

Supporting Information

Electrochemical Oxidative Site-selective Direct C–H Activation of Tanshinone IIA

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General information

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. The instrument for electrolysis was dual display potentiostat (DJS-292B) (made in China). The anodic electrode was graphite rod (ϕ 6 mm) and cathodic electrode was platinum plate (15 mm \times 15 mm \times 0.3 mm). Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (boiling point was between 60-90 °C). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum to the indicated solvent, and they were listed as volume/volume ratios. NMR spectra were recorded on a Bruker spectrometer at 400 MHz (^1H NMR), 101 MHz (^{13}C NMR), 376 MHz (^{19}F NMR). Chemical shifts were reported relative to tetramethylsilane, chloroform-D (7.26 ppm for ^1H , 77.16 ppm for ^{13}C), respectively. And all ^1H , ^{13}C and ^{19}F NMR data spectra were reported in delta (δ) units, parts per million (ppm) downfield from the internal standard. Coupling constants were reported in Hertz (Hz). LC-MS spectra were recorded on AB SCIEX Triple TOF 5600⁺.

Experimental procedure

General procedure for the preparation of 2a-2y:

In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, Tanshinone IIA (0.3 mmol, 88.3 mg), diselenides **1** (0.3 mmol), $n\text{-Bu}_4\text{NBF}_4$ (0.3 mmol, 98.9 mg), MeCN (7 mL) was added. The bottle was equipped with graphite rod (ϕ 6 mm, about 15 mm immersion depth in solution) as the anode and platinum plate (15 mm \times 15 mm \times 0.3 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current of 25 mA under Ar atmosphere at room temperature for 8 h. After completion of the reaction, as indicated by TLC and LC-MS, the crude mixture product was obtained by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100: 1).

When we use diphenyl disulfide as the substrate, we slightly reduced the current to 15 mA to mitigate the risk of electrochemical degradation in the reaction system.

General procedure for the preparation of 2z-2za:

In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, Tanshinone IIA (0.3 mmol, 88.3 mg), KCl or KBr (3.0 mmol), MeCN/H₂O (6/1 mL) was added. The bottle was equipped with graphite rod (ϕ 6 mm, about 15 mm immersion depth in solution) as the anode and platinum plate (15 mm \times 15 mm \times 0.3 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current of 15 mA under Ar atmosphere at room temperature for 10 h. After completion of the reaction, as indicated by TLC and LC-MS, the crude mixture product was obtained by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 300: 1).

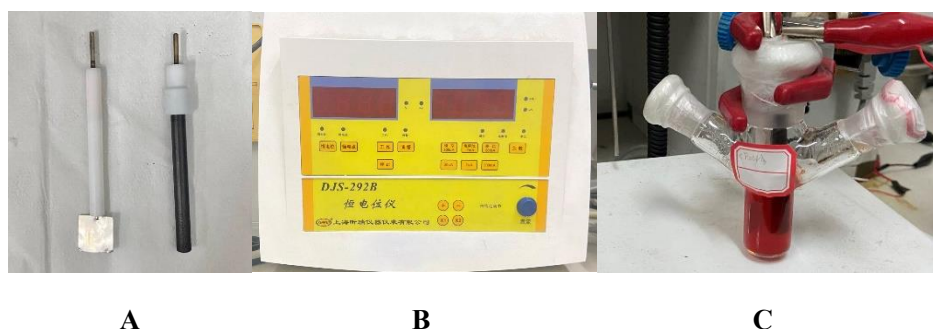


Figure S1. The experimental setup for electrolysis. (A, B, C: The electrochemical reaction apparatus used.)

Procedure for gram scale synthesis of 2a:

In an oven-dried undivided beaker (100 mL) equipped with a stir bar, Tanshinone IIA (5.0 mmol, 1471.7 mg), 1,2-diphenyldislane **1a** (5.0 mmol, 1560.7 mg), $n\text{Bu}_4\text{NBF}_4$ (5.0 mmol, 1646.0 mg), MeCN (130 mL) was added. The bottle was equipped with graphite rod (ϕ 6 mm, about 15 mm immersion depth in solution) as the anode and platinum plate (15 mm \times 15 mm \times 0.3 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current of 25 mA under Ar atmosphere at room temperature for 96 h, after completion of the reaction, as indicated by TLC and LC-MS. The pure product **2a** (yield 72%, red solid, 1.62 g) was obtained by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1).

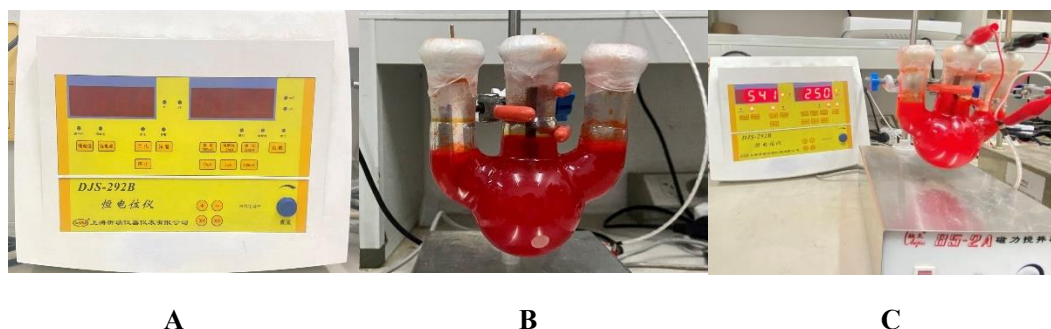
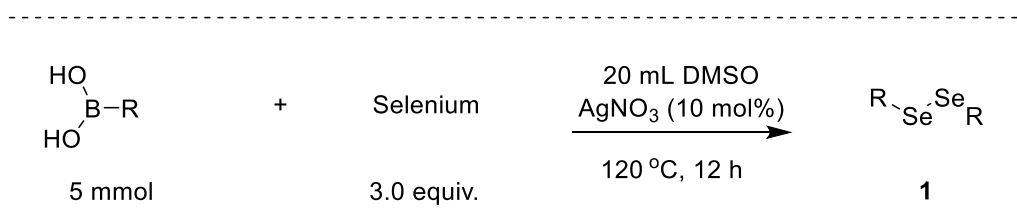


Figure S2. The experimental setup for electrolysis. (A, B, C: The electrochemical reaction apparatus used.)

General procedure for the preparation of **1**:¹



In a 25 mL schlenk flask was charged with substituted aryl boronic acid (5 mmol, 1.0 equiv.), selenium (15 mmol, 3.0 equiv.) and AgNO_3 (10 mol%), then 20 mL of dimethyl sulfoxide was added. Stir the reaction mixture at 120 °C for 12 hours. After completion of the reaction, as indicated by TLC. The contents cooled, dilute the reaction mixture with H_2O (20 mL), the resulting mixture was extracted with EtOAc (3 \times 20 mL). Wash the combined organic phase with water and brine (30 mL). Dry over anhydrous Na_2SO_4 . After remove the solvent under reduced pressure, the residue was purified by silica-gel column chromatography to give the products **1** (petroleum ether: ethyl acetate = 1000:1).

Procedure of antitumor activity of tanshinone derivatives:²

A549 Cells (5×10^3 cells/well) cultured in 96-well plates were treated with Tanshinone IIA and derivatives (10 μ M) for 24 h. After adding 100 μ L of CCK-8 mixture and culturing for another 1 h and the absorbance at 450 nm was detected using a multilabel microplate reader (Vermont, Bio Tek, USA). We found that compounds **2k**, **2q**, and **2w** showed better effects than Tanshinone IIA at a concentration of 10 μ M.

Table 1 Viability of IIA, **2a-2za** and **3a** on A549 cells at a concentration of 10 μ M.

Compound	Viability	Compound	Viability
2a	6%	2p	11%
2b	9%	2q	51%
2c	12%	2r	3%
2d	13%	2s	0%
2e	0%	2t	0%
2f	12%	2u	30%
2g	3%	2v	6%
2h	0%	2w	65%
2i	0%	2x	30%
2j	17%	2y	27%
2k	41%	2z	18%
2l	5%	2za	18%
2m	0%	3a	16%
2n	27%	Tanshinone IIA	31%
2o	9%		

To further ascertain the antitumor activity of compounds **2k**, **2q**, and **2w**, we assessed the impact of varying concentrations on A549 cells. The findings revealed that compounds **2k** (IC_{50} =19.39 μ M), **2q** (IC_{50} =13.55 μ M), and **2w** (IC_{50} =6.03 μ M) notably suppressed the proliferation of A549 cancer cells in a dose-dependent and time-dependent manner. These compounds exhibited enhanced antitumor activity relative to the parent compound, Tanshinone IIA (IC_{50} =24.57 μ M).

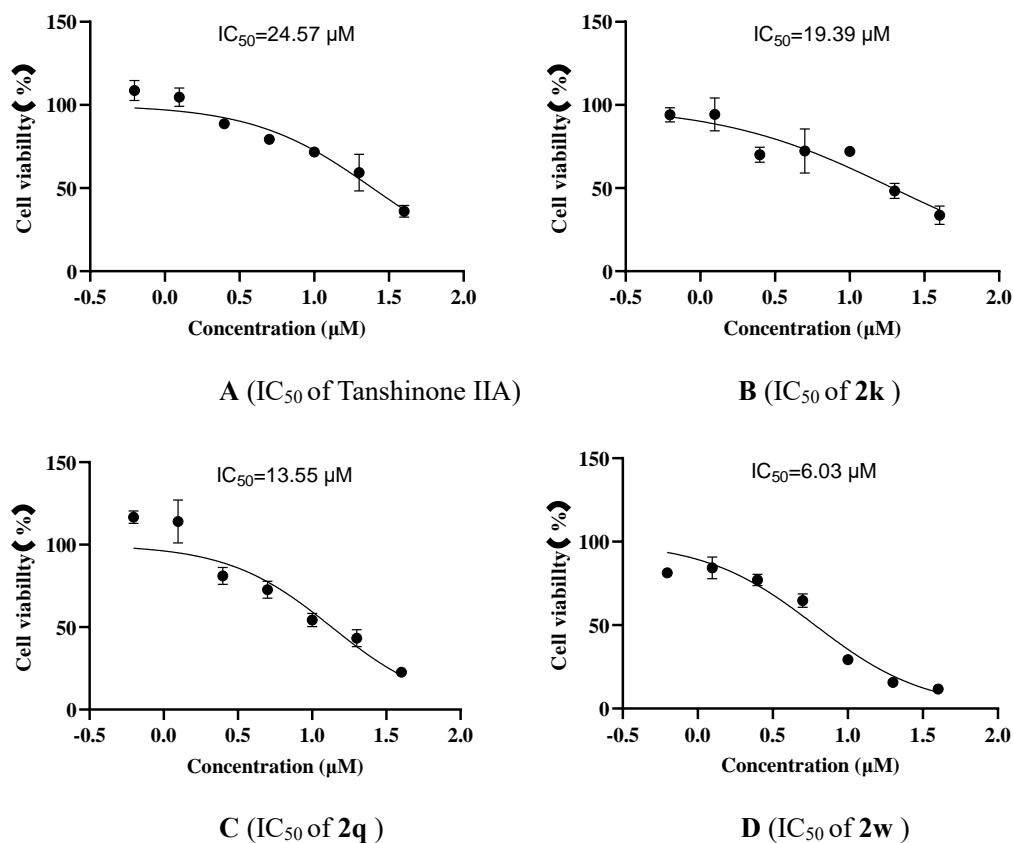
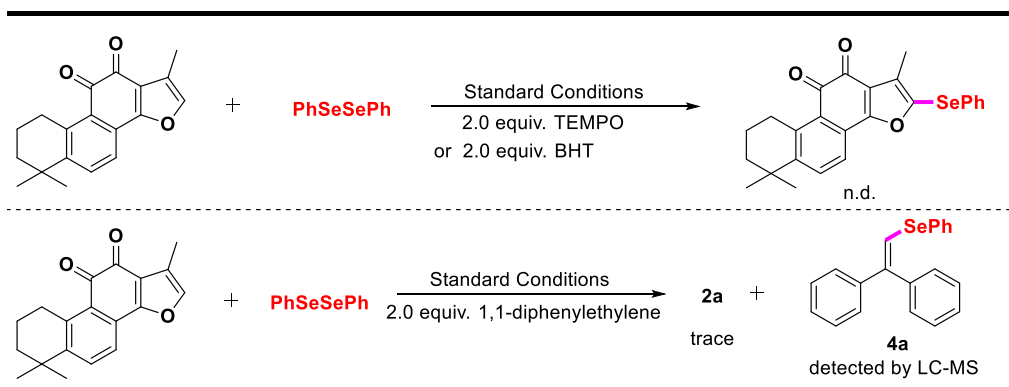


Figure S3. Cells were treated with different concentrations of tanshinone IIA, 2k, 2q 2w for 24 h, then assayed by CCK-8 method.

Mechanism research

In order to investigate the possible mechanism of this transformation, a series of control experiments were carried out. When stoichiometric amounts of radical scavengers, such as 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) or butylated hydroxytoluene (BHT) were introduced into the reaction environment, the conversion was significantly reduced. The observation of adducts **4a** indicated that the reaction likely followed a radical mechanism, potentially involving selenium radicals in the transformation.



Scheme 1. Control experiments.

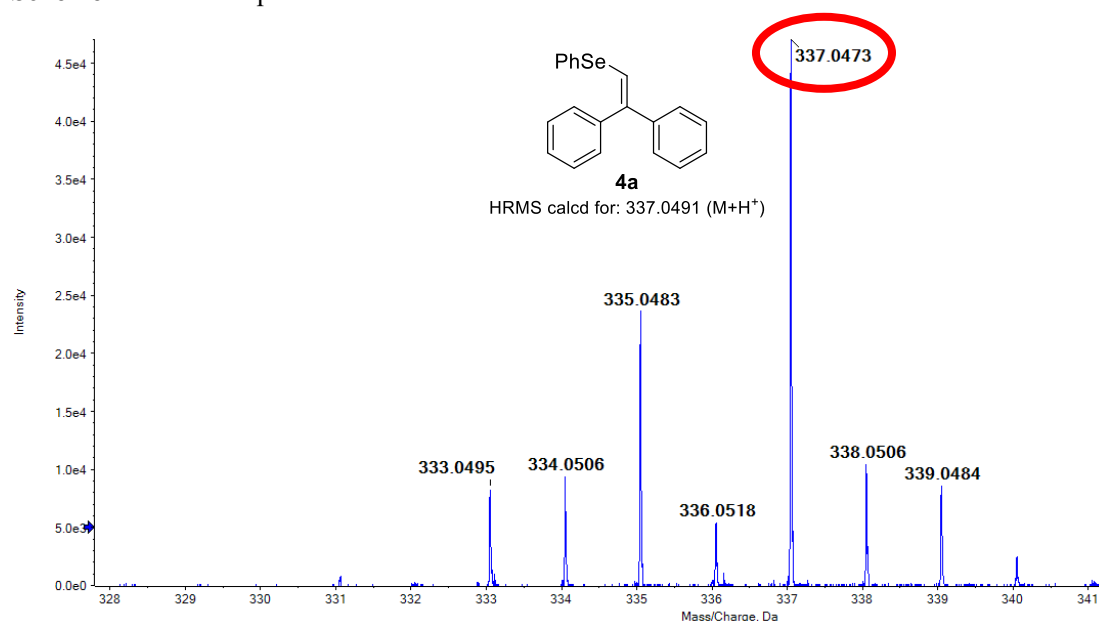


Figure S4. Free radical capture experiment (DPE-SePh)

General procedure for cyclic voltammetry (CV):

Cyclic voltammetry was performed in a three-electrode cell connected to a schlenk line under air at room temperature. The working electrode was a glassy carbon electrode, the counter electrode a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. 10 mL of CH₃CN containing 0.01 M *n*Bu₄NBF₄ were poured into the electrochemical cell in all experiments. The scan rate is 0.1 V/s, ranging from 0 V to 3.5 V. The peak potentials vs. Ag/AgCl for used. Distinct anodic peaks for Tanshinone IIA was observed at potentials of 2.29 V. Furthermore, the cyclic voltammetry curve of compound **1a** in acetonitrile displayed two oxidation peaks, located at 1.92 V and 2.82 V. These findings suggest that compound **1a** undergoes preferential oxidation at the anode within this electrochemical setup.

