Supporting Information for

Electrochemical Regioselective Selenylation/Oxidation of *N*-Alkylisoquinolinium Salts via Double C(sp2)−H Bond Functionalization

Xiang Liu,† Yajun Wang,† Dan Song, Yuhan Wang, and Hua Cao *

School of Chemistry and Chemical Engineering and Guangdong Cosmetics Engineering & Technology Research Center, Guangdong Pharmaceutical University, Zhongshan 528458, P. R. of China

E-mail: caohua@gdpu.edu.cn

Table of Contents:

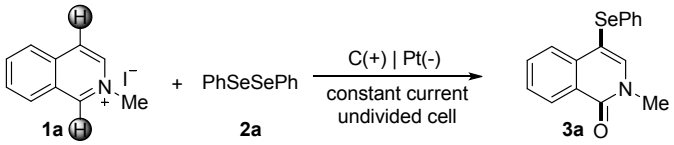
1. General considerations

^{1}H and ^{13}C NMR spectra were recorded using a Bruker DRX-400 spectrometer using $CDCl_3$ as solvent. Chemical shifts were recorded in parts per million (ppm, δ) relative to tetramethylsilane (δ 0.00) or chloroform (δ = 7.26, singlet). The data of HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). IR spectra were obtained either as potassium bromide pellets or as liquid films between two potassium bromide pellets with a Bruker TENSOR 27 spectrometer. Melting points were determined with a Büchi Melting Point B-545 instrument. The instrument for electrolysis is dual display potentiostat (CHI 660E) (made in China). The anode electrode is vitreous carbon plate (10 mm×10 mm×1 mm) and cathodic electrode was platinum plate (10 mm×10 mm×0.1 mm). Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification.

2. Experimental procedures and characterization data

2.1 Conditions optimization

Table S1. Optimization of reaction conditions[a]



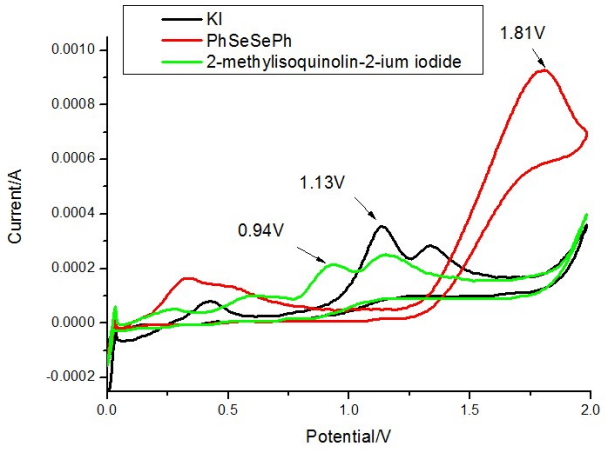
entry	solvent	electrolyte	base	yield [b](%)
1	CH_3CN/H_2O [c]	KI	/	n. d.
2	CH_3CN/H_2O [c]	KI	Na_2CO_3	55
3	CH_3CN/H_2O [c]	KI	KH_2PO_4	72
4	CH_3CN/H_2O [c]	KI	K_2CO_3	60
5	CH_3CN/H_2O [c]	KI	Cs_2CO_3	74
6	CH_3CN/H_2O [c]	KBr	Cs_2CO_3	66
7	CH_3CN/H_2O [c]	NH_4I	Cs_2CO_3	27
8	CH_3CN/H_2O [c]	$^nBu_4NI$	Cs_2CO_3	45
9	CH_3CN/H_2O [c]	$^nBu_4NBF_4$	Cs_2CO_3	35
10	CH_3CN/H_2O [c]	Et_4NPF_6	Cs_2CO_3	15
11	THF/H_2O [c]	KI	Cs_2CO_3	31
12	DMF/H_2O [c]	KI	Cs_2CO_3	n. d.
13	CH_3CN	KI	Cs_2CO_3	55
14 [d]	**CH_3CN/H_2O** [c]	**KI**	**Cs_2CO_3**	**83**
15 [d,e]	CH_3CN/H_2O [c]	KI	Cs_2CO_3	50
16 [d,f]	CH_3CN/H_2O [c]	KI	Cs_2CO_3	n. d.

[a] Standard conditions: vitreous carbon plate anode (10 mm × 10 mm × 1 mm), platinum plate cathode (10 mm × 10 mm × 0.1 mm), constant current = 10 mA, **1a** (0.1 mmol), **2a** (0.1 mmol), electrolyte (0.5 mmol), base (0.15 mmol), solvents (5.0 mL), undivided cell, open to air, r.t., 10 h. [b] Determined by GC analysis, n. d. = not detected. [c] Solvent/H_2O = 4: 1. [d] O_2 atmosphere. [e] Constant current = 5 mA. [f] No electric current.

2.2 Cyclic voltammetry

Cyclic voltammetry was performed in a three-electrode cell connected to a schlenk line under nitrogen at room temperature. The working electrode was a steady vitreous carbon plate electrode, the counter electrode was a platinum plate. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution, and separated from reaction by a salt bridge. Then 10 mL electrolyte solution containing 0.05 M *n*-Bu_4NPF_6 in CH_3CN was poured into electrochemical cell. The concentration of samples was 0.01 M. The scan rate was 0.1 V/s, ranging from -0.5 V to 2.0 V.

Figure S1. Cyclic voltammetry of 2-methylisoquinolin-2-ium iodide **1a**, KI and diphenyl diselenide **2a**



2.3 Spectroscopic data

Considering the practical applications as fluorescent materials of many isoquinolone derivatives, it is important to know the spectral property of selenide isoquinolones prepared by present method. So, a series of photophysical experiments of compound **3l** were carried out (Table S2 and Figure S2).

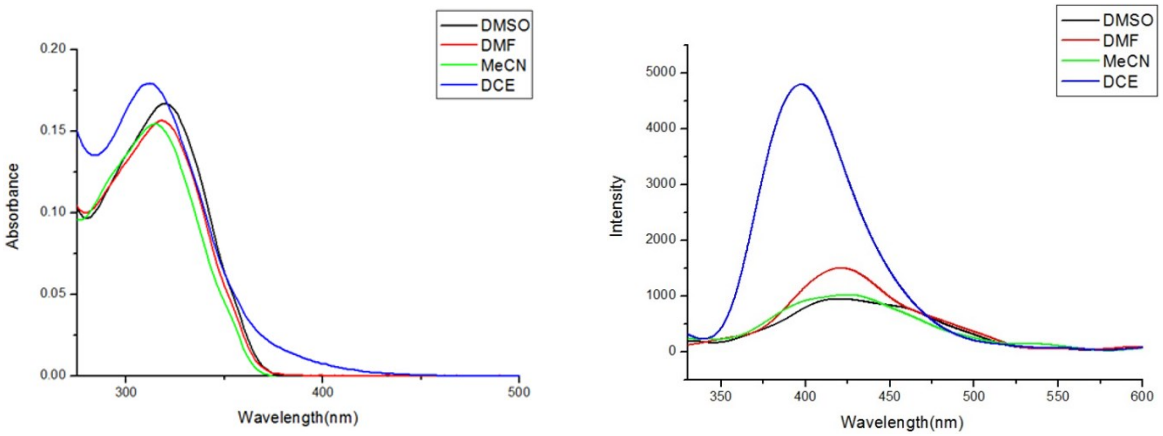
Weigh compound **3l** of 0.0391g, add 1 mL DMSO into EP tube to dissolve, then transfer to 100 ml volumetric bottle, continue to dilute with DMSO to scale, shake well, and set aside. Take 1mL of the above solution, transfer it to a 100 mL volumetric bottle and dilute it to the scale, then mix it into 10^{-5} mol·L^{-1} standard reserve solution for fluorescence test. Turn on the power, turn on the fluorophotometer and the computer, preheat the instrument, initialize the instrument, and measure the fluorescence intensity according to the excitation and emission fluorescence spectrometry. Determine the fluorescence intensity of compound **3l** in different solvents, replace DMSO with other solvents and repeat the above experimental steps.

Table S2. Spectroscopic data of compound **3l** in different solvent [a]

solvent	DMSO	DMF	MeCN	DCE
λabs [a] (nm)	320	318	314	312
λem [b] (nm)	420	421	425	397
λ_{abs} [c] (ε in L mol $^{-1}$ cm $^{-1}$)	16710	15657	15455	17954

[a] Longest wavelength absorption maximum. [b] Excited at the longest wavelength absorption maximum. [c] The extinction coefficients.

Figure S2. Absorption and emission spectra of compound **3l**



The strong UV–visible absorption of **3l** in DMSO, DMF, MeCN, and DCE were observed at about 315 nm. And its fluorescence emission (λem) was at a range of violet–blue light wavelengths in the region 400-425 nm in DMSO, DMF, MeCN, and DCE. It revealed that compound **3l** displayed high fluorescence absorption and emission intensity, which might have potential applications in luminescent materials.

2.4 The test of antiviral activity

Table S3. Antiviral activities of the target compounds against TMV [a]

compound	percentage inhibition	toxic regression equation	R	(μg mL^{-1})
3j	90%	Y=2.848X + 1.2	0.9961	62.06
3m	44.7%	Y=2.351X + 1.0	0.9949	368.87
6b	28.6%	--	--	--
Ningnanmycin	64.1%	--	--	--

[a] Tested and calculated at the drug test concentrations of 500 μg mL^{-1}. The data are average of three replicates. Agents ningnanmycin is commercial.

Figure S3. The test of antiviral activity against TMV

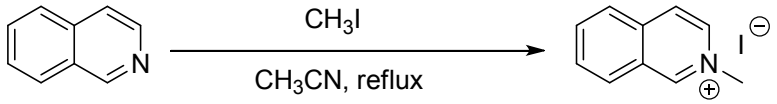
The experiments were carried out in two steps. (1) Purification of Tobacco Mosaic Virus. Using Gooding's method, the upper leaves of Nicotiana tabacum L. inoculated with TMV were selected and ground in phosphate buffer and then filtered through double-layer pledget. The filtrate was centrifuged at 10000g,

treated with PEG twice, and centrifuged again. The whole experiment was processed at 4 °C. Absorbance value was estimated at 260 nm by ultraviolet spectrophotometer. (2) Inhibition Effect of Compounds (**3j**, **3m**, **6b**) on TMV in Vivo. The virus was inhibited by mingling with the compounds (**3j**, **3m**, **6b**) solution at the same volume for 30 min. The mixture was then inoculated on the left side of the leaves of N. tabacum L., whereas the right side of the leaves was inoculated with the mixture of solvent and the virus for control. The local lesion numbers were recorded 3-4 days after inoculation. Three repetitions were conducted for each compound.

2.5 Experimental procedures

Synthesis of substrate 1 according to the following procedure:

The procedure for the synthesis of *N*-alkylisoquinolinium salts was based on the known procedure.[1] Compounds **1a-1l**, **1n-1o, 1q-1t, 4a-4g, 4i-4o** are known and their spectral data are in accordance with those reported in the literature.[1] As exemplified for **1a**:



1a

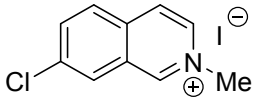
The oven-dried round-bottom flask were charged with CH_3CN (15 mL), isoquinoline (5 mmol, 1.0 equiv), CH_3I (10 mmol, 2.0 eq). The reaction mixture was refluxed for 12 hours, and then cooled to room temperature. When ethyl acetate was added to the system, the isoquinoline salt precipitated quickly as a solid, which was filtered and washed with ethyl acetate to give pure product **1a**.

Synthesis of product 3 according to the following procedure:

As exemplified for **3a**: 2-methylisoquinolin-2-ium iodide (0.3 mmol, 1.0 equiv), diphenyl diselenide (0.3 mmol, 1.0 equiv), KI (1.5 mmol), Cs_2CO_3 (0.45 mmol), CH_3CN(4 mL) and H_2O (1 mL) were placed in a 20 mL undivided electrolytic cell with a vitreous carbon plate anode (10 mm×10 mm×1 mm) and a platinum plate cathode (10 mm×10 mm×0.1 mm) under oxygen. The electrolysis was carried out at room temperature under a constant current of 10 mA for 10 hours (monitored by TLC). When the reaction was finished, the resulting reaction solution was quenched with 100 mL brine and extracted with 4×60 mL ethyl acetate. The extract was dried with Na_2SO_4. The solvent was removed with a rotary evaporator. The pure product was obtained by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 3: 1).

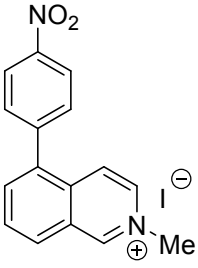
2.6 Characterization data

7-Chloro-2-methylisoquinolin-2-ium iodide (1m)



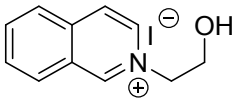
Yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 9.93 (s, 1H), 8.75 (d, J = 5.5 Hz, 1H), 8.65 – 8.57 (m, 2H), 8.40 (d, J = 8.8 Hz, 1H), 8.28 (dd, J = 8.8, 2.1 Hz, 1H), 4.48 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ ppm 150.1, 137.1, 136.6, 135.6, 135.4, 129.7, 128.6 128.0, 125.6, 48.3. HRMS MALDI (m/z): calcd for $C_{10}H_9ClN^+$ [M + H]$^+$: 178.0424, found: 178.0421.

2-Methyl-5-(4-nitrophenyl)isoquinolin-2-ium iodide (1p)



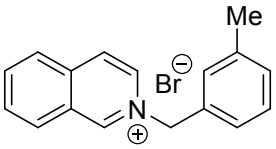
Yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 10.14 (s, 1H), 8.68 (dd, J = 7.0, 1.5 Hz, 1H), 8.60 (d, J = 8.2 Hz, 1H), 8.47 (d, J = 8.7 Hz, 2H), 8.31 – 8.26 (m, 2H), 8.21 – 8.17 (m, 1H), 7.87 (d, J = 8.7 Hz, 2H), 4.51 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ ppm 151.3, 147.6, 143.5, 137.3, 137.1, 136.7, 134.3, 131.5, 131.1, 127.7, 124.2, 123.1, 48.0. HRMS MALDI (m/z): calcd for $C_{16}H_{13}N_2O_2^+$ [M + H]$^+$: 265.0977, found: 265.0975.

2-(Hydroxymethyl)isoquinolin-2-ium iodide (4h)



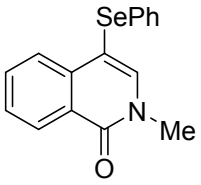
Brown solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 10.04 (s, 1H), 8.78 (dd, J = 6.8, 1.4 Hz, 1H), 8.62 (d, J = 6.8 Hz, 1H), 8.54 (d, J = 8.2 Hz, 1H), 8.37 (d, J = 8.2 Hz, 1H), 8.28 – 8.24 (m, 1H), 8.10 – 8.06 (m, 1H), 5.23 (t, J = 5.4 Hz, 1H), 4.81 – 4.77 (m, 2H), 3.96 (q, J = 5.3 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ ppm 150.4, 137.1, 136.9, 135.3, 131.2, 130.4, 127.3, 127.1, 125.7, 63.3, 60.0. HRMS MALDI (m/z): calcd for $C_{11}H_{12}NO^+$ [M + H]$^+$: 174.0919, found: 174.0914.

2-(3-Methylbenzyl)isoquinolin-2-ium bromide (4p)



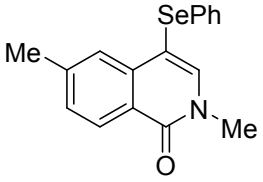
Brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 11.20 (s, 1H), 8.68 (dd, J = 17.5, 7.5 Hz, 2H), 8.20 (d, J = 6.7 Hz, 1H), 8.10 – 8.05 (m, 2H), 7.93 – 7.89 (m 1H), 7.45 (d, J = 8.8 Hz, 2H), 7.23 (d, J = 7.5 Hz, 1H), 7.15 (d, J = 7.6 Hz, 1H), 6.28 (s, 2H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 150.5, 139.5, 137.2, 137.1, 133.9, 132.9, 131.5, 131.3, 130.7, 130.0, 129.4, 127.8, 126.9, 126.6, 126.0, 64.1, 21.3. HRMS MALDI (m/z): calcd for $C_{17}H_{16}N^+$ [M + H]$^+$: 234.1283, found: 234.1279.

2-Methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3a)



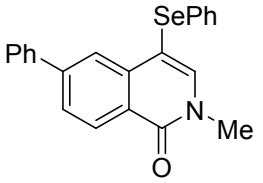
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3a**. Yellow solid (78.4 mg, 83%), mp 135-136 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.46 (d, J = 8.9 Hz, 1H), 7.93 (d, J = 7.8 Hz, 1H), 7.71 (s, 1H), 7.63 (t, J = 8.4 Hz, 1H), 7.51 (t, J = 8.1 Hz, 1H), 7.24 (d, J = 1.5 Hz, 2H), 7.21 – 7.14 (m, 3H), 3.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.6, 140.9, 137.9, 132.8, 132.3, 129.3, 129.0, 128.1, 127.5, 127.3, 126.4, 104.1, 37.0. HRMS MALDI (m/z): calcd for $C_{16}H_{13}NOSe$ $[M + H]^+$: 316.0241, found: 316.0240.

2,6-Dimethyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3b)



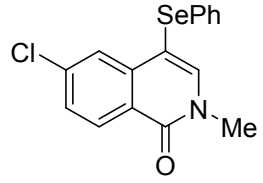
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3b**. Yellow solid (80.9 mg, 82%), mp 135.8-136.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.35 (d, J = 8.2 Hz, 1H), 7.73 (s, 1H), 7.67 (s, 1H), 7.32 (d, J = 7.5 Hz, 1H), 7.24 (t, J = 1.6 Hz, 2H), 7.21 – 7.13 (m, 3H), 3.62 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.6, 143.5, 141.1, 138.0, 132.5, 129.3, 129.0, 128.9, 128.1, 126.9, 126.3, 124.1, 103.9, 36.9, 22.0. HRMS MALDI (m/z): calcd for $C_{17}H_{15}NOSe$ $[M + H]^+$: 330.0397, found: 330.0400.

2-Methyl-6-phenyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3c)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3c**. Yellow solid (90.3 mg, 77%), mp 160.0-160.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.49 (d, J = 8.3 Hz, 1H), 8.12 (d, J = 1.7 Hz, 1H), 7.70 (d, J = 11.1 Hz, 2H), 7.51 (d, J = 7.0 Hz, 2H), 7.42 – 7.28 (m, 5H), 7.20 – 7.13 (m, 3H), 3.61 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.5, 145.4, 141.2, 140.0, 138.2, 132.3, 129.4, 128.9, 128.7, 128.2, 127.5, 126.6, 126.5, 125.5, 125.2, 104.5, 37.0. HRMS MALDI (m/z): calcd for $C_{22}H_{17}NOSe$ $[M + H]^+$: 392.0554, found: 392.0555.

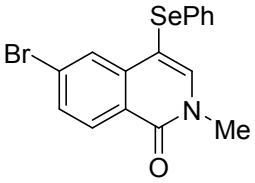
6-Chloro-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3d)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3d**. Yellow solid (78.5mg, 75%), mp 138 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.38 (d, J = 8.6 Hz, 1H), 7.94 (d, J = 2.1 Hz, 1H), 7.72 (s, 1H), 7.44 (dd, J = 8.6, 2.0 Hz, 1H), 7.26 – 7.16 (m, 5H), 3.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm

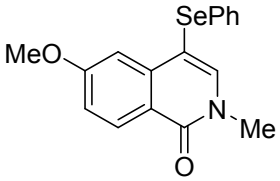
162.0, 142.3, 139.7, 139.5, 131.8, 130.0, 129.4, 129.2, 128.1, 126.7, 126.7, 124.7, 103.2, 37.1. HRMS MALDI (m/z): calcd for $C_{16}H_{12}ClNOSe$ $[M + H]^+$: 349.9851, found: 349.9855.

6-Bromo-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3e)



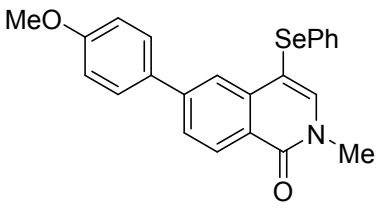
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3e**. Yellow solid (90.8 mg, 77%), mp 139.0-140.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.29 (d, J = 8.6 Hz, 1H), 8.12 (d, J = 1.9 Hz, 1H), 7.71 (s, 1H), 7.60 – 7.57 (m, 1H), 7.26 – 7.16 (m, 5H), 3.62 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.1, 142.2, 139.6, 131.8, 130.8, 129.9, 129.9, 129.4, 129.3, 128.4, 126.7, 125.0, 103.1, 37.1. HRMS MALDI (m/z): calcd for $C_{16}H_{12}BrNOSe$ $[M + H]^+$: 393.9346, found: 393.9348.

6-Methoxy-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3f)



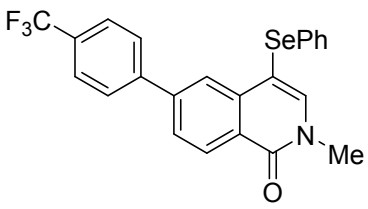
Flash column chromatography on silica gel (eluent: PE/EtOAc = 15/1, v/v) to afford **3f**. Yellow solid (74.5 mg, 72%), mp 161.0-161.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.86 – 7.82 (m, 2H), 7.57 (s, 1H), 7.23 – 7.13 (m, 6H), 3.91 (s, 3H), 3.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.3, 159.2, 138.5, 132.4, 131.8, 129.3, 129.0, 129.0, 127.5, 126.3, 123.0, 108.0, 104.0, 55.7, 37.1. HRMS MALDI (m/z): calcd for $C_{17}H_{15}NO_2Se$ $[M + H]^+$: 346.0346, found: 346.0355.

6-(4-Methoxyphenyl)-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3g)



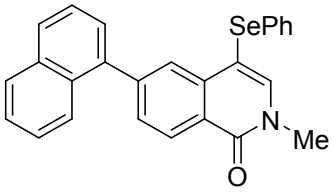
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3g**. Yellow solid (92.3 mg, 77%), mp 177.0-177.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.47 (d, J = 8.3 Hz, 1H), 8.07 (d, J = 1.8 Hz, 1H), 7.71 – 7.67 (m, 2H), 7.47 (d, J = 8.8 Hz, 2H), 7.30 (d, J = 6.5 Hz, 2H), 7.21 – 7.14 (m, 3H), 6.95 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H), 3.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.5, 159.9, 145.0, 141.1, 138.2, 132.3, 132.3, 129.3, 128.7, 128.6, 126.5, 126.1, 124.8, 124.7, 114.4, 104.5, 55.4, 37.0. HRMS MALDI (m/z): calcd for $C_{23}H_{19}NO_2Se$ $[M + H]^+$: 422.0659, found: 422.0666.

2-Methyl-4-(phenylselanyl)-6-(4-(trifluoromethyl)phenyl)isoquinolin-1(2*H*)-one (3h)



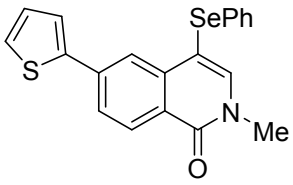
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3h**. Green solid (103.3 mg, 75%), mp 193.1-193.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.52 (d, J = 8.3 Hz, 1H), 8.10 (d, J = 1.8 Hz, 1H), 7.74 (s, 1H), 7.66 (d, J = 8.5 Hz, 3H), 7.58 (d, J = 8.2 Hz, 2H), 7.30 (dd, J = 8.1, 1.6 Hz, 2H), 7.22 – 7.16 (m, 3H), 3.65 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 162.3, 143.8, 143.5, 141.4, 138.2, 132.0, 130.2 (q, J = 32.6 Hz), 129.4, 129.0, 127.8, 126.6, 126.4, 126.0, 125.8 (q, J = 3.8 Hz), 124.1 (q, J = 272.1 Hz), 104.3, 37.0. HRMS MALDI (m/z): calcd for $C_{23}H_{16}F_3NOSe$ $[M + H]^+$: 460.0427, found: 460.0434.

2-Methyl-6-(naphthalen-1-yl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3i)



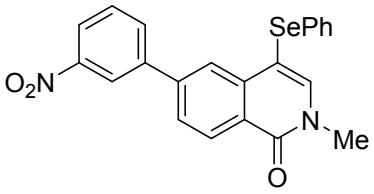
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3i**. Yellow solid (95.3 mg, 72%), mp 136.1-136.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.57 (d, J = 8.2 Hz, 1H), 8.08 (d, J = 1.7 Hz, 1H), 7.86 (t, J = 8.0 Hz, 2H), 7.75 (s, 1H), 7.66 – 7.61 (m, 2H), 7.51 – 7.43 (m, 2H), 7.34 (dd, J = 7.1, 1.3 Hz, 1H), 7.26 – 7.23 (m, 3H), 7.19 (d, J = 3.8 Hz, 3H), 3.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.6, 145.3, 141.3, 139.0, 137.7, 133.8, 132.2, 131.1, 129.7, 129.4, 129.3, 128.8, 128.4, 128.4, 128.3, 127.3, 126.5, 126.4, 125.9, 125.4, 125.4, 125.3, 104.3, 37.1. HRMS MALDI (m/z): calcd for $C_{26}H_{19}NOSe$ $[M + H]^+$: 442.0710, found: 442.0715.

2-Methyl-4-(phenylselanyl)-6-(thiophen-2-yl)isoquinolin-1(2*H*)-one (3j)



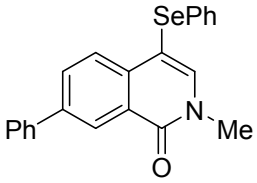
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3j**. Yellow solid (76.2 mg, 64%), mp 191.1-191.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.41 (d, J = 9.0 Hz, 1H), 8.12 (s, 1H), 7.70 (d, J = 9.0 Hz, 2H), 7.36 – 7.31 (m, 4H), 7.21 – 7.13 (m, 3H), 7.06 (t, J = 3.7 Hz, 1H), 3.61 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.3, 143.1, 141.3, 138.4, 132.0, 129.7, 129.4, 128.9, 128.3, 126.7, 126.6, 125.1, 125.0, 124.8, 123.8, 104.4, 37.0. HRMS MALDI (m/z): calcd for $C_{20}H_{15}NOSSe$ $[M + H]^+$: 398.0118, found: 398.0119.

2-Methyl-6-(3-nitrophenyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3k)



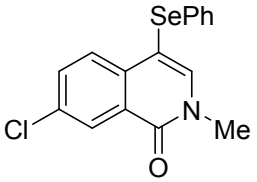
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3k**. Yellow solid (78.5 mg, 60%), mp 220.3-220.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.55 (d, J = 8.3 Hz, 1H), 8.33 (t, J = 2.0 Hz, 1H), 8.25 – 8.20 (m, 1H), 8.13 (d, J = 1.8 Hz, 1H), 7.83 (d, J = 7.6 Hz, 1H), 7.78 (s, 1H), 7.72 (dd, J = 8.3, 1.8 Hz, 1H), 7.61 (t, J = 8.0 Hz, 1H), 7.38 – 7.32 (m, 2H), 7.26 – 7.17 (m, 3H), 3.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.3, 148.7, 142.7, 141.7, 141.3, 138.3, 133.4, 131.7, 129.9, 129.7, 129.5, 129.3, 126.8, 126.2, 126.1, 126.0, 122.9, 122.4, 104.4, 37.1. HRMS MALDI (m/z): calcd for $C_{22}H_{16}N_2O_3Se$ $[M + H]^+$: 437.0404, found: 437.0401.

2-Methyl-7-phenyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3l)



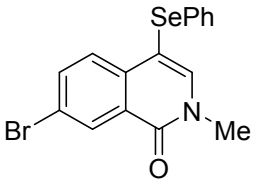
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3l**. Yellow solid (88.0 mg, 75%), mp 151.4-152.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.70 (s, 1H), 7.97 (d, J = 8.4 Hz, 1H), 7.85 (d, J = 8.1 Hz, 1H), 7.71 – 7.66 (m, 3H), 7.45 (t, J = 7.6 Hz, 2H), 7.36 (t, J = 7.3 Hz, 1H), 7.27 (d, J = 7.5 Hz, 2H), 7.16 (dd, J = 9.4, 6.9 Hz, 3H), 3.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.7, 140.8, 140.2, 139.7, 136.9, 132.3, 131.7, 129.4, 129.1, 129.0, 128.0, 127.9, 127.2, 126.7, 126.4, 126.0, 103.9, 37.1. HRMS MALDI (m/z): calcd for $C_{22}H_{17}NOSe$ $[M + H]^+$: 392.0554, found: 392.0554.

7-Chloro-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3m)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3m**. Yellow solid (81.7mg, 78%), mp 131.5-131.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.41 (s, 1H), 7.85 (d, J = 8.7 Hz, 1H), 7.68 (s, 1H), 7.54 (d, J = 8.7 Hz, 1H), 7.24 – 7.15 (m, 5H), 3.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.6, 141.0, 136.3, 133.6, 133.2, 131.9, 129.4, 129.1, 129.1, 127.5, 127.35, 126.6, 103.6, 37.1. HRMS MALDI (m/z): calcd for $C_{16}H_{12}ClNOSe$ $[M + H]^+$: 349.9851, found: 349.9850.

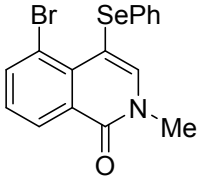
7-Bromo-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3n)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3n**. Yellow solid (94.3mg, 80%), mp 145.2-145.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.58 (d, J = 2.1 Hz, 1H), 7.79 (d, J = 8.7 Hz, 1H), 7.71 – 7.67 (m, 2H), 7.24 –

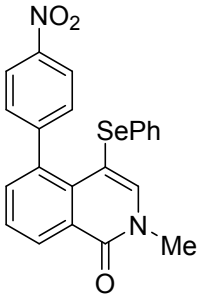
7.16 (m, 5H), 3.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.5, 141.2, 136.7, 136.0, 131.9, 130.6, 129.4, 129.2, 129.1, 127.6, 126.6, 121.6, 103.7, 37.2. HRMS MALDI (m/z): calcd for $C_{16}H_{12}BrNOSe$ [M + H]$^+$: 393.9346, found: 393.9345.

5-Bromo-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3o)



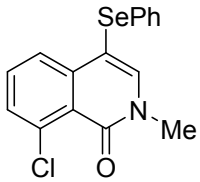
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3o**. Yellow solid (86.1 mg, 73%), mp 134.4-134.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.56 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 7.7 Hz, 1H), 7.42 (d, J = 1.6 Hz, 1H), 7.37 – 7.32 (m, 3H), 7.25 (d, J = 2.0 Hz, 3H), 3.52 (d, J = 1.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.5, 141.7, 139.8, 135.6, 134.6, 130.8, 129.5, 129.0, 128.6, 127.8, 127.0, 120.0, 103.2, 36.8. HRMS MALDI (m/z): calcd for $C_{16}H_{12}BrNOSe$ [M + H]$^+$: 393.9346, found: 393.9342.

2-Methyl-5-(4-nitrophenyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3p)



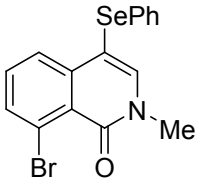
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3p**. Green solid (82.4 mg, 63%), mp 195.4-195.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.65 (d, J = 9.5 Hz, 1H), 8.09 (d, J = 8.2 Hz, 2H), 7.57 (t, J = 7.7 Hz, 1H), 7.47 (dd, J = 7.3, 1.5 Hz, 1H), 7.45 (s, 1H), 7.29 (s, 2H), 7.13 (t, J = 3.5 Hz, 3H), 6.91 – 6.84 (m, 2H), 3.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.0, 148.6, 147.2, 142.7, 138.0, 135.6, 135.6, 134.6, 130.5, 129.3, 129.2, 129.1, 127.7, 126.6, 122.9, 102.0, 36.9. ^{77}Se NMR (76 MHz, $CDCl_3$) δ ppm 395.9. HRMS MALDI (m/z): calcd for $C_{22}H_{16}N_2O_3Se$ [M + H]$^+$: 437.0404, found: 437.0399.

8-Chloro-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3q)



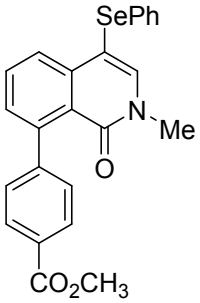
Flash column chromatography on silica gel (eluent: PE/EtOAc = 15/1, v/v) to afford **3q**. Green solid (75.4 mg, 72%); mp 155.4-155.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.98 (dd, J = 8.2, 1.2 Hz, 1H), 7.80 – 7.75 (m, 2H), 7.37 (t, J = 7.9 Hz, 1H), 7.24 – 7.15 (m, 5H), 3.61 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 160.8, 141.9, 140.7, 134.7, 132.6, 132.0, 129.4, 128.92, 127.6, 126.5, 123.6, 123.2, 103.2, 37.6. HRMS MALDI (m/z): calcd for $C_{16}H_{12}ClNOSe$ [M + H]$^+$: 349.9851, found: 349.9851.

8-Bromo-2-methyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (3r)



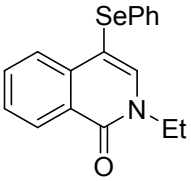
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3r**. Yellow solid (86.1 mg, 73%), mp 145.1-145.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.92 (dd, J = 7.9, 1.5 Hz, 1H), 7.76 (s, 1H), 7.51 (dd, J = 7.8, 1.5 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 7.23 – 7.16 (m, 5H), 3.60 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 160.8, 142.0, 140.7, 135.6, 132.4, 132.0, 130.8, 129.4, 128.9, 126.8, 126.5, 122.7, 103.1, 37.5. ^{77}Se NMR (76 MHz, $CDCl_3$) δ ppm 308.1. HRMS MALDI (m/z): calcd for $C_{16}H_{12}BrNOSe$ $[M + H]^+$: 393.9346, found: 393.9344.

Methyl 4-(2-methyl-1-oxo-4-(phenylselanyl)-1,2-dihydroisoquinolin-8-yl)benzoate (3s)



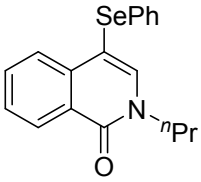
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **3s**. Brown solid (94.3 mg, 70%), mp 119.6-120.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.08 (t, J = 8.4 Hz, 3H), 7.78 (s, 1H), 7.64 – 7.59 (m, 1H), 7.36 (d, J = 7.8 Hz, 2H), 7.30 – 7.26 (m, 3H), 7.23 – 7.17 (m, 3H), 3.93 (s, 3H), 3.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 167.2, 161.8, 148.5, 143.7, 141.7, 139.3, 132.3, 131.8, 130.6, 129.4, 129.0, 128.8, 128.3, 128.2, 127.9, 126.5, 123.3, 103.5, 52.0, 37.3. HRMS MALDI (m/z): calcd for $C_{24}H_{19}NO_3Se$ $[M + H]^+$: 450.0608, found: 450.0605.

2-Ethyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5a)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5a**. Brown oil (78.0 mg, 79%), mp 124.3-124.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.46 (d, J = 7.8 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.70 (s, 1H), 7.62 (t, J = 7.9 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.24 (d, J = 1.6 Hz, 2H), 7.17 (q, J = 7.8, 7.0 Hz, 3H), 4.10 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.0, 139.8, 137.7, 132.8, 132.3, 129.3, 129.0, 128.2, 127.4, 127.2, 126.6, 126.3, 104.3, 44.5, 14.7. HRMS MALDI (m/z): calcd for $C_{17}H_{15}NOSe$ $[M + H]^+$: 330.0397, found: 330.0398.

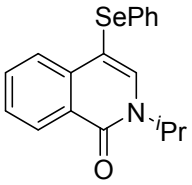
4-(Phenylselanyl)-2-propylisoquinolin-1(2*H*)-one (5b)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5b**. Yellow solid (79.2 mg, 77%), mp 99.3-99.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.46 (d, J = 9.3 Hz, 1H), 7.91 (d, J = 8.2 Hz, 1H), 7.68 (s, 1H), 7.60 (t, J = 8.3 Hz, 1H), 7.48 (t, J = 8.2 Hz, 1H), 7.23 (s, 2H), 7.17 (t, J = 7.0 Hz, 3H), 4.01 – 3.97 (m, 2H), 1.84 (q, J

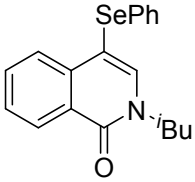
= 7.4 Hz, 2H), 0.99 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.1, 140.4, 137.7, 132.8, 132.3, 129.3, 129.0, 128.2, 127.4, 127.2, 126.6, 126.4, 103.9, 51.0, 22.6, 11.3. ^{77}Se NMR (77 MHz, $CDCl_3$) δ ppm 307.4. HRMS MALDI (m/z): calcd for $C_{18}H_{17}NOSe$ $[M + H]^+$: 344.0554, found: 344.0560.

2-Isopropyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5c)



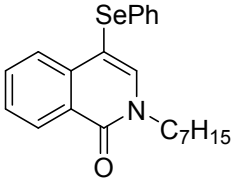
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5c**. Yellow solid (77.2 mg, 75%), mp 132.3-132.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.47 (d, *J* = 9.4 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.72 (s, 1H), 7.60 (t, *J* = 8.3 Hz, 1H), 7.48 (t, *J* = 8.2 Hz, 1H), 7.25 – 7.22 (m, 2H), 7.20 – 7.12 (m, 3H), 5.39 (p, *J* = 6.8 Hz, 1H), 1.42 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.8, 137.2, 135.7, 132.8, 132.4, 129.3, 129.0, 128.4, 127.4, 127.1, 126.58, 126.3, 104.4, 46.4, 21.9. HRMS MALDI (m/z): calcd for $C_{18}H_{17}NOSe$ $[M + H]^+$: 344.0554, found: 344.0555.

2-Isobutyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5d)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 15/1, v/v) to afford **5d**. Green solid (77.1 mg, 72%), mp 157.7-158.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.46 (d, *J* = 9.5 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.65 (s, 1H), 7.61 (d, *J* = 8.3 Hz, 1H), 7.49 (t, *J* = 8.2 Hz, 1H), 7.26 – 7.23 (m, 2H), 7.20 – 7.14 (m, 3H), 3.85 (d, *J* = 7.4 Hz, 2H), 2.25 (dt, *J* = 13.8, 6.9 Hz, 1H), 0.98 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.3, 140.9, 137.7, 132.8, 132.3, 129.3, 129.0, 128.3, 127.4, 127.2, 126.6, 126.4, 103.7, 56.7, 28.3, 20.0. ^{77}Se NMR (76 MHz, $CDCl_3$) δ ppm 307.6. HRMS MALDI (m/z): calcd for $C_{19}H_{19}NOSe$ $[M + H]^+$: 358.0710, found: 358.0717.

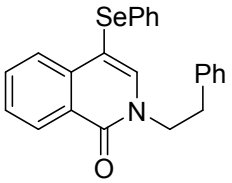
2-Heptyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5e)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 15/1, v/v) to afford **5e**. Green solid (92.2 mg, 72%), mp 67.2-67.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.46 (d, *J* = 9.4 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.68 (s, 1H), 7.60 (t, *J* = 8.4 Hz, 1H), 7.48 (t, *J* = 8.2 Hz, 1H), 7.26 – 7.22 (m, 2H), 7.20 – 7.13 (m, 3H), 4.05 – 3.99 (m, 2H), 1.80 (p, *J* = 7.3 Hz, 2H), 1.38 – 1.25 (m, 8H), 0.89 – 0.85 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm

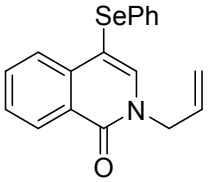
162.1, 140.4, 137.7, 132.8, 132.4, 129.3, 129.0, 128.2, 127.4, 127.2, 126.6, 126.3, 104.0, 49.6, 31.7, 29.3, 29.0, 26.8, 22.6, 14.1. HRMS MALDI (m/z): calcd for $C_{22}H_{25}NOSe$ $[M + H]^+$: 400.1180, found: 400.1181.

2-Phenethyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5f)



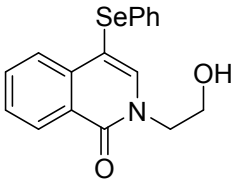
Flash column chromatography on silica gel (eluent: PE/EtOAc = 15/1, v/v) to afford **5f**. Yellow solid (87.5 mg, 72%), mp 103.3-103.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.48 (d, J = 8.0 Hz, 1H), 7.88 (dd, J = 8.1, 1.1 Hz, 1H), 7.61 (t, J = 7.2 Hz, 1H), 7.50 (t, J = 7.4 Hz, 1H), 7.36 (s, 1H), 7.28 – 7.24 (m, 2H), 7.22 – 7.13 (m, 8H), 4.24 (t, J = 7.2 Hz, 2H), 3.13 (t, J = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.1, 140.6, 137.9, 137.8, 132.9, 132.1, 129.3, 129.2, 129.0, 128.8, 128.2, 127.4, 127.3, 126.8, 126.5, 126.4, 103.7, 51.6, 35.1. HRMS MALDI (m/z): calcd for $C_{23}H_{19}NOSe$ $[M + H]^+$: 406.0710, found: 406.0709.

2-Allyl-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5g)



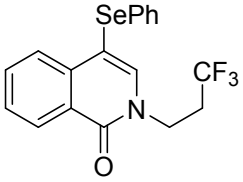
Flash column chromatography on silica gel (eluent: PE/EtOAc = 15/1, v/v) to afford **5g**. Green solid (71.6 mg, 70%), mp 95.1-95.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.47 (d, J = 7.7 Hz, 1H), 7.92 (d, J = 7.7 Hz, 1H), 7.66 (s, 1H), 7.62 (t, J = 7.7 Hz, 1H), 7.50 (t, J = 7.5 Hz, 1H), 7.24 (d, J = 1.5 Hz, 2H), 7.17 (q, J = 7.3, 6.7 Hz, 3H), 6.05 – 5.95 (m, 1H), 5.31 – 5.23 (m, 2H), 4.67 (d, J = 5.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.0, 139.6, 137.7, 133.0, 132.4, 132.2, 129.3, 129.1, 128.3, 127.5, 127.3, 126.6, 126.4, 118.7, 104.5, 50.7. HRMS MALDI (m/z): calcd for $C_{18}H_{15}NOSe$ $[M + H]^+$: 342.0397, found: 342.0400.

2-(2-Hydroxyethyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5h)



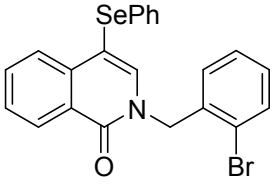
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5h**. Green solid (67.3 mg, 65%), mp 125.5-126.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.41 (d, J = 7.9 Hz, 1H), 7.93 (d, J = 8.2 Hz, 1H), 7.75 (s, 1H), 7.63 (t, J = 7.6 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.26 (s, 2H), 7.16 (t, J = 6.9 Hz, 3H), 4.20 (t, J = 4.8 Hz, 2H), 4.01 (t, J = 4.9 Hz, 2H), 2.34 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.2, 140.8, 137.9, 133.1, 132.1, 129.3, 129.2, 128.1, 127.5, 127.4, 126.46, 126.2, 104.7, 61.8, 52.7. HRMS MALDI (m/z): calcd for $C_{17}H_{15}NO_2Se$ $[M + H]^+$: 346.0346, found: 346.0346.

4-(Phenylselanyl)-2-(3,3,3-trifluoropropyl)isoquinolin-1(2*H*)-one (5i)



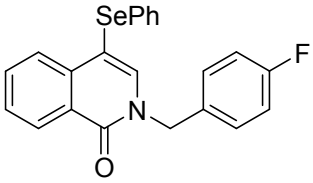
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5i**. Green solid (89.3 mg, 75%), mp 127.1-127.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.43 (d, J = 7.5 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.66 (s, 1H), 7.63 (t, J = 7.7 Hz, 1H), 7.50 (t, J = 7.4 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.21 – 7.13 (m, 3H), 4.23 (t, J = 6.8 Hz, 2H), 2.76 – 2.65 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm δ 162.0, 139.9, 137.7, 133.2, 131.8, 129.3, 129.2, 128.0, 127.7, 127.5, 126.5, 126.2, 126.0 (q, J = 277.0 Hz), 105.0, 43.9 (q, J = 3.5 Hz), 32.7 (q, J = 28.7 Hz). HRMS MALDI (m/z): calcd for $C_{18}H_{14}F_3NOSe$ $[M + H]^+$: 398.0271, found: 398.0272.

