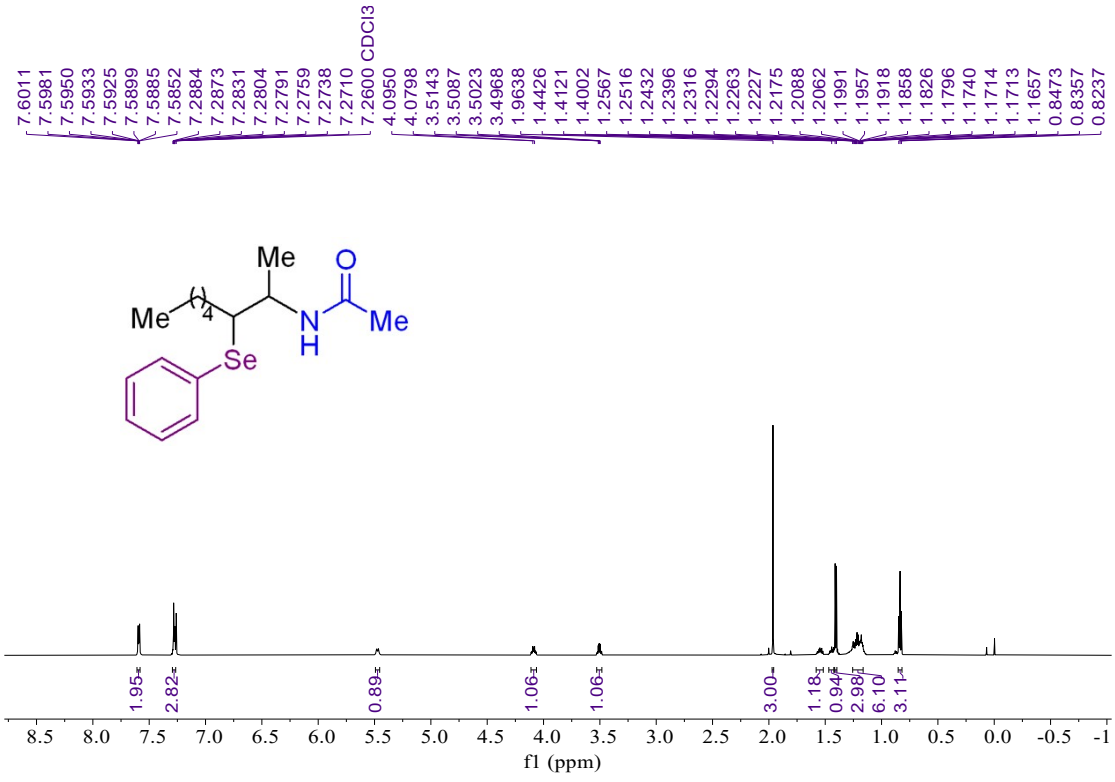
^{1}H NMR of product 3j in $CDCl_3$ (600 MHz)



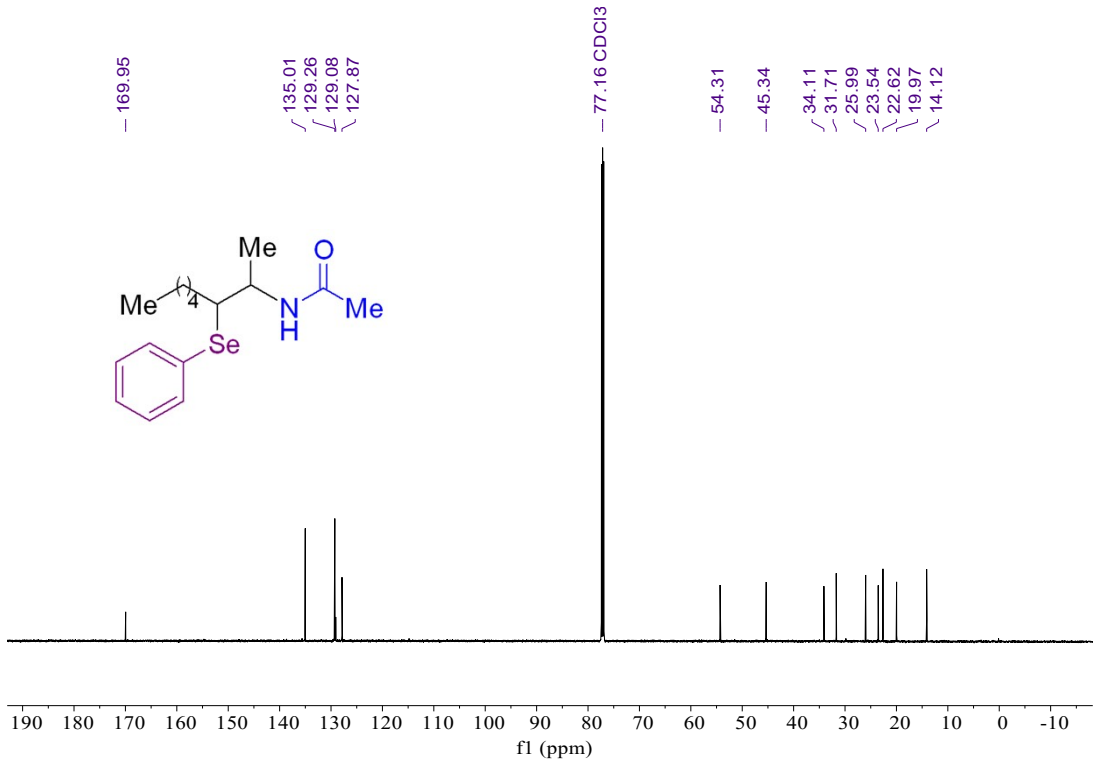
^{13}C NMR of product 3j in $CDCl_3$ (151 MHz)



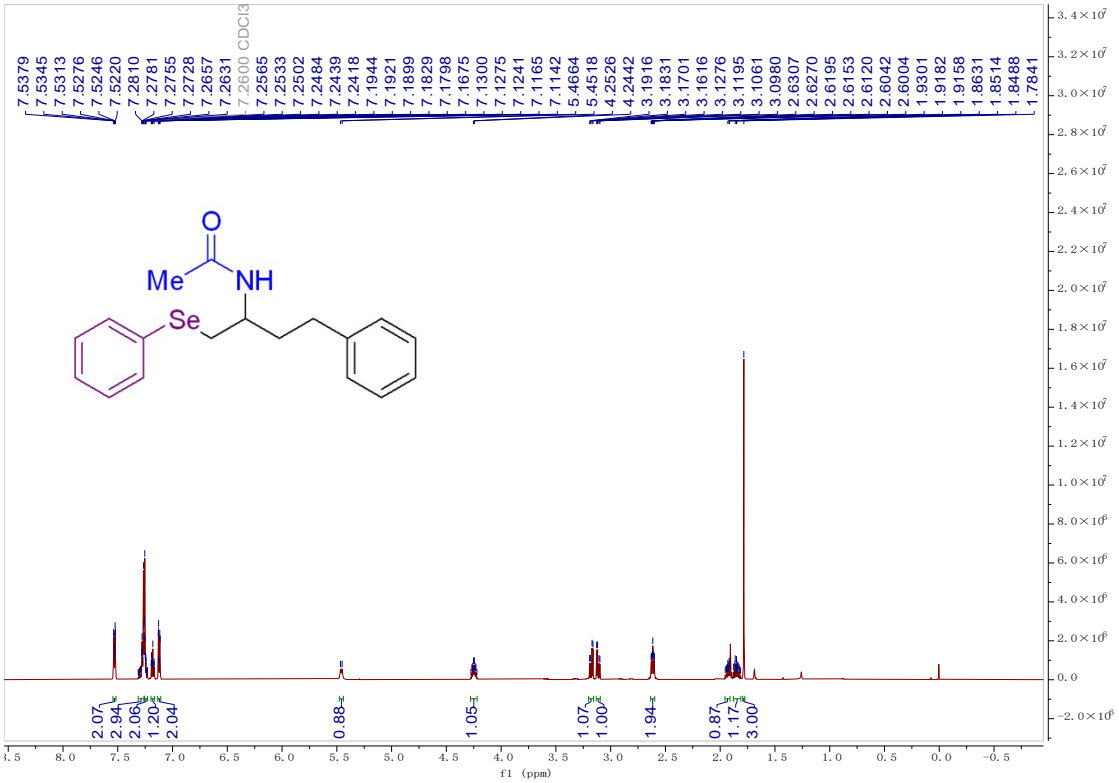
^{1}H NMR of product 3j` in $CDCl_3$ (600 MHz)



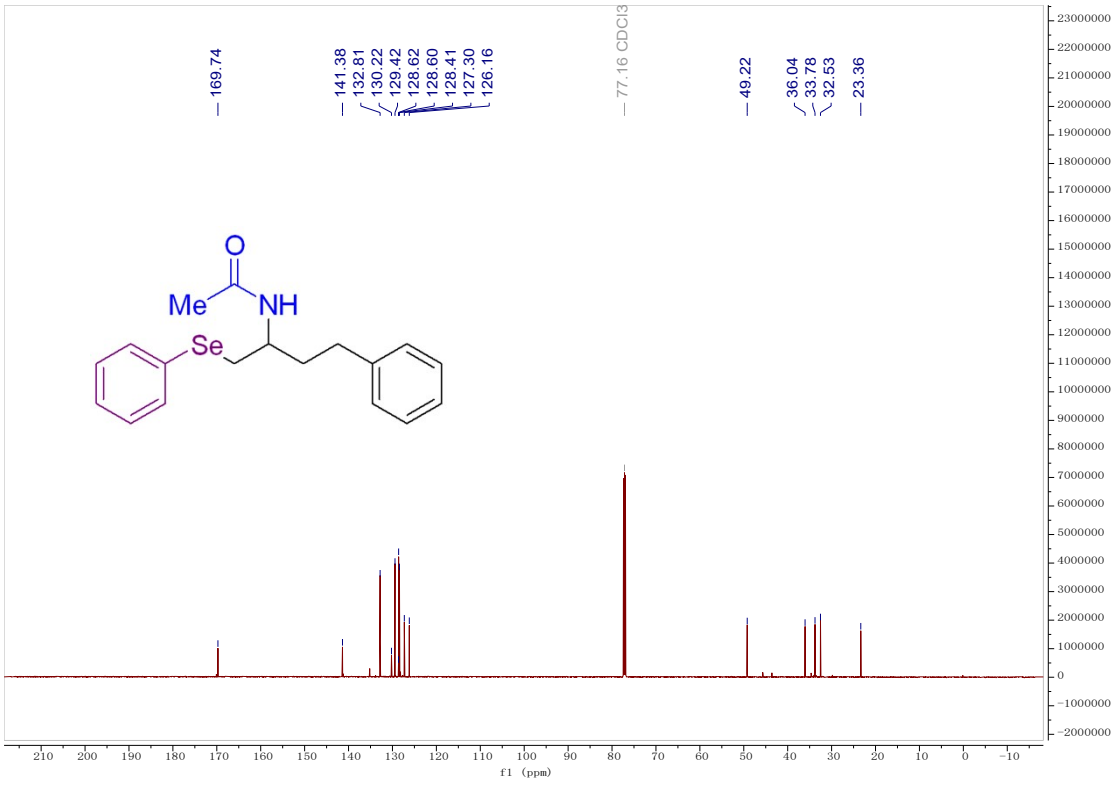
^{13}C NMR of product 3j` in $CDCl_3$ (151 MHz)



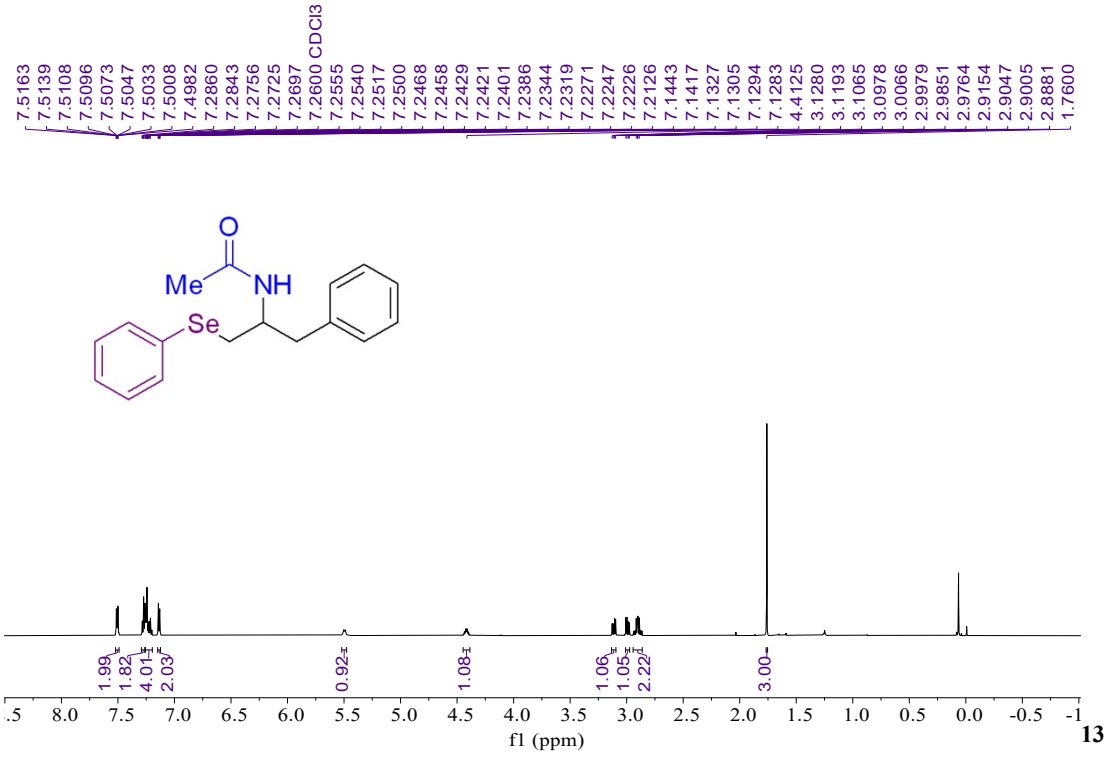
^{1}H NMR of product 3k in $CDCl_3$ (600 MHz)



^{13}C NMR of product 3k in $CDCl_3$ (151 MHz)

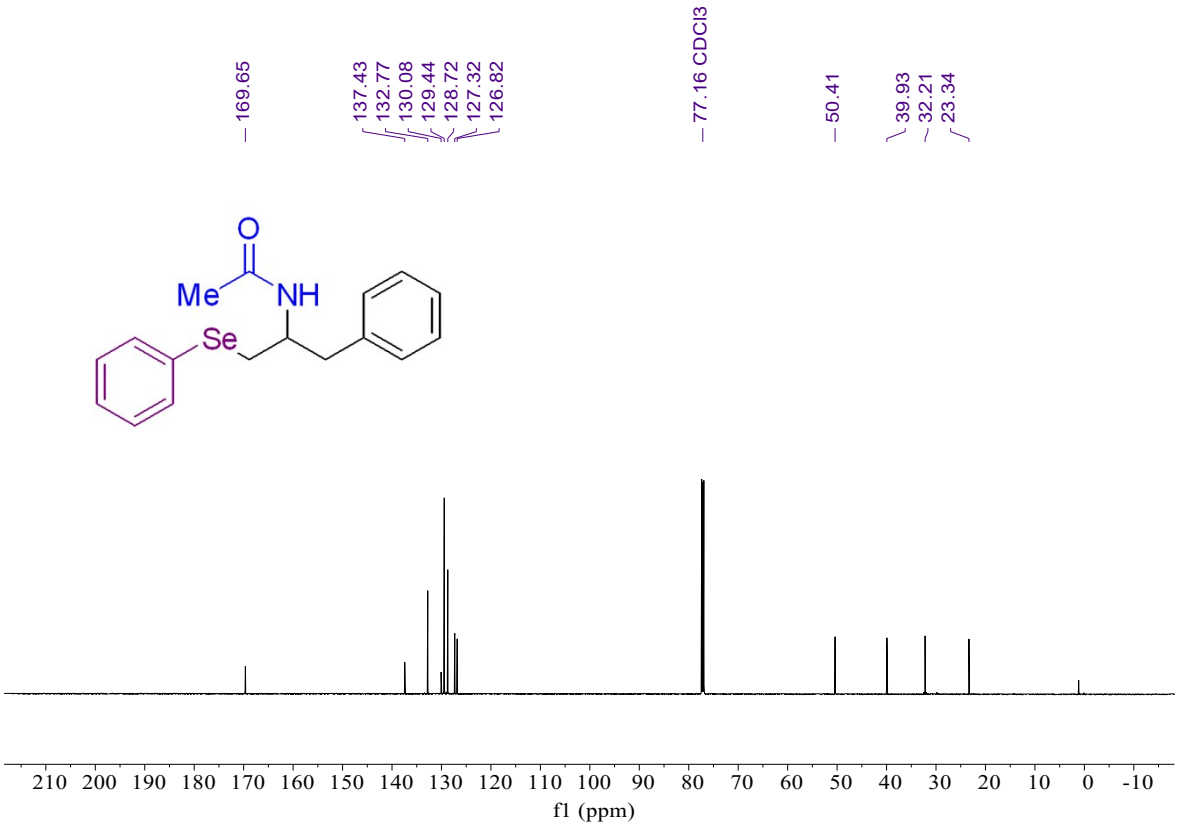


^{1}H NMR of product 3l in $CDCl_3$ (600 MHz)