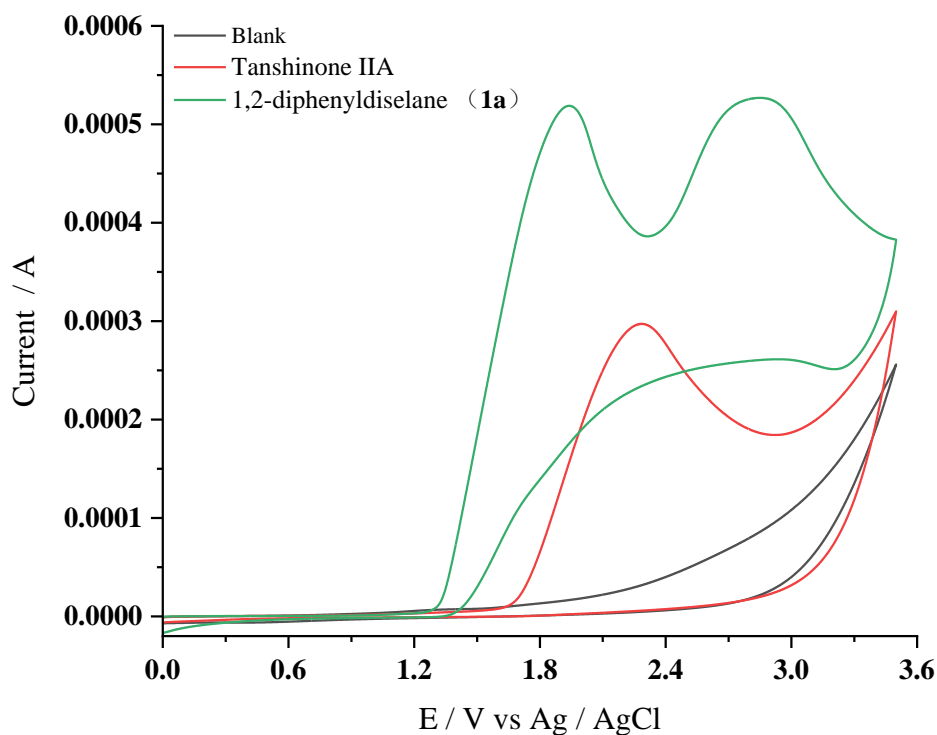
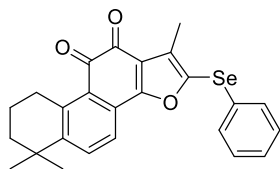


Figure S5 Cyclic voltammetry

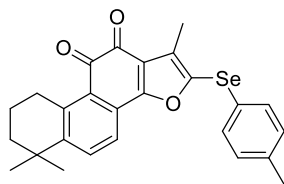
Detail descriptions for products



1,6,6-trimethyl-2-(phenylselanyl)-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2a).

(Red solid was obtained in 92% isolated yield, 124.7 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.58 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 20.0$ Hz), 7.37-7.36 (m, 2H), 7.27-7.22 (m, 3H), 3.16 (t, 2H, $J = 8.0$ Hz), 2.36 (s, 3H), 1.81-1.75 (m, 2H), 1.66-1.63 (m, 2H), 1.30 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.07, 175.04, 163.98, 150.81, 144.63, 140.93, 133.52, 130.50, 130.47, 130.26, 129.58, 127.41, 126.85, 126.66, 120.81, 120.52, 37.80, 34.74, 31.84, 29.95, 19.11, 10.91.

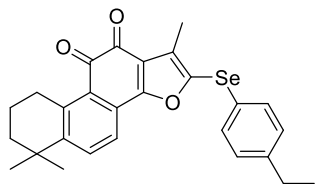
HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{22}\text{O}_3\text{Se}$: 451.0809 ($\text{M}+\text{H}^+$), found: 451.0811.



1,6,6-trimethyl-2-(p-tolylselanyl)-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2b).

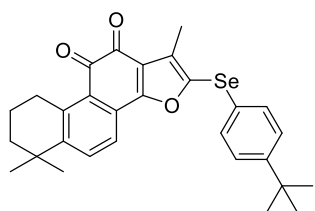
(Red solid was obtained in 59% isolated yield, 82.1 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.52 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 7.22 (d, 2H, $J = 8.0$ Hz), 7.00 (d, 2H, $J = 8.0$ Hz), 3.10 (t, 2H, $J = 8.0$ Hz), 2.29 (s, 3H), 2.22 (s, 3H), 1.75-1.70 (m, 2H), 1.59-1.56 (m, 2H), 1.23 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.17, 174.11, 162.83, 149.69, 143.58, 140.42, 136.61, 132.47, 130.10, 129.31, 128.66, 125.90, 125.63, 125.45, 119.76, 119.49, 36.77, 33.69, 30.80, 28.91, 20.03, 18.07, 9.85.

HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{24}\text{O}_3\text{Se}$: 465.0965 ($\text{M}+\text{H}^+$), found: 465.0954.



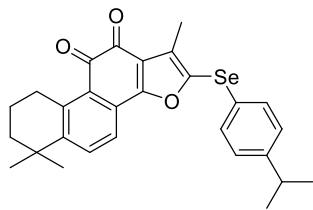
2-((4-ethylphenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2c). (Red solid was obtained in 33% isolated yield, 47.6 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.62 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 7.32 (d, 2H, $J = 8.0$ Hz), 7.10 (d, 2H, $J = 8.0$ Hz), 3.18 (t, 2H, $J = 8.0$ Hz), 2.60 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 2.37 (s, 3H), 1.81-1.78 (m, 2H), 1.67-1.64 (m, 2H), 1.30 (s, 6H), 1.20 (t, 3H, $J = 8.0$ Hz); ^{13}C NMR (101 MHz, CDCl_3) δ 183.23, 175.16, 163.90, 150.73, 144.62, 143.97, 141.42, 133.51, 132.22, 131.12, 129.79, 129.19, 126.96, 126.77, 126.68, 120.82, 120.53, 37.81, 34.73, 31.84, 29.95, 28.45, 19.11, 15.45, 10.89.

HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{26}\text{O}_3\text{Se}$: 501.0941 ($\text{M}+\text{Na}^+$), found: 501.0934.



2-((4-(tert-butyl)phenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2d). (Red solid was obtained in 32% isolated yield, 47.8 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.63 (t, 2H, $J = 8.0$ Hz), 7.31 (q, 4H, $J_1 = 8.0$ Hz, $J_2 = 16.0$ Hz), 3.18 (t, 2H, $J = 8.0$ Hz), 2.38 (s, 3H), 1.82-1.76 (m, 2H), 1.67-1.65 (m, 2H), 1.31 (s, 6H), 1.28 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.25, 175.18, 163.93, 150.83, 150.74, 144.63, 141.29, 133.52, 130.65, 129.96, 128.86, 126.96, 126.74, 126.69, 120.83, 120.53, 37.81, 34.73, 34.57, 31.84, 31.21, 29.95, 19.11, 10.94.

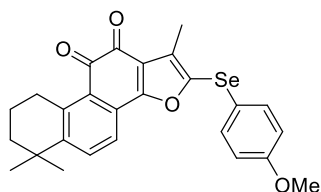
HRMS (ESI) calcd for $\text{C}_{29}\text{H}_{30}\text{O}_3\text{Se}$: 529.1255 ($\text{M}+\text{Na}^+$), found: 529.1267.



2-((4-isopropylphenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-

10,11-dione (2e). (Red solid was obtained in 54% isolated yield, 79.8 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.60 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 7.32 (d, 2H, $J = 8.0$ Hz), 7.12 (d, 2H, $J = 8.0$ Hz), 3.17 (t, 2H, $J = 8.0$ Hz), 2.90-2.80 (m, 1H), 2.37 (s, 3H), 1.80-1.77 (m, 2H), 1.67-1.64 (m, 2H), 1.30 (s, 6H), 1.21 (s, 3H), 1.20 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.18, 175.11, 163.87, 150.73, 148.58, 144.61, 141.39, 133.51, 131.06, 129.85, 127.78, 126.93, 126.91, 126.66, 120.81, 120.53, 37.81, 34.73, 33.76, 31.84, 29.95, 23.87, 19.11, 10.93.

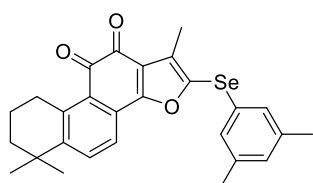
HRMS (ESI) calcd for $\text{C}_{28}\text{H}_{28}\text{O}_3\text{Se}$: 493.1278 ($\text{M}+\text{H}^+$), found: 493.1275.



2-((4-methoxyphenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-

10,11-dione (2f). (Red solid was obtained in 32% isolated yield, 33.3 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.61 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 7.44-7.40 (m, 2H), 6.83-6.79 (m, 2H), 3.77 (s, 3H), 3.17 (t, 2H, $J = 8.0$ Hz), 2.37 (s, 3H), 1.82-1.77 (m, 2H), 1.66-1.64 (m, 2H), 1.30 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.24, 175.17, 163.69, 159.65, 150.66, 144.61, 142.09, 133.78, 133.51, 128.94, 126.98, 126.64, 120.76, 120.52, 119.93, 115.21, 55.35, 37.80, 34.72, 31.85, 29.95, 19.10, 10.90.

HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{24}\text{O}_4\text{Se}$: 481.0914 ($\text{M}+\text{H}^+$), found: 481.0901.

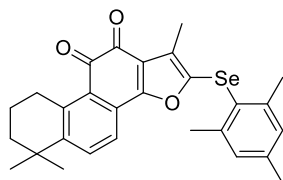


2-((3,5-dimethylphenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-

10,11-dione (2g). (Red solid was obtained in 33% isolated yield, 46.7 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.62 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 8.0$ Hz), 6.98 (s, 2H), 6.87 (s, 1H), 3.18 (t, 2H, $J = 8.0$ Hz),

2.37 (s, 3H), 2.25 (s, 6H), 1.83-1.77 (m, 2H), 1.67-1.64 (m, 2H), 1.31 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.25, 175.20, 163.99, 150.74, 144.64, 141.15, 139.31, 133.54, 130.14, 129.90, 129.31, 128.09, 126.97, 126.69, 120.86, 120.55, 37.81, 34.74, 31.85, 29.98, 21.28, 19.11, 10.97.

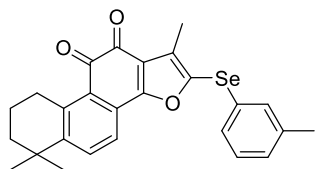
HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{26}\text{O}_3\text{Se}$: 479.1121 ($\text{M}+\text{H}^+$), found: 479.1117.



2-((4-methoxyphenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-

10,11-dione (2h). (Red solid was obtained in 41% isolated yield, 59.7 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.50 (d, 1H, $J = 8.0$ Hz), 7.35 (d, 1H, $J = 8.0$ Hz), 6.84 (s, 2H), 3.06 (t, 2H, $J = 8.0$ Hz), 2.50 (s, 6H), 2.21 (s, 3H), 2.16 (s, 3H), 1.72-1.66 (m, 2H), 1.57-1.54 (m, 2H), 1.20 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.17, 174.00, 162.11, 149.30, 143.42, 141.65, 141.12, 138.17, 132.39, 127.98, 125.98, 125.70, 125.56, 125.35, 119.36, 119.33, 36.75, 33.62, 30.78, 28.84, 23.50, 19.90, 18.05, 9.65.

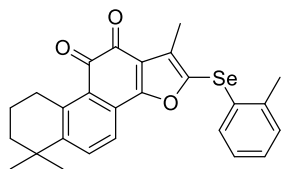
HRMS (ESI) calcd for $\text{C}_{28}\text{H}_{28}\text{O}_3\text{Se}$: 493.1278 ($\text{M}+\text{H}^+$), found: 493.1265.



1,6,6-trimethyl-2-(m-tolylselanyl)-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2i).

(Red solid was obtained in 42% isolated yield, 58.1 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.54 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 16.0$ Hz), 7.13-7.06 (m, 2H), 7.03 (d, 1H, $J = 8.0$ Hz), 6.98-6.94 (m, 1H), 3.12 (t, 2H, $J = 8.0$ Hz), 2.39 (s, 3H), 2.28 (s, 3H), 1.74-1.71 (m, 2H), 1.60-1.57 (m, 2H), 1.23 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.16, 174.09, 163.23, 149.80, 143.64, 139.03, 136.53, 132.51, 130.32, 129.74, 129.53, 129.10, 126.35, 126.02, 125.87, 125.65, 119.79, 119.54, 36.77, 33.71, 30.80, 28.92, 20.68, 18.07, 9.82.

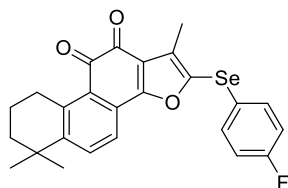
HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{24}\text{O}_3\text{Se}$: 465.0965 ($\text{M}+\text{H}^+$), found: 465.0962.



1,6,6-trimethyl-2-(o-tolylselanyl)-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2j).

(Red solid was obtained in 33% isolated yield, 46.0 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.54 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 7.12 (s, 1H), 7.08-7.04 (m, 2H), 6.99-6.96 (m, 1H), 3.11 (t, 2H, $J = 8.0$ Hz), 2.30 (s, 3H), 2.22 (s, 3H), 1.75-1.70 (m, 2H), 1.59-1.57 (m, 2H), 1.23 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.15, 174.11, 162.95, 149.74, 143.60, 140.01, 138.48, 132.49, 130.00, 129.13, 128.33, 127.25, 126.57, 126.51, 125.88, 125.65, 119.79, 119.50, 36.77, 33.70, 30.80, 28.91, 20.35, 18.06, 9.88.

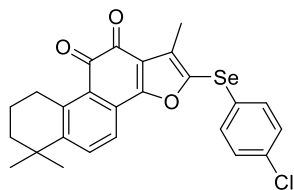
HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{24}\text{O}_3\text{Se}$: 465.0965 ($\text{M}+\text{H}^+$), found: 465.0956.