2-(2-Bromobenzyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5j)



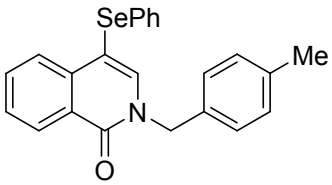
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5j**. Green solid (106.9mg, 76%), mp 173.5-174.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.48 (d, J = 7.9 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.72 (s, 1H), 7.66 – 7.57 (m, 2H), 7.50 (t, J = 7.5 Hz, 1H), 7.28 – 7.25 (m, 2H), 7.24 – 7.20 (m, 2H), 7.20 – 7.11 (m, 4H), 5.33 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.3, 139.9, 137.7, 135.4, 133.1, 132.0, 129.8, 129.6, 129.3, 129.3, 128.5, 127.9, 127.6, 127.4, 126.5, 123.5, 105.0, 52.0. HRMS MALDI (m/z): calcd for $C_{22}H_{16}BrNOSe$ $[M + H]^+$: 469.9659, found: 469.9656.

2-(4-Fluorobenzyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5k)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5k**. Green solid (89.6 mg, 73%), mp 110.4-111.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.47 (d, J = 7.8 Hz, 1H), 7.91 (d, J = 8.1 Hz, 1H), 7.68 (s, 1H), 7.64 – 7.59 (m, 1H), 7.52 – 7.47 (m, 1H), 7.34 (dd, J = 8.4, 5.4 Hz, 2H), 7.22 (dd, J = 7.5, 2.3 Hz, 2H), 7.18 – 7.12 (m, 3H), 7.01 (t, J = 8.6 Hz, 2H), 5.19 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.5 (d, J = 246.9 Hz), 162.2, 139.5, 137.7, 133.1, 132.3 (d, J = 3.3 Hz), 132.0, 130.0, 129.9, 129.3, 129.2, 128.4, 127.7, 127.4, 126.6, 126.5, 115.9 (d, J = 21.8 Hz), 105.0, 51.3. HRMS MALDI (m/z): calcd for $C_{22}H_{16}FNOSe$ $[M + H]^+$: 410.0459, found: 410.0455.

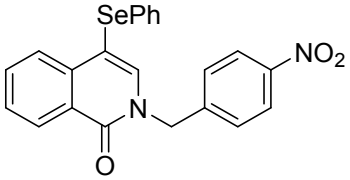
2-(4-Methylbenzyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5l)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5l**. Green solid (93.6 mg, 77%), mp 120.1-120.3 °C. ^{1}H NMR (400

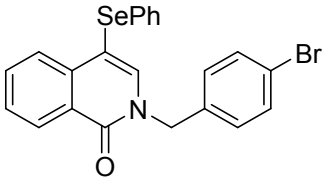
MHz, $CDCl_3$) δ ppm 8.48 (d, J = 7.9 Hz, 1H), 7.90 (d, J = 8.1 Hz, 1H), 7.69 (s, 1H), 7.61 (t, J = 6.9 Hz, 1H), 7.49 (t, J = 7.2 Hz, 1H), 7.25 – 7.19 (m, 4H), 7.17 – 7.12 (m, 5H), 5.20 (s, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.2, 139.8, 137.9, 137.7, 133.4, 132.9, 132.1, 129.6, 129.3, 129.1, 128.43, 128.1, 127.5, 127.3, 126.7, 126.4, 104.6, 51.6, 21.2. HRMS MALDI (m/z): calcd for $C_{23}H_{19}NOSe$ $[M + H]^+$: 406.0710, found: 406.0714.

2-(4-Nitrobenzyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5m)



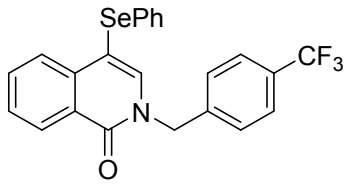
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5m**. Green solid (89.0 mg, 68%), mp 120.4-120.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.45 (d, J = 8.4 Hz, 1H), 8.18 (d, J = 7.9 Hz, 2H), 7.93 (dd, J = 13.8, 8.0 Hz, 1H), 7.72 – 7.64 (m, 2H), 7.51 (dd, J = 18.3, 7.6 Hz, 4H), 7.24 – 7.10 (m, 4H), 5.31 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.2, 147.7, 143.7, 139.2, 137.7, 133.5, 133.4, 133.3, 131.8, 130.0, 129.4, 129.3, 128.6, 128.4, 127.9, 127.6, 126.7, 126.4, 124.1, 105.7, 51.6. HRMS MALDI (m/z): calcd for $C_{22}H_{16}N_2O_3Se$ $[M + H]^+$: 437.0404, found: 437.0410.

2-(4-Bromobenzyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5n)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5n**. Green solid (101.3 mg, 72%), mp 116.4-116.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.46 (d, J = 7.7 Hz, 1H), 7.91 (d, J = 8.2 Hz, 1H), 7.66 (s, 1H), 7.62 (t, J = 6.9 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.44 (d, J = 8.4 Hz, 2H), 7.24 – 7.19 (m, 4H), 7.19 – 7.06 (m, 3H), 5.16 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.2, 139.4, 137.7 135.5, 133.3, 133.1, 132.1, 132.0, 129.8, 129.4, 129.2, 128.4, 127.7, 127.4, 126.5, 122.2, 105.1, 51.4. HRMS MALDI (m/z): calcd for $C_{22}H_{16}BrNOSe$ $[M + H]^+$: 469.9659, found: 469.9655.

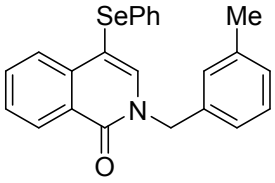
4-(Phenylselanyl)-2-(4-(trifluoromethyl)benzyl)isoquinolin-1(2*H*)-one (5o)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5o**. Green solid (99.2 mg, 72%), mp 123.1-123.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.47 (d, J = 8.0 Hz, 1H), 7.94 (d, J = 8.1 Hz, 1H), 7.69 (s, 1H), 7.66 – 7.58 (m, 3H), 7.54 – 7.49 (m, 1H), 7.45 (d, J = 8.0 Hz, 2H), 7.22 (d, J = 1.9 Hz, 2H), 7.16 (dd, J = 5.1, 2.1 Hz, 3H), 5.28 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm

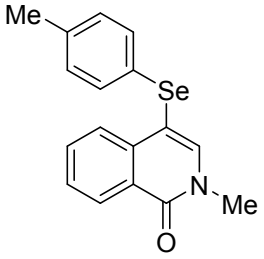
162.2, 140.4, 140.4, 139.4, 137.7, 133.2, 131.9, 130.3 (q, J = 32.5 Hz), 129.4, 129.3, 128.4, 128.2, 127.8, 127.5, 126.6, 126.5, 125.9 (q, J = 3.8 Hz), 124.0 (q, J = 272.2 Hz), 105.4, 51.6. HRMS MALDI (m/z): calcd for $C_{23}H_{16}F_3NOSe$ $[M + H]^+$: 460.0427, found: 460.0428.

2-(3-Methylbenzyl)-4-(phenylselanyl)isoquinolin-1(2*H*)-one (5p)



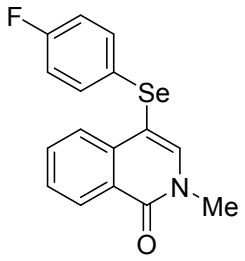
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **5p**. Green solid (88.7 mg, 73%), mp 119.2-119.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.49 (d, J = 8.1 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.69 (s, 1H), 7.61 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.24 – 7.19 (m, 3H), 7.17 – 7.08 (m, 6H), 5.20 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.3, 139.9, 138.7, 137.7, 136.4, 133.0, 132.2, 129.3, 129.1, 128.9, 128.8, 128.7, 128.5, 127.5, 127.3, 126.7, 126.4, 125.1, 104.7, 51.7, 21.5. HRMS MALDI (m/z): calcd for $C_{23}H_{19}NOSe$ $[M + H]^+$: 406.0710, found: 406.0717.

2-Methyl-4-(p-tolylselanyl)isoquinolin-1(2*H*)-one (6a)



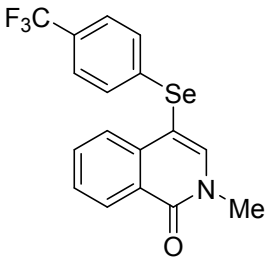
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **6a**. Green solid (69.1 mg, 70%), mp 137.1-137.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.45 (d, J = 9.4 Hz, 1H), 7.94 (d, J = 7.6 Hz, 1H), 7.68 (s, 1H), 7.63 (t, J = 8.4 Hz, 1H), 7.49 (t, J = 7.0 Hz, 1H), 7.18 (d, J = 8.2 Hz, 2H), 7.00 (d, J = 7.9 Hz, 2H), 3.63 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.6, 140.6, 137.9, 136.5, 132.8, 130.1, 129.5, 128.2, 128.0, 127.4, 127.3, 126.4, 104.7, 37.0, 21.0. HRMS MALDI (m/z): calcd for $C_{17}H_{15}NOSe$ $[M + H]^+$: 330.0397, found: 330.0406.

4-((4-Fluorophenyl)selanyl)-2-methylisoquinolin-1(2*H*)-one (6b)



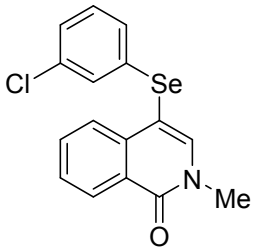
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **6b**. Green solid (70.9 mg, 71%), mp 148.2-148.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.45 (d, J = 8.3 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.69 (s, 1H), 7.63 (t, J = 8.1 Hz, 1H), 7.50 (t, J = 8.2 Hz, 1H), 7.28 (s, 1H), 7.26 – 7.23 (m, 1H), 6.90 (t, J = 8.8 Hz, 2H), 3.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.5, 161.9 (d, J = 246.2 Hz), 140.7, 137.6, 132.8, 131.3 (d, J = 7.8 Hz), 128.1, 127.5, 127.1, 126.4, 126.4, 116.5 (d, J = 21.8 Hz), 104.5, 37.0. HRMS MALDI (m/z): calcd for $C_{16}H_{12}FNOSe$ $[M + H]^+$: 334.0146, found: 334.0155.

2-Methyl-4-((4-(trifluoromethyl)phenyl)selanyl)isoquinolin-1(2*H*)-one (6c)



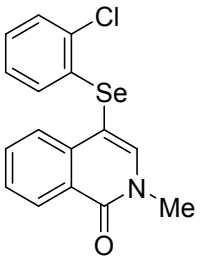
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **6c**. Green solid (77.0 mg, 67%), mp 89.3-90.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.49 (d, J = 6.7 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.73 (s, 1H), 7.65 (t, J = 6.9 Hz, 1H), 7.54 (t, J = 7.0 Hz, 1H), 7.41 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.3 Hz, 2H), 3.66 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.6, 141.5, 137.9, 137.5, 133.1, 128.5 (q, J = 11.2 Hz), 128.4, 128.3, 128.3, 127.8, 127.0, 126.4, 126.0 (q, J = 3.7 Hz), 124.0 (q, J = 271.8 Hz), 102.8, 37.1. HRMS MALDI (m/z): calcd for $C_{17}H_{12}F_3NOSe$ [M + H]$^+$: 384.0114, found: 384.0110.

4-((3-Chlorophenyl)selanyl)-2-methylisoquinolin-1(2*H*)-one (6d)



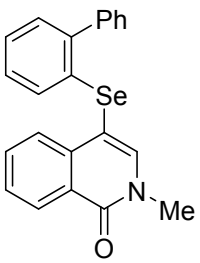
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **6d**. Green solid (72.2 mg, 69%), mp 125.3-125.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.46 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 2.6 Hz, 1H), 7.65 – 7.60 (m, 1H), 7.53 – 7.47 (m, 1H), 7.21 (s, 1H), 7.12 – 7.06 (m, 3H), 3.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.6, 141.3, 137.5, 135.1, 134.1, 133.0, 130.3, 128.5, 128.1, 127.6, 127.0, 126.9, 126.6, 126.4, 103.3, 37.1. HRMS MALDI (m/z): calcd for $C_{16}H_{12}ClNOSe$ [M + H]$^+$: 349.9851, found: 349.9854.

4-((2-Chlorophenyl)selanyl)-2-methylisoquinolin-1(2*H*)-one (6e)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **6e**. Green solid (71.2 mg, 68%), mp 231.8-232.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.49 (d, J = 7.7 Hz, 1H), 7.84 (d, J = 8.3 Hz, 1H), 7.73 (s, 1H), 7.64 (t, J = 7.2 Hz, 1H), 7.53 (t, J = 7.2 Hz, 1H), 7.34 (d, J = 7.1 Hz, 1H), 7.08 (t, J = 6.9 Hz, 1H), 6.94 (t, J = 7.2 Hz, 1H), 6.71 (d, J = 6.6 Hz, 1H), 3.66 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.7, 141.8, 137.7, 133.2, 133.1, 132.3, 129.4, 128.7, 128.2, 127.7, 127.4, 127.1, 127.0, 126.4, 102.7, 37.1. HRMS MALDI (m/z): calcd for $C_{16}H_{12}ClNOSe$ [M + H]$^+$: 349.9851, found: 349.9857.

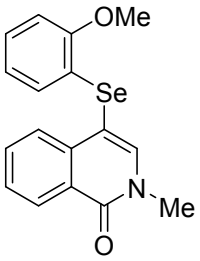
4-([1,1'-Biphenyl]-2-ylselanyl)-2-methylisoquinolin-1(2*H*)-one (6f)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **6f**. Green solid (84.5 mg, 72%), mp 117.4-117.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm

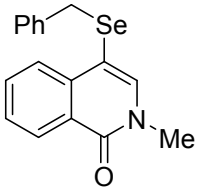
8.45 (d, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 6.9 Hz, 1H), 7.50 – 7.46 (m, 6H), 7.26 – 7.17 (m, 3H), 7.06 (t, *J* = 6.5 Hz, 1H), 7.00 (d, *J* = 6.7 Hz, 1H), 3.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.6, 142.1, 141.2, 141.1, 137.9, 132.8, 132.1, 130.2, 129.0, 128.8, 128.4, 128.1, 128.0, 127.9, 127.4, 127.3, 126.4, 126.2, 104.1, 37.0. HRMS MALDI (m/z): calcd for $C_{22}H_{17}NOSe$ $[M + H]^+$: 392.0554, found: 392.0554.

4-((2-Methoxyphenyl)selanyl)-2-methylisoquinolin-1(2*H*)-one (6g)



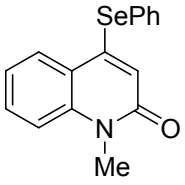
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **6g**. Green solid (77.6 mg, 74%), mp 150.1-150.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.48 (d, *J* = 7.3 Hz, 1H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.69 (s, 1H), 7.62 (t, *J* = 6.9 Hz, 1H), 7.51 (t, *J* = 7.0 Hz, 1H), 7.15 – 7.11 (m, 1H), 6.85 (d, *J* = 7.0 Hz, 1H), 6.71 – 6.64 (m, 2H), 3.95 (s, 3H), 3.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.8, 156.0, 141.5, 138.2, 132.9, 128.1, 128.0, 127.5, 127.4, 127.0, 126.4, 121.9, 121.8, 110.2, 102.0, 55.9, 37.0. HRMS MALDI (m/z): calcd for $C_{17}H_{15}NO_2Se$ $[M + H]^+$: 346.0346, found: 346.0352.

4-(Benzylselanyl)-2-methylisoquinolin-1(2*H*)-one (6h)



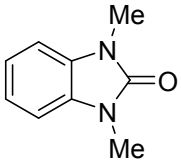
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **6h**. Yellow oil (73.0 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.44 (d, *J* = 8.1 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 7.4 Hz, 3H), 7.01 (s, 1H), 6.94 (d, *J* = 6.1 Hz, 2H), 3.86 (s, 2H), 3.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.5, 140.6, 138.7, 138.2, 132.6, 129.0, 128.2, 128.1, 127.1, 127.1, 126.8, 126.0, 103.8, 36.7, 31.9. HRMS MALDI (m/z): calcd for $C_{17}H_{15}NOSe$ $[M + H]^+$: 330.0397, found: 330.0398.

1-Methyl-4-(phenylselanyl)quinolin-2(1*H*)-one (7b)



Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **7b**. Brown solid (51.0 mg, 54%), mp 116.5-116.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.73 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.50 – 7.42 (m, 4H), 7.34 (d, *J* = 8.5 Hz, 1H), 7.27 (d, *J* = 1.6 Hz, 1H), 7.15 (t, *J* = 8.0 Hz, 1H), 7.06 (s, 1H), 3.79 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 160.1, 138.1, 137.2, 133.6, 131.8, 129.9, 129.3, 129.2, 127.3, 126.7, 122.3, 121.36, 114.1, 30.1. HRMS MALDI (m/z): calcd for $C_{16}H_{13}NOSe$ $[M + H]^+$: 316.0241, found: 316.0242.

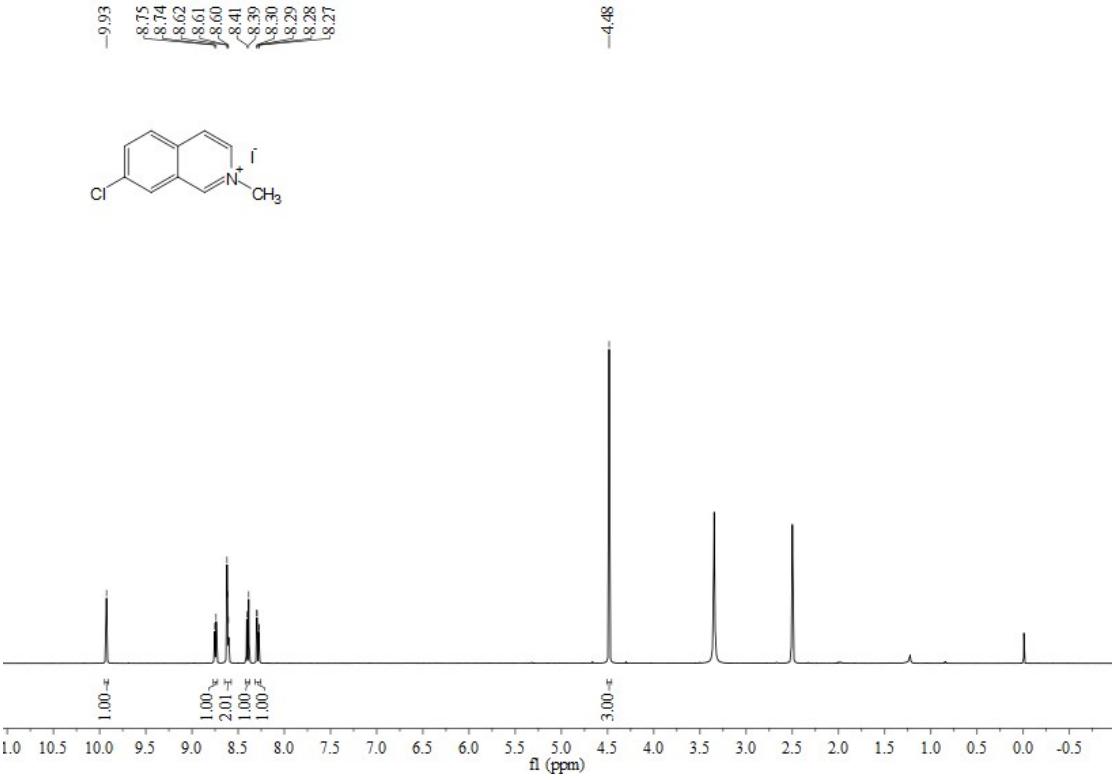
1,3-Dimethyl-1,3-dihydro-2*H*-benzo[*d*]imidazol-2-one (8b)



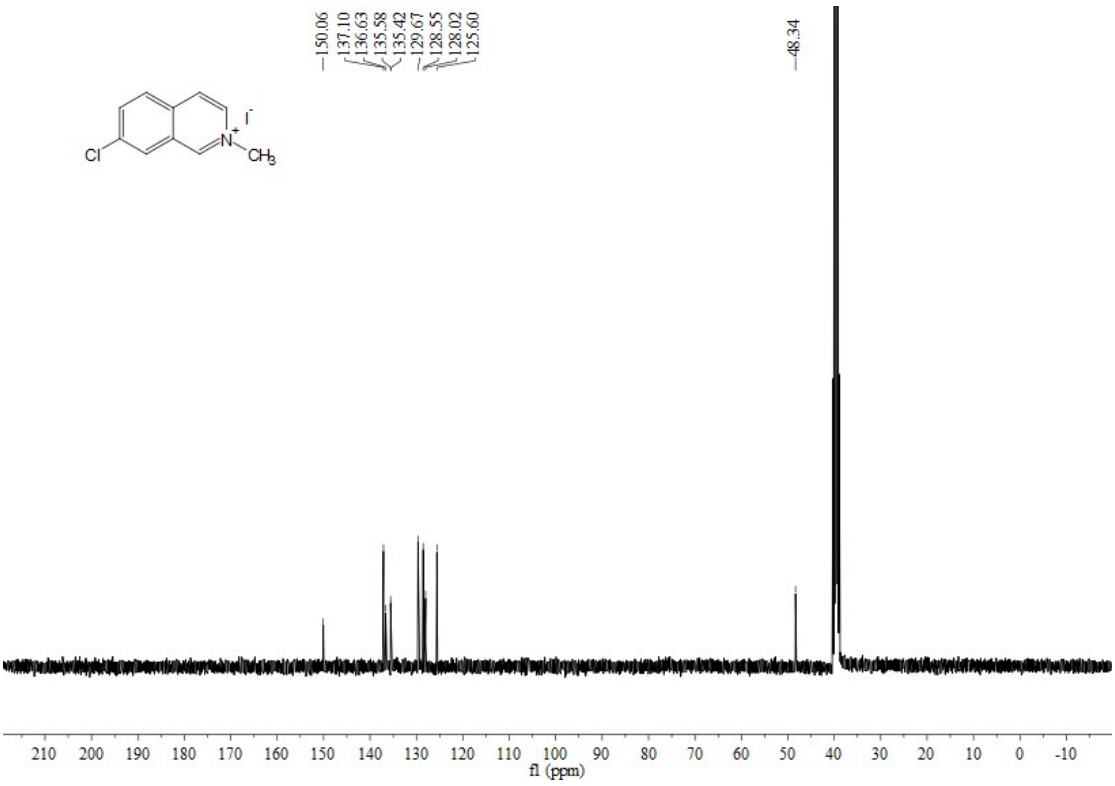
Flash column chromatography on silica gel (eluent: PE/EtOAc = 3/1, v/v) to afford **8b**. Brown solid (45.7 mg, 94%), mp 84.2-84.6 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.08 (dd, J = 5.7, 3.2 Hz, 2H), 6.95 (dd, J = 5.7, 3.3 Hz, 2H), 3.40 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 155.0, 129.9, 121.2, 107.4, 27.2. HRMS MALDI (m/z): calcd for $C_9H_{10}N_2O$ $[M + H]^+$: 163.0871, found: 163.0869.

3. NMR spectra for new compounds

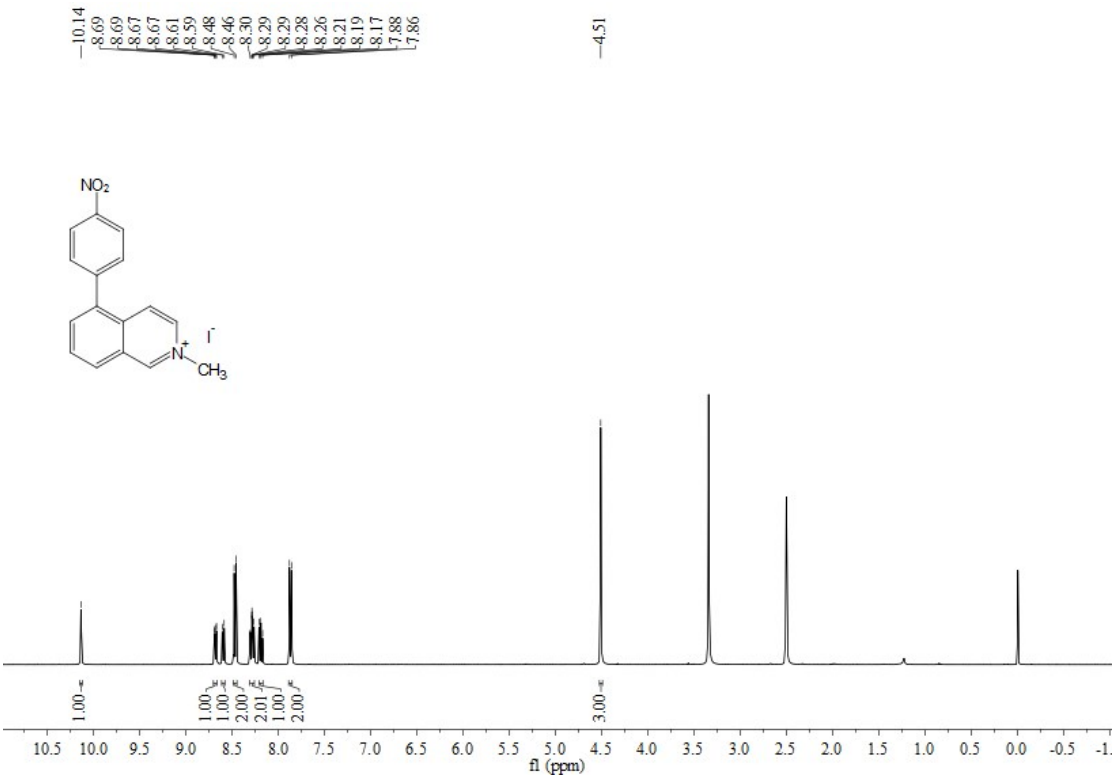
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **1m**



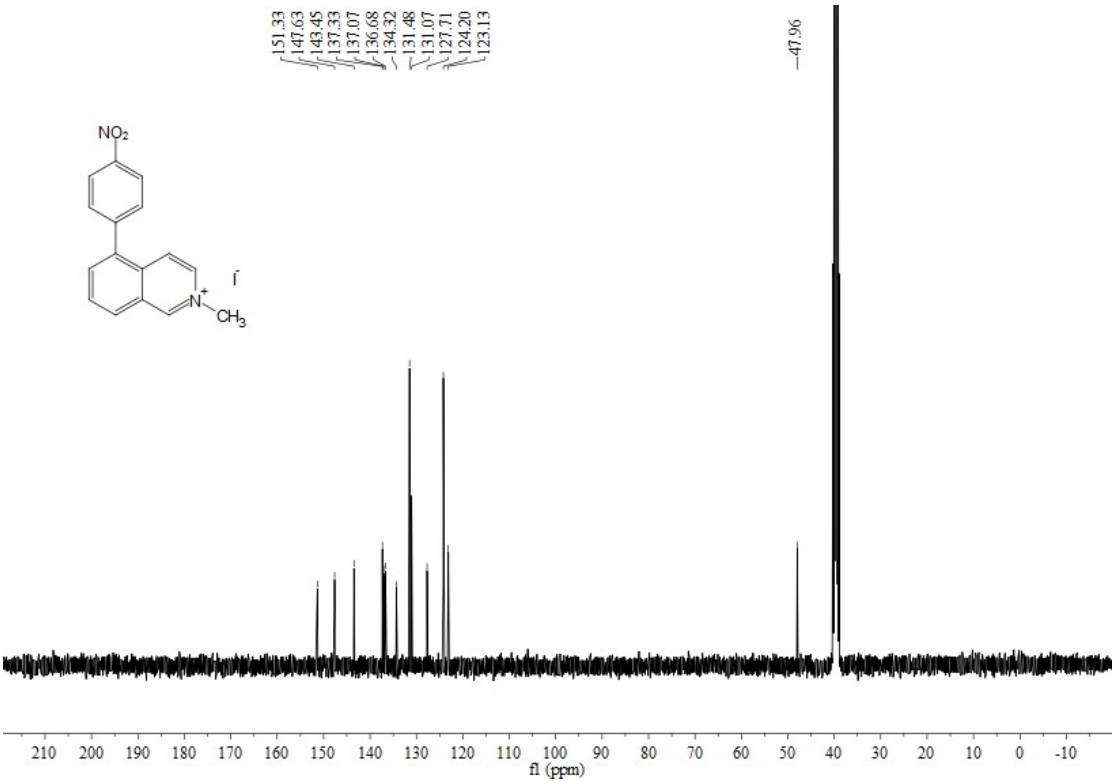
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **1m**



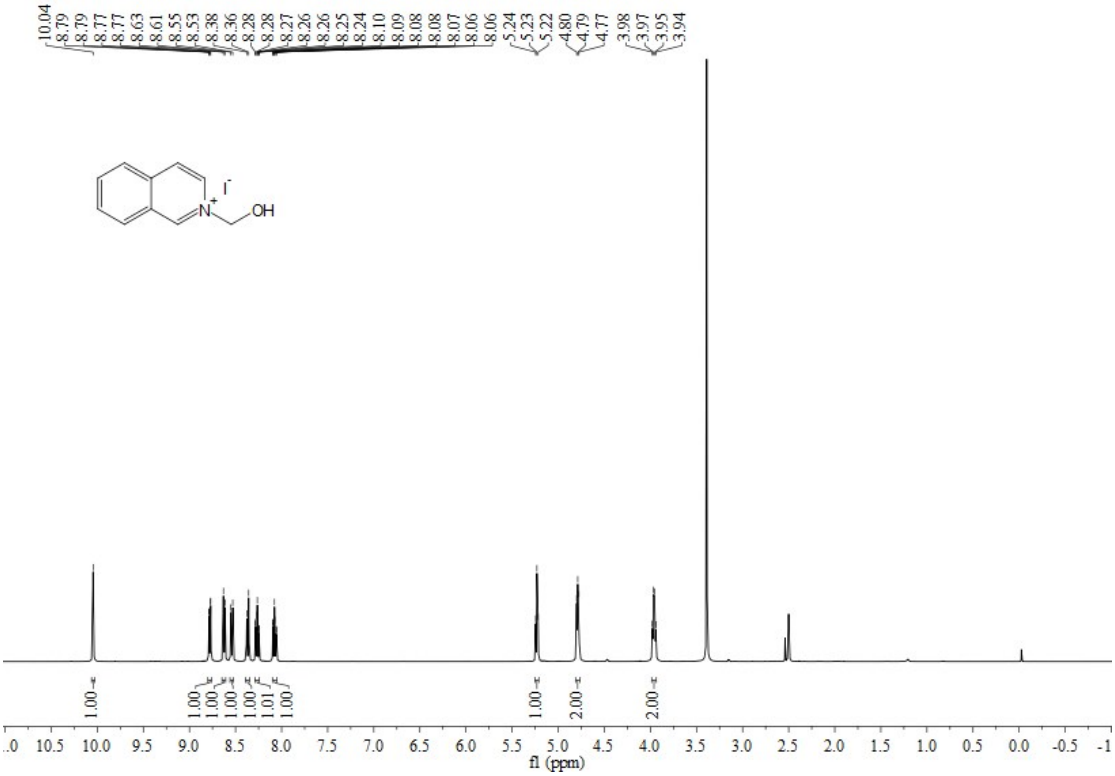
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **1p**



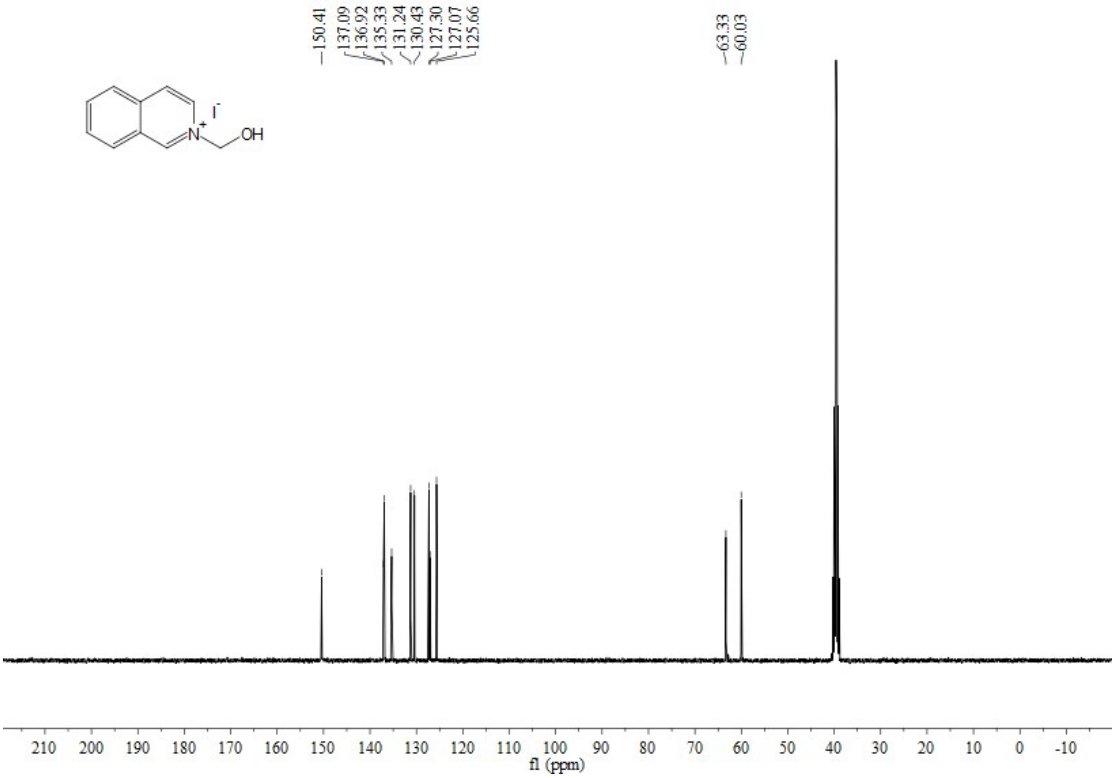
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **1p**



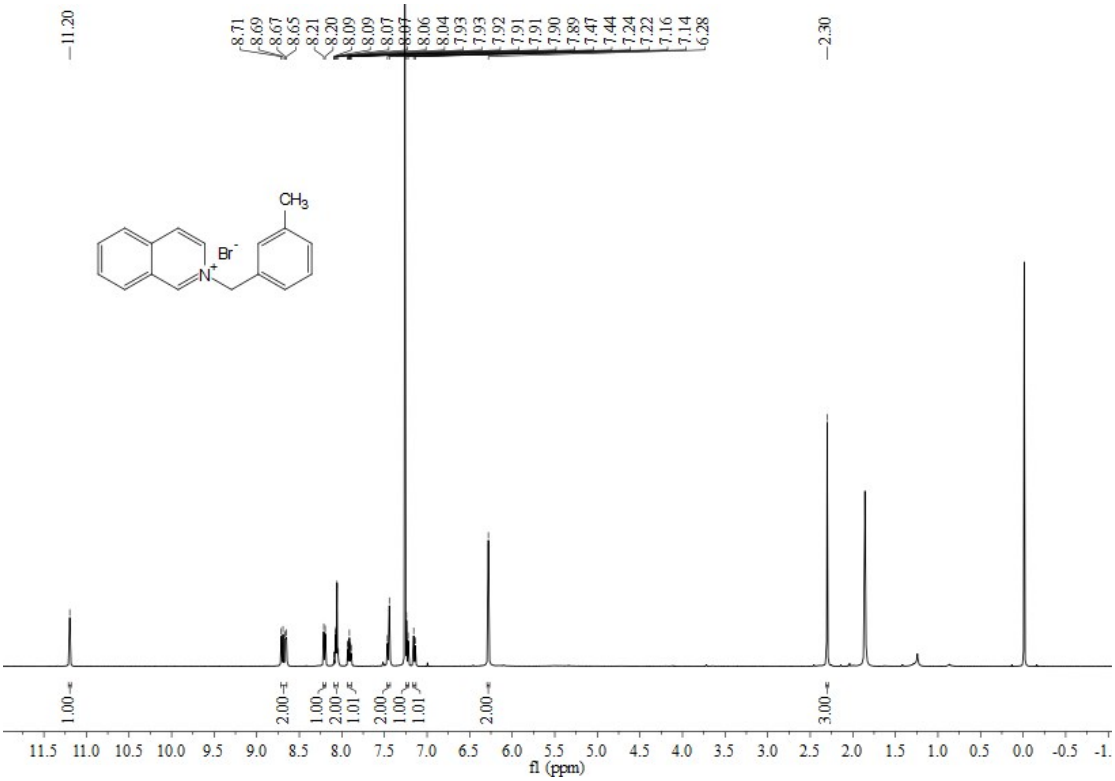
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4h**



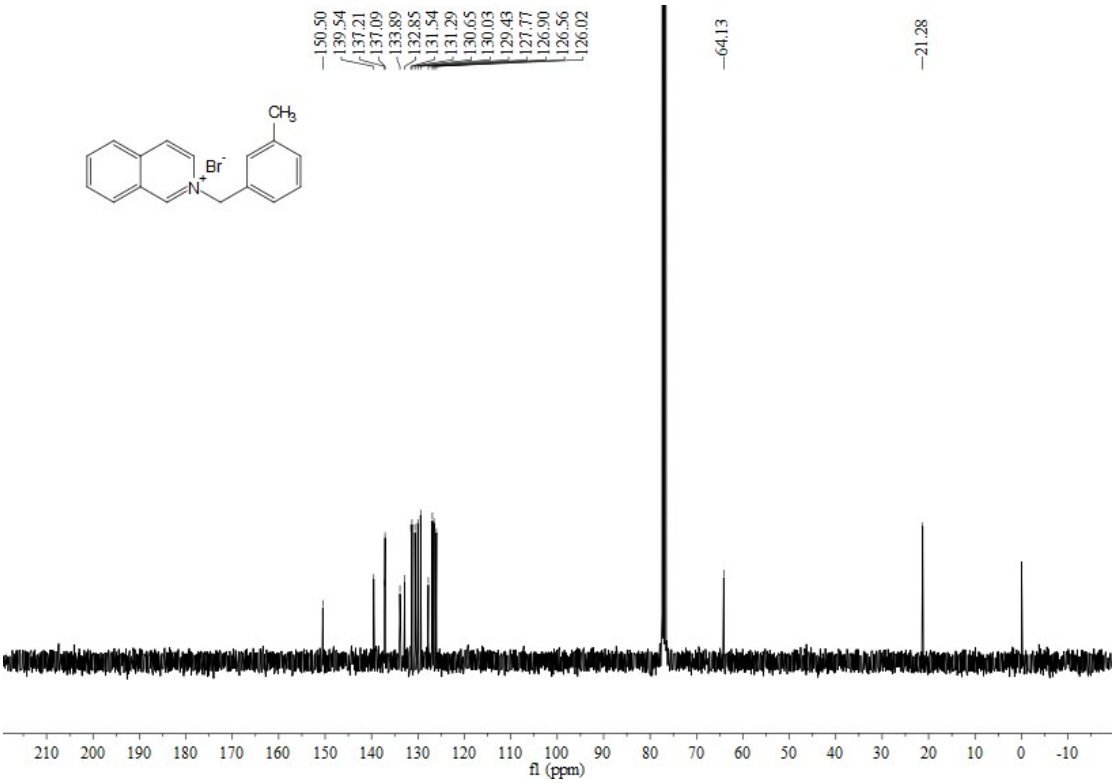
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **4h**



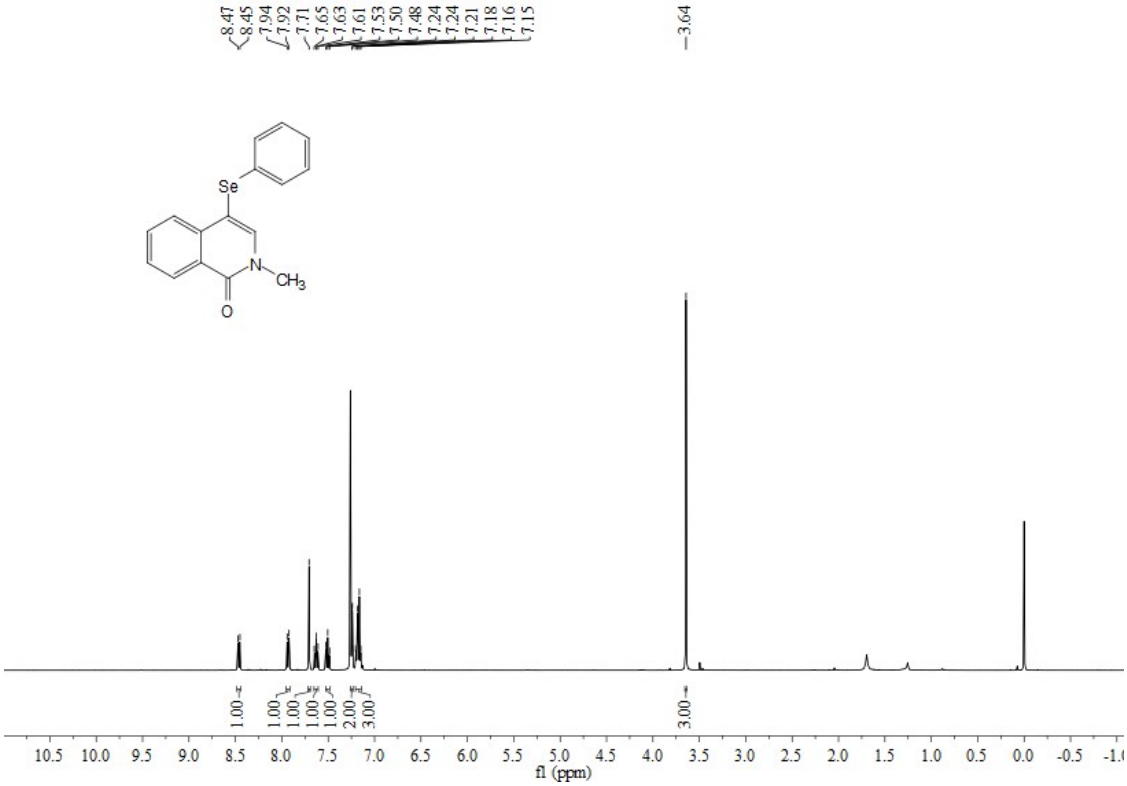
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4p**



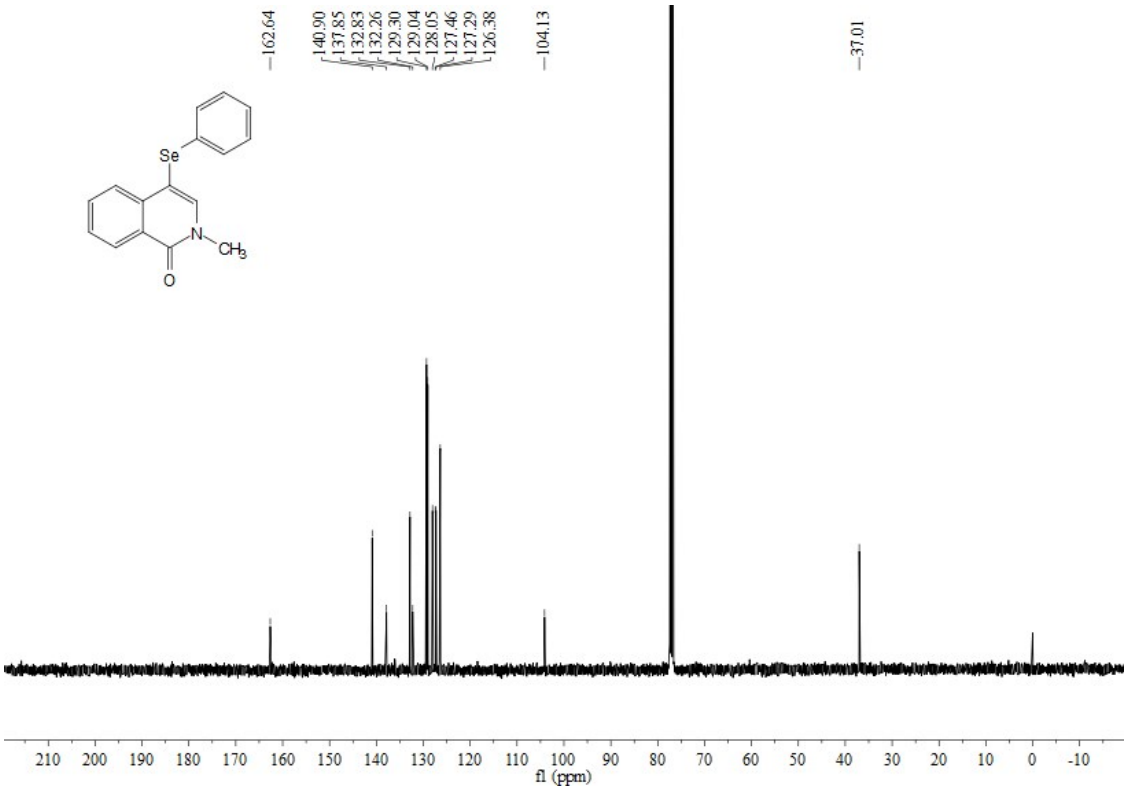
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4p**



