Supporting Information

Electrochemical synthesis of selenyl imidazo[2,1-*b*]thiazinones *via* three-component reactions

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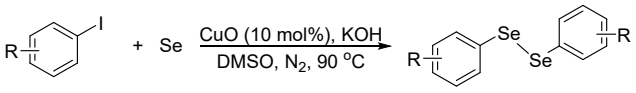
1. General Information

The ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker AVANCE NEO-600 (600 MHz, 150 MHz and 565 MHz respectively) NMR spectrometer. ^{1}H and ^{13}C NMR chemical shifts were determined relative to internal standard $CDCl_3$ (δ (^{1}H), 7.26 ppm; δ (^{13}C), 77.16 ppm). Chemical shifts (δ) were reported as parts per million (ppm) downfield from tetramethylsilane and the following abbreviations were used to identify the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, m = multiplet, dd = doublet of doublets and all combinations thereof can be explained by their integral parts. Coupling constant (*J*) was reported in hertz unit (Hz). Melting point (m.p.) was recorded on BÜCHI (M-560). High-resolution mass spectra (HRMS) were recorded on a Thermo Fisher Scientific Q-Exactive (ESI-Orbitrap). Cyclic voltammetry (CV) was carried out on a CHI660E electrochemical workstation (CH Instruments, INS). Analytical thin layer chromatography (TLC) was performed on 0.25 mm silica gel 60 F254 plates and viewed by UV light (254 nm). Column chromatographic purification was performed using 200-300 mesh silica gel.

Materials. All commercial reagents and solvents were purchased from commercial sources and used as received unless otherwise indicated.

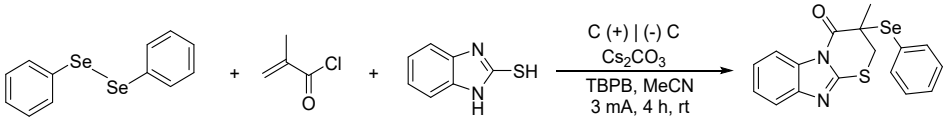
2 Experimental Procedures

2.1 General procedure for the synthesis of diselenides



According to the literature[1], we have prepared a series of diselenide compounds. To a stirred solution of Se^0 powder (156 mg, 2.0 mmol) and iodobenzene (204 mg, 1.0 mmol) in dry DMSO (2.0 mL) was added CuO (10 mol%) followed by KOH (112 mg, 2.0 mmol) under nitrogen atmosphere at 90 °C for 2 h. 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 diselenide.

2.2 General procedure for the synthesis of products (taking 4a as an example)

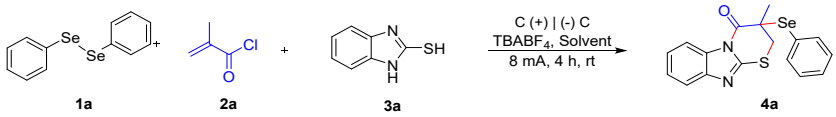


1a **2a** **3a** **4a**

A mixture of diphenyl diselenide **1a** (15.6 mg, 0.05 mmol), methacryloyl chloride **2a** (42 μL, 0.4 mmol), 2-mercaptobenzimidazole **3a** (30.0 mg, 0.2 mmol), TBPB (67.9 mg, 0.2 mmol), Cs_2CO_3 (32.6 mg, 0.1 mmol) and CH_3CN (4.0 mL), were added in an undivided bottle (10 mL). The bottle was equipped with graphite plates as anode and cathode. The resulting mixture was stirred and electrolyzed with constant current 3 mA at room temperature for 4 h. After the reaction finished, the resulting mixture were evaporated under reduced pressure. The resultant residue was purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 10:1, v/v) to afford the desired product **4a** in 90% yield.

2.3 Optimization of reaction conditions

Table S1 Screening of solvents[a]

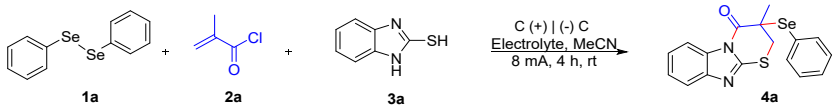


1a 2a 3a 4a

Entry	Solvent	Yield (%)[b]
1	MeCN	29
2	MeOH	trace
3	DMF	7
4	DMSO	trace
5	DCE	24
6	NMP	N.D.

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), **3a** (0.2 mmol), $TBABF_4$ (0.2 mmol), solvent (4 mL), C (15 mm×10 mm×1 mm) cathode, C plate (15 mm×10 mm×1 mm) anode, undivided cell, current = 8 mA, rt, 4 h. [b] Isolated yields. N.D. = not detected

Table S2 Screening of electrolytes[a]

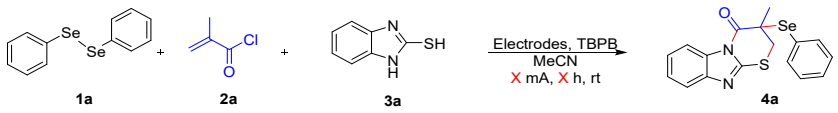


1a 2a 3a 4a

Entry	Electrolyte	Yield (%)[b]
1	TBAI	26
2	$TBAClO_4$	37
3	$TBAPF_6$	32
4	TBAOAc	29
5	$Mg(ClO_4)_2$	16
6	$EMImClO_4$	35
7	$TBAHSO_4$	11
8	TBPB	46
9	$EMImBF_4$	21
10	TBAOH	trace

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), **3a** (0.2 mmol), electroyte (0.2 mmol), MeCN (4 mL), C (15 mm×10 mm×1 mm) cathode, C plate (15 mm×10 mm×1 mm) anode, undivided cell, current = 8 mA, rt, 4 h. [b] Isolated yields.

Table S3 Screening of electrodes, times and currents[a]

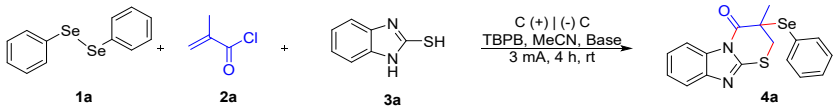


1a 2a 3a 4a

Entry	Electrode	Time (h)	Current (mA)	Yields (%)[b]
1	C (+) | C (-)	4	8	46
2	C (+) | Ni (-)	4	8	26
3	C (+) | Pt (-)	4	8	34
4	Pt (+) | Pt (-)	4	8	36
5	Ni (+) | Pt (-)	4	8	trace
6	C (+) | C (-)	3	8	33
7	C (+) | C (-)	5	8	25
8	C (+) | C (-)	4	2	47
9	C (+) | C (-)	4	3	54
10	C (+) | C (-)	4	4	44

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), **3a** (0.2 mmol), TBPB (0.2 mmol), MeCN (4 mL), cathode, anode, undivided cell, constant current, rt. [b] Isolated yields.

Table S4 Screening of bases[a]

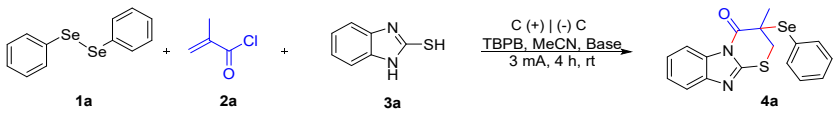


1a 2a 3a 4a

Entry	Base (mmol)	Yields (%)[b]
1	TEA	35
2	Py	24
3	Cs_2CO_3	61
4	DMAP	44
5	DBU	42
6	TBD	37
7	^{t}BuOK	34
8	^{t}BuONa	26
9	K_2CO_3	53
10	CsCl	52
11	CsF	58

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), **3a** (0.2 mmol), TBPB (0.2 mmol), base (0.2 mmol), MeCN (4 mL), C (15 mm×10 mm×1 mm) cathode, C plate (15 mm×10 mm×1 mm) anode, undivided cell, current = 3 mA, rt, 4 h. [b] Isolated yields.

Table S5 Screening of reaction ratio[a]



1a 2a 3a 4a

Entry	1a (mmol)	3a (mmol)	Cs_2CO_3 (mmol)	TBPB (mmol)	Yields (%)[b]
1	0.1	0.2	0.2	0.2	39
2	0.09	0.2	0.2	0.2	54
3	0.08	0.2	0.2	0.2	57
4	0.07	0.2	0.2	0.2	60
5	0.06	0.2	0.2	0.2	63
6	0.05	0.2	0.2	0.2	85
7	0.05	0.2	0.18	0.2	49
8	0.05	0.2	0.16	0.2	49
9	0.05	0.2	0.14	0.2	81
10	0.05	0.2	0.12	0.2	81
11	0.05	0.2	0.1	0.2	90
12	0.05	0.2	0.08	0.2	73
13	0.05	0.2	0.1	0.15	69
14	0.05	0.2	0.1	0.1	52
15	0.05	0.15	0.1	0.2	76
16	0.05	0.1	0.1	0.2	50

[a] Reaction conditions: **1a** (X mmol), **2a** (0.4 mmol), **3a** (X mmol), TBPB (X mmol), Cs_2CO_3 (X mmol), MeCN (4 mL), C (15 mm×10 mm×1 mm) cathode, C plate (15 mm×10 mm×1 mm) anode, undivided cell, current = 3 mA, rt, 4 h. [b] Isolated yields.

3 Mechanistic studies

3.1 Cyclic voltammetry experiments

Cyclic voltammograms were recorded with a CHI660E electrochemical workstation at room temperature in MeCN. Scan rate 0.05 V/s, ranging from -1 V-1.7 V, a glassy carbon-disk (R = 5.5 mm, h = 10 mm) was used as the working electrode. The Pt disk (R = 5.5 mm, h = 10 mm) and Ag/AgCl (R = 5.0 mm, h = 10 mm) was used as counter and reference electrode, respectively. A: MeCN (4 mL) + TBPB (0.2 mmol) + Cs_2CO_3 (0.1 mmol); b: MeCN (4 mL) + TBPB (0.2 mmol) + Cs_2CO_3 (0.1 mmol) + **1a** (0.2 mmol).

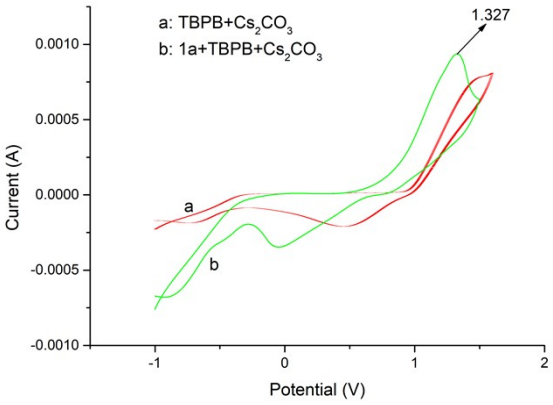
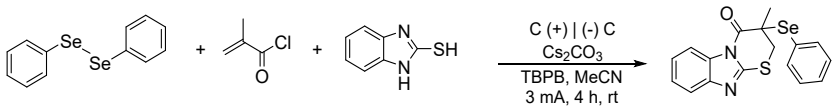


Fig. S1 Cyclic voltammetry experiments

3.2 Radical trapping experiments[a]

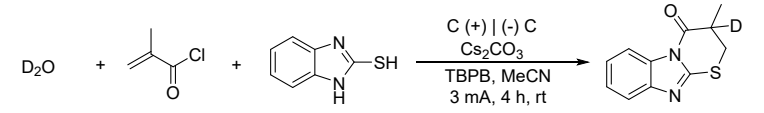


1a **2a** **3a** **4a**

Entry	Radical scavenger (mmol)	Yield of 4a (%)[b]
1	none	90
2	TEMPO (0.8)	80
3	TEMPO (1.2)	54
4	BHT (0.8)	70
5	BHT (1.2)	65
6	DPE (0.8)	67
7	DPE (1.2)	60

[a] Reaction conditions: **1a** (0.05 mmol), **2a** (0.4 mmol), **3a** (0.2 mmol), TBPB (0.2 mmol), Cs_2CO_3 (0.2 mmol), MeCN (4 mL), C (15 mm×10 mm×1 mm) cathode, C plate (15 mm×10 mm×1 mm) anode, undivided cell, current = 3 mA, rt, 4 h. [b] Isolated yields.

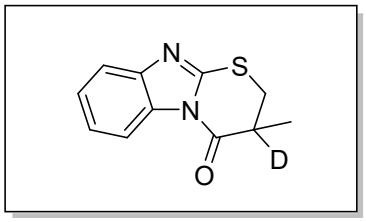
3.2 Deuterium labeling study



10 equiv. **2a** **3a** **6-*d***, 95%
96% D-incorporation

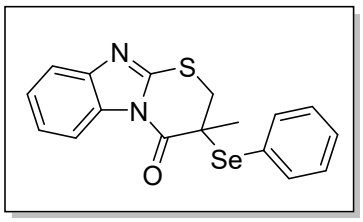
A mixture of D_2O (36 μL, 2.0 mmol), methacryloyl chloride **2a** (42 μL, 0.4 mmol), **3a** (30.0 mg, 0.2 mmol), TBPB (67.9 mg, 0.2 mmol), Cs_2CO_3 (32.6 mg, 0.1 mmol) and CH_3CN (4.0 mL), were added in an undivided bottle (10 mL). The bottle was equipped with graphite plates as anode and cathode. The resulting mixture was stirred and electrolyzed with constant current 3 mA at room temperature for 4 h. After the reaction

finished, the resulting mixture were evaporated under reduced pressure. The resultant residue was purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 10:1, v/v) to afford the desired product **6-*d*** in 95% yield, D incorporation was determined by ^{1}H NMR: 96%.

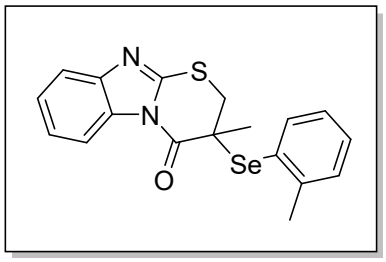


3-Methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one-3-*d* (6-*d*): ^{1}H NMR ($CDCl_3$, 600 MHz) δ 8.19-8.18 (m, 1H), 7.59-7.58 (m, 1H), 7.33 (td, *J* = 7.5, 1.3 Hz, 1H), 7.28 (td, *J* = 8.0, 1.3 Hz, 1H), 3.23 (d, *J* = 1.3 Hz, 2.04H), 1.52 (s, 3H).. **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 169.9, 150.8, 143.1, 132.8, 125.6, 124.6, 118.6, 115.5, 39.1 (t, *J* = 21 Hz), 31.0, 15.3. **HRMS** (APCI) m/z calcd for $C_{11}H_{10}DN_2OS$ $[M+H]^+$: 220.0649; Found: 220.0644.

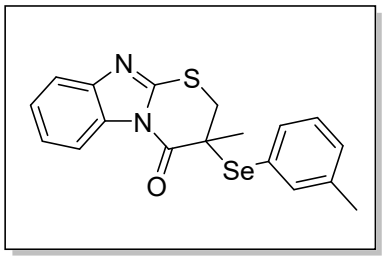
4 Analytical data



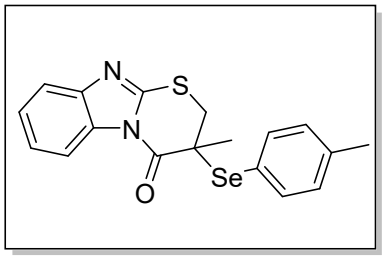
3-Methyl-3-(phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4a): New compound, 33.7 mg, 90% yield. White solid, m.p.: 128.3-128.9 °C. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21-8.20 (m, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.53-7.51 (m, 2H), 7.41-7.38 (m, 1H), 7.36-7.34 (m, 1H), 7.32-7.28 (m, 3H), 3.79 (d, *J* = 14.0 Hz, 1H), 3.35 (d, *J* = 13.9 Hz, 1H), 1.70 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.0, 149.7, 143.1, 138.4, 133.2, 130.1, 129.2, 125.4, 125.4, 124.6, 118.7, 115.6, 47.2, 37.8, 24.3. **HRMS** (ESI) m/z calcd for $C_{17}H_{15}N_2OSSe$ $[M+H]^+$: 375.0065; Found: 375.0058.



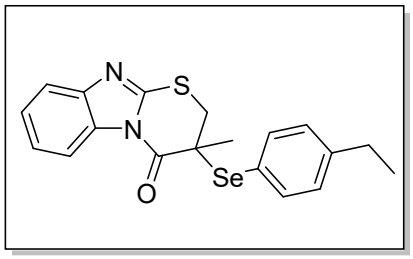
3-Methyl-3-(*o*-tolylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4b): New compound, 29.2 mg, 75% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.20 (d, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.32-7.28 (m, 3H), 7.10-7.08 (m, 1H), 3.84 (d, *J* = 13.9 Hz, 1H), 3.39 (d, *J* = 13.9 Hz, 1H), 2.37 (s, 3H), 1.69 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.2, 149.8, 144.3, 143.2, 140.3, 133.3, 130.8, 130.6, 126.6, 126.5, 125.5, 124.7, 118.8, 115.6, 47.3, 38.1, 24.1, 23.5. **HRMS** (ESI) m/z calcd for $C_{18}H_{17}N_2OSSe$ $[M+H]^+$: 389.0222; Found: 389.0218.



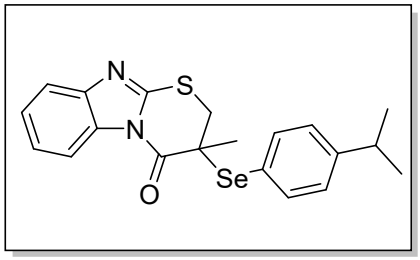
3-Methyl-3-(*m*-tolylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4c): New compound, 31.1 mg, 80% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.20 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 7.7, 1H), 7.37-7.30 (m, 4H), 7.18-7.17 (m, 2H), 3.80 (d, *J* = 14.0 Hz, 1H), 3.35 (d, *J* = 14.0 Hz, 1H), 2.27 (s, 3H), 1.74 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.1, 149.9, 143.1, 139.1, 139.0, 135.4, 133.2, 131.0, 129.0, 125.5, 125.2, 124.6, 118.7, 115.6, 47.3, 37.9, 24.5, 21.3. **HRMS** (ESI) m/z calcd for $C_{18}H_{17}N_2OSSe$ $[M+H]^+$: 389.0222; Found: 389.0220.



3-Methyl-3-(*p*-tolylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4d): New compound, 37.0 mg, 95% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21-8.20 (m, 1H), 7.62-7.61 (m, 1H), 7.40-7.39 (m, 2H), 7.36-7.34 (m, 1H), 7.32-7.29 (m, 1H), 7.10 (d, *J* = 7.7 Hz, 2H), 3.79 (d, *J* = 13.9 Hz, 1H), 3.34 (d, *J* = 14.0 Hz, 1H), 2.33 (s, 3H), 1.70 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.1, 149.8, 143.1, 140.5, 138.4, 138.3, 133.3, 132.4, 130.1, 125.4, 124.6, 121.9, 118.7, 115.7, 47.1, 37.8, 24.4, 21.4. **HRMS** (ESI) m/z calcd for $C_{18}H_{17}N_2OSSe$ $[M+H]^+$: 389.0222; Found: 389.0218.

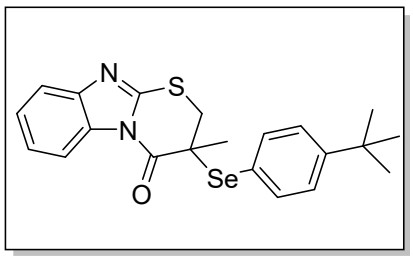


3-((4-Ethylphenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4e): New compound, 32.2 mg, 80% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.20 (d, *J* = 7.9 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 2H), 7.36-7.33 (m, 1H), 7.31-7.29 (m, 1H), 7.11 (d, *J* = 7.9 Hz, 2H), 3.79 (d, *J* = 14.0 Hz, 1H), 3.34 (d, *J* = 13.9 Hz, 1H), 2.62 (q, *J* = 7.6 Hz, 2H), 1.70 (s, 3H), 1.20 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.1, 149.8, 146.7, 143.2, 138.5, 133.3, 128.9, 125.4, 124.6, 122.2, 118.7, 115.7, 47.1, 37.9, 28.7, 24.4, 15.3. **HRMS** (ESI) m/z calcd for $C_{19}H_{19}N_2OSSe$ $[M+H]^+$: 403.0378; Found: 403.0378.

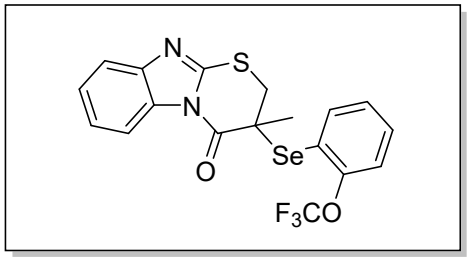


3-((4-Isopropylphenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4f): New compound, 19.1 mg, 46% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21 (d, *J* = 7.7 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.45 (d, *J* = 8.1 Hz, 2H), 7.36-7.33 (m, 1H), 7.32-7.29 (m, 1H), 7.13

(d, *J* = 8.0 Hz, 2H), 3.80 (d, *J* = 14.0 Hz, 1H), 3.35 (d, *J* = 13.9 Hz, 1H), 2.87 (sept, J = 6.9 Hz, 1H), 1.72 (s, 3H), 1.21 (dd, *J* = 7.0, 1.3 Hz, 6H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.2, 151.3, 149.8, 143.2, 138.5, 133.3, 127.5, 125.5, 124.6, 122.3, 118.8, 115.7, 47.2, 38.0, 34.1, 24.5, 23.9, 23.9. **HRMS** (ESI) m/z calcd for $C_{20}H_{21}N_2OSSe$ $[M+H]^+$: 417.0535; Found: 417.0529.

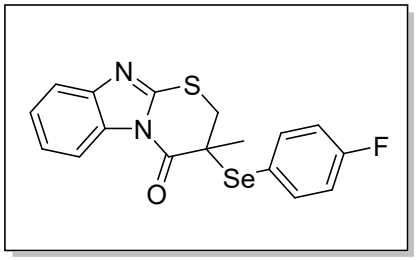


3-((4-(*tert*-Tutyl)phenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4g): New compound, 25.4 mg, 59% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21 (d, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.36-7.33 (m, 1H), 7.32-7.27 (m, 3H), 3.80 (d, *J* = 13.9 Hz, 1H), 3.36 (d, *J* = 13.9 Hz, 1H), 1.73 (s, 3H), 1.27 (s, 9H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.2, 153.6, 149.9, 143.0, 138.2, 133.2, 131.5, 130.3, 126.4, 125.5, 124.6, 122.1, 118.7, 115.7, 47.2, 38.1, 34.9, 31.3, 24.5. **HRMS** (ESI) m/z calcd for $C_{21}H_{23}N_2OSSe$ $[M+H]^+$: 431.0691; Found: 431.0687.

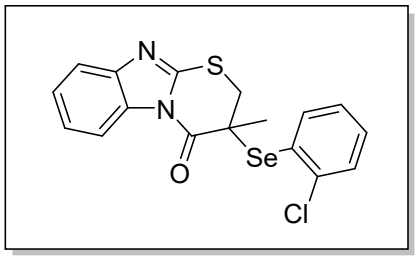


3-Methyl-3-((2-(trifluoromethoxy)phenyl)selanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4h): New compound, 31.1 mg, 68% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21-8.20 (m, 1H), 7.64-7.63 (m, 1H), 7.58 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.50-7.47 (m, 1H), 7.38-7.31 (m, 3H), 7.25-7.22 (m, 1H), 3.82 (d, *J* = 14.0 Hz, 1H), 3.44 (d, *J* = 14.0 Hz, 1H), 1.70 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) *δ* 167.8, 151.5, 149.5, 143.2, 141.2, 133.3, 132.5, 127.3, 125.6, 124.7, 120.7, 120.4 (q, *J* = 258.0 Hz), 119.2, 118.8, 115.7, 48.3, 37.7, 24.0. **^{19}F NMR**

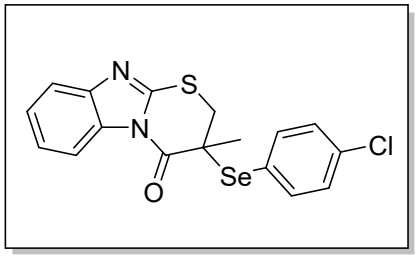
(565 MHz, $CDCl_3$) δ: 20.9. **HRMS** (ESI) m/z calcd for $C_{18}H_{14}F_3N_2O_2SSe$ $[M+H]^+$: 458.9888; Found: 458.9881.



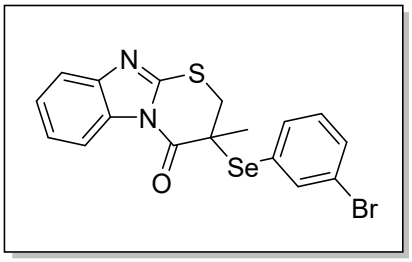
3-((4-Fluorophenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4i): New compound, 31.4 mg, 80% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.20 (d, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.50-7.48 (m, 2H), 7.38-7.35 (m, 1H), 7.33-7.31 (m, 1H), 7.00-6.97 (m, 2H), 3.83 (d, *J* = 14.0 Hz, 1H), 3.35 (d, *J* = 14.0 Hz, 1H), 1.70 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.9, 164.3 (d, *J* = 250.5 Hz), 149.7, 143.1, 140.5 (d, *J* = 7.5 Hz), 133.2, 125.6, 124.8, 120.3 (d, *J* = 3.0 Hz), 118.8, 116.7, 116.6, 115.7, 47.4, 37.7, 24.4. **^{19}F NMR** (565 MHz, $CDCl_3$) δ: -32.1. **HRMS** (ESI) m/z calcd for $C_{17}H_{14}FN_2OSSe$ $[M+H]^+$: 392.9971; Found: 392.9970.



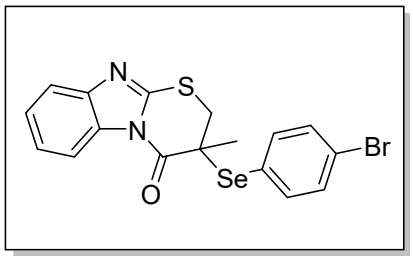
3-((2-Chlorophenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4j): New compound, 21.6 mg, 53% yield. White solid, m.p.: 150.8-151.4 °C. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.22 (d, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.57 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.37-7.35 (m, 2H), 7.33-7.31 (m, 1H), 7.20-7.17 (m, 1H), 3.84 (d, *J* = 14.0 Hz, 1H), 3.47 (d, *J* = 14.0 Hz, 1H), 1.74 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.8, 149.5, 143.2, 141.4, 141.2, 133.3, 132.0, 130.1, 127.4, 126.0, 125.5, 124.7, 118.8, 115.8, 48.5, 37.8, 23.8. **HRMS** (ESI) m/z calcd for $C_{17}H_{14}ClN_2OSSe$ $[M+H]^+$: 408.9675; Found: 408.9669.



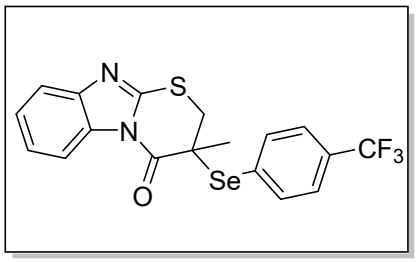
3-((4-Chlorophenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4k): New compound, 29.4 mg, 72% yield. White solid, m.p.: 93.2-93.8 °C. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.20 (d, *J* = 7.7 Hz, 1H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.44-7.43 (m, 2H), 7.38-7.35 (m, 1H), 7.33-7.31 (m, 1H), 7.28-7.25 (m, 2H), 3.83 (d, *J* = 14.0 Hz, 1H), 3.35 (d, *J* = 14.0 Hz, 1H), 1.70 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.9, 149.5, 143.2, 139.7, 137.0, 133.2, 129.6, 125.6, 124.8, 123.6, 118.8, 115.7, 47.6, 37.8, 24.4. **HRMS** (ESI) m/z calcd for $C_{17}H_{14}ClN_2OSSe$ $[M+H]^+$: 408.9675; Found: 408.9674.