2-((4-fluorophenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-

dione (2k). (Red solid was obtained in 77% isolated yield, 107.8 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.53 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 20.0$ Hz), 7.35-7.30 (m, 2H), 6.89 (t, 2H, $J = 8.0$ Hz), 3.09 (t, 2H, $J = 8.0$ Hz), 2.29 (s, 3H), 1.74-1.69 (m, 2H), 1.59-1.56 (m, 2H), 1.22 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 181.98, 173.99, 162.89, 161.49 (d, $J = 249.47$ Hz), 149.84, 143.64, 140.06, 132.49, 132.22 (d, $J = 8.08$ Hz), 128.79, 125.75, 125.63, 123.60, 123.57, 119.72, 115.72 (d, $J = 22.2$ Hz), 36.74, 33.70, 30.79, 28.90, 18.04, 9.83. ^{19}F NMR (376 MHz, CDCl_3) δ -113.77.

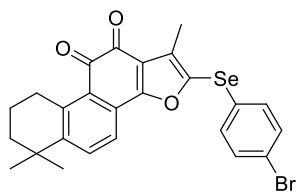
HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{21}\text{O}_3\text{FSe}$: 469.0714 ($\text{M}+\text{H}^+$), found: 469.0713.



2-((4-chlorophenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-

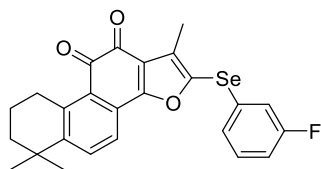
dione (2l). (Red solid was obtained in 91% isolated yield, 131.5 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.55 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 16.0$ Hz), 7.25-7.22 (m, 2H), 7.18-7.14 (m, 2H), 3.11 (t, 2H, $J = 8.0$ Hz), 2.30 (s, 3H), 1.74-1.70 (m, 2H), 1.60-1.58 (m, 2H), 1.24 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.04, 174.06, 163.13, 149.96, 143.72, 139.39, 132.73, 132.53, 130.91, 129.41, 128.69, 127.50, 125.73, 125.71, 119.80, 119.44, 36.75, 33.73, 30.80, 28.93, 18.06, 9.85.

HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{21}\text{O}_3\text{ClSe}$: 485.0416 ($\text{M}+\text{H}^+$), found: 485.0417.



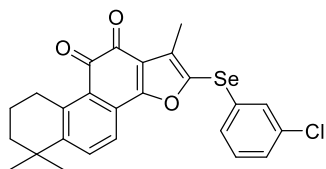
2-((4-bromophenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2m). (Red solid was obtained in 79% isolated yield, 125.5 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.55 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 16.0$ Hz), 7.25-7.22 (m, 2H), 7.18-7.14 (m, 2H), 3.11 (t, 2H, $J = 8.0$ Hz), 2.30 (s, 3H), 1.74-1.70 (m, 2H), 1.60-1.58 (m, 2H), 1.24 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.01, 174.04, 163.15, 149.97, 143.72, 139.23, 132.53, 131.60, 131.29, 131.08, 131.01, 129.51, 128.27, 125.71, 119.80, 119.43, 36.75, 33.73, 30.80, 28.93, 18.05, 9.85.

HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{21}\text{O}_3\text{BrSe}$: 528.9911 ($\text{M}+\text{H}^+$), found: 528.9904.



2-((3-fluorophenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2n). (Red solid was obtained in 44% isolated yield, 61.9 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.62 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 16.0$ Hz), 7.25-7.20 (m, 1H), 7.11 (d, 1H, $J = 8.0$ Hz), 7.04-7.01 (m, 1H), 6.95-6.90 (m, 1H), 3.18 (t, 2H, $J = 8.0$ Hz), 2.37 (s, 3H), 1.81-1.78 (m, 2H), 1.67-1.64 (m, 2H), 1.31 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.93, 174.98, 162.99 (d, $J = 254.52$ Hz), 151.03, 144.74, 140.00, 133.56, 132.32 (d, $J = 7.07$ Hz), 130.98, 130.85, 130.76, 126.72, 125.65, 125.62, 120.85, 120.46, 117.12 (d, $J = 23.23$ Hz), 114.42 (d, $J = 21.21$ Hz), 37.78, 34.76, 31.83, 29.96, 19.09, 10.89. ^{19}F NMR (376 MHz, CDCl_3) δ -110.80.

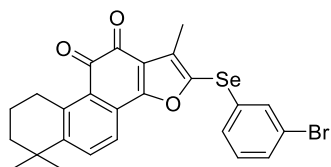
HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{21}\text{O}_3\text{FSe}$: 469.0714 ($\text{M}+\text{H}^+$), found: 469.0710.



2-((3-chlorophenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2o). (Red solid was obtained in 25% isolated yield, 36.8 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.62 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 7.32 (d, 1H, $J = 4.0$ Hz), 7.24-7.16 (m, 3H), 3.19 (t, 2H, J

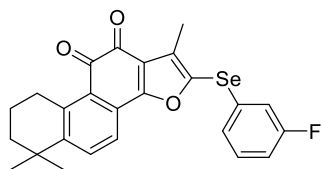
= 8.0 Hz), 2.38 (s, 3H), 1.83-1.78 (m, 2H), 1.67-1.65 (m, 2H), 1.31 (s, 6H) ; ^{13}C NMR (101 MHz, CDCl_3) δ 183.03, 175.08, 164.29, 151.04, 144.75, 139.95, 135.30, 133.57, 132.11, 130.97, 130.54, 129.95, 128.26, 127.61, 126.78, 126.74, 120.88, 120.48, 37.79, 34.77, 31.84, 29.97, 19.09, 10.92.

HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{21}\text{O}_3\text{ClSe}$: 485.0416 ($\text{M}+\text{H}^+$), found: 485.0417.



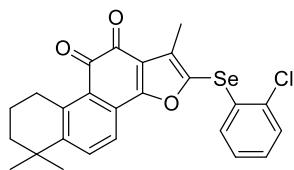
2-((3-bromophenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2p). (Red solid was obtained in 29% isolated yield, 45.8 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.62 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 7.49 (d, 1H, $J = 8.0$ Hz), 7.37 (d, 1H, $J = 8.0$ Hz), 7.28-7.25 (m, 1H), 7.12 (t, 1H, $J = 8.0$ Hz), 3.18 (t, 2H, $J = 8.0$ Hz), 2.38 (s, 3H), 1.83-1.78 (m, 2H), 1.67-1.64 (m, 2H), 1.31 (s, 6H) ; ^{13}C NMR (101 MHz, CDCl_3) δ 183.00, 175.04, 164.28, 151.04, 144.75, 139.98, 133.58, 132.77, 132.40, 130.94, 130.87, 130.51, 128.77, 126.75, 126.72, 123.41, 120.88, 120.47, 37.79, 34.76, 31.84, 29.97, 19.09, 10.94.

HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{21}\text{O}_3\text{BrSe}$: 528.9911 ($\text{M}+\text{H}^+$), found: 528.9907.



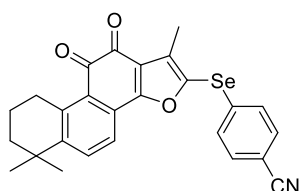
2-((2-fluorophenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2q). (Red solid was obtained in 41% isolated yield, 57.0 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.61 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 16.0$ Hz), 7.24-7.20 (m, 1H), 7.15-7.11 (m, 1H), 7.06 (t, 1H, $J = 8.0$ Hz), 7.01 (t, 1H, $J = 8.0$ Hz), 3.18 (t, 2H, $J = 8.0$ Hz), 2.37 (s, 3H), 1.81-1.78 (m, 2H), 1.67-1.64 (m, 2H), 1.31 (s, 6H) ; ^{13}C NMR (101 MHz, CDCl_3) δ 182.98, 174.97, 164.34, 160.32 (d, $J = 245.43$ Hz), 150.98, 144.69, 141.31, 138.58, 133.56, 131.80, 129.36 (d, $J = 7.07$ Hz), 126.74, 125.23, 125.20, 120.85, 120.23, 117.37 (d, $J = 22.22$ Hz), 115.85 (d, $J = 22.22$ Hz), 37.78, 34.75, 31.84, 29.95, 19.09, 10.86. ^{19}F NMR (376 MHz, CDCl_3) δ -105.75.

HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{21}\text{O}_3\text{FSe}$: 469.0714 ($\text{M}+\text{H}^+$), found: 469.0710.



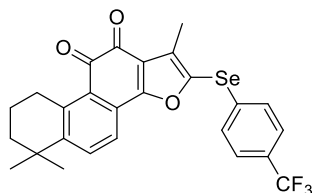
2-((2-chlorophenyl)selanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2r). (Red solid was obtained in 21% isolated yield, 30.5 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.65 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 7.35 (d, 1H, $J = 8.0$ Hz), 7.16 (t, 1H, $J = 8.0$ Hz), 7.08 (t, 1H, $J = 8.0$ Hz), 6.87 (d, 1H, $J = 8.0$ Hz) 3.20 (t, 2H, $J = 8.0$ Hz), 2.37 (s, 3H), 1.82-1.79 (m, 2H), 1.68-1.65 (m, 2H), 1.31 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.06, 175.07, 164.79, 151.14, 144.79, 139.11, 133.62, 132.59, 132.45, 131.79, 129.80, 129.10, 127.87, 127.77, 126.79, 126.73, 120.95, 120.55, 37.79, 34.79, 31.84, 29.98, 19.10, 10.87.

HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{21}\text{O}_3\text{ClSe}$: 485.0416 ($\text{M}+\text{H}^+$), found: 485.0398.



4-((1,6,6-trimethyl-10,11-dioxo-6,7,8,9,10,11-hexahydrophenanthro[1,2-b]furan-2-yl)selanyl)benzonitrile (2s). (Red solid was obtained in 30% isolated yield, 42.7 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.63 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 20.0$ Hz), 7.51 (d, 2H, $J = 12.0$ Hz), 7.36 (d, 2H, $J = 8.0$ Hz), 3.20 (t, 2H, $J = 8.0$ Hz), 2.38 (s, 3H), 1.84-1.78 (m, 2H), 1.68-1.65 (m, 2H), 1.32 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.84, 174.97, 164.69, 151.36, 144.92, 138.53, 138.35, 133.63, 132.85, 132.06, 129.46, 126.82, 126.52, 120.90, 120.44, 118.38, 110.69, 37.75, 34.81, 31.84, 29.99, 19.07, 10.89.

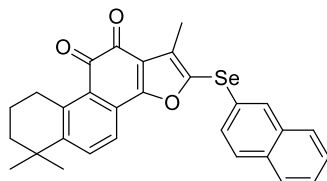
HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{21}\text{NOSe}$: 476.0761 ($\text{M}+\text{H}^+$), found: 476.0759.



1,6,6-trimethyl-2-((4-(trifluoromethyl)phenyl)selanyl)-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2t). (Red solid was obtained in 46% isolated yield, 71.1 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.63 (q, 2H, $J_1 = 12.0$ Hz, $J_2 = 16.0$ Hz), 7.50 (d, 2H, $J = 8.0$ Hz), 7.41 (d, 2H, $J =$

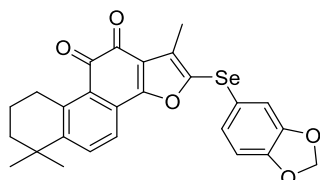
8.0 Hz), 3.19 (t, 2H, $J = 8.0$ Hz), 2.38 (s, 3H), 1.83-1.79 (m, 2H), 1.68-1.65 (m, 2H), 1.31 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.91, 174.99, 164.45, 151.18, 144.82, 139.34, 135.91, 133.59, 131.45, 129.67, 129.44 (q, $J_1 = 32.3$ Hz, $J_2 = 65.6$ Hz), 126.77, 126.63, 126.32 (q, $J_1 = 4.0$ Hz, $J_2 = 8.1$ Hz), 123.90 (q, $J_1 = 272.7$ Hz, $J_2 = 546.4$ Hz), 120.87, 120.46, 37.76, 34.78, 31.83, 29.97, 19.08, 10.90. ^{19}F NMR (376 MHz, CDCl_3) δ -62.69.

HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{21}\text{O}_3\text{F}_3\text{Se}$: 519.0683 ($\text{M}+\text{H}^+$), found: 519.0677.



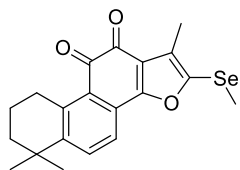
1,6,6-trimethyl-2-(naphthalen-2-ylselanyl)-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2u). (Red solid was obtained in 67% isolated yield, 100.5 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.85 (s, 1H), 7.76-7.74 (m, 1H), 7.70 (d, 2H, $J = 8.0$ Hz), 7.60-7.57 (m, 2H), 7.47-7.43 (m, 2H), 7.40 (d, 1H, $J = 8.0$ Hz), 3.16 (t, 2H, $J = 8.0$ Hz), 2.40 (s, 3H), 1.79-1.76 (m, 2H), 1.65-1.62 (m, 2H), 1.29 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.06, 175.06, 164.03, 150.81, 144.62, 141.30, 140.92, 133.94, 133.50, 132.35, 130.31, 129.43, 129.15, 127.92, 127.83, 127.71, 127.31, 126.84, 126.79, 126.66, 126.35, 120.82, 37.80, 34.73, 31.83, 29.95, 19.10, 10.95.

HRMS (ESI) calcd for $\text{C}_{29}\text{H}_{24}\text{O}_3\text{Se}$: 501.0966 ($\text{M}+\text{H}^+$), found: 501.0967.



2-(benzo[d][1,3]dioxol-5-ylselanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2v). (Red solid was obtained in 33% isolated yield, 48.3 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.62 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 8.0$ Hz), 6.98 (dd, 1H, $J_1 = 4.0$ Hz, $J_2 = 8.0$ Hz), 6.92 (s, 1H), 6.72 (d, 1H, $J = 8.0$ Hz), 5.94 (s, 2H), 3.17 (t, 2H, $J = 8.0$ Hz), 2.37 (s, 3H), 1.81-1.78 (m, 2H), 1.67-1.64 (m, 2H), 1.30 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.06, 175.06, 164.03, 150.81, 144.62, 141.30, 140.92, 133.94, 133.50, 132.35, 130.31, 129.43, 129.15, 127.92, 127.83, 127.71, 127.31, 126.84, 126.79, 126.66, 126.35, 120.82, 37.80, 34.73, 31.83, 29.95, 19.10, 10.95.

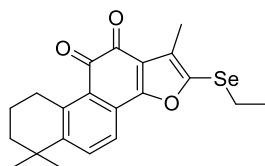
HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{22}\text{O}_5\text{Se}$: 495.0707 ($\text{M}+\text{H}^+$), found: 495.0708.



1,6,6-trimethyl-2-(methyiselanyl)-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2w).

(Red solid was obtained in 59% isolated yield, 68.3 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.54 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 16.0$ Hz), 3.10 (t, 2H, $J = 8.0$ Hz), 2.23 (d, 6H, $J = 8.0$ Hz), 1.73-1.70 (m, 2H), 1.60-1.57 (m, 2H), 1.24 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.28, 175.11, 163.40, 150.47, 144.56, 141.65, 133.48, 127.49, 127.04, 126.48, 120.53, 120.24, 37.82, 34.70, 31.84, 29.93, 19.11, 10.70, 9.17.