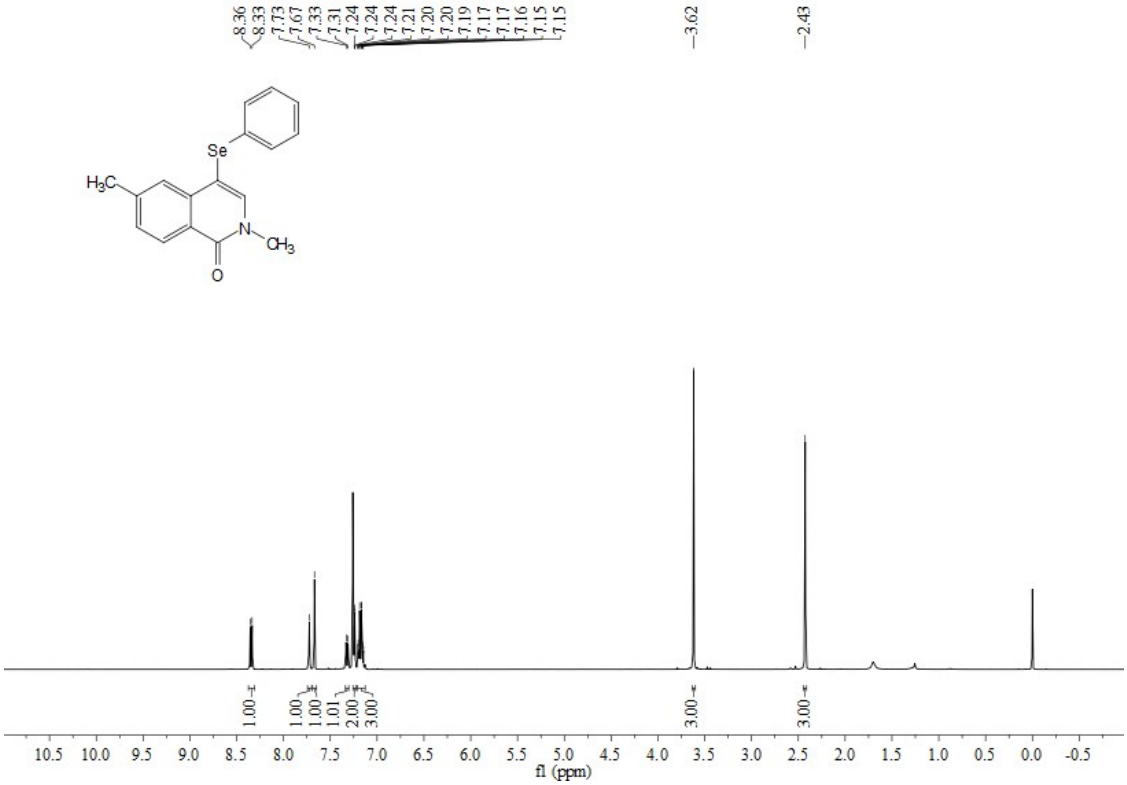
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3a**



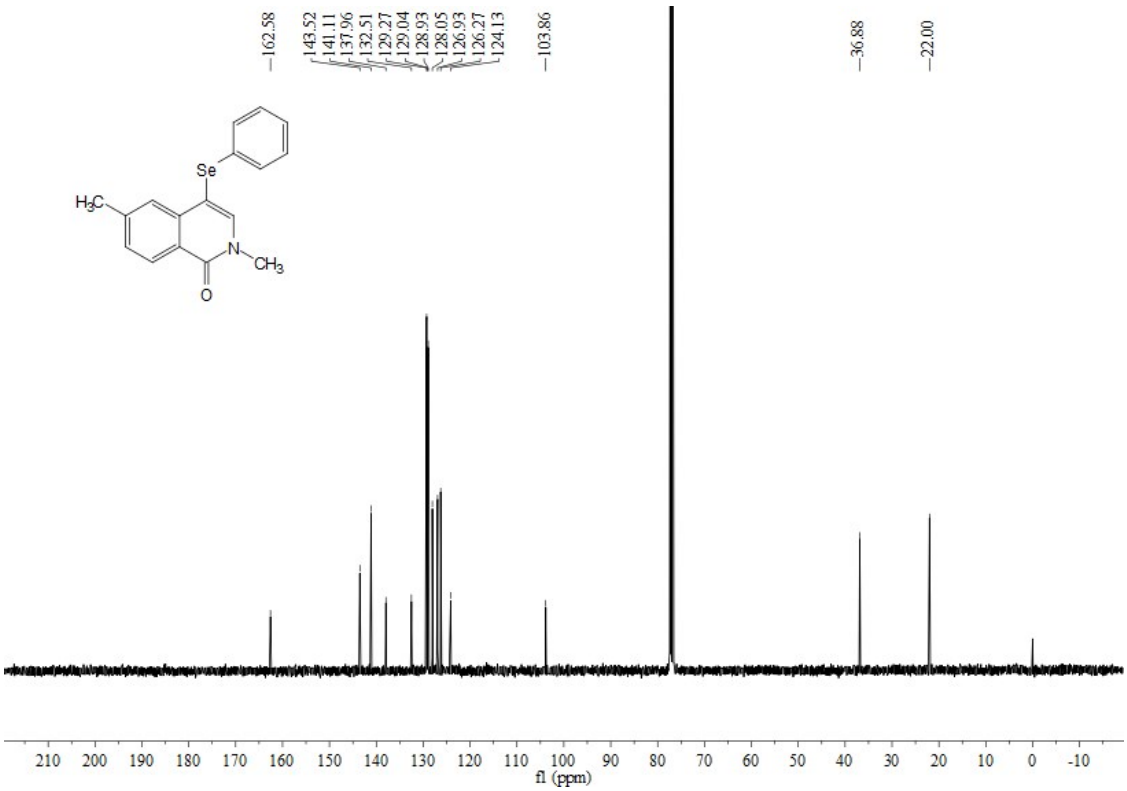
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3a**



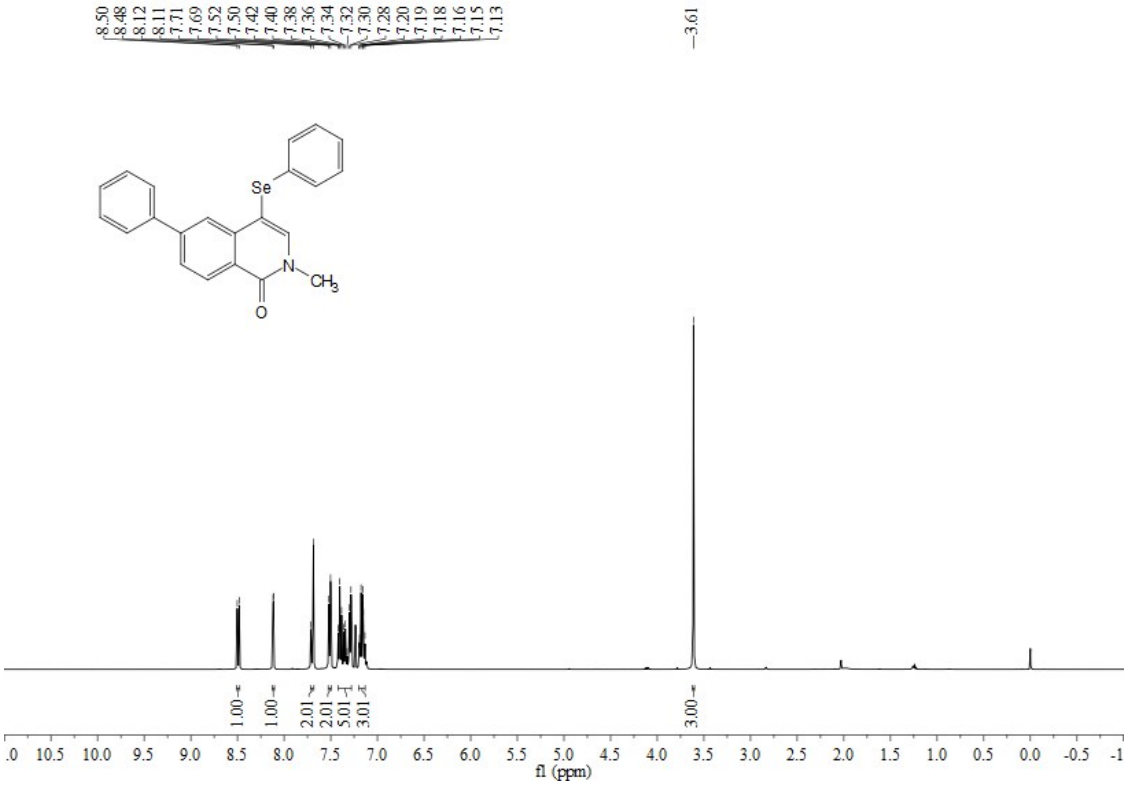
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3b**



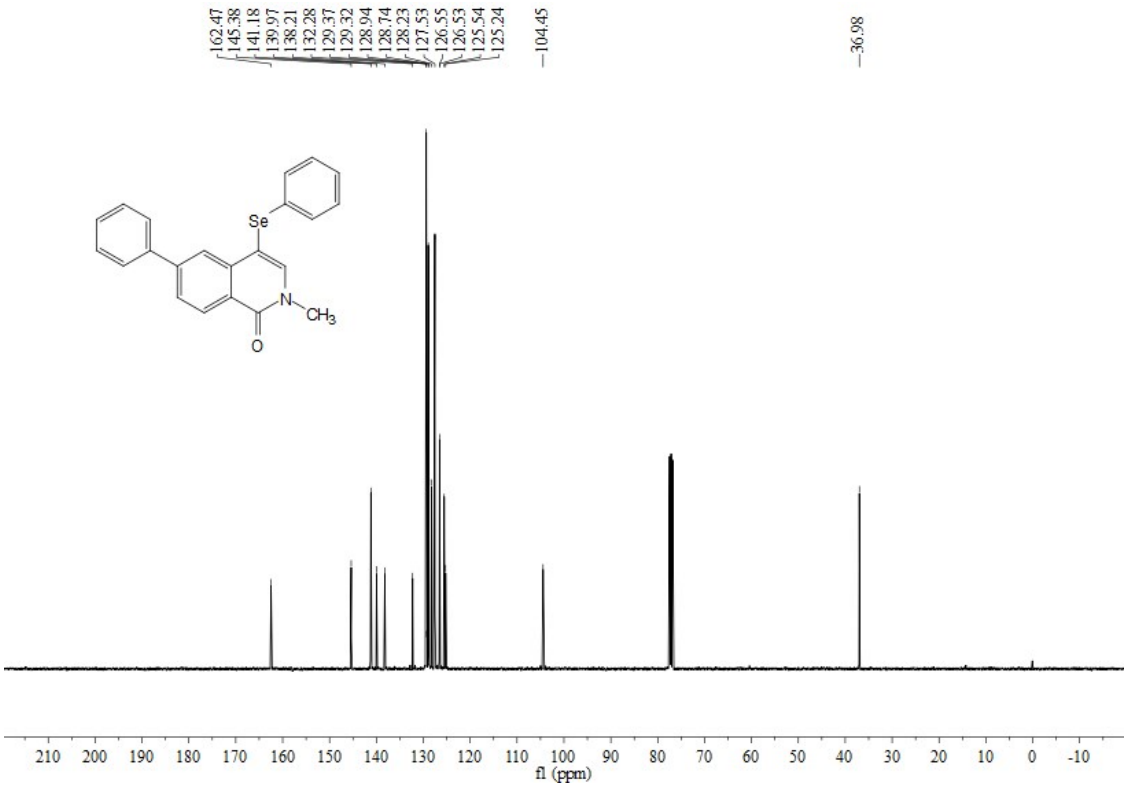
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3b**



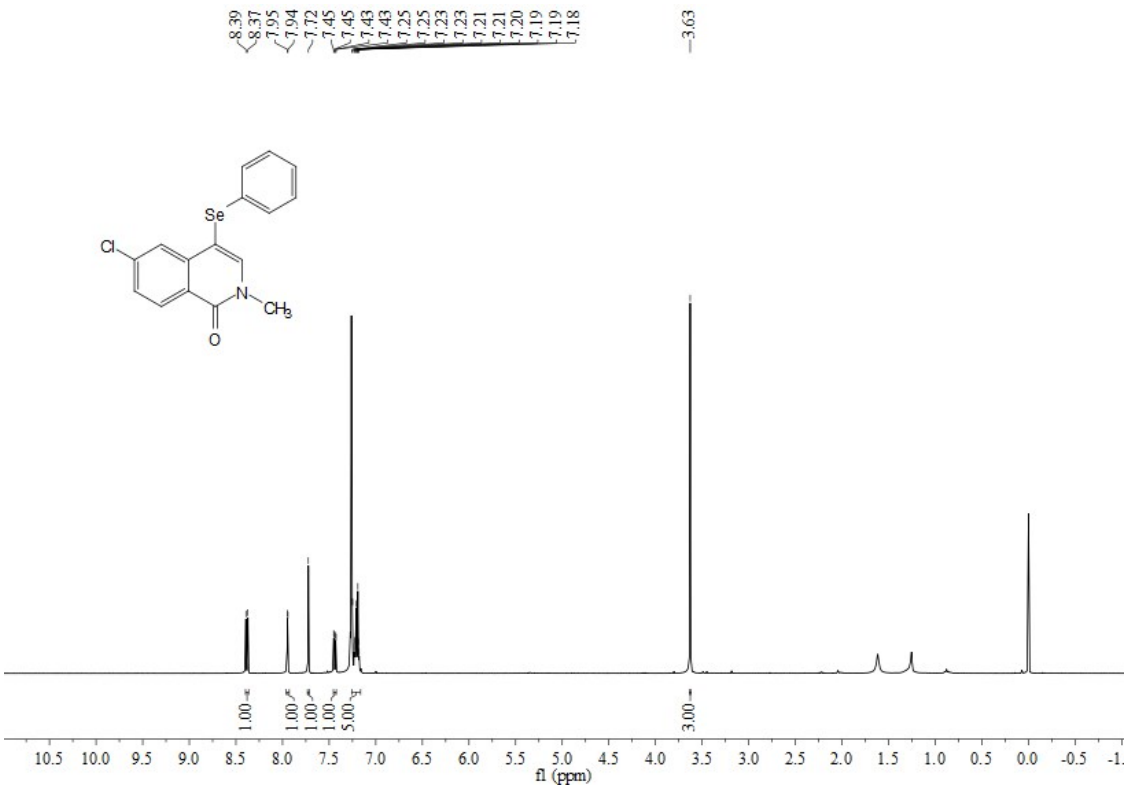
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3c**



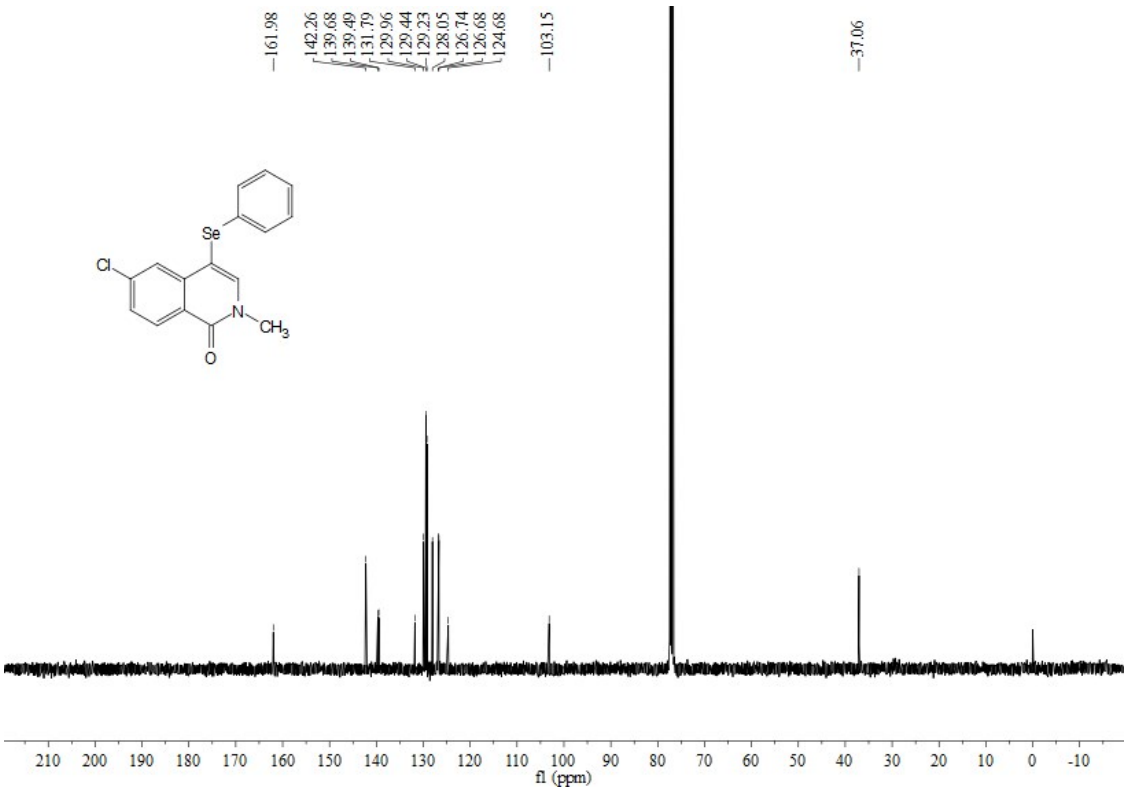
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3c**



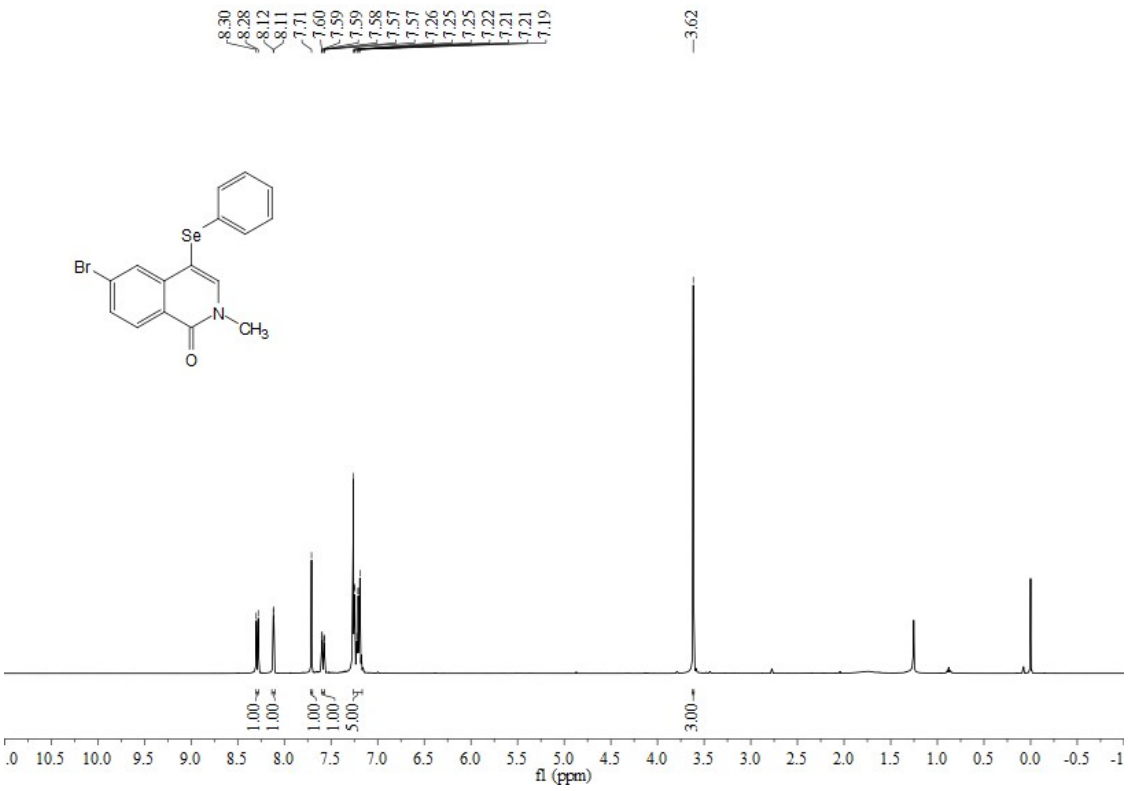
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3d**



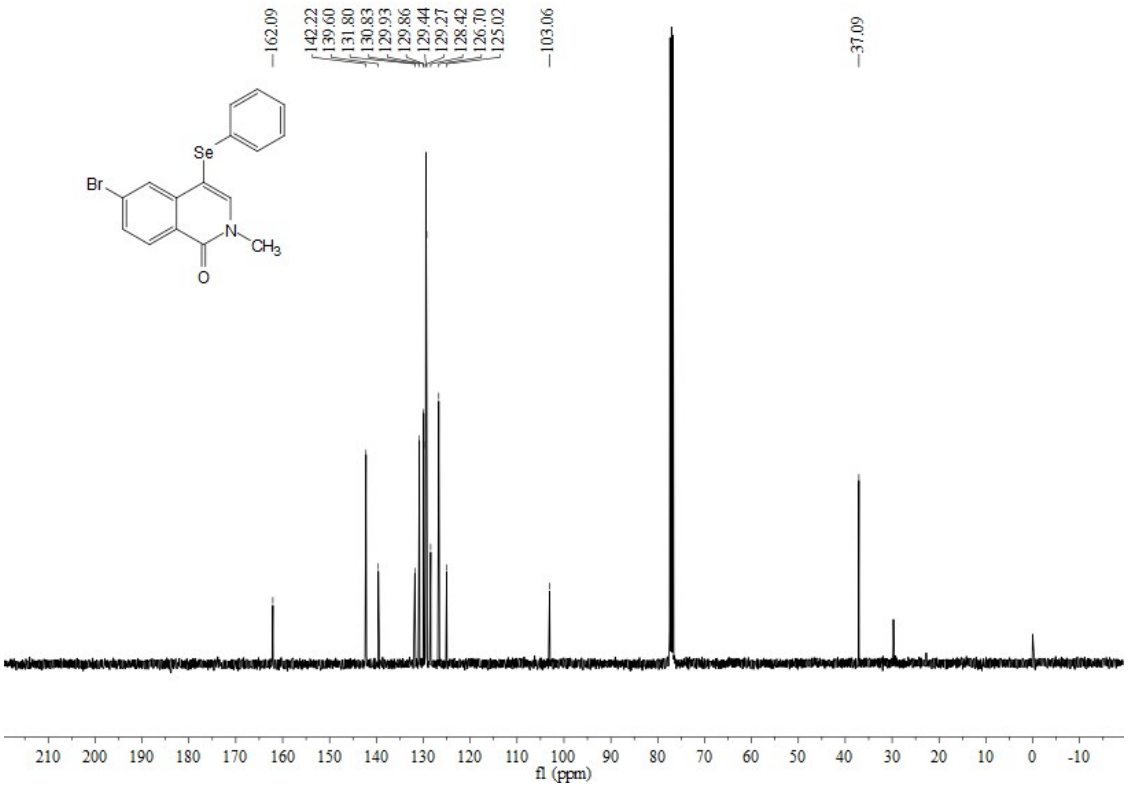
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3d**



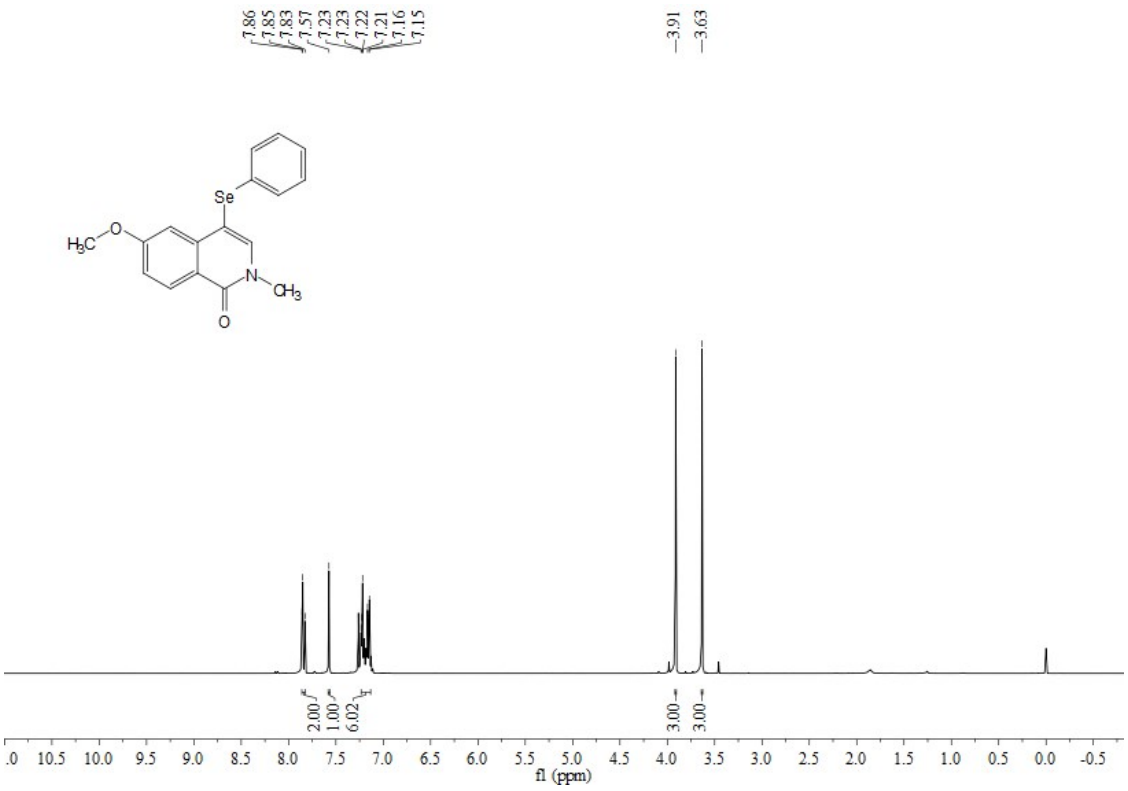
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3e**



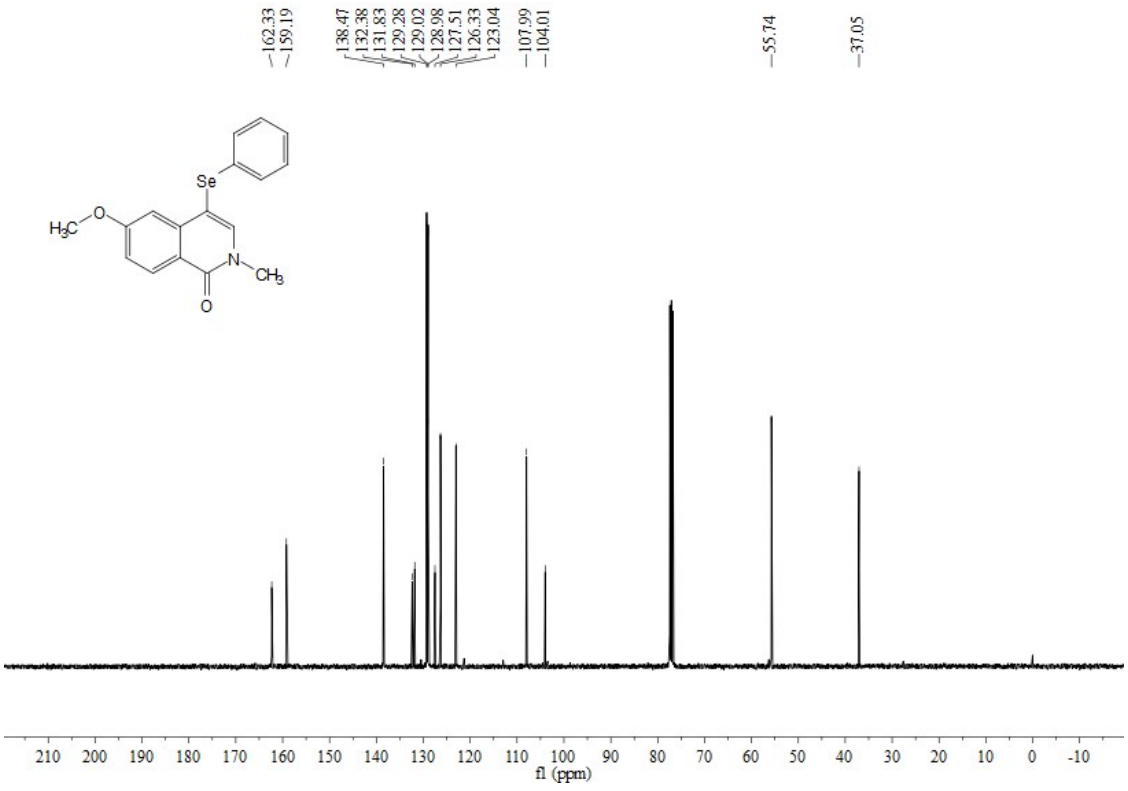
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3e**



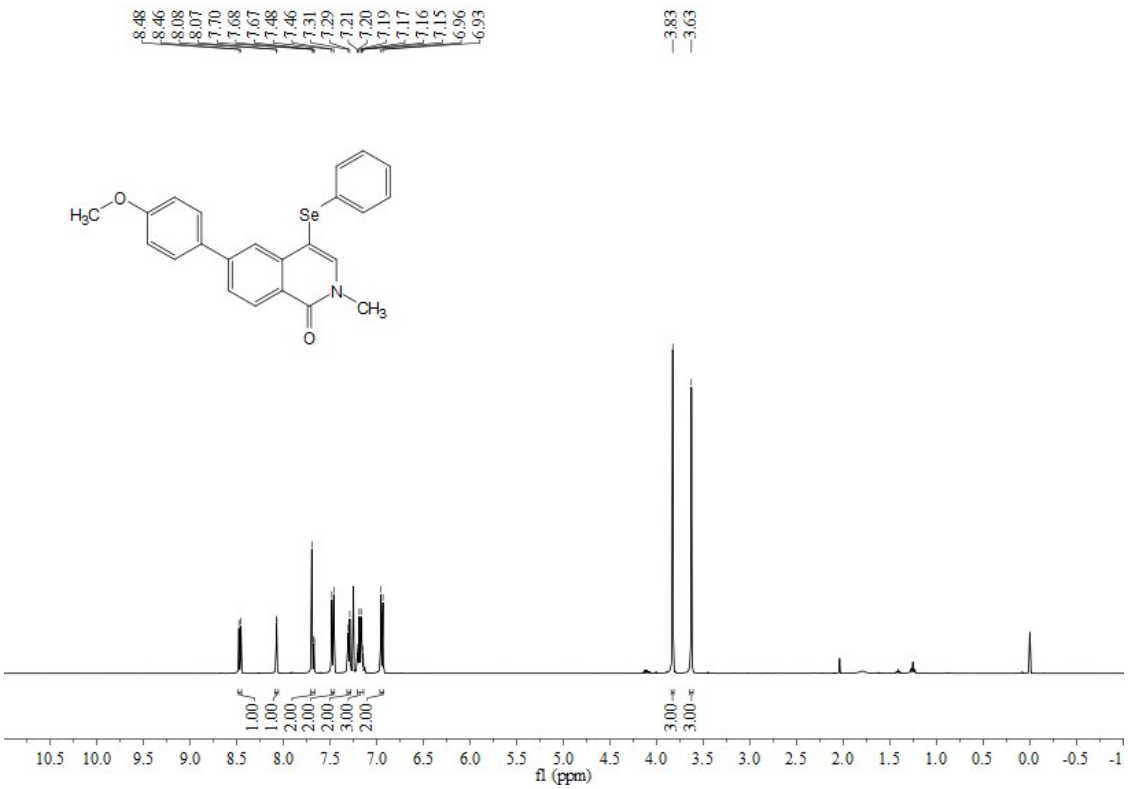
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3f**



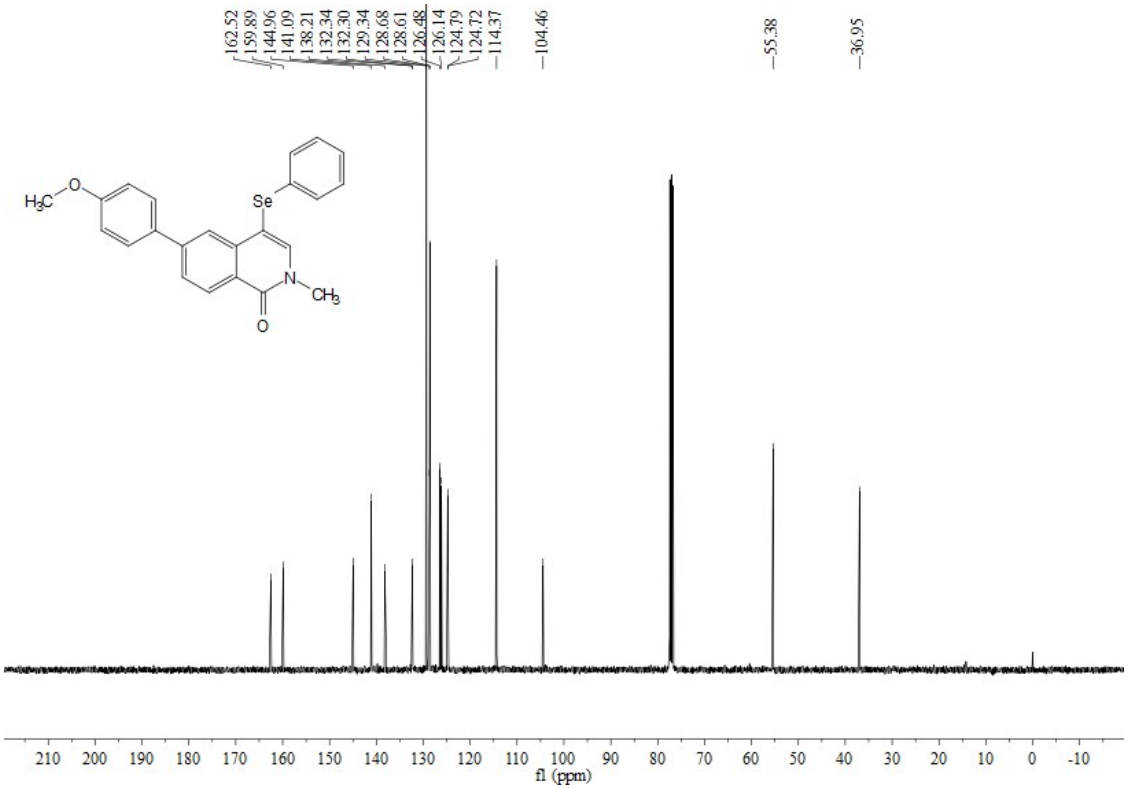
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3f**



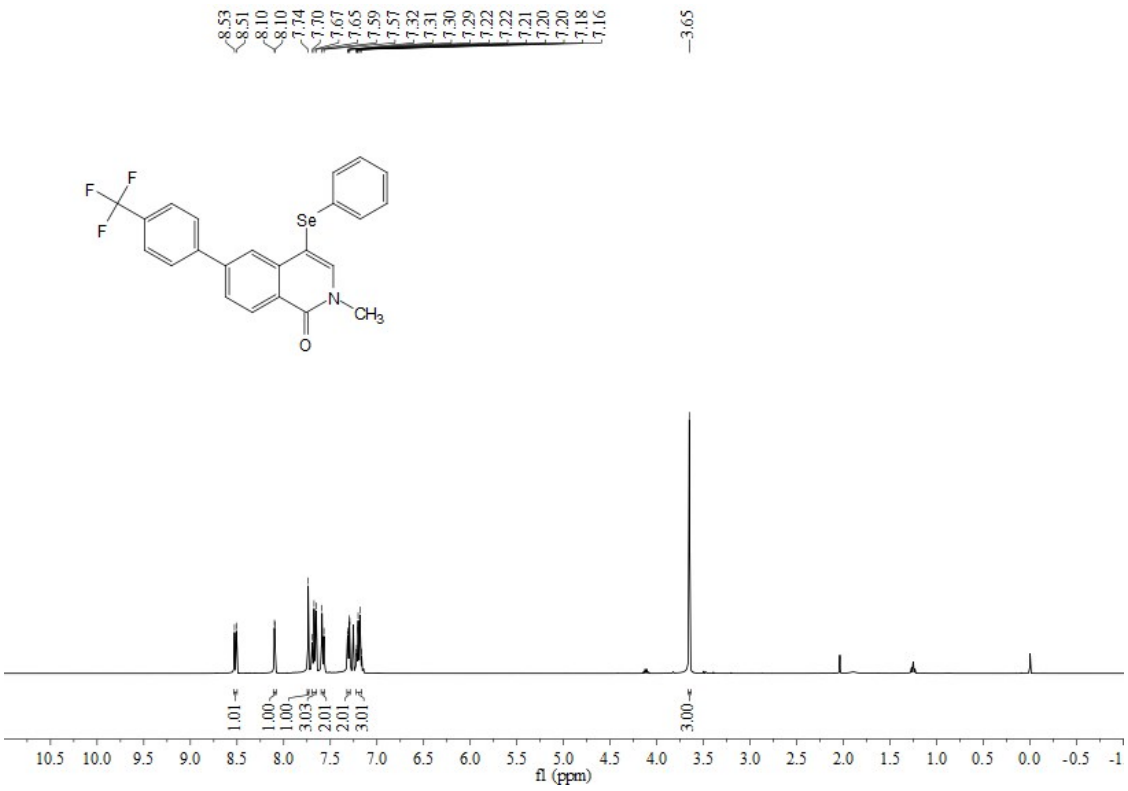
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3g**



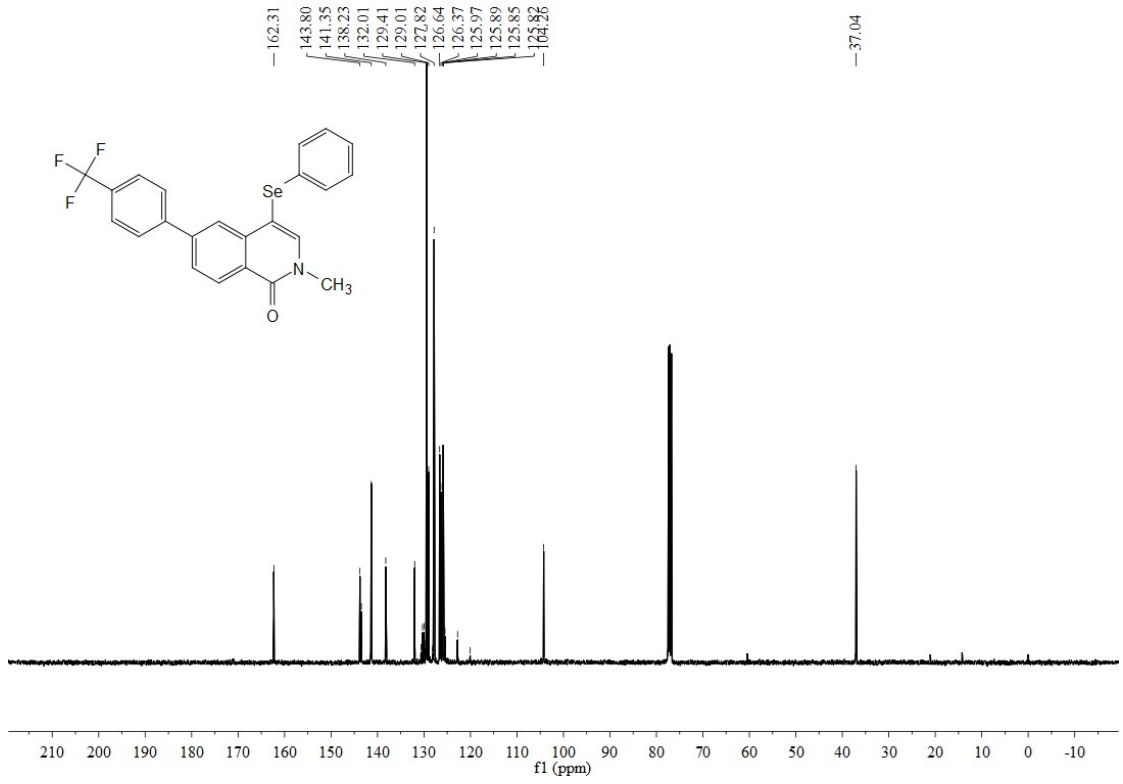
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3g**



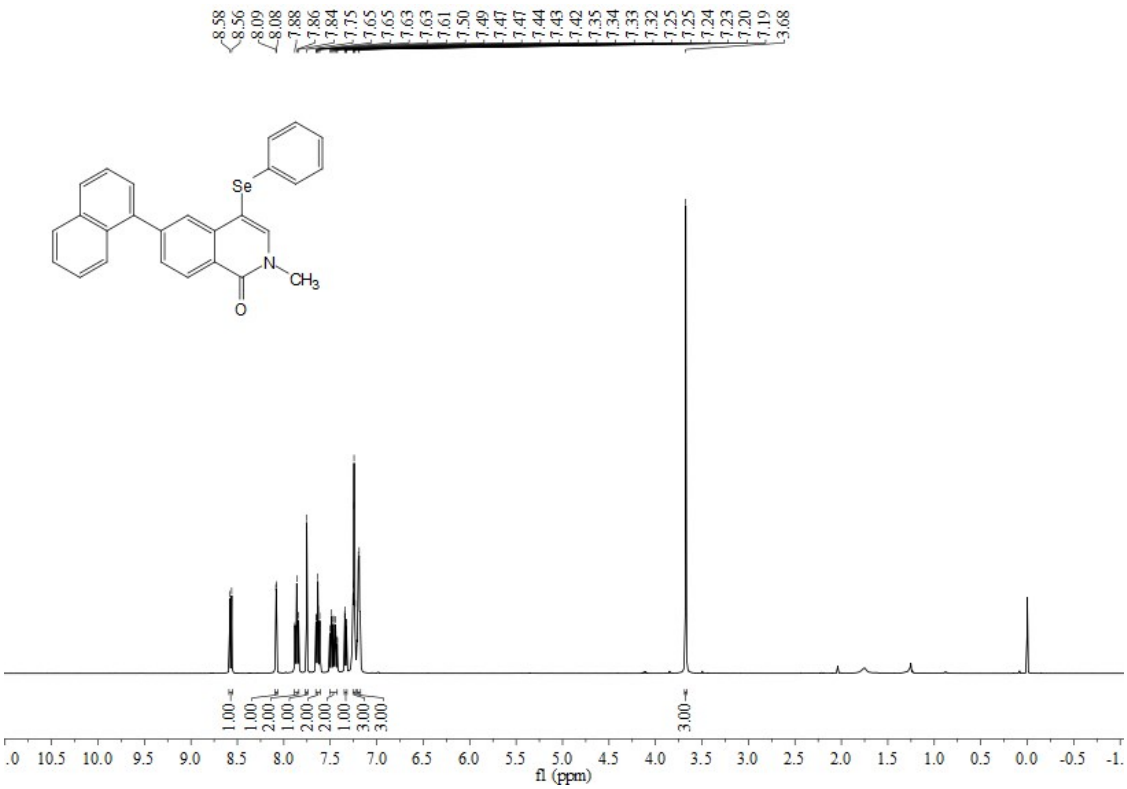
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3h**