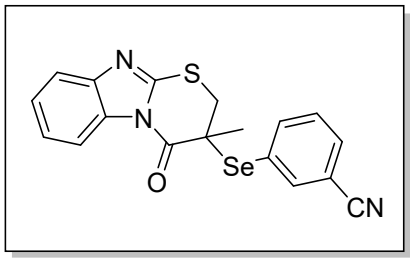
3-((3-Bromophenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4l): New compound, 27.1 mg, 60% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21 (d, *J* = 7.9 Hz, 1H), 7.69 (s, 1H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.1 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.9 Hz, 1H), 3.83 (d, *J* = 14.0 Hz, 1H), 3.37 (d, *J* = 14.0 Hz, 1H), 1.74 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.8, 149.5, 143.1, 140.7, 136.9, 133.3, 133.2, 130.6, 127.1, 125.7, 124.8, 122.7, 118.8, 115.7, 47.9, 37.8, 24.5. **HRMS** (ESI) m/z calcd for $C_{17}H_{14}BrN_2OSSe$ $[M+H]^+$: 452.9170; Found: 452.9160.



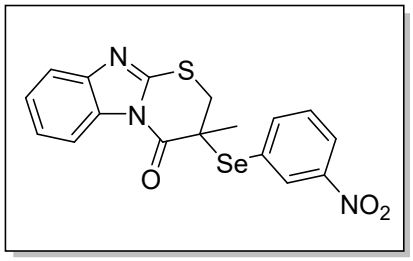
3-((4-Bromophenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4m): New compound, 33.9 mg, 75% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.20 (d, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.43-7.35 (m, 5H), 7.32 (t, *J* = 7.7 Hz, 1H), 3.83 (d, *J* = 14.0 Hz, 1H), 3.35 (d, *J* = 14.0 Hz, 1H), 1.70 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.8, 149.5, 143.1, 139.9, 133.2, 132.5, 125.6, 125.4, 124.8, 124.2, 118.8, 115.6, 47.6, 37.8, 24.4. **HRMS** (ESI) m/z calcd for $C_{17}H_{14}BrN_2OSSe$ $[M+H]^+$: 452.9170; Found: 452.9163.



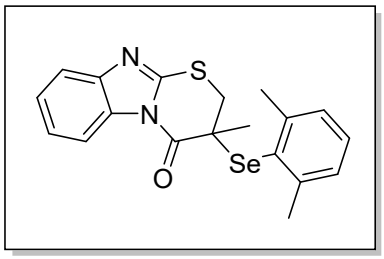
3-Methyl-3-((4-(trifluoromethyl)phenyl)selanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4n): New compound, 37.1 mg, 84% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.20-8.17 (m, 1H), 7.63-7.61 (m, 1H), 7.42-7.40 (m, 2H), 7.37-7.34 (m, 3H), 7.33-7.30 (m, 1H), 3.82 (dd, *J* = 14.1, 3.0 Hz, 1H), 3.34 (dd, *J* = 14.0, 4.6 Hz, 1H), 1.69 (d, *J* = 4.0 Hz, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.8, 149.4, 143.1, 138.6, 133.1, 132.2 (q, *J* = 31.5 Hz), 130.0, 125.9 (q, *J* = 3.0 Hz), 125.7, 124.9, 123.9 (q, *J* = 271.5 Hz), 118.9, 115.7, 48.0, 37.9, 24.5. **^{19}F NMR** (565 MHz, $CDCl_3$) δ: 14.9. **HRMS** (ESI) m/z calcd for $C_{18}H_{14}F_3N_2OSSe$ $[M+H]^+$: 442.9939; Found: 442.9933.



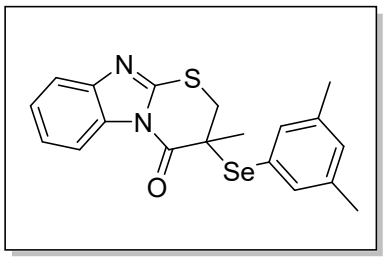
3-((3-Methyl-4-oxo-3,4-dihydro-2*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-3-yl)selanyl)benzonitrile (4o): New compound, 22.7 mg, 57% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.19-8.18 (m, 1H), 7.81-7.81 (m, 1H), 7.74-7.73 (m, 1H), 7.67-7.65 (m, 1H), 7.62-7.61 (m, 1H), 7.41-7.38 (m, 1H), 7.37-7.35 (m, 1H), 7.35-7.32 (m, 1H), 3.88 (d, *J* = 14.1 Hz, 1H), 3.38 (d, *J* = 14.1 Hz, 1H), 1.71 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.6, 149.2, 143.1, 142.6, 141.3, 133.5, 133.1, 129.8, 126.9, 125.8, 125.0, 118.9, 117.8, 115.6, 113.4, 48.3, 37.7, 24.5. **HRMS** (ESI) m/z calcd for $C_{18}H_{14}N_3OSSe$ $[M+H]^+$: 400.0018; Found: 400.0017.



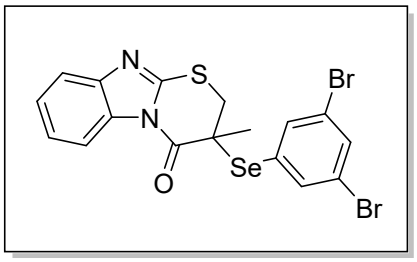
3-Methyl-3-((3-nitrophenyl)selanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4p): New compound, 15.1 mg, 36% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.40 (t, *J* = 1.9 Hz, 1H), 8.24-8.23 (m, 1H), 8.20-8.19 (m, 1H), 7.84-7.82 (m, 1H), 7.64-7.62 (m, 1H), 7.48 (t, *J* = 7.9 Hz, 1H), 7.39-7.36 (m, 1H), 7.35-7.32 (m, 1H), 3.90 (d, *J* = 14.1 Hz, 1H), 3.41 (d, *J* = 14.1 Hz, 1H), 1.75 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.6, 149.2, 148.1, 144.1, 143.1, 133.1, 132.9, 130.0, 127.1, 125.8, 125.0, 125.0, 119.0, 115.7, 48.6, 37.8, 24.6. **HRMS** (ESI) m/z calcd for $C_{17}H_{14}N_3O_3SSe$ $[M+H]^+$: 419.9916; Found: 419.9918.



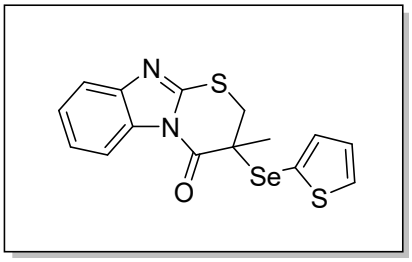
3-((2,6-Dimethylphenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4q): New compound, 28.9 mg, 72% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.18 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.27 (s, 1H), 7.15 (d, *J* = 7.7 Hz, 1H), 7.07 (d, *J* = 7.6 Hz, 1H), 3.83 (d, *J* = 13.9 Hz, 1H), 3.37 (d, *J* = 13.9 Hz, 1H), 2.33 (s, 3H), 2.20 (s, 3H), 1.72 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.0, 149.9, 143.1, 141.0, 140.6, 136.1, 133.2, 131.5, 130.2, 126.2, 125.5, 124.6, 118.7, 115.6, 47.3, 38.0, 24.2, 23.0, 20.6. **HRMS** (ESI) m/z calcd for $C_{19}H_{19}N_2OSSe$ $[M+H]^+$: 403.0378; Found: 403.0378.



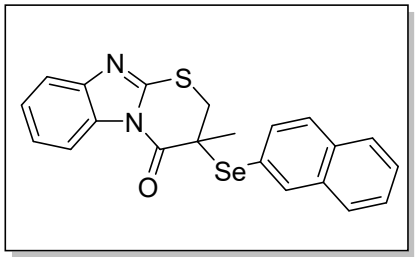
3-((3,5-Dimethylphenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4r): New compound, 25.3 mg, 63%. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.18 (d, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.35-7.33 (m, 1H), 7.31-7.28 (m, 1H), 7.12 (s, 2H), 6.96 (s, 1H), 3.77 (d, *J* = 14.0 Hz, 1H), 3.33 (d, *J* = 14.0 Hz, 1H), 2.23 (s, 6H), 1.75 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.0, 149.9, 143.2, 138.8, 136.0, 133.2, 131.9, 129.1, 125.4, 124.9, 124.5, 118.7, 115.5, 47.3, 37.9, 24.5, 21.1. **HRMS** (ESI) m/z calcd for $C_{19}H_{19}N_2OSSe$ $[M+H]^+$: 403.0378; Found: 403.0378.



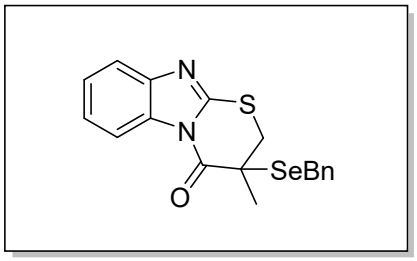
3-((3,5-Dibromophenyl)selanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4s): New compound, 37.1 mg, 70% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21-8.19 (m, 1H), 7.64 (t, *J* = 1.7 Hz, 1H), 7.62-7.61 (m, 1H), 7.59 (d, *J* = 1.7 Hz, 2H), 7.37-7.35 (m, 1H), 7.34-7.31 (m, 1H), 3.84 (d, *J* = 14.1 Hz, 1H), 3.36 (d, *J* = 14.1 Hz, 1H), 1.75 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.5, 149.2, 143.1, 139.2, 135.7, 133.0, 128.2, 125.7, 124.9, 122.9, 118.9, 115.7, 48.7, 37.7, 24.5. **HRMS** (ESI) m/z calcd for $C_{17}H_{13}Br_2N_2OSSe$ $[M+H]^+$: 532.8255; Found: 532.8255.



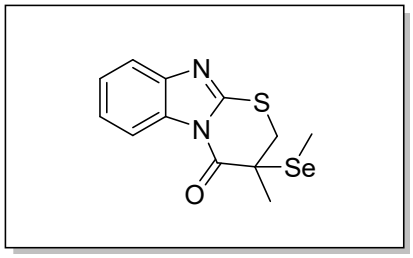
3-Methyl-3-(thiophen-2-ylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4t): New compound, 32.3 mg, 85% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21 (d, *J* = 7.8 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.52-7.51 (m, 1H), 7.37-7.34 (m, 1H), 7.33-7.30 (m, 1H), 7.22-7.21 (m, 1H), 7.06-7.04 (m, 1H), 3.72 (d, *J* = 14.1 Hz, 1H), 3.38 (d, *J* = 14.0 Hz, 1H), 1.77 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.9, 149.5, 143.1, 140.1, 134.4, 133.2, 128.7, 125.6, 124.8, 119.3, 118.8, 115.7, 49.0, 37.3, 24.1. **HRMS** (ESI) m/z calcd for $C_{15}H_{13}N_2OS_2Se$ $[M+H]^+$: 380.9629; Found: 380.9628.



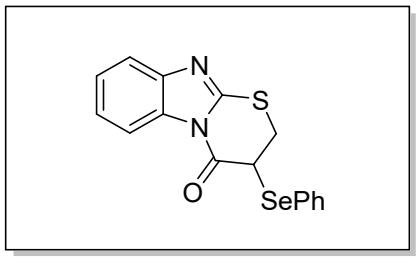
3-Methyl-3-(naphthalen-2-ylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4u): New compound, 33.9 mg, 80% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21 (d, *J* = 7.9 Hz, 1H), 8.05 (s, 1H), 7.82 (d, *J* = 7.5 Hz, 1H), 7.75 (t, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.56-7.49 (m, 3H), 7.36-7.34 (m, 1H), 7.32-7.30 (m, 1H), 3.79 (d, *J* = 13.9 Hz, 1H), 3.38 (d, *J* = 13.9 Hz, 1H), 1.73 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.1, 149.7, 143.2, 138.9, 134.3, 133.6, 133.6, 133.3, 128.7, 128.1, 127.9, 127.5, 126.7, 125.5, 124.6, 122.8, 118.7, 115.6, 47.6, 37.8, 24.5. **HRMS** (ESI) m/z calcd for $C_{21}H_{17}N_2OSSe$ $[M+H]^+$: 425.0222; Found: 425.0216.



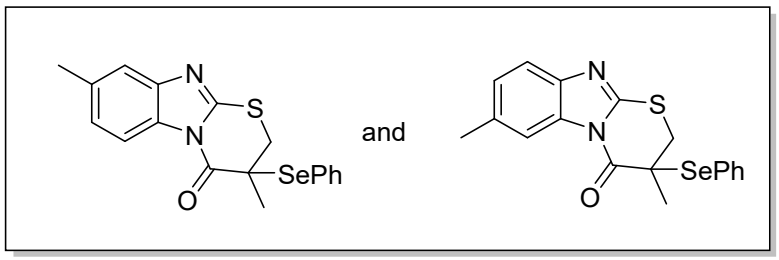
3-(Benzylselanyl)-3-methyl-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4v): New compound, 32.2 mg, 83% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.27 (d, *J* = 7.4 Hz, 1H), 7.63 (d, *J* = 8.1 Hz, 1H), 7.38-7.32 (m, 2H), 7.25-7.21 (m, 4H), 7.19-7.18 (m, 1H), 4.07 (d, *J* = 10.6 Hz, 1H), 3.99 (d, *J* = 10.8 Hz, 1H), 3.79 (d, *J* = 14.0 Hz, 1H), 3.25 (d, *J* = 14.0 Hz, 1H), 2.01 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.0, 149.7, 143.2, 136.4, 133.4, 129.4, 129.2, 128.8, 127.4, 125.5, 124.9, 124.7, 118.9, 115.8, 45.0, 37.7, 27.8, 24.5. **HRMS** (ESI) m/z calcd for $C_{18}H_{17}N_2OSSe$ $[M+H]^+$: 389.0222; Found: 389.0218.



3-Methyl-3-(methylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (4w): New compound, 25.0 mg, 80% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21-8.20 (m, 1H), 7.60-7.59 (m, 1H), 7.34-7.31 (m, 1H), 7.30-7.27 (m, 1H), 3.78 (d, *J* = 14.0 Hz, 1H), 3.21 (d, *J* = 14.0 Hz, 1H), 2.10 (s, 3H), 1.88 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.5, 149.7, 143.1, 133.3, 125.4, 124.5, 118.7, 115.7, 42.5, 37.6, 23.5, 3.6. **HRMS** (ESI) m/z calcd for $C_{12}H_{13}N_2OSSe$ $[M+H]^+$: 312.9909; Found: 312.9903.

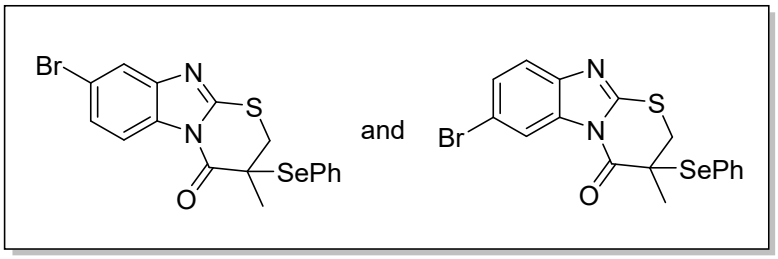


3-(Phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (5a): New compound, 7.2 mg, 20% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.21-8.19 (m, 1H), 7.69-7.68 (m, 2H), 7.63-7.61 (m, 1H), 7.38-7.31 (m, 5H), 4.47 (dd, *J* = 5.9, 3.1 Hz, 1H), 3.83 (dd, *J* = 13.7, 3.1 Hz, 1H), 3.48 (dd, *J* = 13.7, 5.9 Hz, 1H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 166.3, 143.0, 136.1, 132.9, 129.7, 129.5, 126.7, 125.8, 124.9, 118.9, 115.8, 43.5, 31.8. **HRMS** (ESI) m/z calcd for $C_{16}H_{13}N_2OSSe$ $[M+H]^+$: 360.9909; Found: 360.9906.

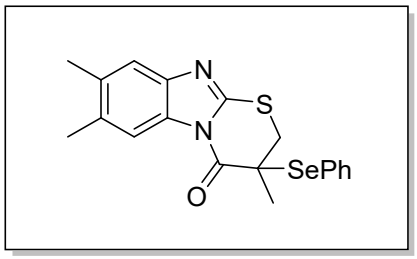


3,7-Dimethyl-3-(phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-

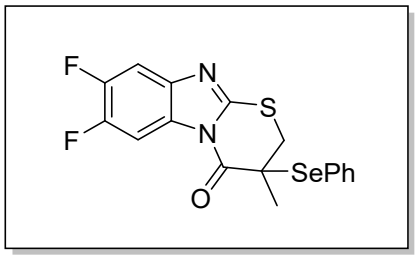
***b*][1,3]thiazin-4-one and 3,8-dimethyl-3-(phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (5b)**: New compound, 26.7 mg, 69% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.06 (d, *J* = 8.2 Hz, 1H), 8.05 (s, 1H), 7.74 (d, *J* = 1.7 Hz, 1H), 7.55-7.52 (m, 4H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.43-7.39 (m, 3H), 7.33-7.29 (m, 4H), 7.18-7.16 (m, 1H), 7.13-7.12 (m, 1H), 3.79-3.77 (m, 2H), 3.36-3.33 (m, 2H), 2.49 (s, 3H), 2.47 (s, 3H), 1.70 (s, 3H), 1.69 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.3, 168.0, 149.6, 148.8, 143.5, 141.2, 138.5, 135.5, 134.9, 133.4, 131.2, 130.1, 129.2, 126.6, 125.7, 125.6, 125.5, 118.8, 118.2, 116.0, 115.1, 47.3, 47.2, 37.9, 37.9, 24.4, 24.4, 21.9, 21.7. **HRMS** (ESI) m/z calcd for $C_{18}H_{17}N_2OSSe$ $[M+H]^+$: 389.0222; Found: 389.0218.



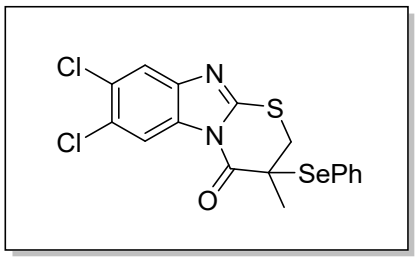
7-Bromo-3-methyl-3-(phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one and 8-bromo-3-methyl-3-(phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (5c): New compound, 34.8 mg, 80% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.39-8.39 (m, 1H), 8.05 (d, *J* = 8.6 Hz, 1H), 7.74 (d, *J* = 1.7 Hz, 1H), 7.52-7.49 (m, 4H), 7.46-7.46 (m, 2H), 7.43-7.39 (m, 3H), 7.33-7.28 (m, 4H), 3.83-3.81 (m, 2H), 3.36-3.34 (m, 2H), 1.70 (s, 3H), 1.69 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.9, 167.8, 151.3, 150.0, 144.4, 142.2, 138.4, 134.1, 132.2, 130.3, 129.3, 129.3, 128.7, 127.5, 125.3, 125.3, 121.7, 119.8, 118.7, 118.6, 118.0, 116.7, 47.1, 47.0, 37.8, 37.8, 24.3, 24.3. **HRMS** (ESI) m/z calcd for $C_{17}H_{14}BrN_2OSSe$ $[M+H]^+$: 452.9170; Found: 452.9163.



3,7,8-Trimethyl-3-(phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (5d): New compound, 27.3 mg, 68% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.00 (s, 1H), 7.55-7.53 (m, 2H), 7.43-7.40 (m, 1H), 7.37 (s, 1H), 7.33-7.30 (m, 2H), 3.77 (d, *J* = 13.9 Hz, 1H), 3.34 (d, *J* = 13.9 Hz, 1H), 2.38 (s, 3H), 2.36 (s, 3H), 1.68 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 168.2, 148.5, 141.6, 138.5, 134.3, 133.7, 131.6, 130.1, 129.2, 125.6, 119.1, 116.1, 47.2, 38.0, 24.4, 20.5, 20.4. **HRMS** (ESI) m/z calcd for $C_{19}H_{19}N_2OSSe$ $[M+H]^+$: 403,0378; Found: 403.0375.

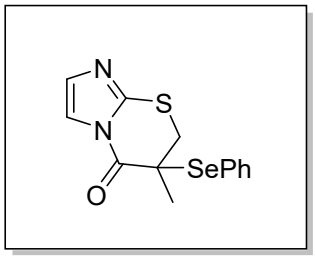


7,8-Difluoro-3-methyl-3-(phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (5e): New compound, 27.5 mg, 67% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.08-8.05 (m, 1H), 7.52-7.50 (m, 2H), 7.43-7.38 (m, 2H), 7.33-7.30 (m, 2H), 3.84 (d, *J* = 14.0 Hz, 1H), 3.37 (d, *J* = 14.0 Hz, 1H), 1.70 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.8, 151.0 (d, *J* = 3.0 Hz), 150.1 (d, *J* = 15.0 Hz), 149.3 (d, *J* = 13.5 Hz), 148.4 (d, *J* = 13.5 Hz), 147.7 (d, *J* = 15.0 Hz), 138.9, 138.8 (d, *J* = 1.5 Hz), 138.5, 130.4, 129.4, 128.5 (d, *J* = 12.0 Hz), 125.2, 106.7 (d, *J* = 19.5 Hz), 104.7 (d, *J* = 25.5 Hz), 47.0, 37.9, 24.3. **^{19}F NMR** (565 MHz, $CDCl_3$) δ: -61.4 (d, *J* = 22.6 Hz), -62.0 (d, *J* = 22.6 Hz). **HRMS** (ESI) m/z calcd for $C_{17}H_{13}F_2N_2OSSe$ $[M+H]^+$: 410.9877; Found: 410.9874.

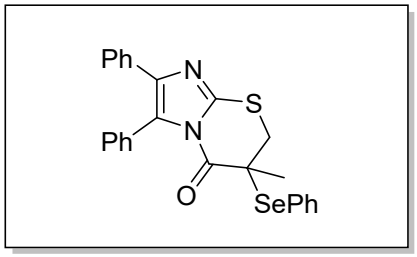


7,8-Dichloro-3-methyl-3-(phenylselanyl)-2,3-dihydro-4*H*-benzo[4,5]imidazo[2,1-*b*][1,3]thiazin-4-one (5f): New compound, 38.4 mg, 87% yield. White solid, m.p.: 147.2-147.9 °C. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.31 (s, 1H),

7.66 (s, 1H), 7.51-7.49 (m, 2H), 7.43-7.40 (m, 1H), 7.32-7.30 (m, 2H), 3.85 (d, *J* = 14.0 Hz, 1H), 3.36 (d, *J* = 14.0 Hz, 1H), 1.69 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.6, 152.0, 142.5, 138.4, 132.2, 130.4, 129.6, 129.4, 128.5, 125.2, 119.8, 117.0, 46.8, 37.8, 24.3. **HRMS** (ESI) m/z calcd for $C_{17}H_{13}Cl_2N_2OSSe$ $[M+H]^+$: 442.9286; Found: 442.9279.



6-Methyl-6-(phenylselanyl)-6,7-dihydro-5*H*-imidazo[2,1-*b*][1,3]thiazin-5-one (5g): New compound, 15.6 mg, 48% yield. Pale yellow oil. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 7.64 (d, *J* = 1.7 Hz, 1H), 7.53 (d, *J* = 7.0 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.02 (d, *J* = 1.7 Hz, 1H), 3.72 (d, *J* = 14.0 Hz, 1H), 3.28 (d, *J* = 14.0 Hz, 1H), 1.63 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 166.7, 143.0, 138.5, 130.8, 130.3, 129.3, 125.3, 117.1, 46.7, 38.3, 24.2. **HRMS** (ESI) m/z calcd for $C_{13}H_{13}N_2OSSe$ $[M+H]^+$: 324.9909; Found: 324.9906.



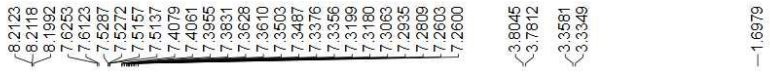
6-Methyl-2,3-diphenyl-6-(phenylselanyl)-6,7-dihydro-5*H*-imidazo[2,1-*b*][1,3]thiazin-5-one (5h): New compound, 19.0 mg, 40% yield. White solid. m.p.: 189.4-189.9 °C. **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 7.53-7.52 (m, 2H), 7.43-7.38 (m, 6H), 7.35-7,34 (m, 2H), 7.28 (t, *J* = 7.7 Hz, 2H), 7.21-7.18 (m, 3H), 3.72 (d, *J* = 13.9 Hz, 1H), 3.36 (d, *J* = 13.9 Hz, 1H), 1.58 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz) δ 167.4, 143.4, 140.0, 138.5, 132.7, 132.5, 131.8, 130.6, 130.1, 129.9, 129.3, 129.3,128.7, 128.6, 128.5, 128.3, 127.6, 127.5, 125.5, 48.0, 37.8, 24.5. **HRMS** (ESI) m/z calcd for $C_{25}H_{21}N_2OSSe$ $[M+H]^+$: 477.0535; Found: 477.0533.

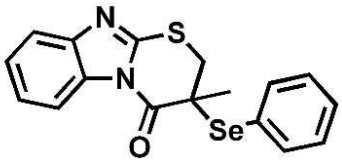
5. References

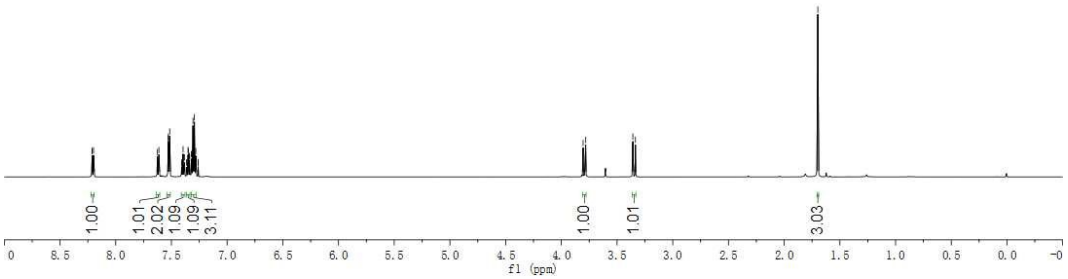
[1] Zhou, J.; Li, W.; Zheng, H.; Pei, Y.; Liu, X. and Cao, H. Visible Light-induced Cascade Cyclization of 3-Aminoindazoles, Ynals, and Chalcogens: Access to Chalcogen-Containing Pyrimido[1,2-*b*]-indazoles. Org. Lett., 2021, **23**, 2754−2759.