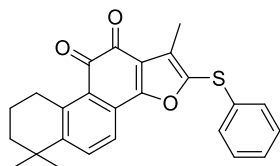
HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{20}\text{O}_3\text{Se}$: 389.0652 ($\text{M}+\text{H}^+$), found: 389.0653.



2-(ethyiselanyl)-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2x).

(Red solid was obtained in 87% isolated yield, 104.3 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.63 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 12.0$ Hz), 3.18 (t, 2H, $J = 8.0$ Hz), 2.84 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 16.0$ Hz), 2.33 (s, 3H), 1.83-1.77 (m, 2H), 1.67-1.64 (m, 2H), 1.44 (t, 3H, $J = 8.0$ Hz), 1.31 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 183.37, 175.19, 163.62, 150.51, 144.57, 141.17, 133.49, 128.92, 127.09, 126.54, 120.61, 120.50, 37.83, 34.71, 31.85, 29.94, 23.33, 19.11, 16.10, 10.90.

HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{22}\text{O}_3\text{Se}$: 403.0808 ($\text{M}+\text{H}^+$), found: 403.0810.

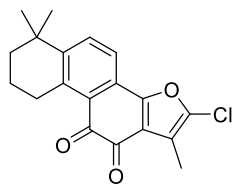


1,6,6-trimethyl-2-(phenylthio)-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2y).

(Red solid was obtained in 36% isolated yield, 43.1 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.55 (q, 2H, $J_1 = 8.0$ Hz, $J_2 = 20.0$ Hz), 7.21-7.19 (m, 2H), 7.16-7.12 (m, 3H), 3.12 (t, 2H, $J = 8.0$ Hz), 2.31 (s, 3H), 1.75-1.69 (m, 2H), 1.60-1.57 (m, 2H), 1.23 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.04, 174.10, 162.12, 149.97, 143.68, 143.01, 133.77, 132.52, 128.67, 128.34, 126.74, 125.87, 125.83,

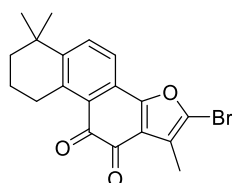
125.77, 119.89, 119.61, 36.76, 33.73, 30.80, 28.93, 18.06, 9.24.

HRMS (ESI) calcd for C₂₅H₂₂O₃S: 403.1362 (M+H⁺), found: 403.1372.



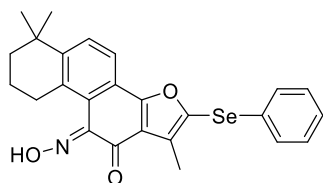
2-chloro-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2z). (Red solid was obtained in 41% isolated yield, 40.1 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.63 (d, 1H, *J* = 8.0 Hz), 7.51 (d, 1H, *J* = 8.0 Hz), 3.16 (t, 2H, *J* = 8.0 Hz), 2.22 (s, 3H), 1.83-1.77 (m, 2H), 1.67-1.64 (m, 2H), 1.31 (s, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 182.61, 174.80, 159.62, 150.60, 144.91, 137.10, 133.61, 126.54, 126.36, 120.64, 120.18, 115.83, 37.77, 34.72, 31.81, 29.98, 19.06, 8.60.

HRMS (ESI) calcd for C₁₉H₁₇ClO₃: 329.0939 (M+H⁺), found: 329.0942.



2-bromo-1,6,6-trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione (2za). (Red solid was obtained in 65% isolated yield, 72.2 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.55 (d, 1H, *J* = 8.0 Hz), 7.43 (d, 1H, *J* = 12.0 Hz), 3.09 (t, 2H, *J* = 8.0 Hz), 2.13 (s, 3H), 1.74-1.71 (m, 2H), 1.60-1.57 (m, 2H), 1.24 (s, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 182.64, 174.66, 161.79, 150.65, 144.88, 133.61, 126.62, 126.30, 124.80, 120.76, 120.48, 120.28, 37.77, 34.73, 31.82, 29.98, 19.07, 9.49.

HRMS (ESI) calcd for C₁₉H₁₇BrO₃: 373.0434 (M+H⁺), found: 373.0437.



(E)-10-(hydroxyimino)-1,6,6-trimethyl-2-(phenylselanyl)-7,8,9,10-tetrahydrophenanthro[1,2-b]furan-11(6H)-one (3a). (Red solid was obtained in 69% isolated yield, 160.8 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.56 (d, 1H, *J* = 8.0 Hz), 7.46 (d, 1H, *J* = 8.0 Hz), 7.23 (d, 2H, *J* = 8.0 Hz), 7.13-7.10 (m, 3H), 3.16 (t, 2H, *J* = 8.0 Hz), 2.25 (s, 3H), 1.72-1.69 (m, 2H), 1.57-1.55 (m, 2H), 1.22 (s, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 185.54, 151.27, 147.43, 144.56, 143.50, 140.26, 134.83,

131.30, 130.07, 129.46, 128.77, 128.65, 127.02, 125.36, 119.29, 117.31, 37.79, 34.66, 31.93, 30.96, 19.39, 12.54.

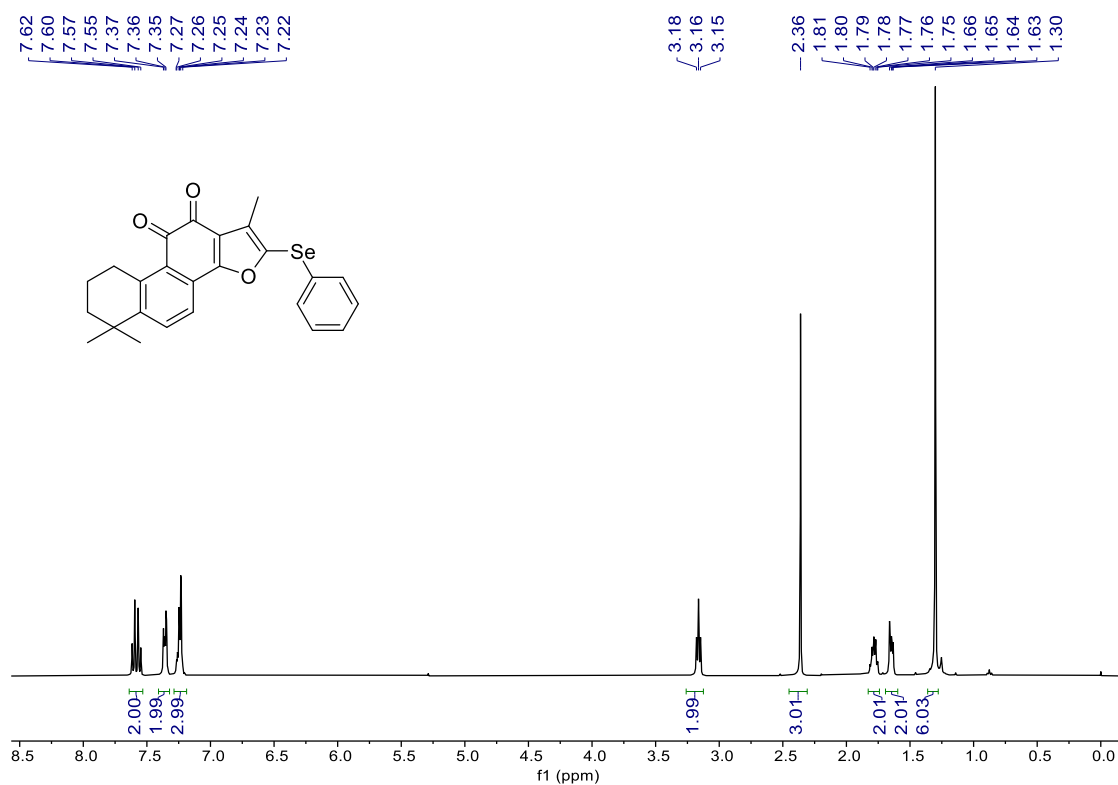
HRMS (ESI) calcd for C₂₅H₂₃NO₃Se: 465.0960 (M+H⁺), found: 465.0962.

References

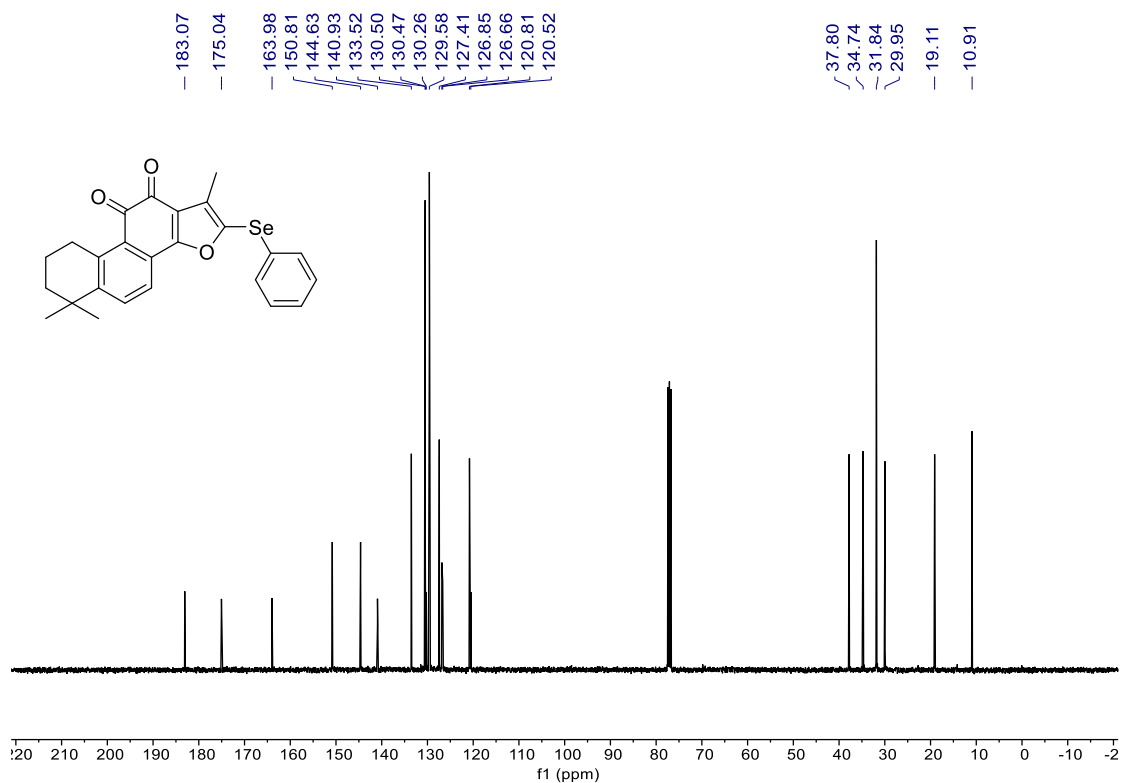
- (1) Dapkekar, Anil Balajirao; Satyanarayana, Gedu. Electrochemical selenofunctionalization of unactivated alkenes: access to β -hydroxy-selenides. *Org. Biomol. Chem.*, **2024**,22,1775-1781.
- (2) Jun Xie , Jiahui Liu , Heng Liu , Shihui Liang , Meigui Lin , Yueyu Gu , Taoli Liu , Dongmei Wang , Hui Ge , Sui-lin Mo. The antitumor effect of tanshinone IIA on anti-proliferation and decreasing VEGF/VEGFR2 expression on the human non-small cell lung cancer A549 cell line. *Acta Pharm. Sin. B.* **2015**,6,554-563.

Copies of ^1H NMR, ^{13}C NMR, ^{19}F NMR and HRMS spectra

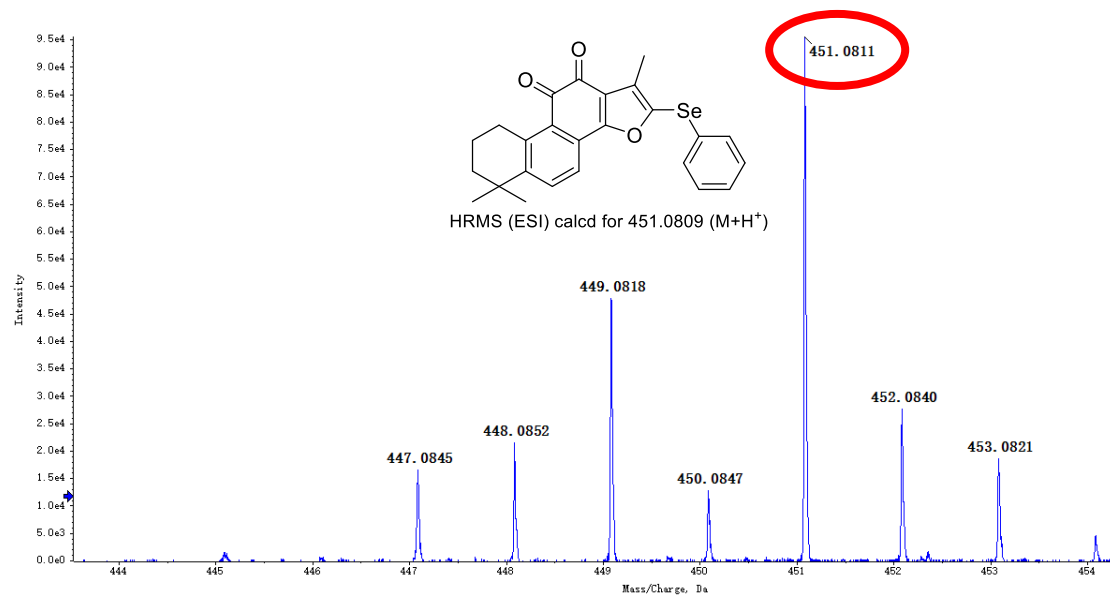
^1H NMR (400 MHz, CDCl_3) of compound **2a**



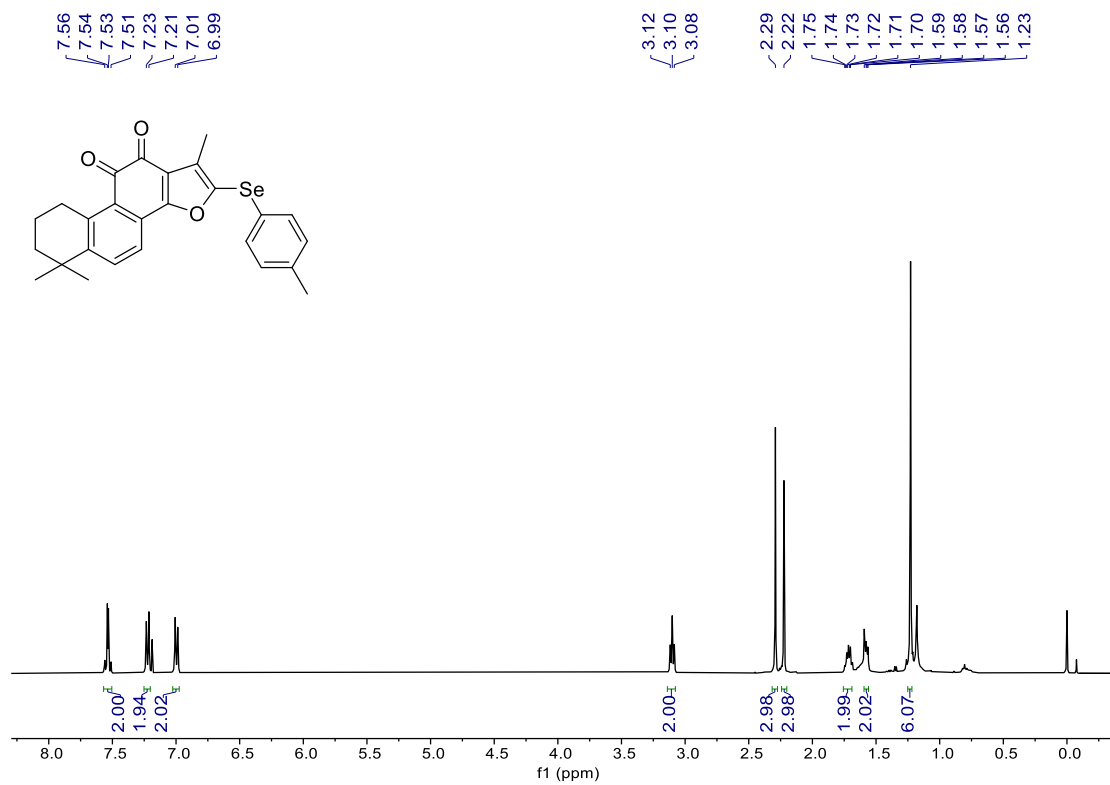
^{13}C NMR (101 MHz, CDCl_3) of compound **2a**