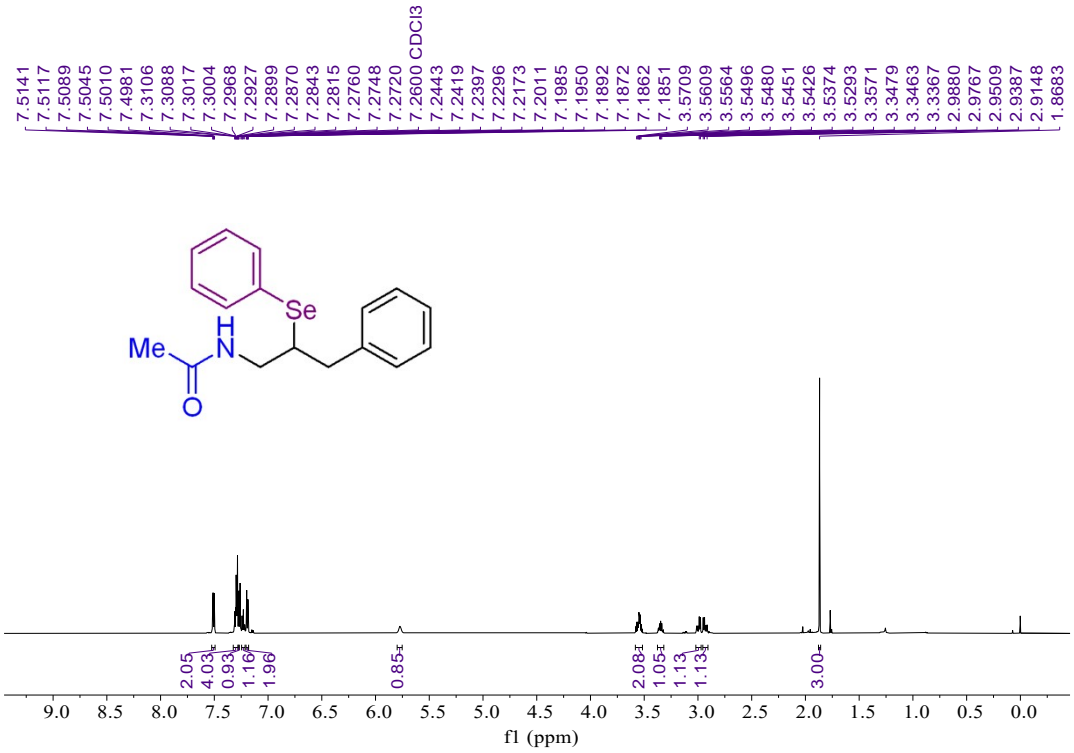


13

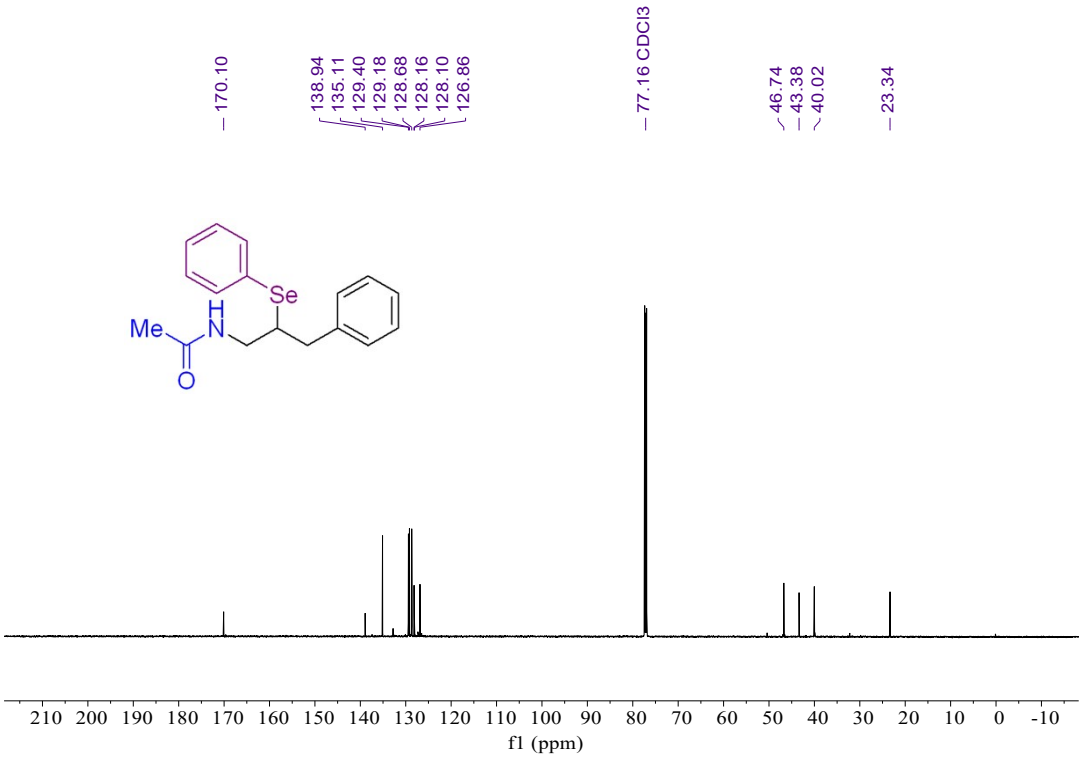
C NMR of product 3l in $CDCl_3$ (151 MHz)



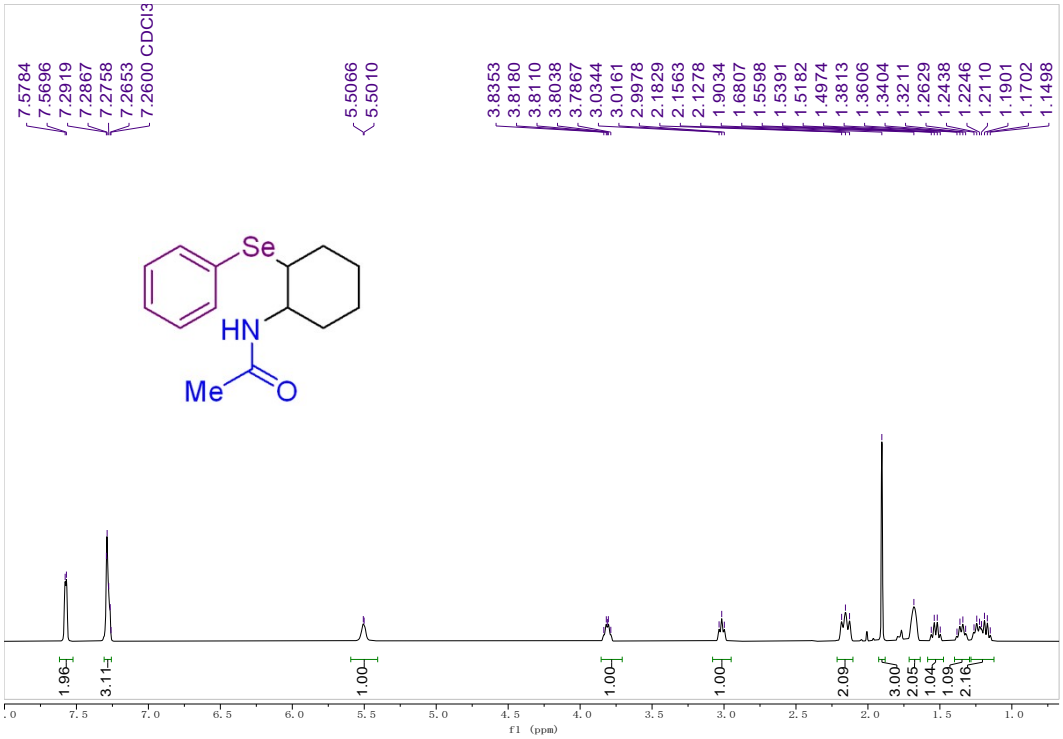
^{1}H NMR of product 3l` in $CDCl_3$ (600 MHz)



^{13}C NMR of product 3l` in $CDCl_3$ (151 MHz)

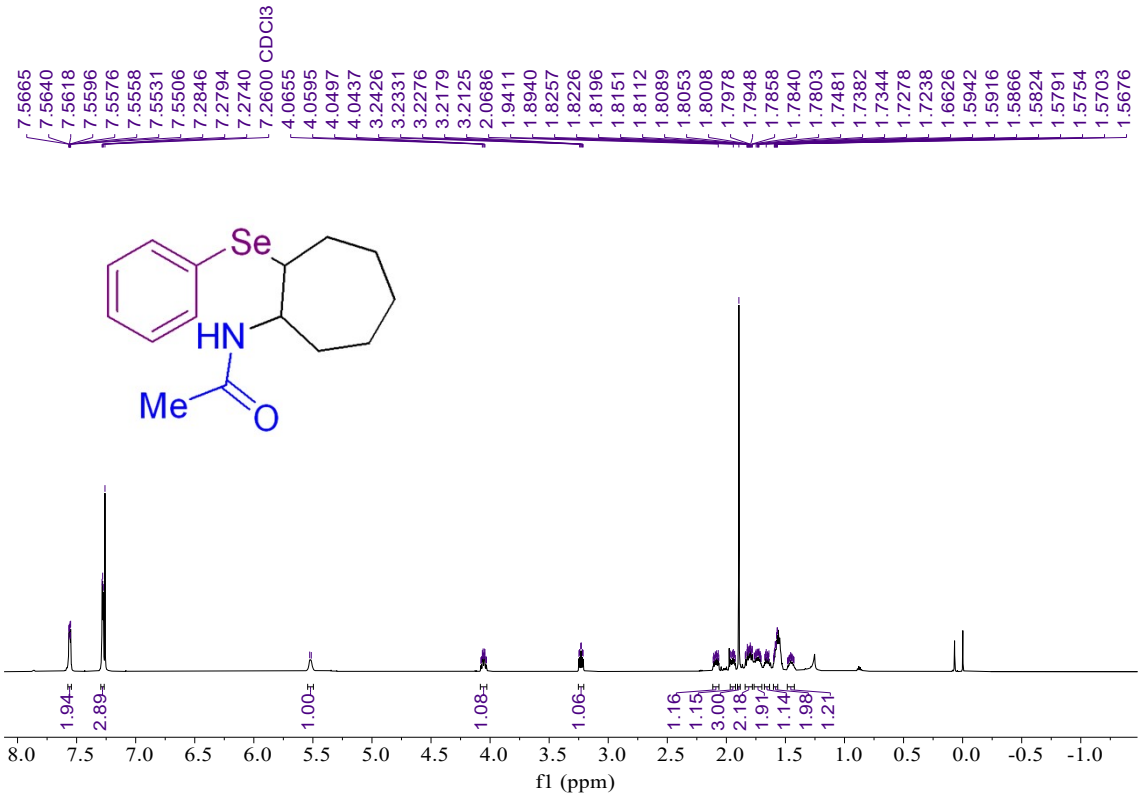


^{1}H NMR of product 3n in $CDCl_3$ (600 MHz)

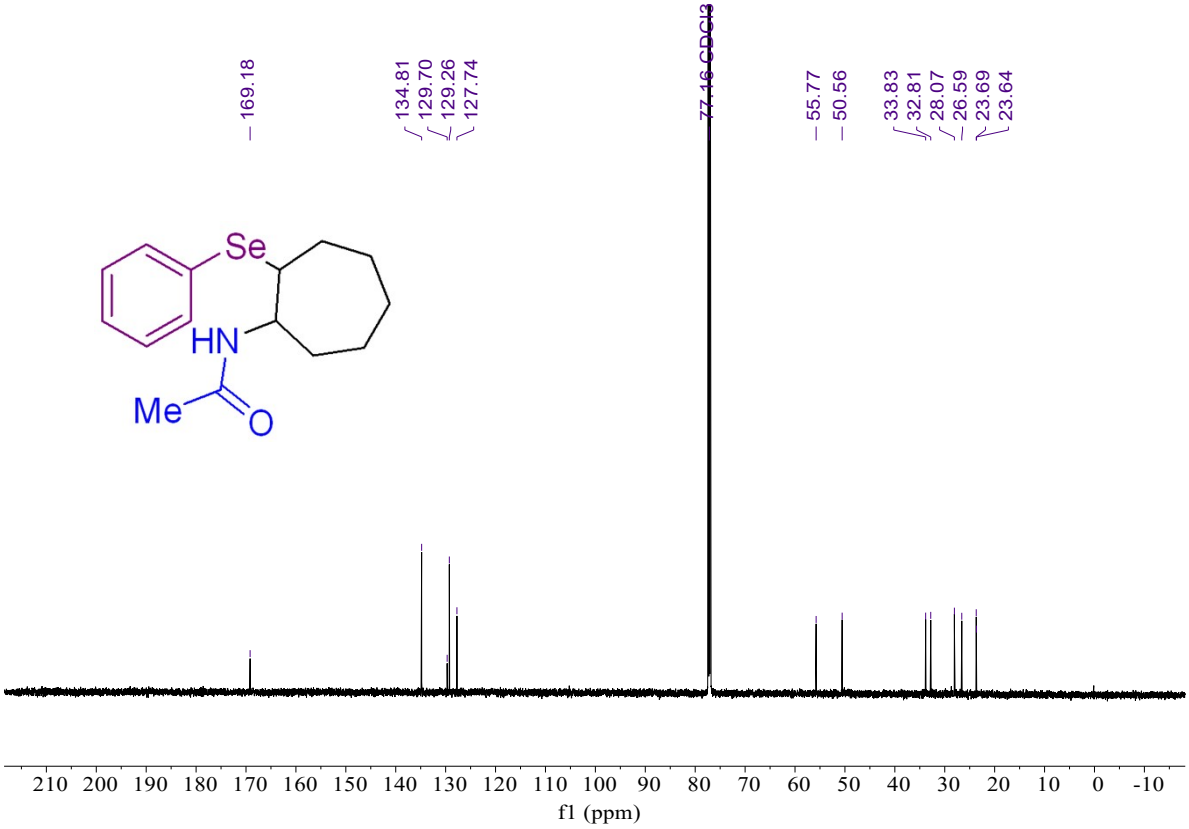


^{13}C NMR of product 3n in $CDCl_3$ (151 MHz)

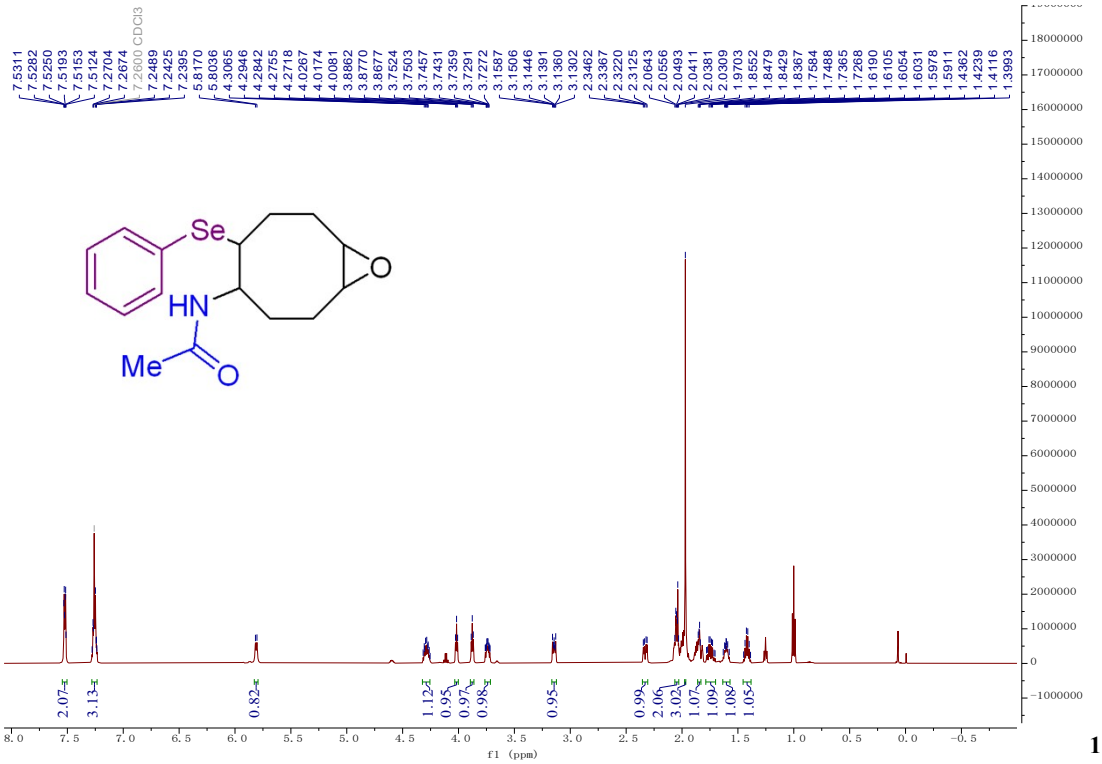
^{1}H NMR of product 3o in $CDCl_3$ (600 MHz)



^{13}C NMR of product 3o in $CDCl_3$ (151 MHz)



^{1}H NMR of product 3p in $CDCl_3$ (600 MHz)