6. Copies of NMR spectra

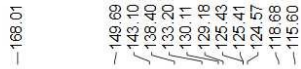
^{1}H NMR of product 4a in $CDCl_3$ (600 MHz)

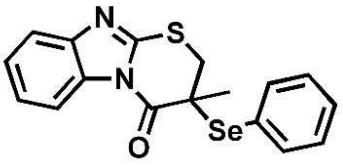


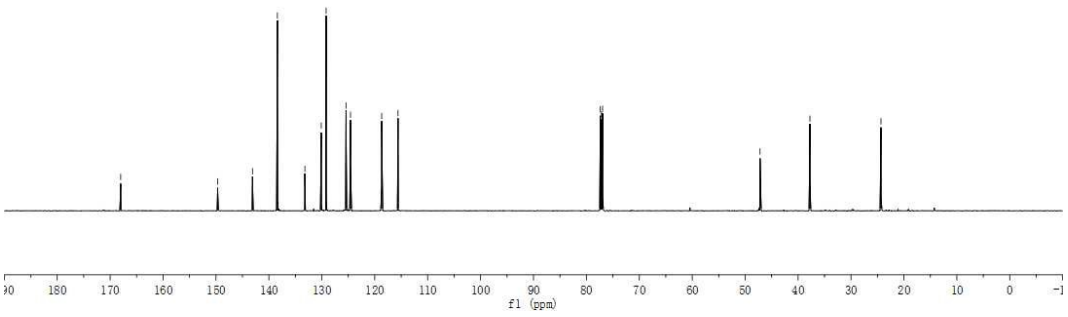




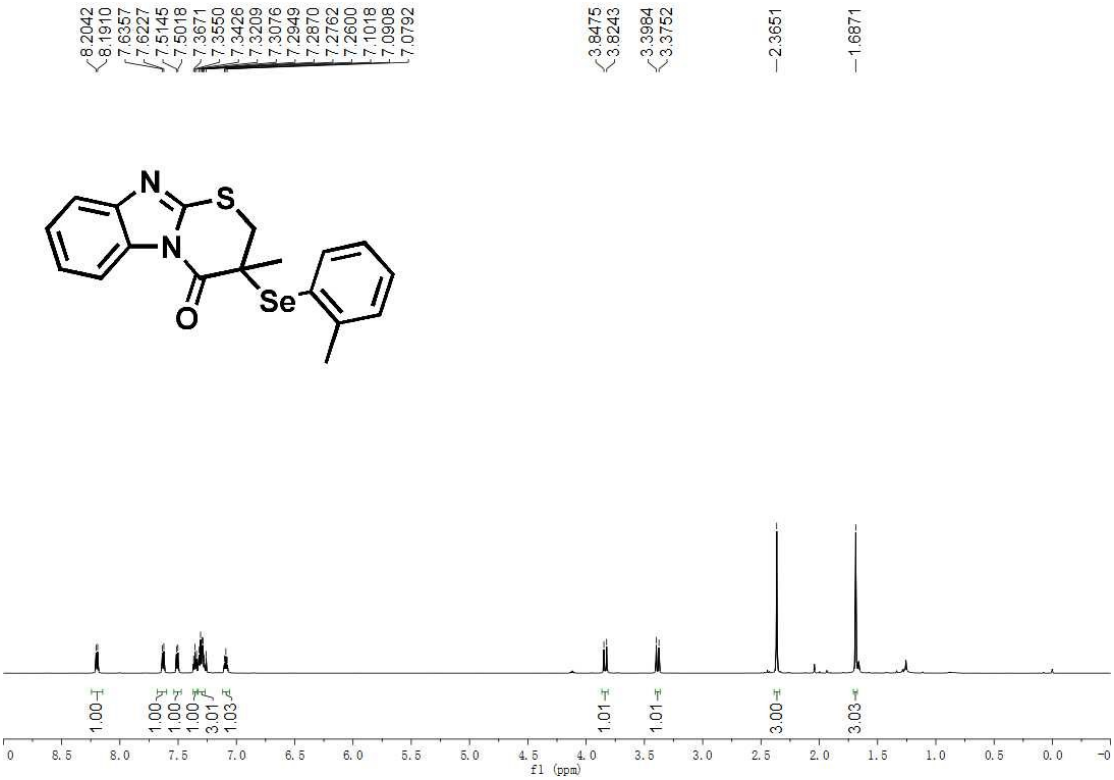
^{13}C NMR of product 4a in $CDCl_3$ (150 MHz)





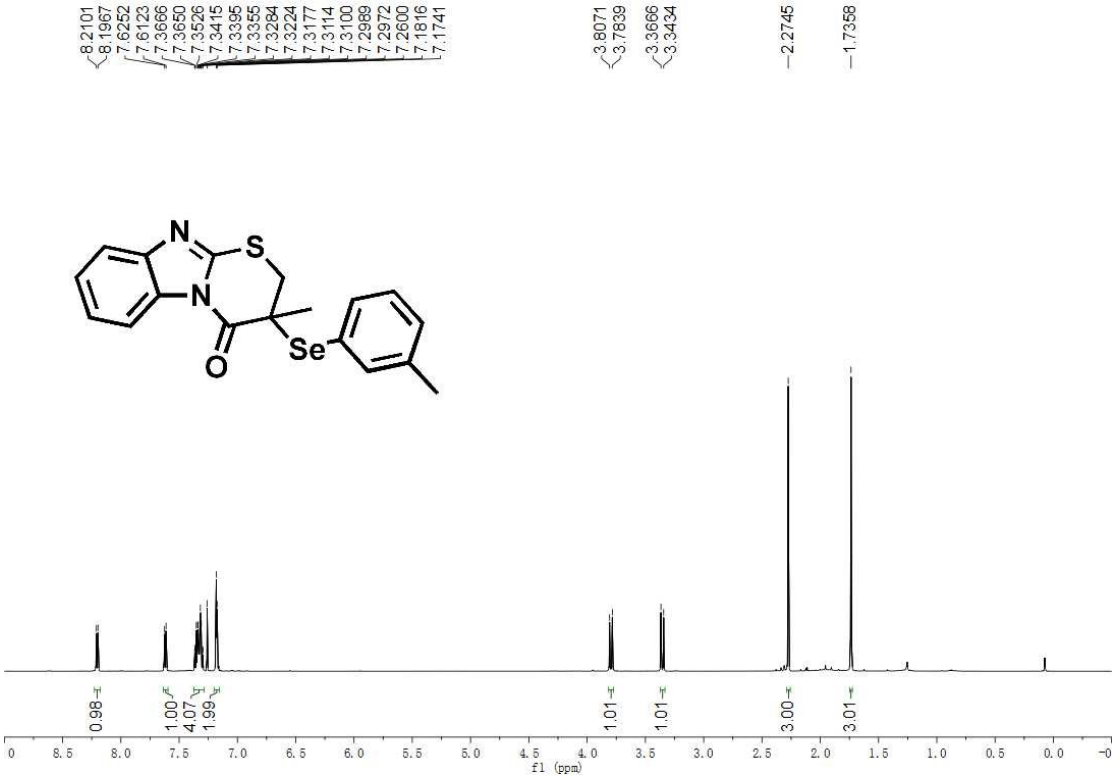


^{1}H NMR of product 4b in $CDCl_3$ (600 MHz)

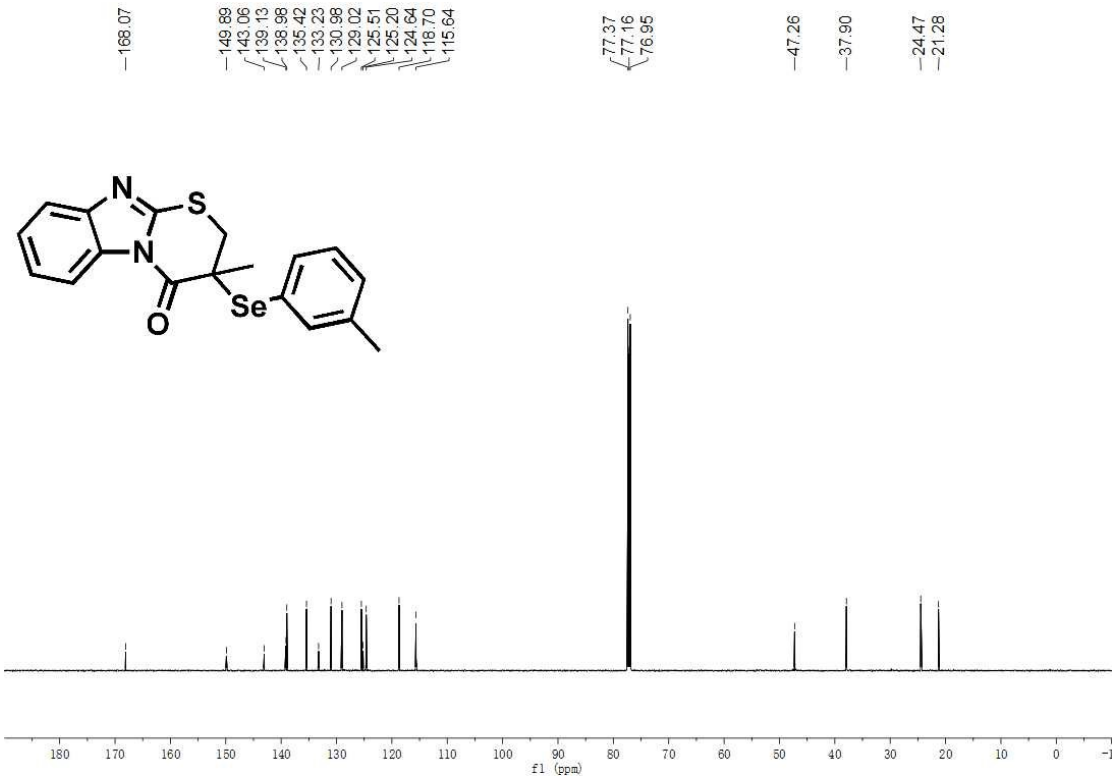


^{13}C NMR of product 4b in $CDCl_3$ (150 MHz)

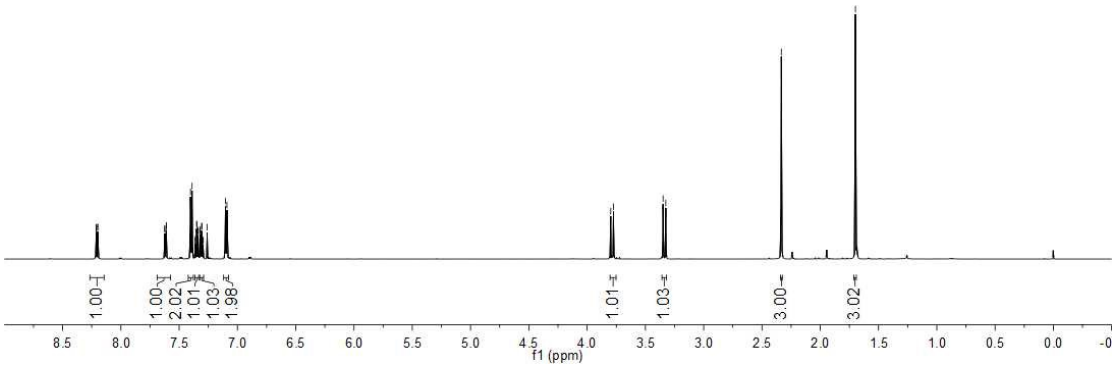
^{1}H NMR of product 4c in $CDCl_3$ (600 MHz)



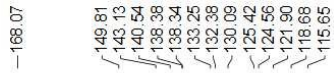
^{13}C NMR of product 4c in $CDCl_3$ (150 MHz)

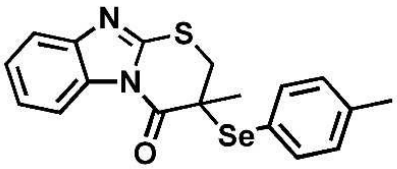


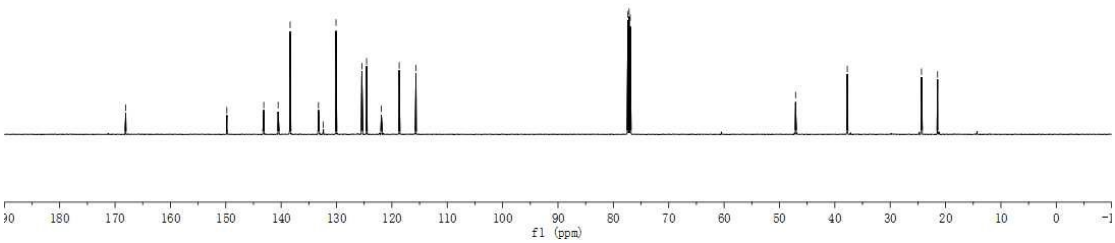
^{1}H NMR of product 4d in $CDCl_3$ (600 MHz)



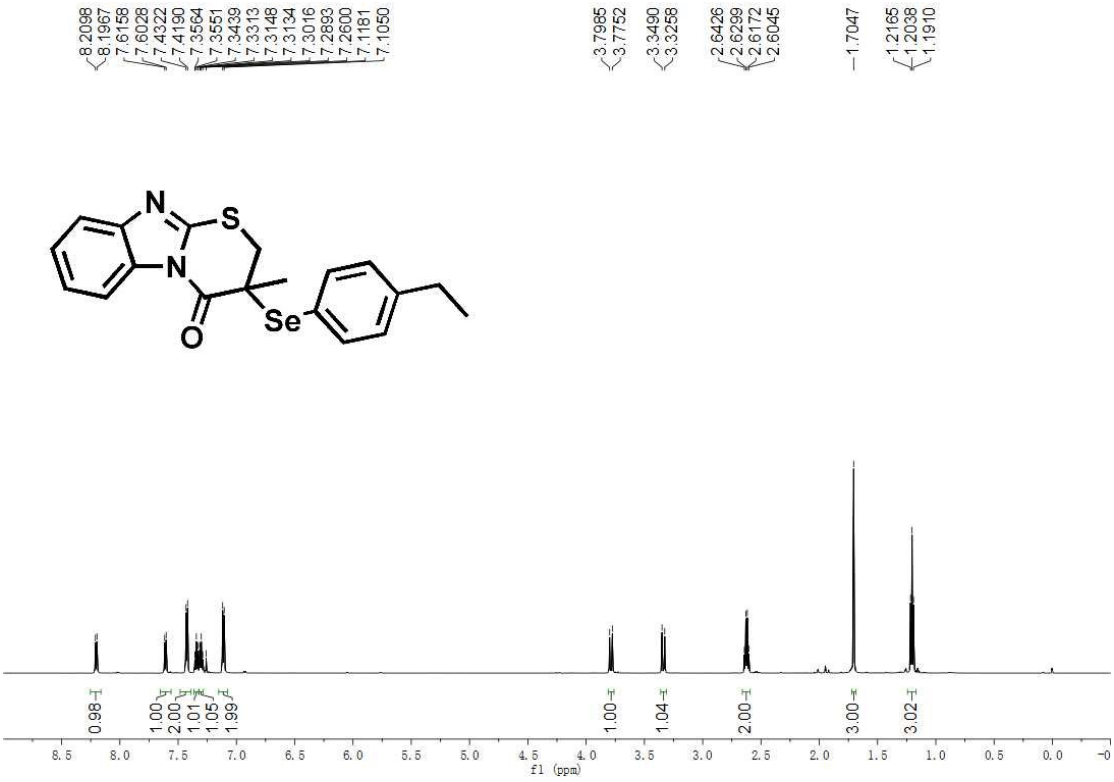
^{13}C NMR of product 4d in $CDCl_3$ (150 MHz)



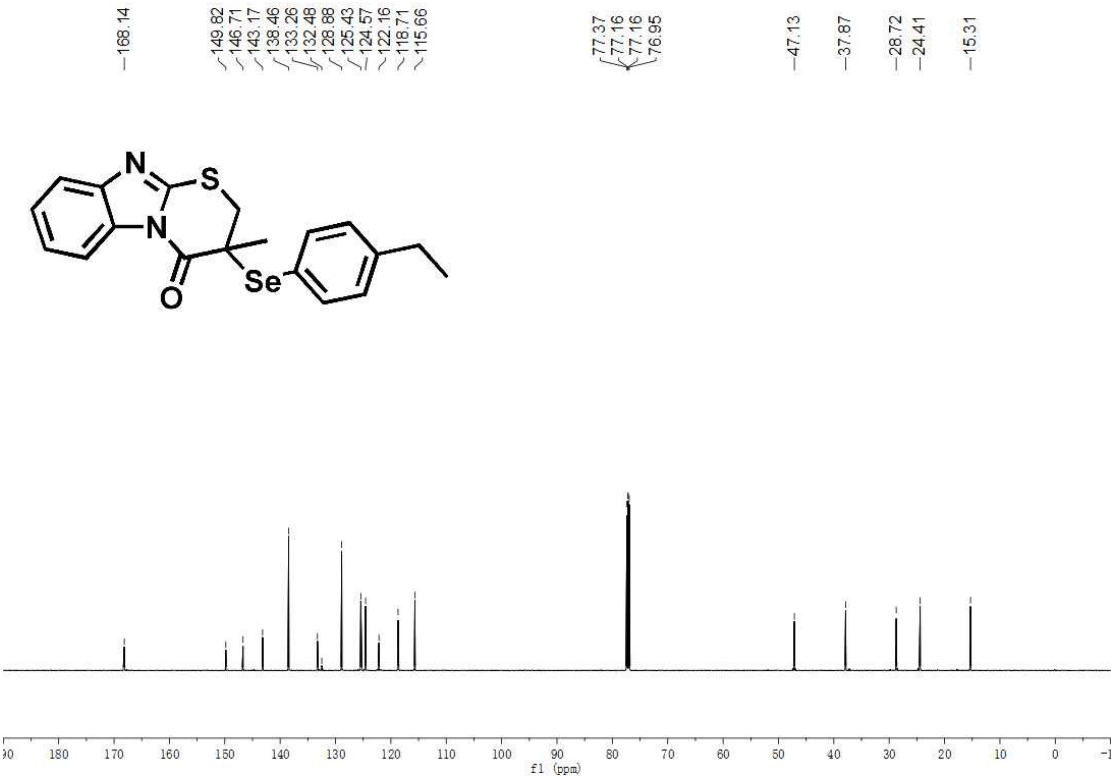




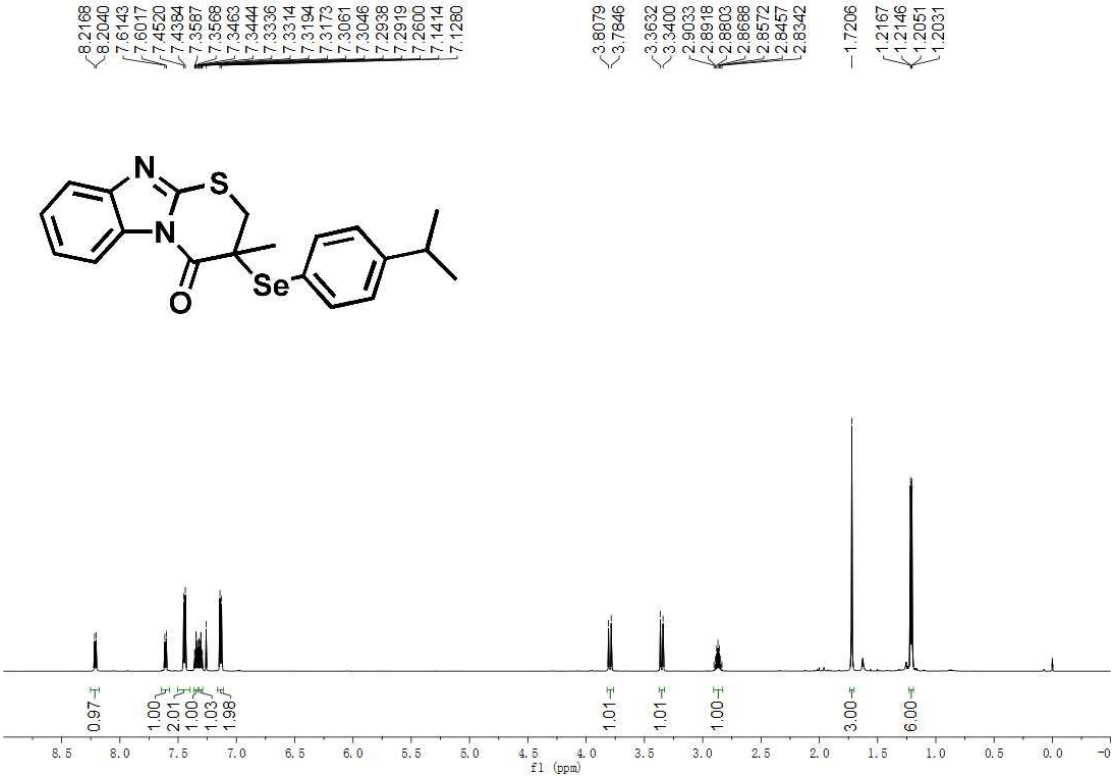
^{1}H NMR of product 4e in $CDCl_3$ (600 MHz)



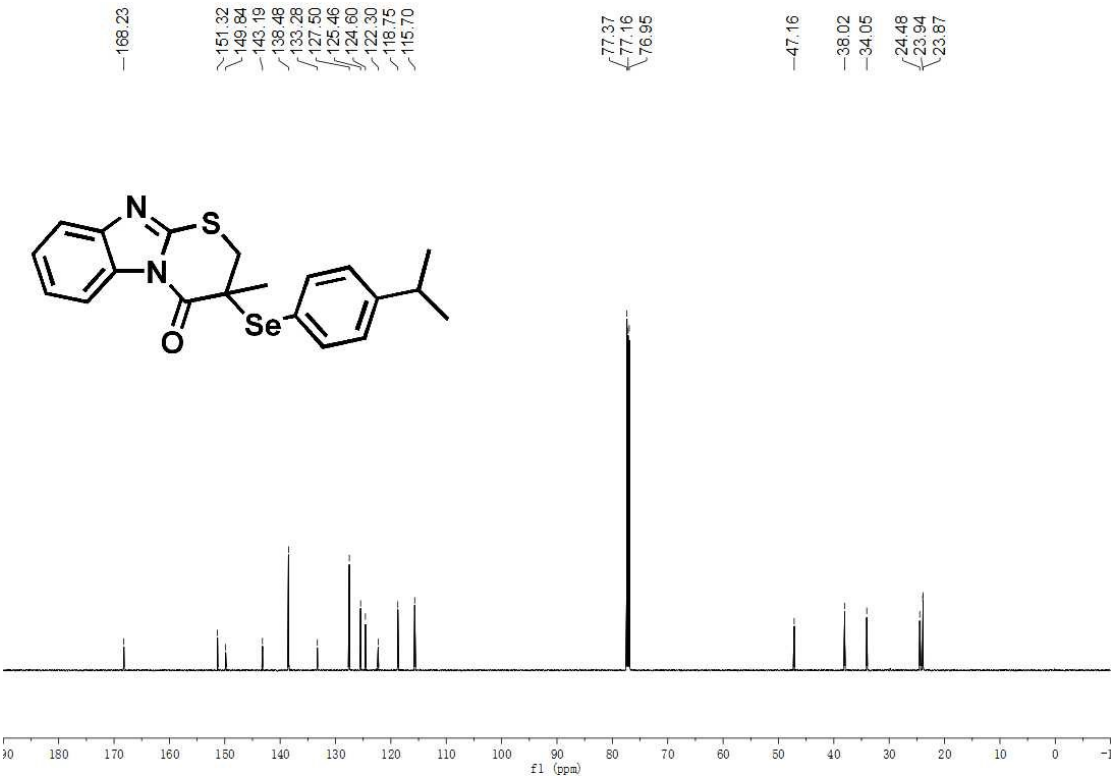
^{13}C NMR of product 4e in $CDCl_3$ (150 MHz)



^{1}H NMR of product 4f in $CDCl_3$ (600 MHz)

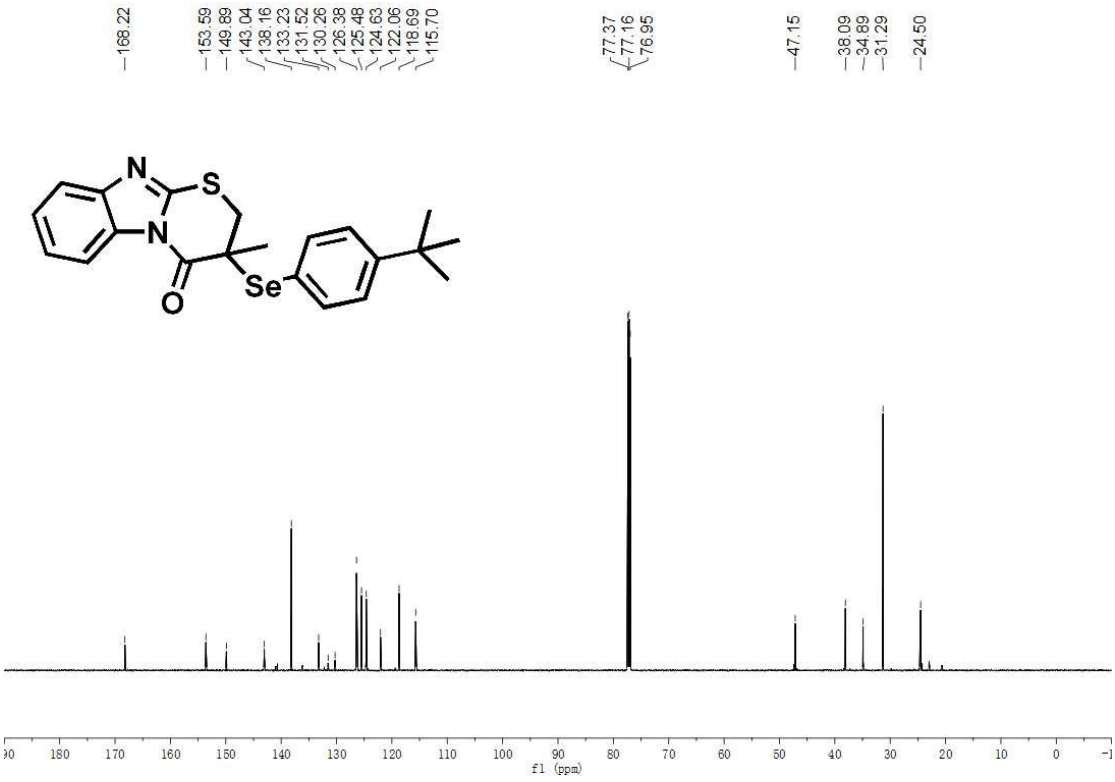


^{13}C NMR of product 4f in $CDCl_3$ (150 MHz)

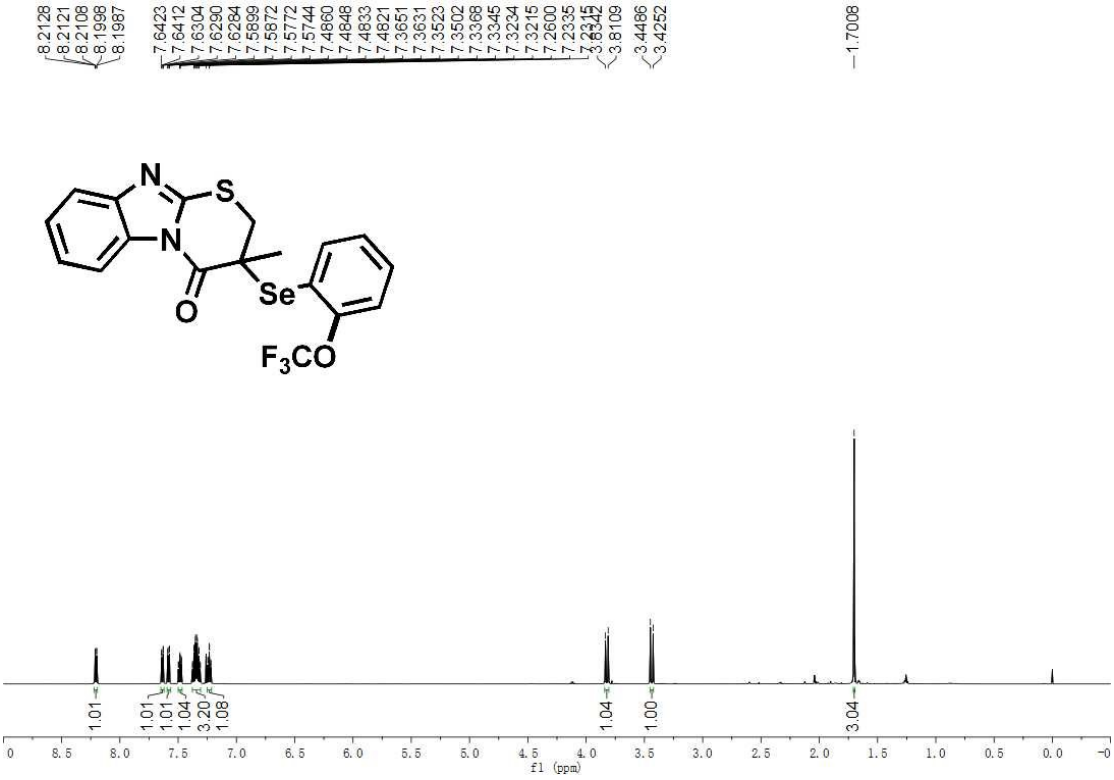


^{1}H NMR of product 4g in $CDCl_3$ (600 MHz)