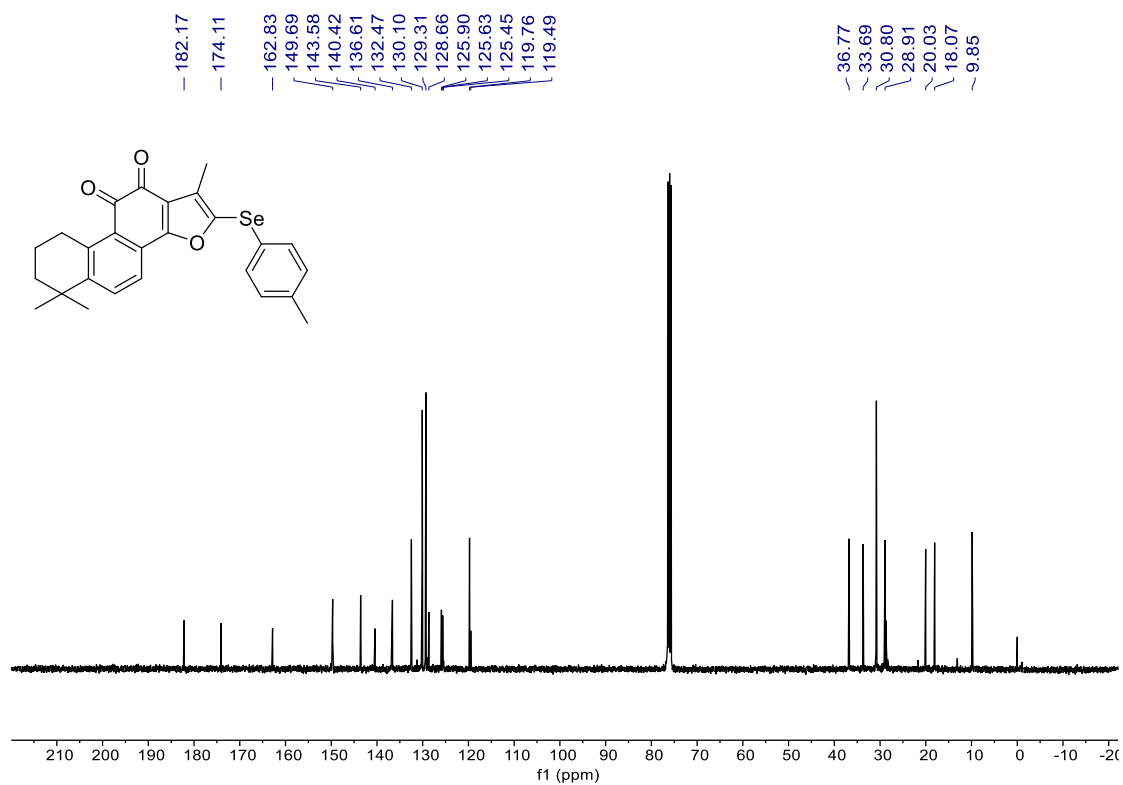
HRMS(ESI) of compound **2a**



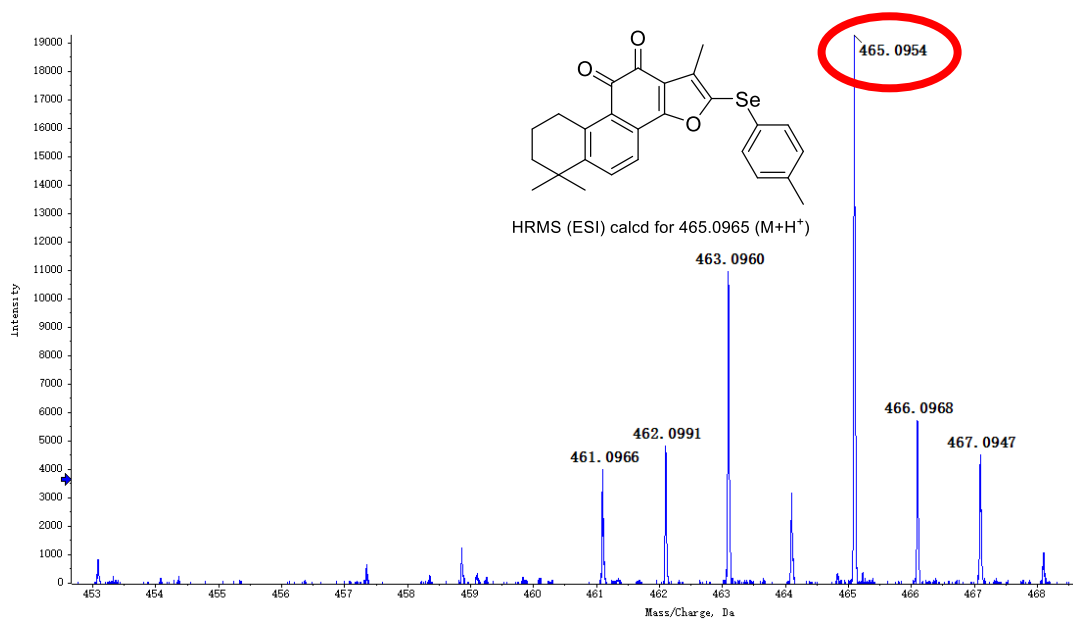
^1H NMR (400 MHz, CDCl_3) of compound **2b**



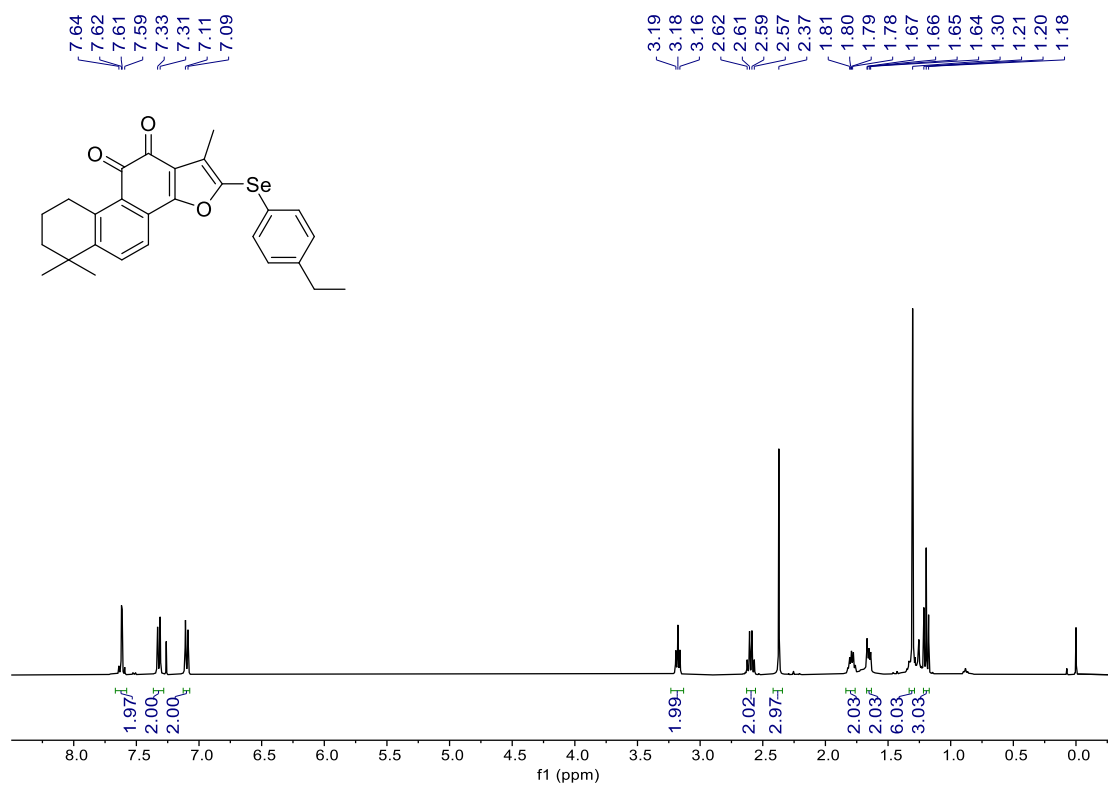
^{13}C NMR (101 MHz, CDCl_3) of compound **2b**



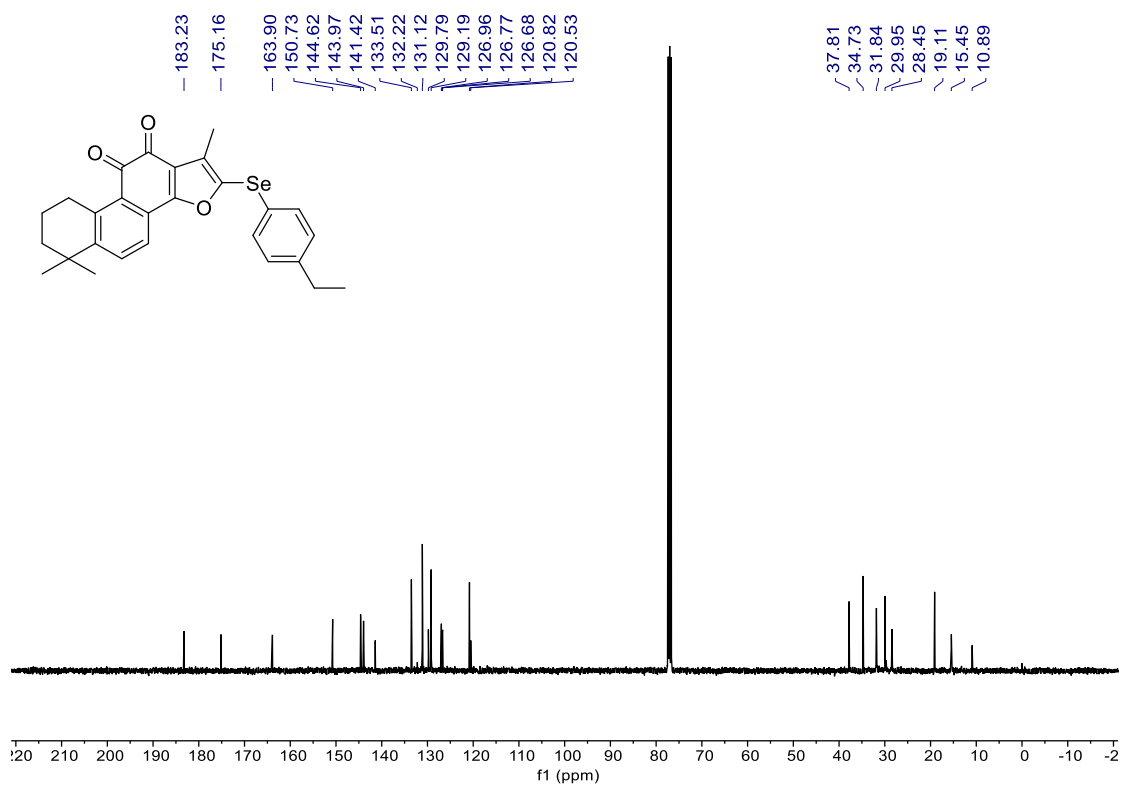
HRMS(ESI) of compound **2b**



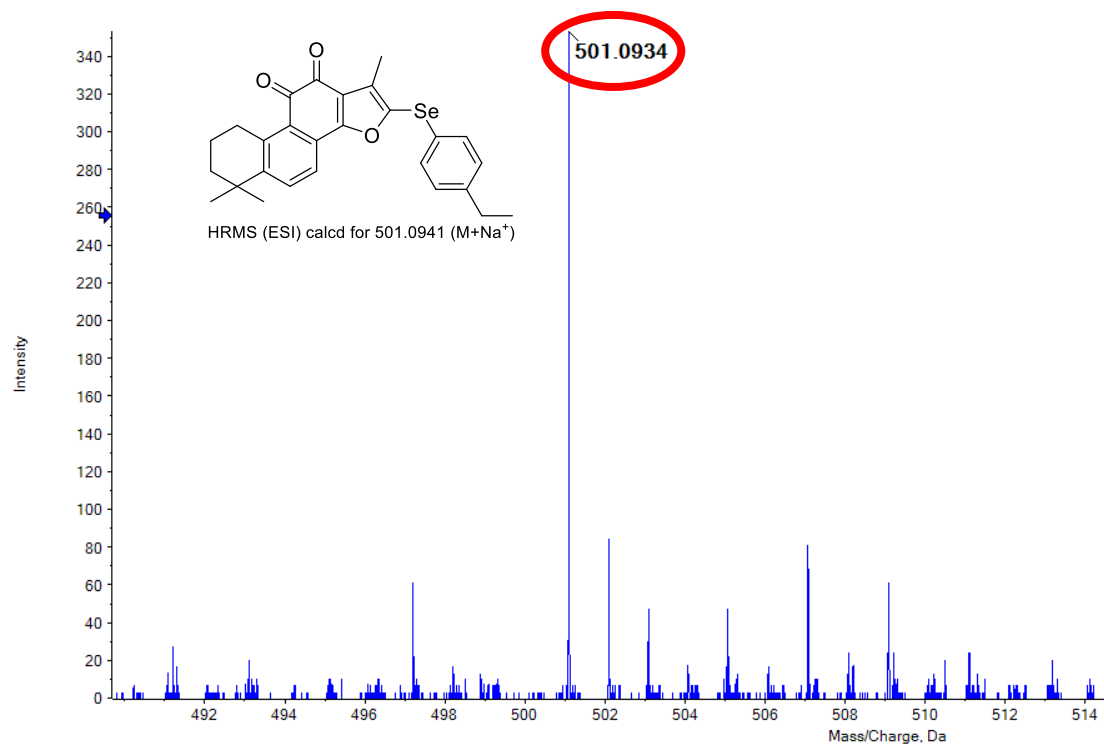
^1H NMR (400 MHz, CDCl_3) of compound **2c**