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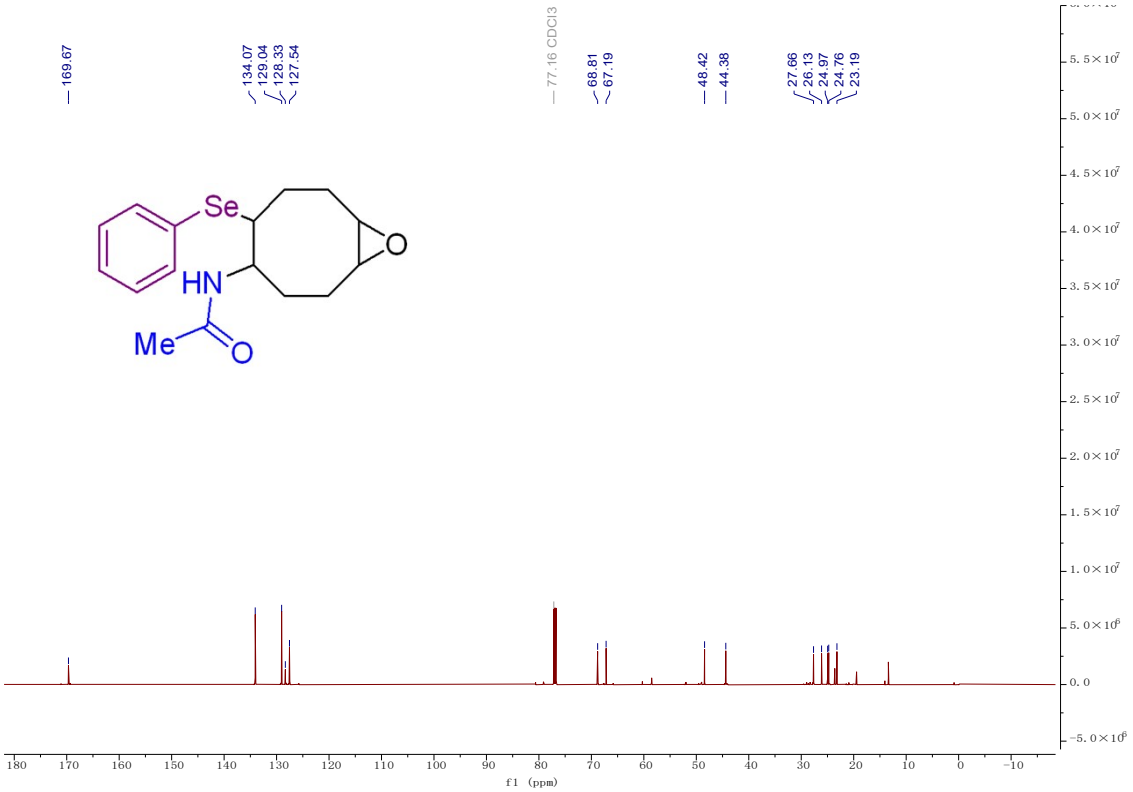
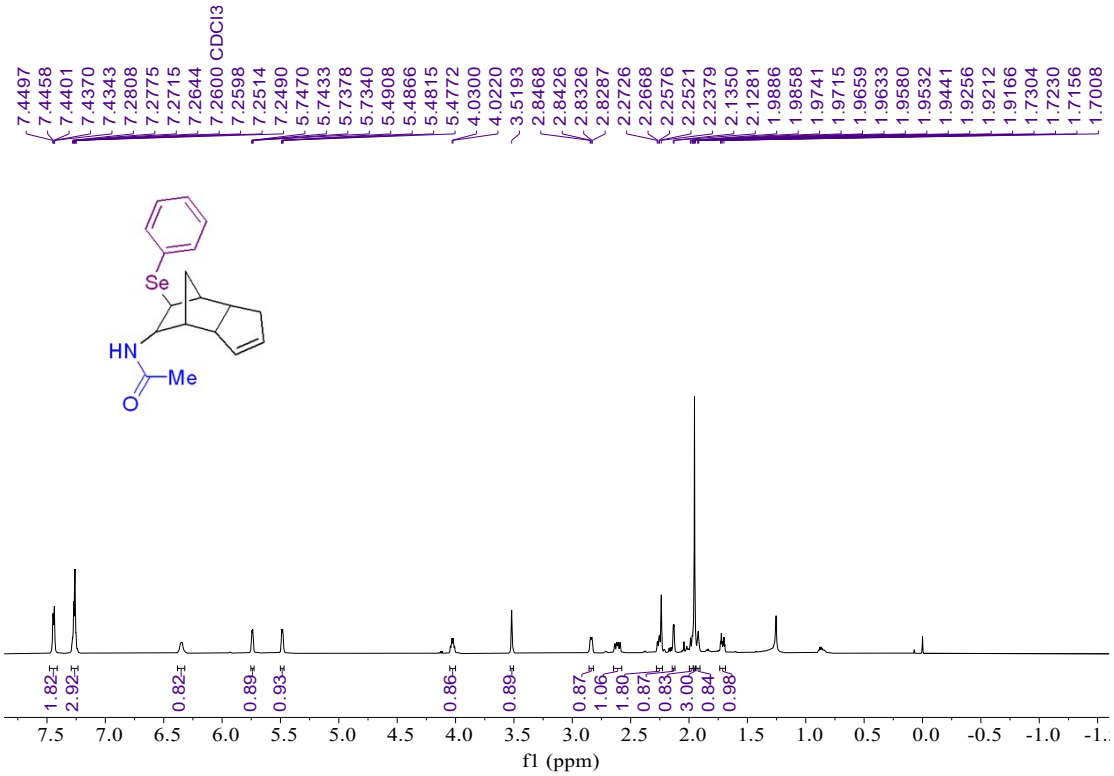
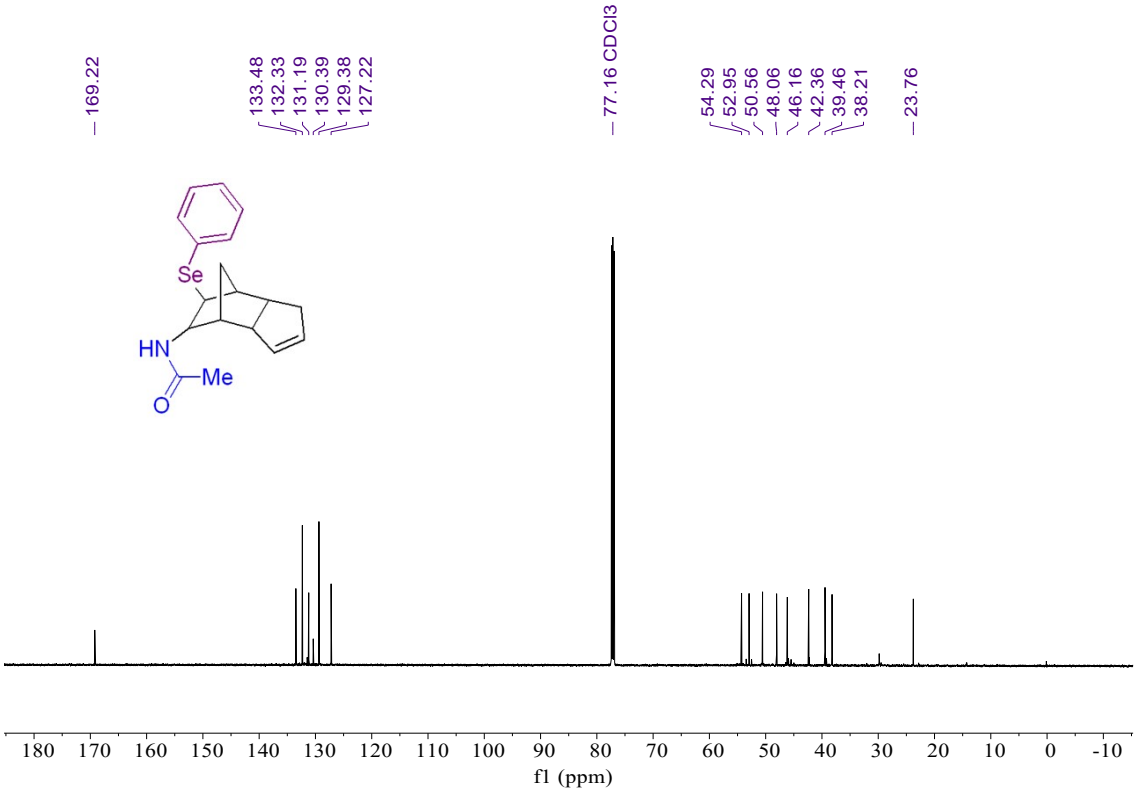
^{3}C NMR of product 3p in $CDCl_3$ (151 MHz)



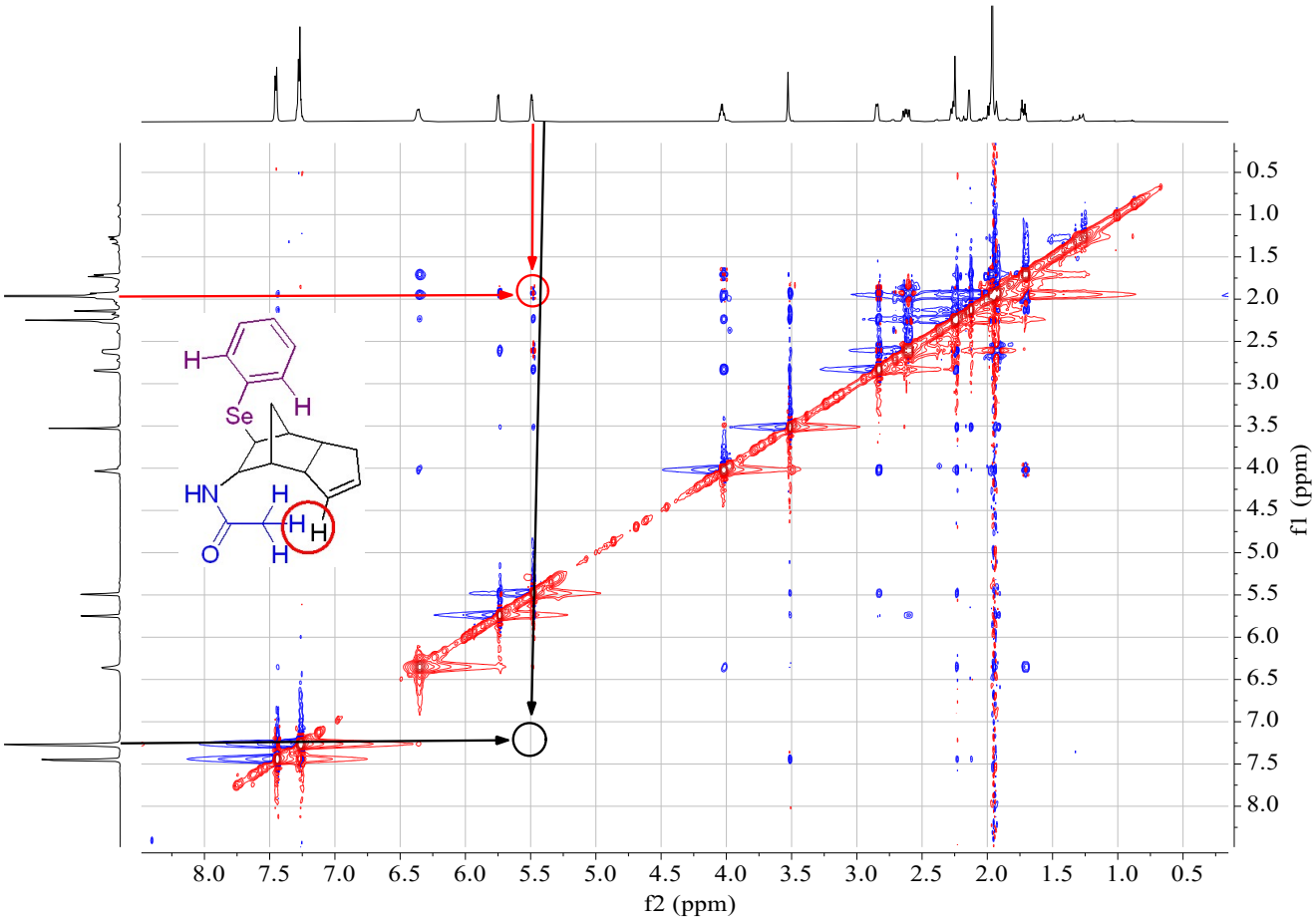
^{1}H NMR of product 3q in $CDCl_3$ (600 MHz)



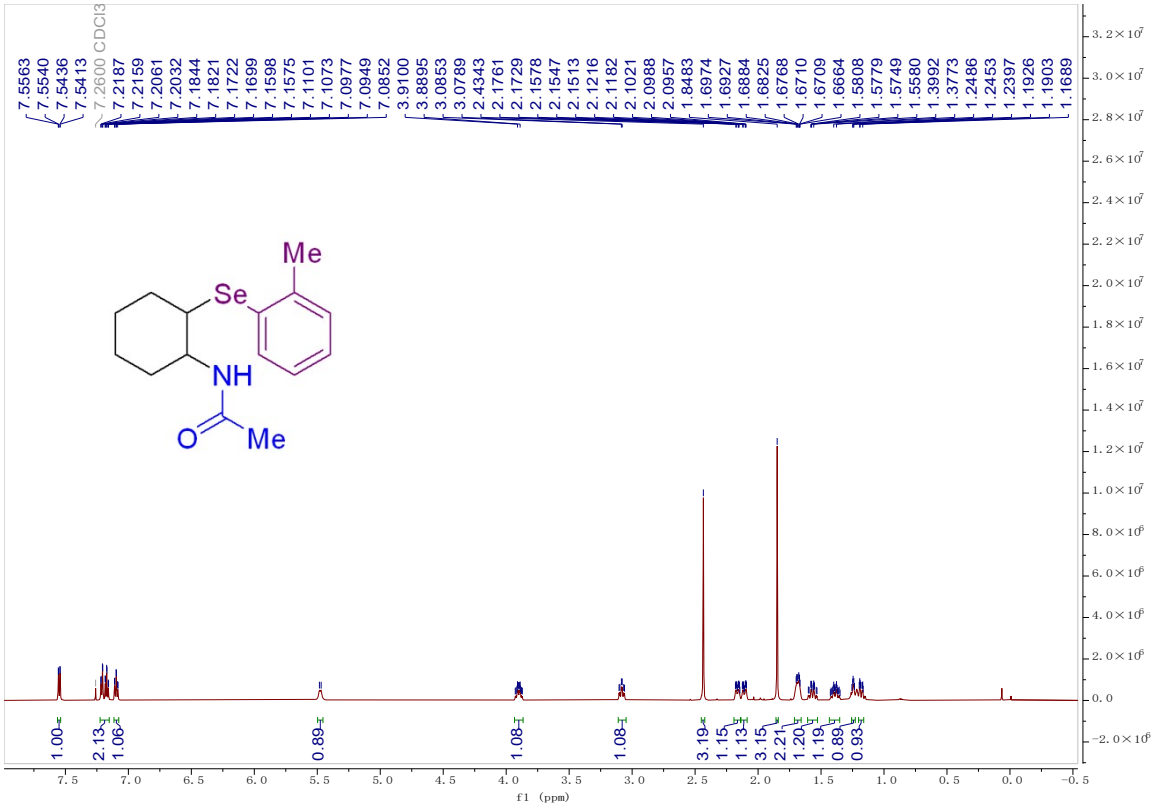
^{13}C NMR of product 3q in $CDCl_3$ (151 MHz)



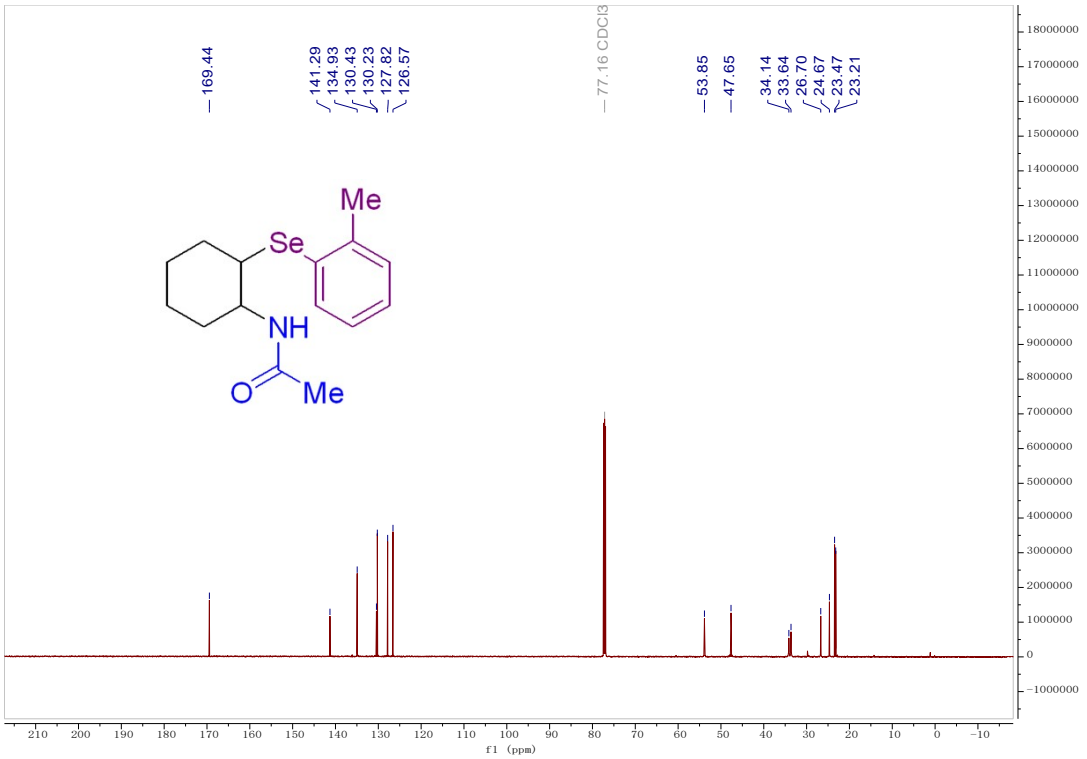
HHCOSY of product 3q in $CDCl_3$ (600 MHz)



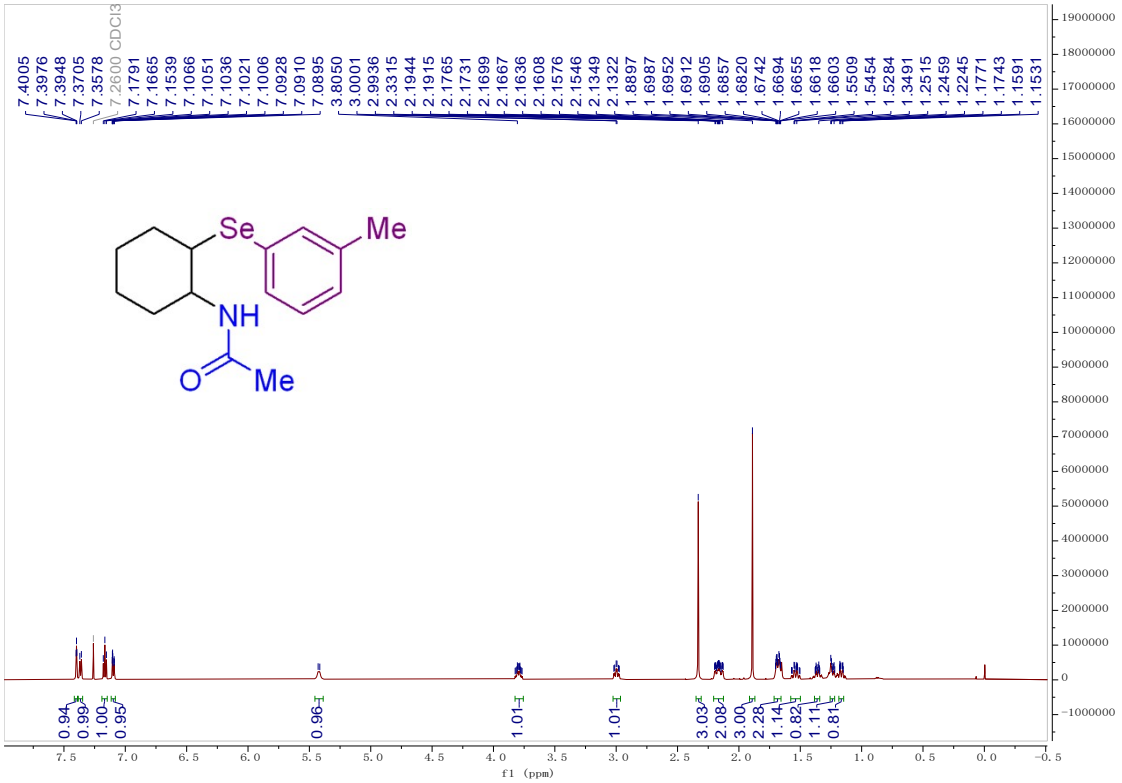
^{1}H NMR of product 3r in $CDCl_3$ (600 MHz)