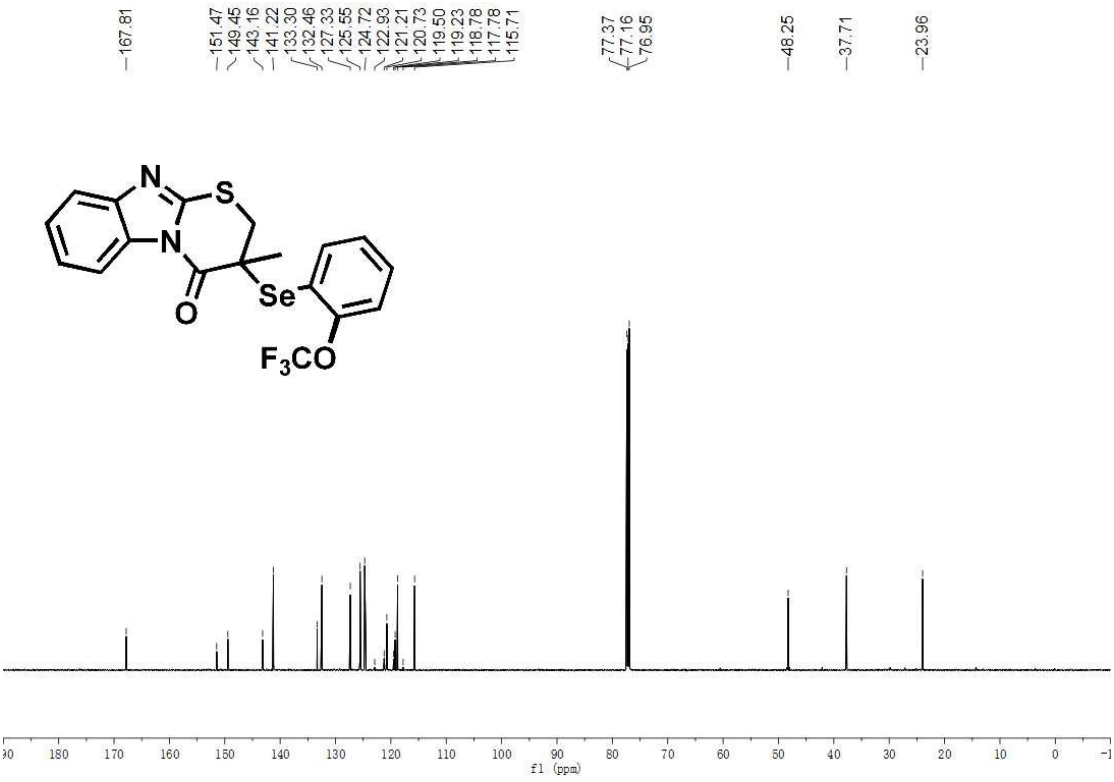
^{13}C NMR of product 4g in $CDCl_3$ (150 MHz)



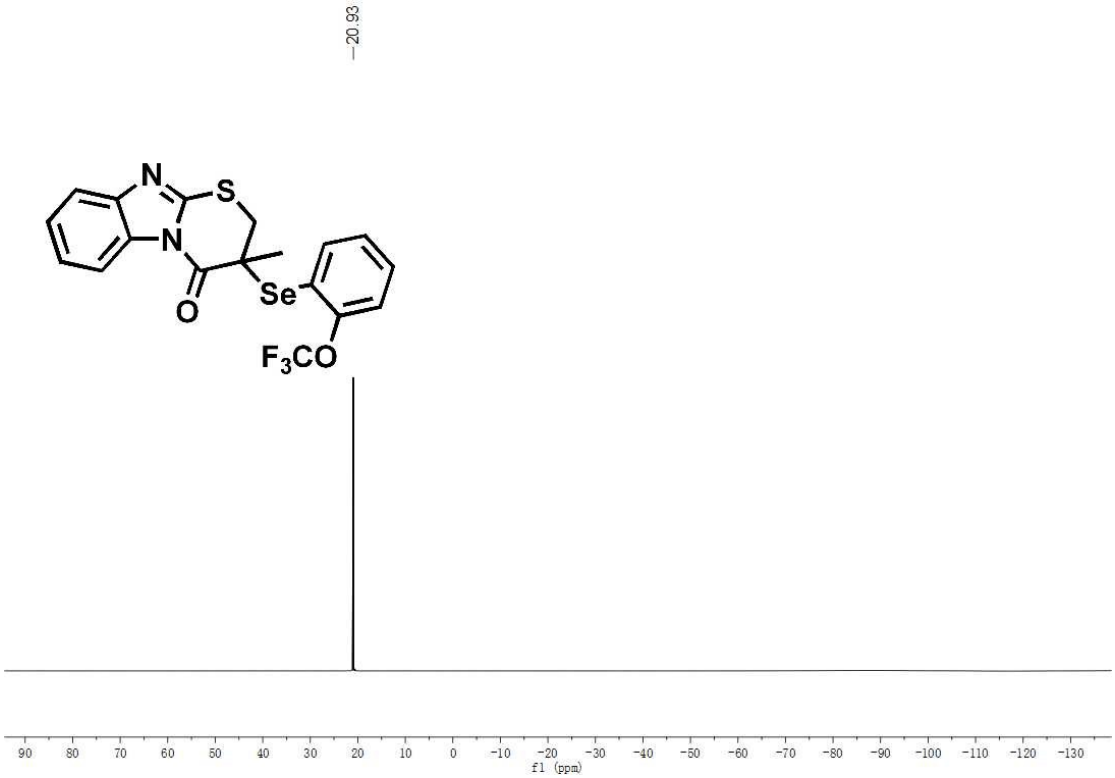
^{1}H NMR of product 4h in $CDCl_3$ (600 MHz)



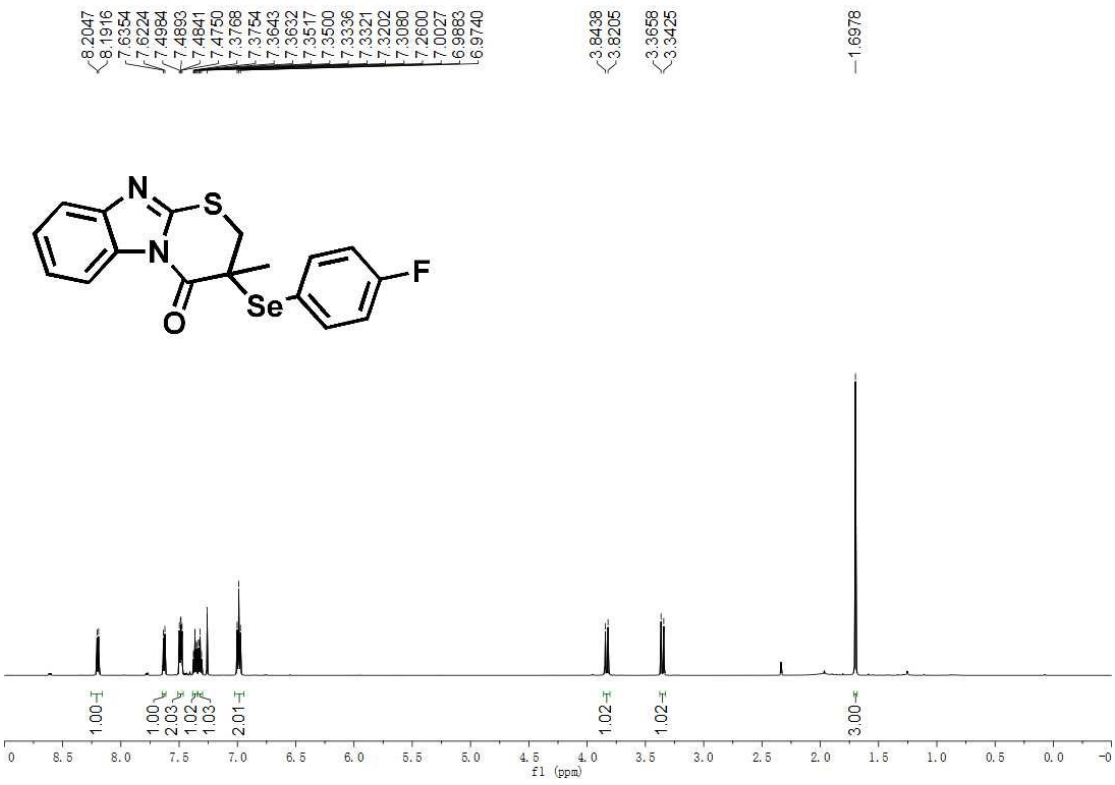
^{13}C NMR of product 4h in $CDCl_3$ (150 MHz)



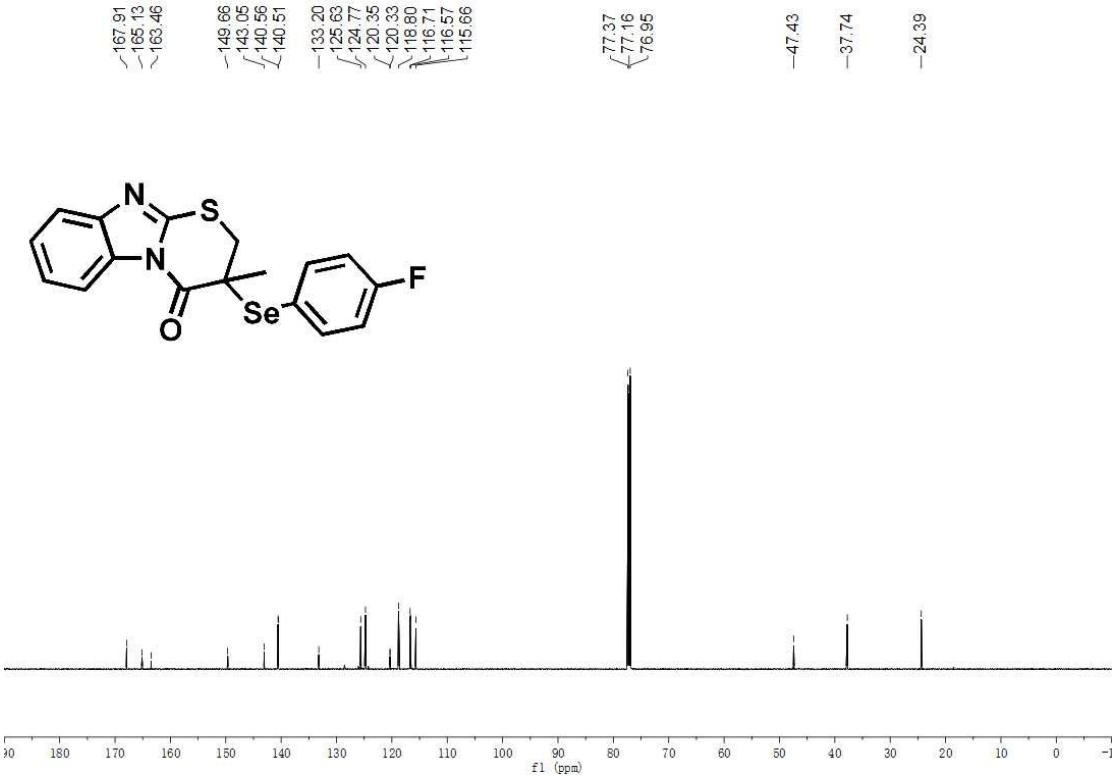
^{19}F NMR of product 4h in $CDCl_3$ (565 MHz)



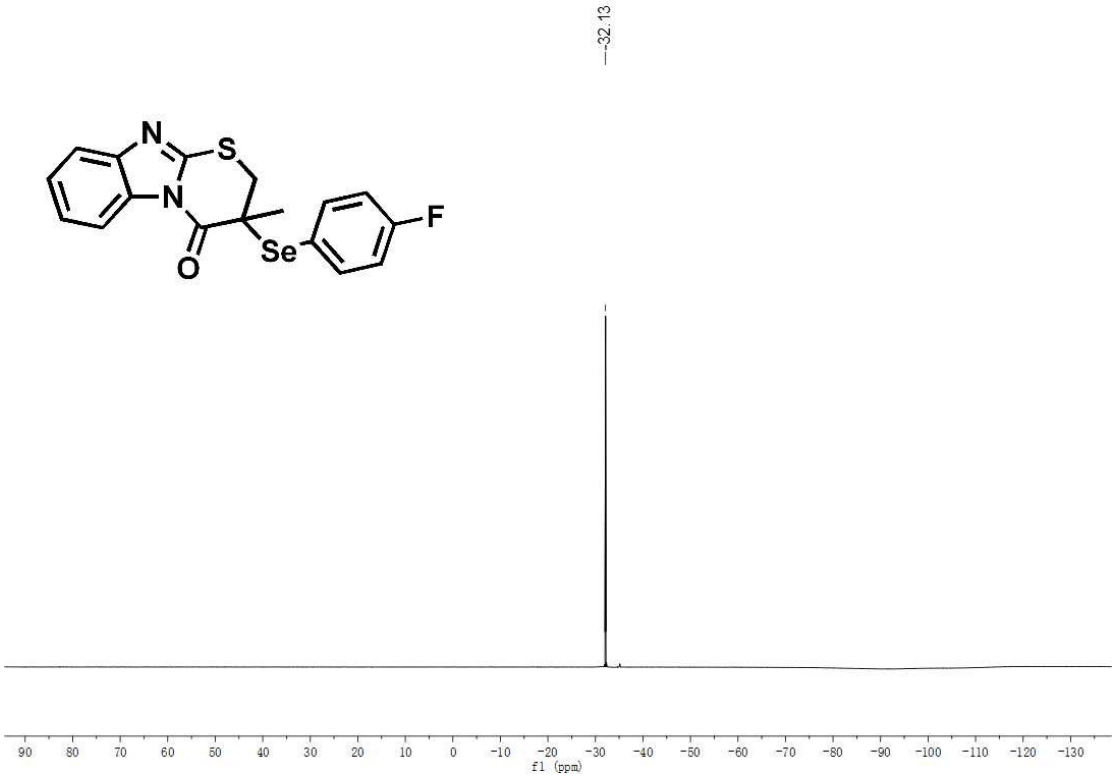
^{1}H NMR of product 4i in $CDCl_3$ (600 MHz)



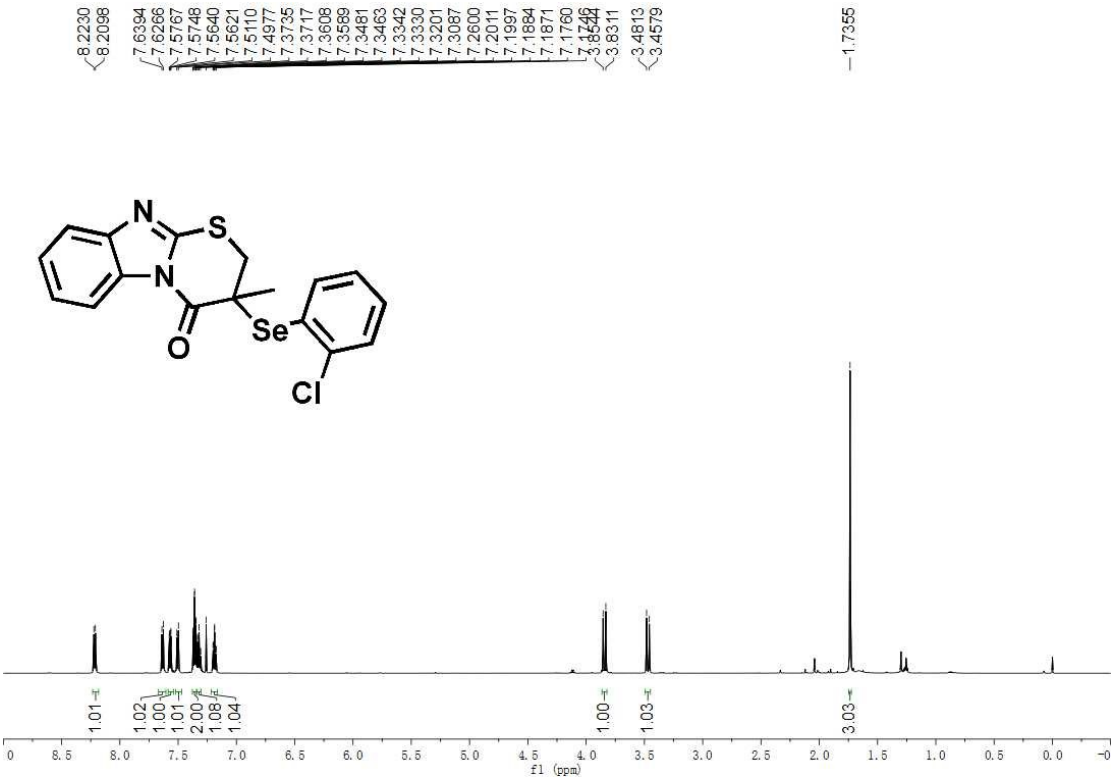
^{13}C NMR of product 4i in $CDCl_3$ (150 MHz)



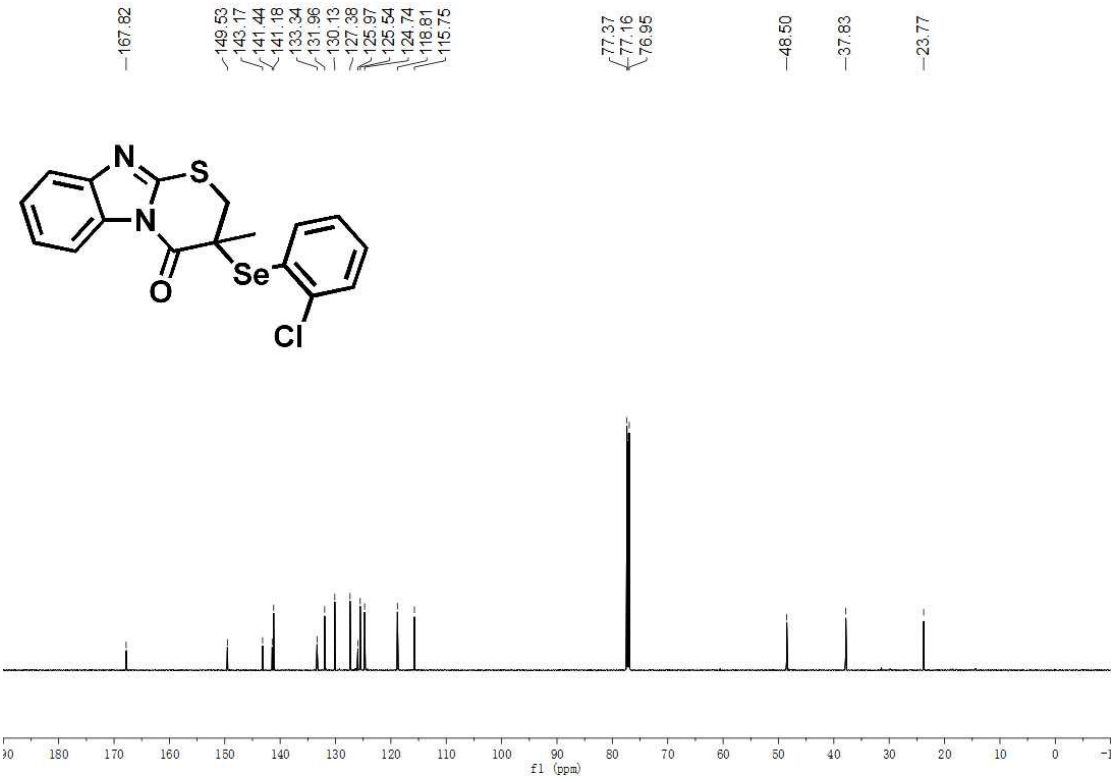
^{19}F NMR of product 4i in $CDCl_3$ (565 MHz)



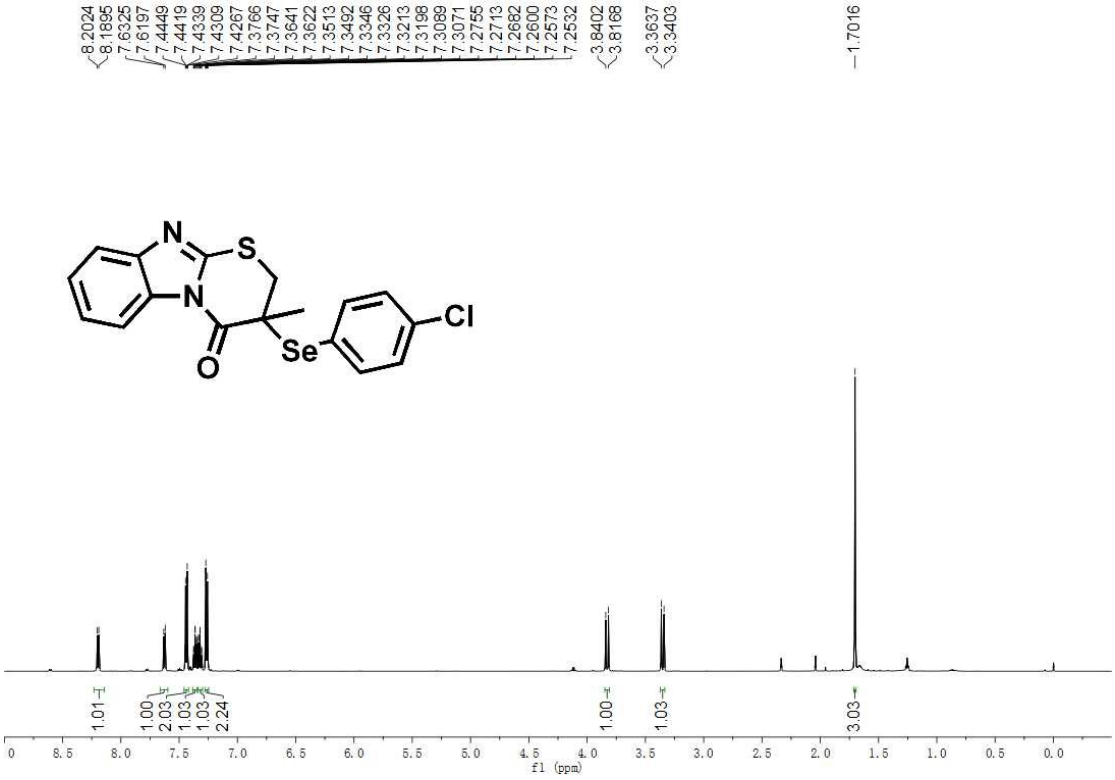
^{1}H NMR of product 4j in $CDCl_3$ (600 MHz)



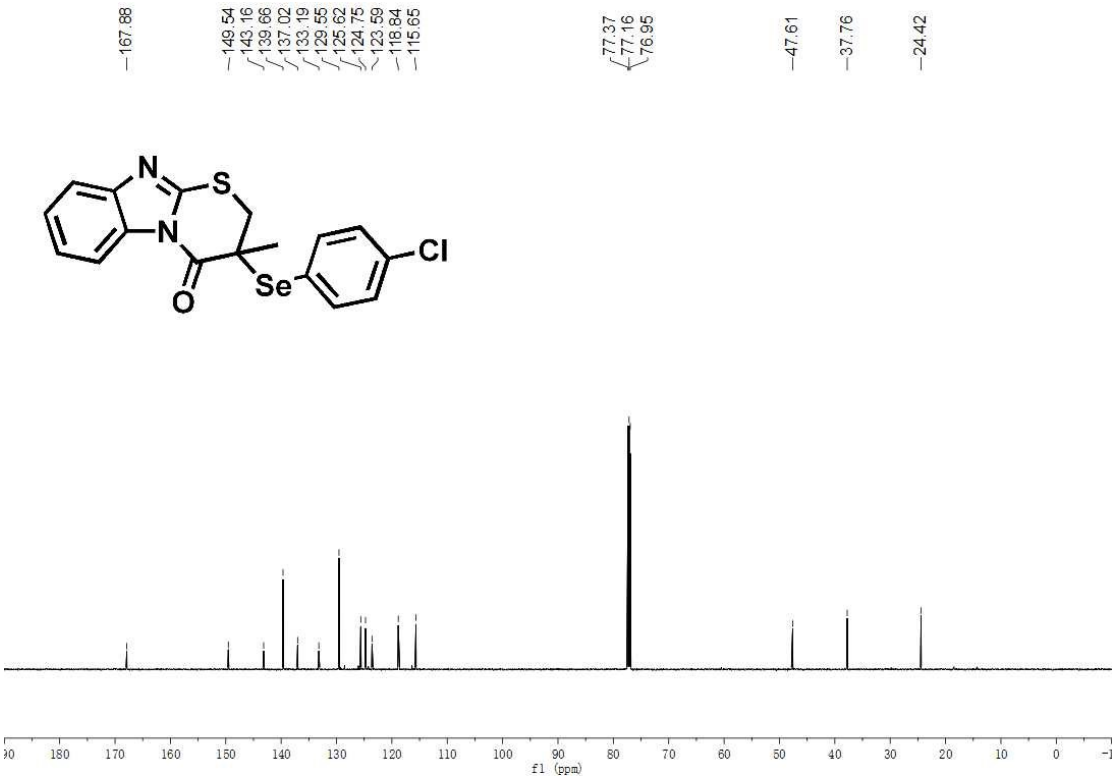
^{13}C NMR of product 4j in $CDCl_3$ (150 MHz)



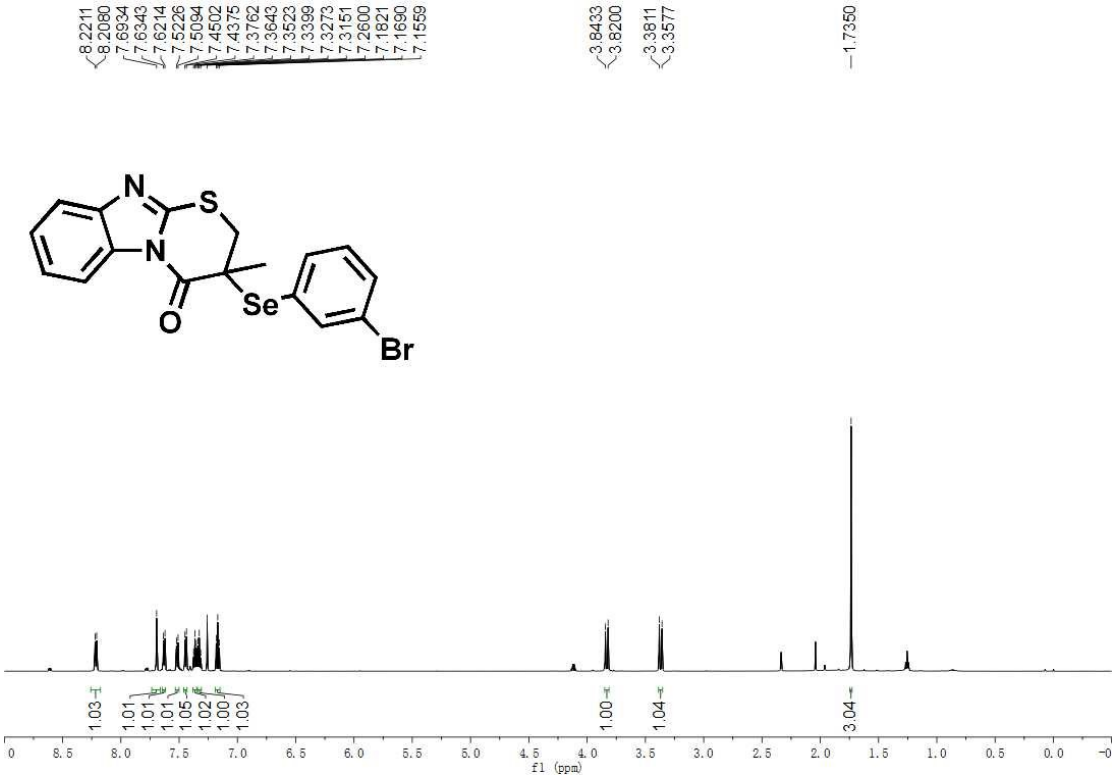
^{1}H NMR of product 4k in $CDCl_3$ (600 MHz)



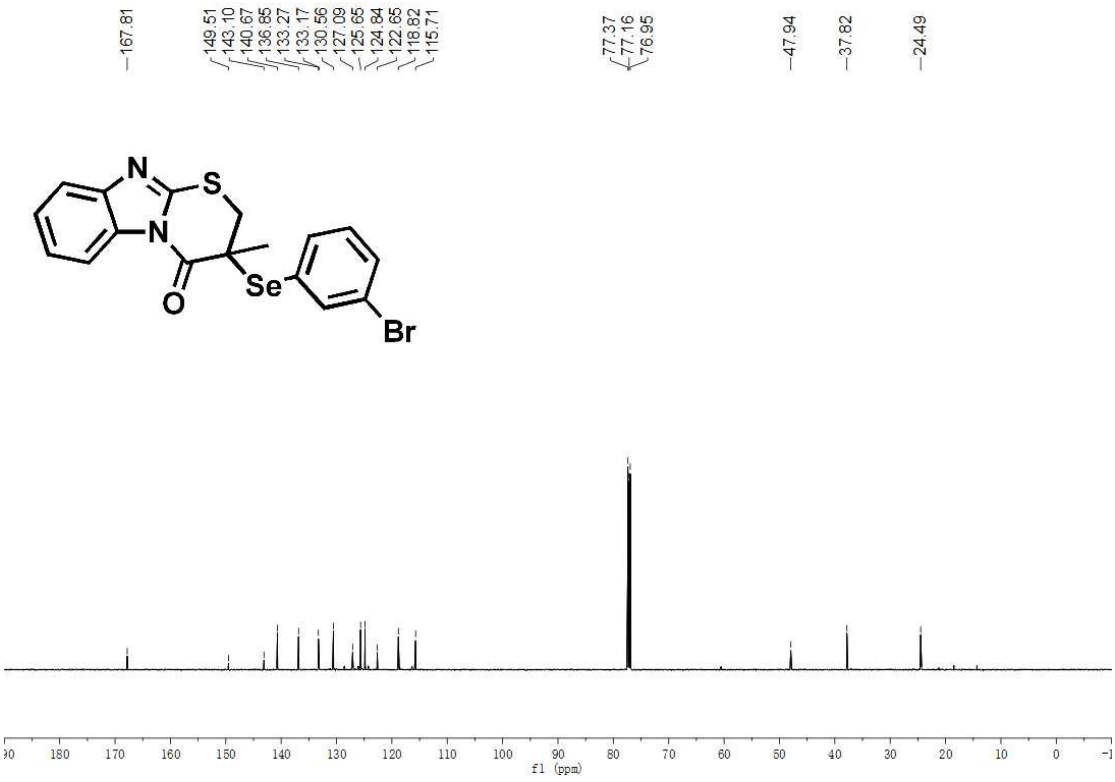
^{13}C NMR of product 4k in $CDCl_3$ (150 MHz)