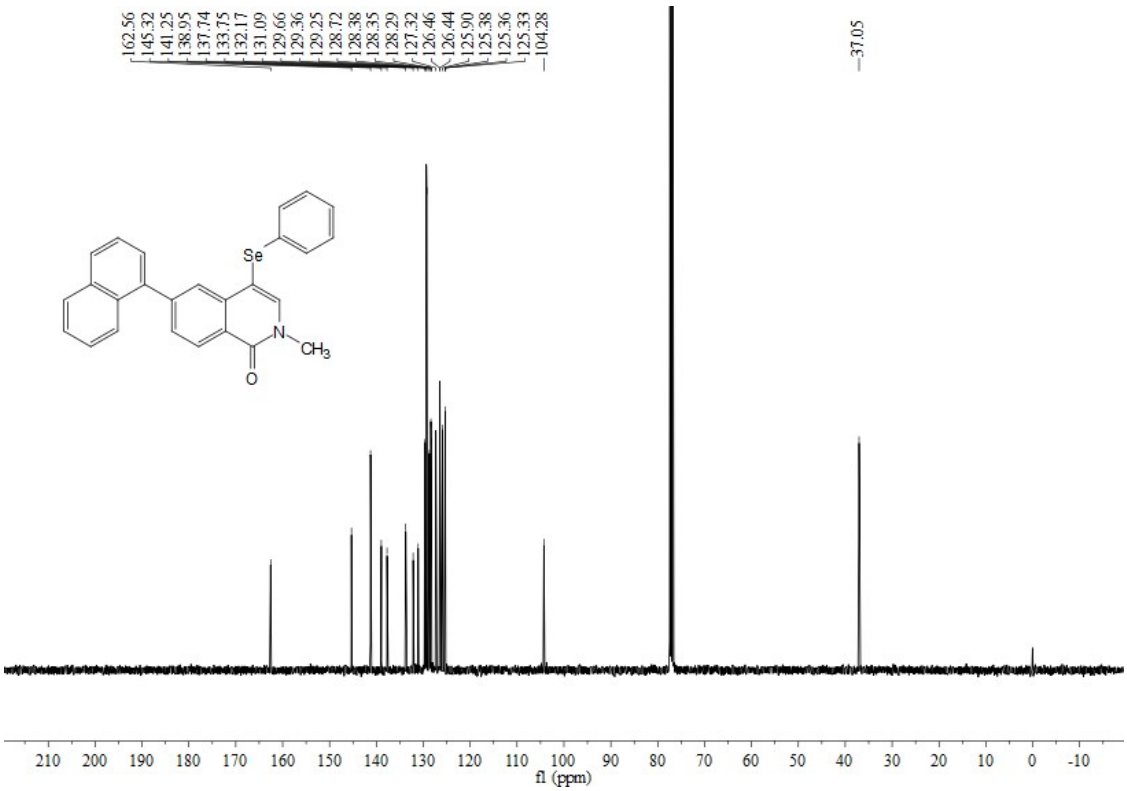
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3h**



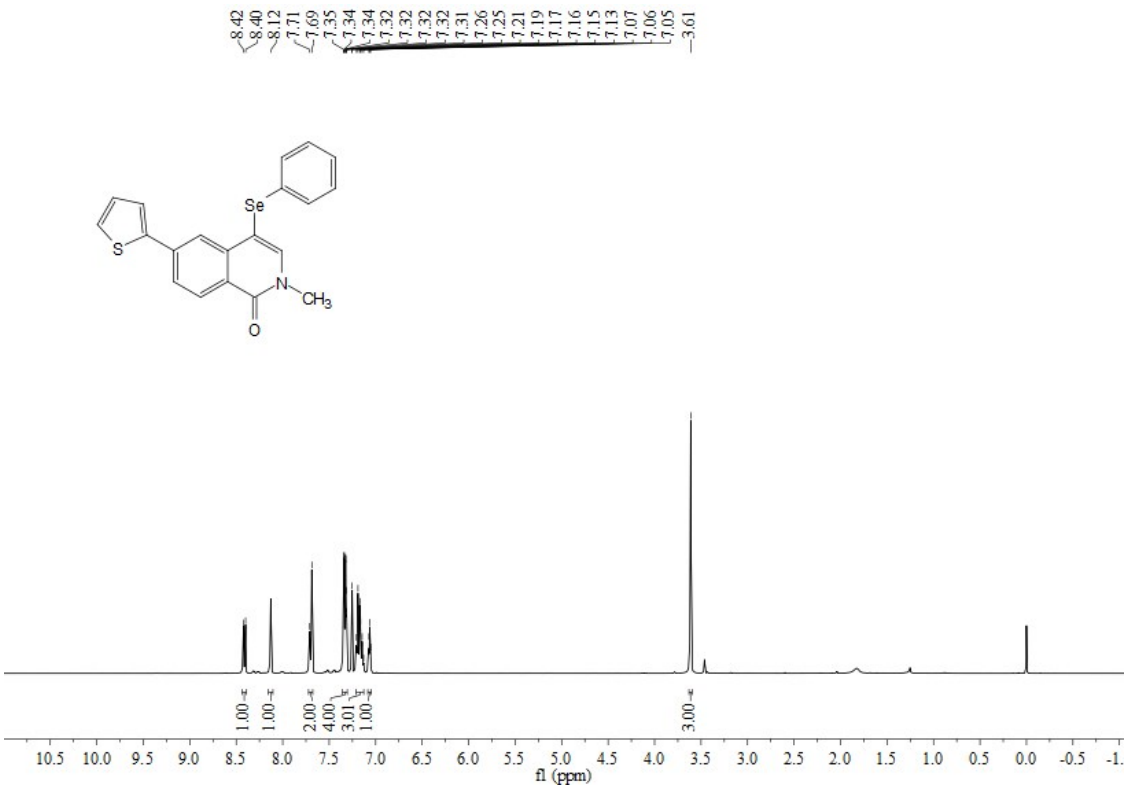
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3i**



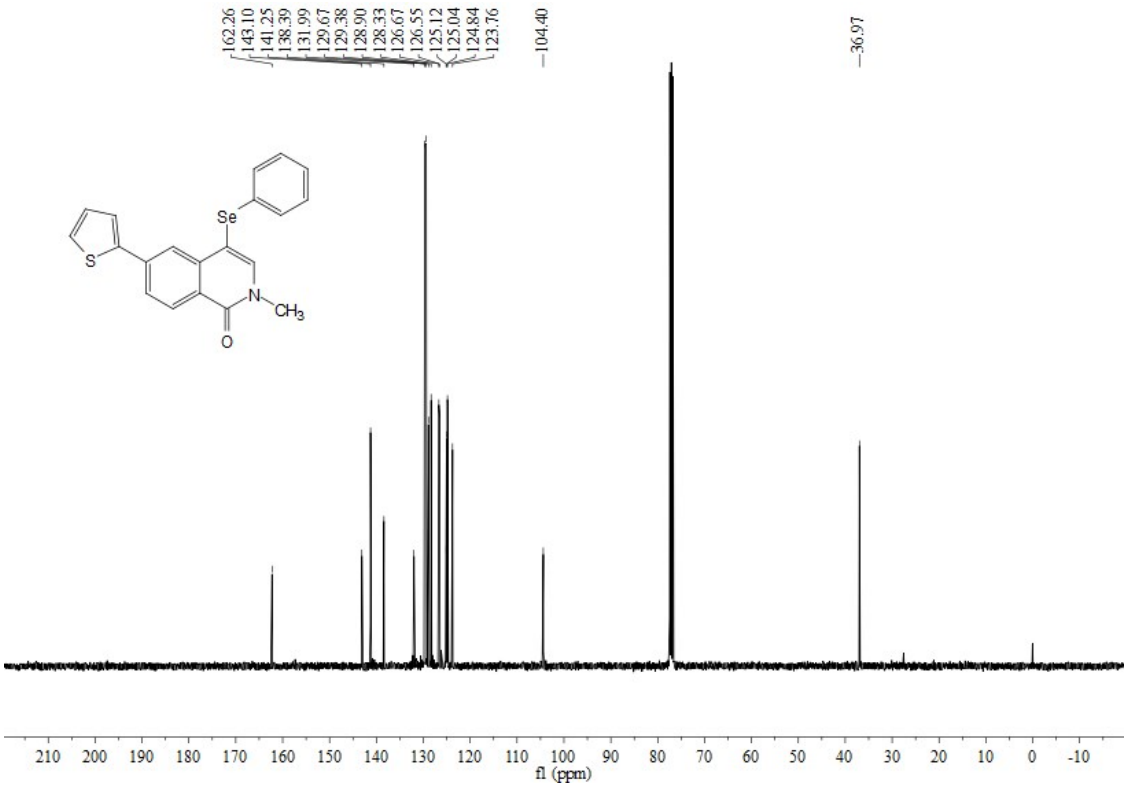
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3i**



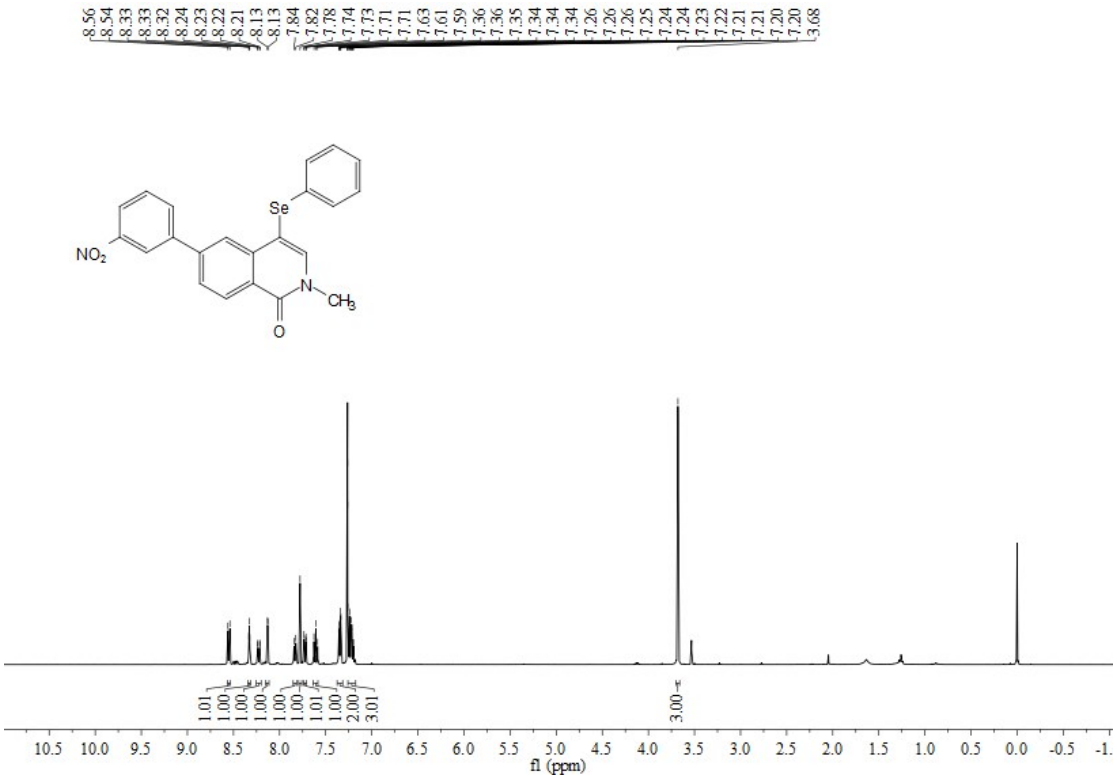
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3j**



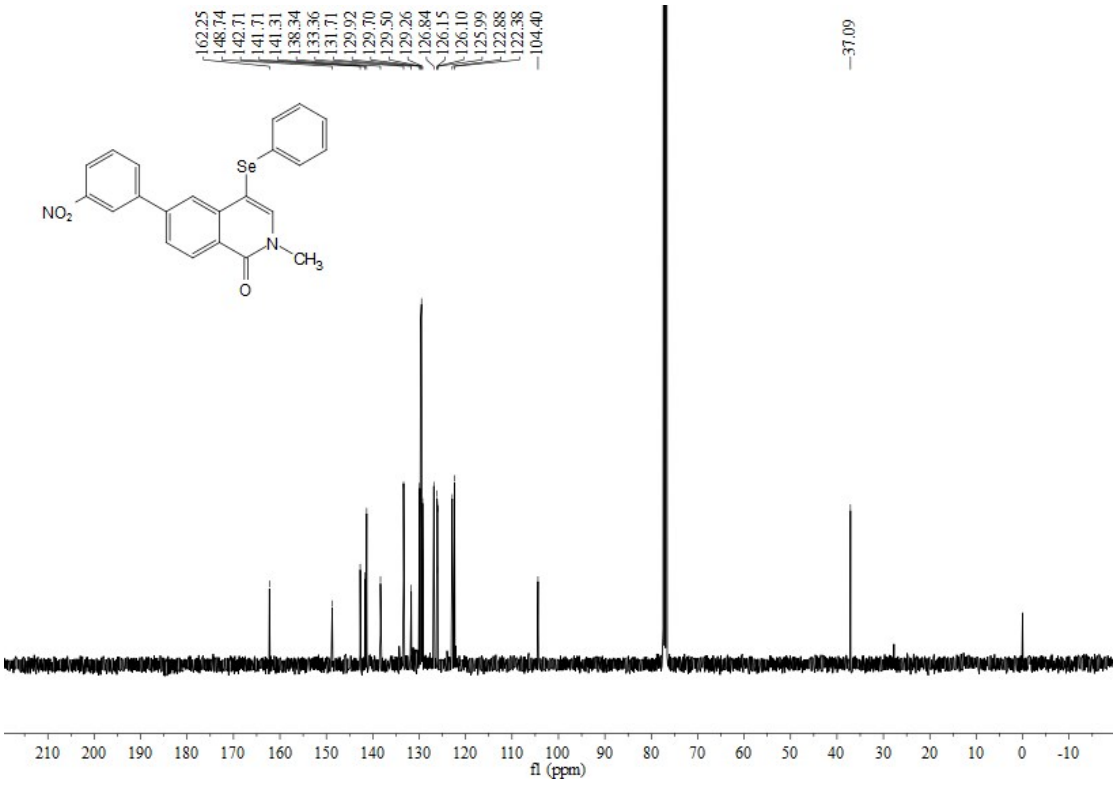
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3j**



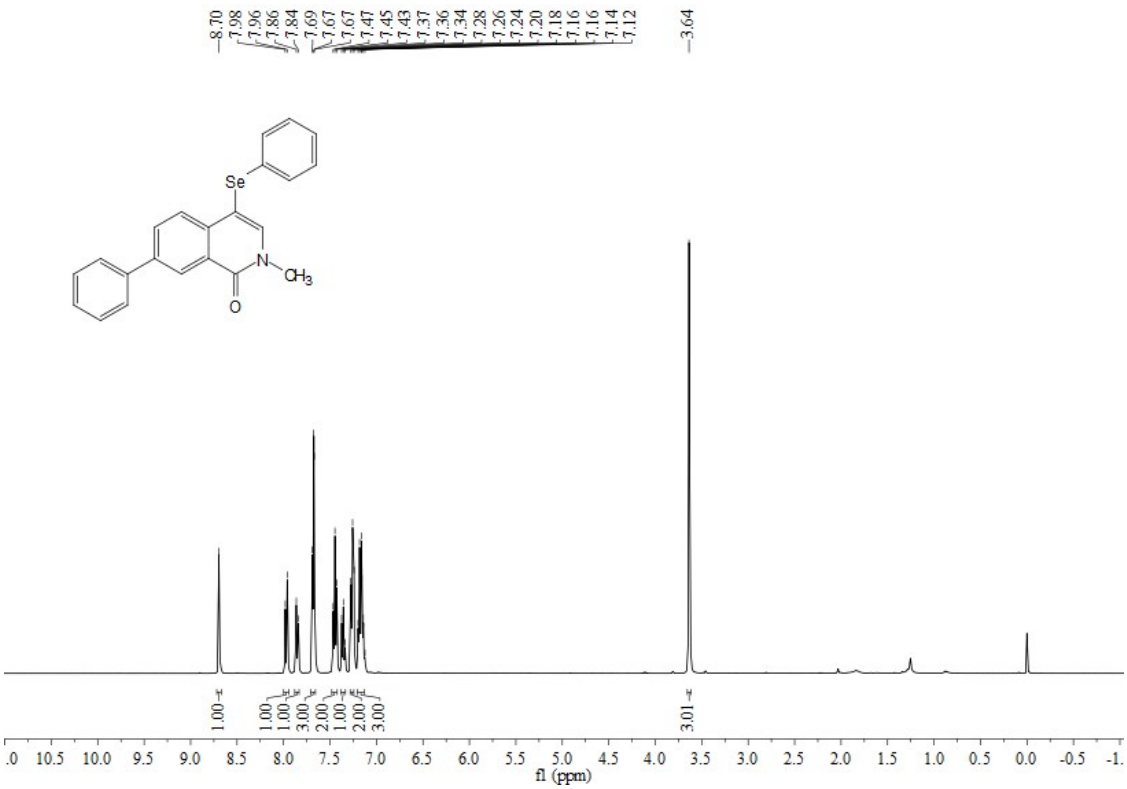
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3k**



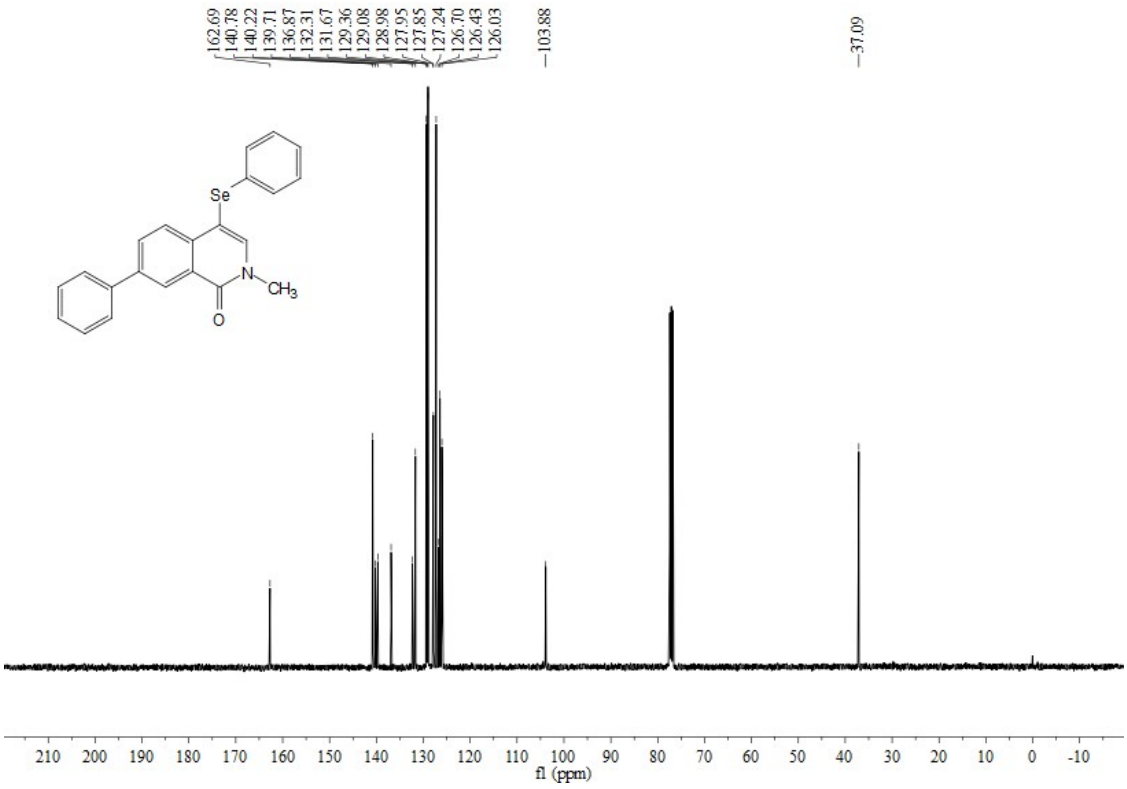
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3k**



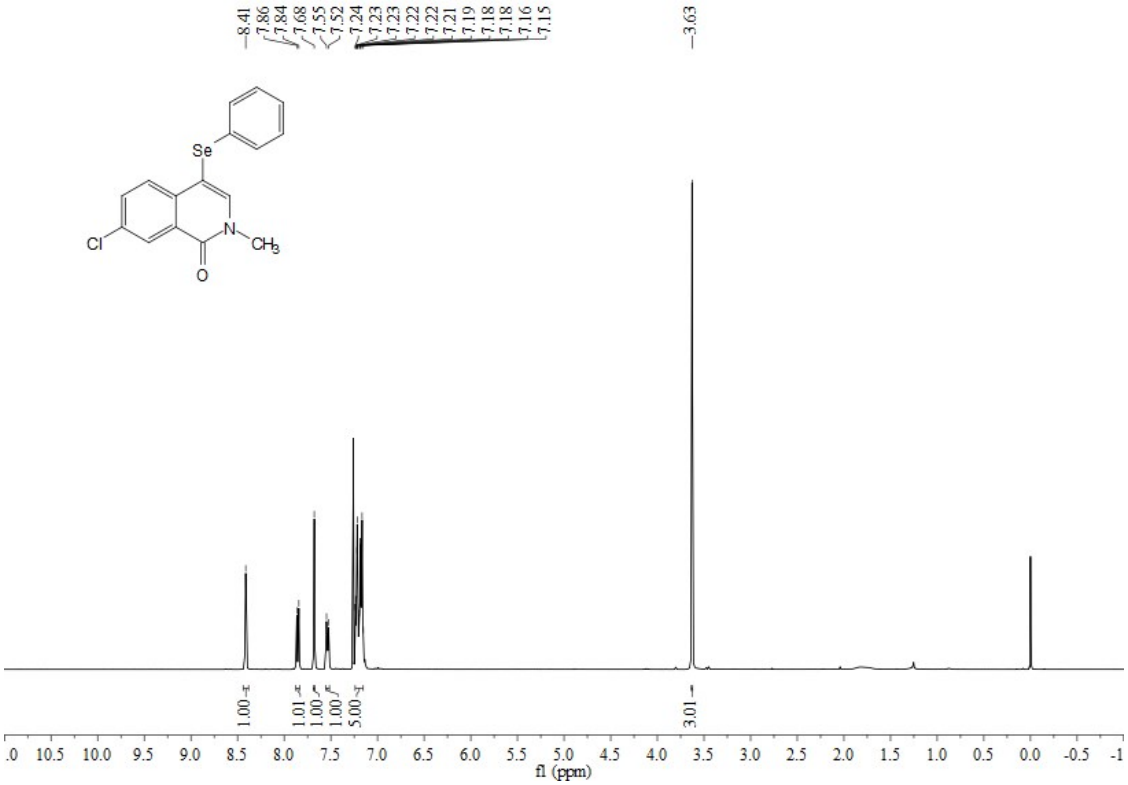
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3l**



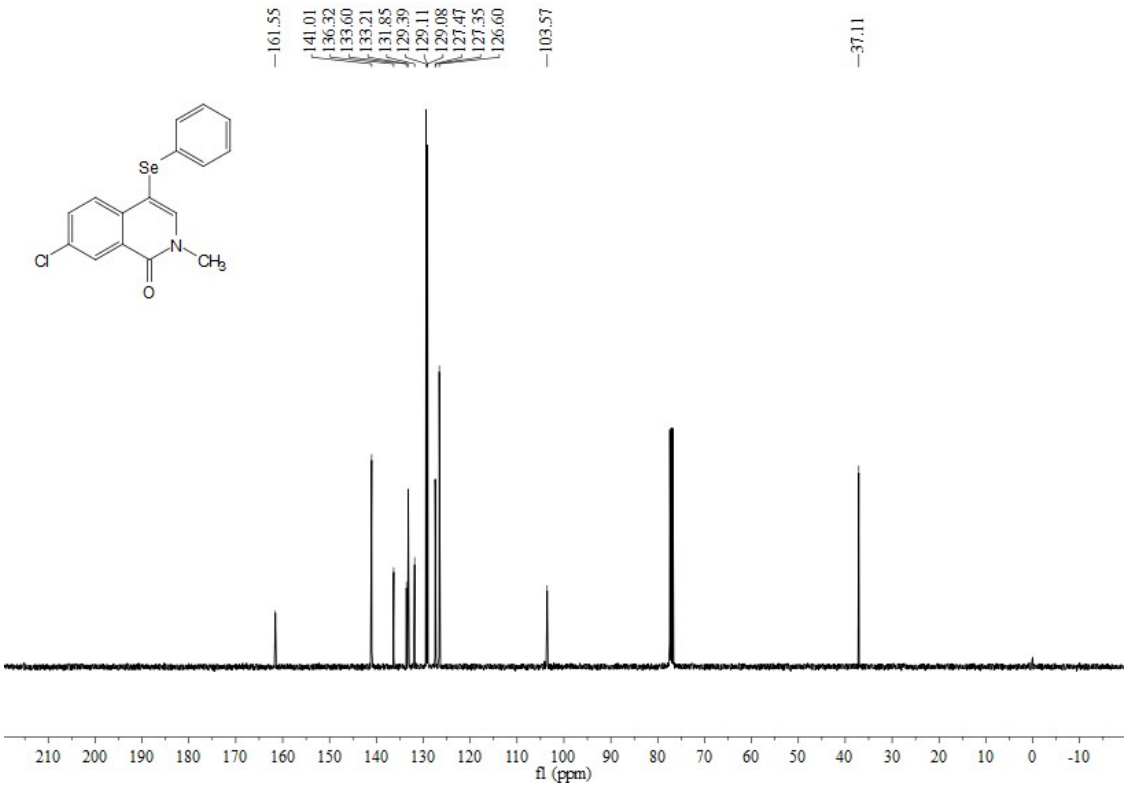
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3l**



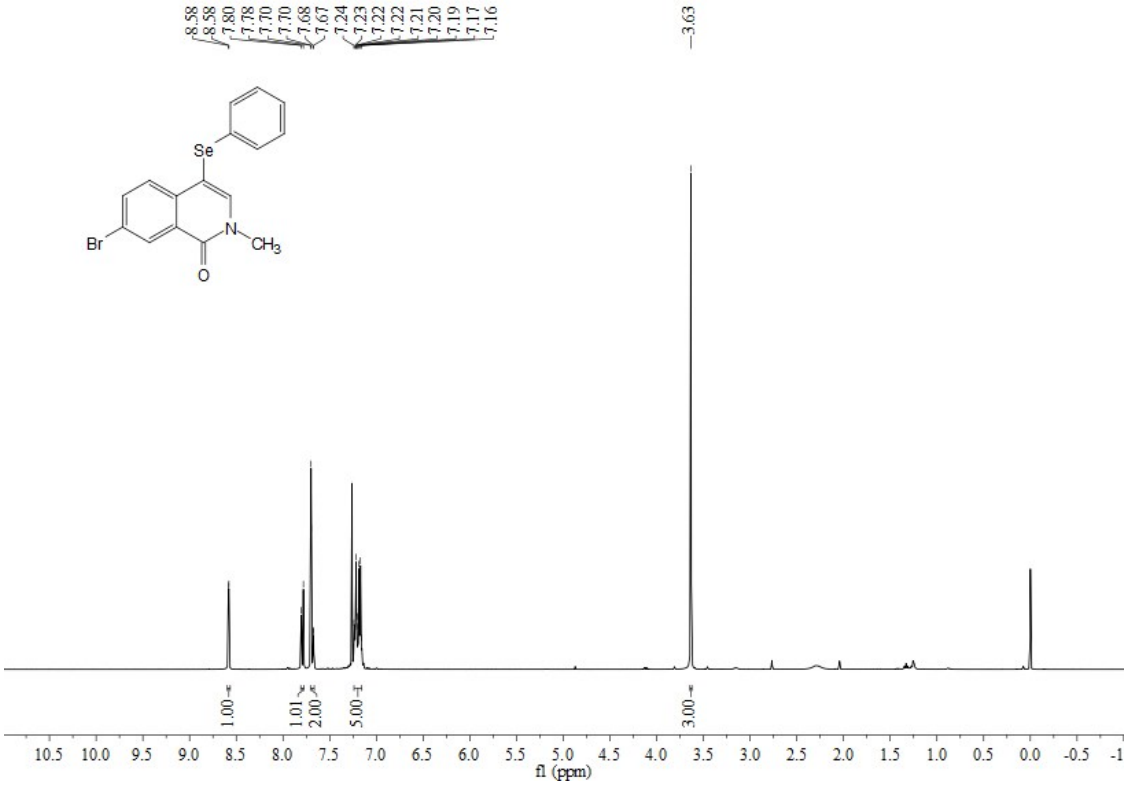
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3m**



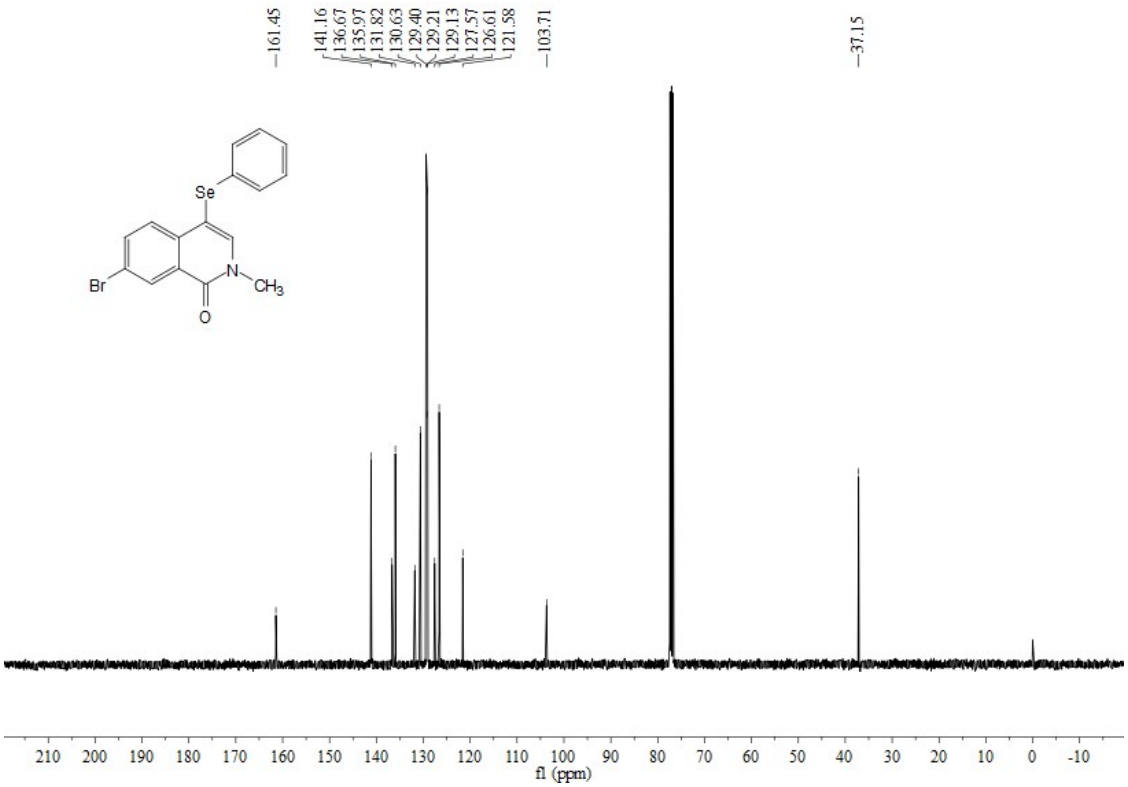
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3m**



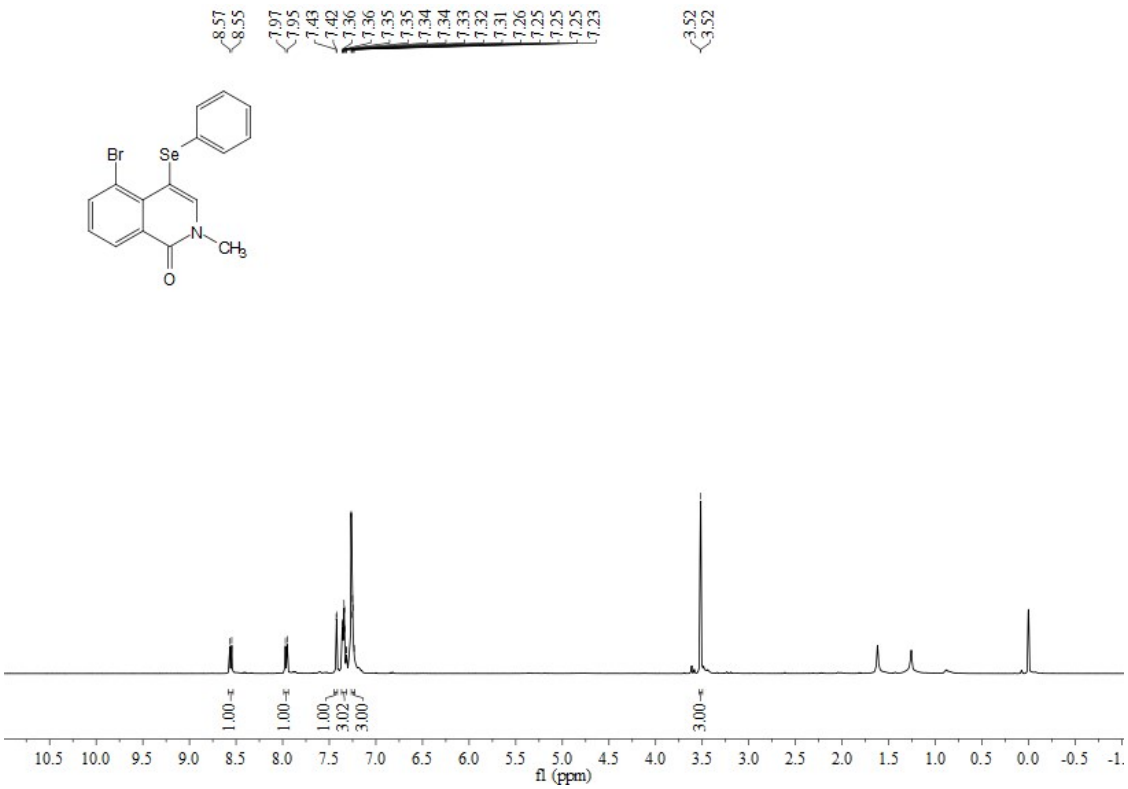
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3n**



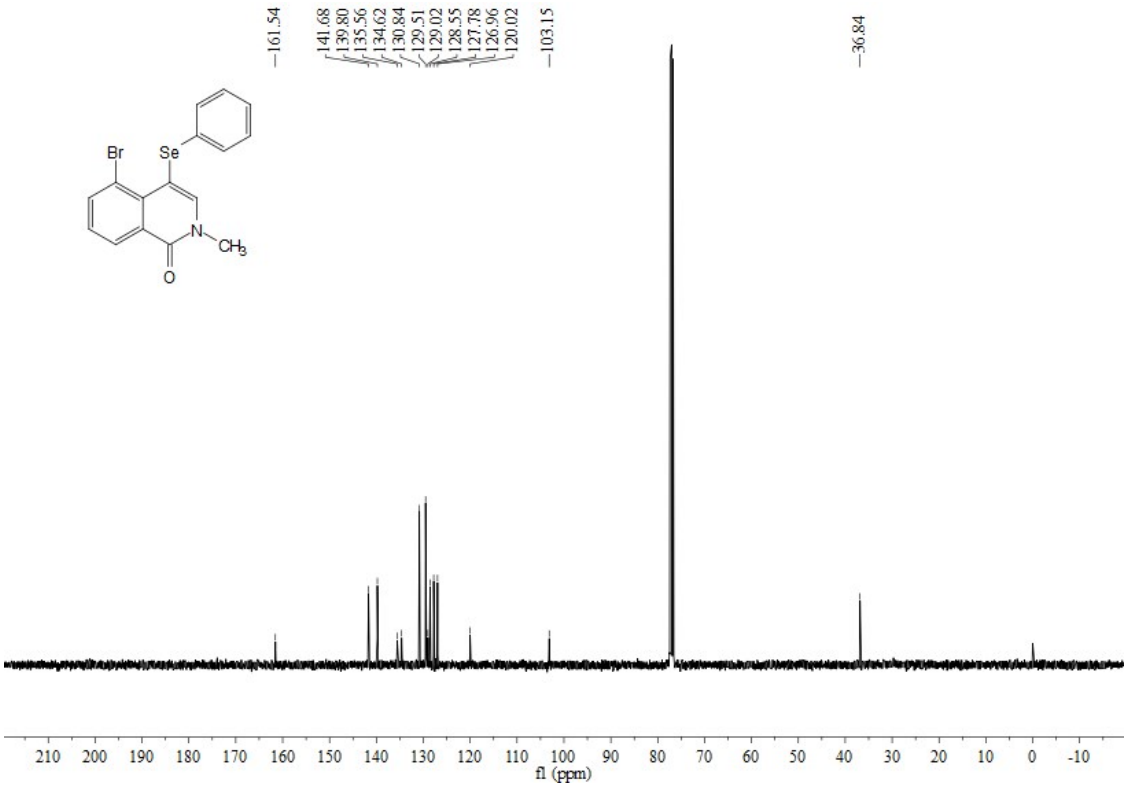
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3n**



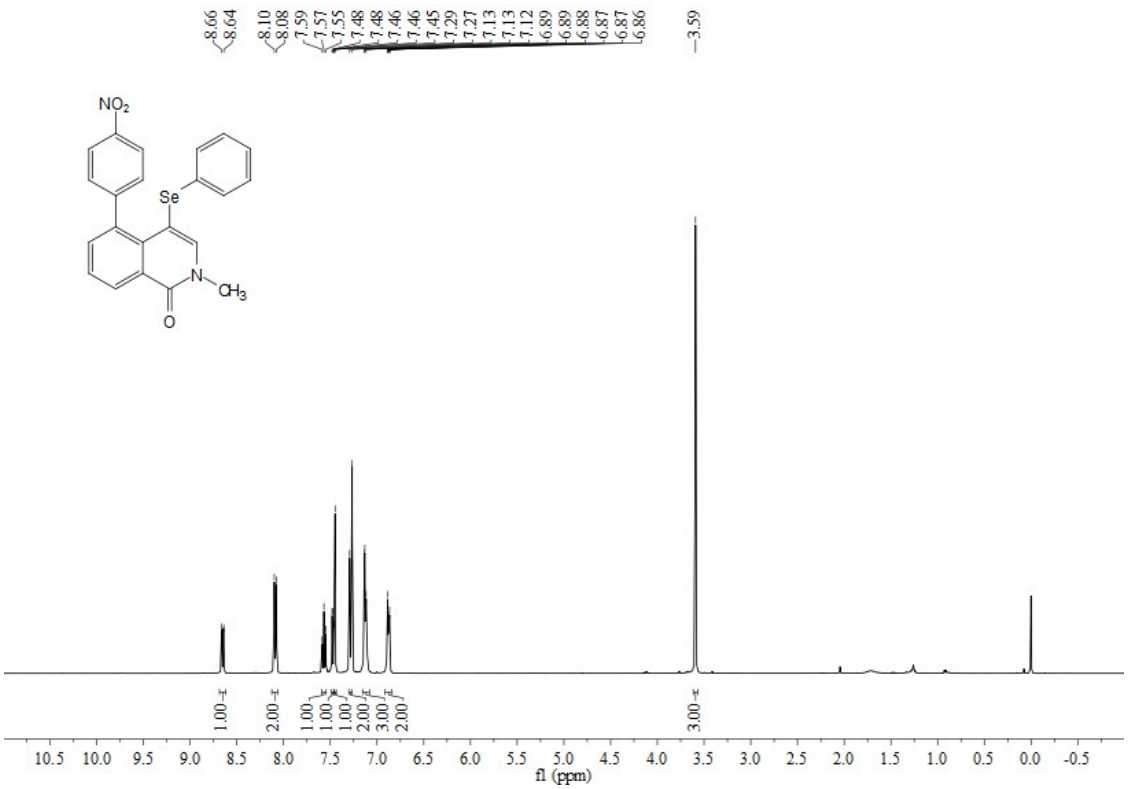
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3o**



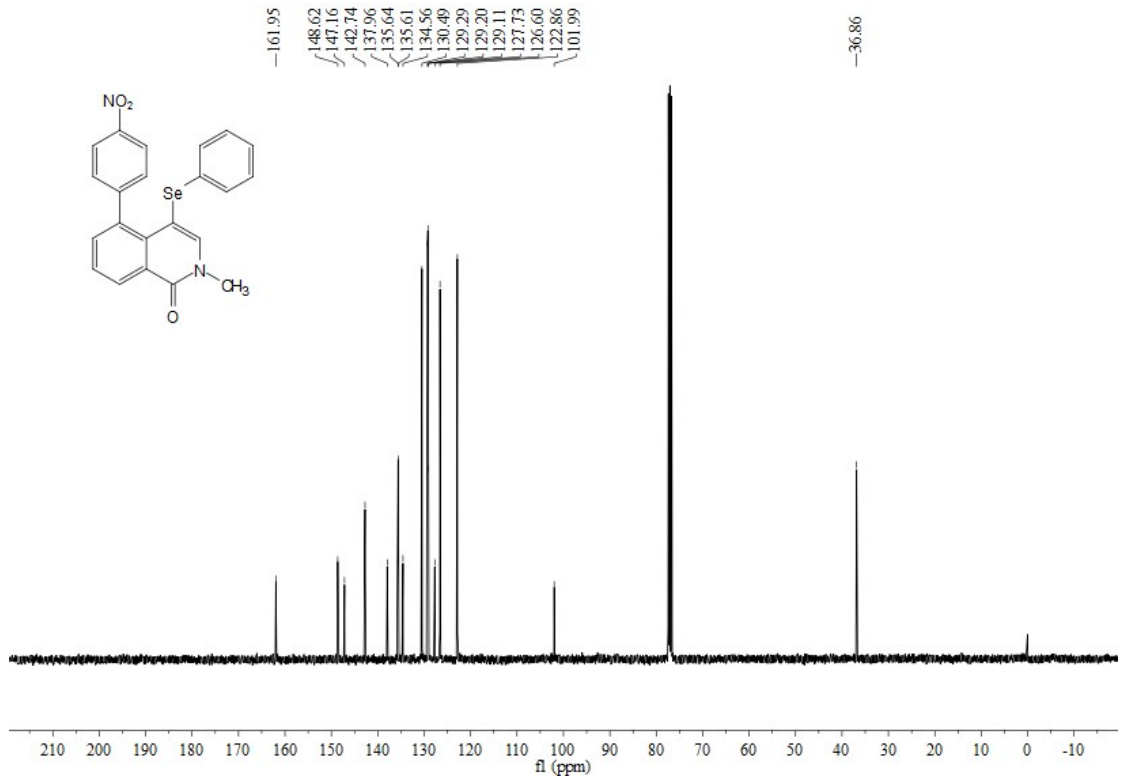
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3o**



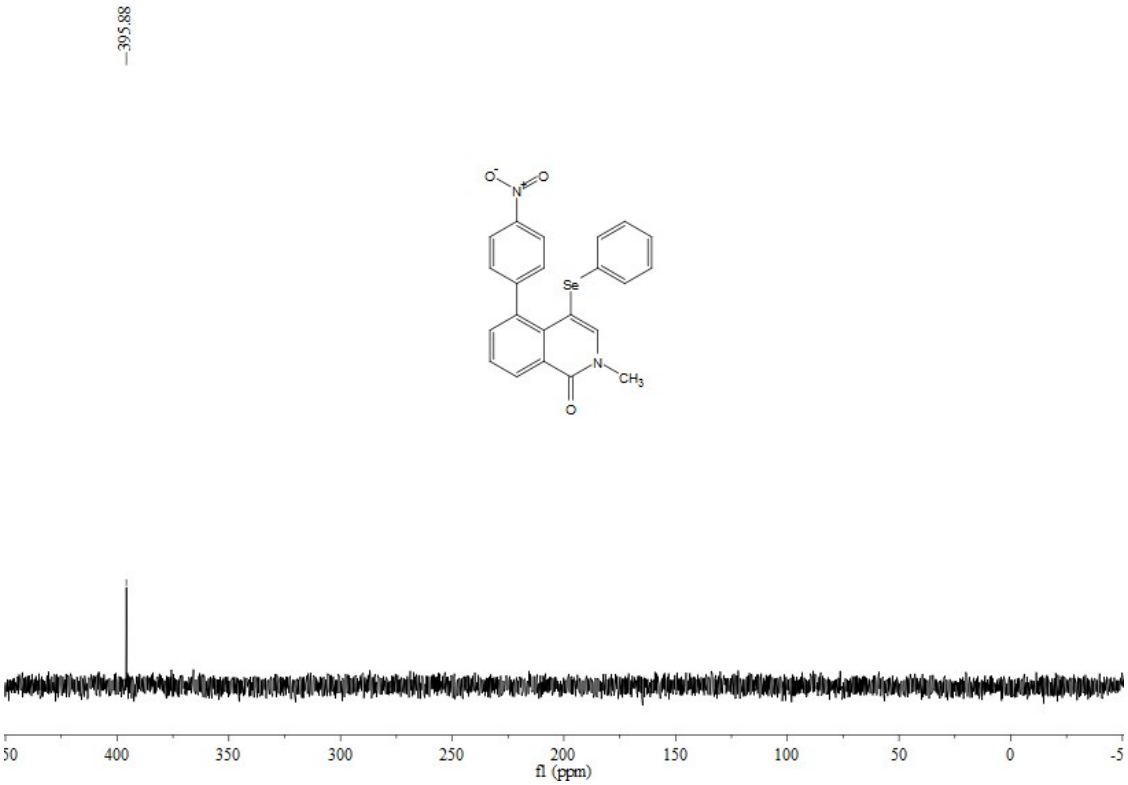
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3p**