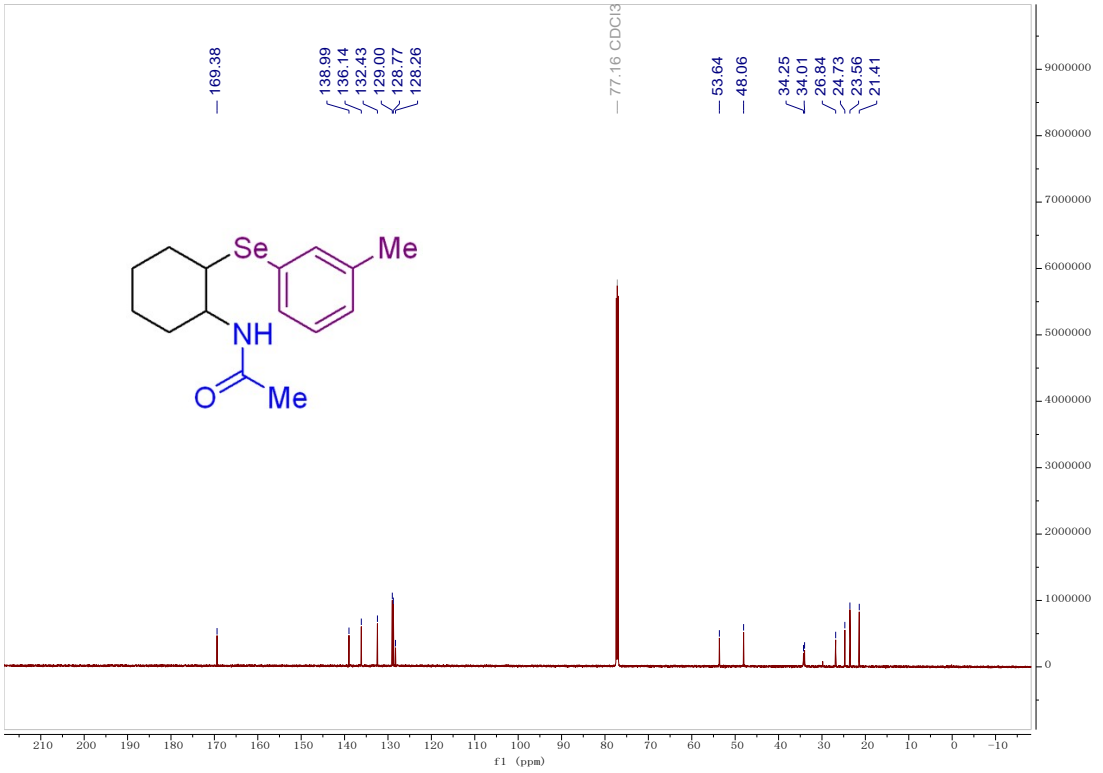
^{13}C NMR of product 3r in $CDCl_3$ (151 MHz)



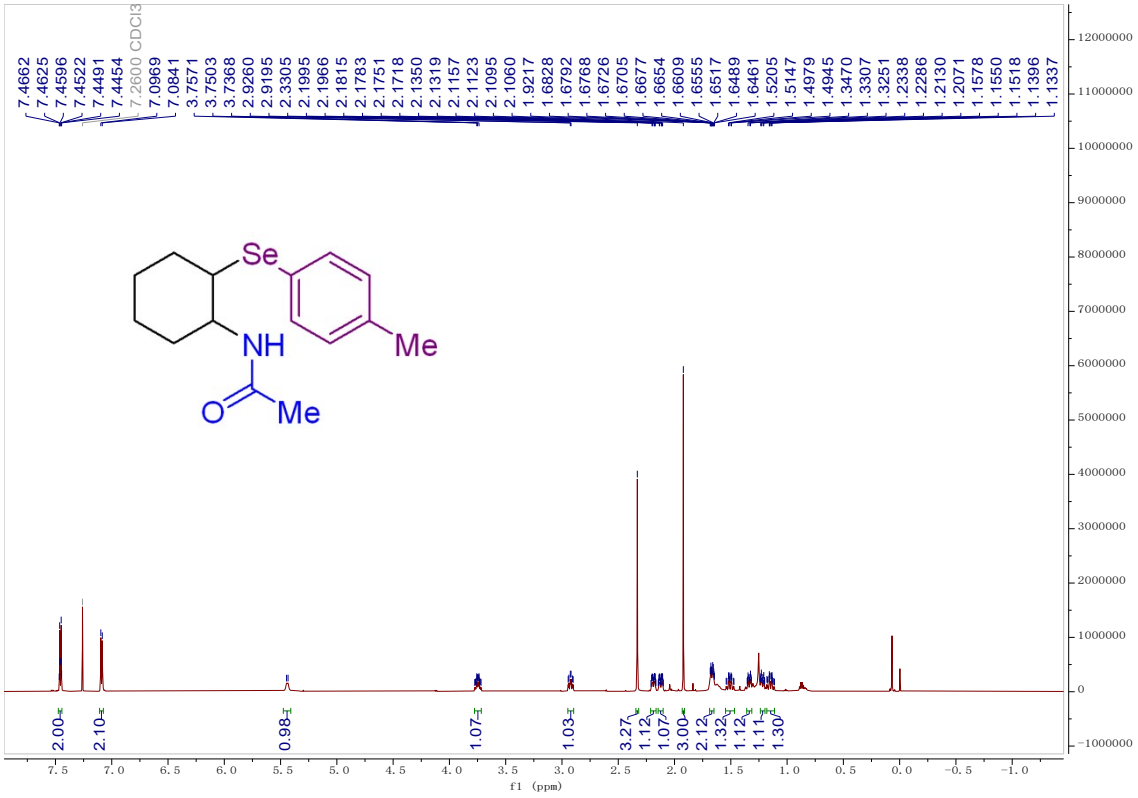
^{1}H NMR of product 3s in $CDCl_3$ (600 MHz)



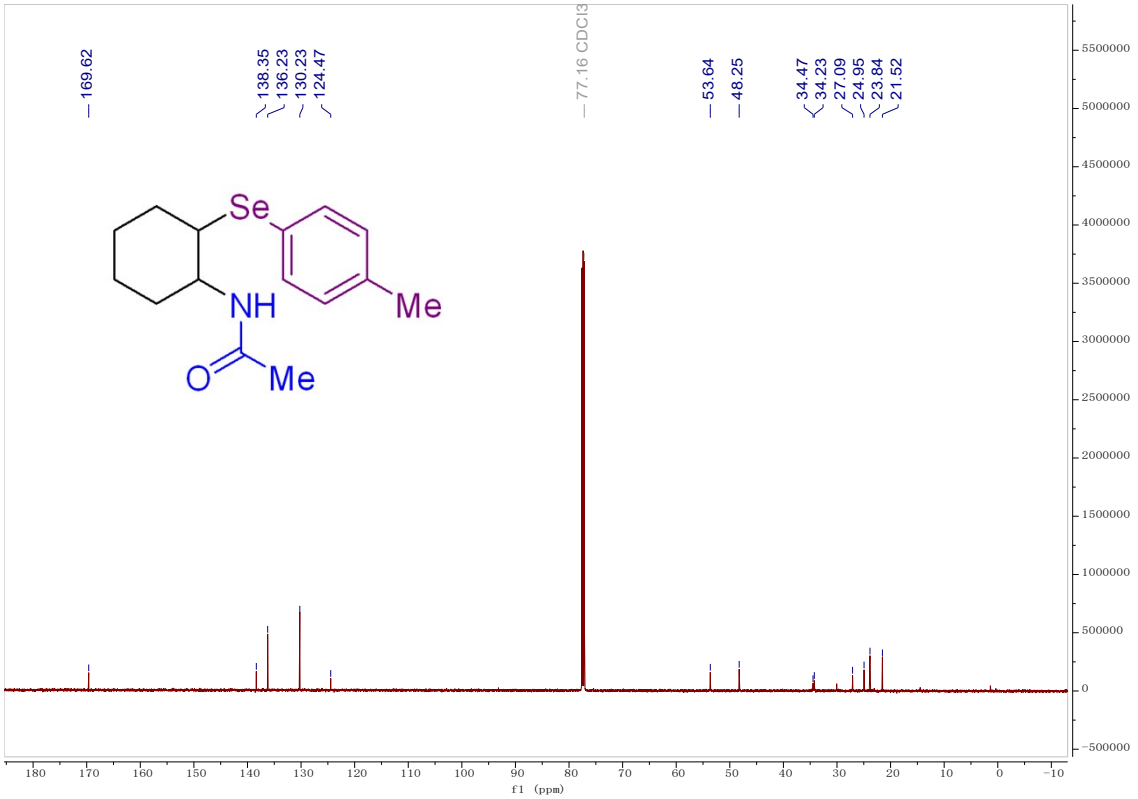
^{13}C NMR of product 3s in $CDCl_3$ (151 MHz)



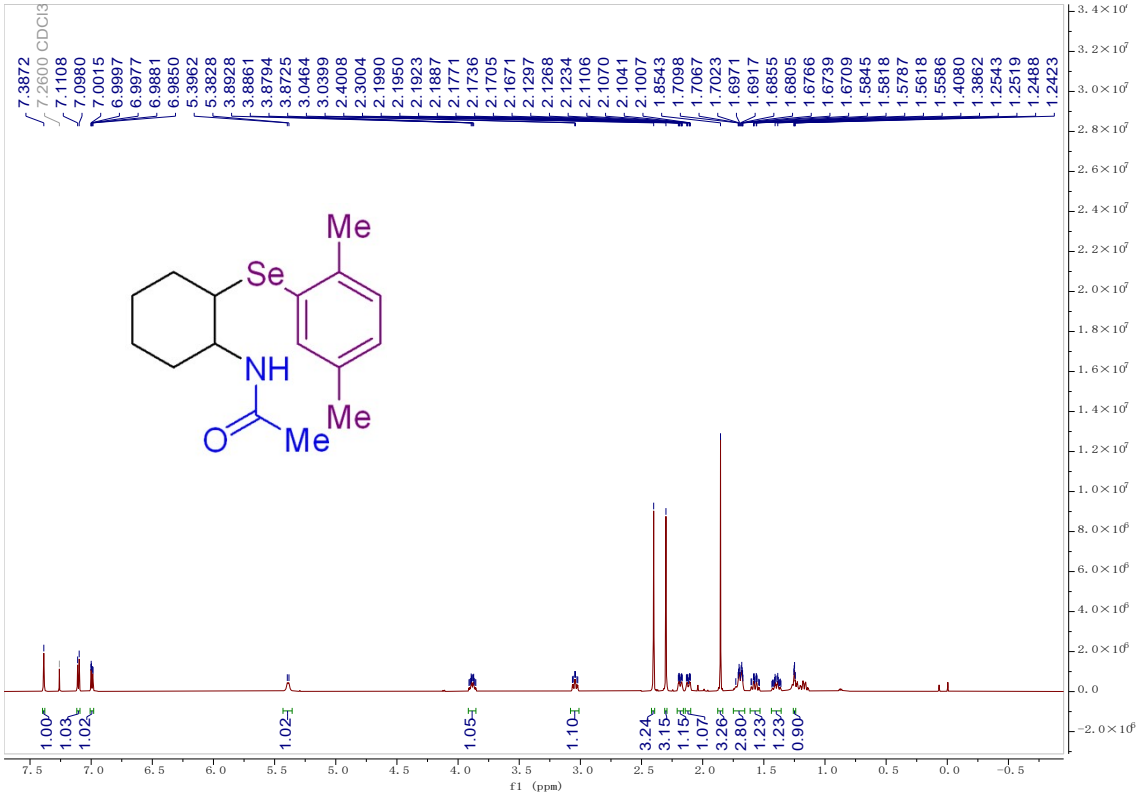
^{1}H NMR of product 3t in $CDCl_3$ (600 MHz)



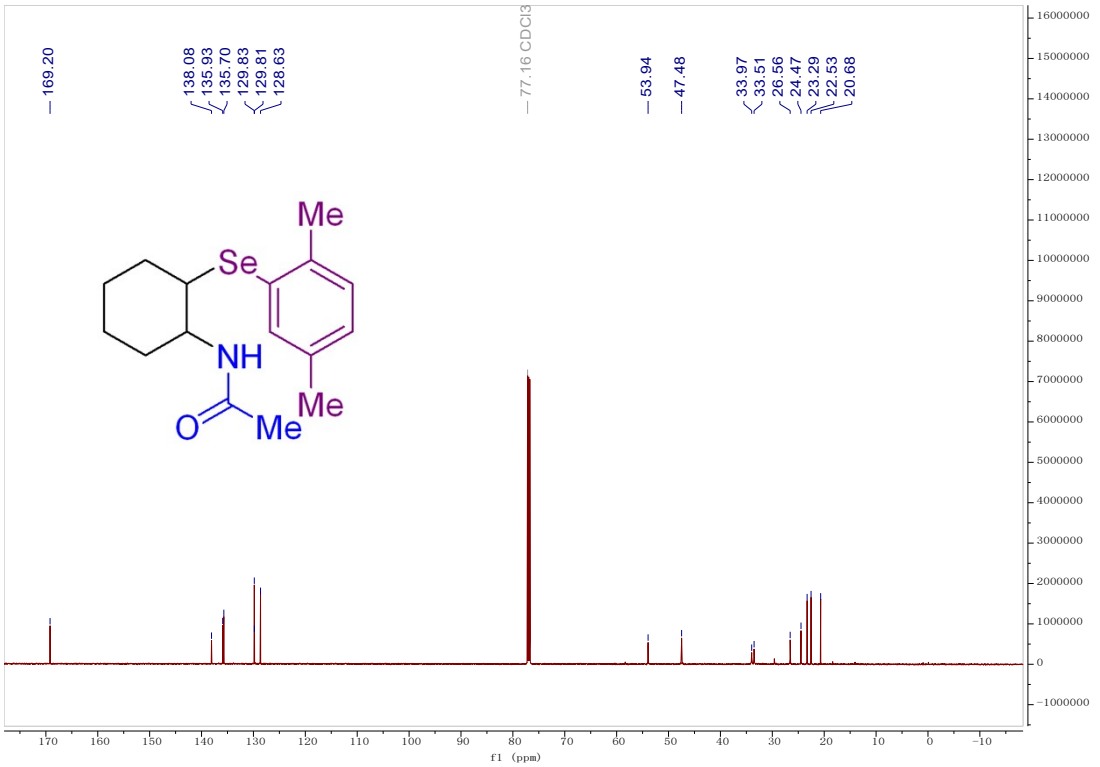
^{13}C NMR of product 3t in $CDCl_3$ (151 MHz)



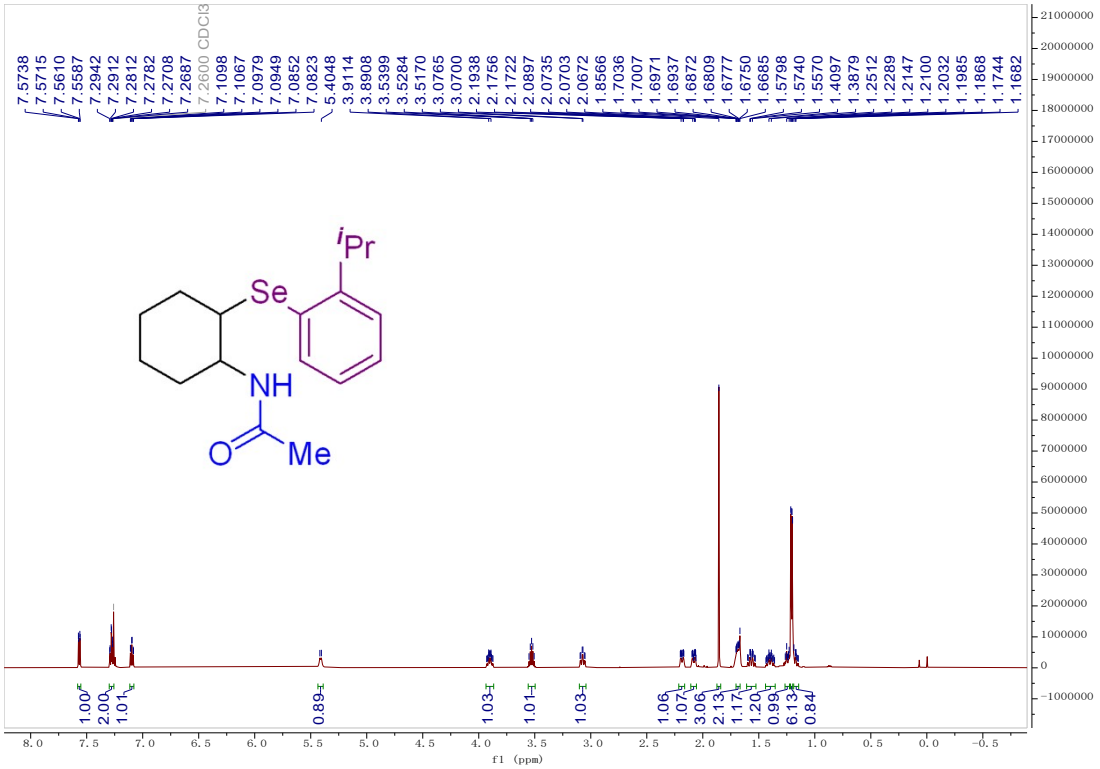
^{1}H NMR of product 3u in $CDCl_3$ (600 MHz)