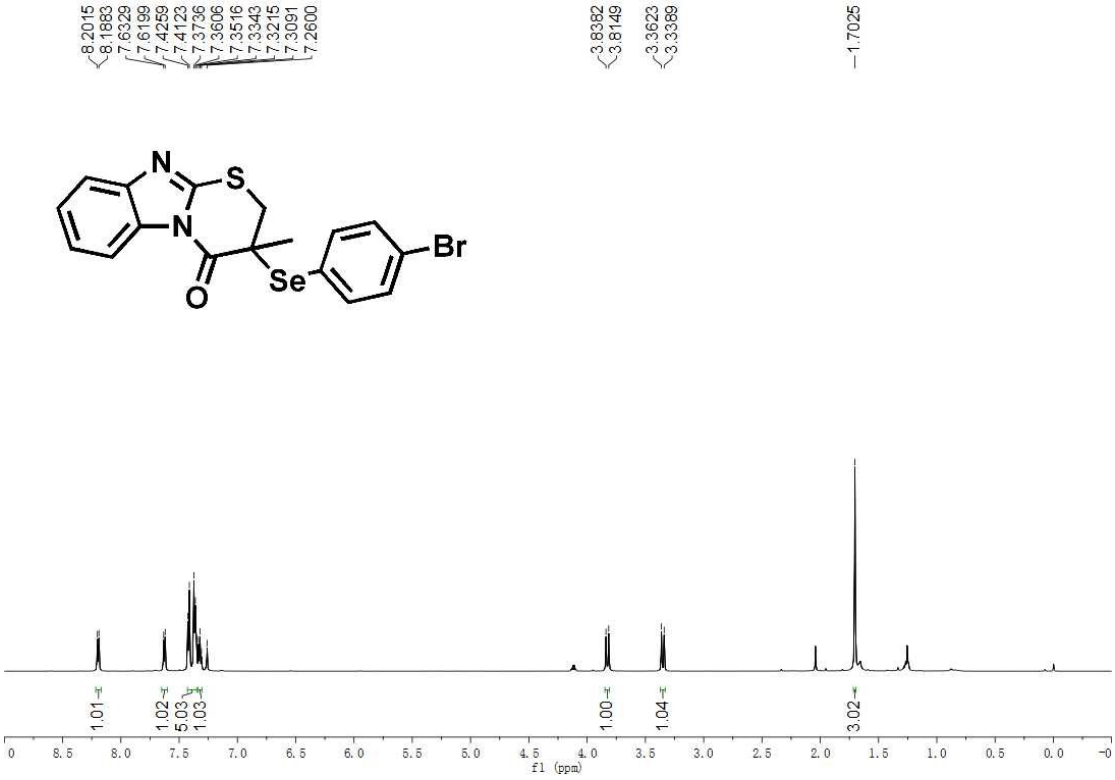
^{1}H NMR of product 4l in $CDCl_3$ (600 MHz)



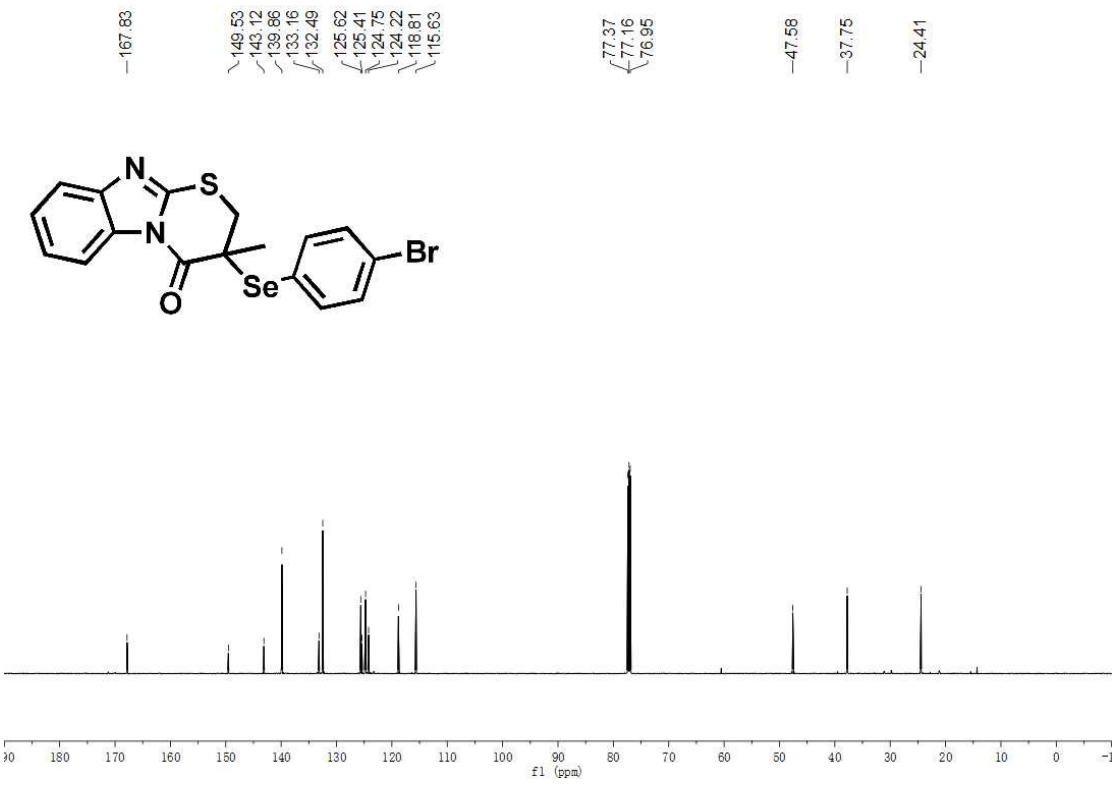
^{13}C NMR of product 4l in $CDCl_3$ (150 MHz)



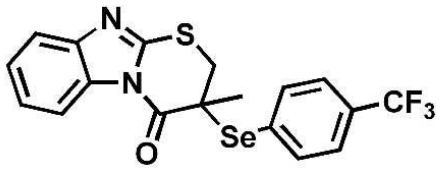
^{1}H NMR of product 4m in $CDCl_3$ (600 MHz)

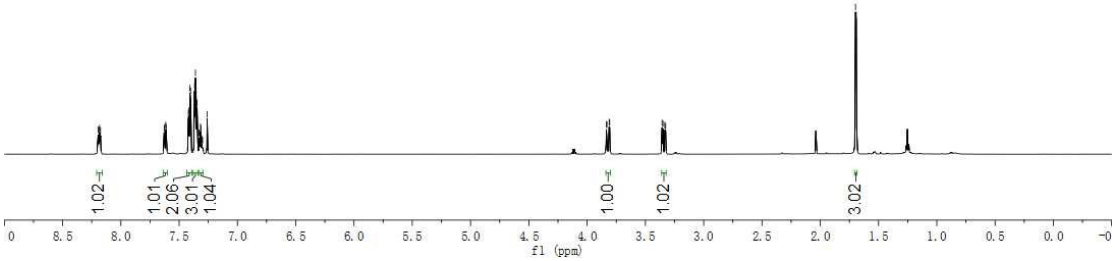


^{13}C NMR of product 4m in $CDCl_3$ (150 MHz)

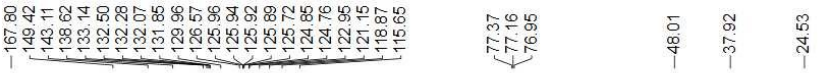


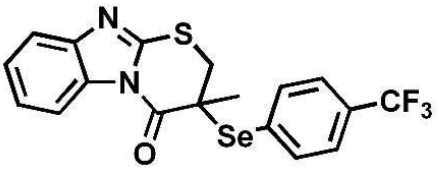
^{1}H NMR of product 4n in $CDCl_3$ (600 MHz)

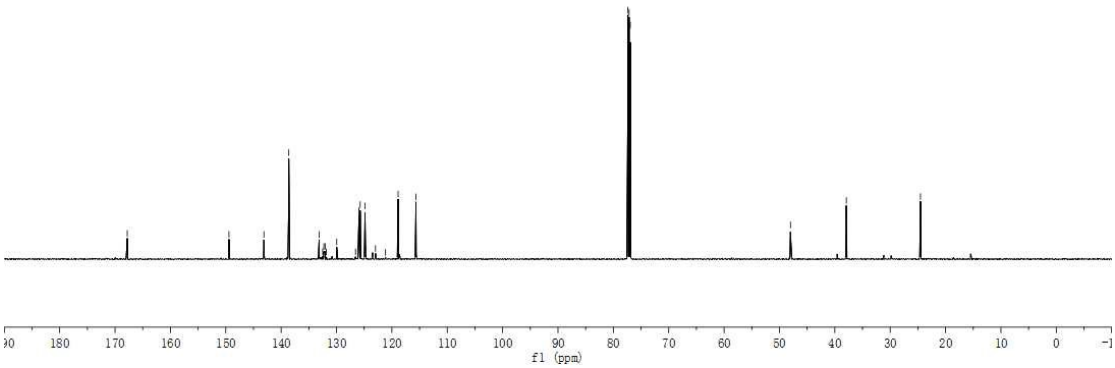




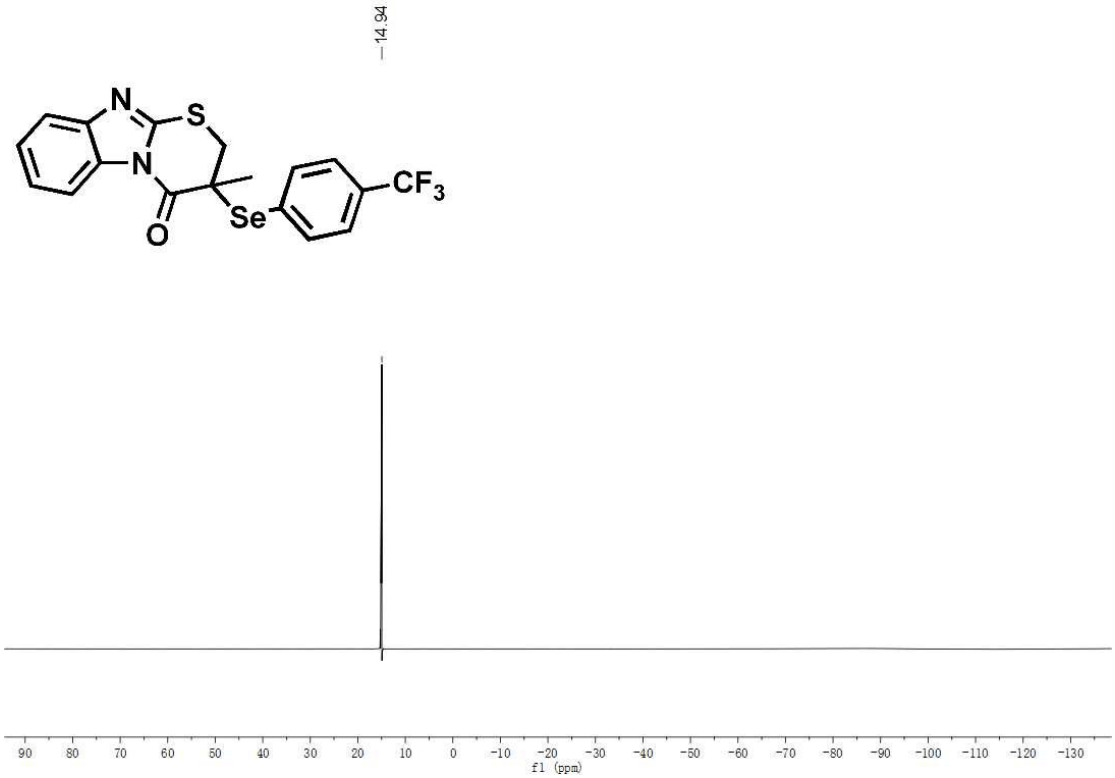
^{13}C NMR of product 4n in $CDCl_3$ (150 MHz)



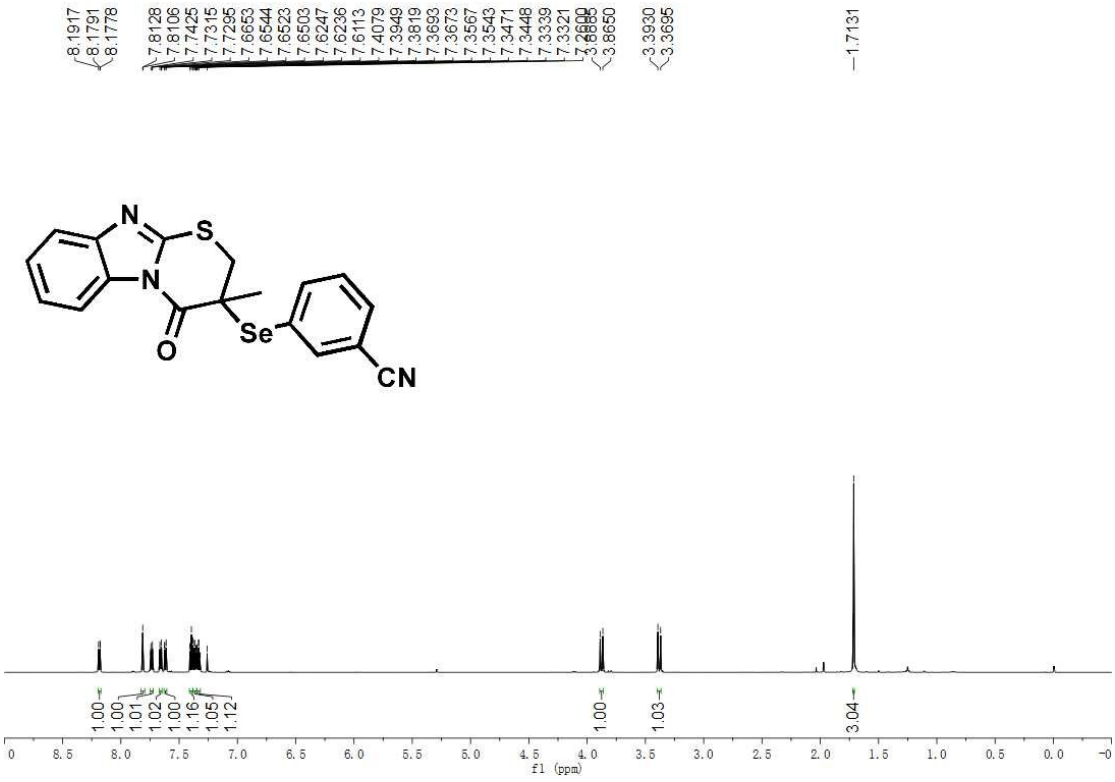




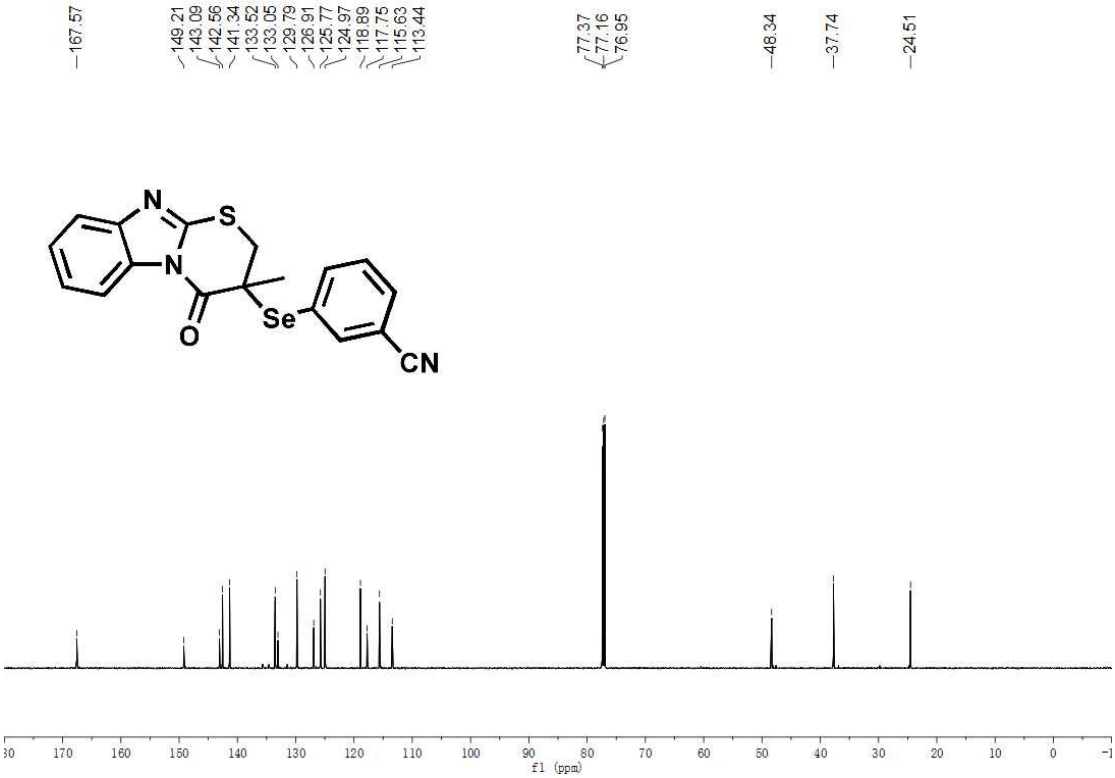
^{19}F NMR of product 4n in $CDCl_3$ (565 MHz)



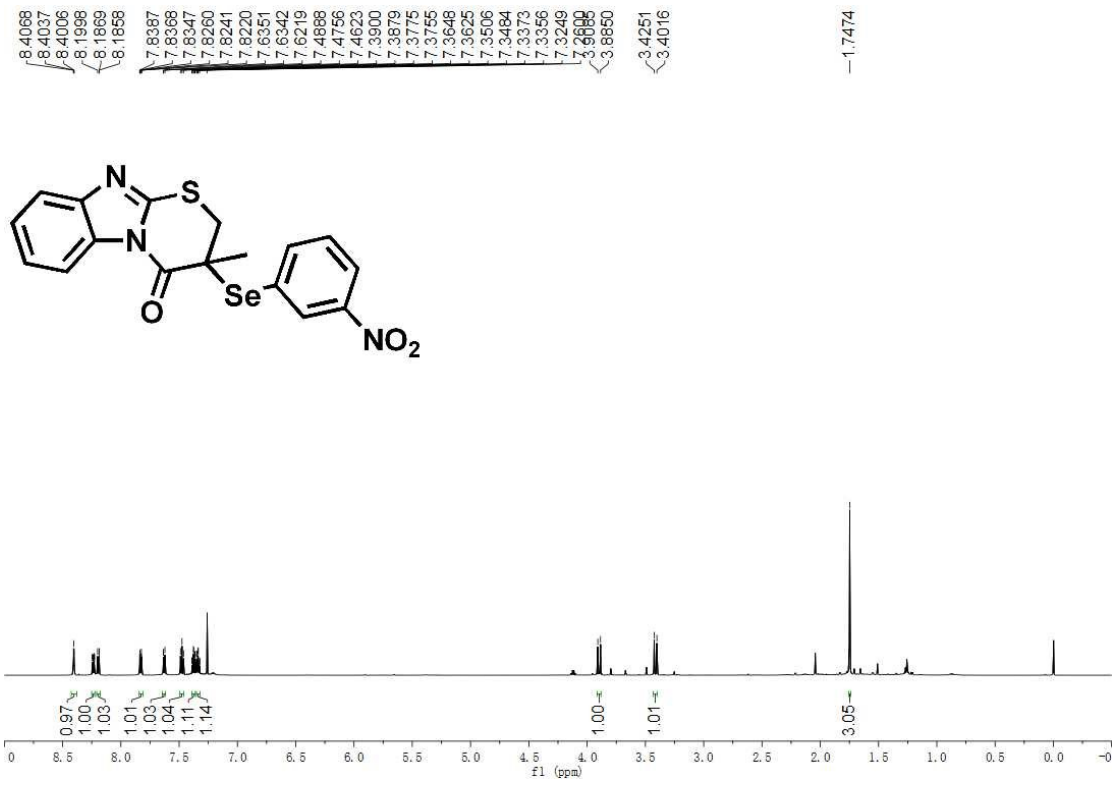
^{1}H NMR of product 4o in $CDCl_3$ (600 MHz)



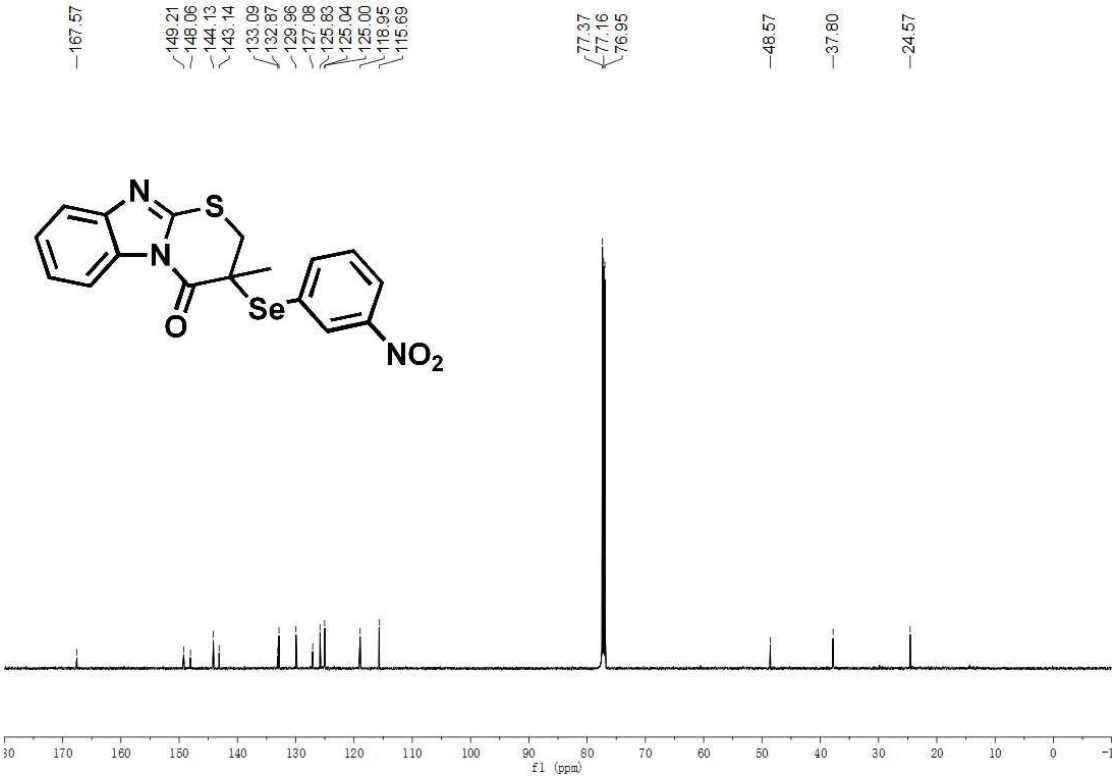
^{13}C NMR of product 4o in $CDCl_3$ (150 MHz)



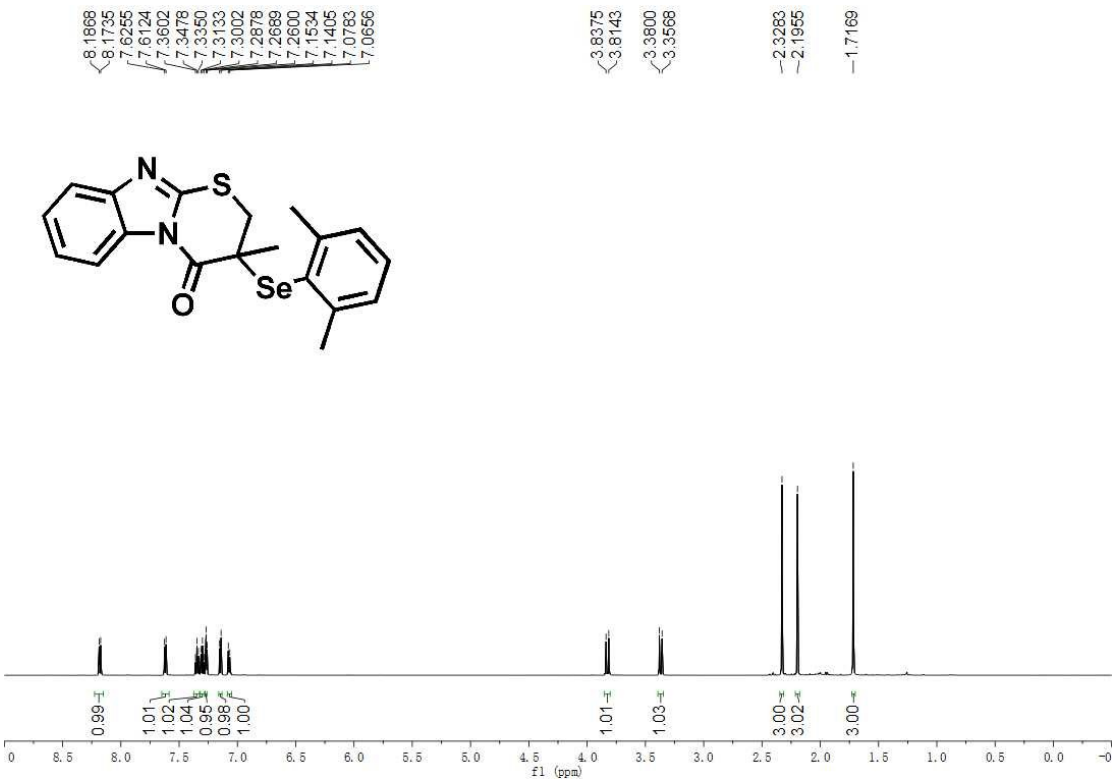
^{1}H NMR of product 4p in $CDCl_3$ (600 MHz)