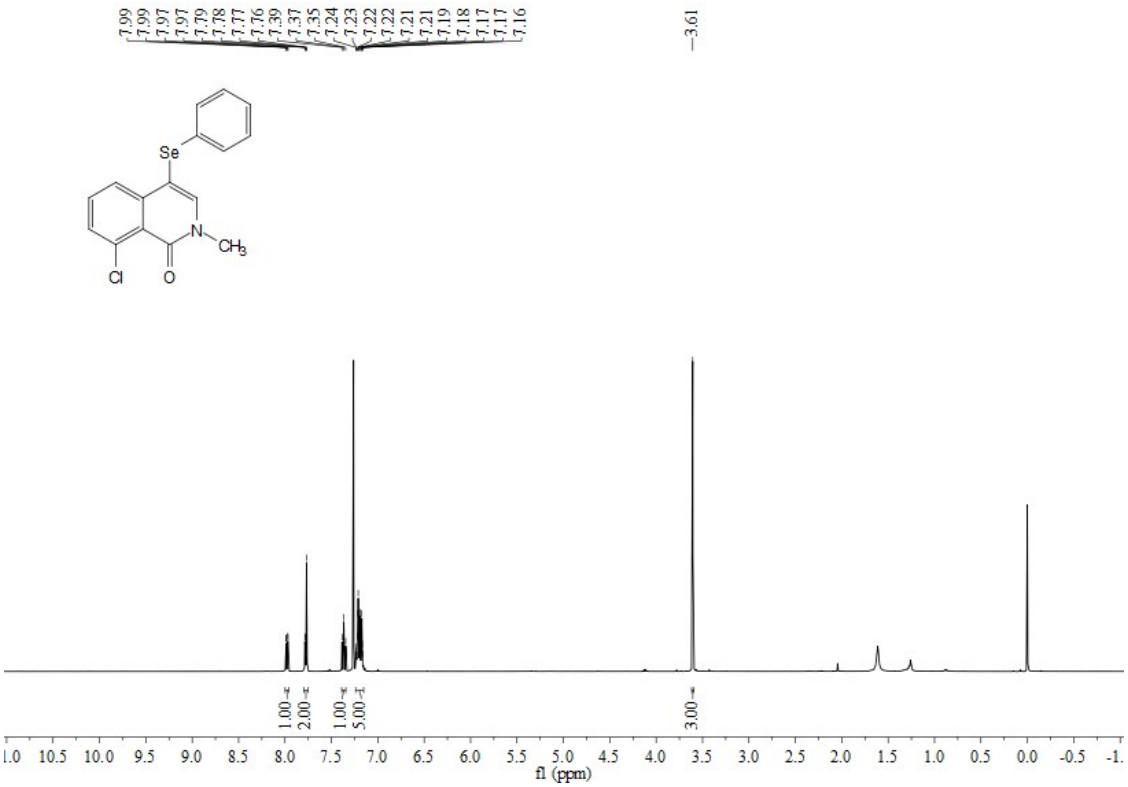
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3p**



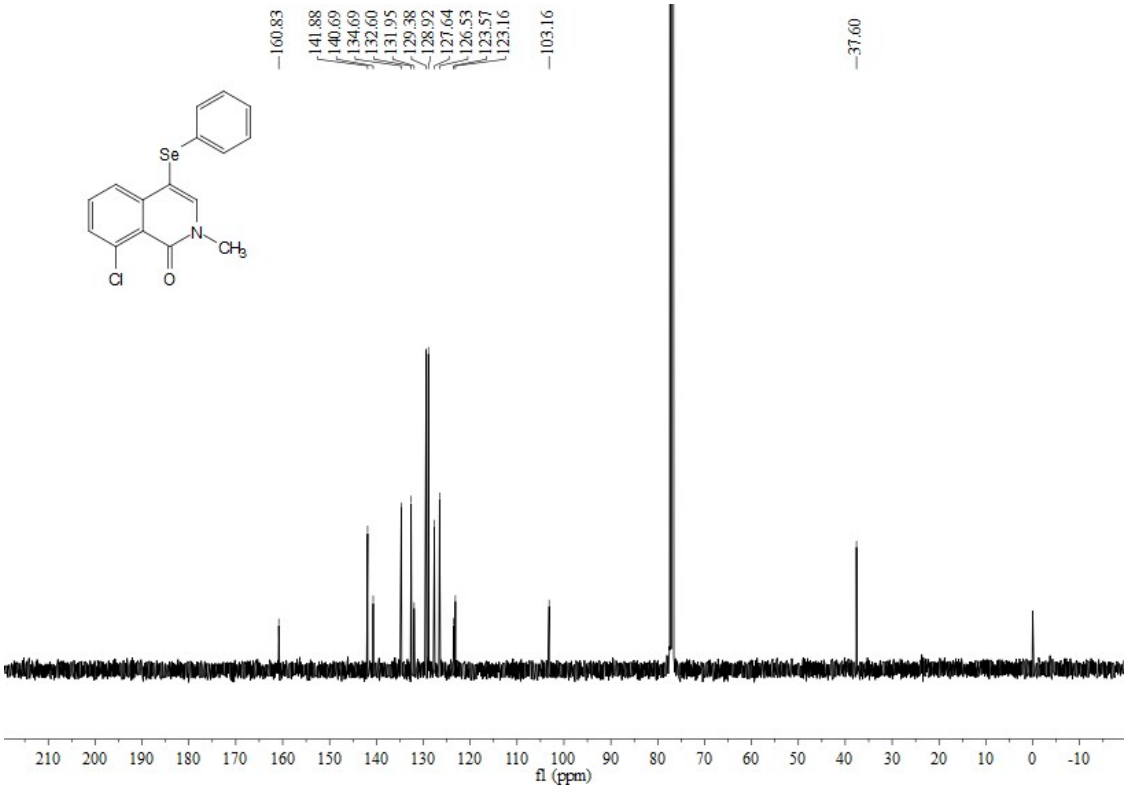
^{77}Se NMR (76 MHz, $CDCl_3$) spectrum of compound **3p**



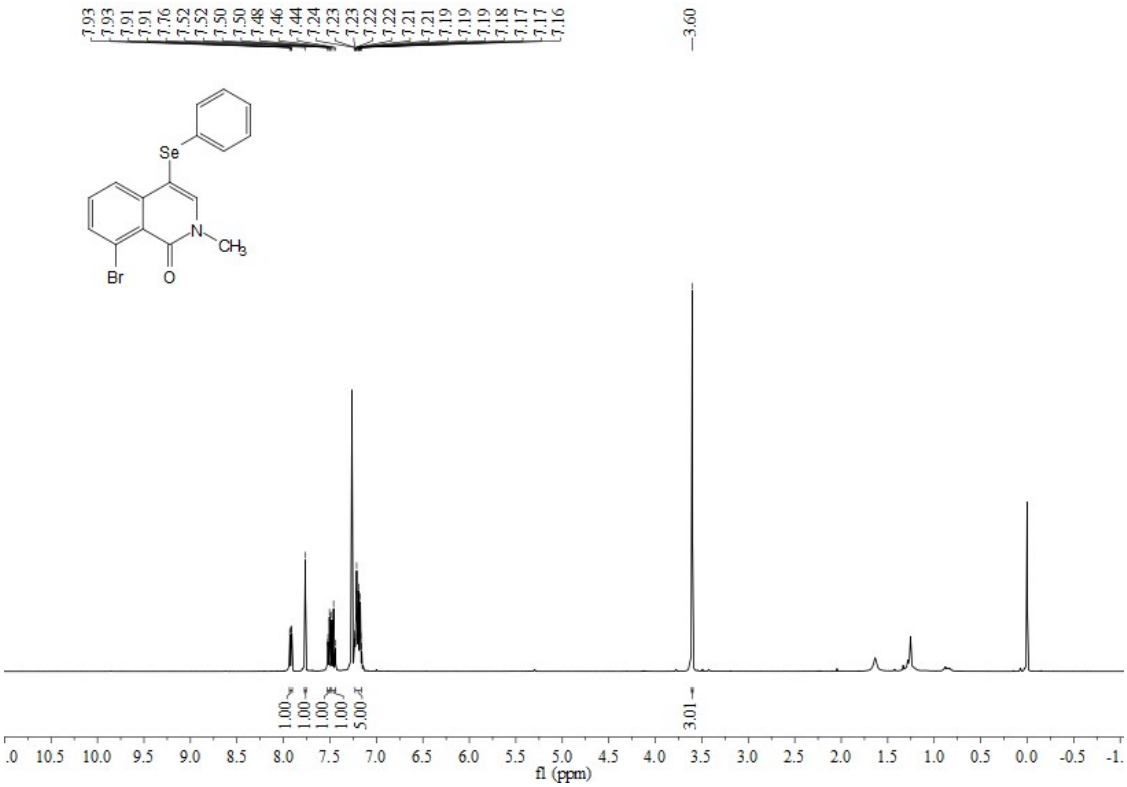
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3q**



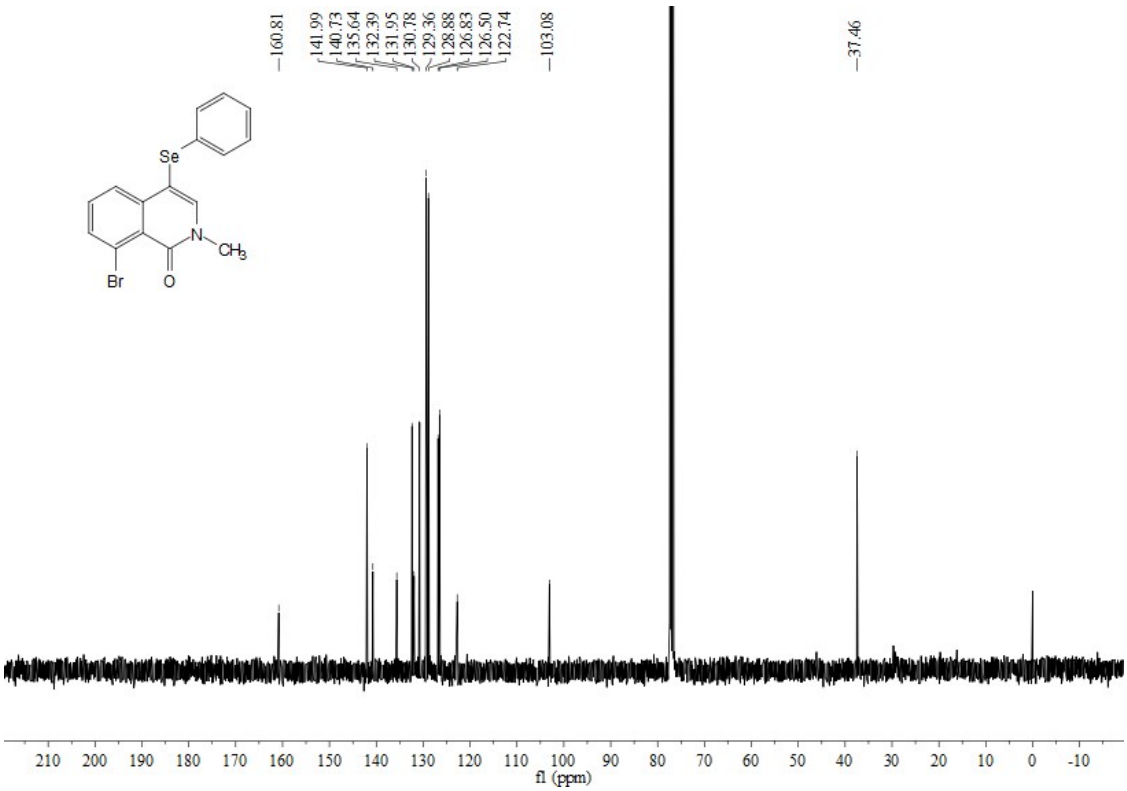
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3q**



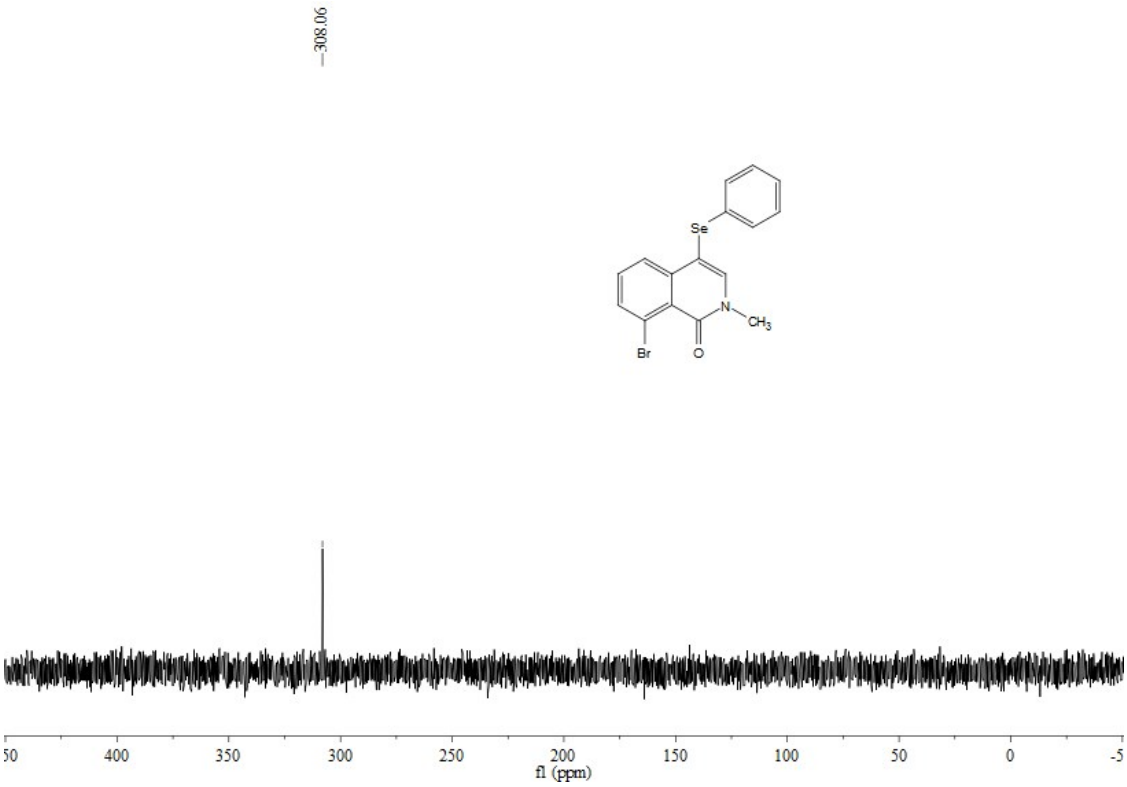
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3r**



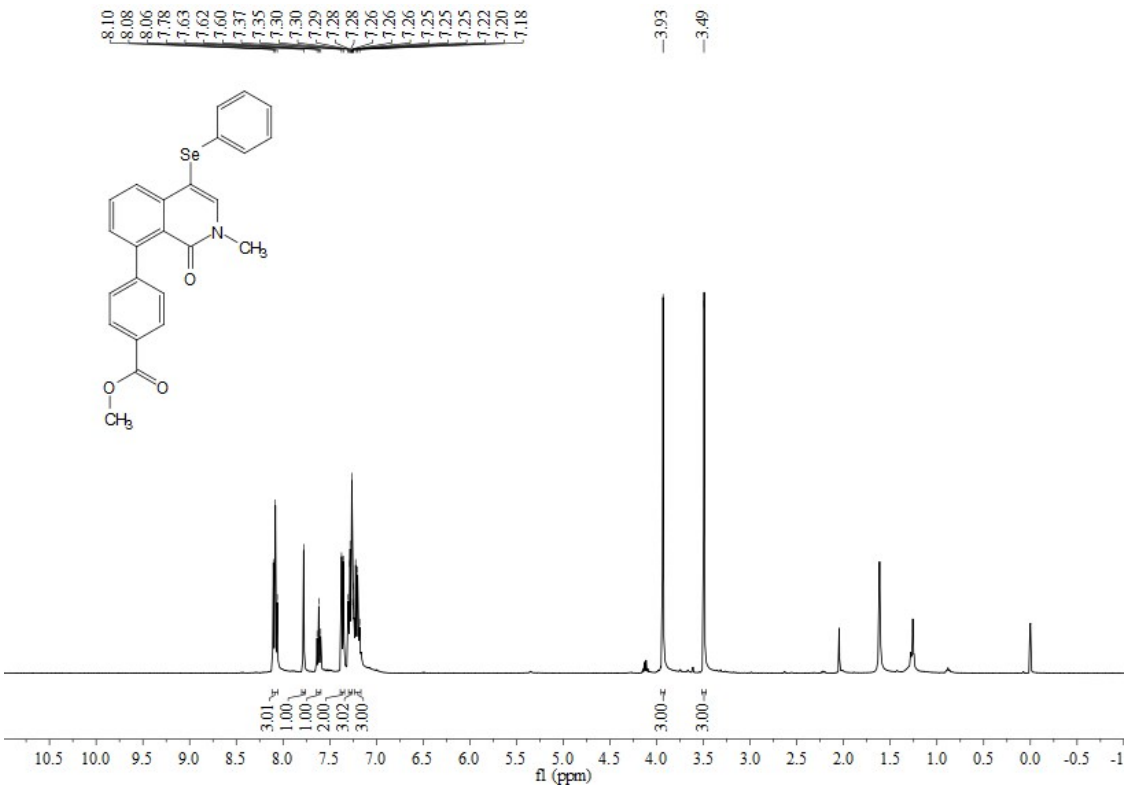
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3r**



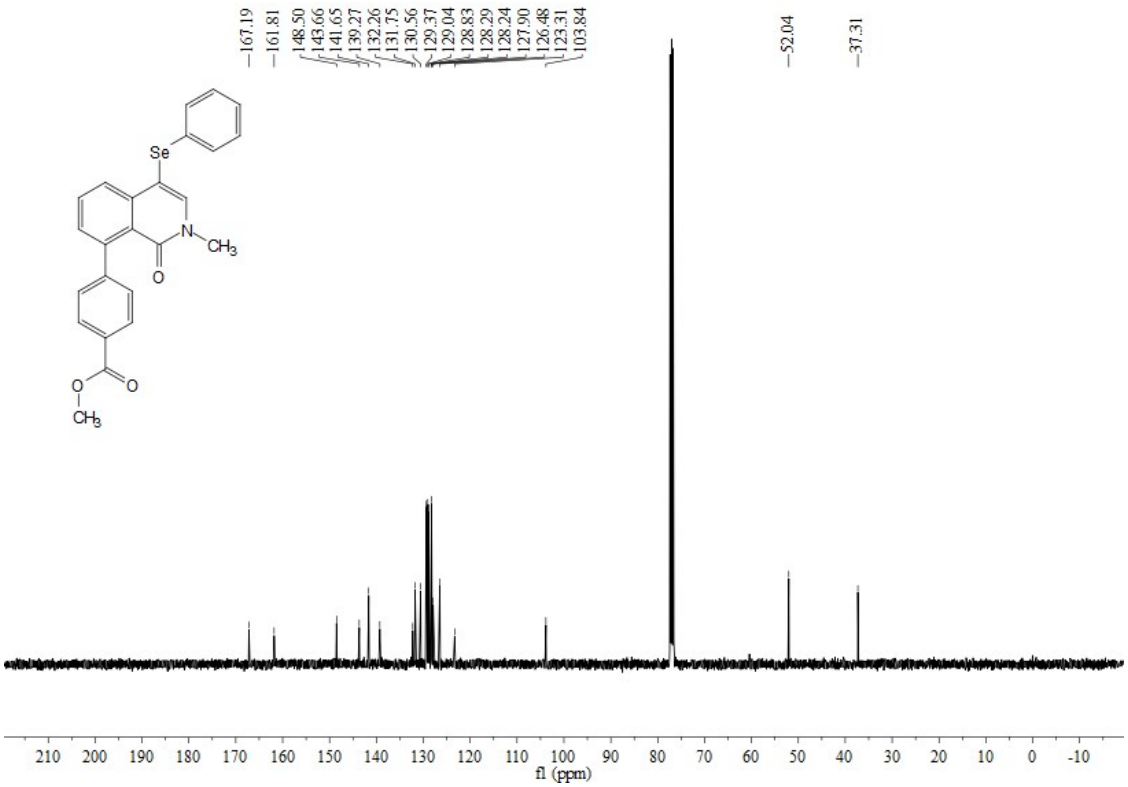
^{77}Se NMR (76 MHz, $CDCl_3$) spectrum of compound **3r**



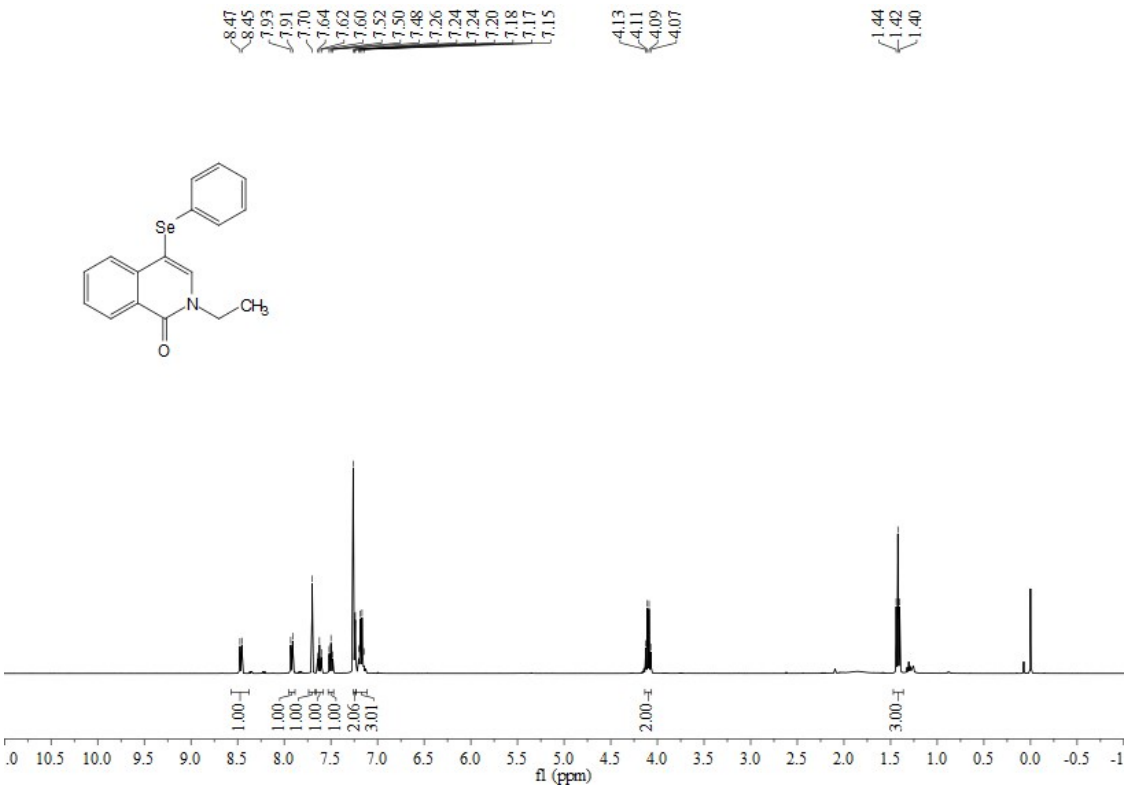
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3s**



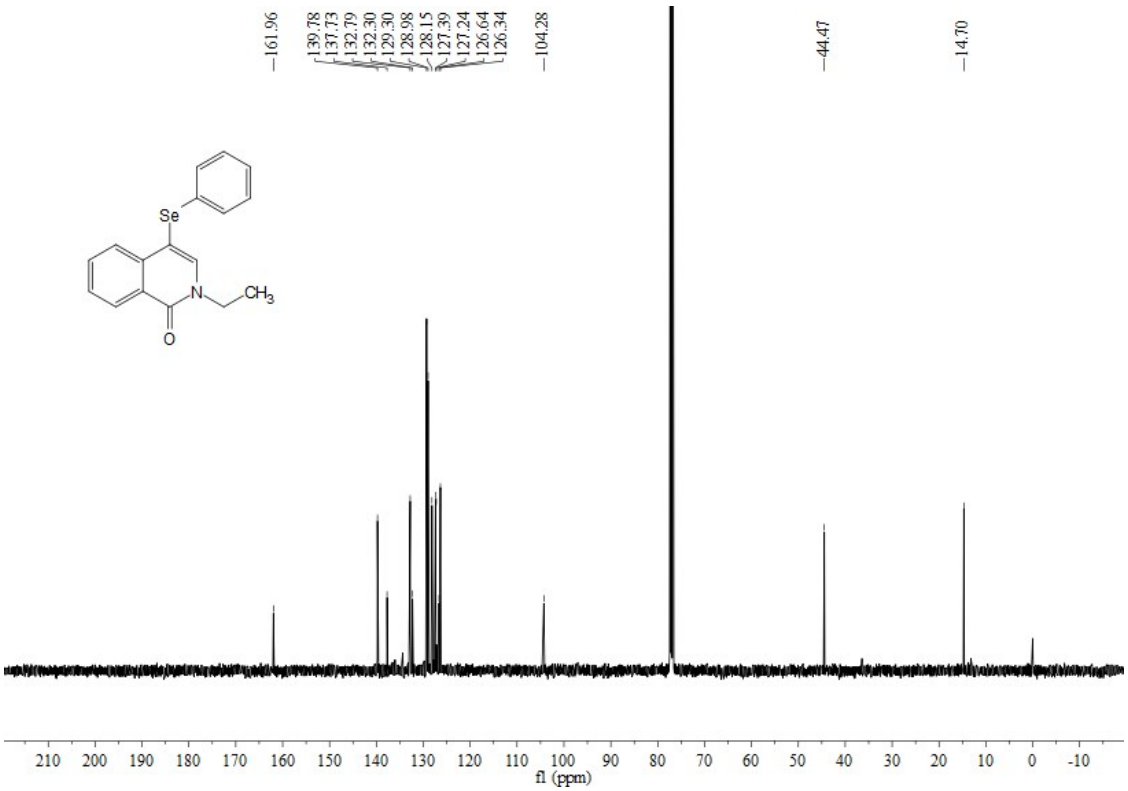
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3s**



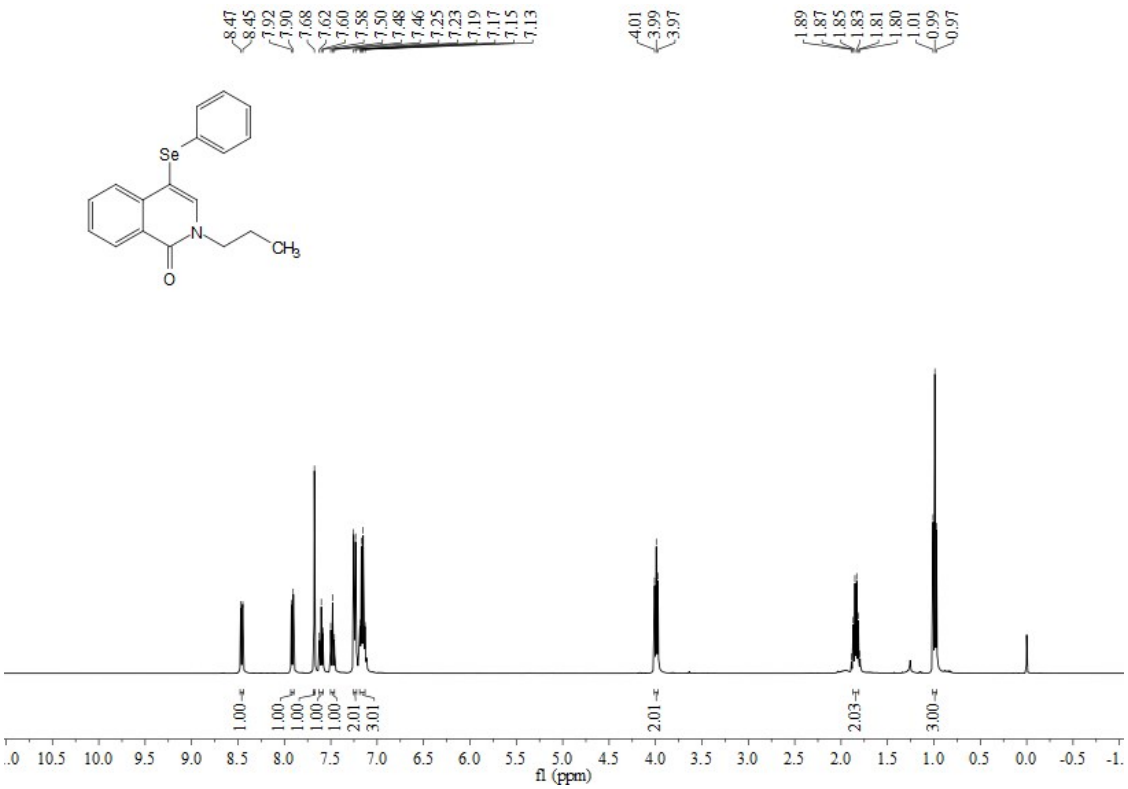
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5a**



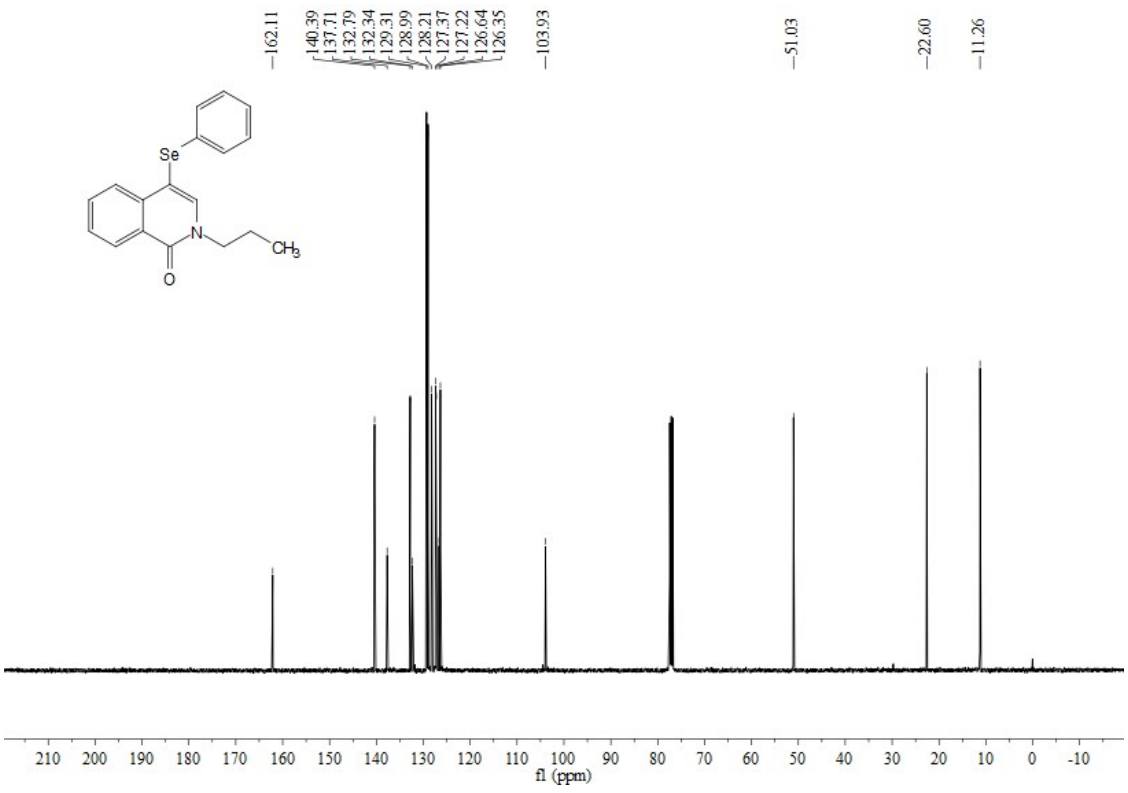
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5a**



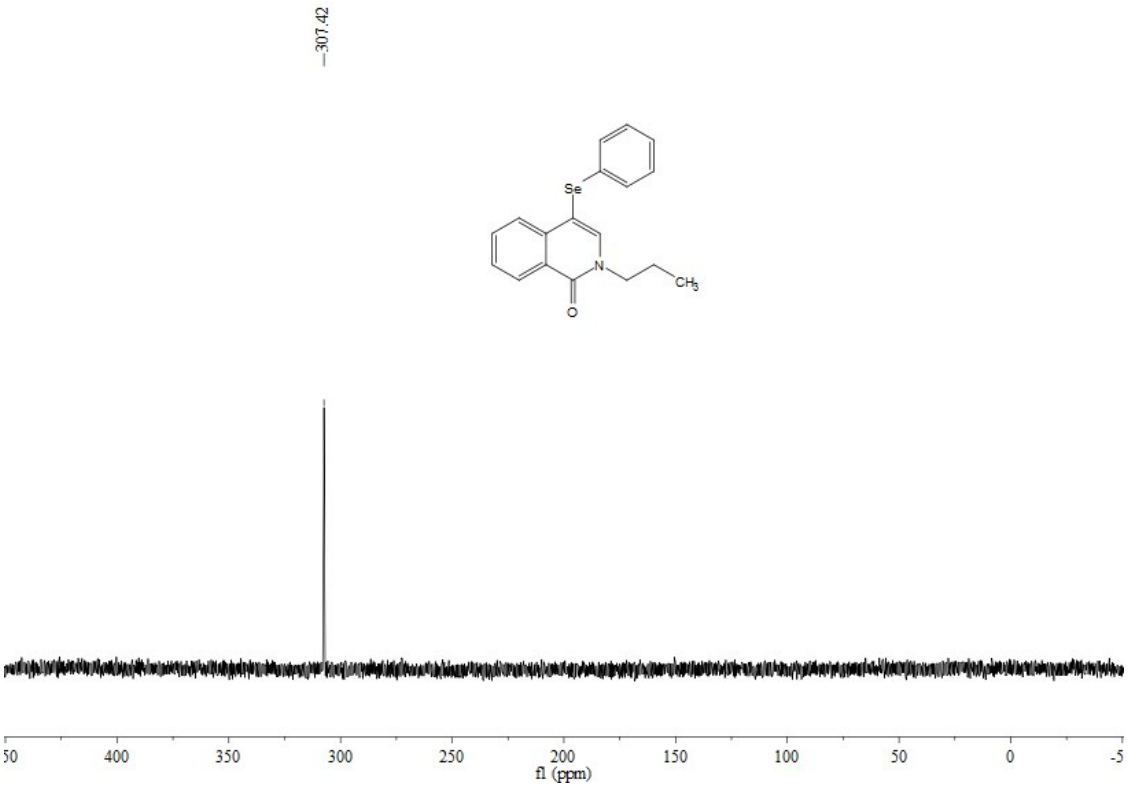
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5b**



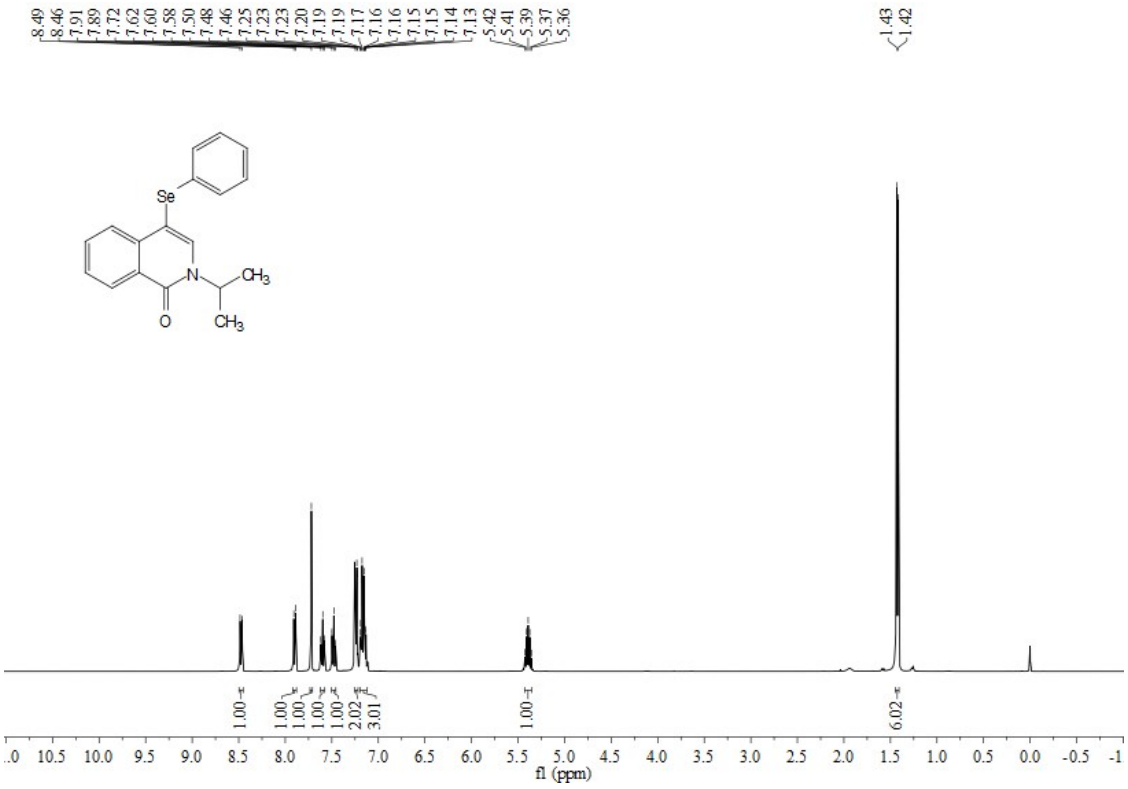
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5b**



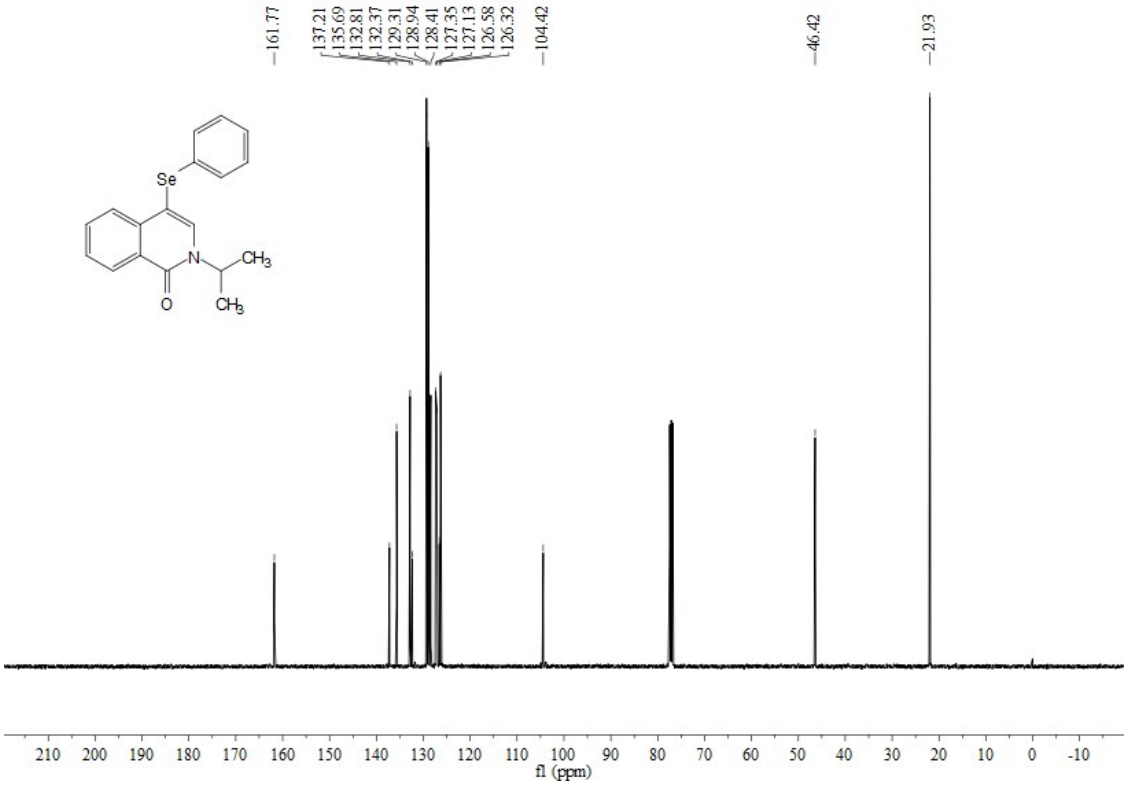
^{77}Se NMR (76 MHz, $CDCl_3$) spectrum of compound **5b**



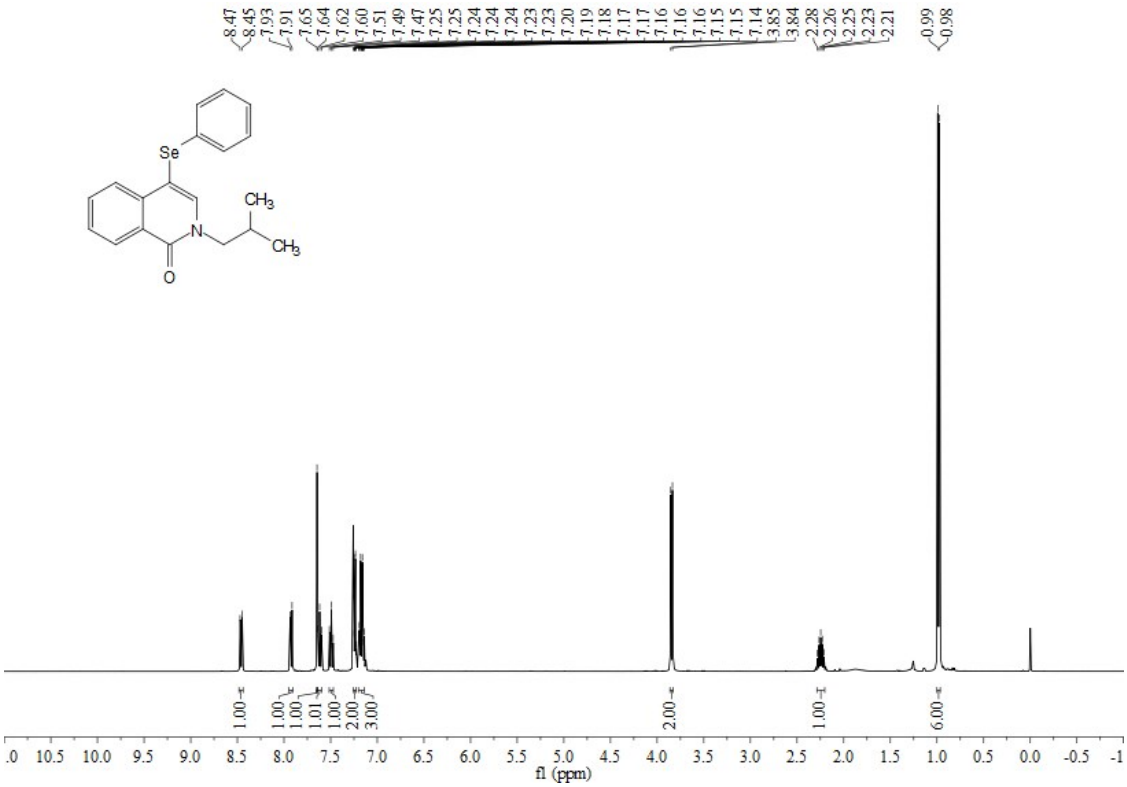
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5c**