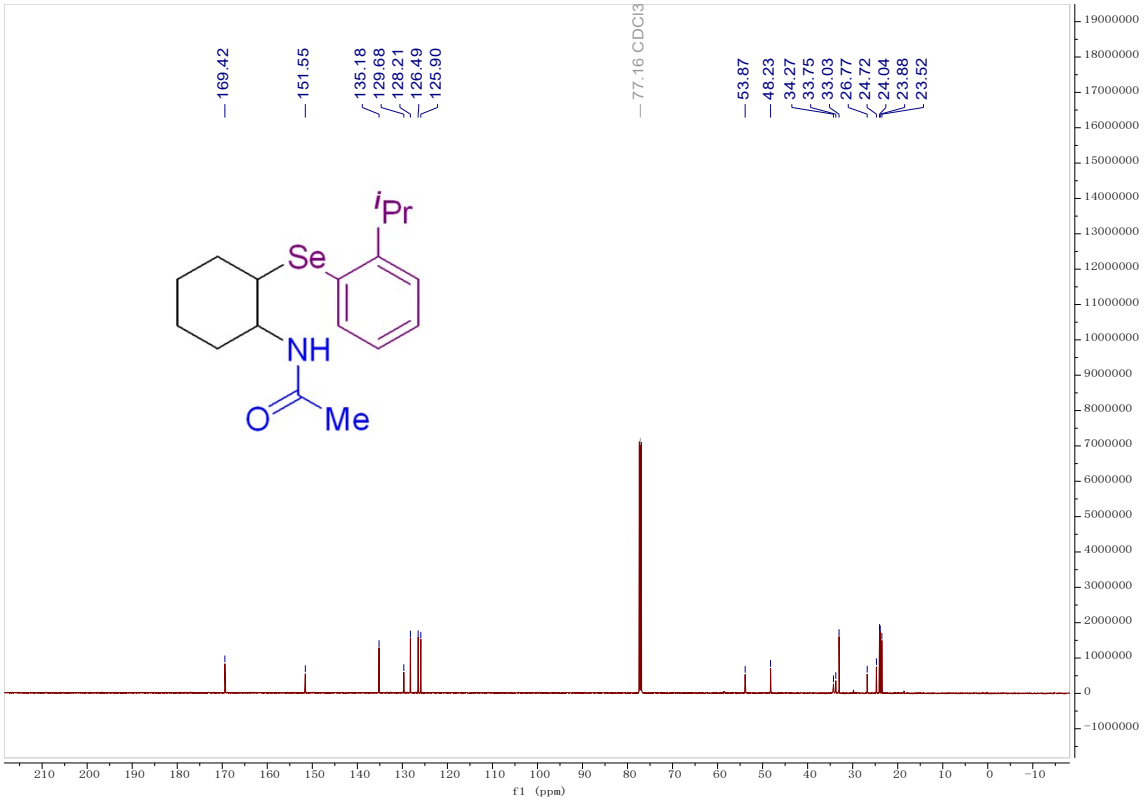
^{13}C NMR of product 3u in $CDCl_3$ (151 MHz)



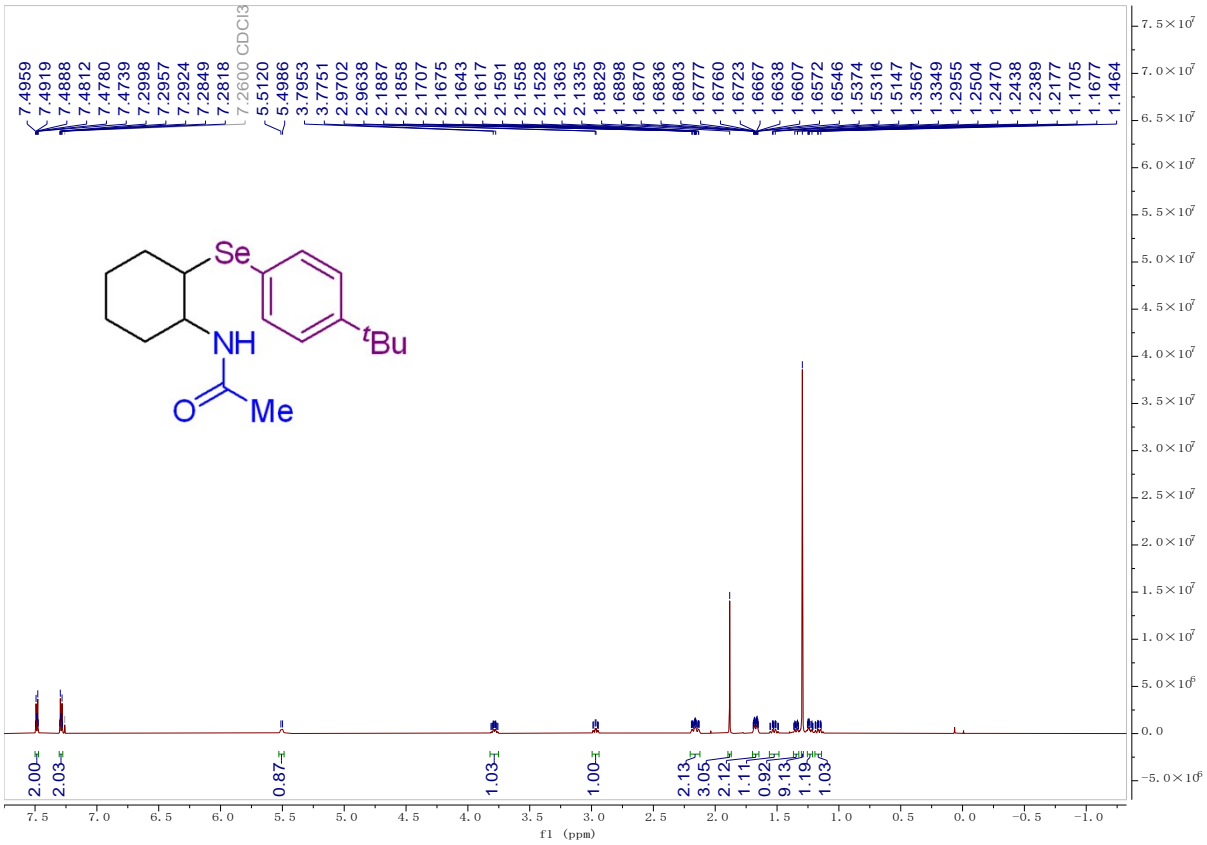
^{1}H NMR of product 3v in $CDCl_3$ (600 MHz)



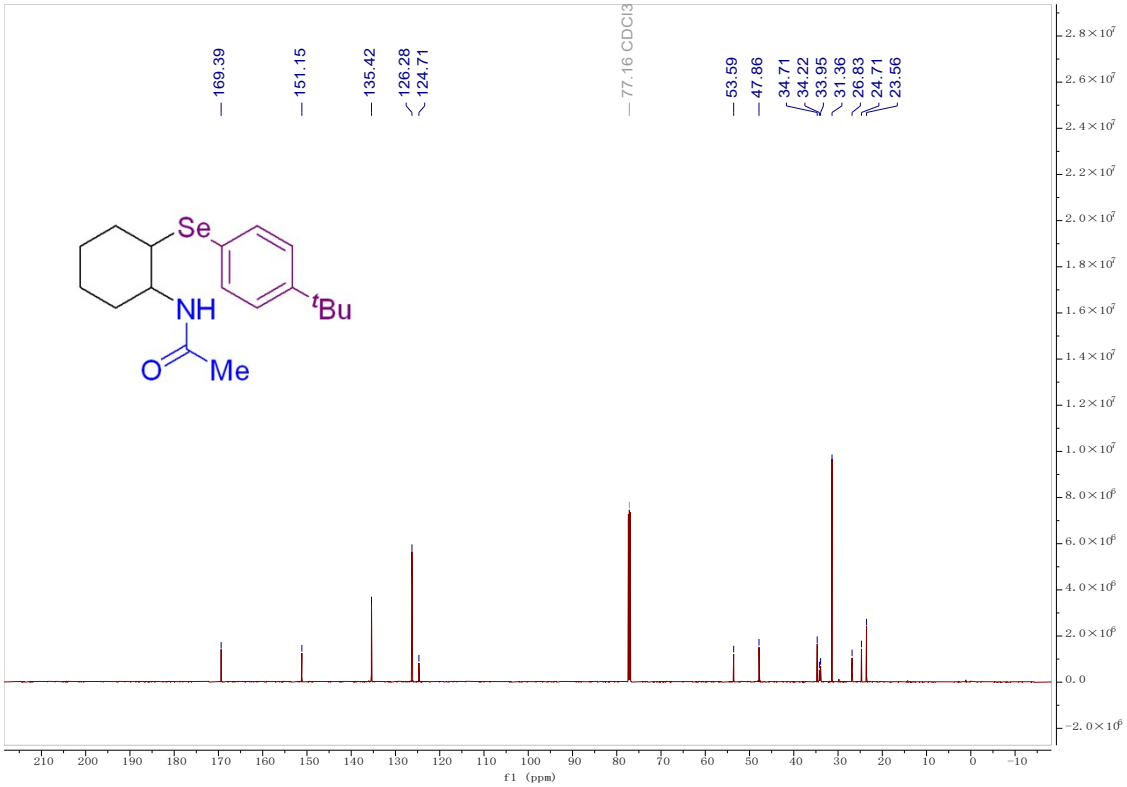
^{13}C NMR of product 3v in $CDCl_3$ (151 MHz)



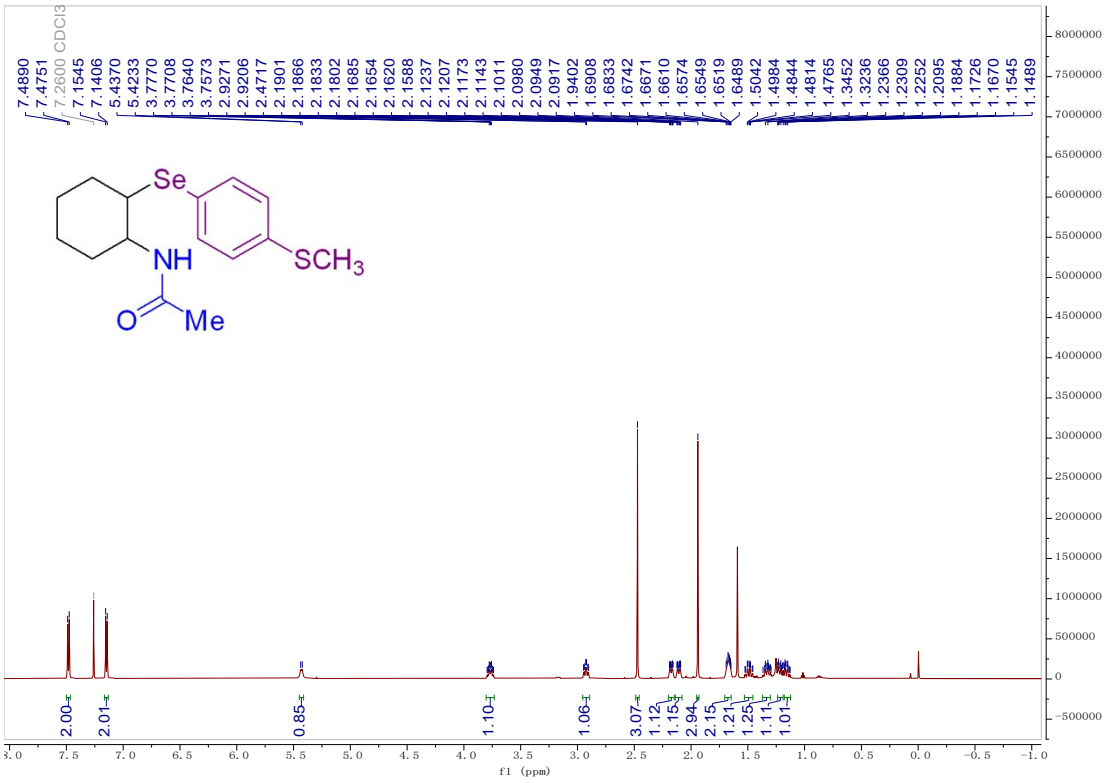
^{1}H NMR of product 3w in $CDCl_3$ (600 MHz)



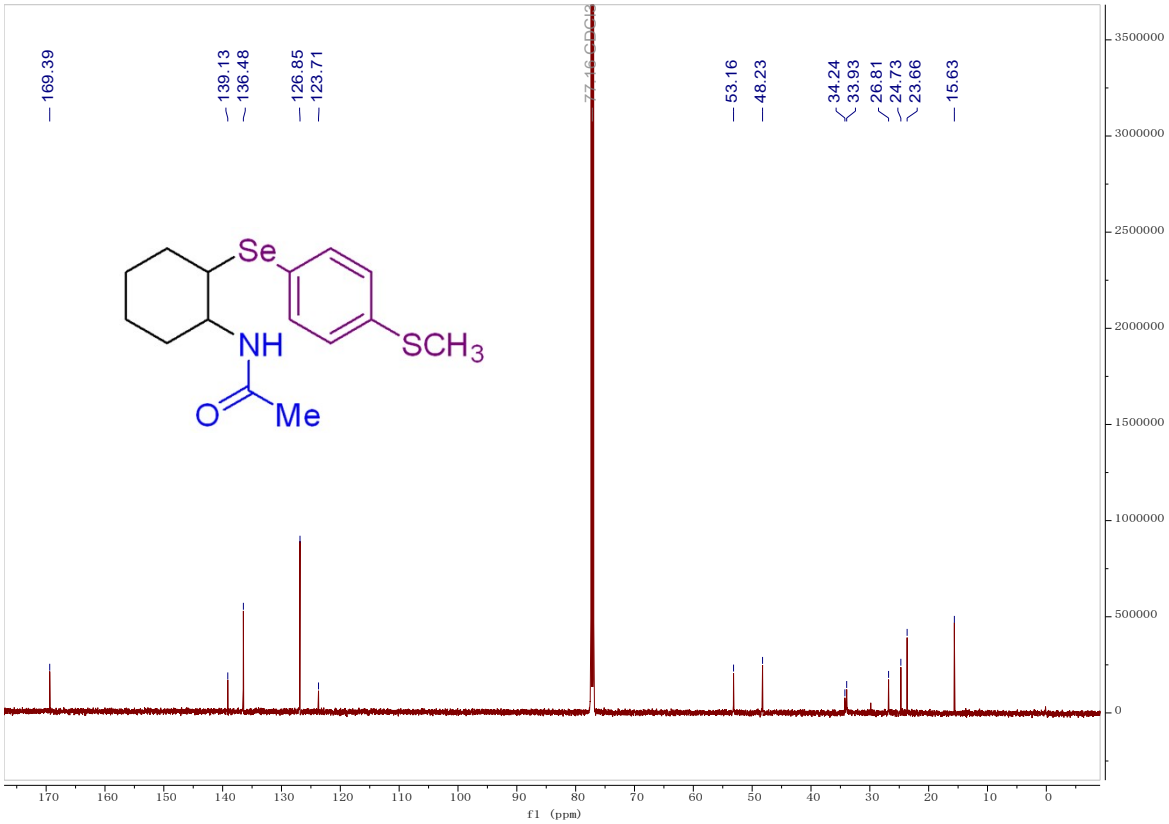
^{13}C NMR of product 3w in $CDCl_3$ (151 MHz)



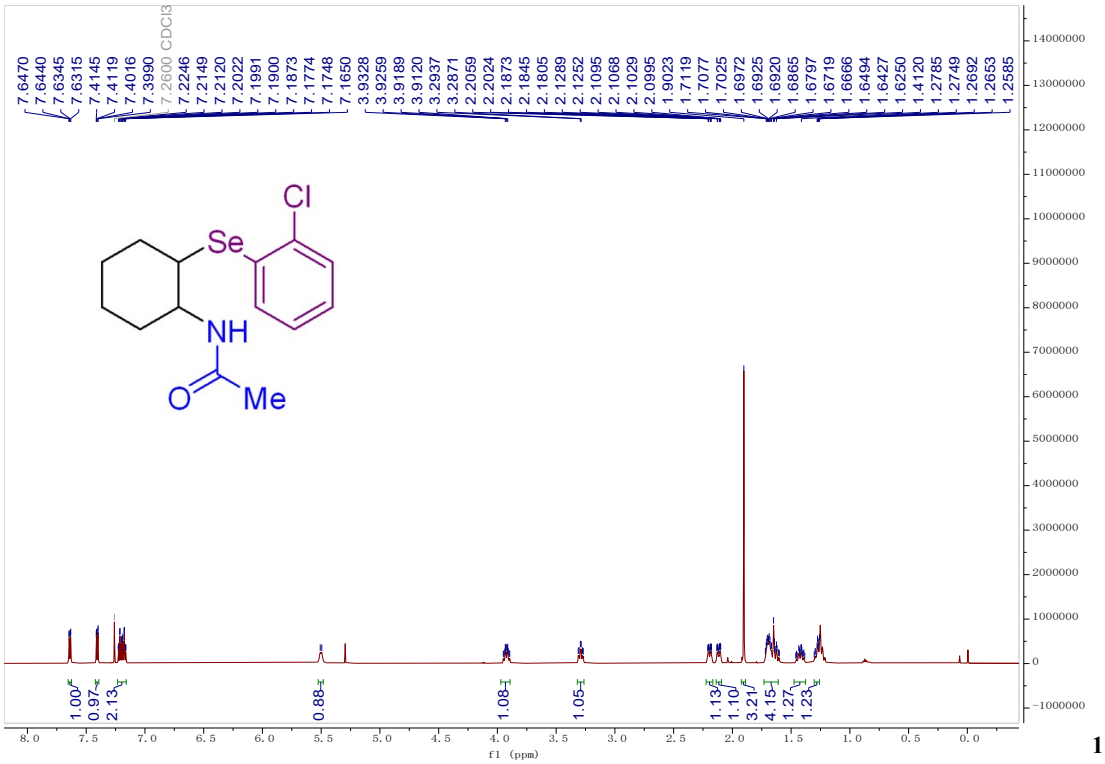
^{1}H NMR of product 3x in $CDCl_3$ (600 MHz)



^{13}C NMR of product 3x in $CDCl_3$ (151 MHz)



^{1}H NMR of product 3y in $CDCl_3$ (600 MHz)