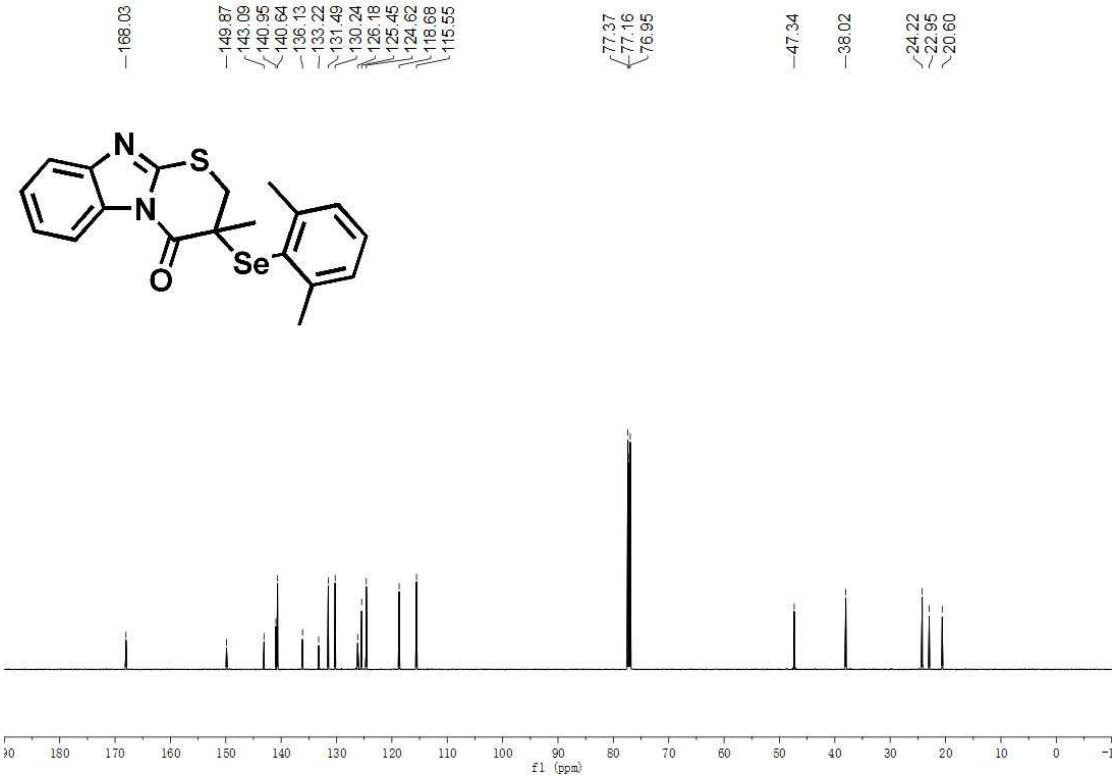
^{13}C NMR of product 4p in $CDCl_3$ (150 MHz)



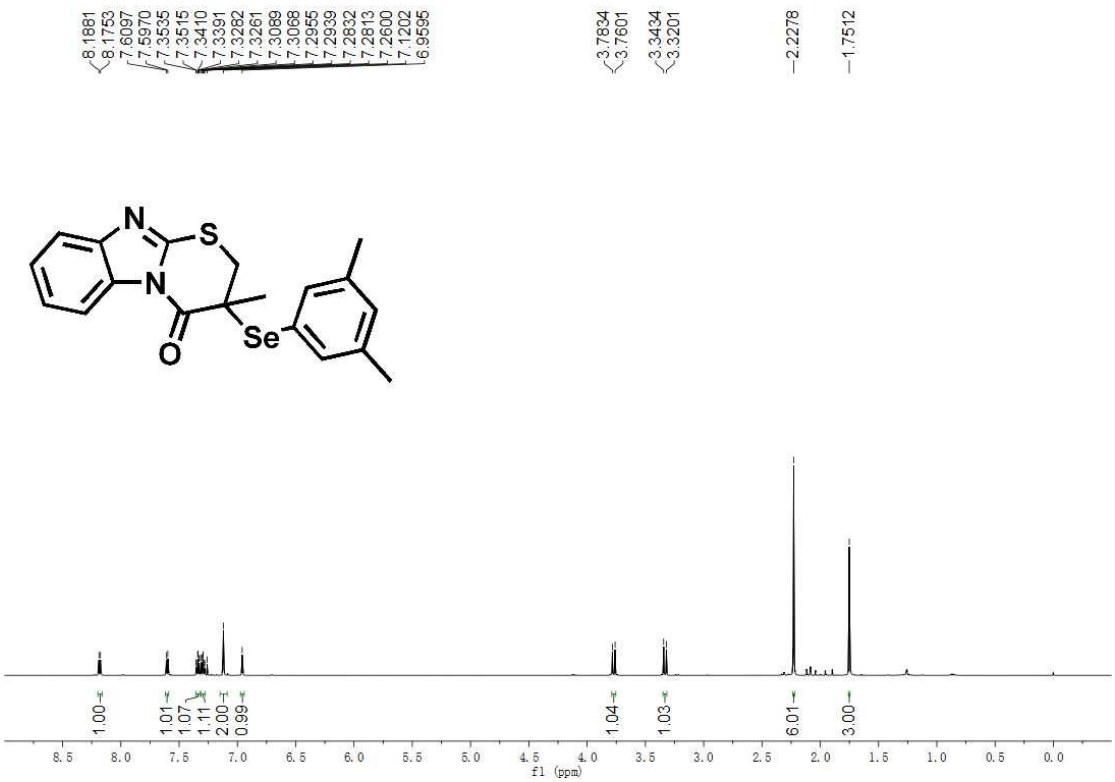
^{1}H NMR of product 4q in $CDCl_3$ (600 MHz)



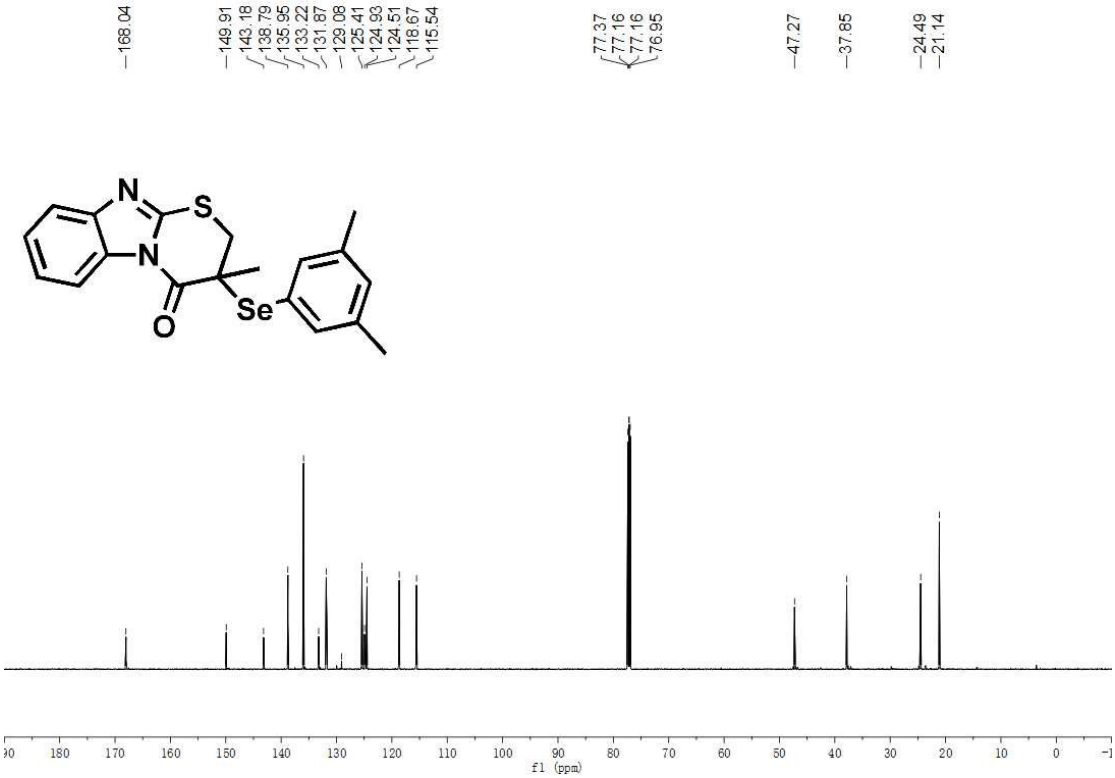
^{13}C NMR of product 4q in $CDCl_3$ (150 MHz)



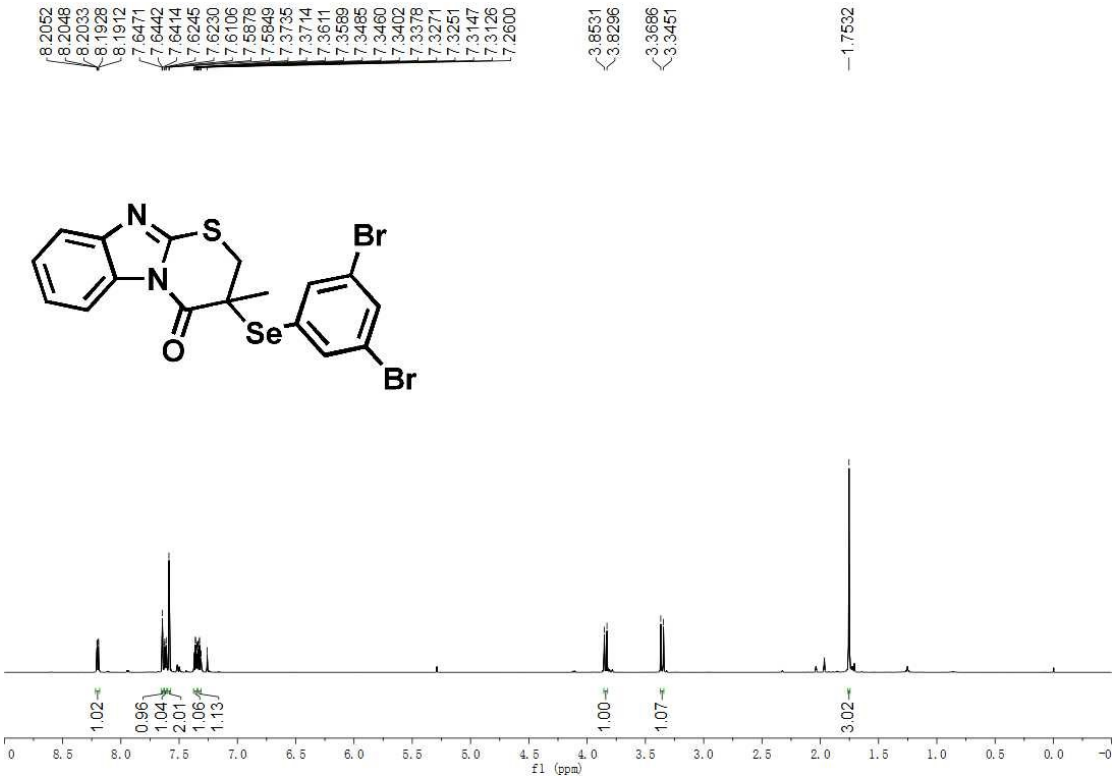
^{1}H NMR of product 4r in $CDCl_3$ (600 MHz)



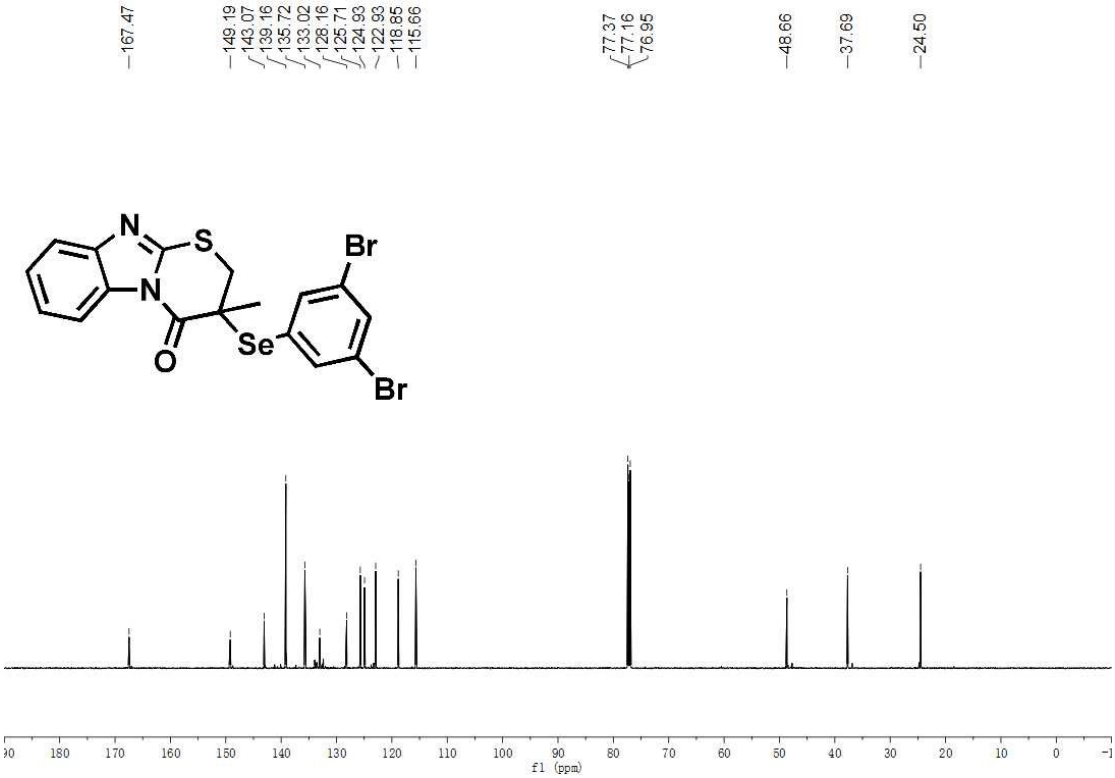
^{13}C NMR of product 4r in $CDCl_3$ (150 MHz)



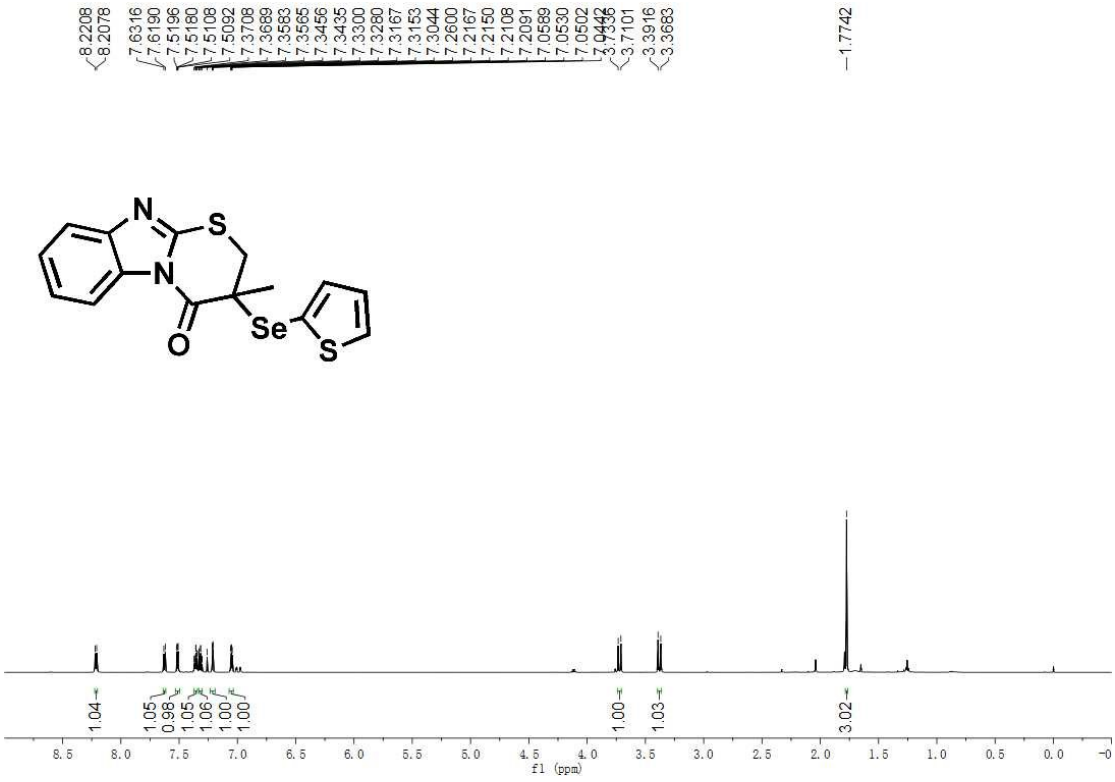
^{1}H NMR of product 4s in $CDCl_3$ (600 MHz)



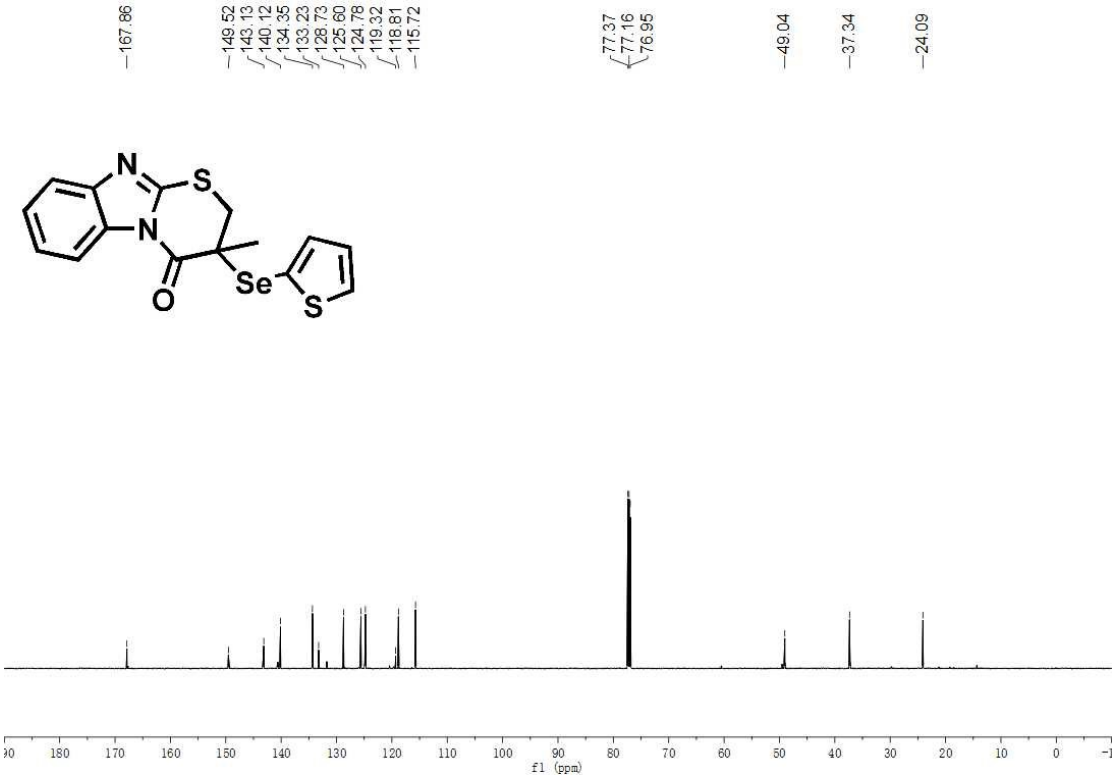
^{13}C NMR of product 4s in $CDCl_3$ (150 MHz)



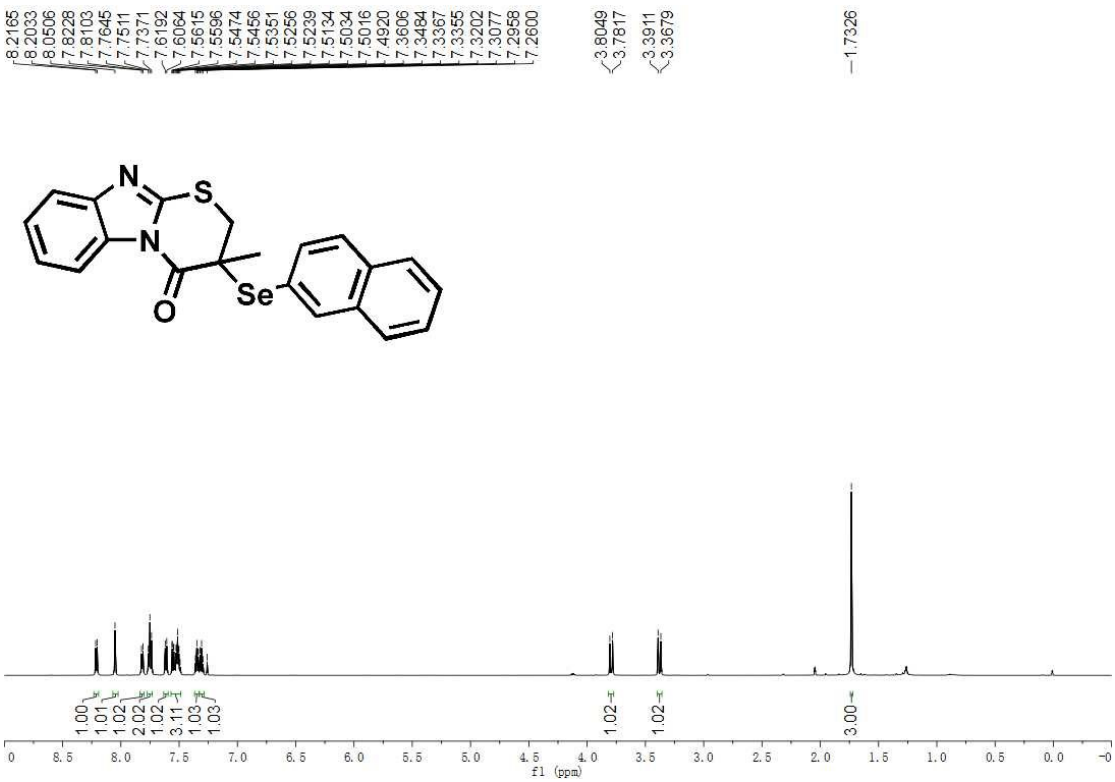
^{1}H NMR of product 4t in $CDCl_3$ (600 MHz)



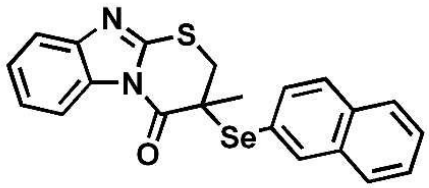
^{13}C NMR of product 4t in $CDCl_3$ (150 MHz)

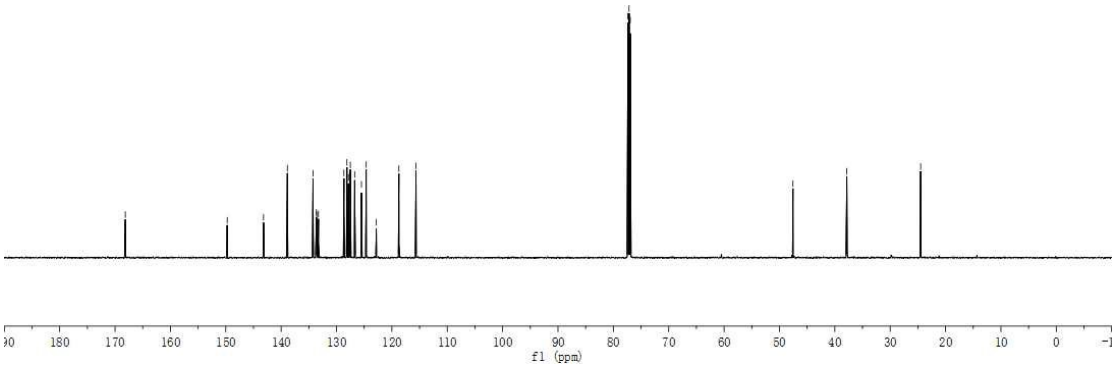


^{1}H NMR of product 4u in $CDCl_3$ (600 MHz)

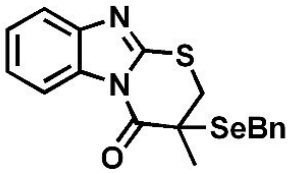


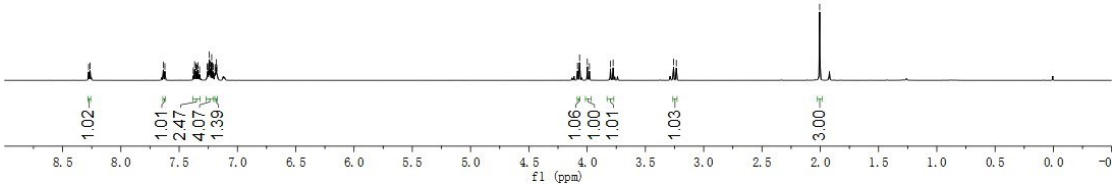
^{13}C NMR of product 4u in $CDCl_3$ (150 MHz)



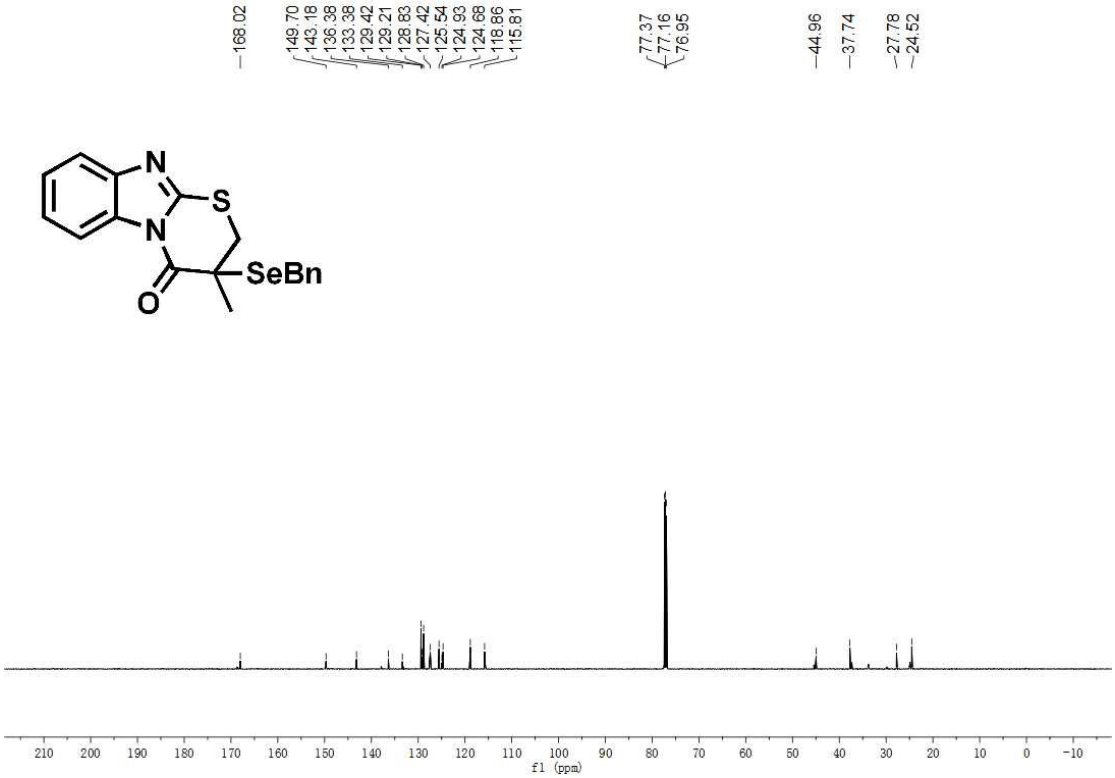


^{1}H NMR of product 4v in $CDCl_3$ (600 MHz)