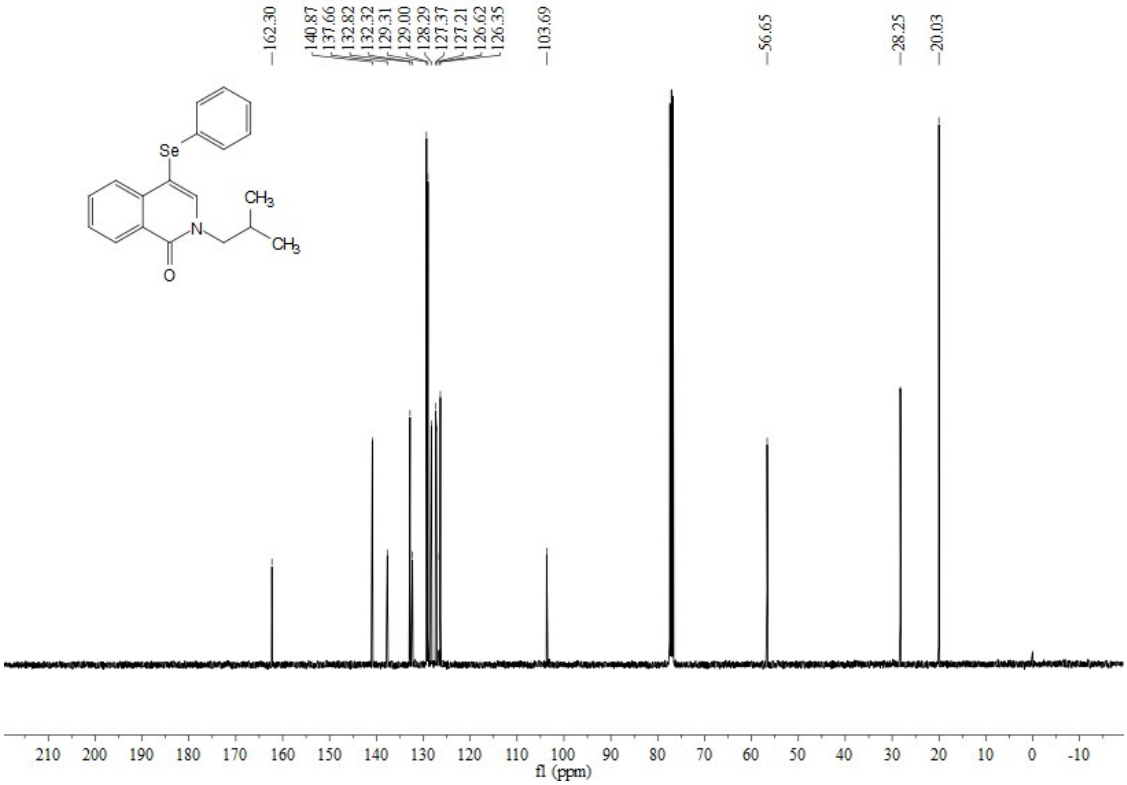
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5c**



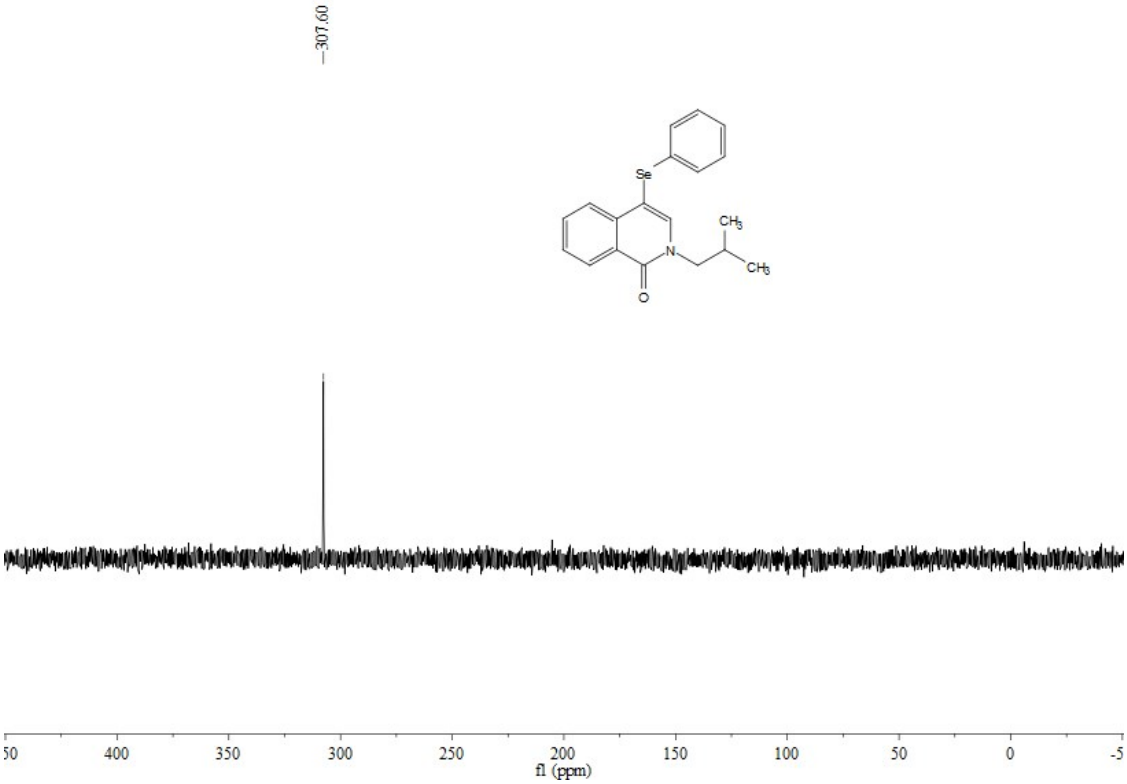
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5d**



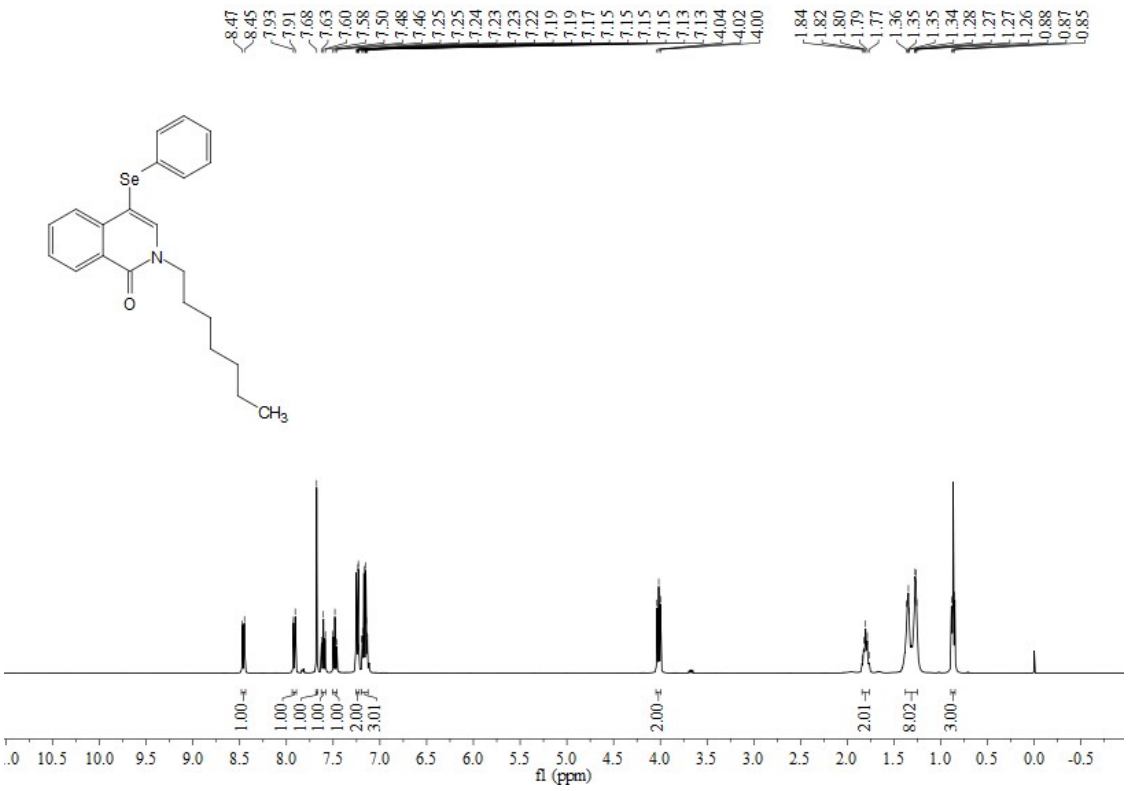
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5d**



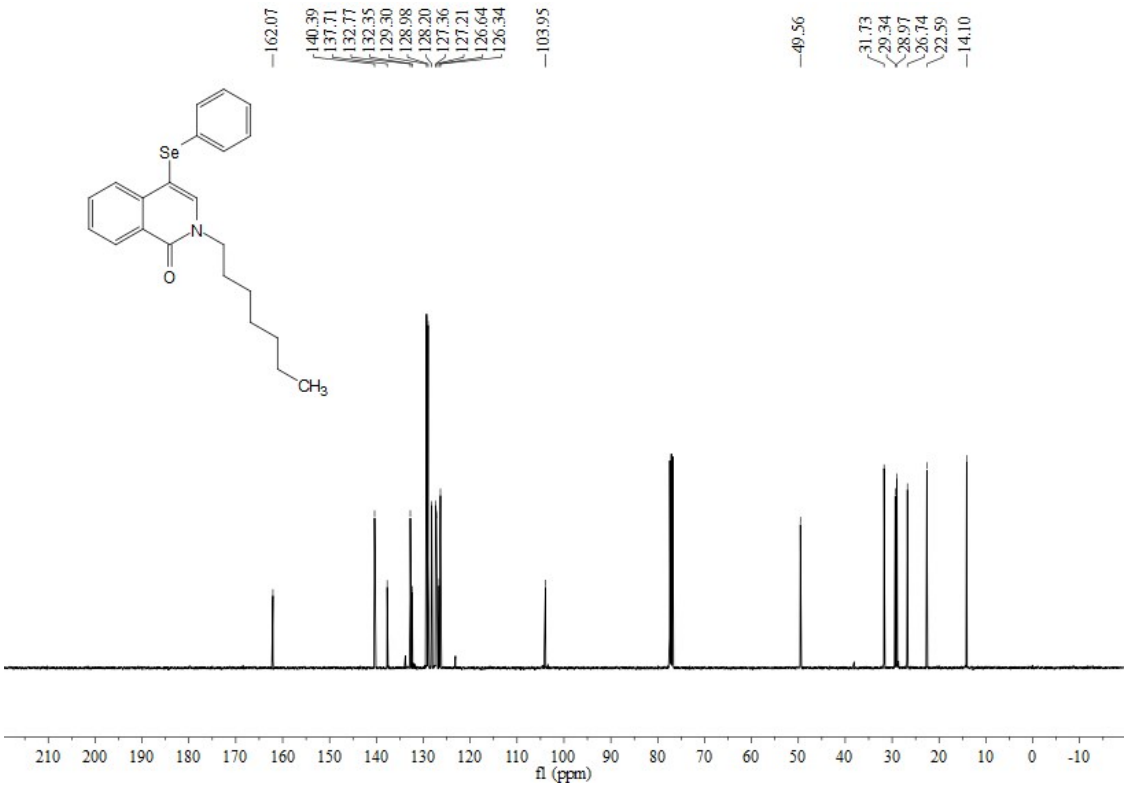
^{77}Se NMR (76 MHz, $CDCl_3$) spectrum of compound **5d**



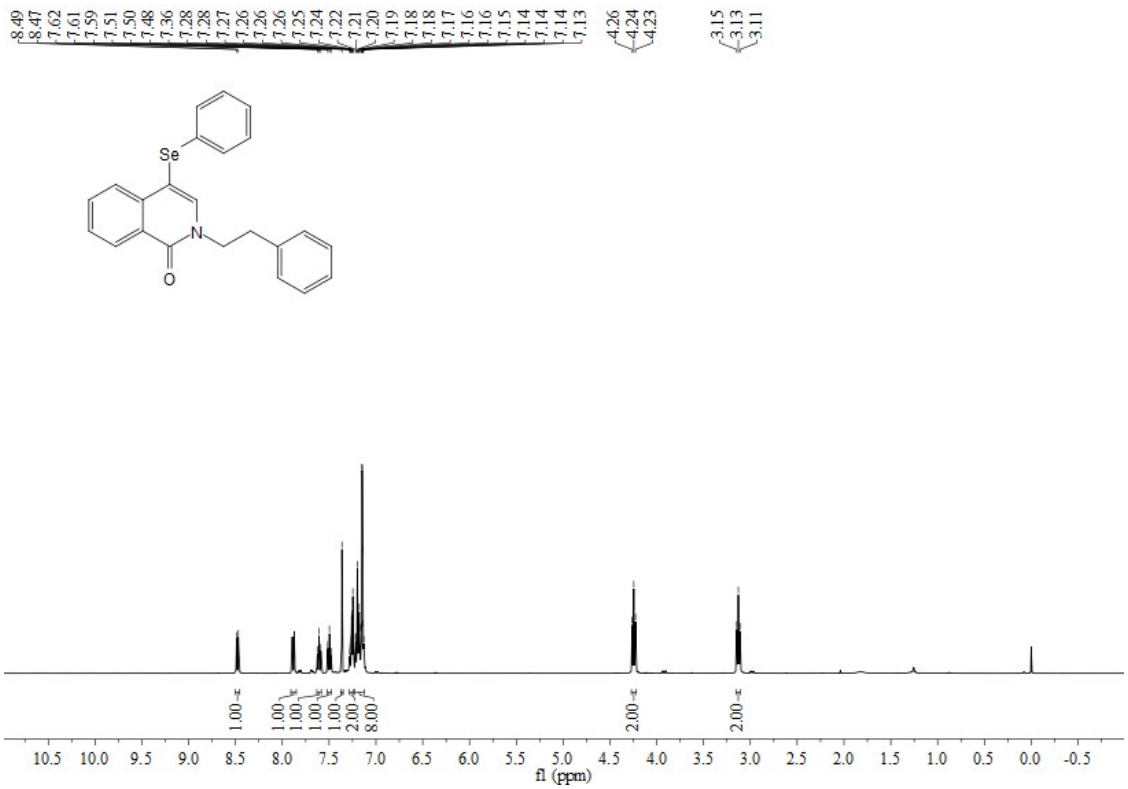
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5e**



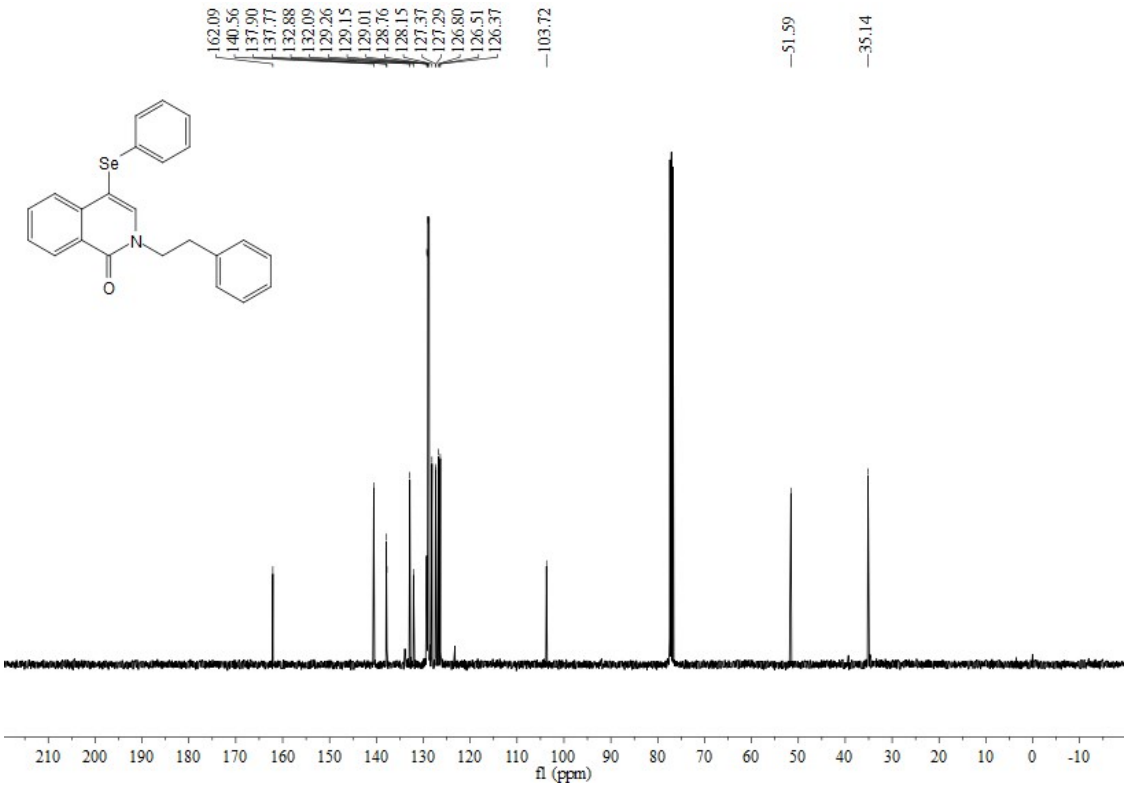
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5e**



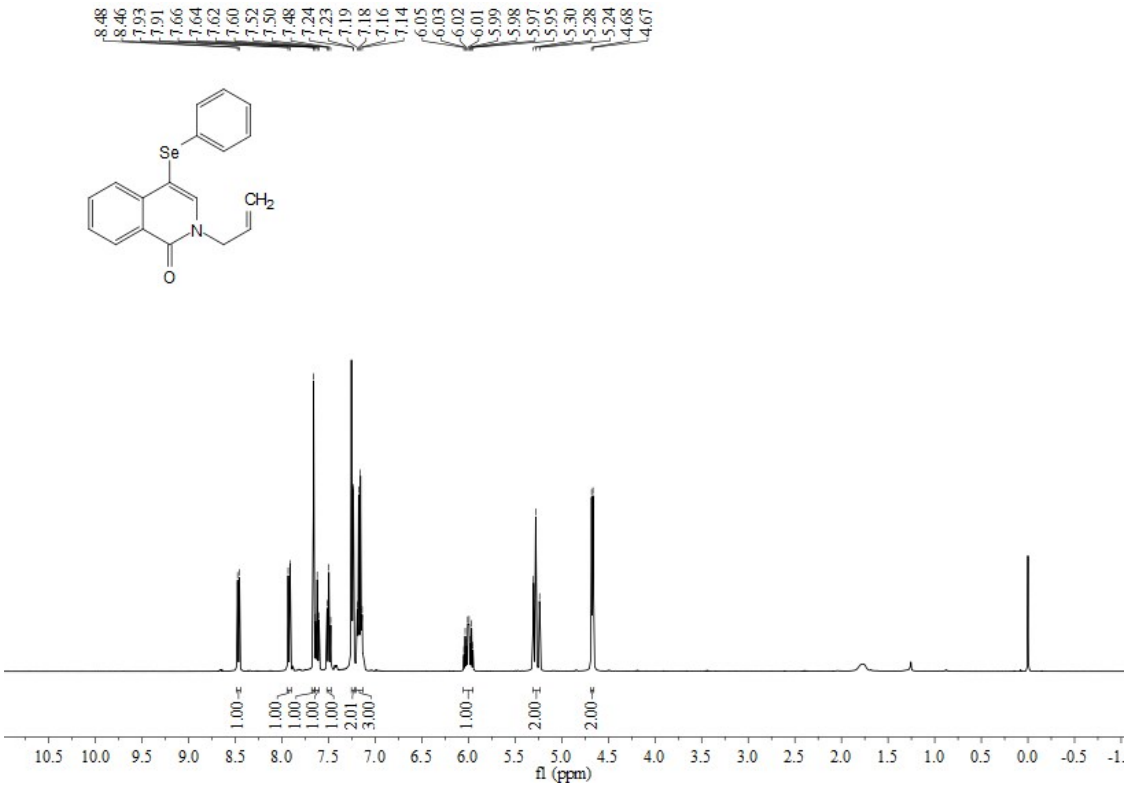
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5f**



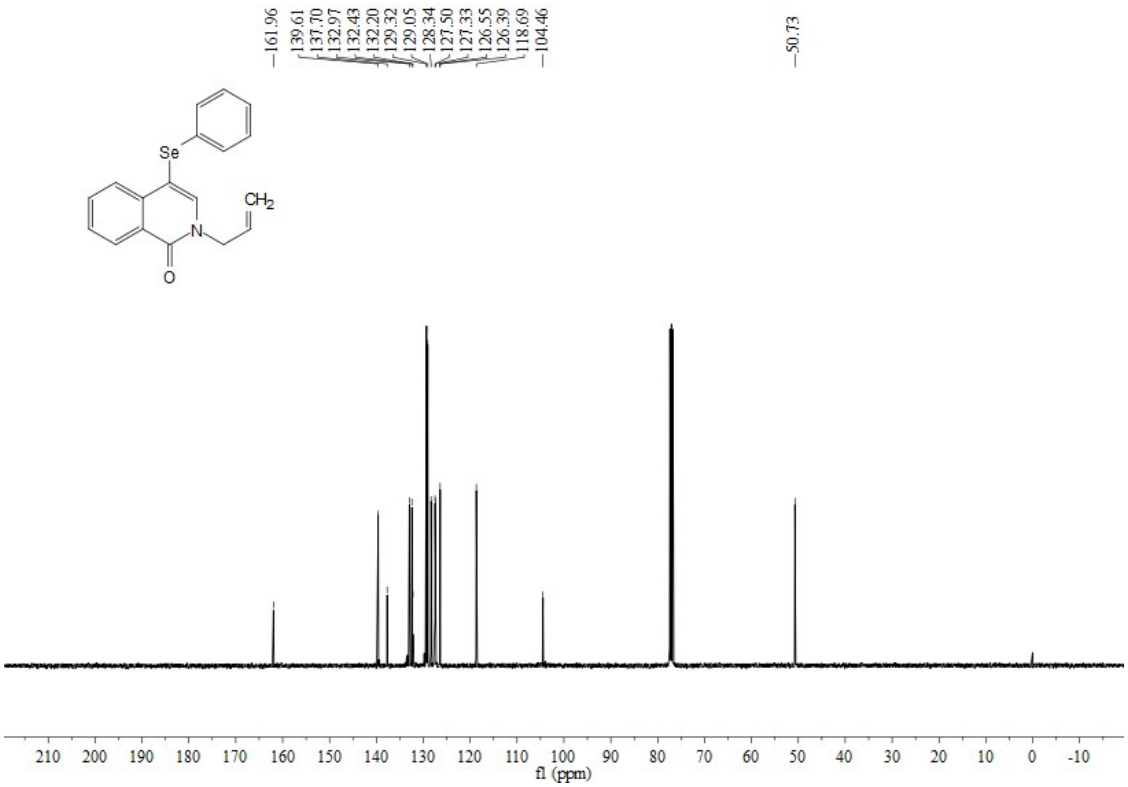
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5f**



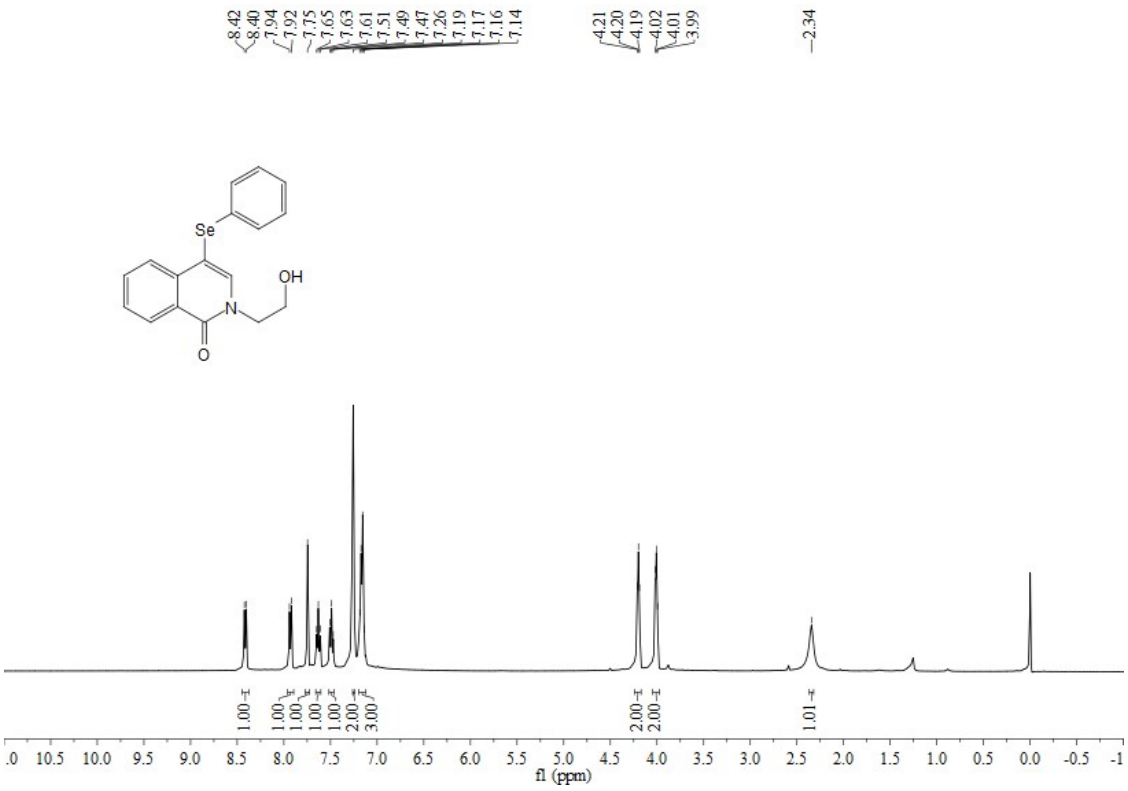
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5g**



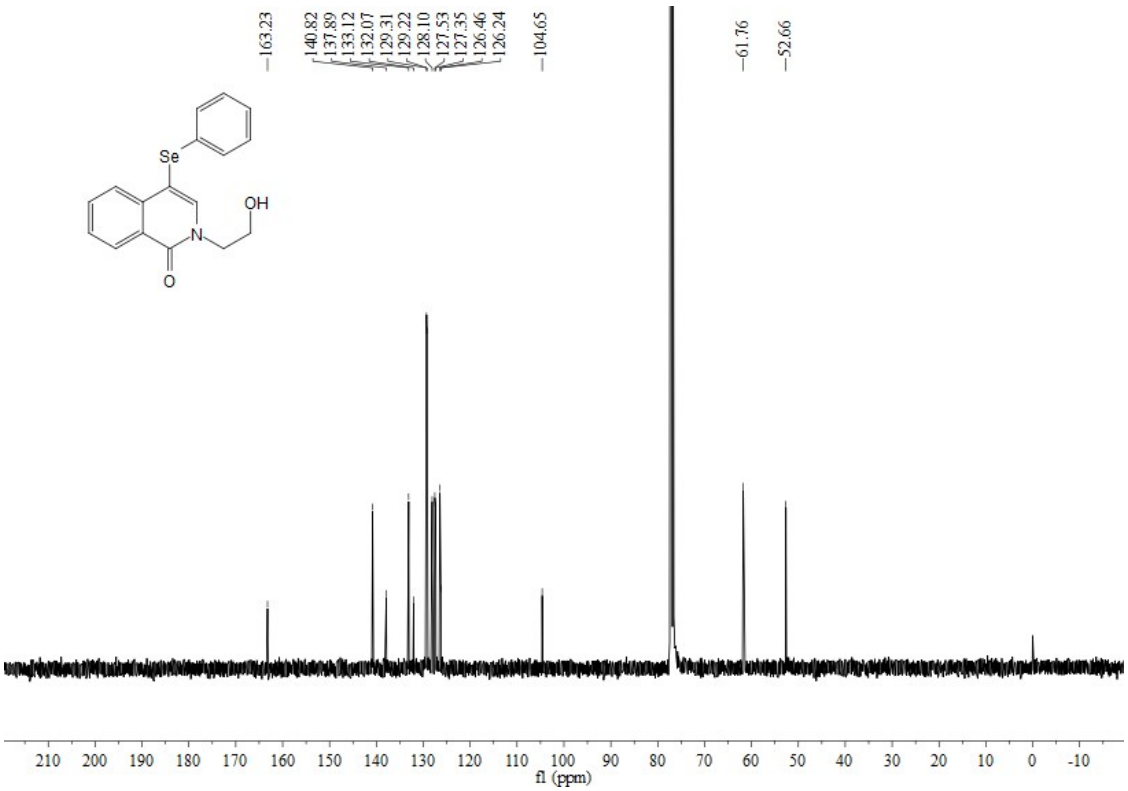
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5g**



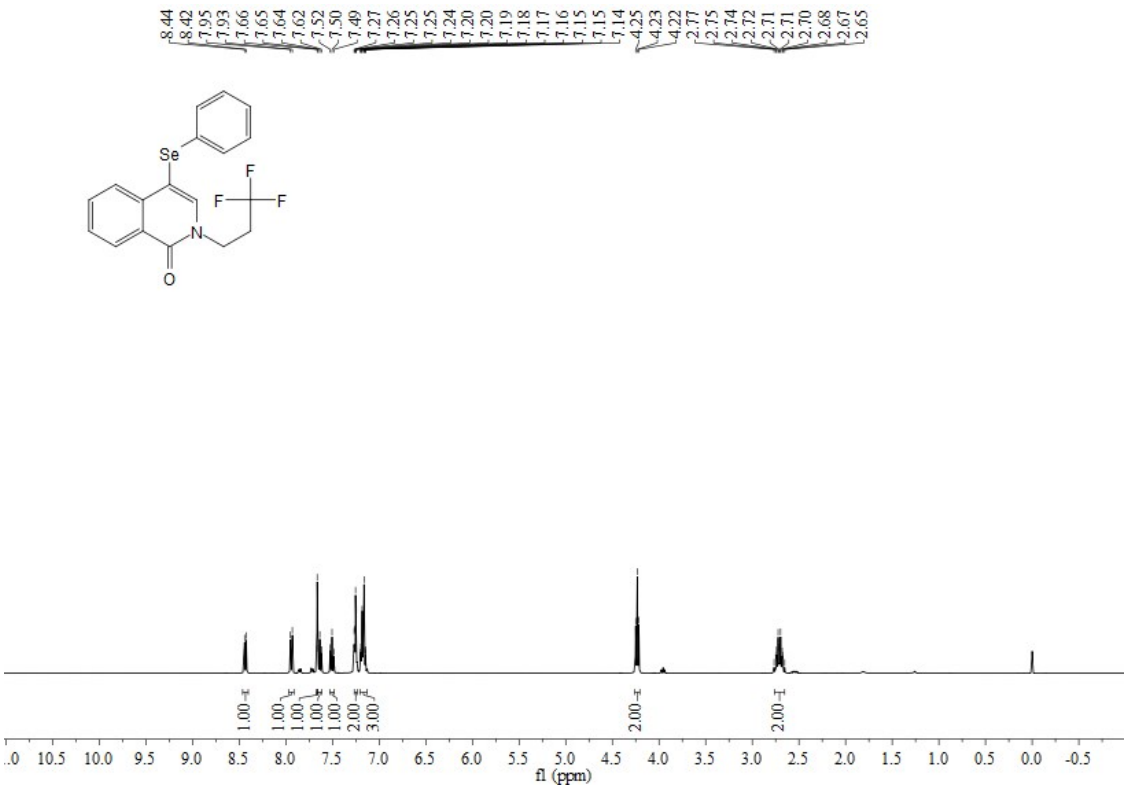
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5h**



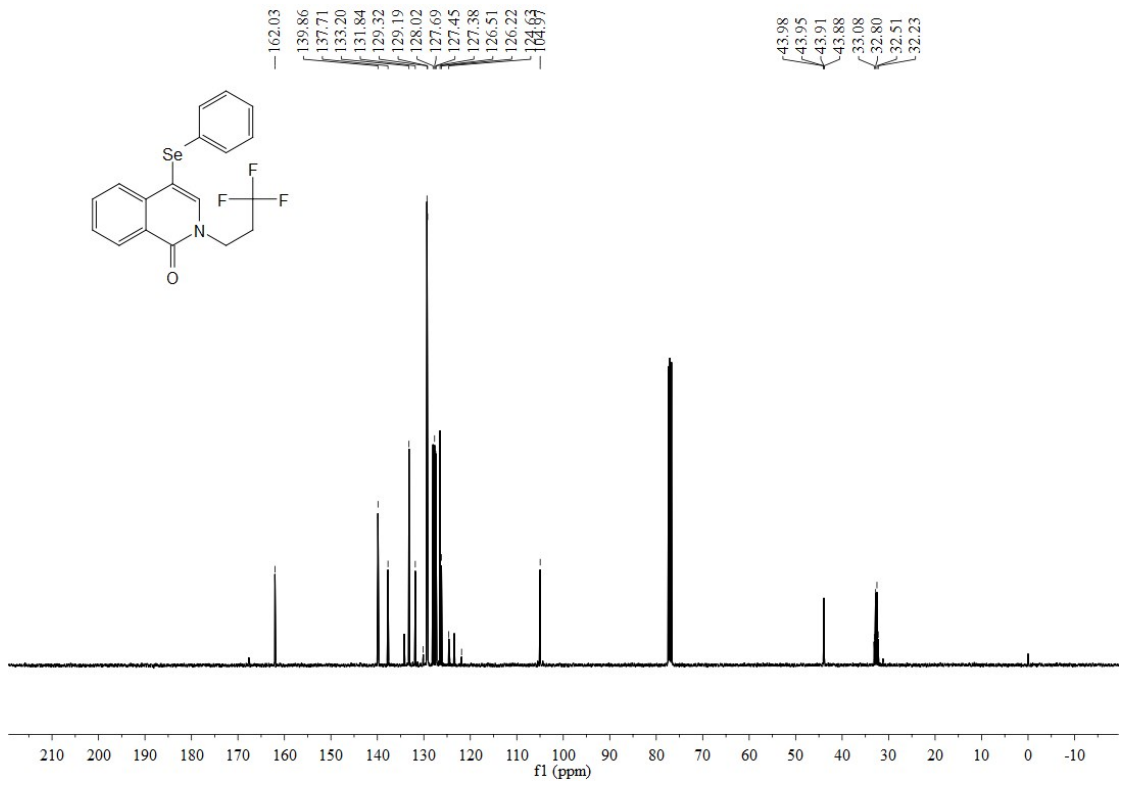
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5h**



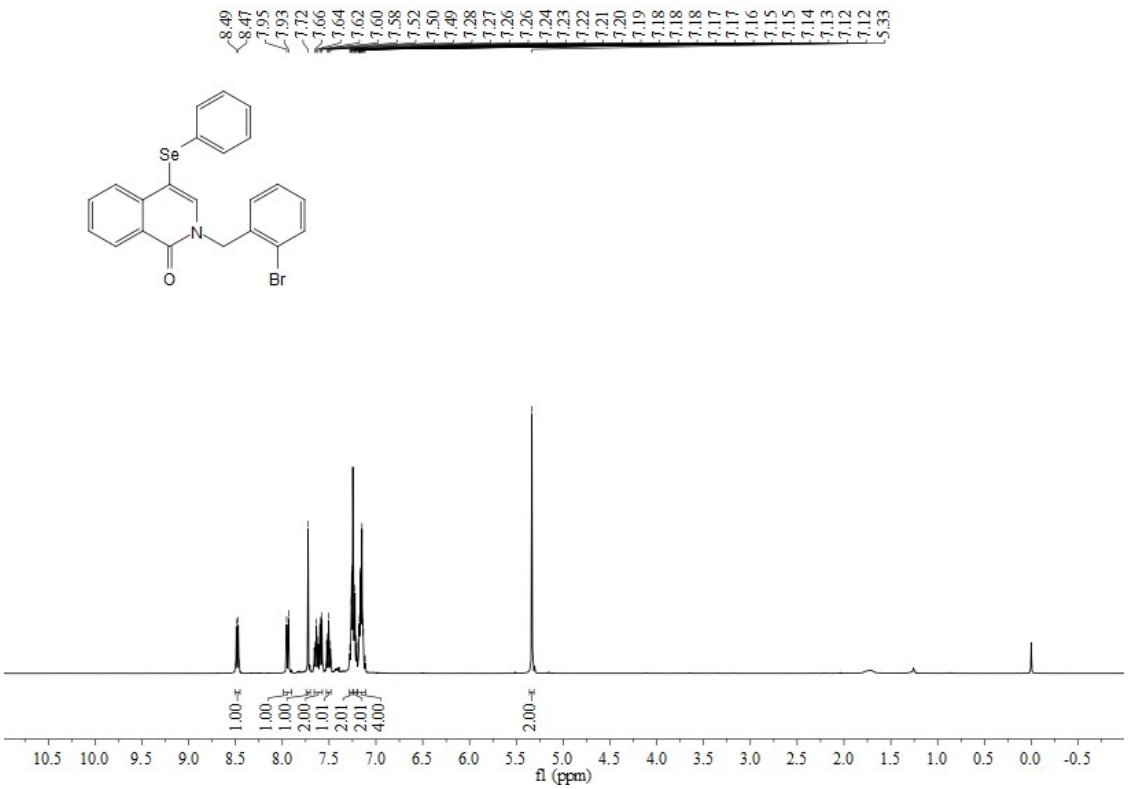
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5i**



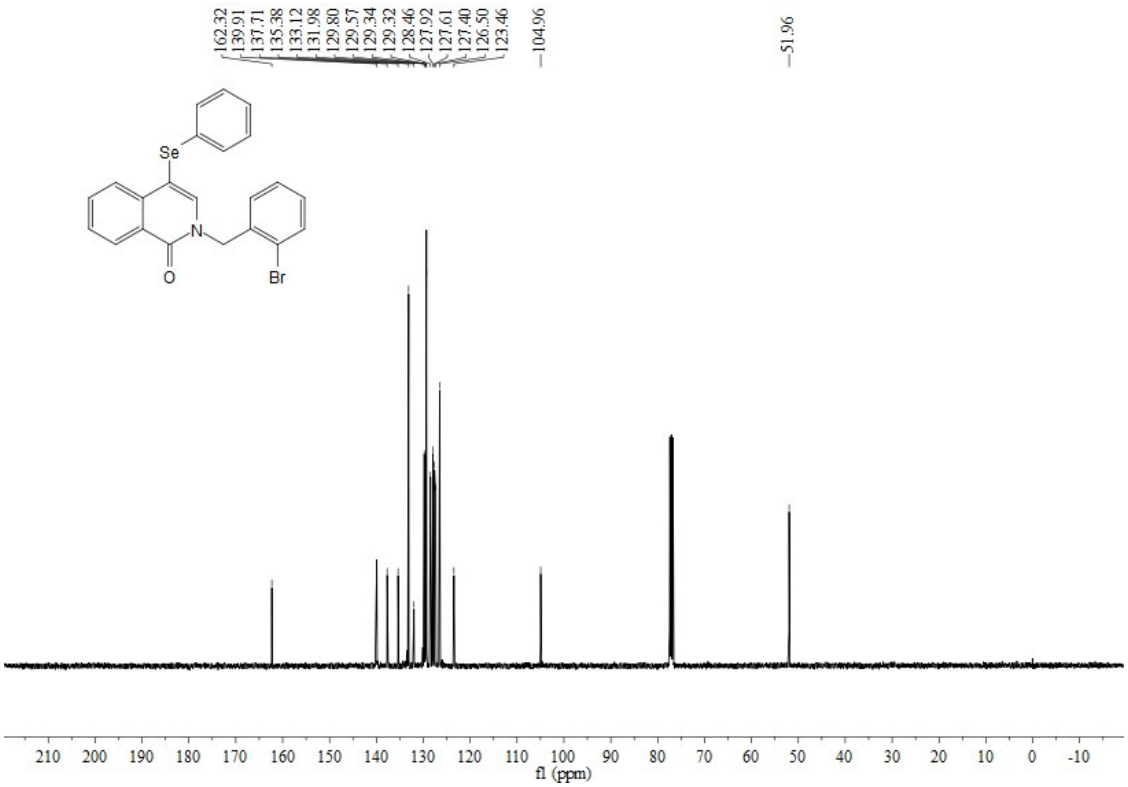
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5i**



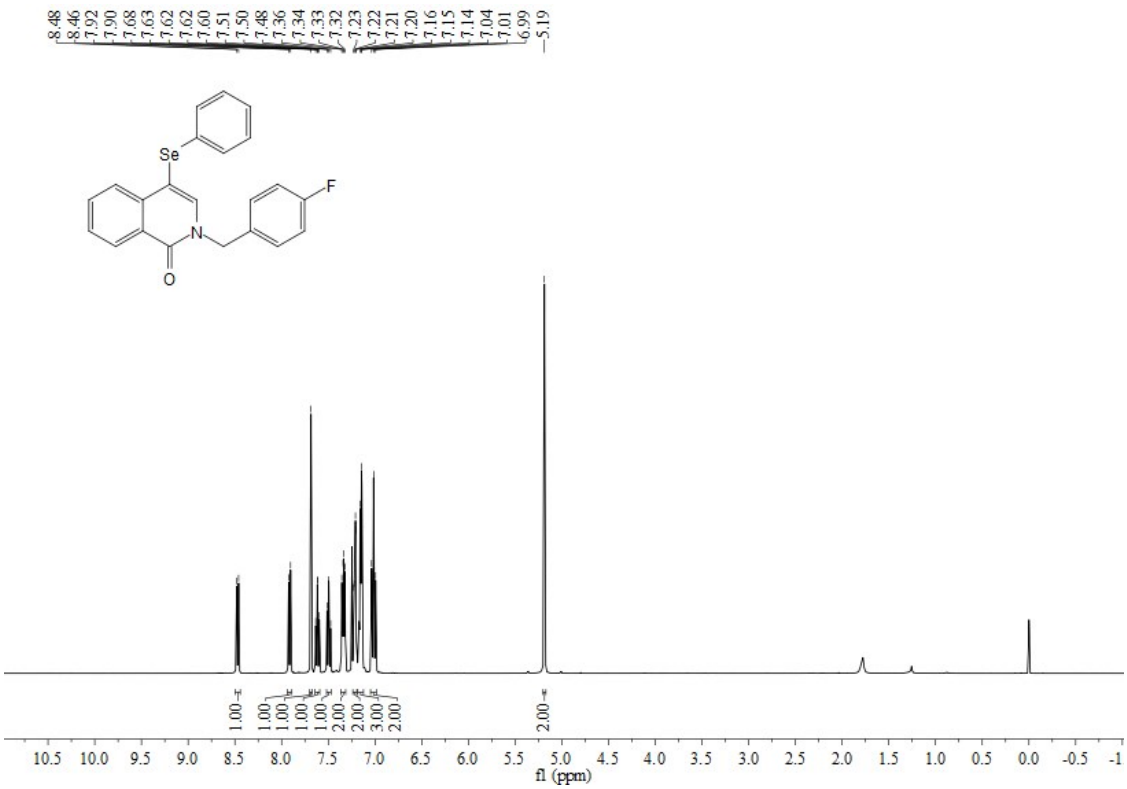
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5j**