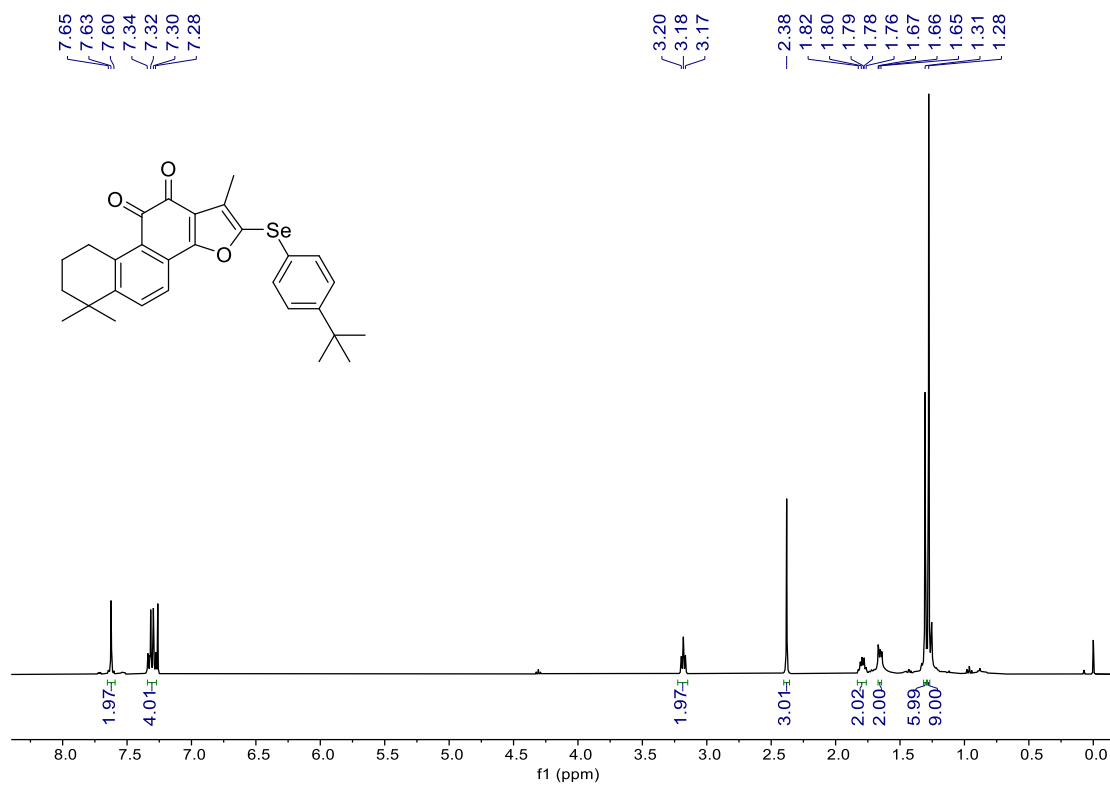
^{13}C NMR (101 MHz, CDCl_3) of compound **2c**



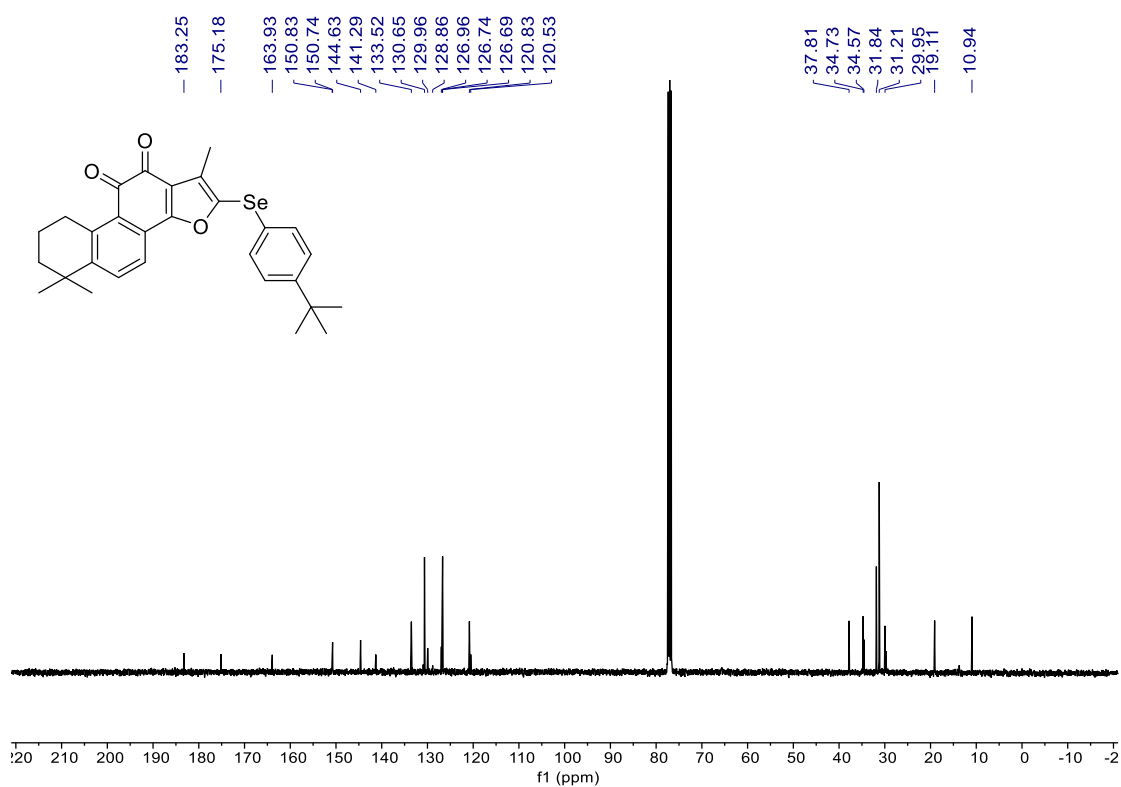
HRMS(ESI) of compound **2c**



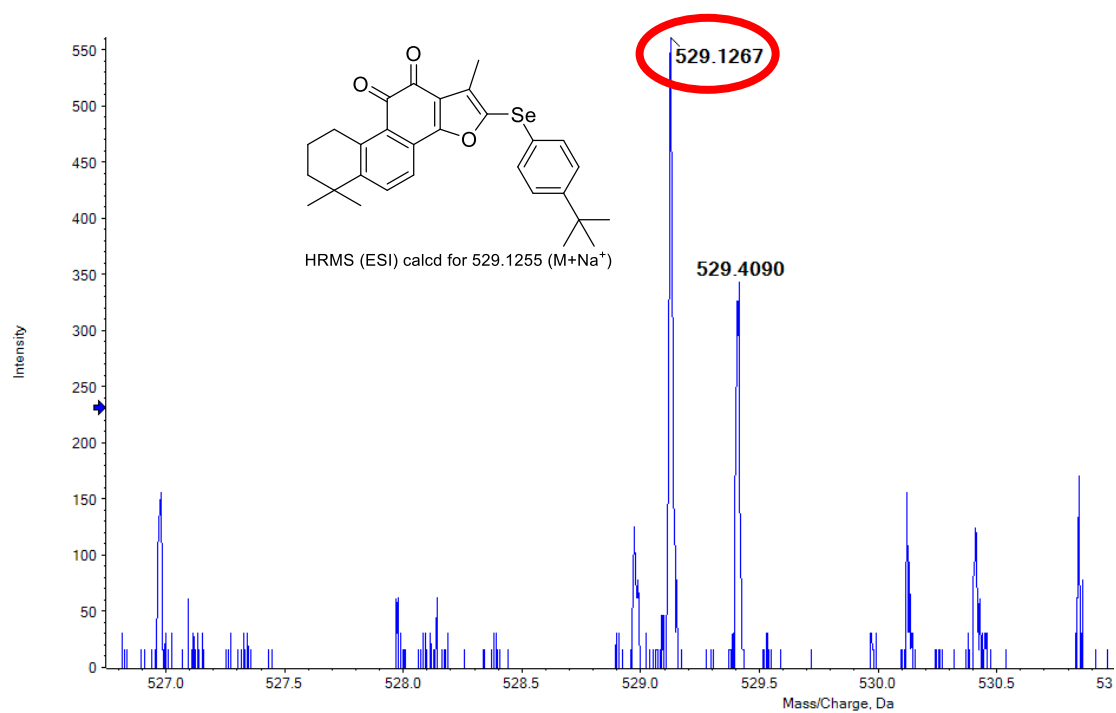
1H NMR (400 MHz, $CDCl_3$) of compound **2d**



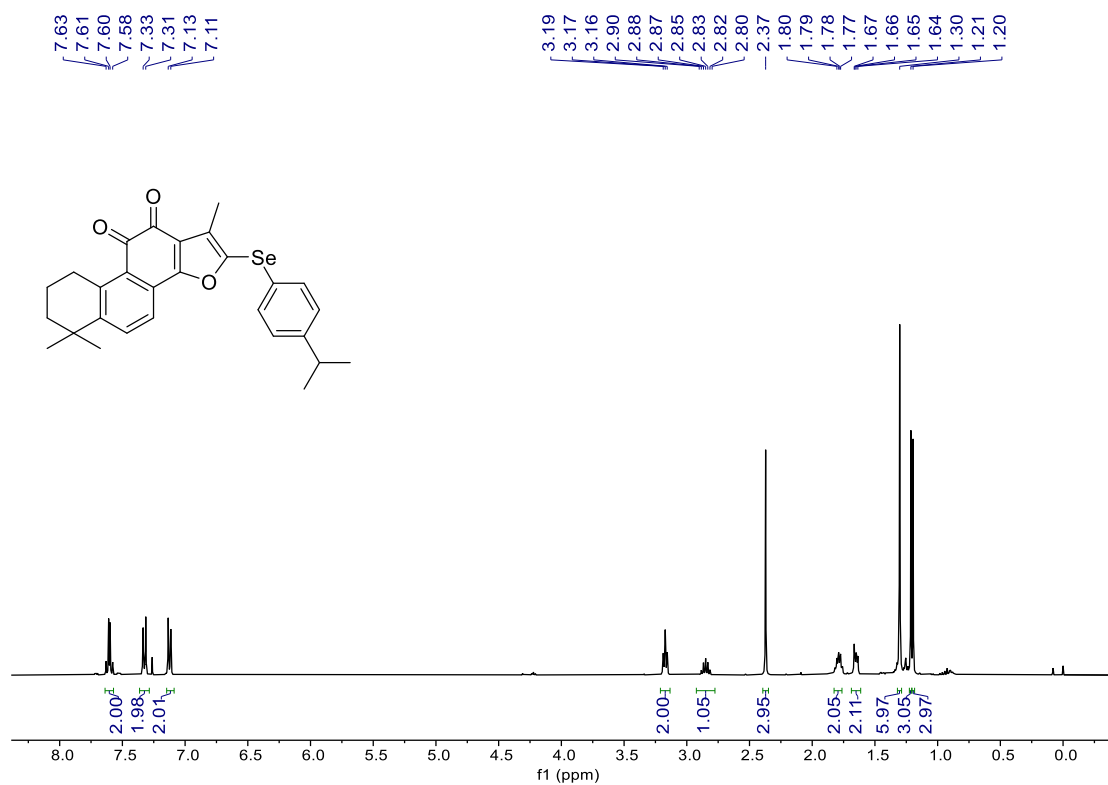
^{13}C NMR (101 MHz, CDCl_3) of compound **2d**



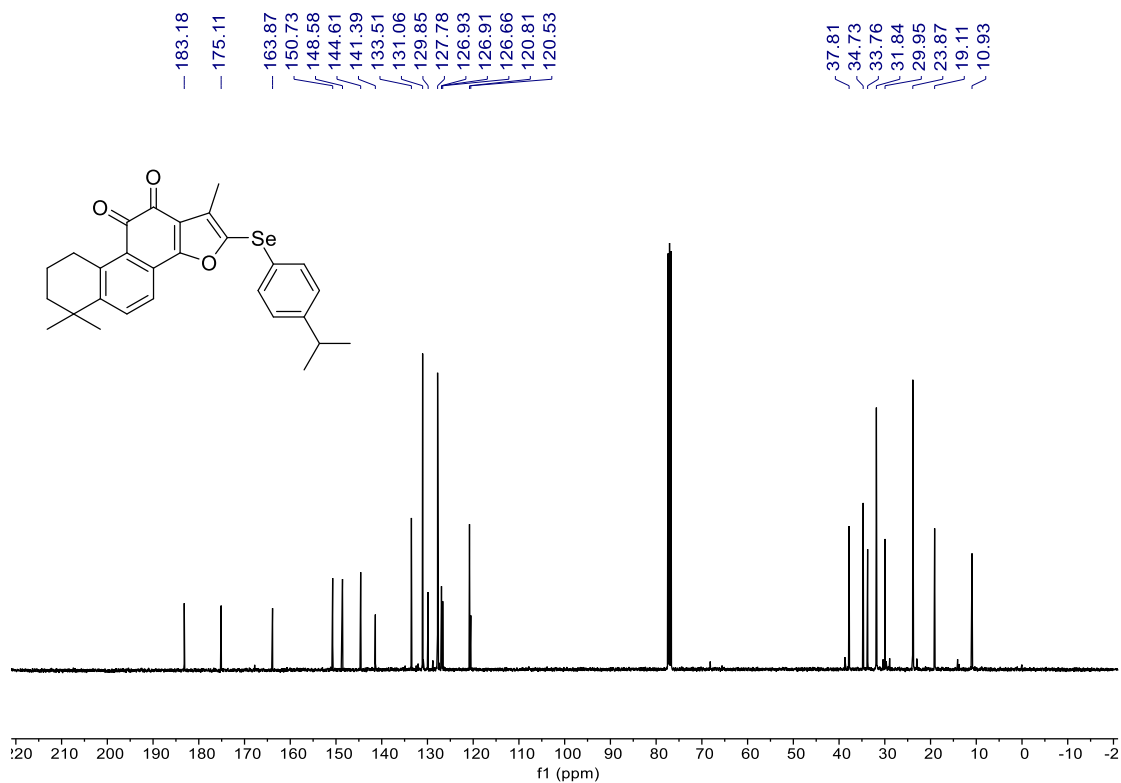
HRMS(ESI) of compound **2d**



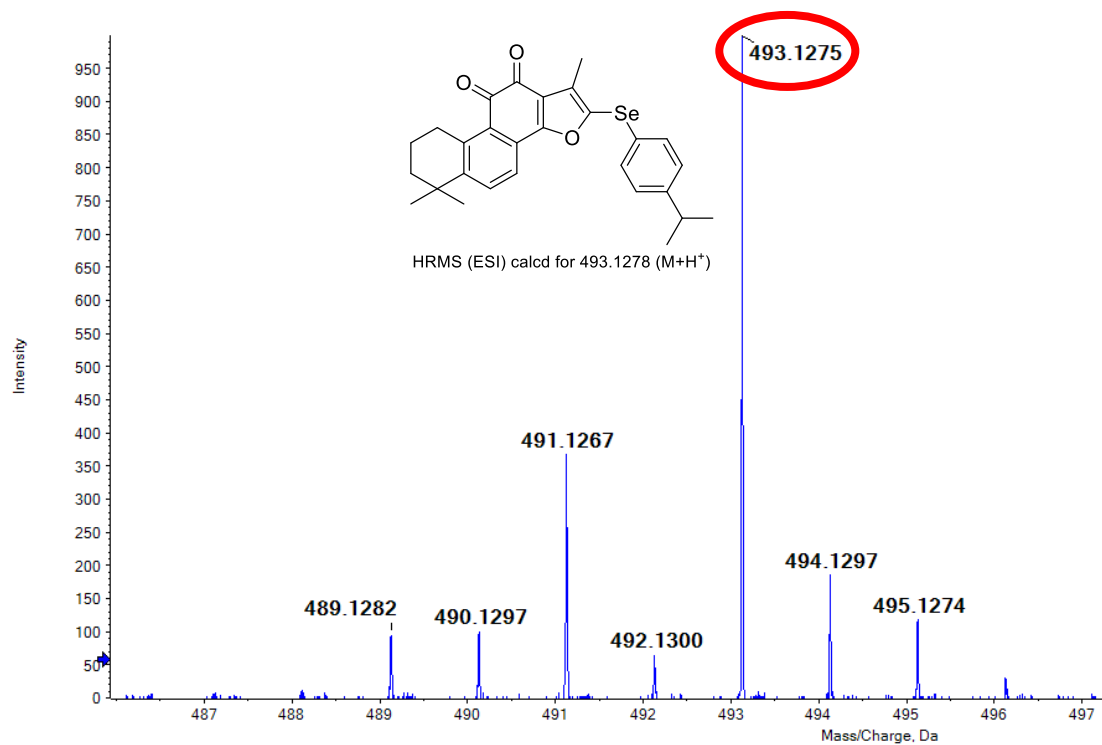
^1H NMR (400 MHz, CDCl_3) of compound **2e**