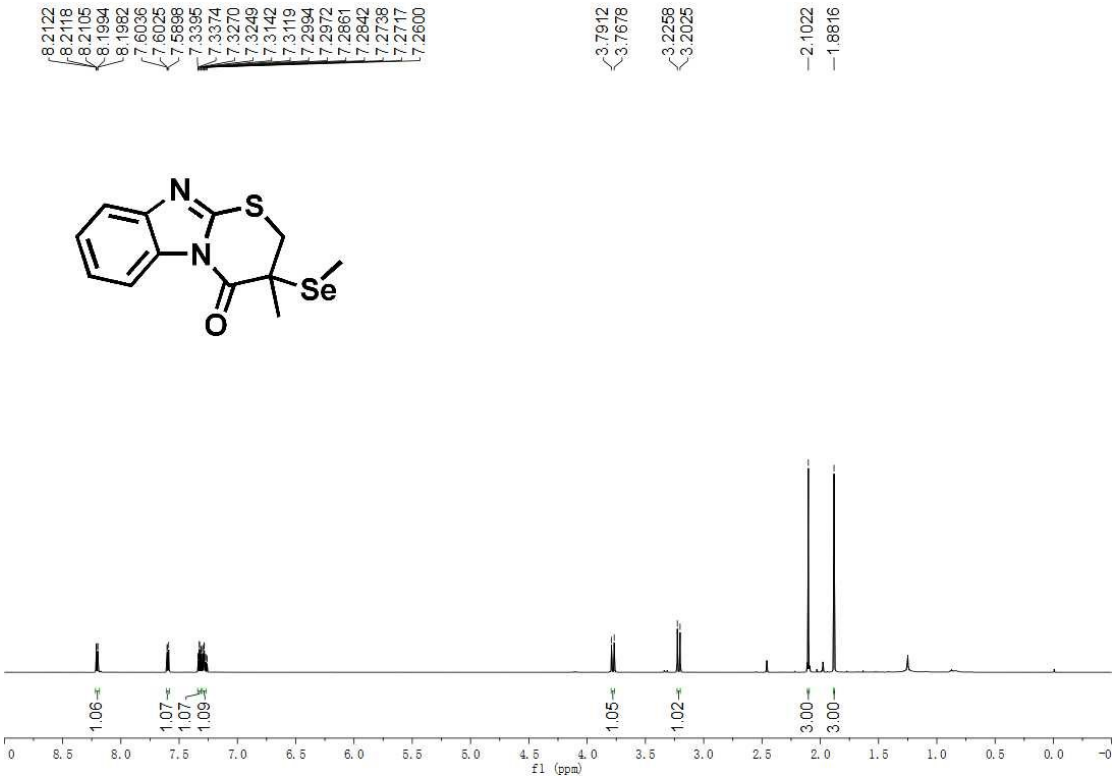




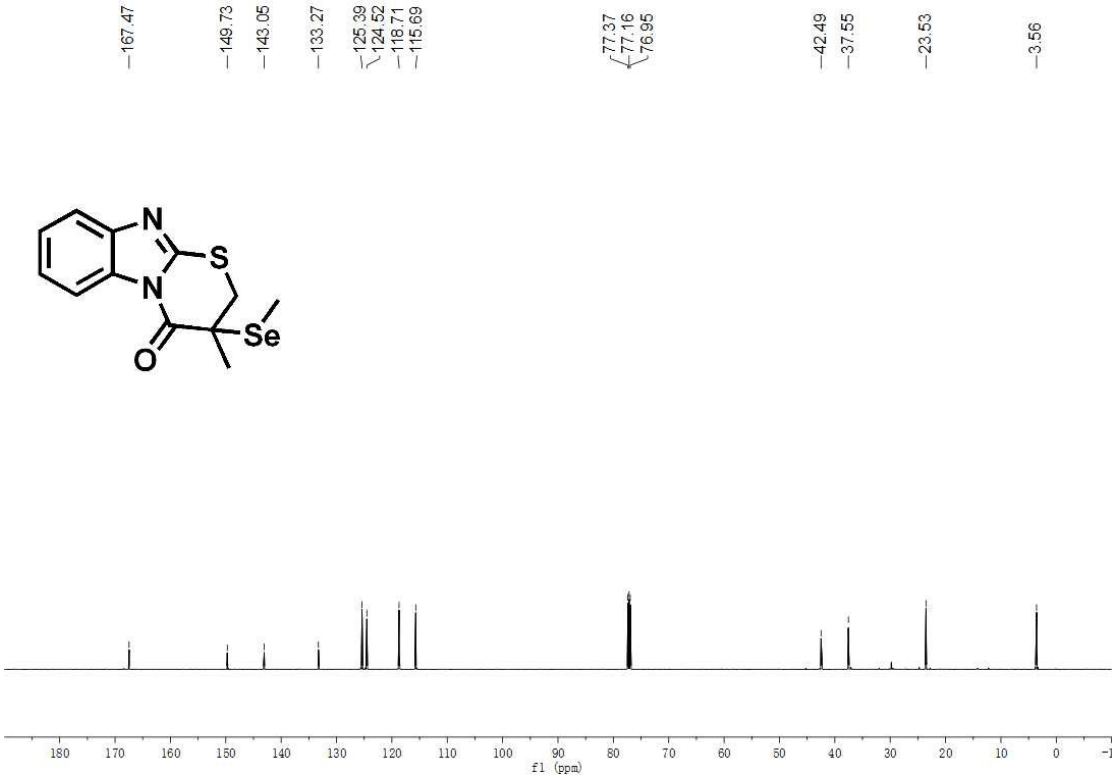
^{13}C NMR of product 4v in $CDCl_3$ (150 MHz)



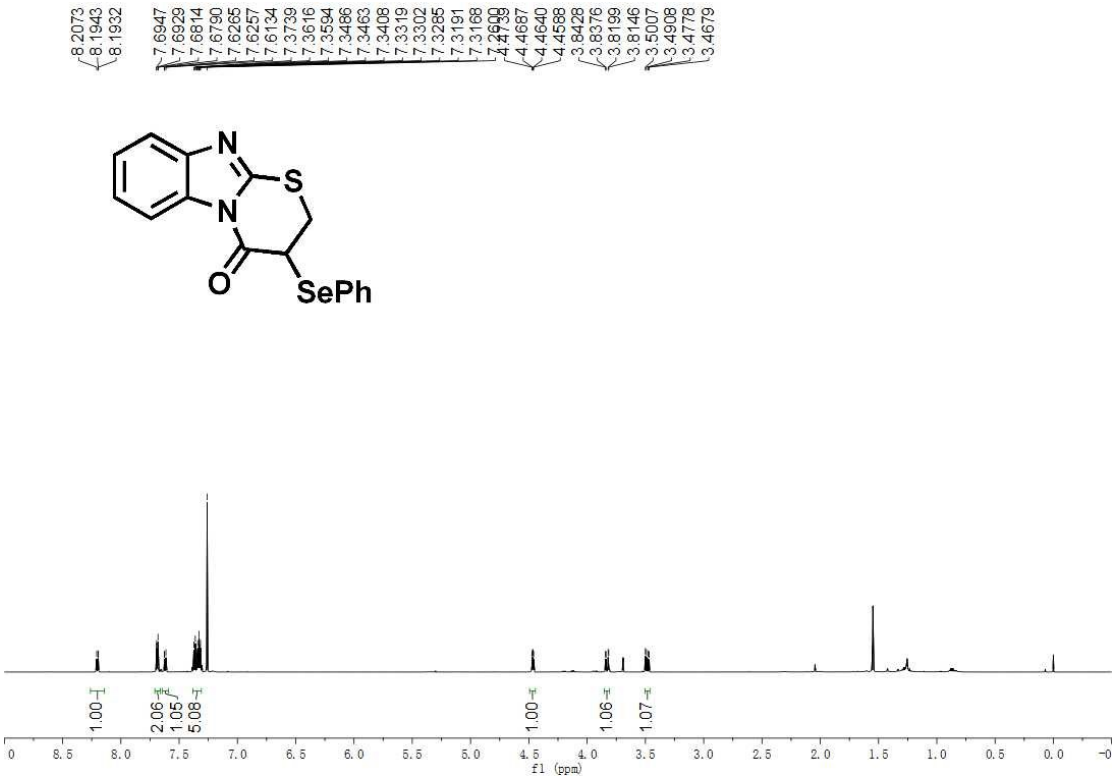
^{1}H NMR of product 4w in $CDCl_3$ (600 MHz)



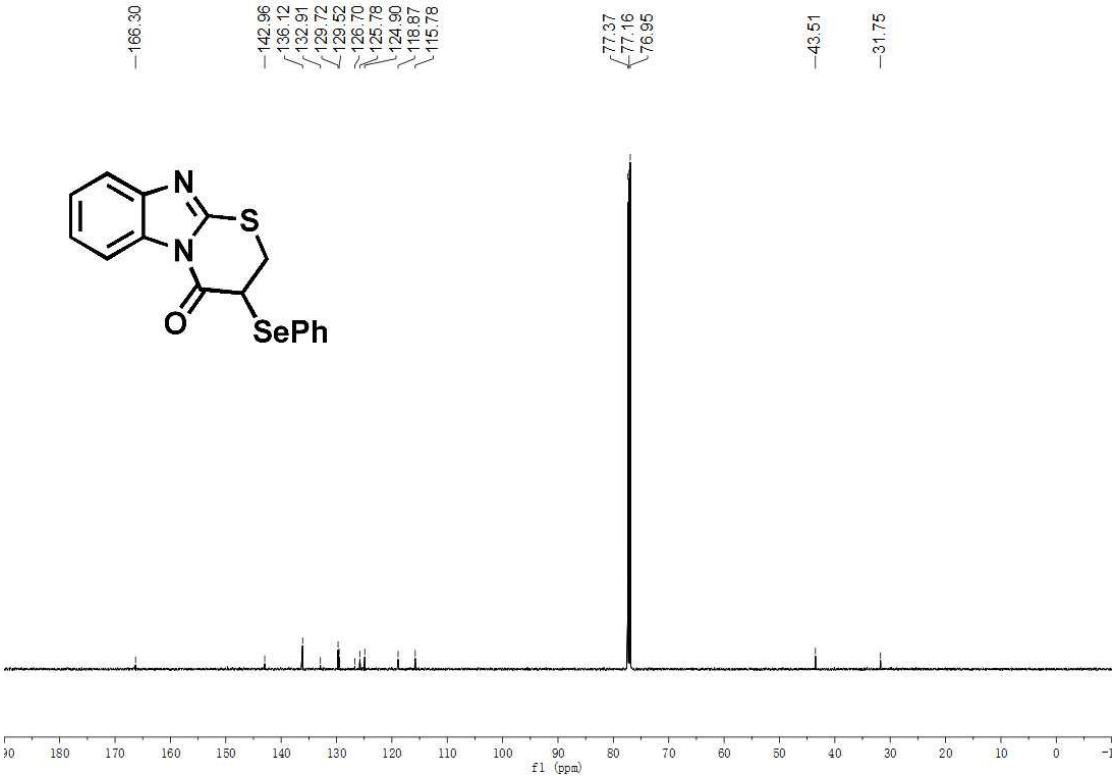
^{13}C NMR of product 4w in $CDCl_3$ (150 MHz)



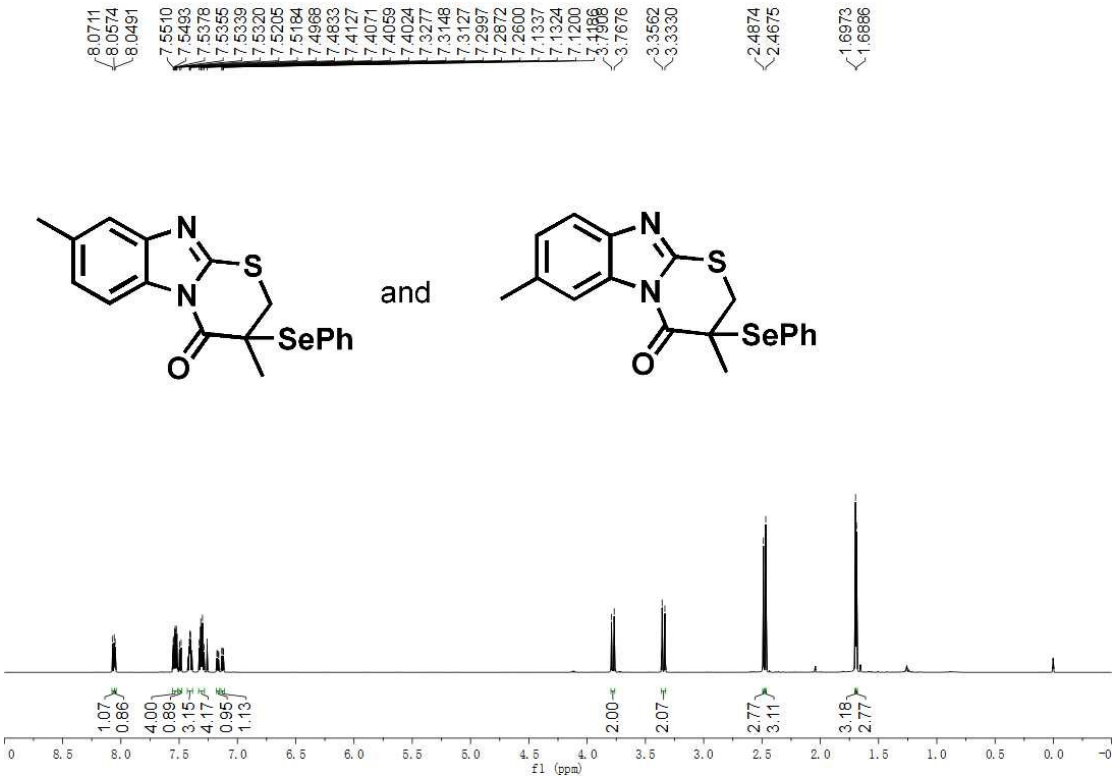
^{1}H NMR of product 5a in $CDCl_3$ (600 MHz)



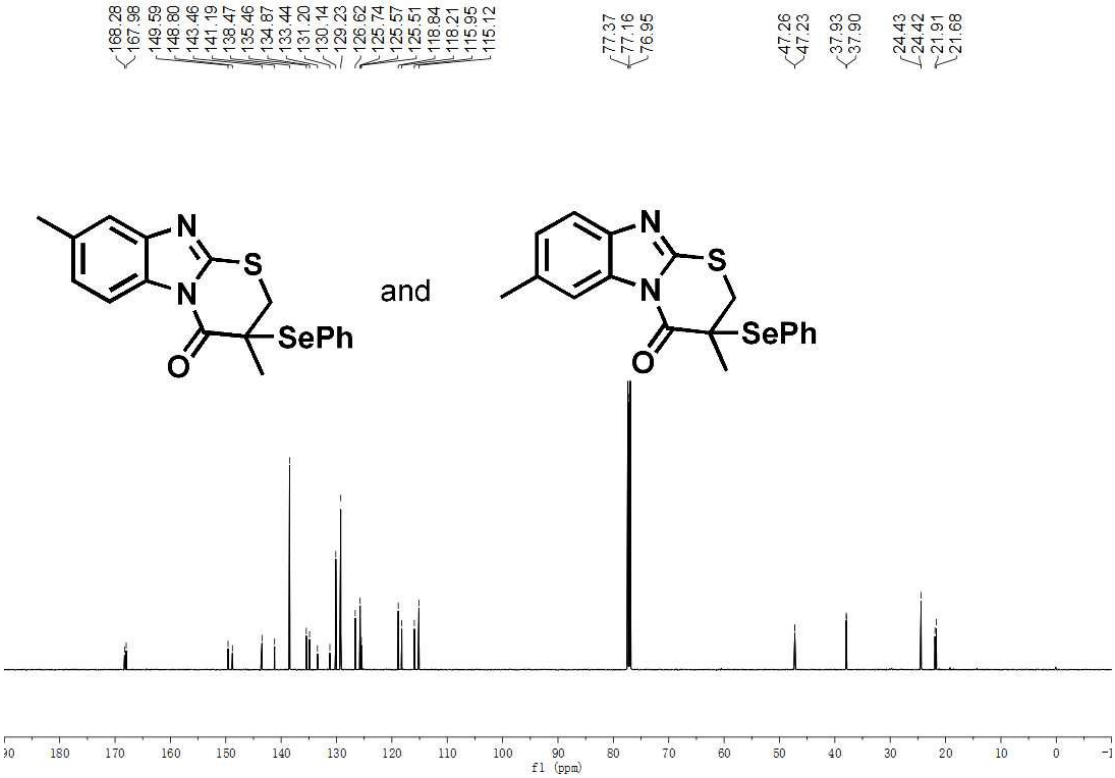
^{13}C NMR of product 5a in $CDCl_3$ (150 MHz)



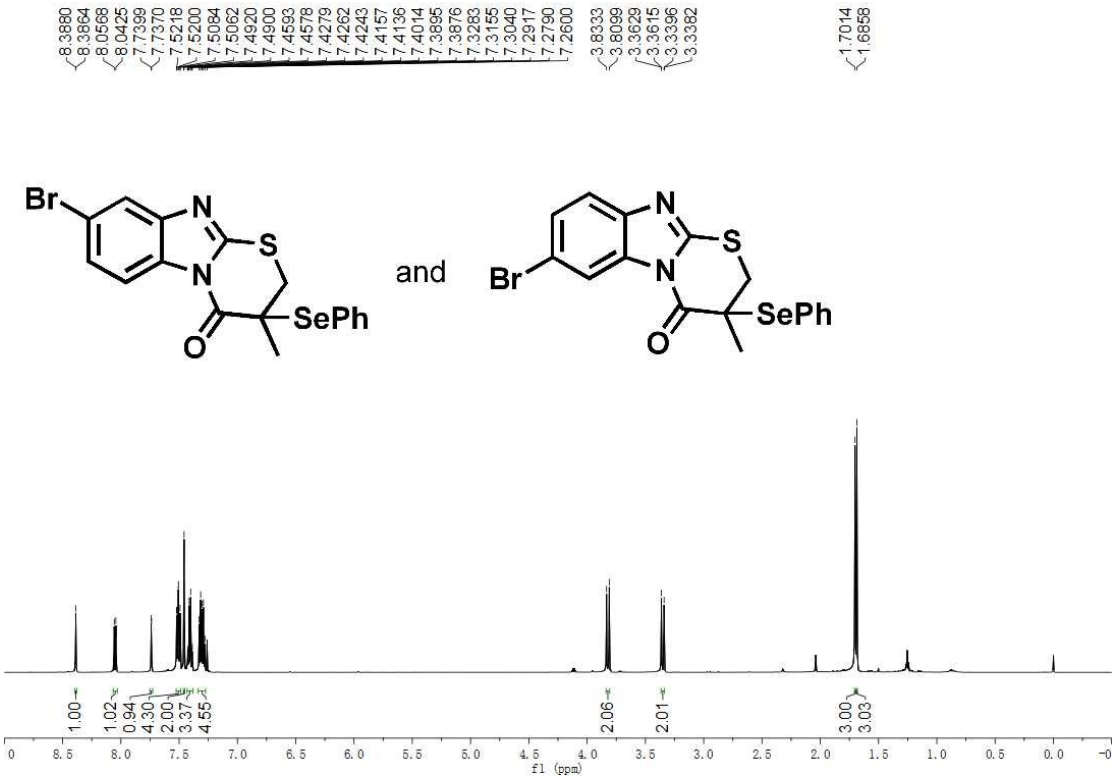
^{1}H NMR of product 5b in $CDCl_3$ (600 MHz)



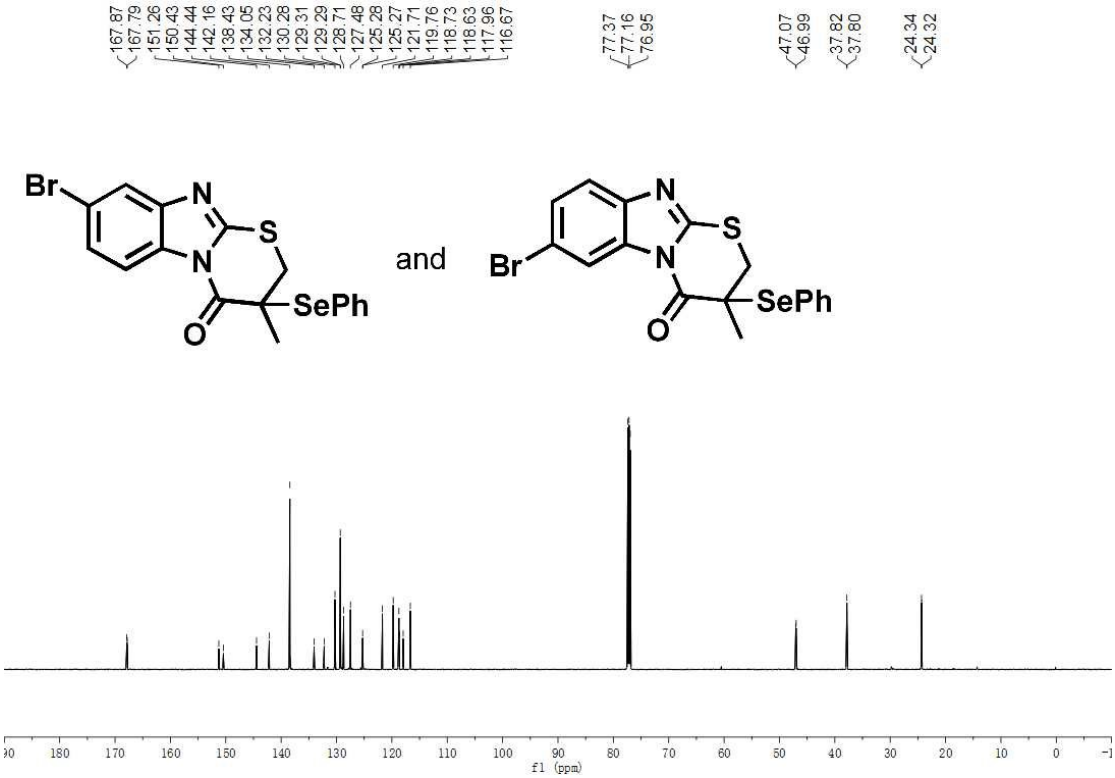
^{13}C NMR of product 5b in $CDCl_3$ (150 MHz)



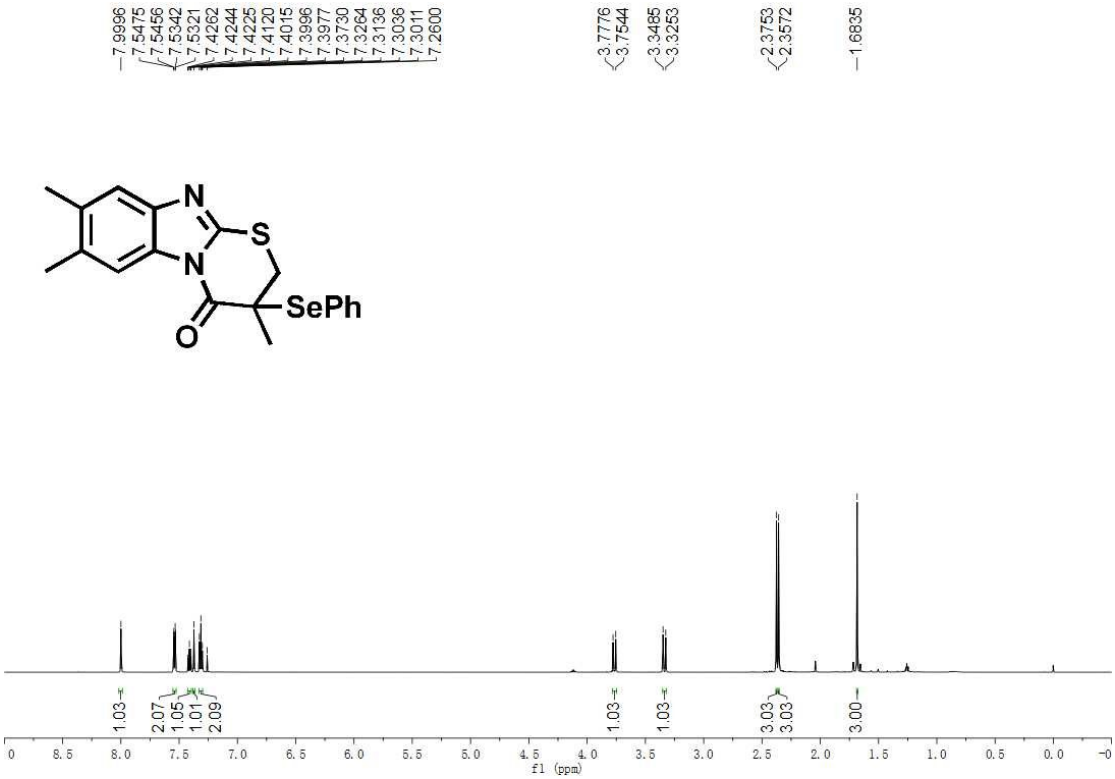
^{1}H NMR of product 5c in $CDCl_3$ (600 MHz)



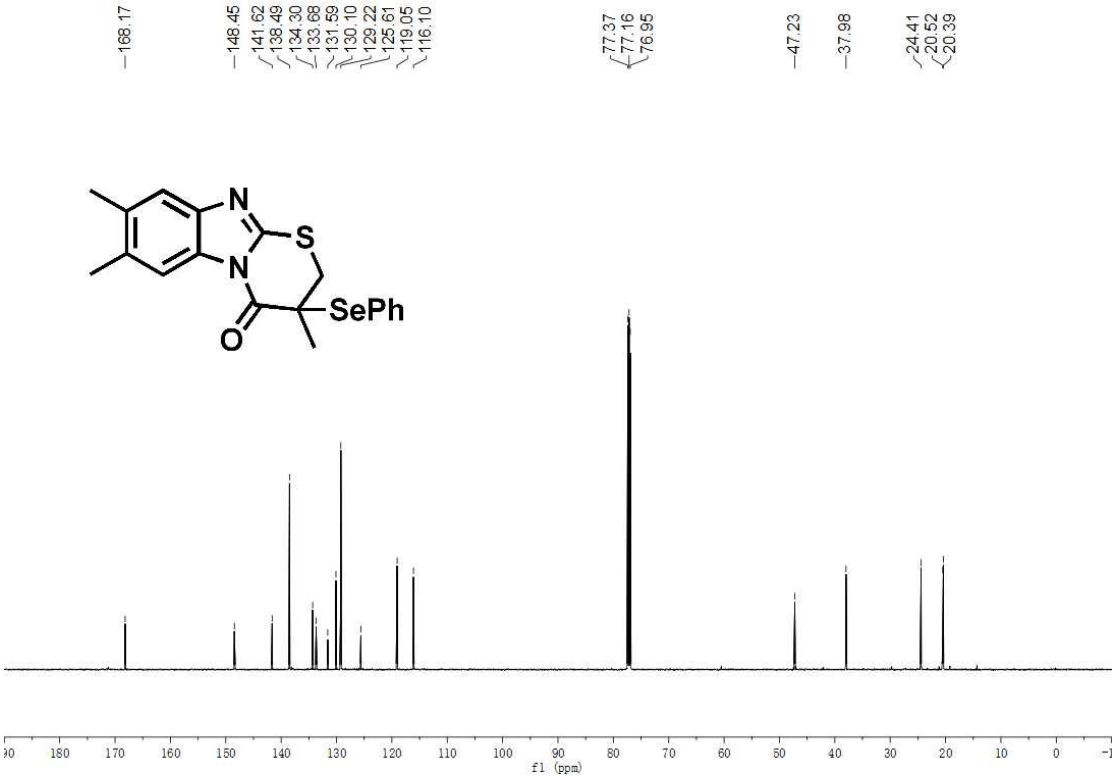
^{13}C NMR of product 5c in $CDCl_3$ (150 MHz)



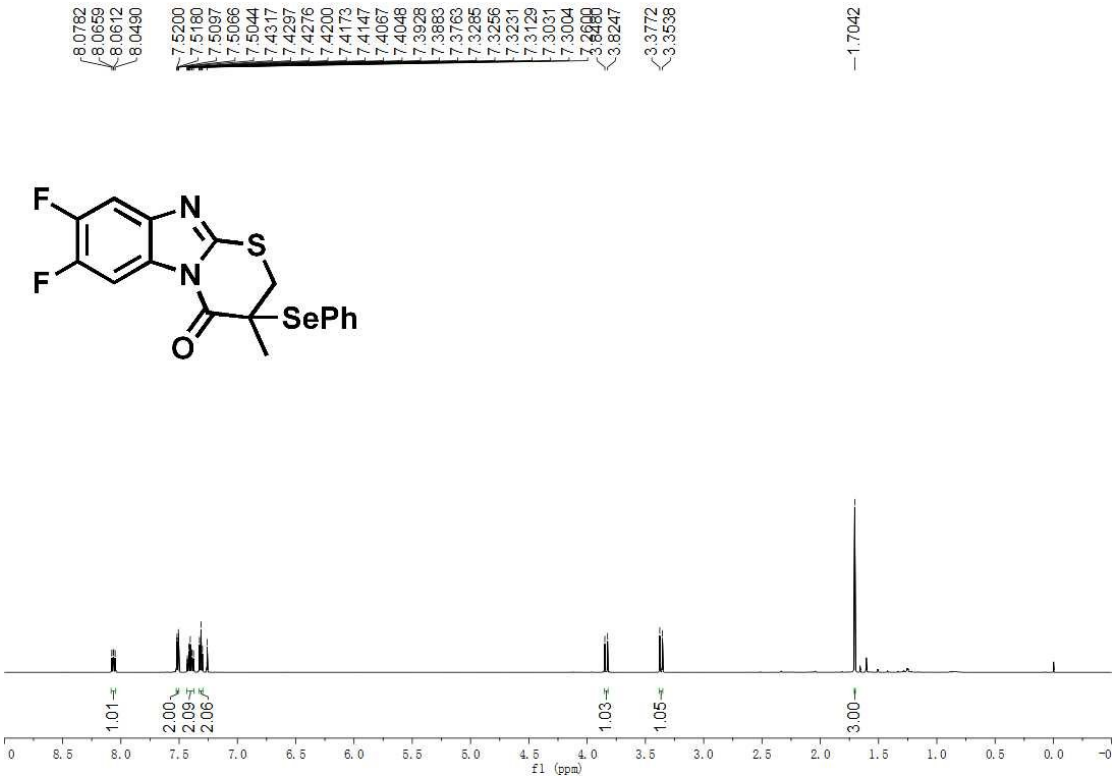
^{1}H NMR of product 5d in $CDCl_3$ (600 MHz)