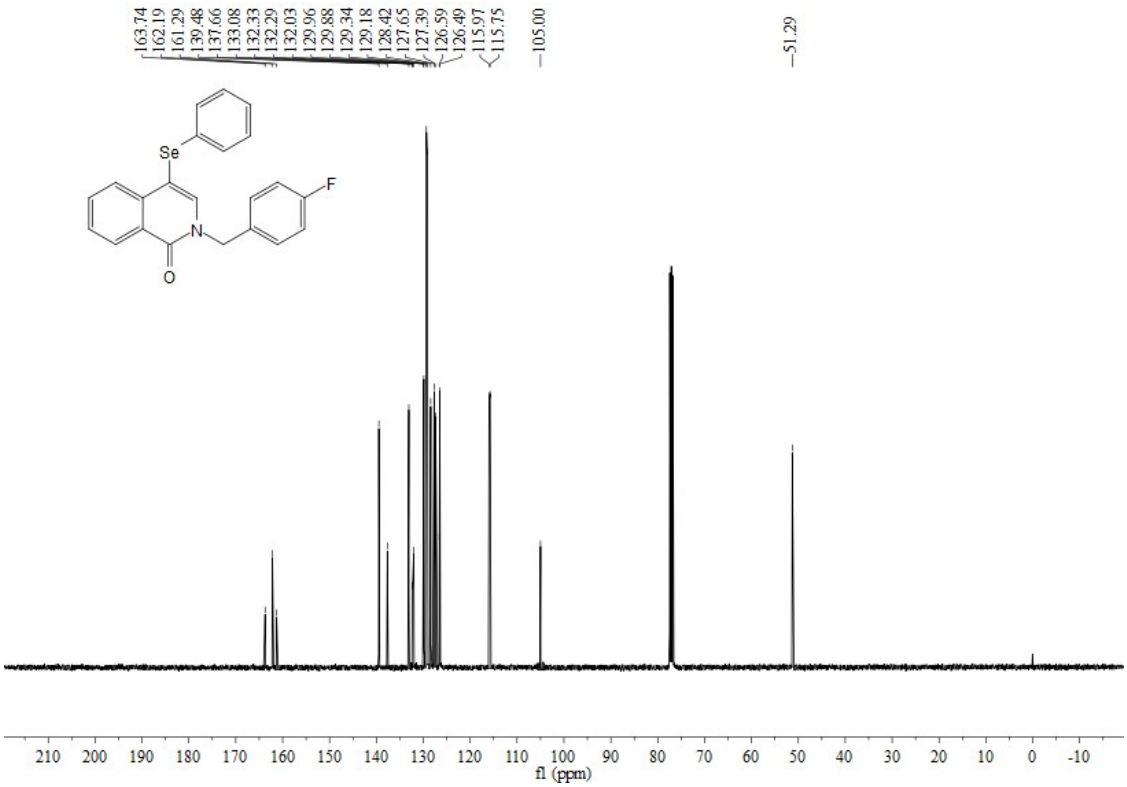
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5j**



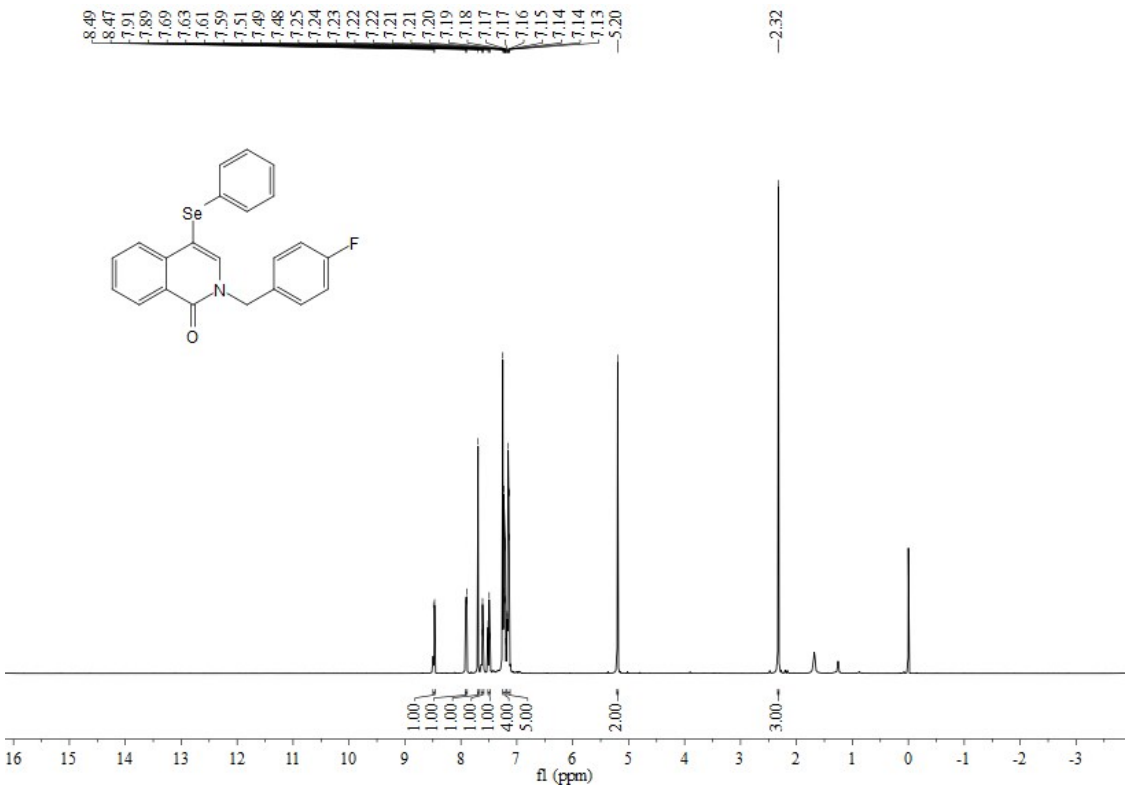
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5k**



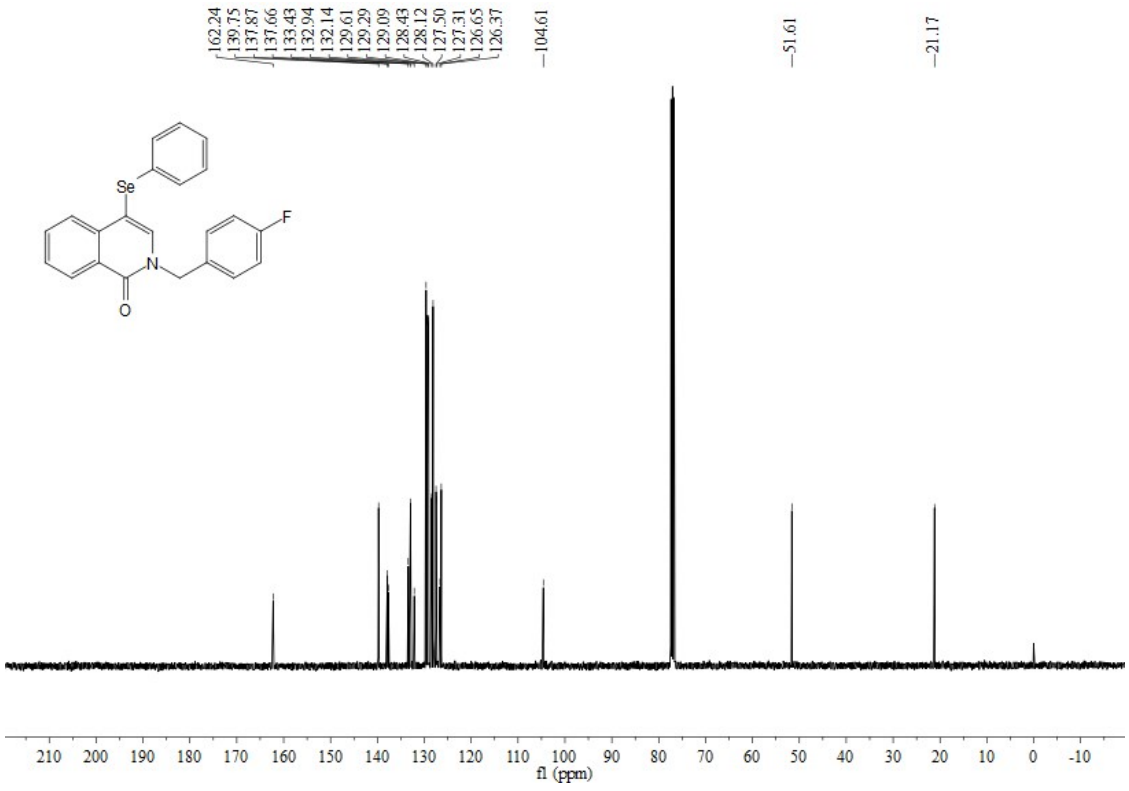
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5k**



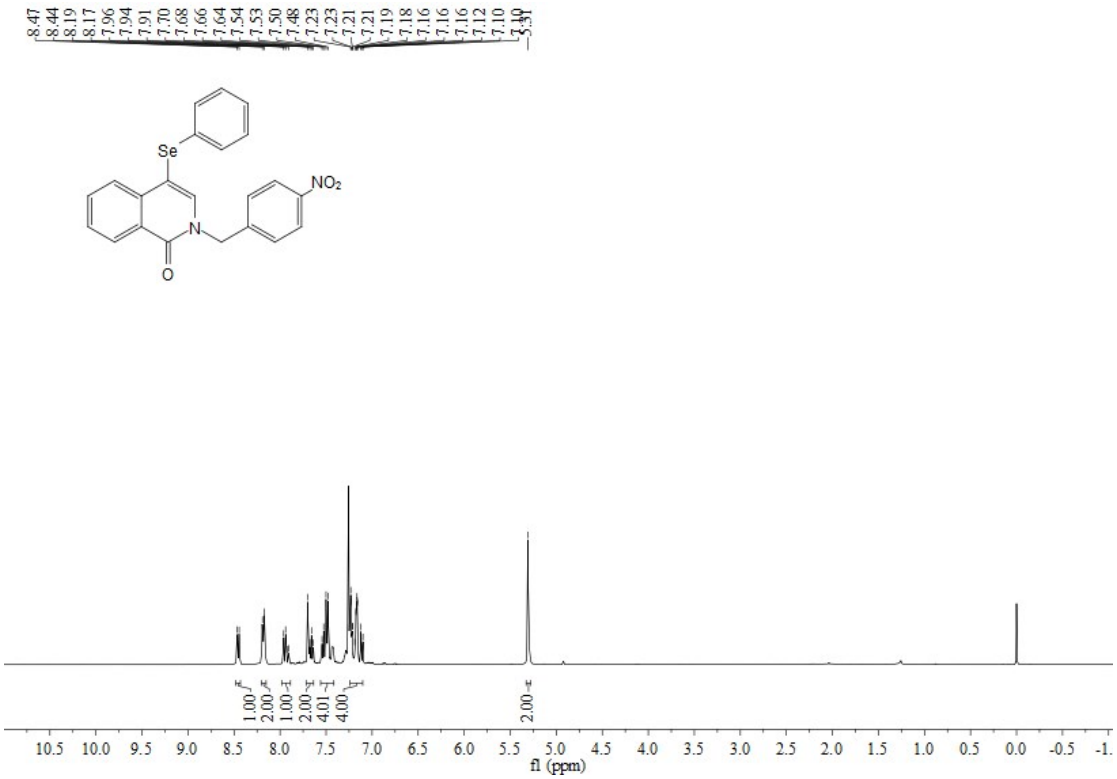
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5l**



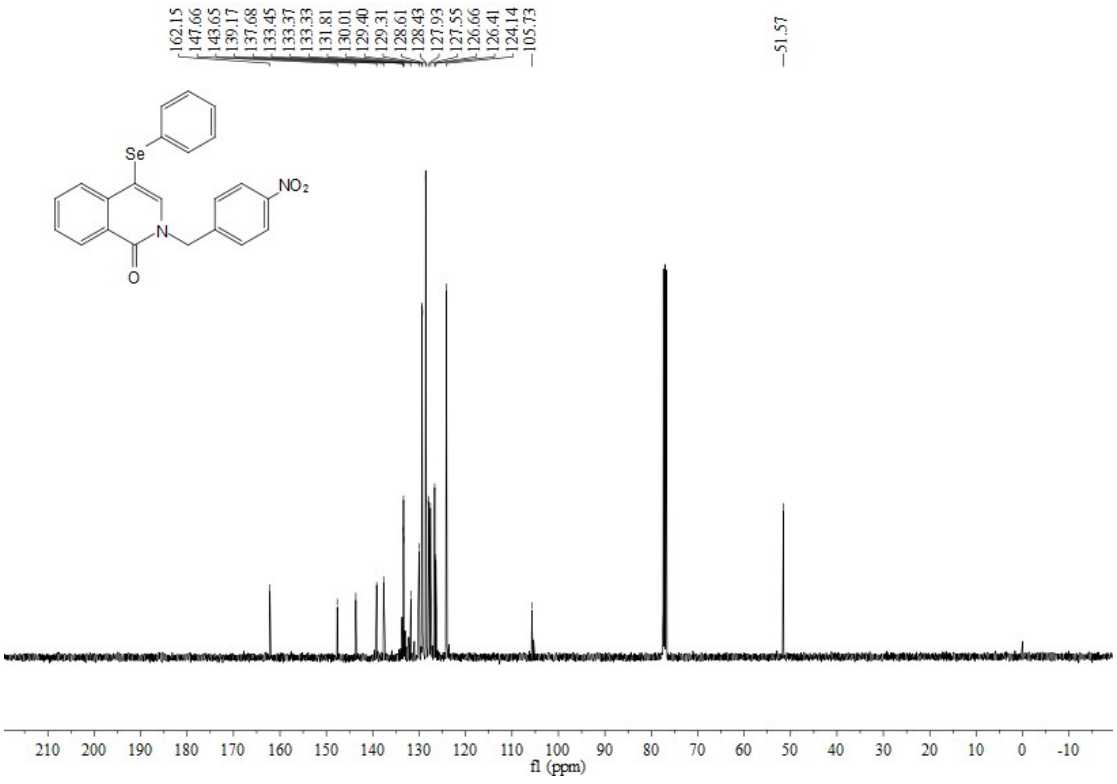
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5l**



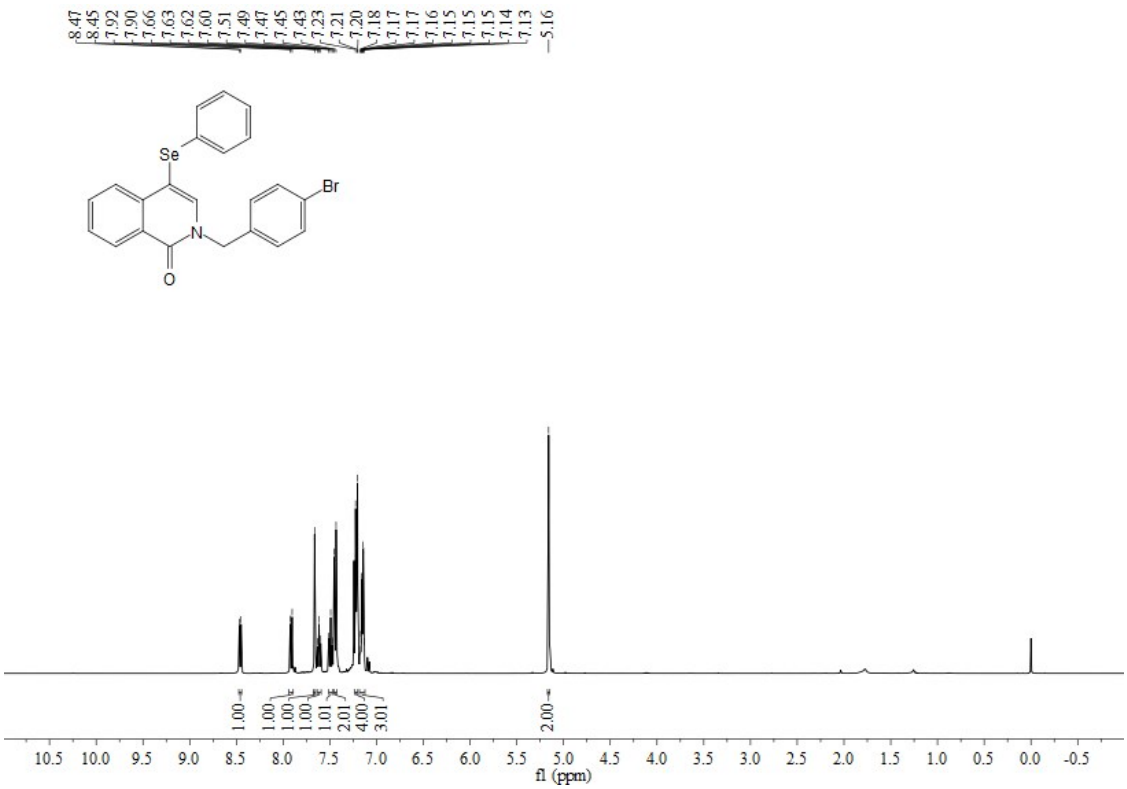
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5m**



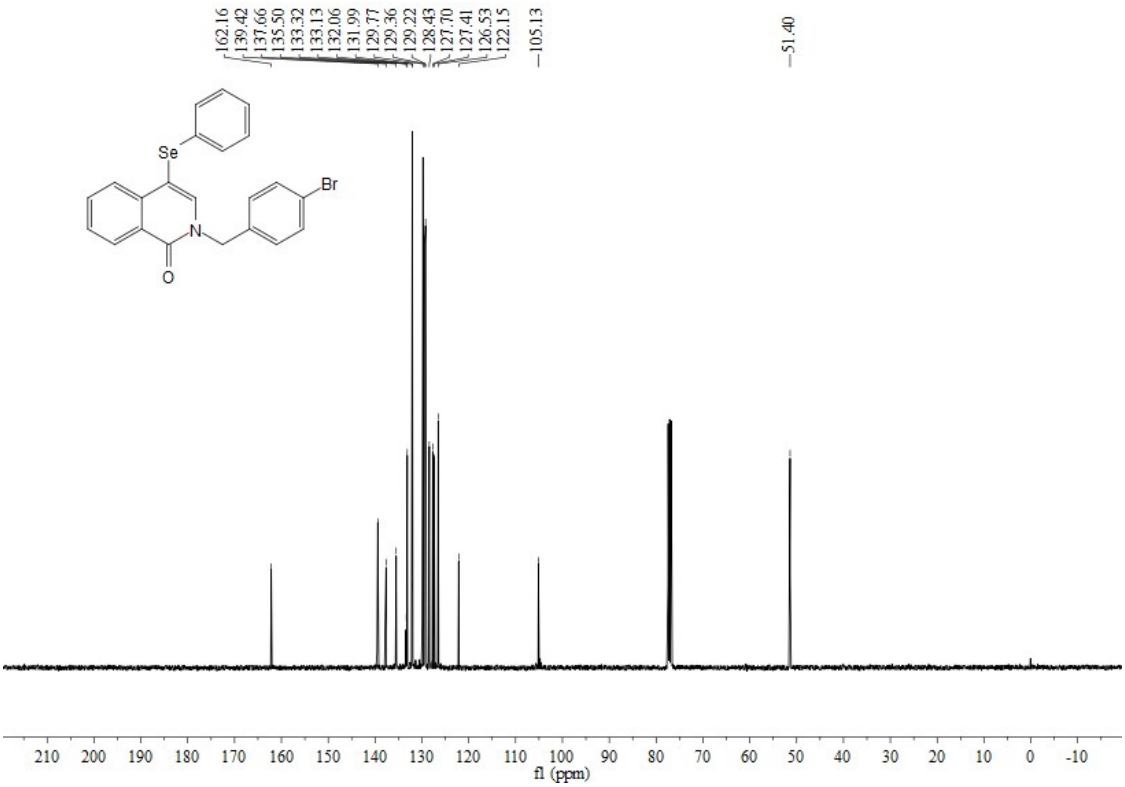
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5m**



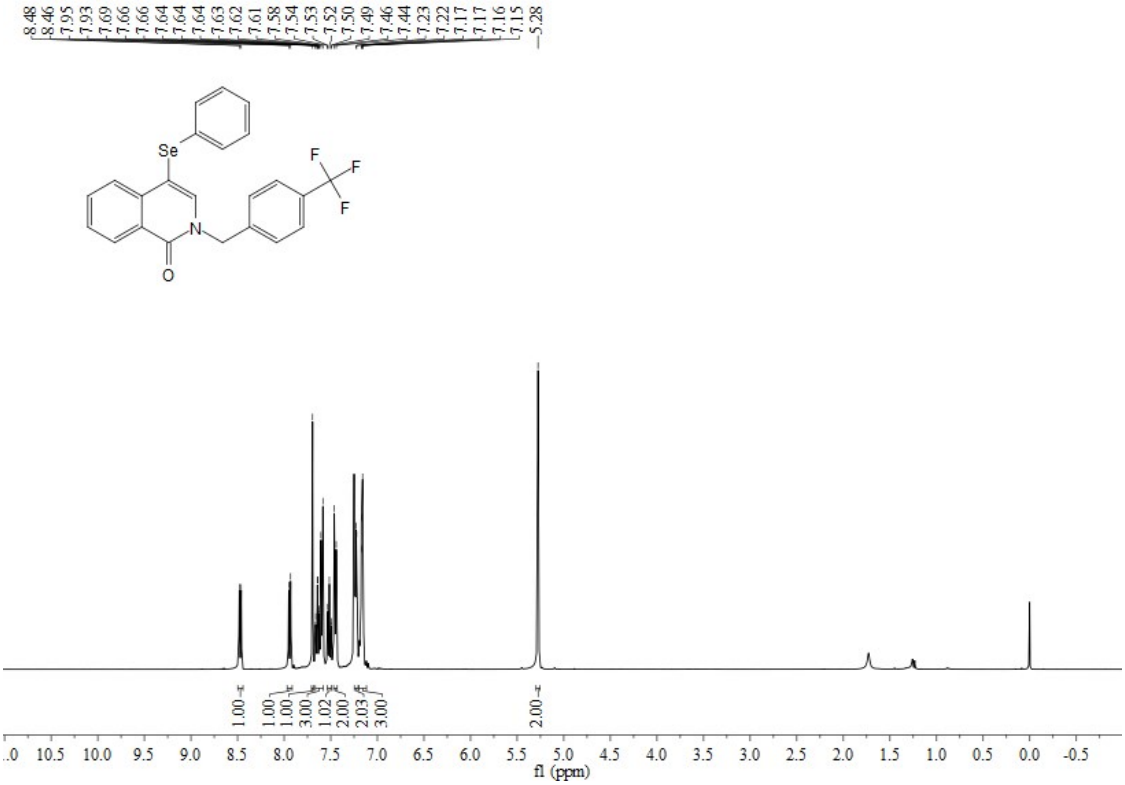
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5n**



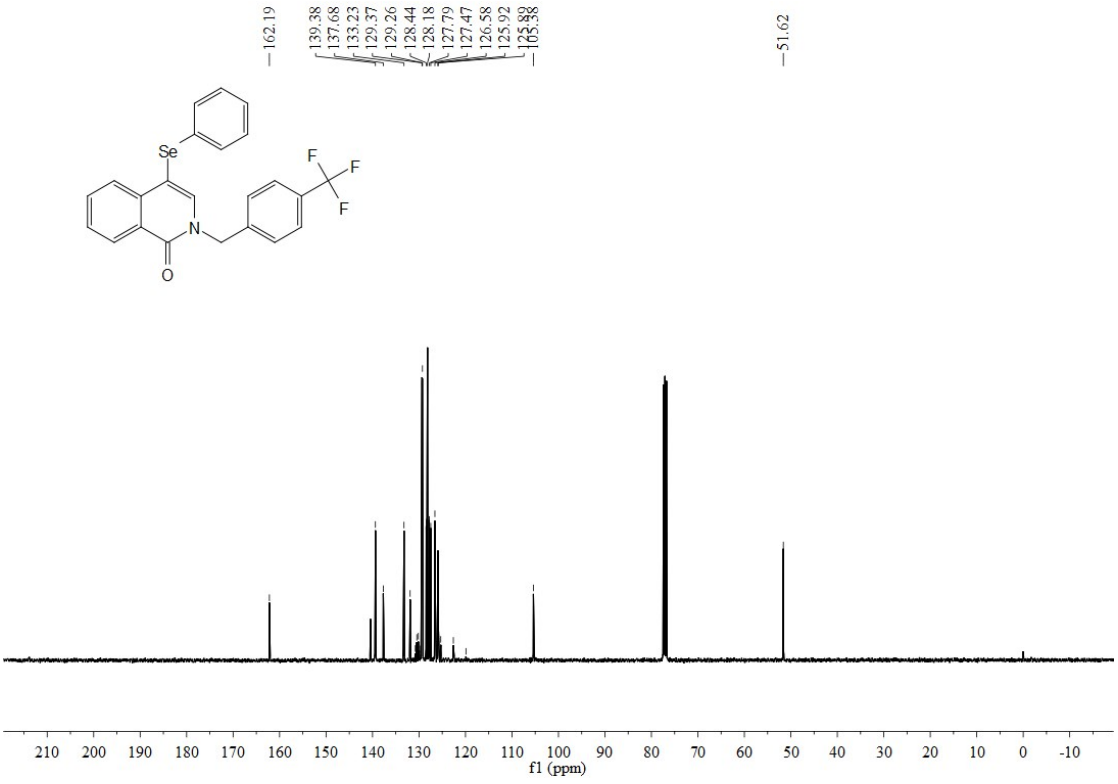
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5n**



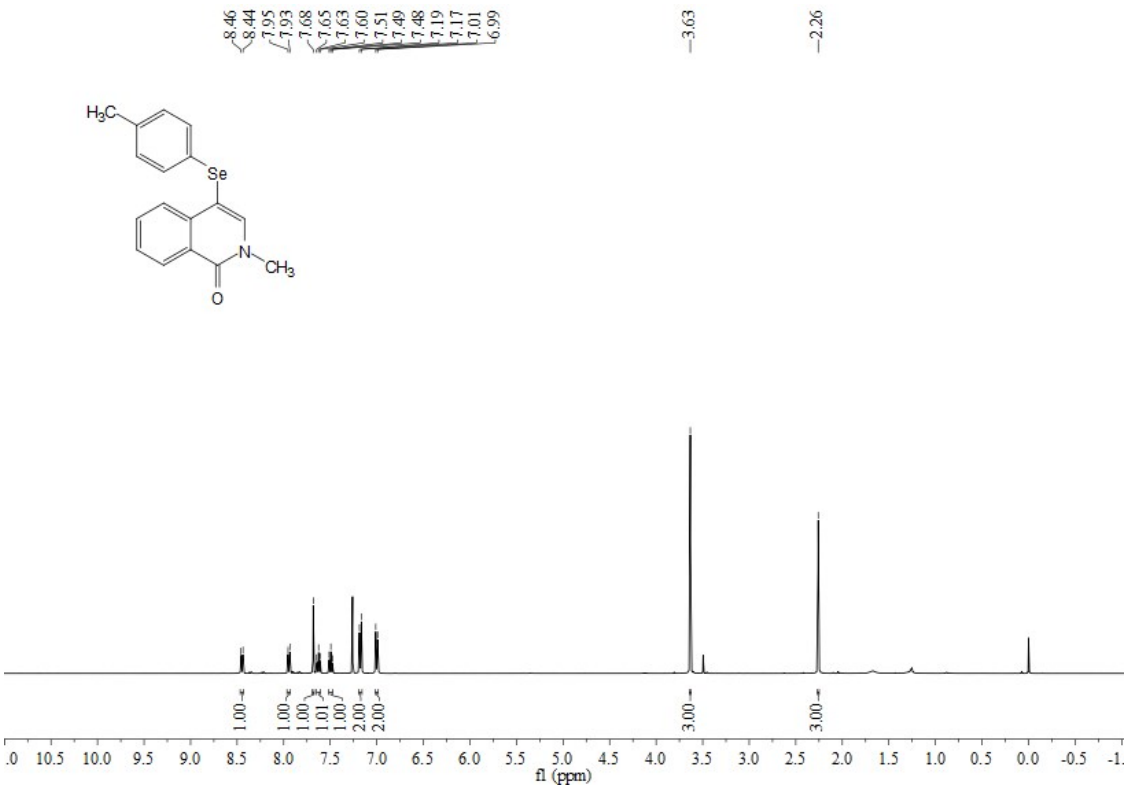
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5o**



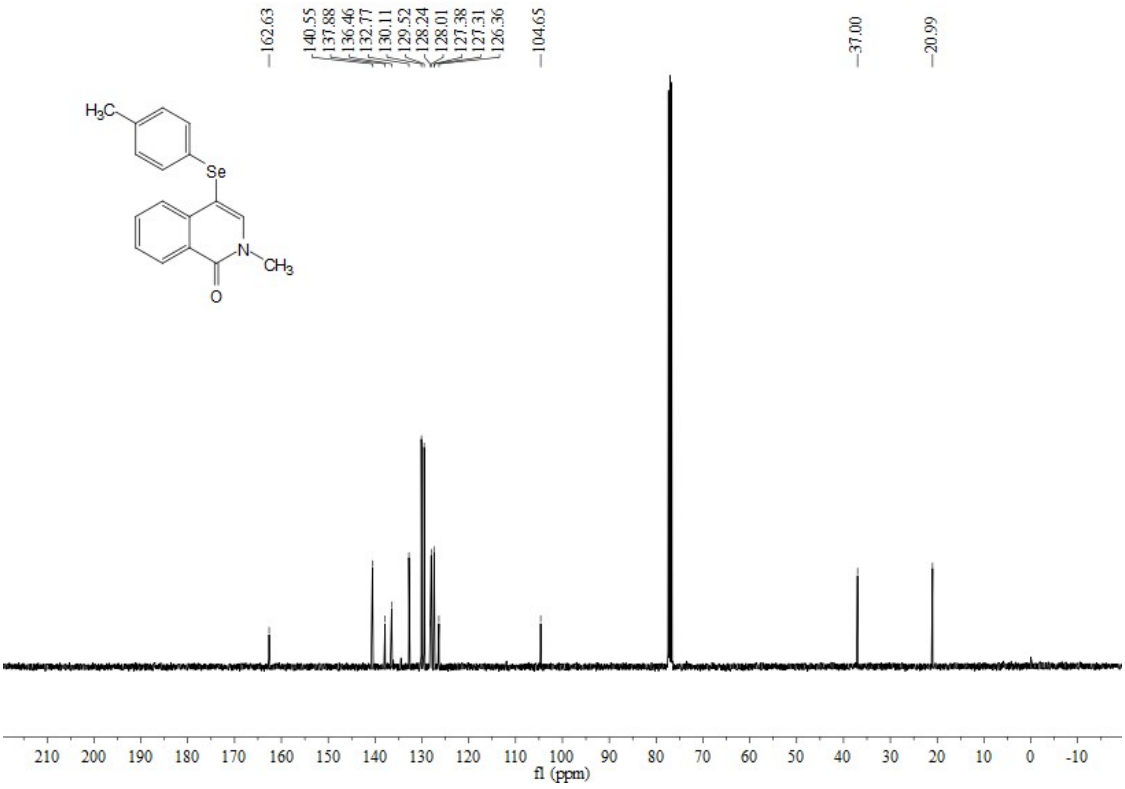
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5o**



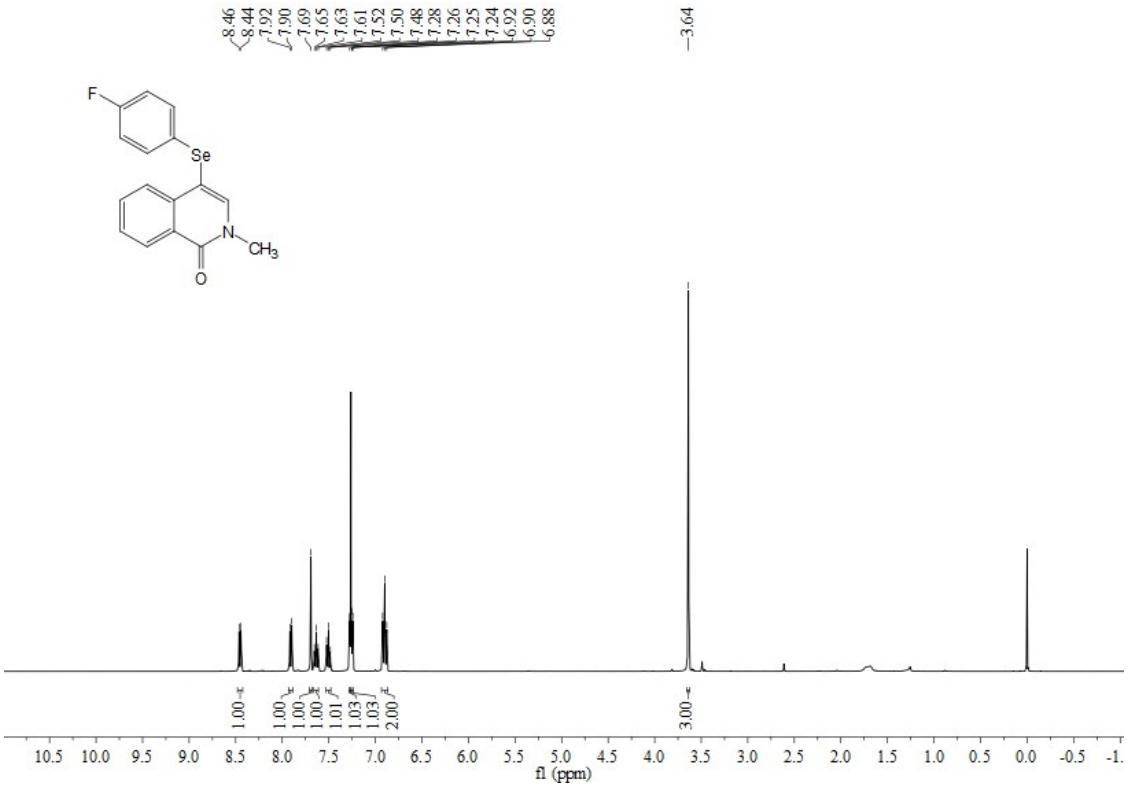
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6a**



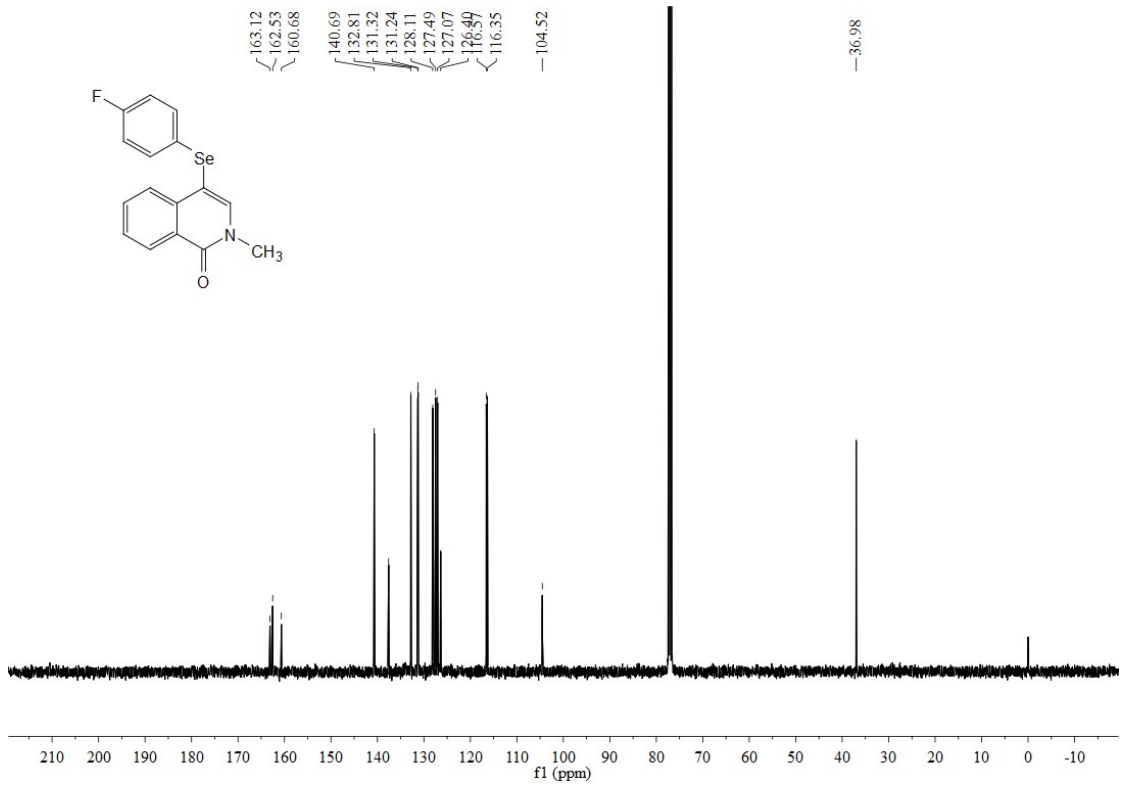
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6a**



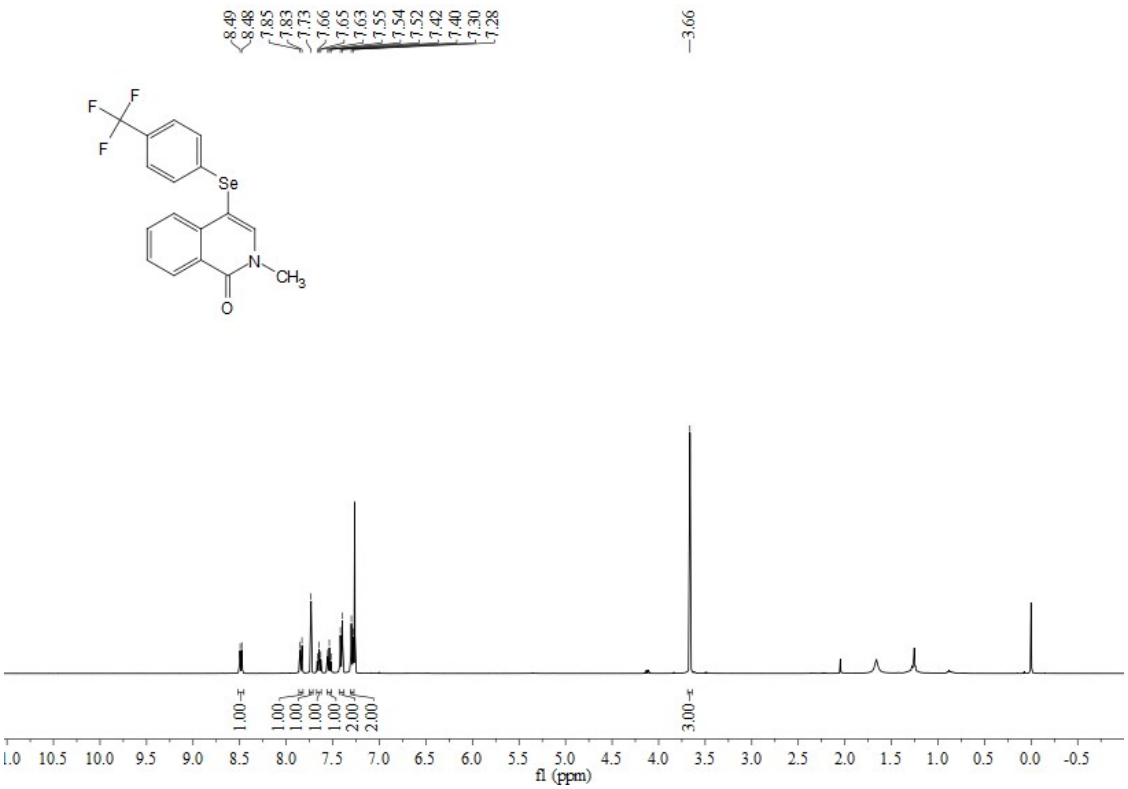
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6b**



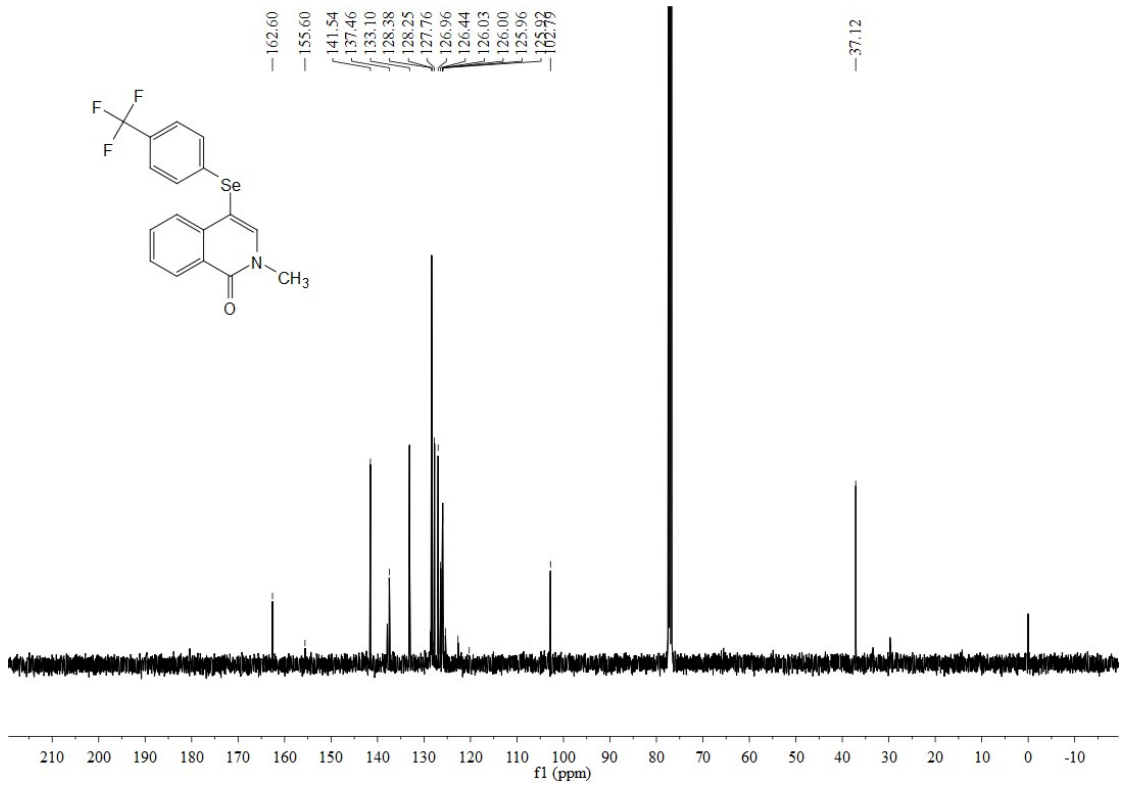
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6b**



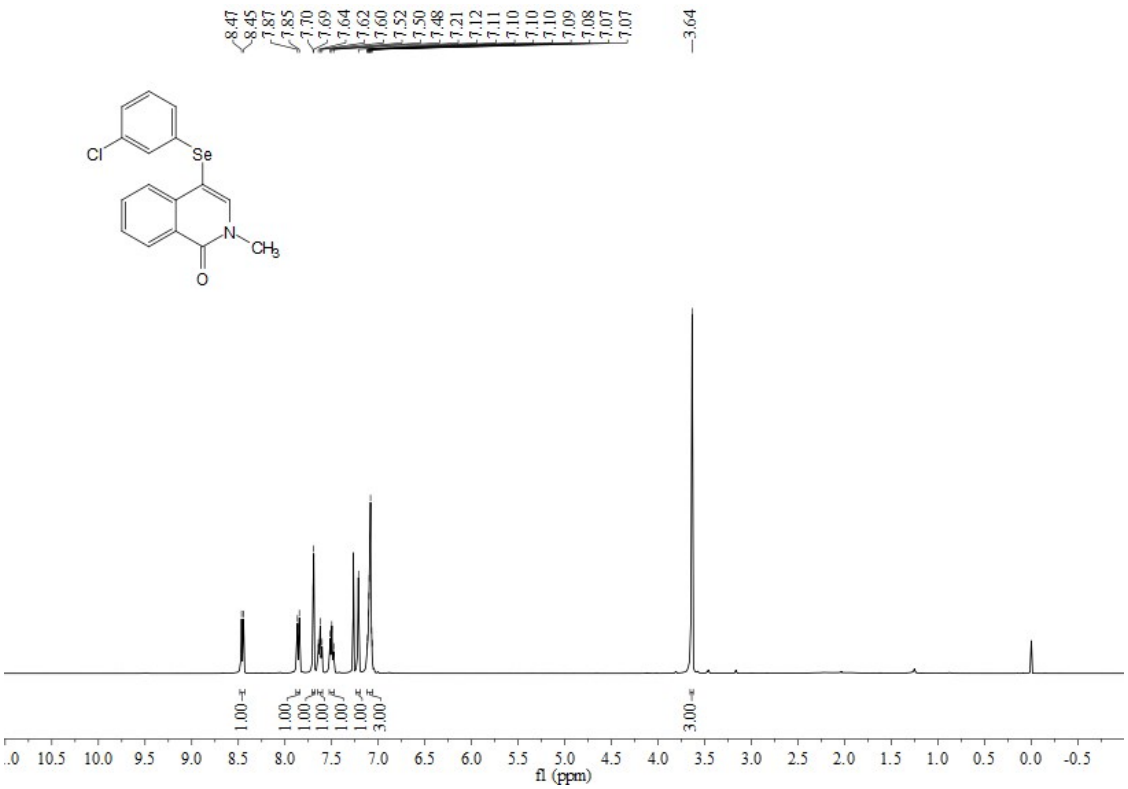
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6c**