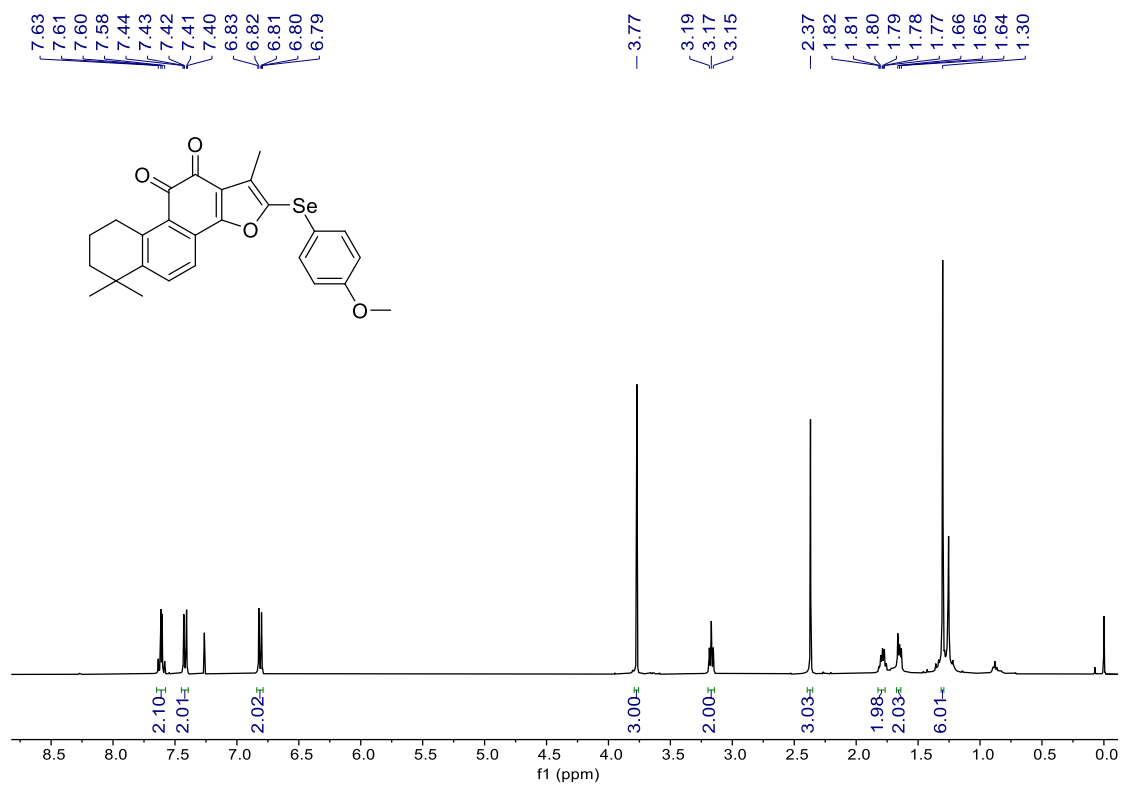
^{13}C NMR (101 MHz, CDCl_3) of compound **2e**



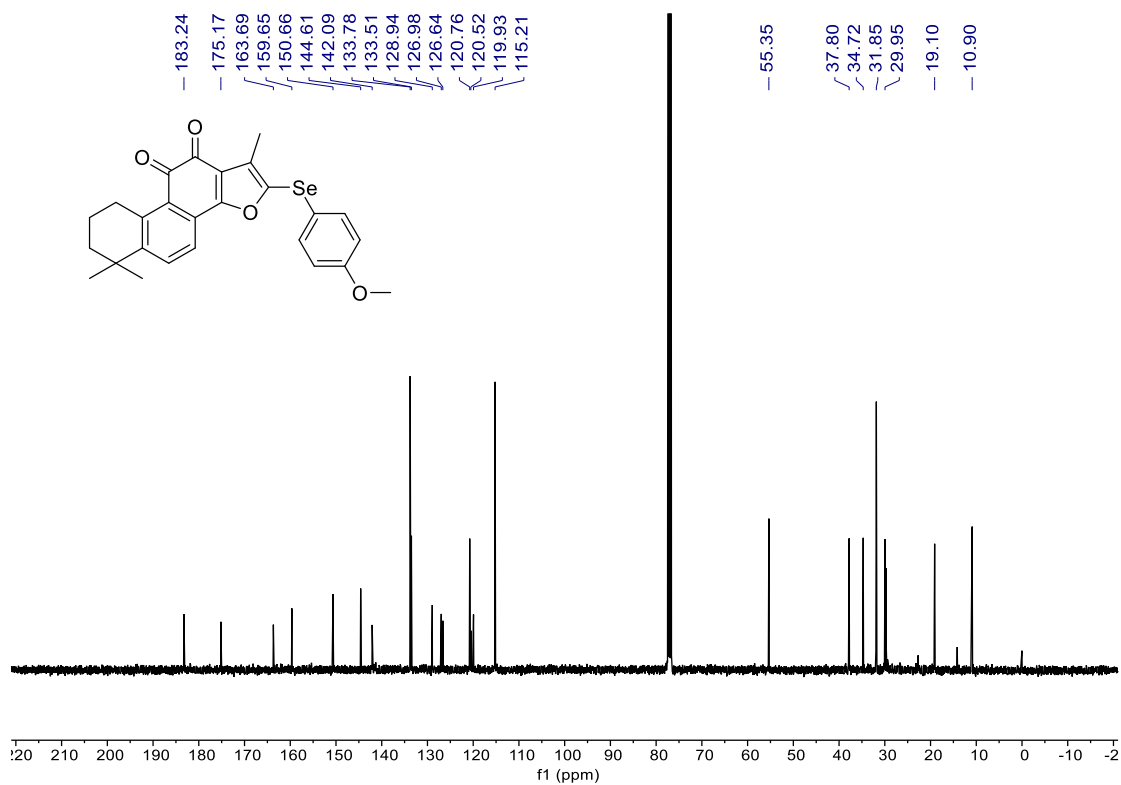
HRMS(ESI) of compound **2e**



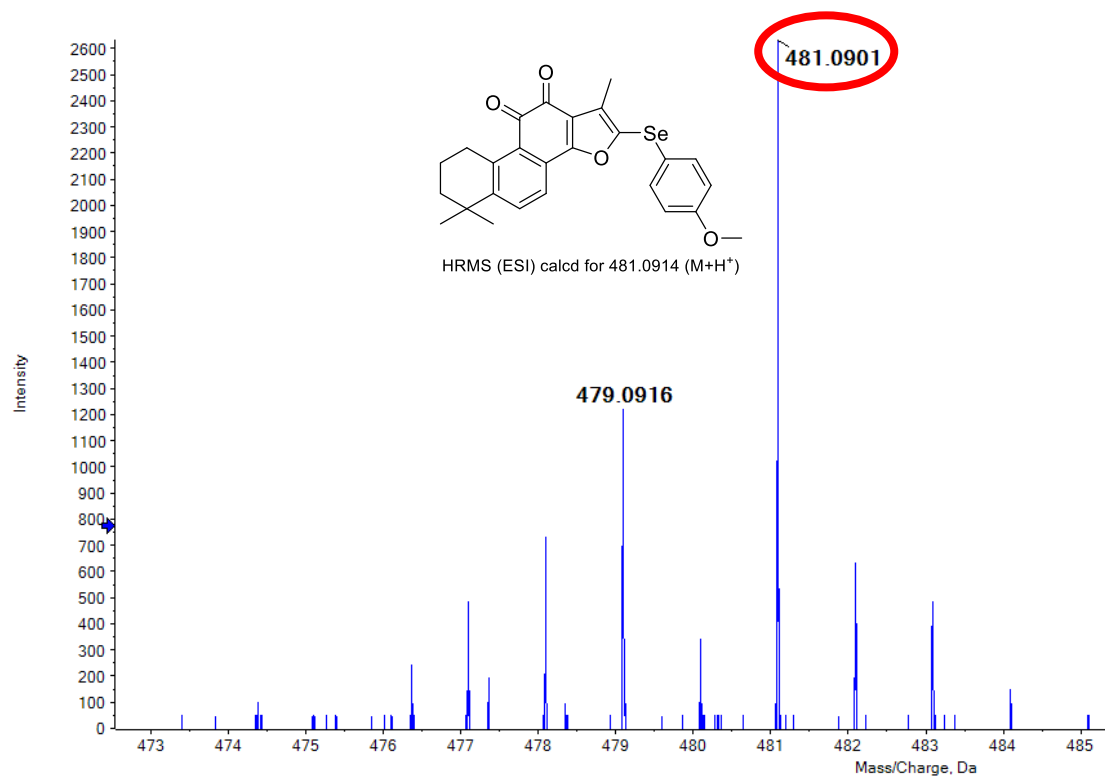
^1H NMR (400 MHz, CDCl_3) of compound **2f**



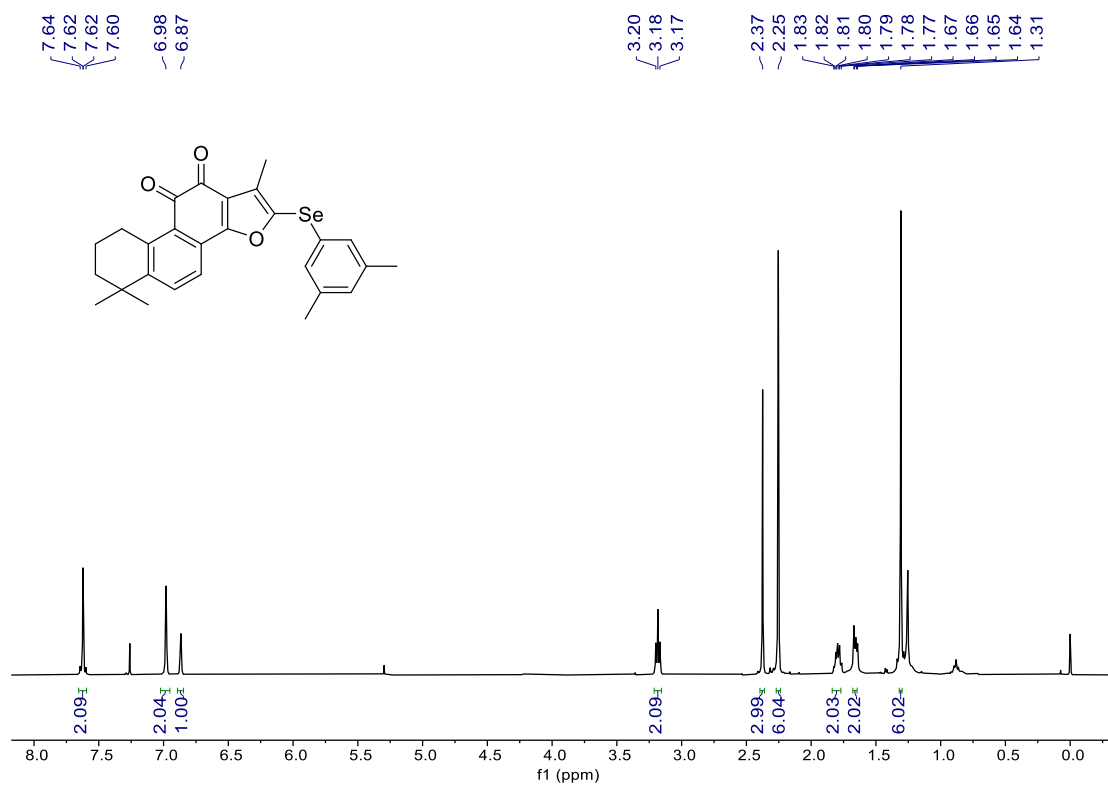
^{13}C NMR (101 MHz, CDCl_3) of compound **2f**