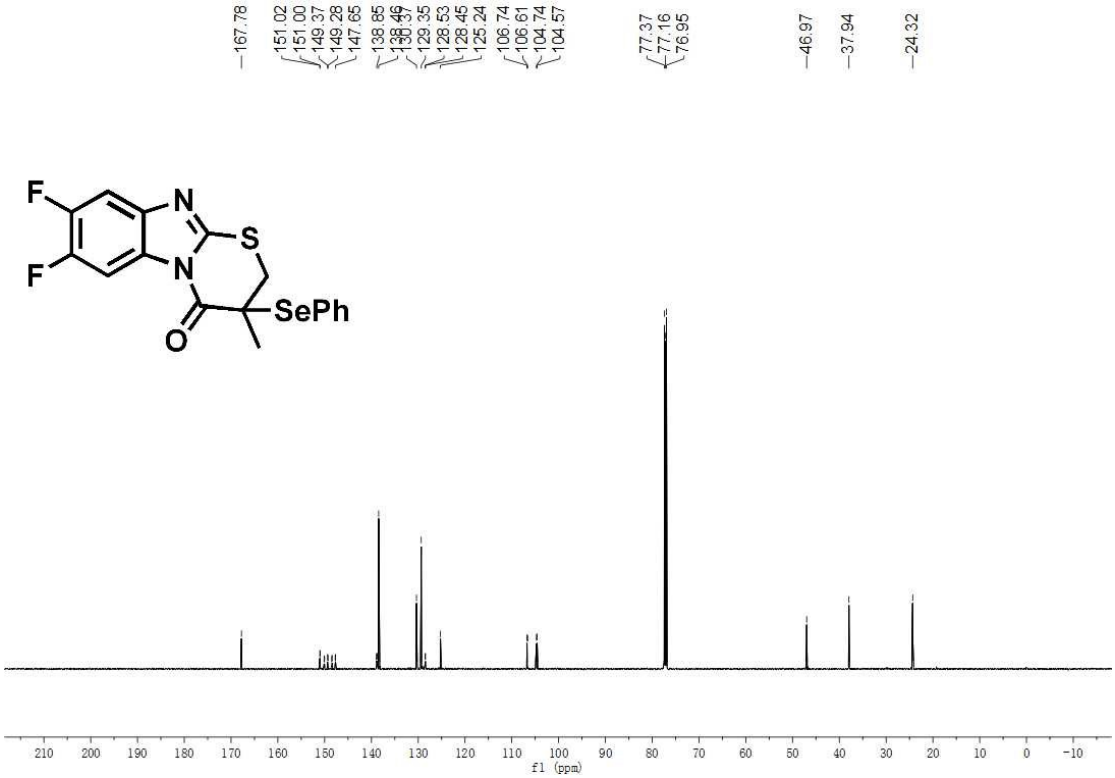
^{13}C NMR of product 5d in $CDCl_3$ (150 MHz)



^{1}H NMR of product 5e in $CDCl_3$ (600 MHz)

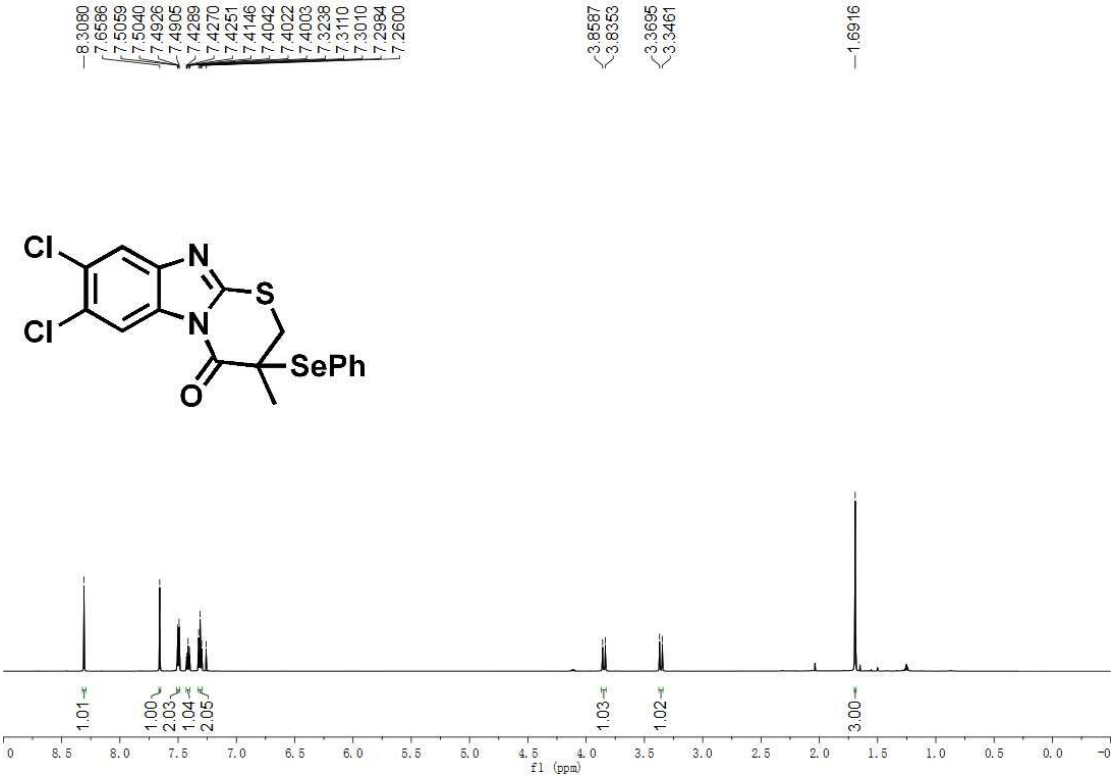


^{13}C NMR of product 5e in $CDCl_3$ (150 MHz)

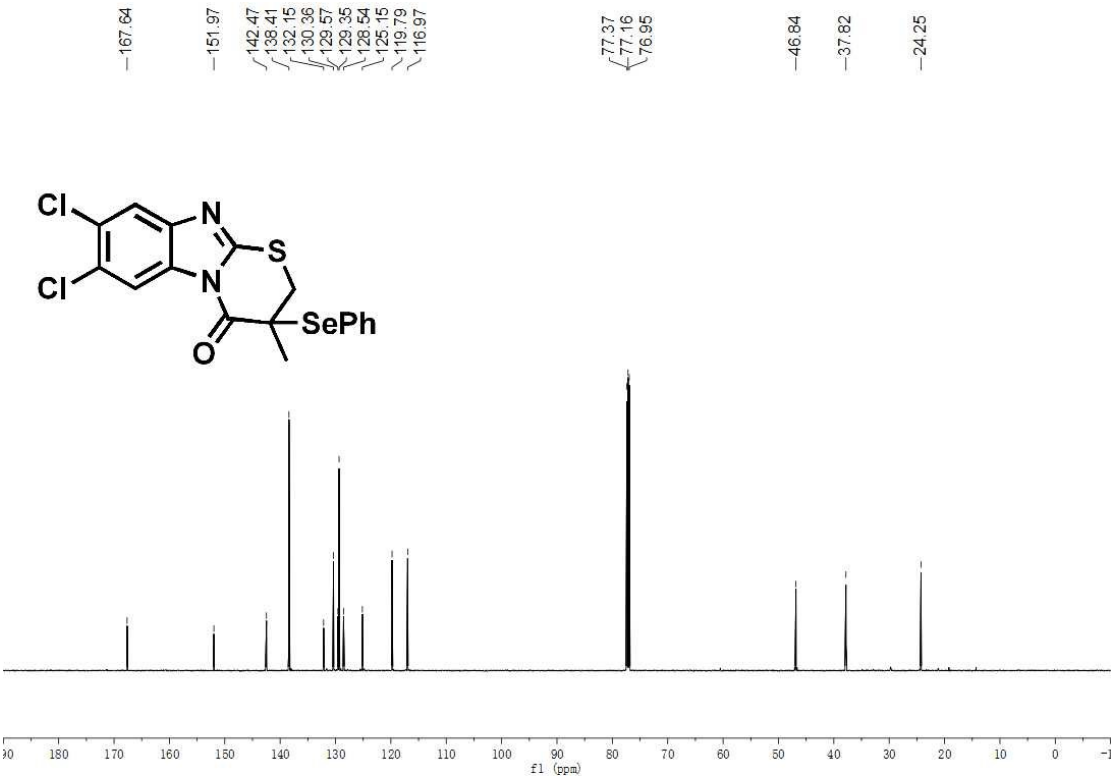


^{19}F NMR of product 5e in $CDCl_3$ (565 MHz)

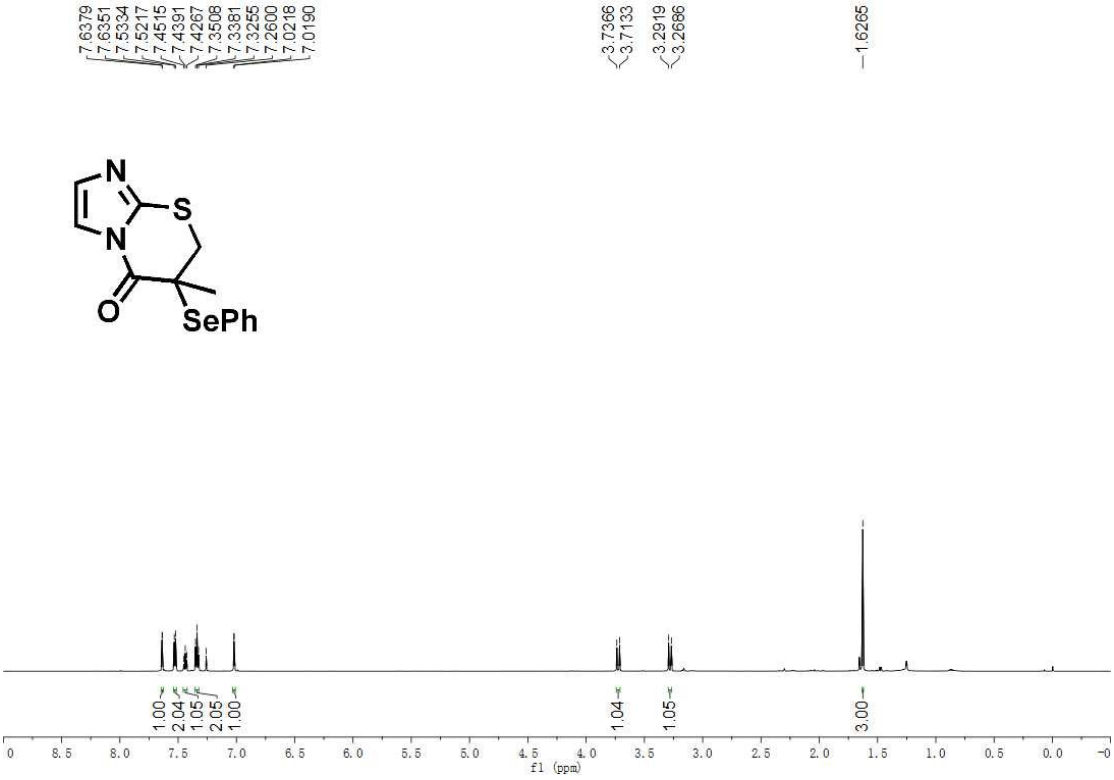
^{1}H NMR of product 5f in $CDCl_3$ (600 MHz)



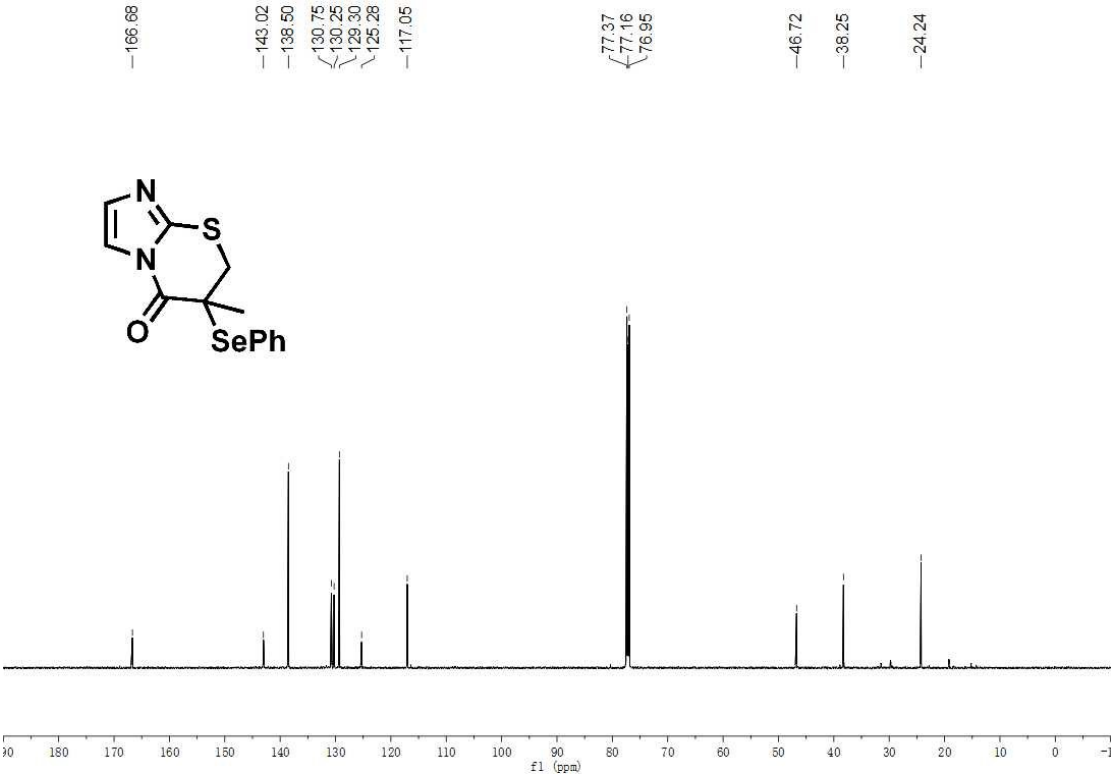
^{13}C NMR of product 5f in $CDCl_3$ (150 MHz)



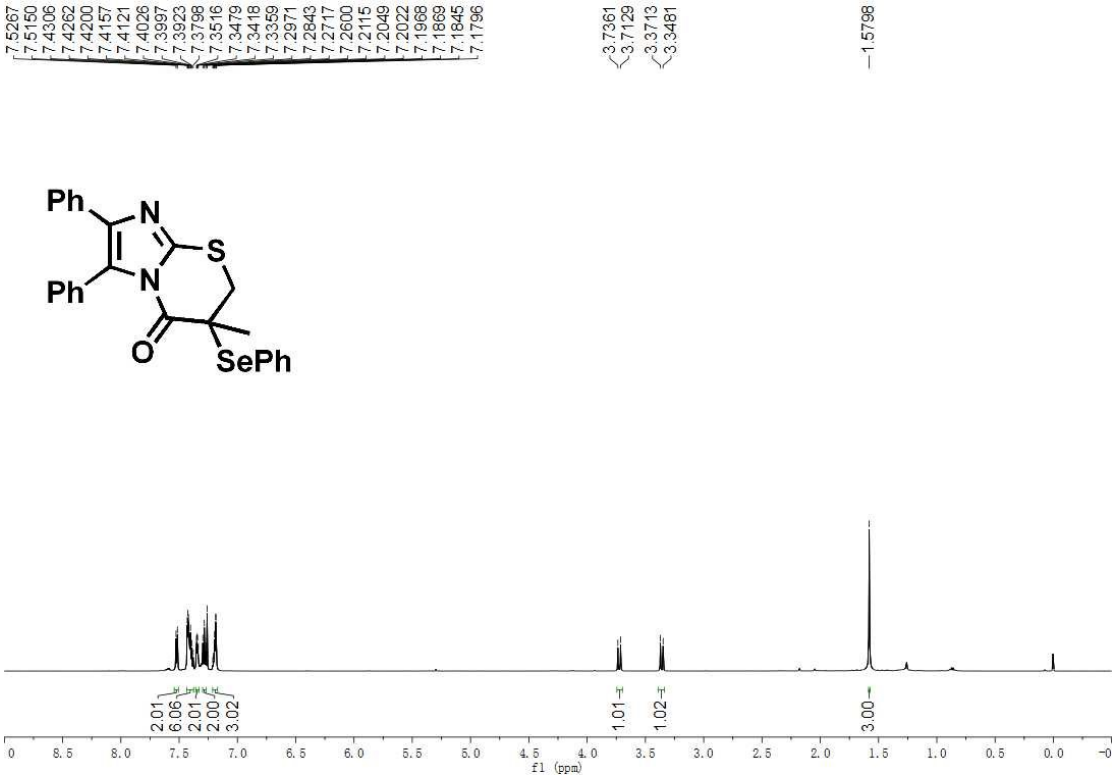
^{1}H NMR of product 5g in $CDCl_3$ (600 MHz)



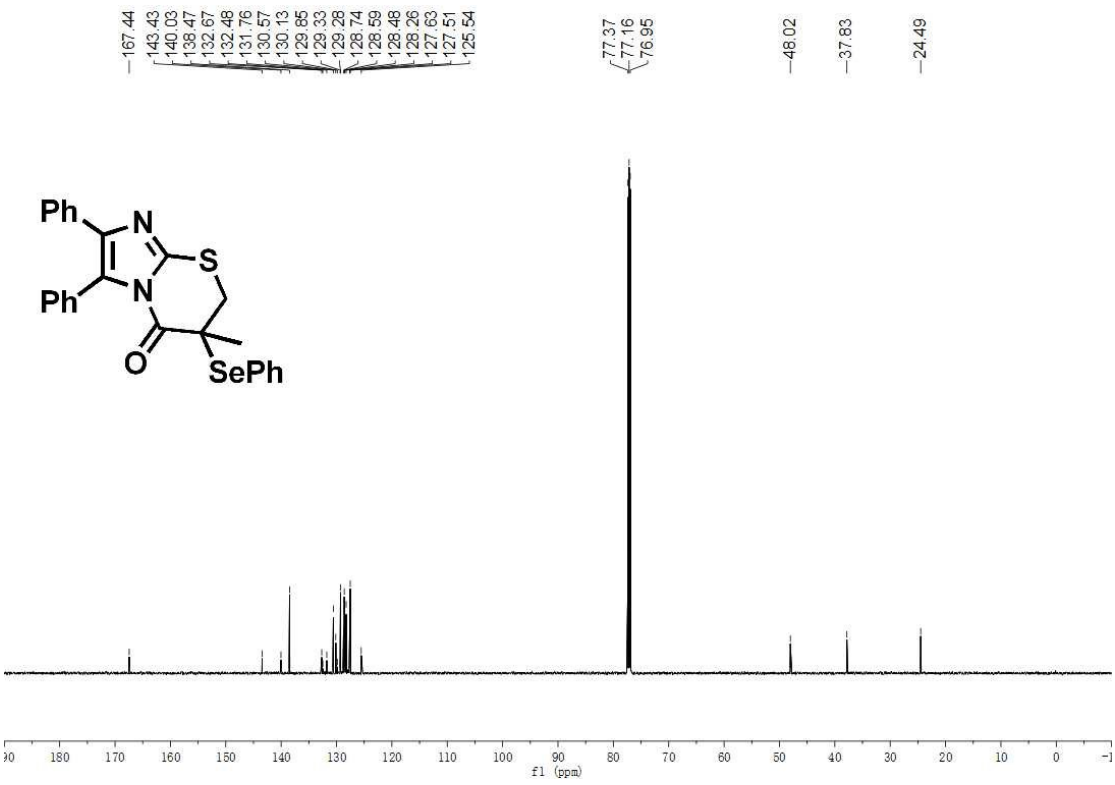
^{13}C NMR of product 5g in $CDCl_3$ (150 MHz)



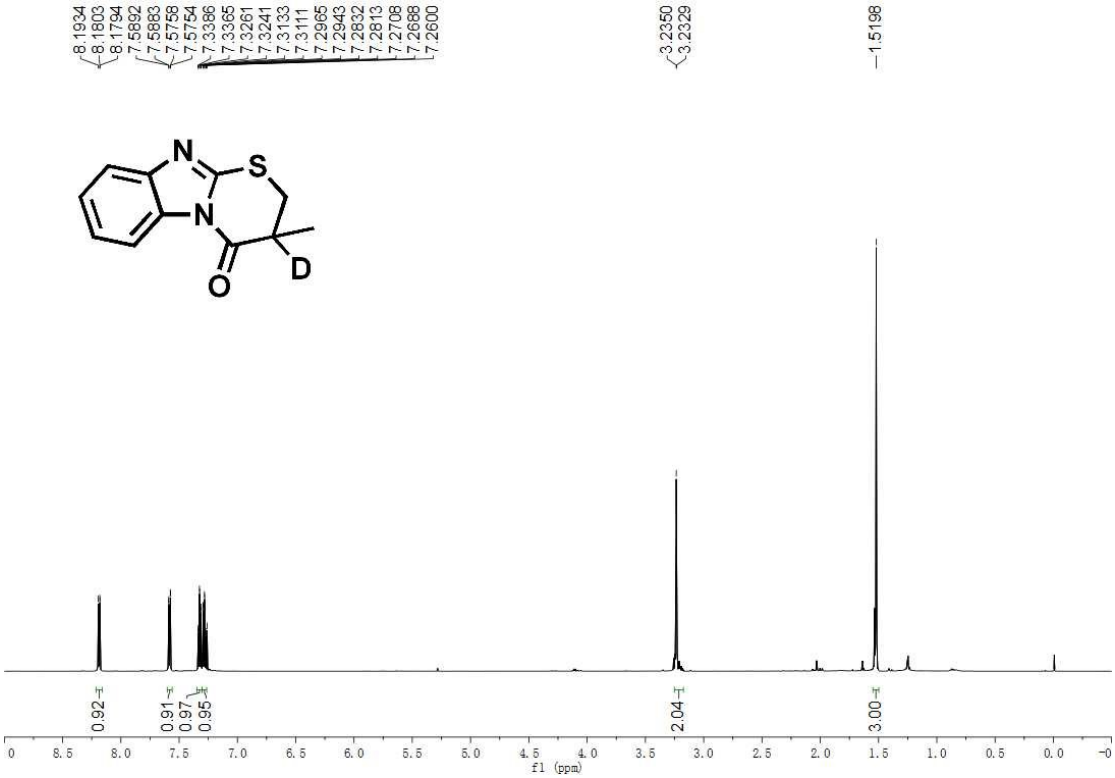
^{1}H NMR of product 5h in $CDCl_3$ (600 MHz)



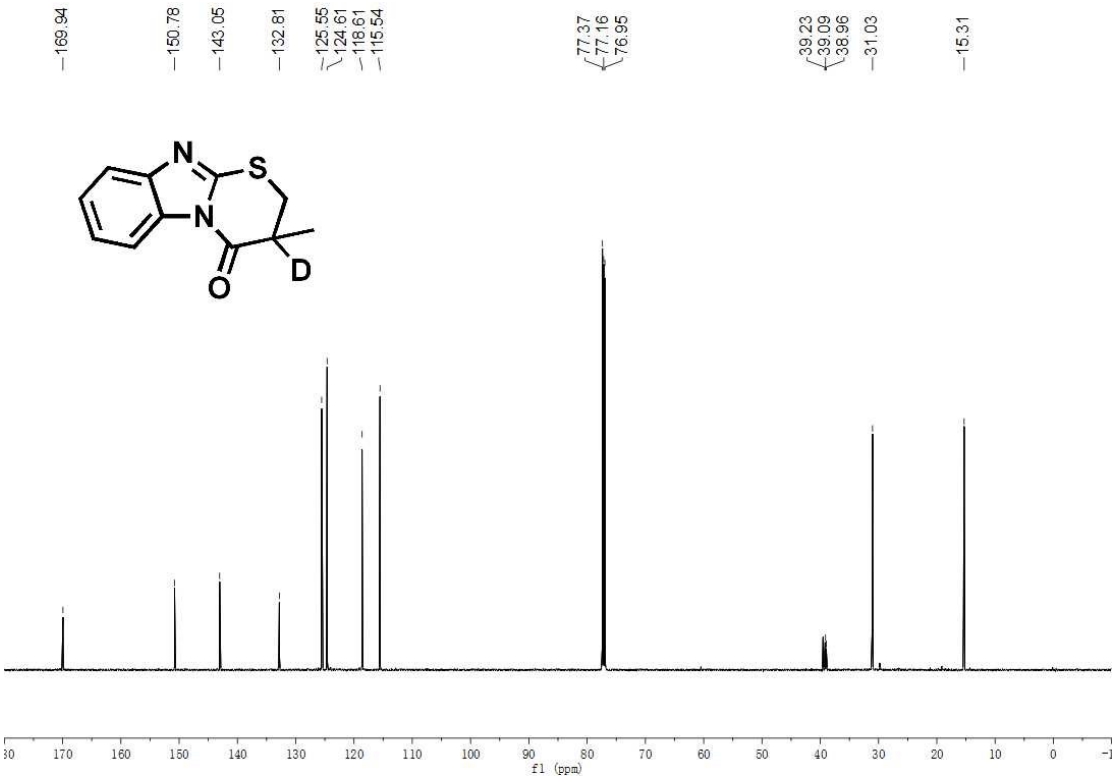
^{13}C NMR of product 5h in $CDCl_3$ (150 MHz)



^{1}H NMR of product 6-*d* in $CDCl_3$ (600 MHz)



^{13}C NMR of product 6-*d* in $CDCl_3$ (150 MHz)



7. X-Ray crystallographic data for 4a (CCDC 2321470)

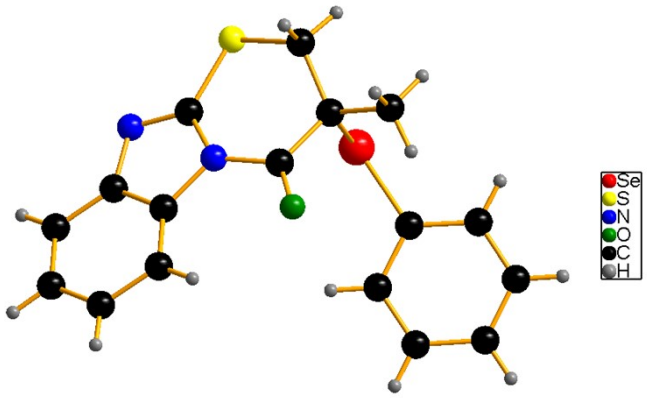
The suitable crystals were selected on a **XtaLAB Synergy**, **Dualflex**, **HyPix** diffractometer. The crystals were kept at 100.03(10) K during data collection. Using Olex2[1], the structures were solved with the ShelXT[2] structure solution program using Intrinsic Phasing and refined with the ShelXL[3] refinement package using Least Squares minimisation.

[1] Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.

[2] Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.

[3] Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Single-crystals suitable for X-ray diffraction analysis were grown from the recrystallization in EA and petroleum ether (1/1, v/v) at 25 °C. Thermal ellipsoids of the crystal structures of **4a** was set at 50%.



Identification code	CCDC 2321470
Empirical formula	$C_{17}H_{14}N_2OSSe$
Formula weight	373.32
Temperature/K	296.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.5195(10)
b/Å	8.3597(13)
c/Å	29.903(5)
α/°	90
β/°	90

γ/°	90
Volume/Å^3	1629.8(4)
Z	4
ρ_{calc}g/cm^3	1.521
μ/mm^{-1}	2.434
F(000)	752.0
Crystal size/mm^3	0.2 × 0.15 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.06 to 55.134
Index ranges	-6 ≤ h ≤ 8, -8 ≤ k ≤ 10, -35 ≤ l ≤ 37
Reflections collected	9718
Independent reflections	3689 [R_{int} = 0.0392, R_{sigma} = 0.0584]
Data/restraints/parameters	3689/0/200
Goodness-of-fit on F^2	1.121
Final R indexes [I>=2σ (I)]	R_1 = 0.0429, wR_2 = 0.0794
Final R indexes [all data]	R_1 = 0.0564, wR_2 = 0.0822
Largest diff. peak/hole / e Å^{-3}	0.45/-0.77