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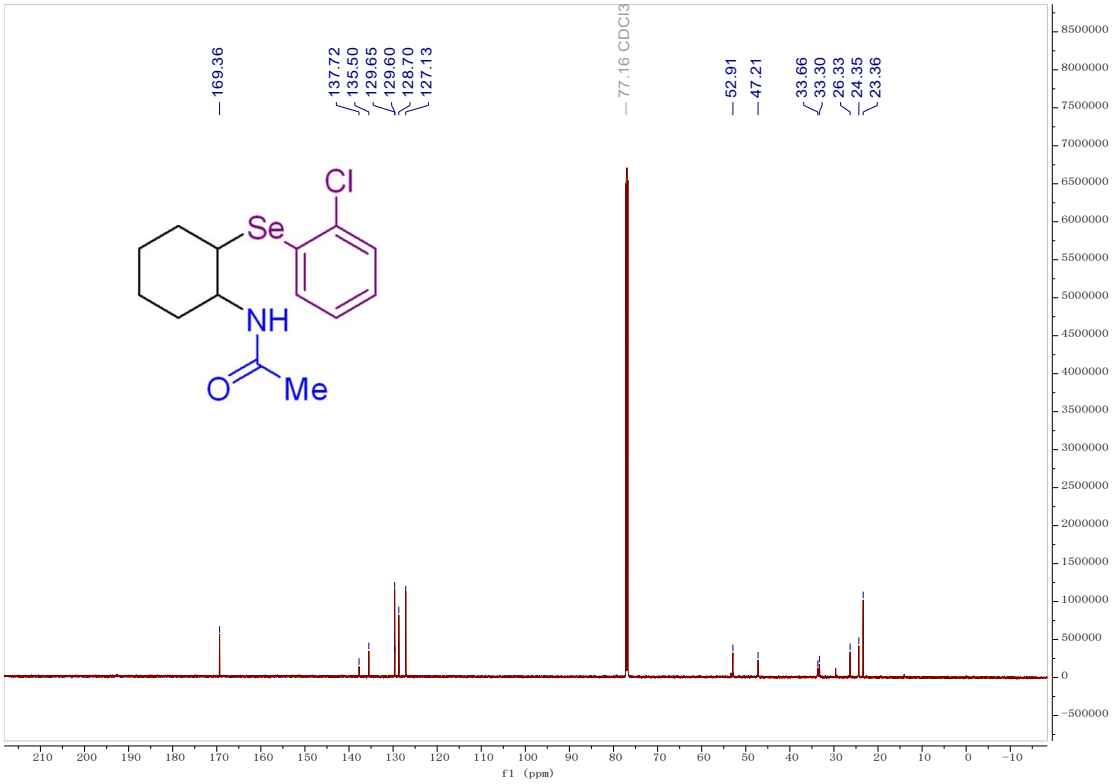
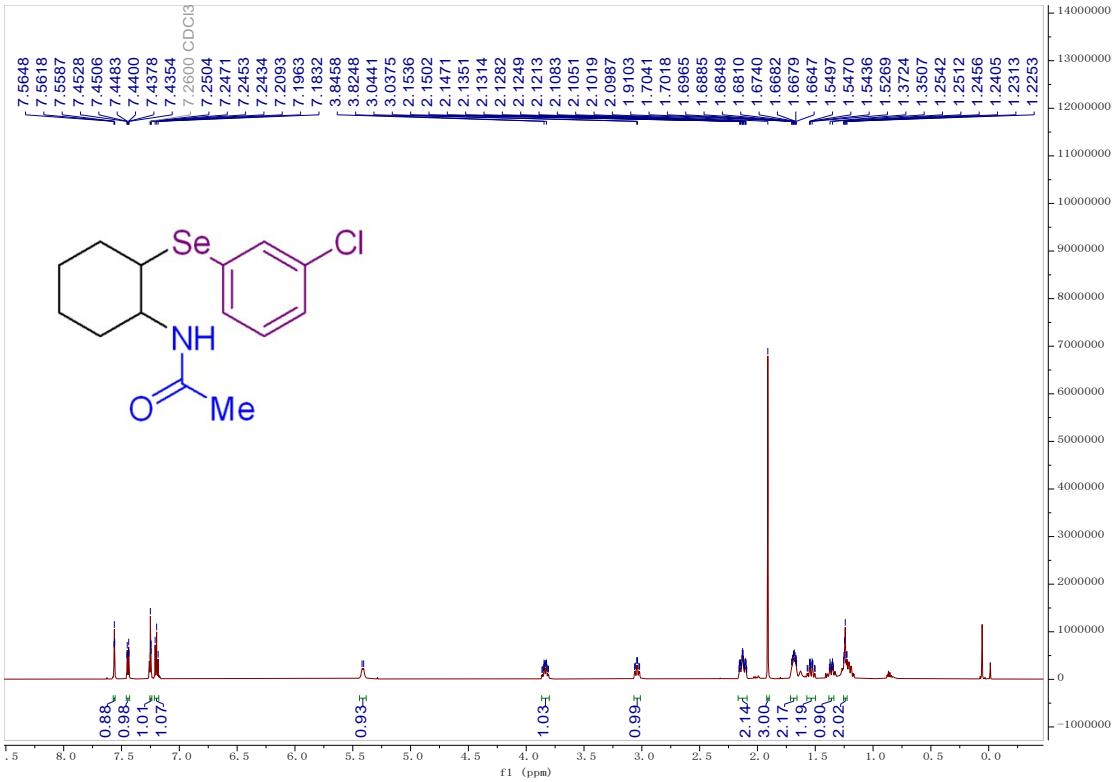
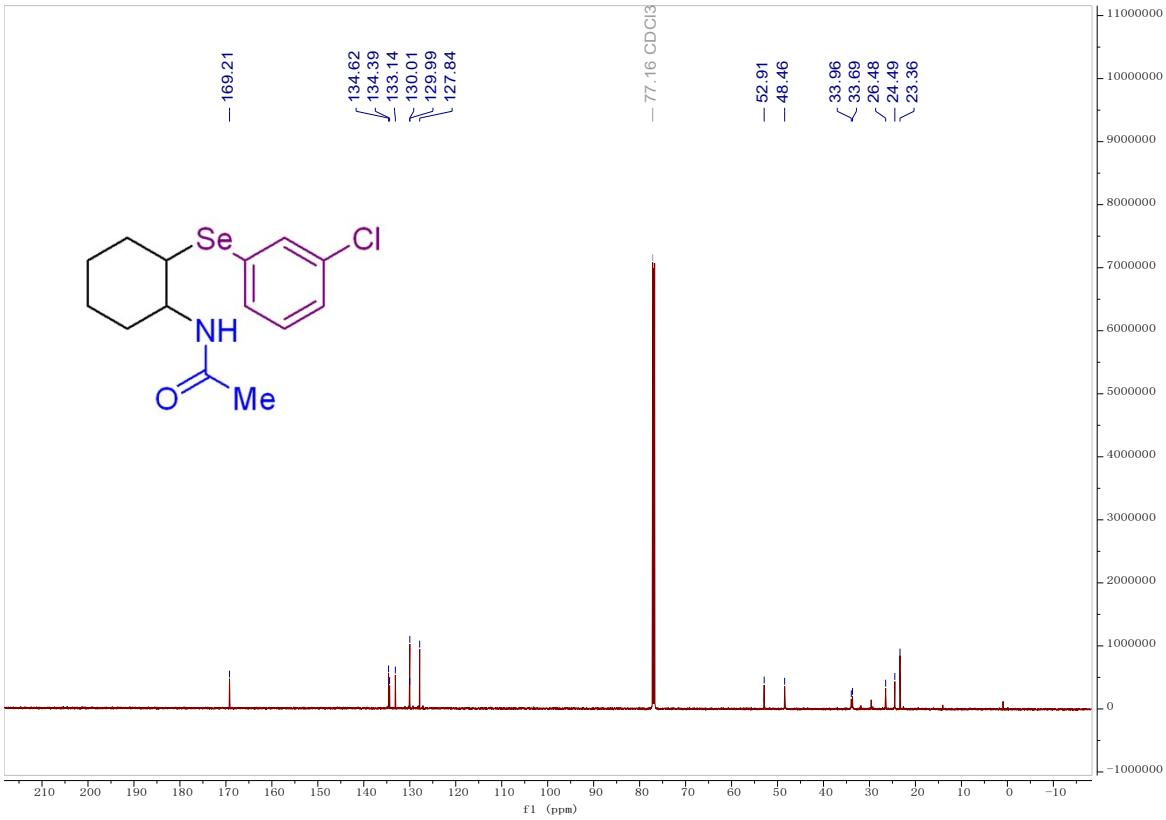
^{3}C NMR of product 3y in $CDCl_3$ (151 MHz)



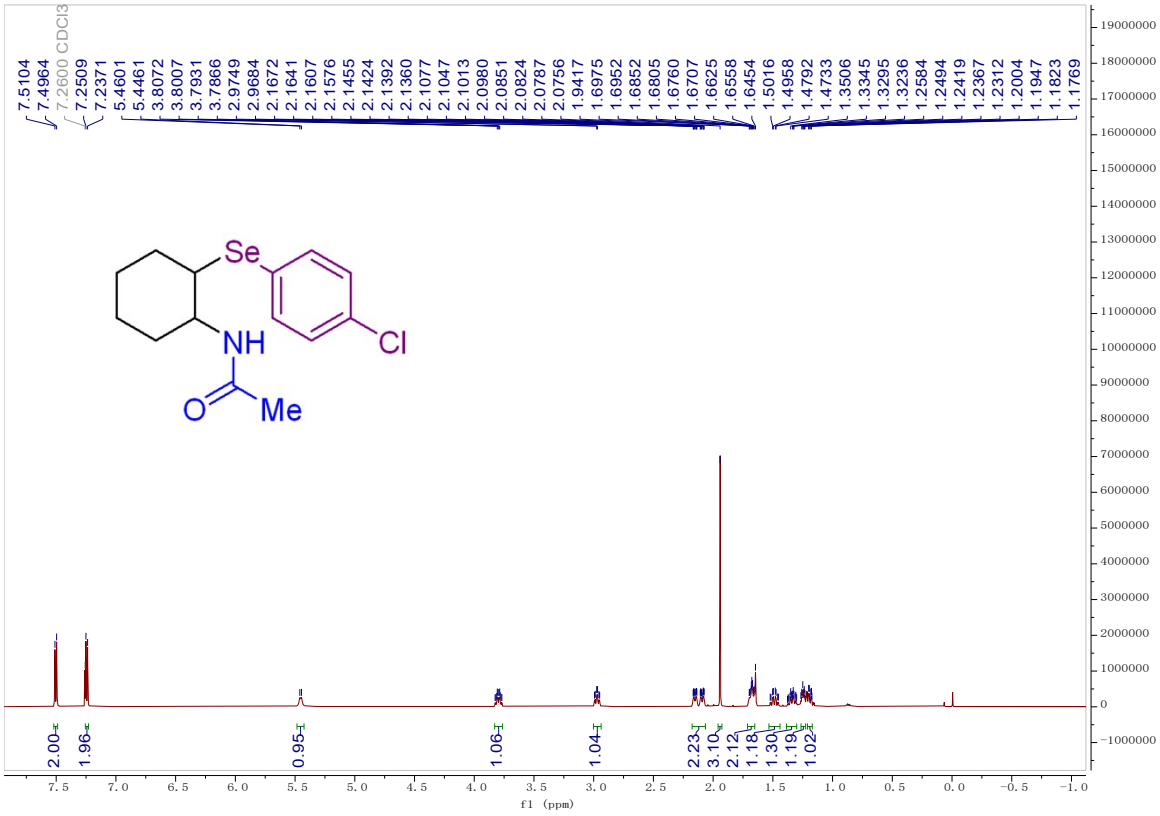
^{1}H NMR of product 3z in $CDCl_3$ (600 MHz)



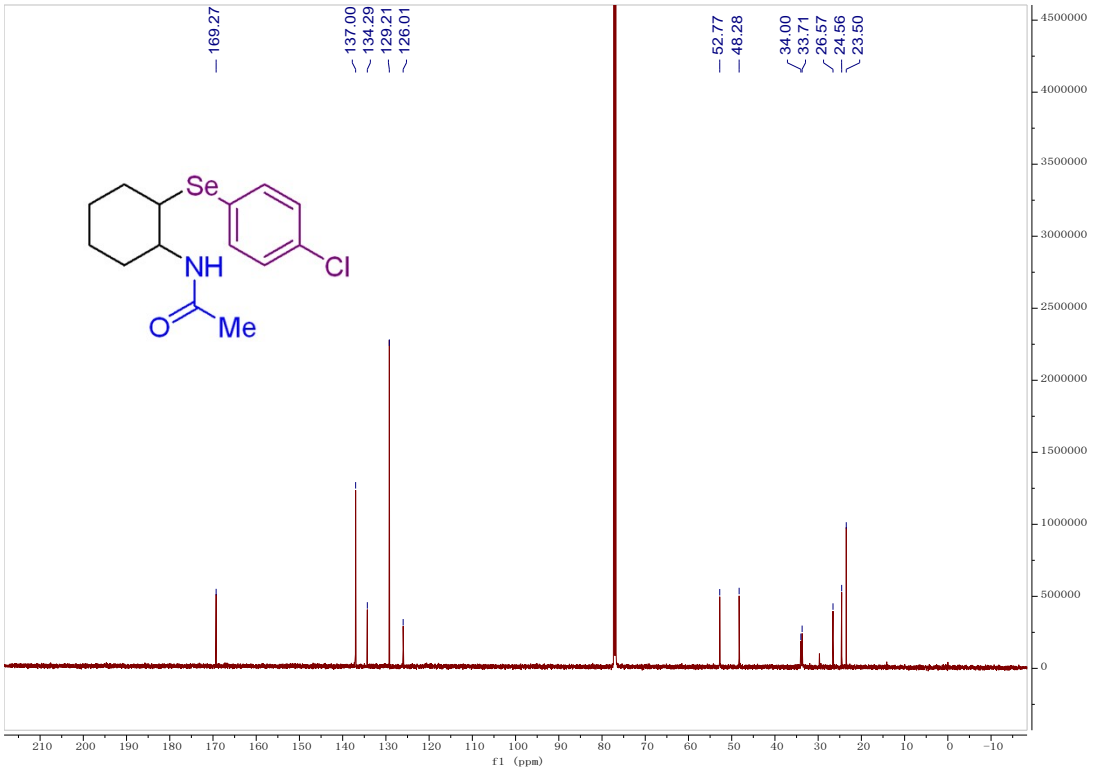
^{13}C NMR of product 3z in $CDCl_3$ (151 MHz)



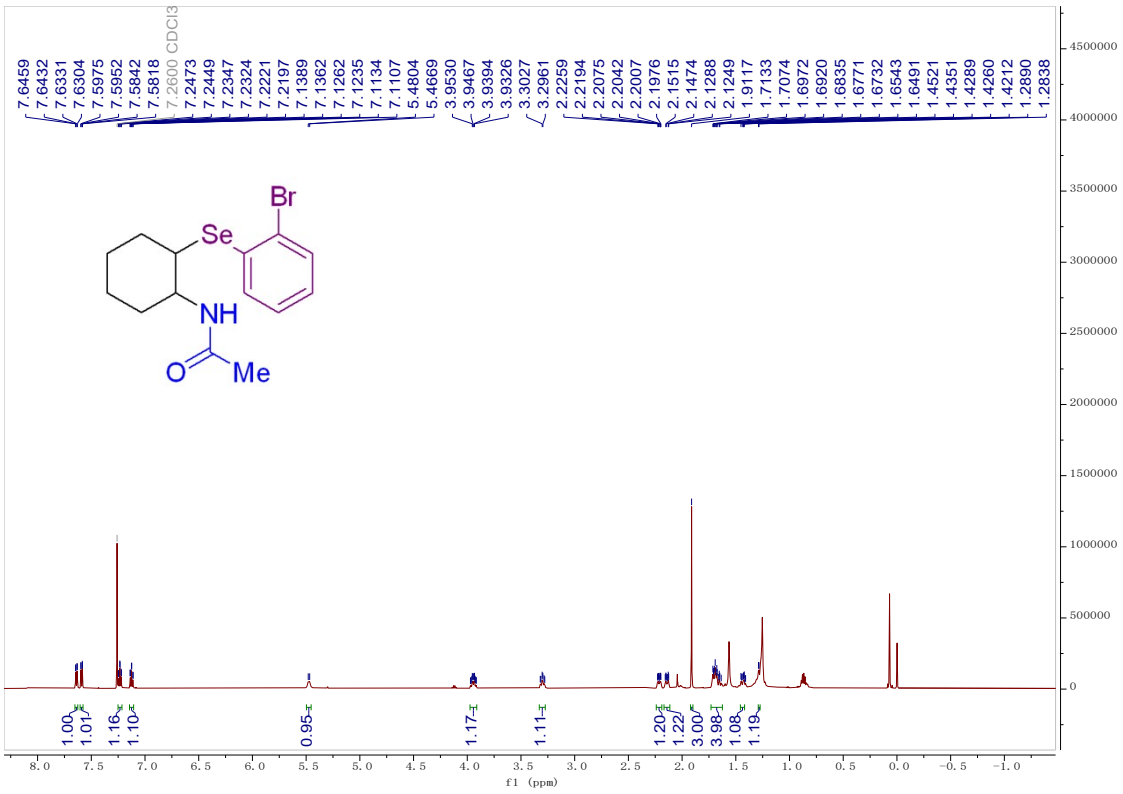
^{1}H NMR of product 3aa in $CDCl_3$ (600 MHz)



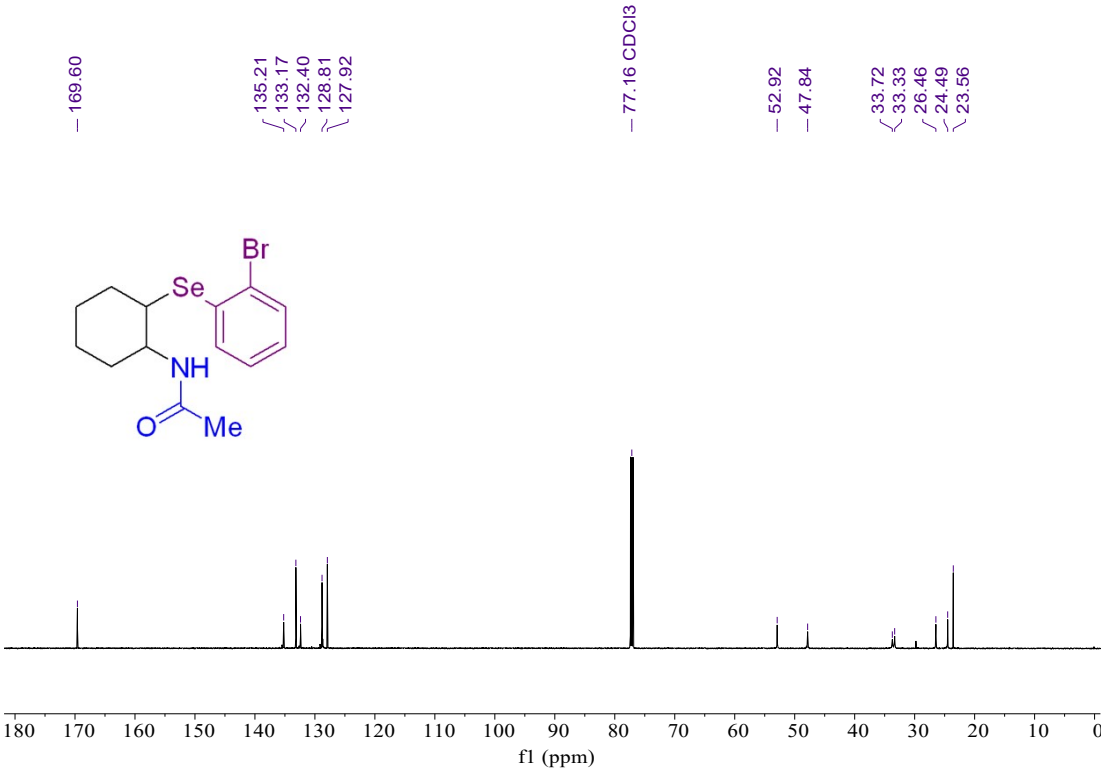
^{13}C NMR of product 3aa in $CDCl_3$ (151 MHz)