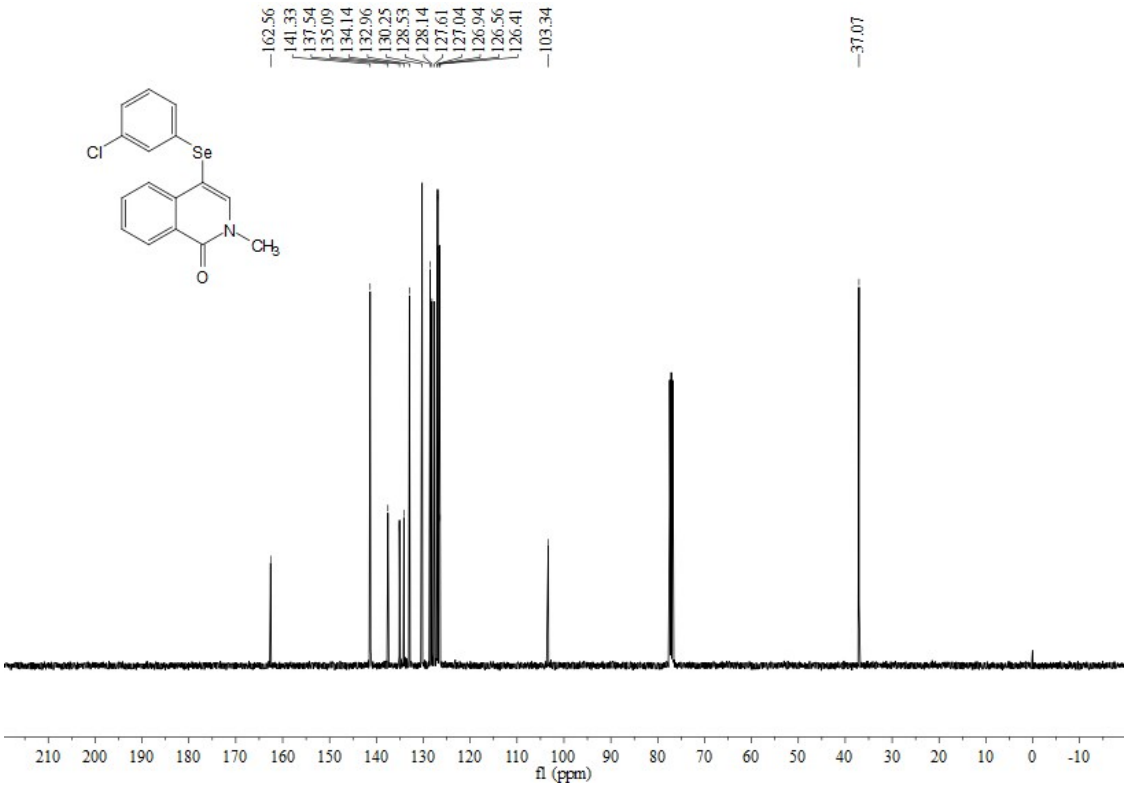
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6c**



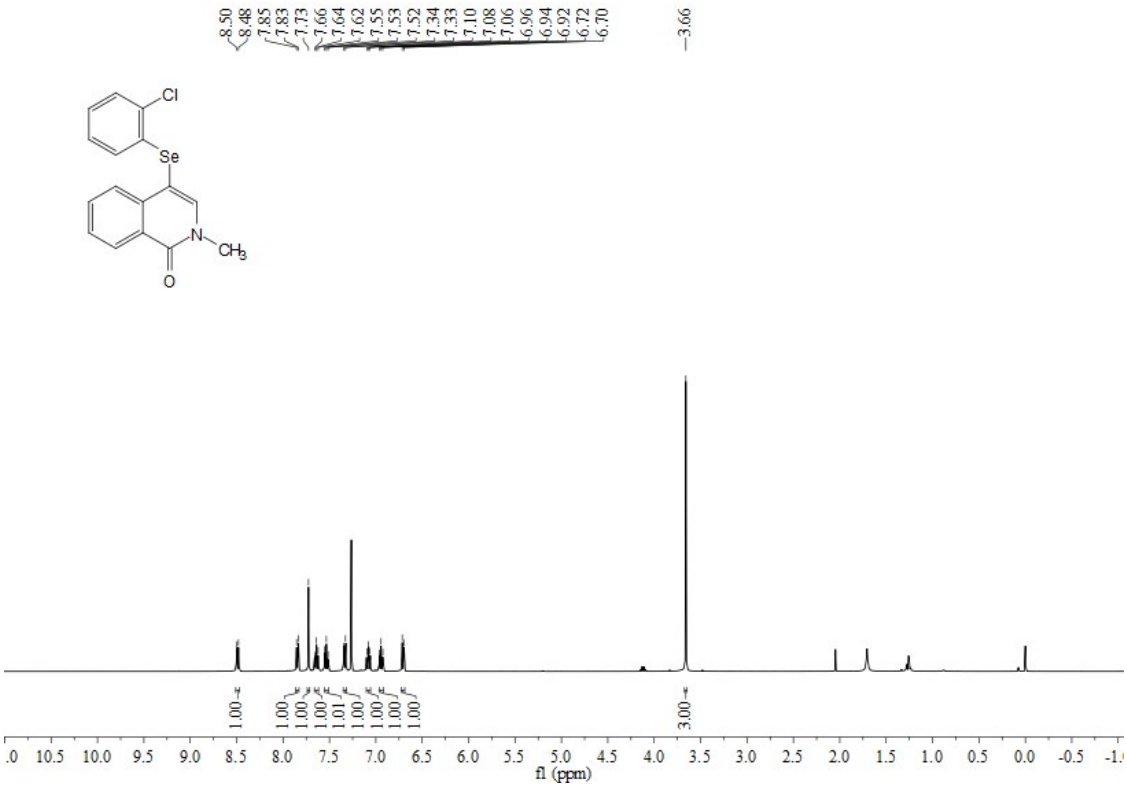
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6d**



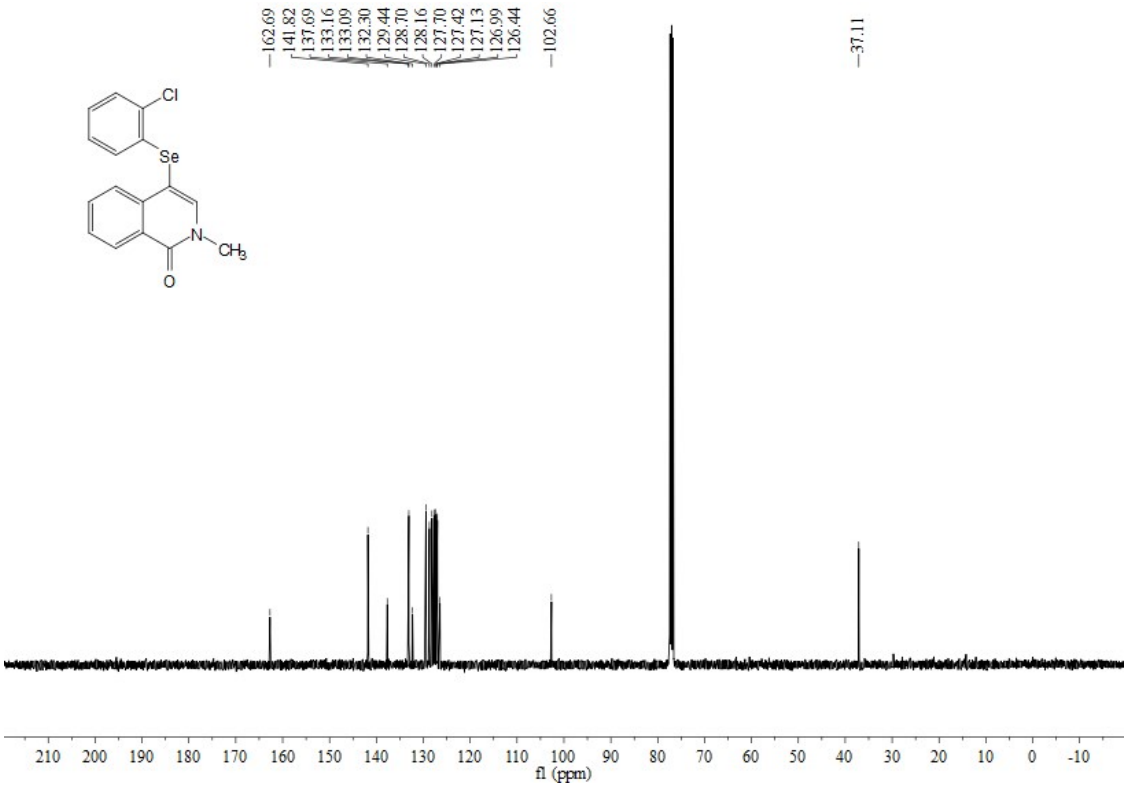
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6d**



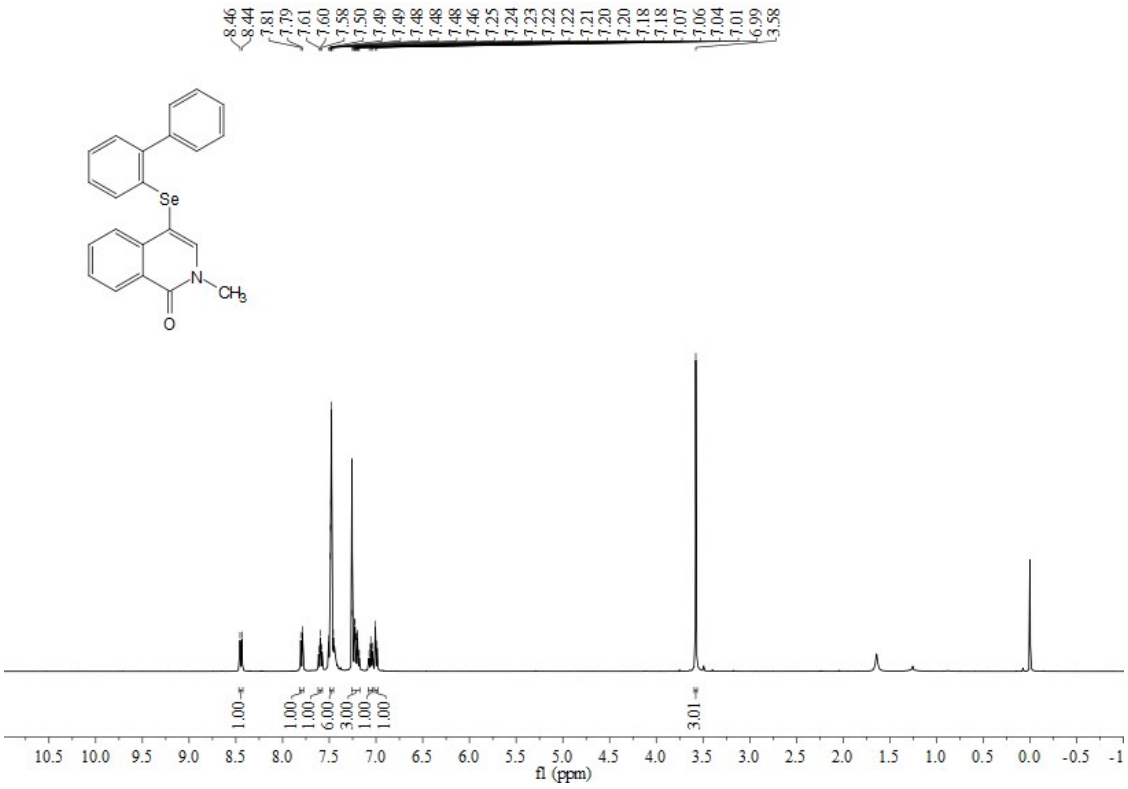
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6e**



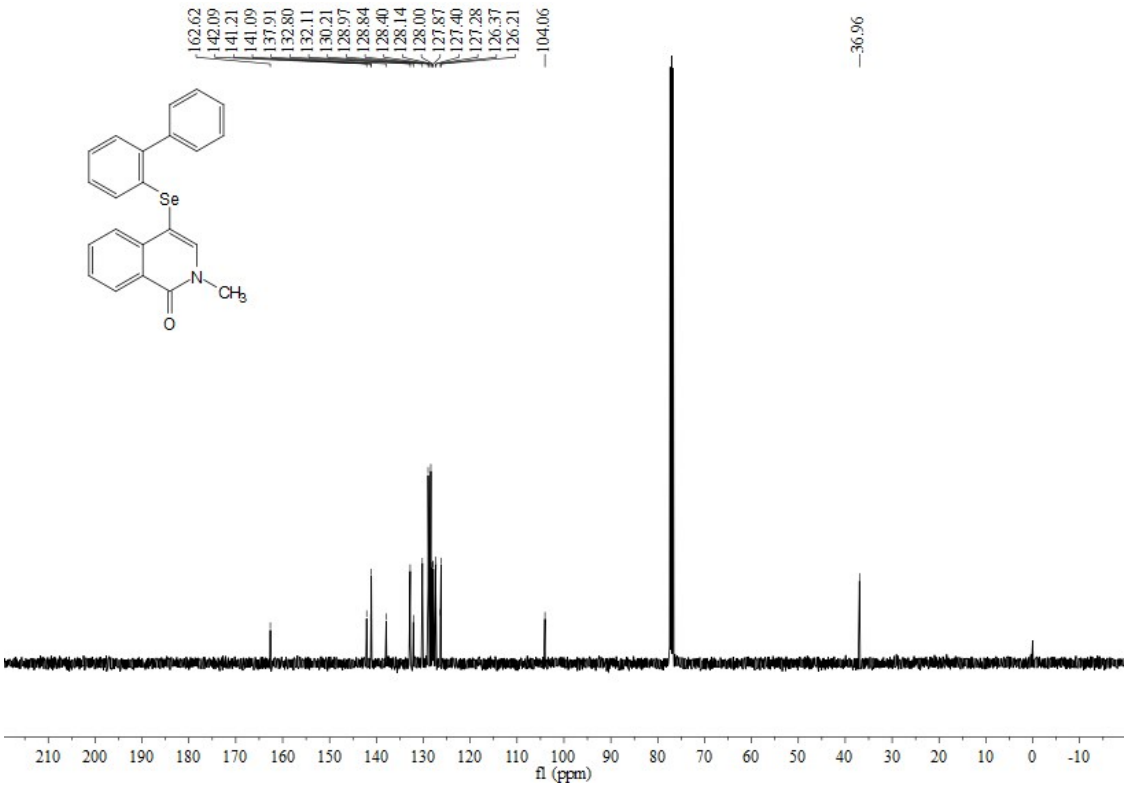
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6e**



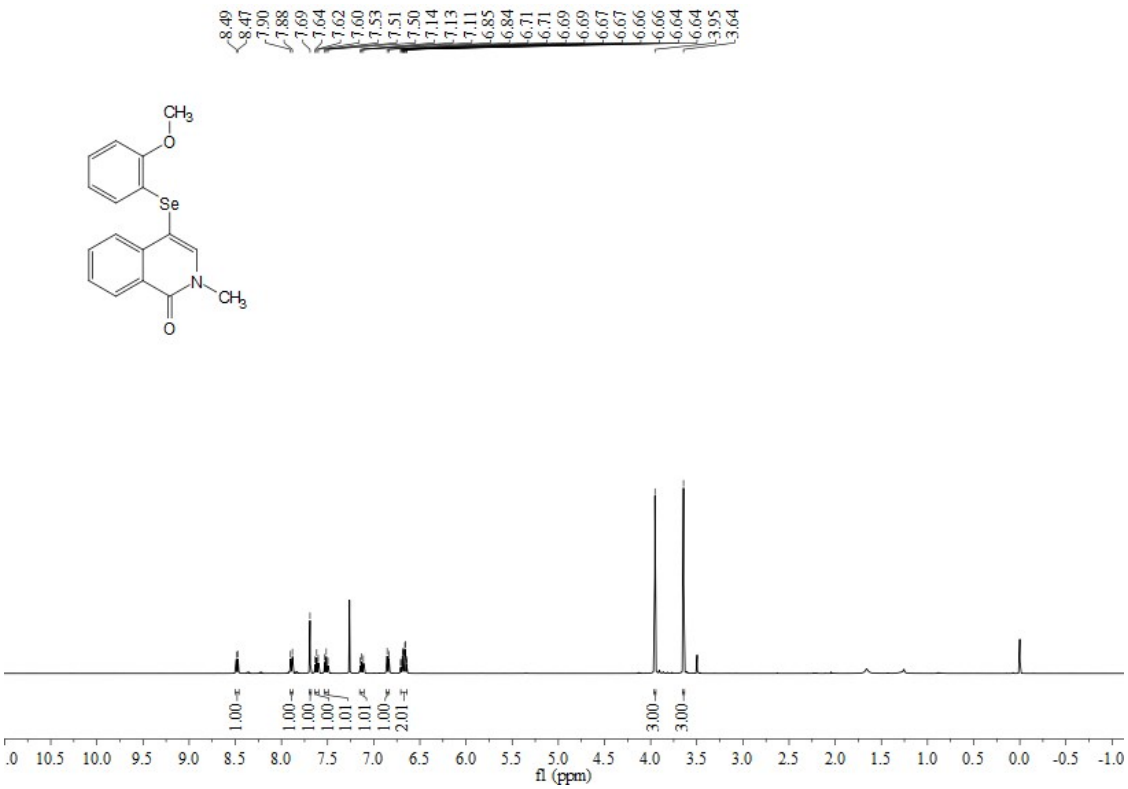
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6f**



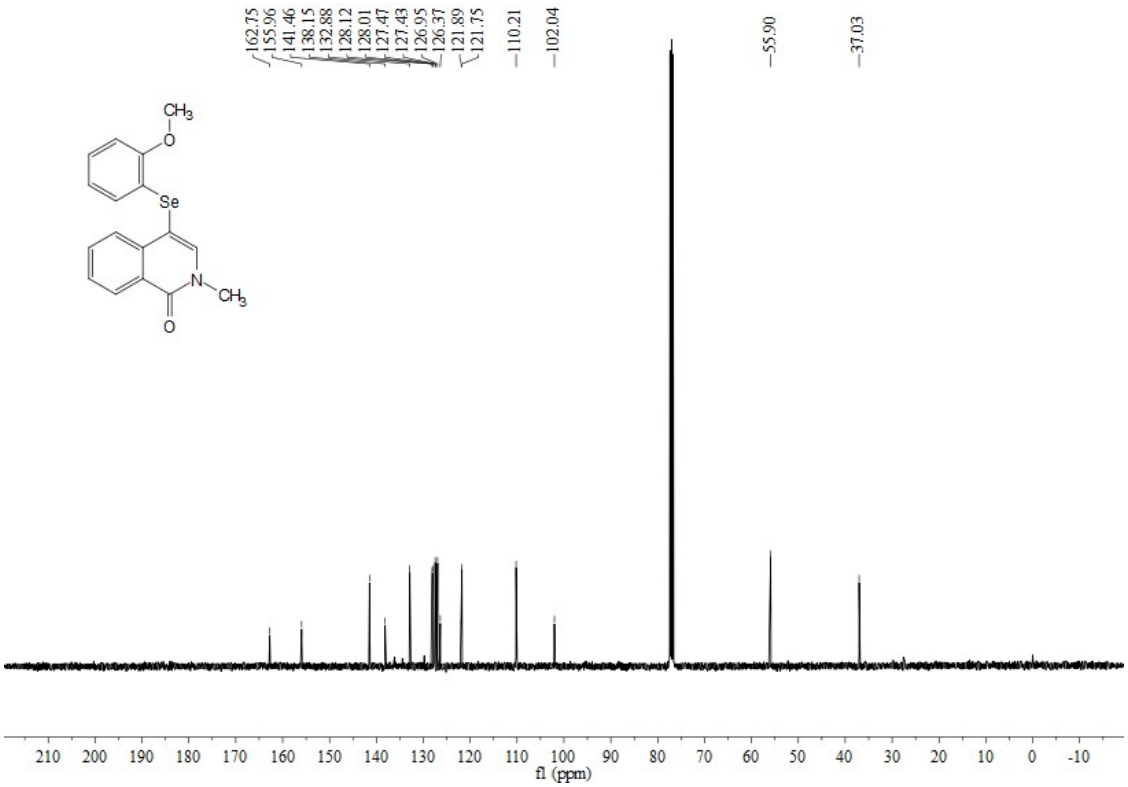
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6f**



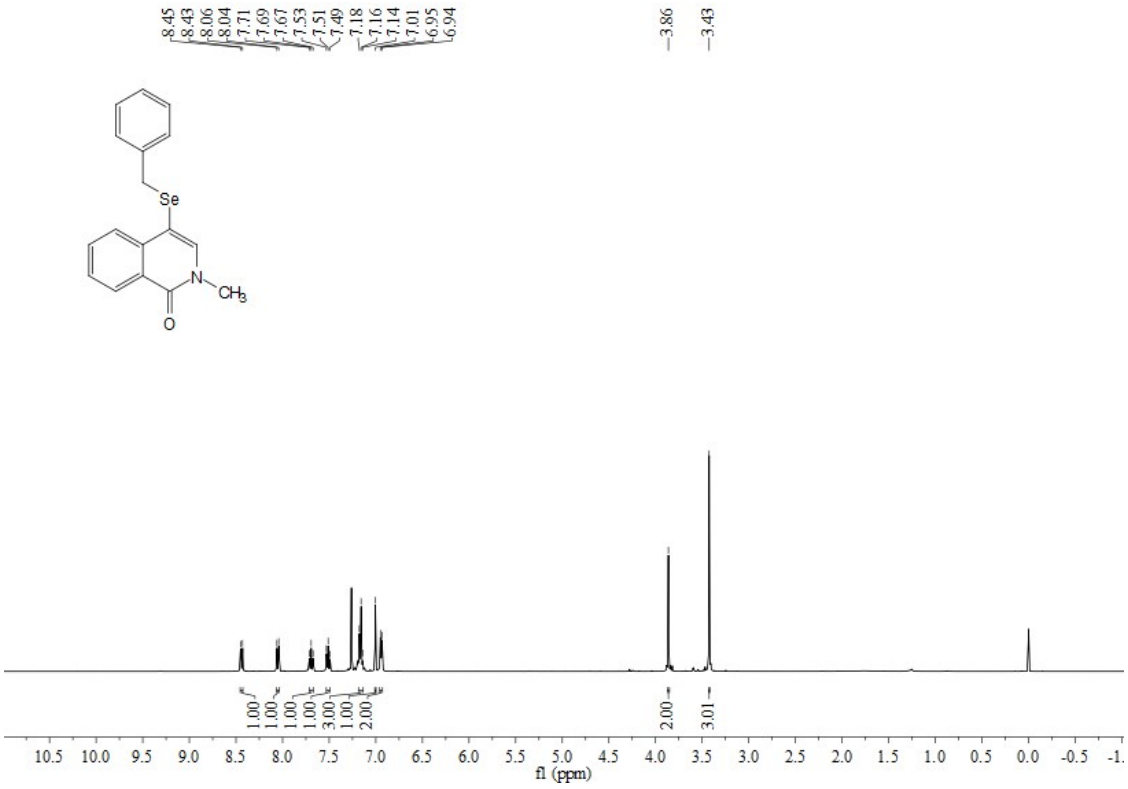
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6g**



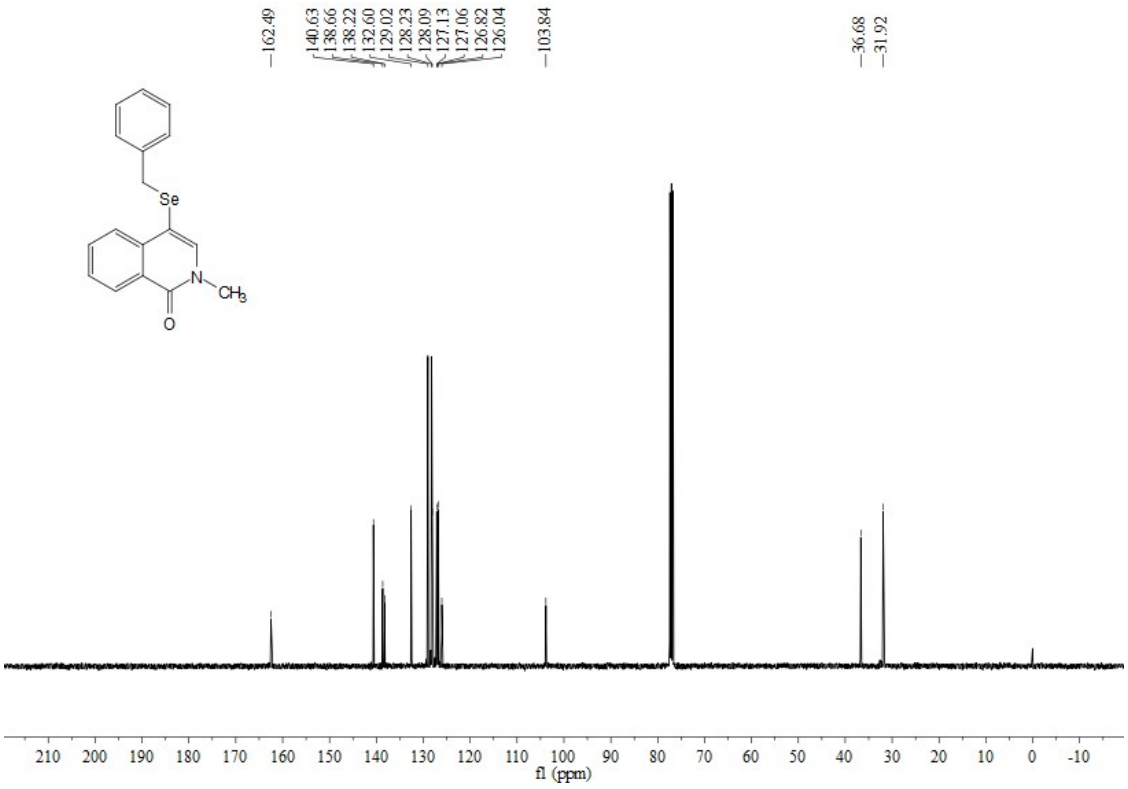
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6g**



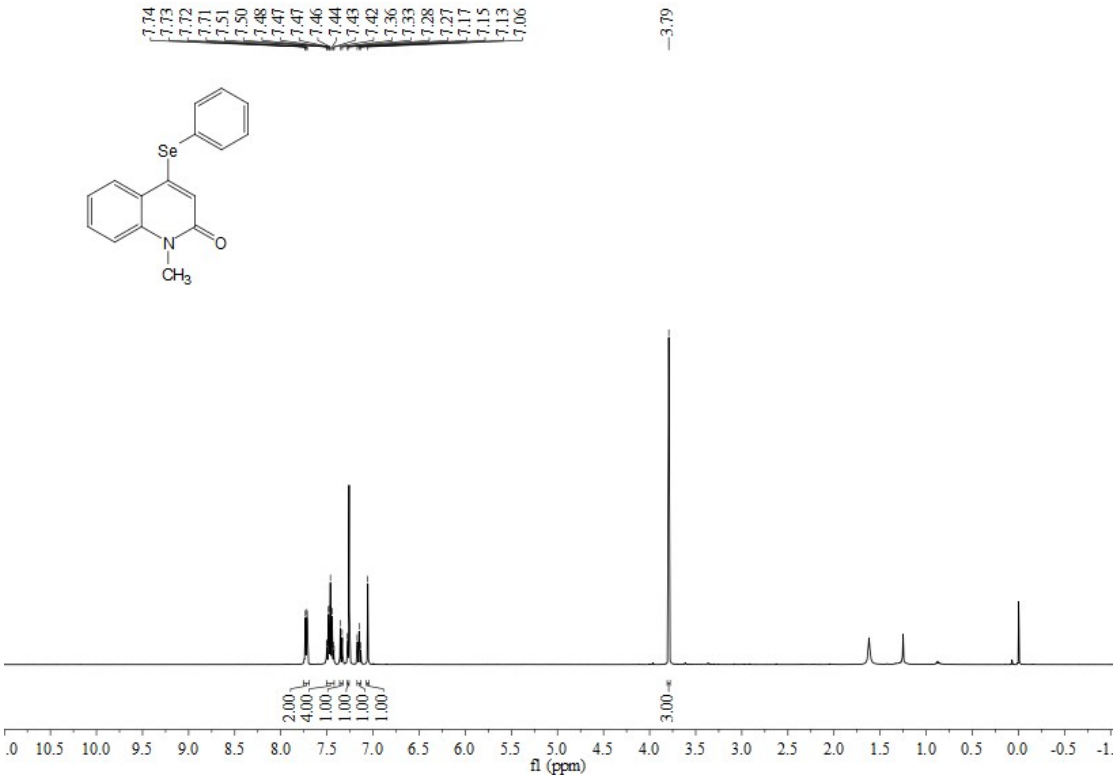
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6h**



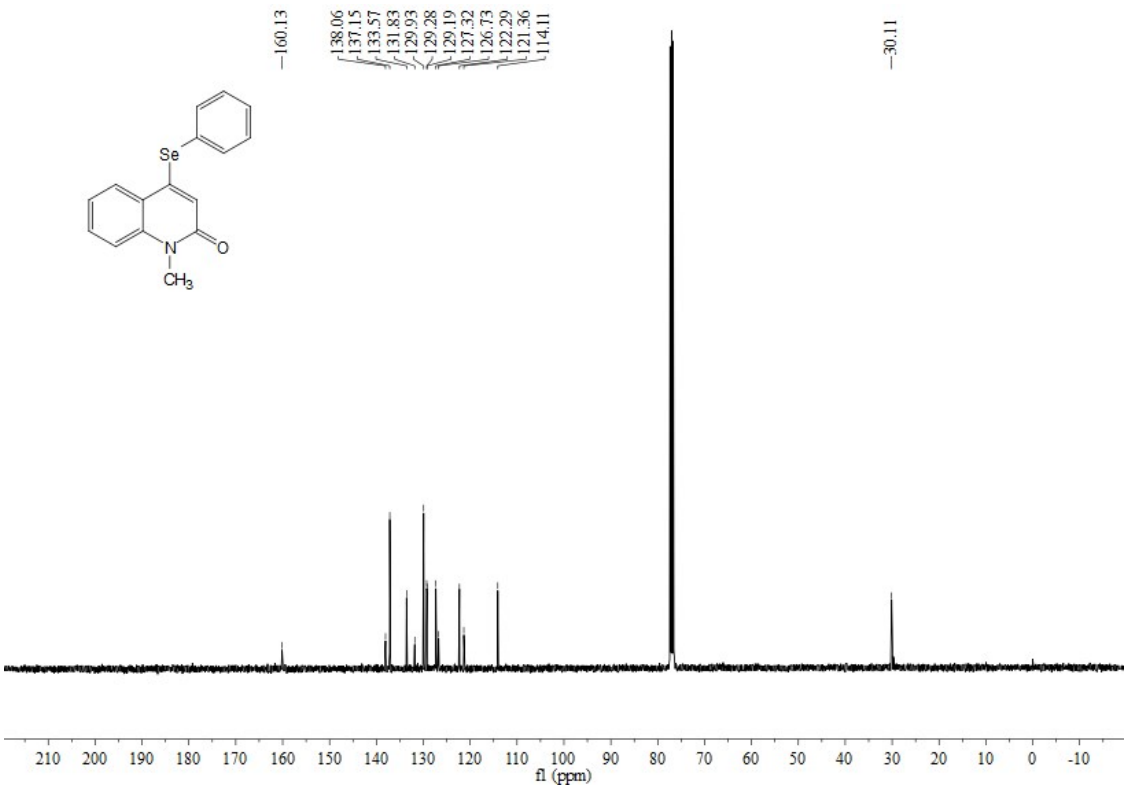
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6h**



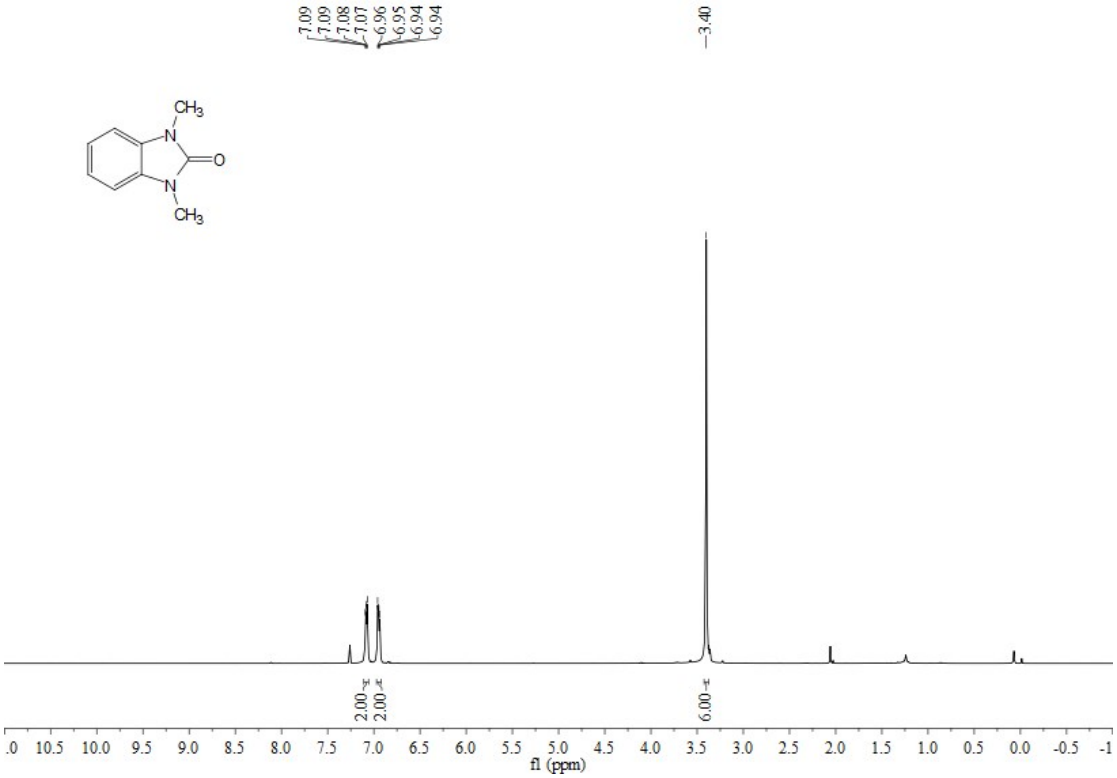
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7b**



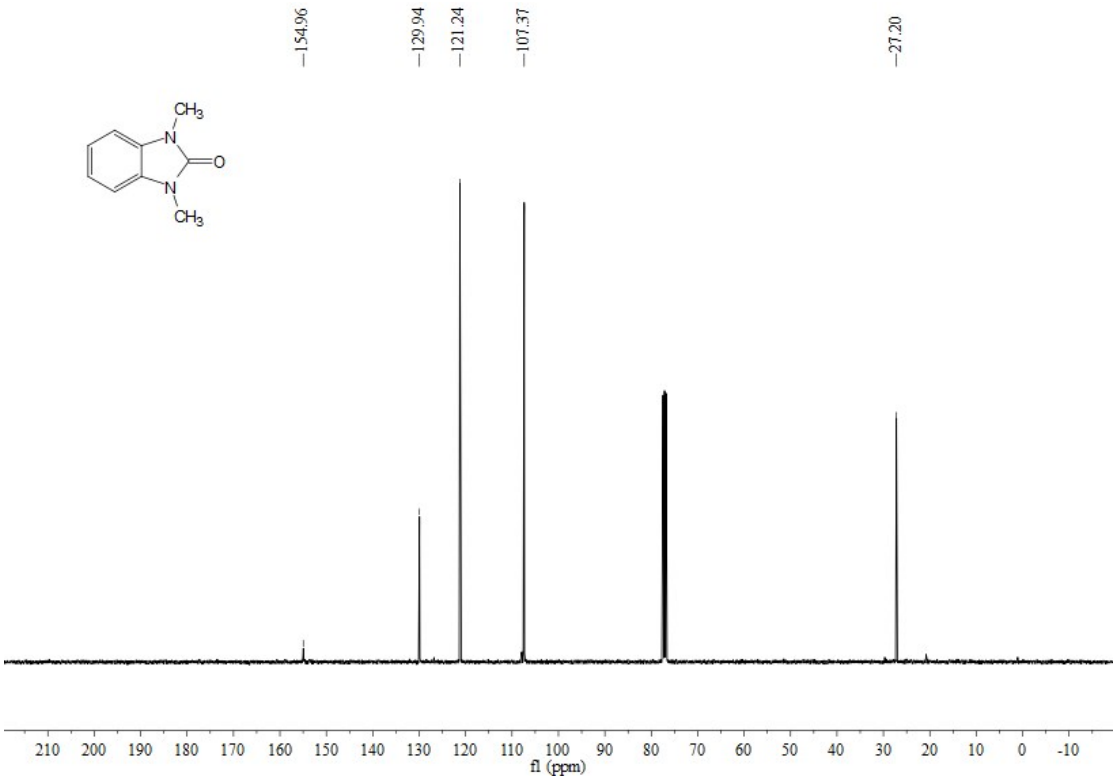
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7b**



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **8b**

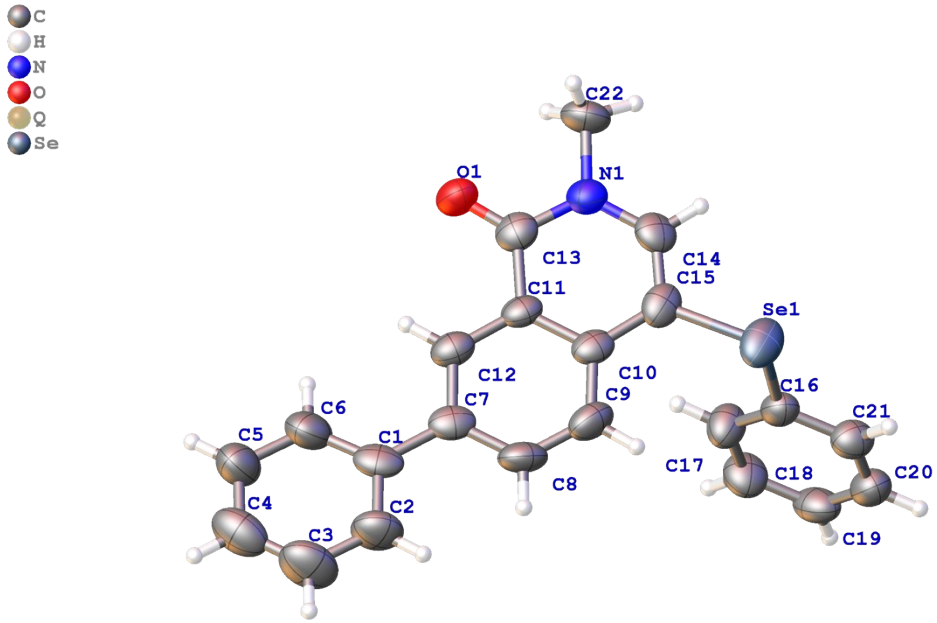


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8b**



4. X-ray crystallographic data

Figure S4 X-ray single crystal structure of **3l**



Single crystals of **3l** were grown by slow evaporation of its DCM/PE solution. Single-crystal X-ray diffraction data were collected with a 'multiwire proportional' diffractometer. The crystal was kept at 293 K during data collection. Using Olex2, the structure was solved with the olex2.solve structure solution program using Charge Flipping and refined with the olex2.refine refinement package using Least Squares minimization. Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2020934).

Table S4 Crystal data and structure refinement for **3l**

Empirical formula	$C_{22}H_{17}NOSe$
Formula weight	390.32
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	5.5032(6)
b/Å	14.7847(17)
c/Å	21.373(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1739.0(3)
Z	4
ρ_{calc}g/cm^3	1.491
μ/mm^{-1}	2.168

F(000)	792.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.704 to 49.996
Index ranges	-6 ≤ h ≤ 6, -12 ≤ k ≤ 17, -25 ≤ l ≤ 23
Reflections collected	7561
Independent reflections	3031 [R_{int} = 0.0609, R_{sigma} = 0.0842]
Data/restraints/parameters	3031/0/227
Goodness-of-fit on F^2	1.011
Final R indexes [I>=2σ (I)]	R_1 = 0.0555, wR_2 = 0.1025
Final R indexes [all data]	R_1 = 0.0918, wR_2 = 0.1190

Table S5 Bond Lengths for **3l**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Se1	C16	1.918(8)	C11	C10	1.411(10)
Se1	C15	1.907(7)	C11	C13	1.474(10)
O1	C13	1.220(9)	C14	C15	1.353(11)
N1	C14	1.366(9)	C21	C20	1.365(10)
N1	C13	1.393(10)	C10	C15	1.438(11)
N1	C22	1.471(10)	C10	C9	1.394(11)
C16	C21	1.369(10)	C20	C19	1.386(11)
C16	C17	1.377(10)	C17	C18	1.378(11)
C12	C7	1.385(10)	C18	C19	1.358(11)
C12	C11	1.407(10)	C8	C9	1.366(11)
C7	C1	1.489(11)	C6	C5	1.405(11)
C7	C8	1.384(11)	C4	C5	1.369(13)
C1	C6	1.368(12)	C4	C3	1.356(13)
C1	C2	1.398(11)	C2	C3	1.381(13)

Table S6 Bond Angles for **3l**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C15	Se1	C16	101.4(3)	C9	C10	C11	117.0(8)
C14	N1	C13	122.7(7)	C9	C10	C15	125.2(8)
C14	N1	C22	120.0(7)	C14	C15	Se1	117.5(7)
C13	N1	C22	117.3(7)	C14	C15	C10	119.1(7)
C21	C16	Se1	116.2(6)	C10	C15	Se1	123.0(7)
C21	C16	C17	119.5(8)	C21	C20	C19	120.5(8)
C17	C16	Se1	124.3(6)	C16	C17	C18	119.4(8)
C7	C12	C11	121.5(7)	O1	C13	N1	120.2(8)
C12	C7	C1	120.7(7)	O1	C13	C11	125.0(8)
C8	C7	C12	116.8(8)	N1	C13	C11	114.8(7)

C8	C7	C1	122.6(8)	C19	C18	C17	121.5(8)
C6	C1	C7	122.7(8)	C9	C8	C7	123.1(8)
C6	C1	C2	116.0(9)	C18	C19	C20	118.6(8)
C2	C1	C7	121.3(8)	C8	C9	C10	121.2(8)
C12	C11	C10	120.4(7)	C1	C6	C5	123.5(10)
C12	C11	C13	117.5(7)	C3	C4	C5	119.5(10)
C10	C11	C13	122.0(7)	C4	C5	C6	118.3(10)
C15	C14	N1	123.5(8)	C3	C2	C1	120.8(10)
C20	C21	C16	120.5(8)	C4	C3	C2	121.8(10)
C11	C10	C15	117.8(8)				

5. References

1. (a) Y. Jin, L. Ou, H. Yang and H. Fu, *J. Am. Chem. Soc.,* 2017, **139**, 14237−14243; (*b*) G. Wang, W. Hu, Z. Hu, Y. Zhang, W. Yao, L. Li, Z. Fu and W. Huang, *Green Chem.,* 2018, **20**, 3302−3307; (*c*) W.-K. Luo, X. Shi, W. Zhou and L. Yang, *Org. Lett.,* 2016, **18**, 2036−2039; (*d*) Z. Fang, Y. Wang and Y. Wang, *Org. Lett.,* 2019, **21**, 434−438.