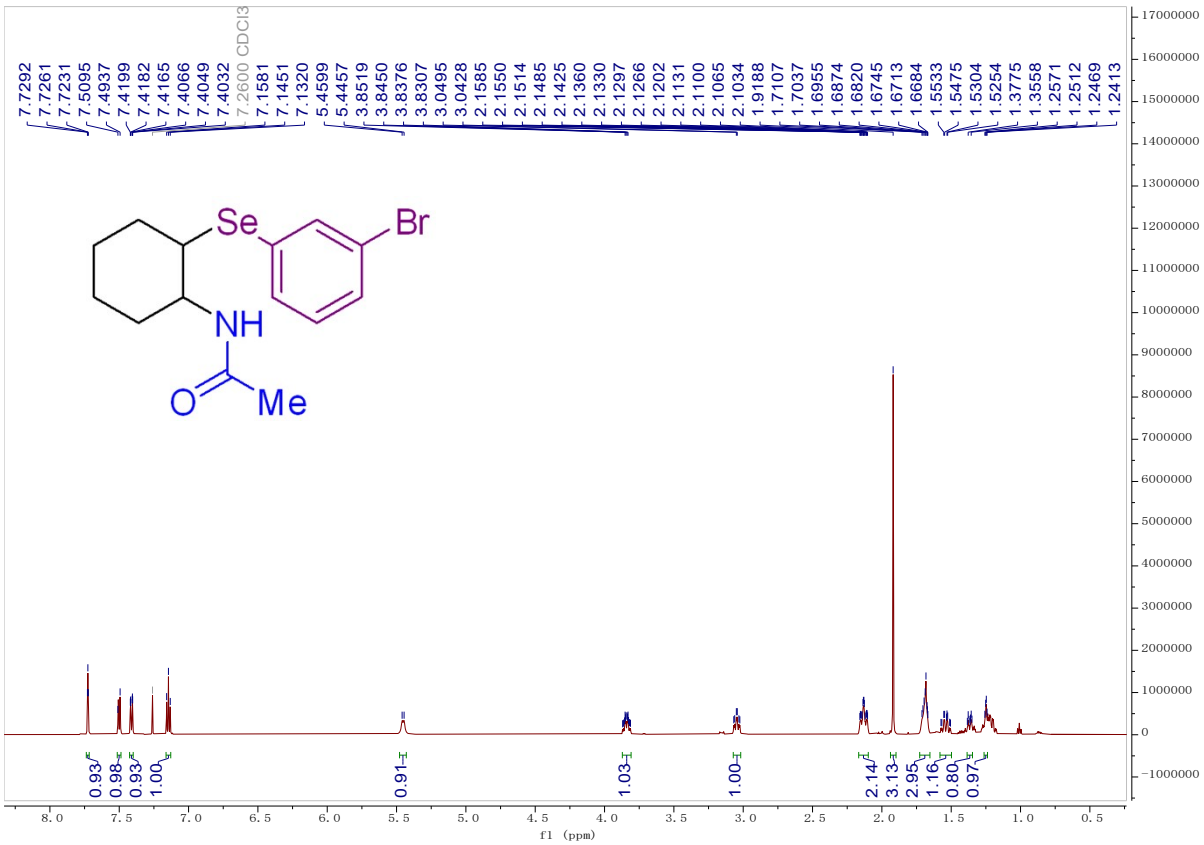
^{1}H NMR of product 3ab in $CDCl_3$ (600 MHz)



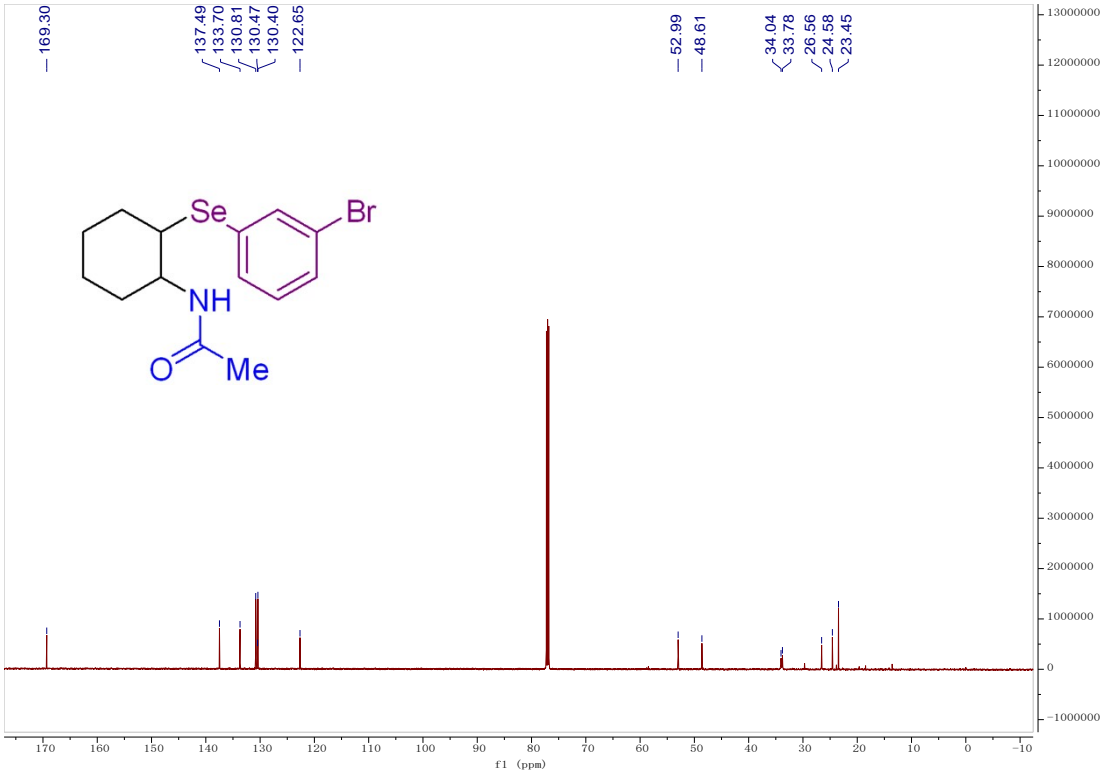
^{13}C NMR of product 3ab in $CDCl_3$ (151 MHz)



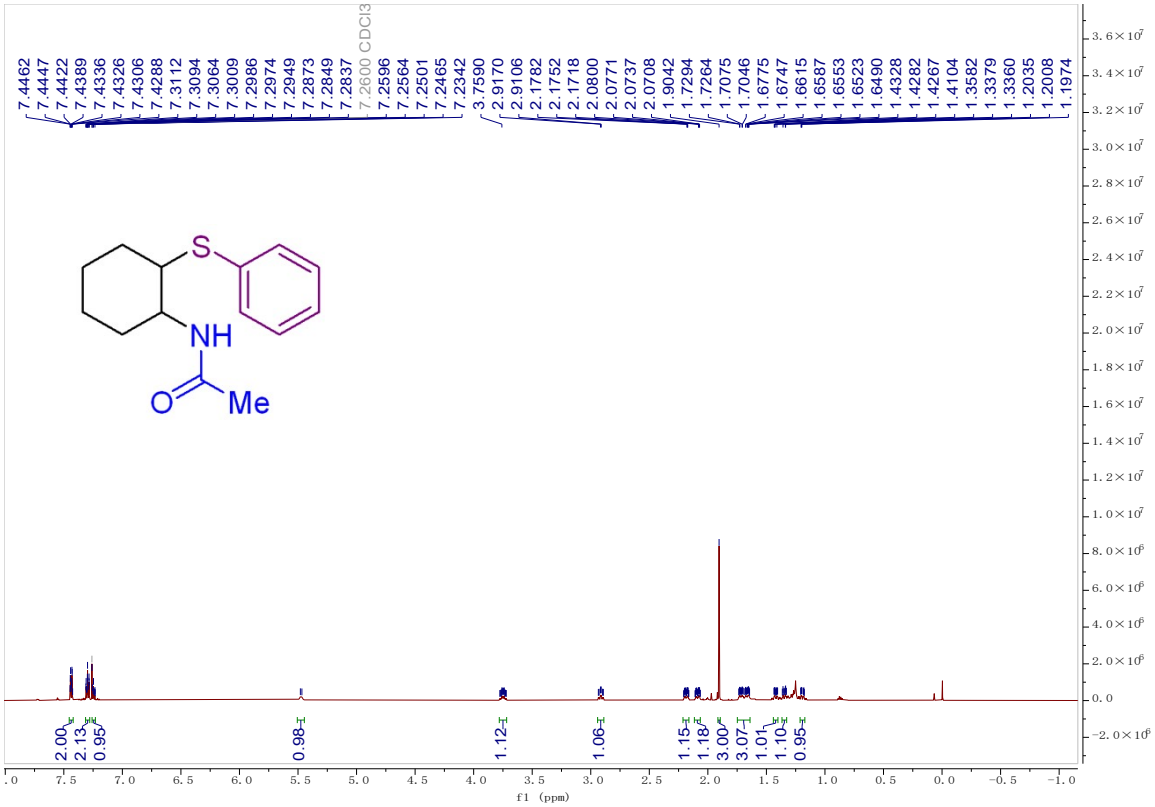
^{1}H NMR of product 3ac in $CDCl_3$ (600 MHz)



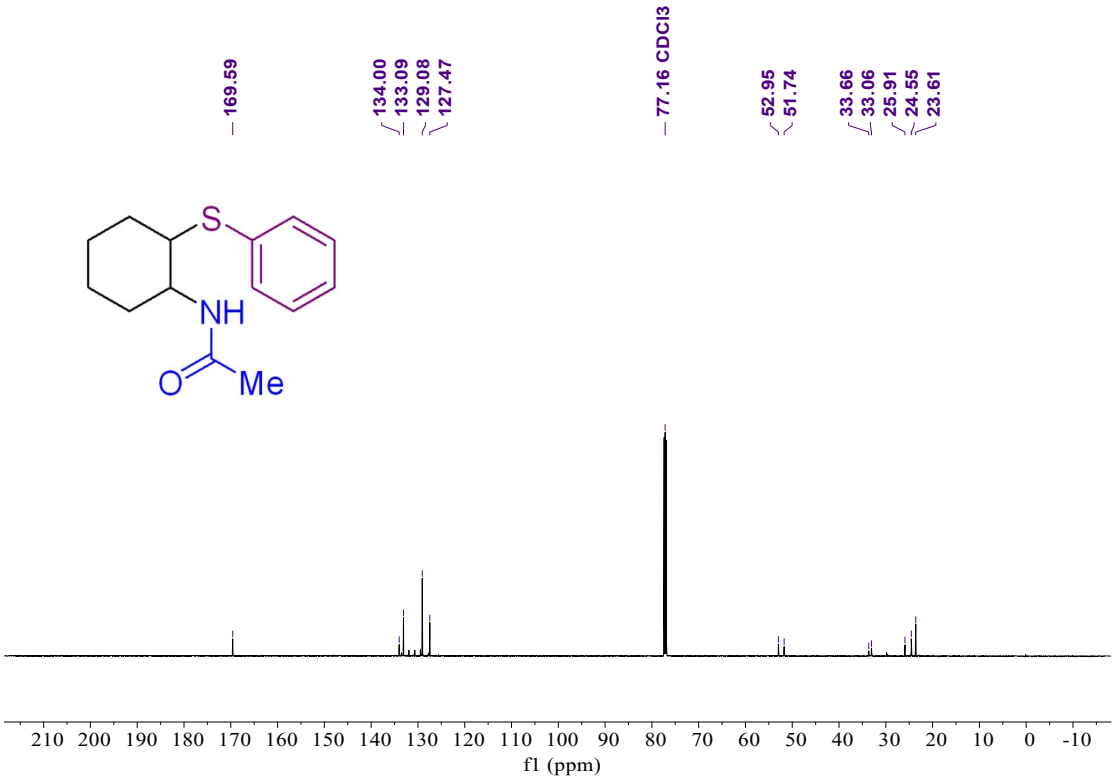
^{13}C NMR of product 3ac in $CDCl_3$ (151 MHz)



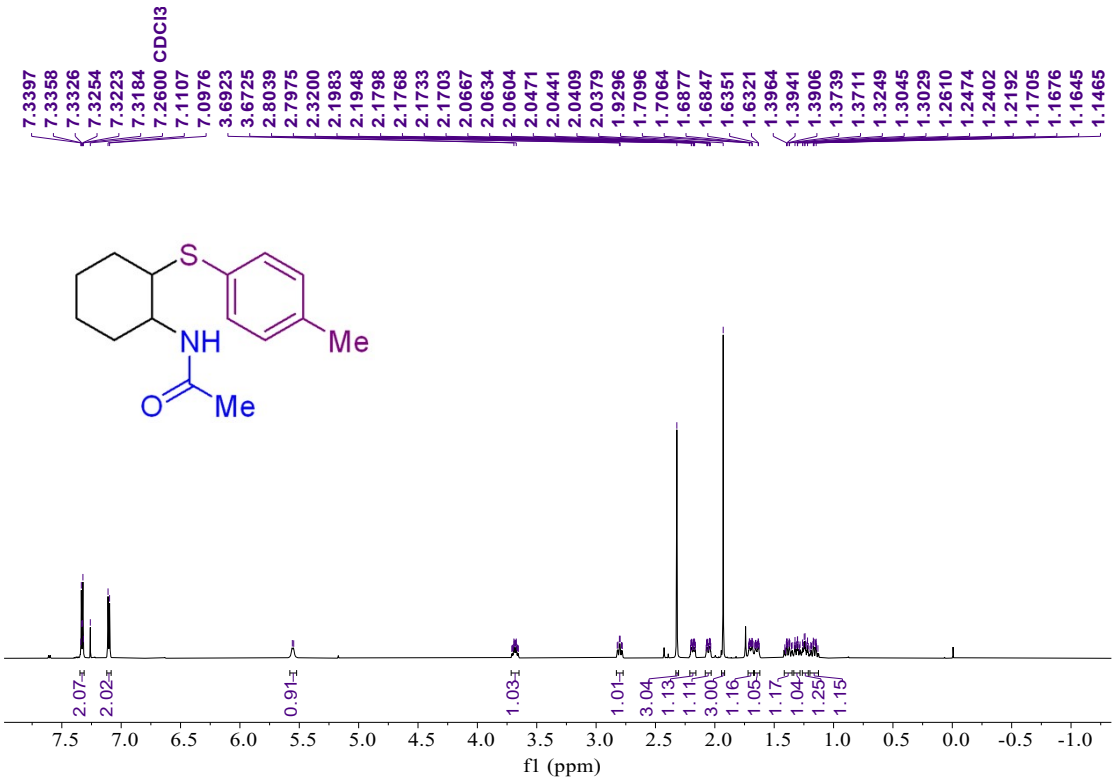
^{1}H NMR of product 3ad in $CDCl_3$ (600 MHz)



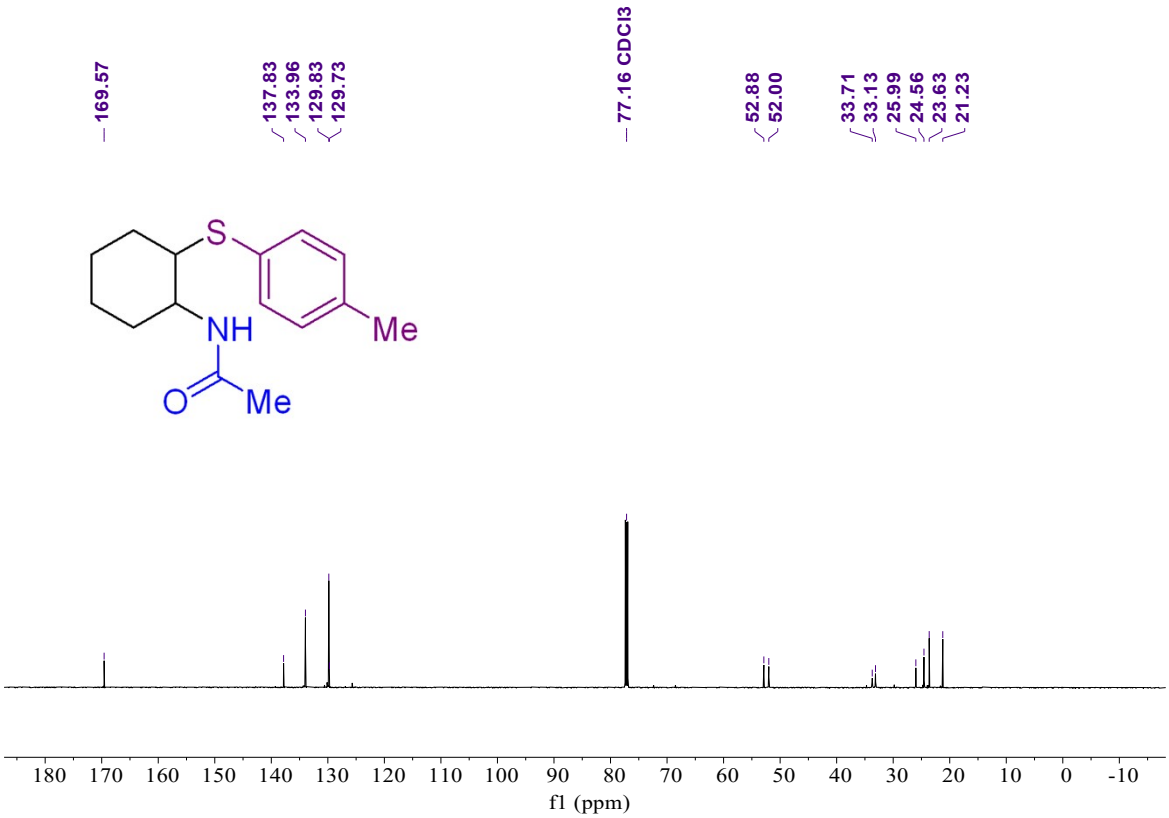
^{13}C NMR of product 3ad in $CDCl_3$ (151 MHz)



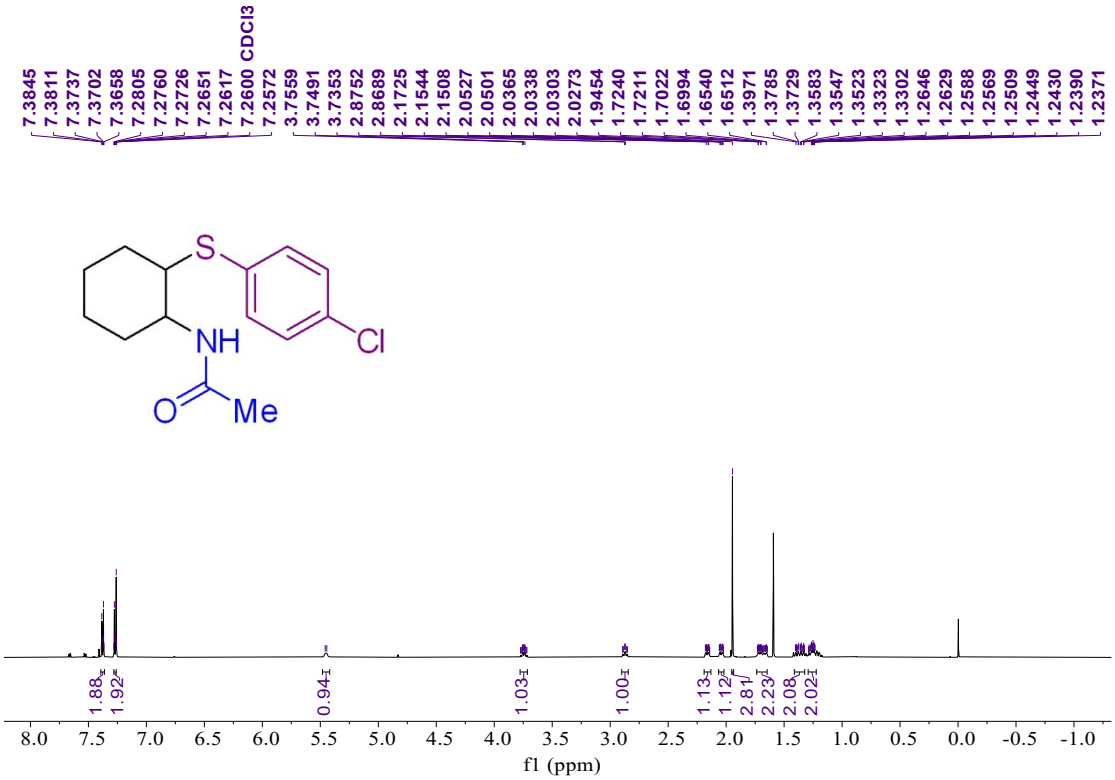
^{1}H NMR of product 3ae in $CDCl_3$ (600 MHz)



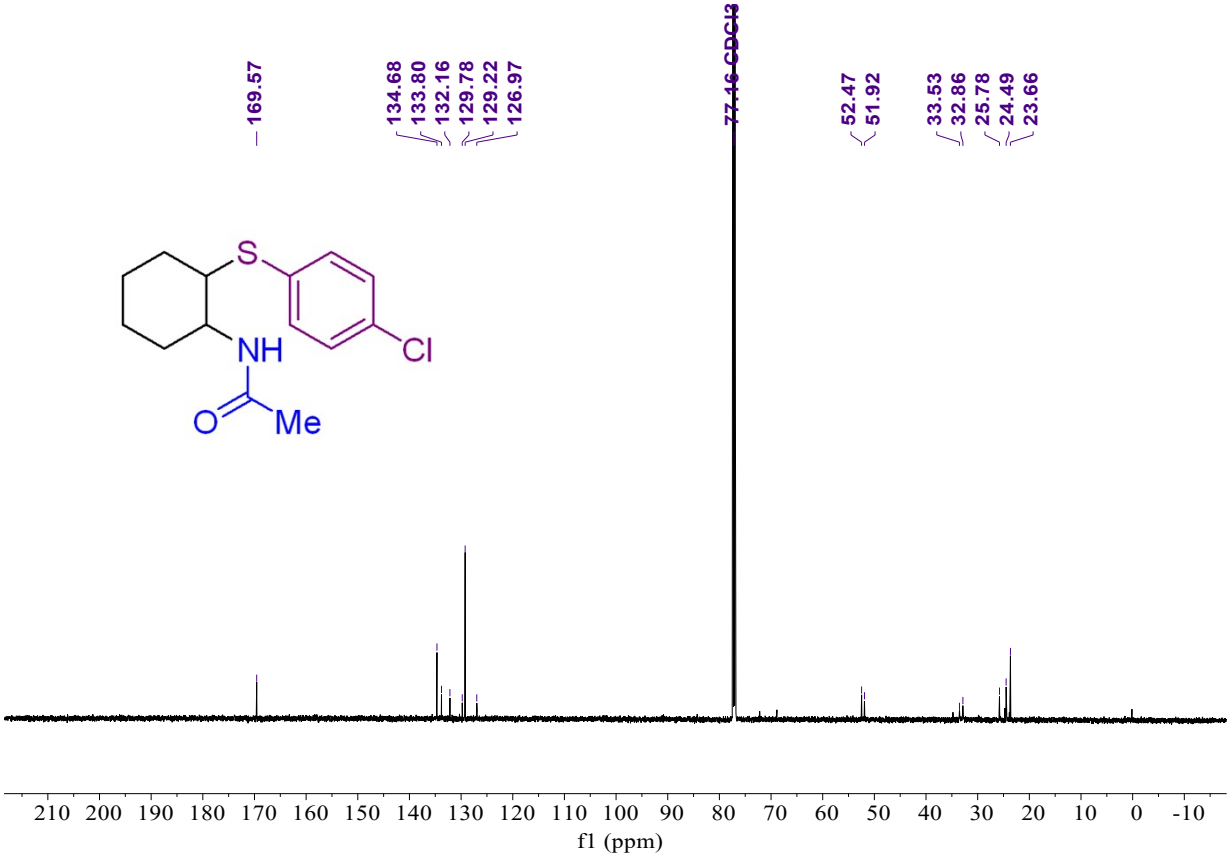
^{13}C NMR of product 3ae in $CDCl_3$ (151 MHz)



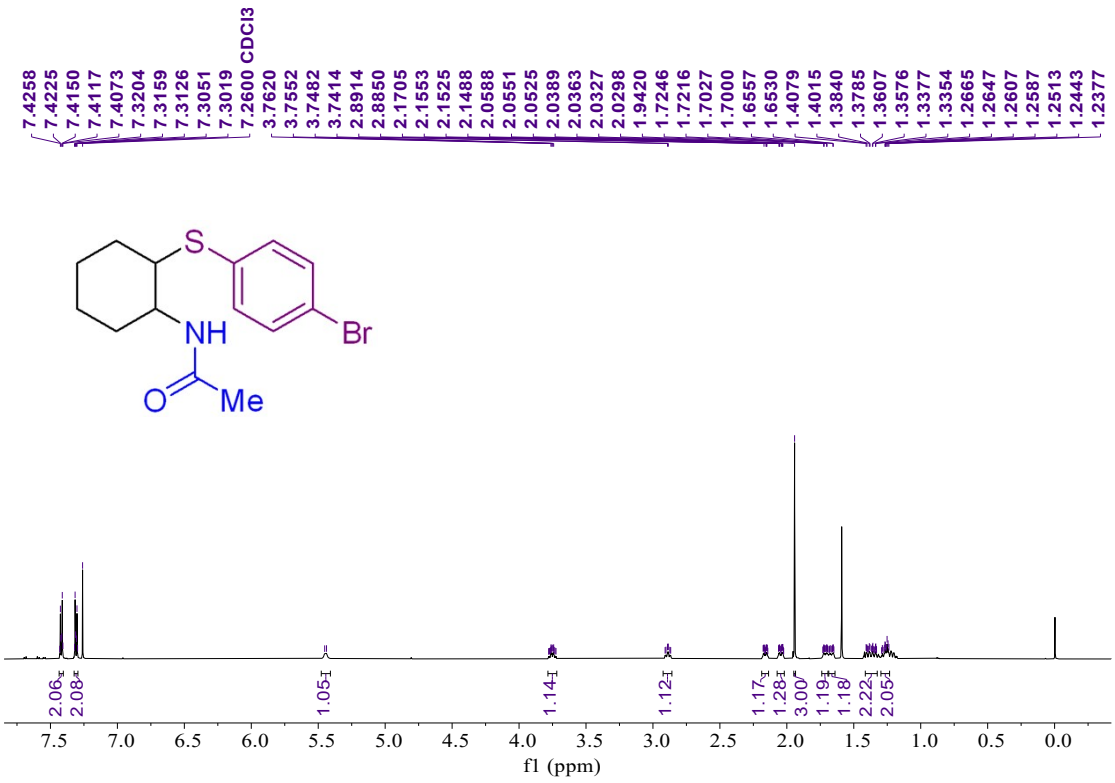
^{1}H NMR of product 3af in $CDCl_3$ (600 MHz)



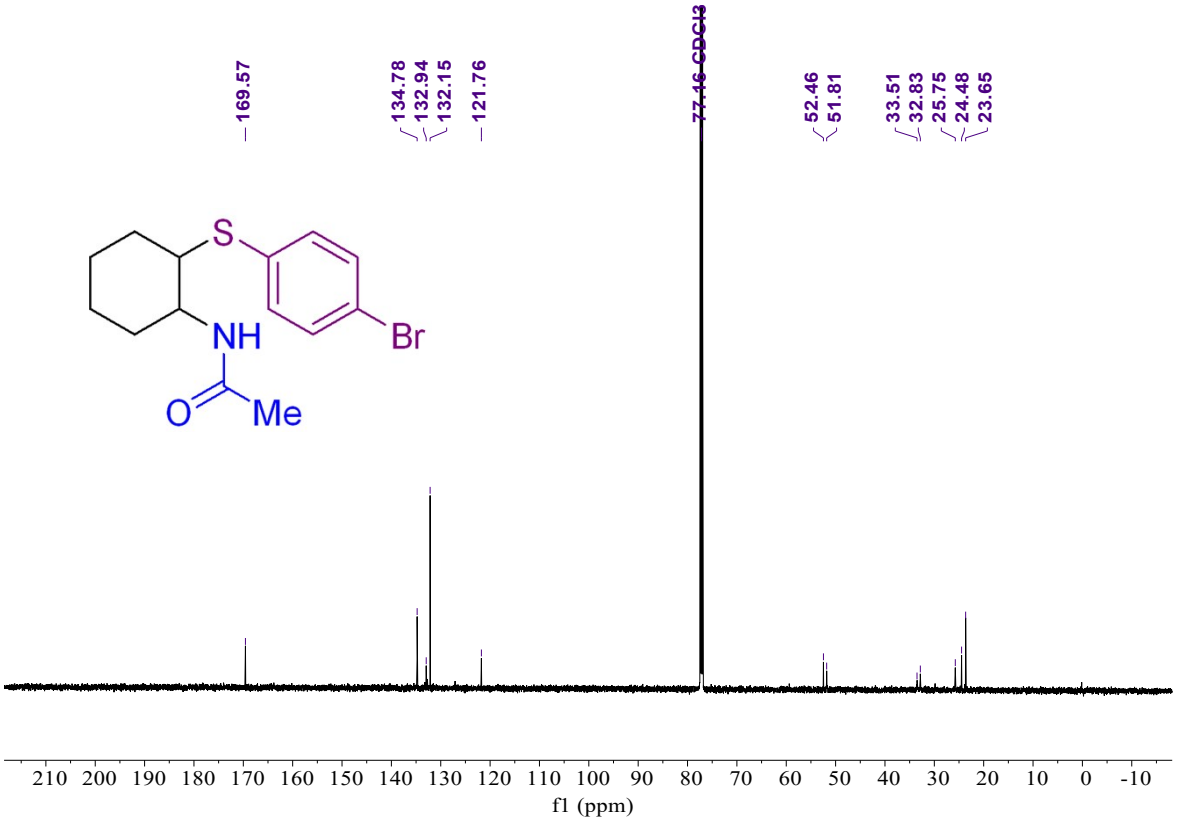
^{13}C NMR of product 3af in $CDCl_3$ (151 MHz)



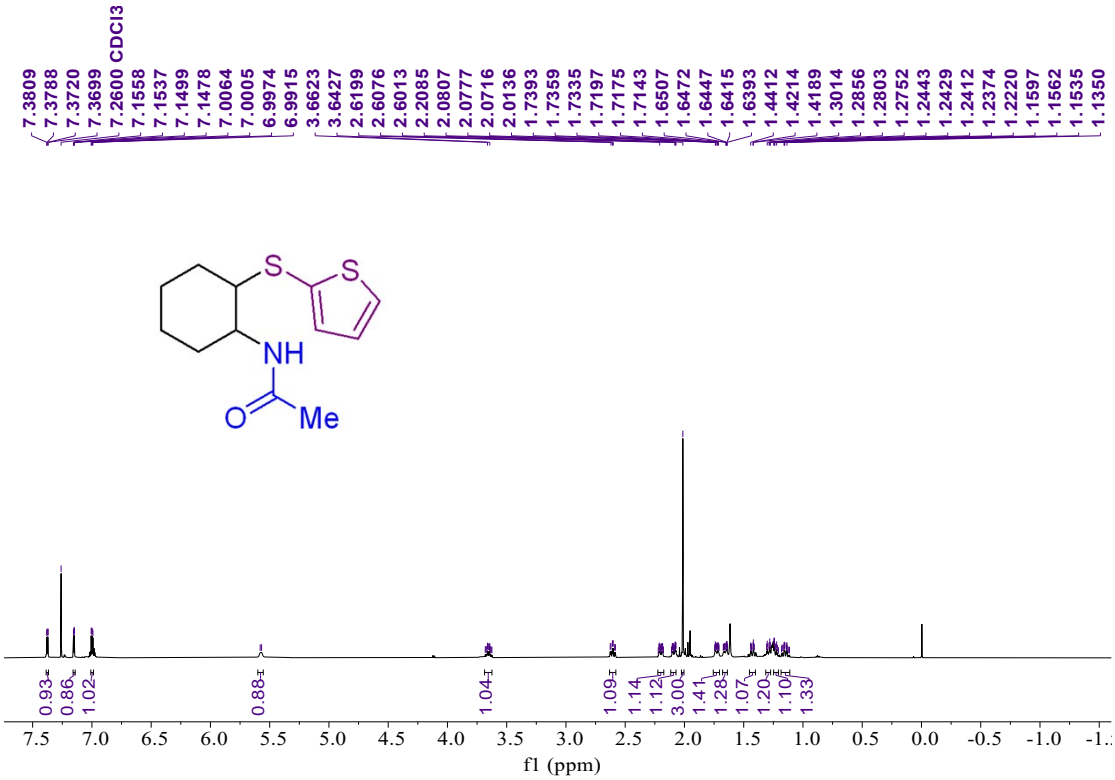
^{1}H NMR of product 3ag in $CDCl_3$ (600 MHz)



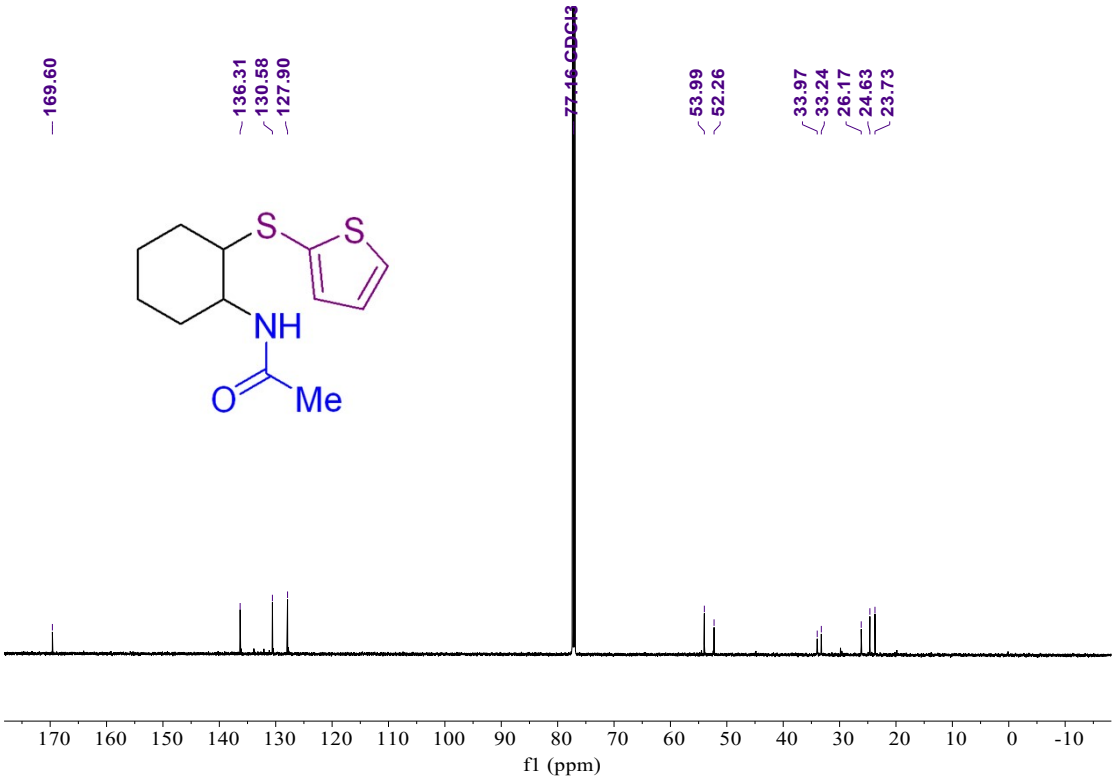
^{13}C NMR of product 3ag in $CDCl_3$ (151 MHz)



^{1}H NMR of product 3ah in $CDCl_3$ (600 MHz)



^{13}C NMR of product 3ah in $CDCl_3$ (151 MHz)


169.60
136.31
130.58
127.90
77.16 CDCl3
53.99
52.26
33.97
33.24
26.17
24.63
23.73
S
S
NH
O
Me
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)