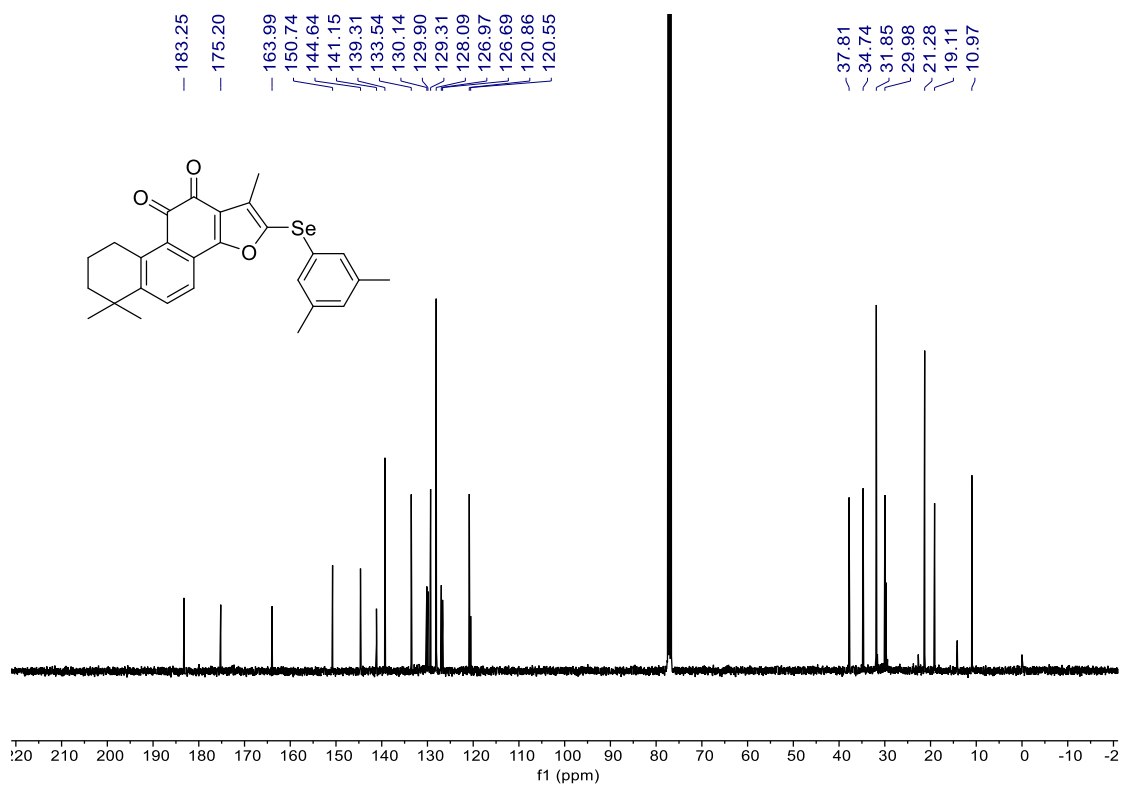
HRMS(ESI) of compound **2f**



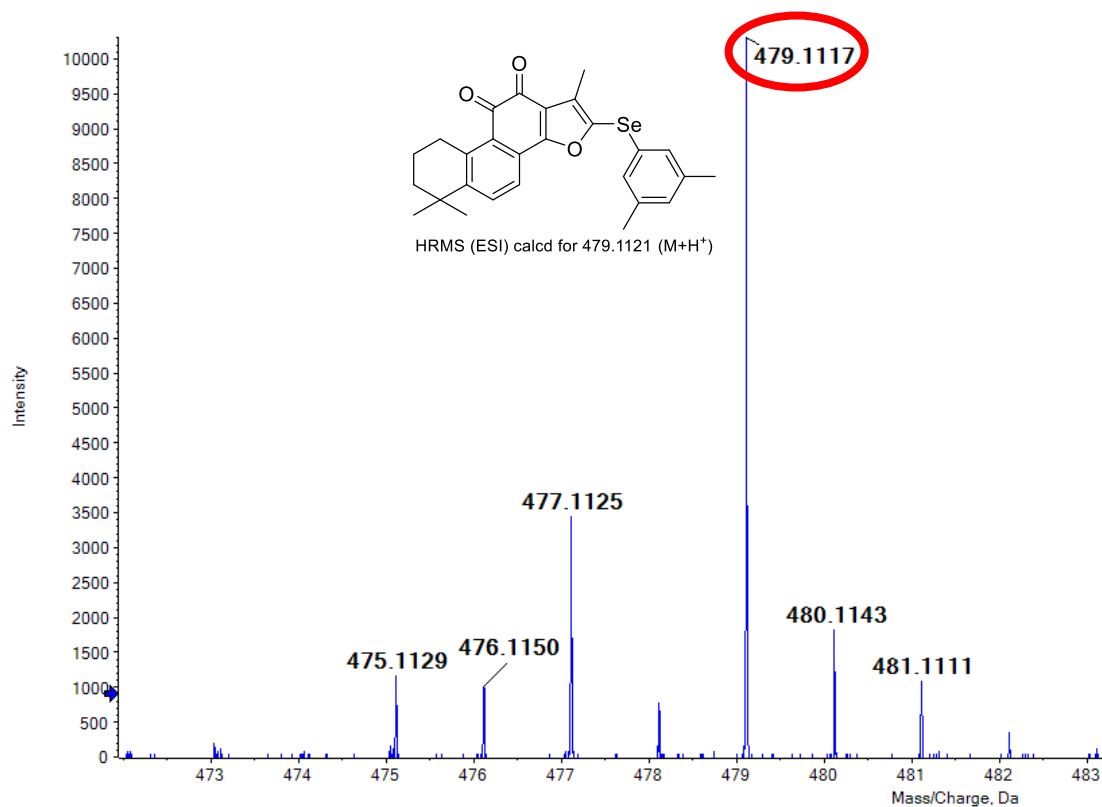
^1H NMR (400 MHz, CDCl_3) of compound **2g**



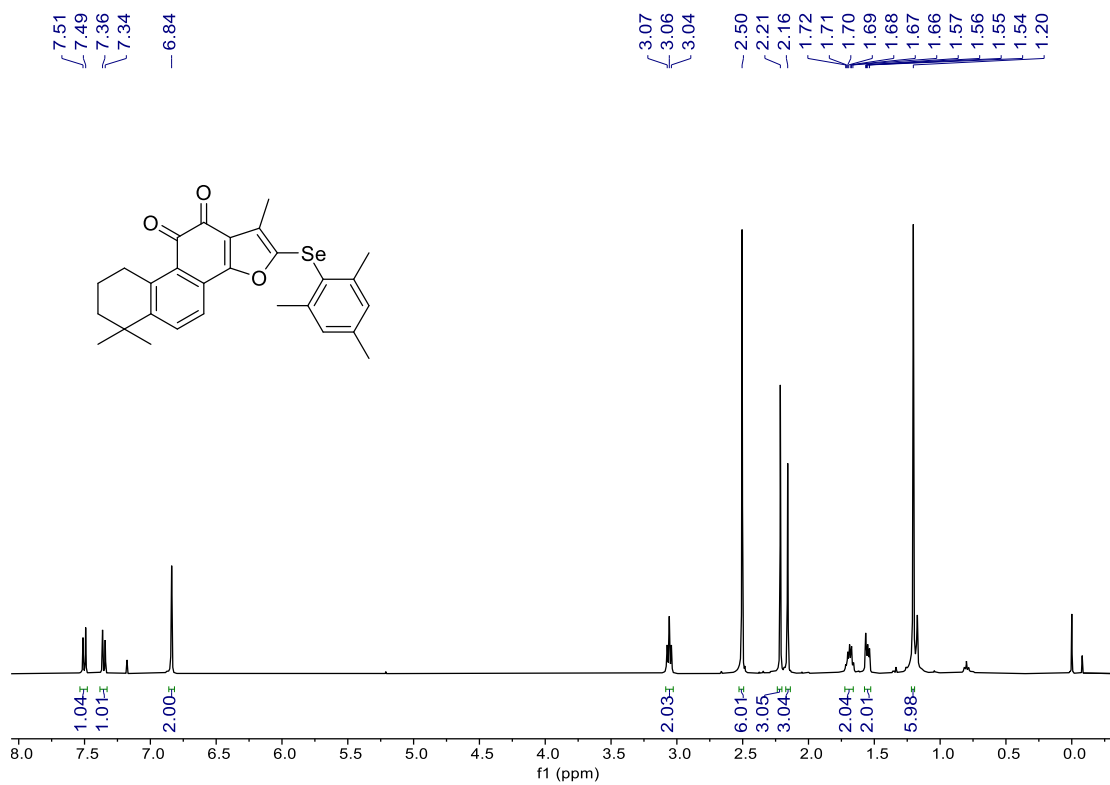
^{13}C NMR (101 MHz, CDCl_3) of compound **2g**



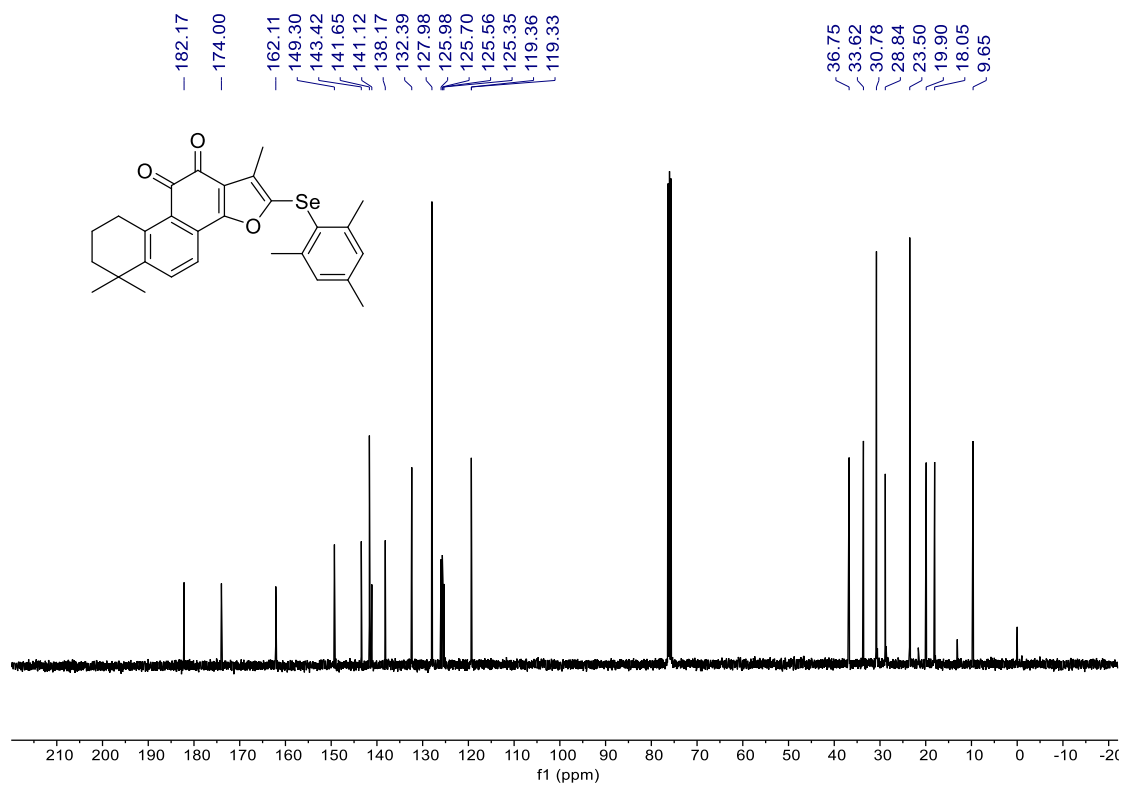
HRMS(ESI) of compound **2g**



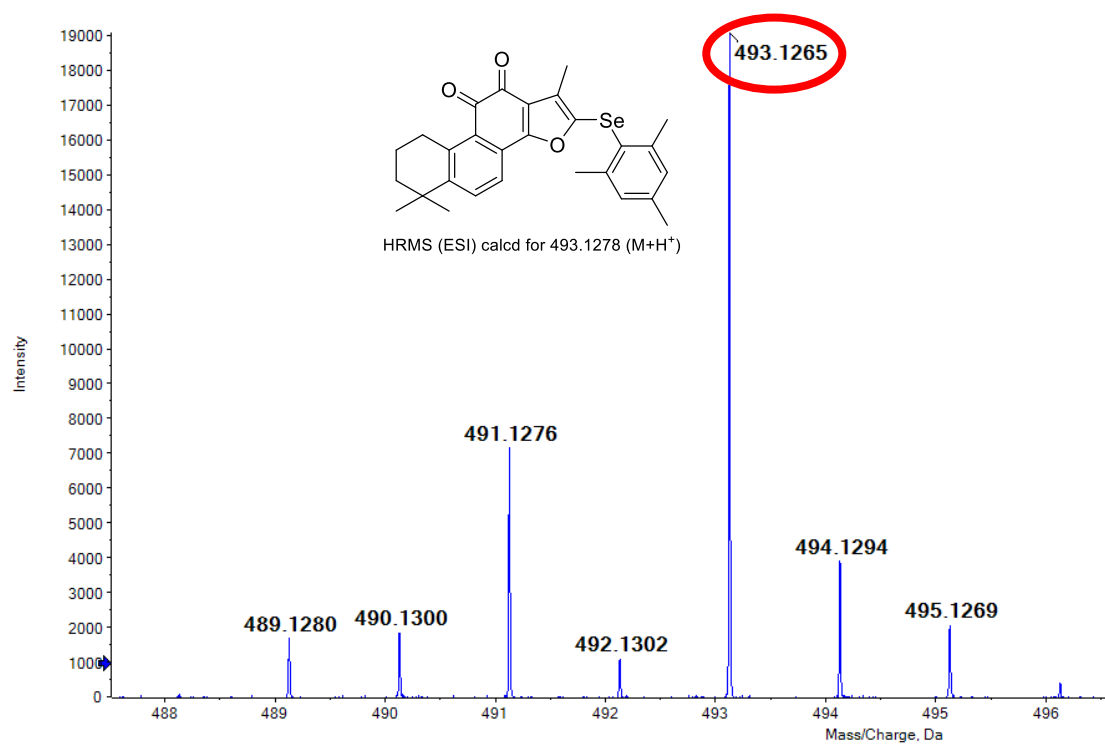
^1H NMR (400 MHz, CDCl_3) of compound **2h**



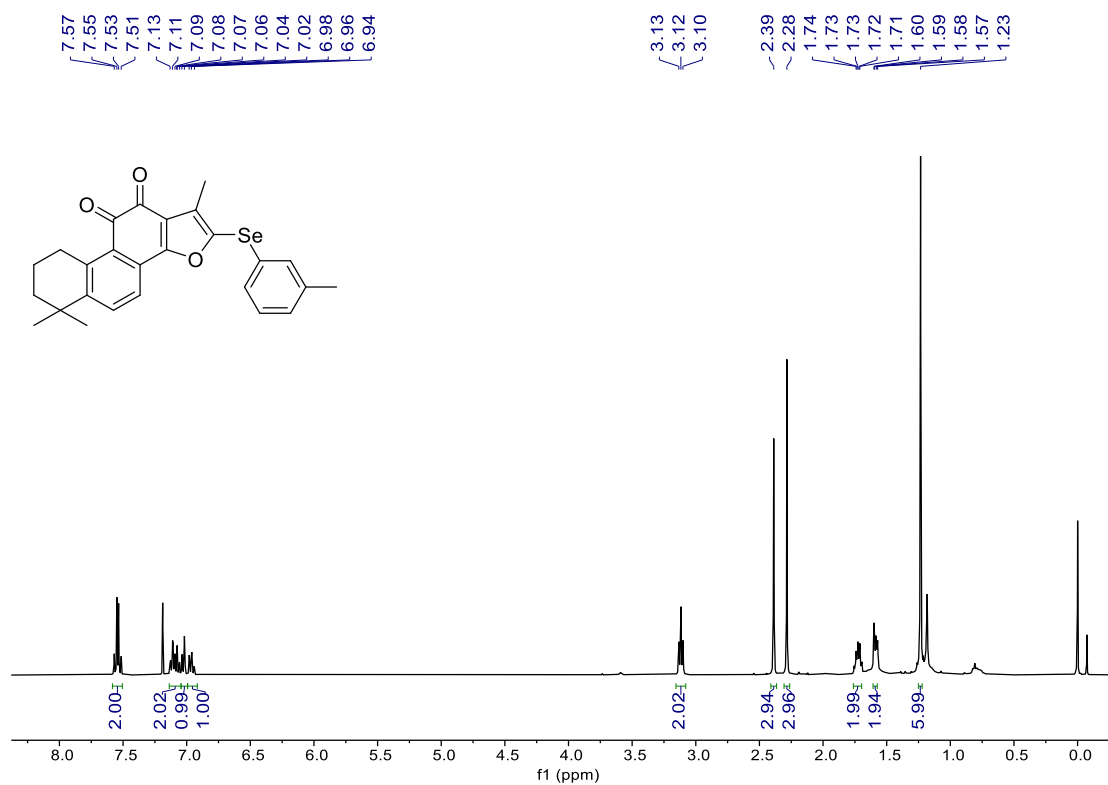
^{13}C NMR (101 MHz, CDCl_3) of compound **2h**



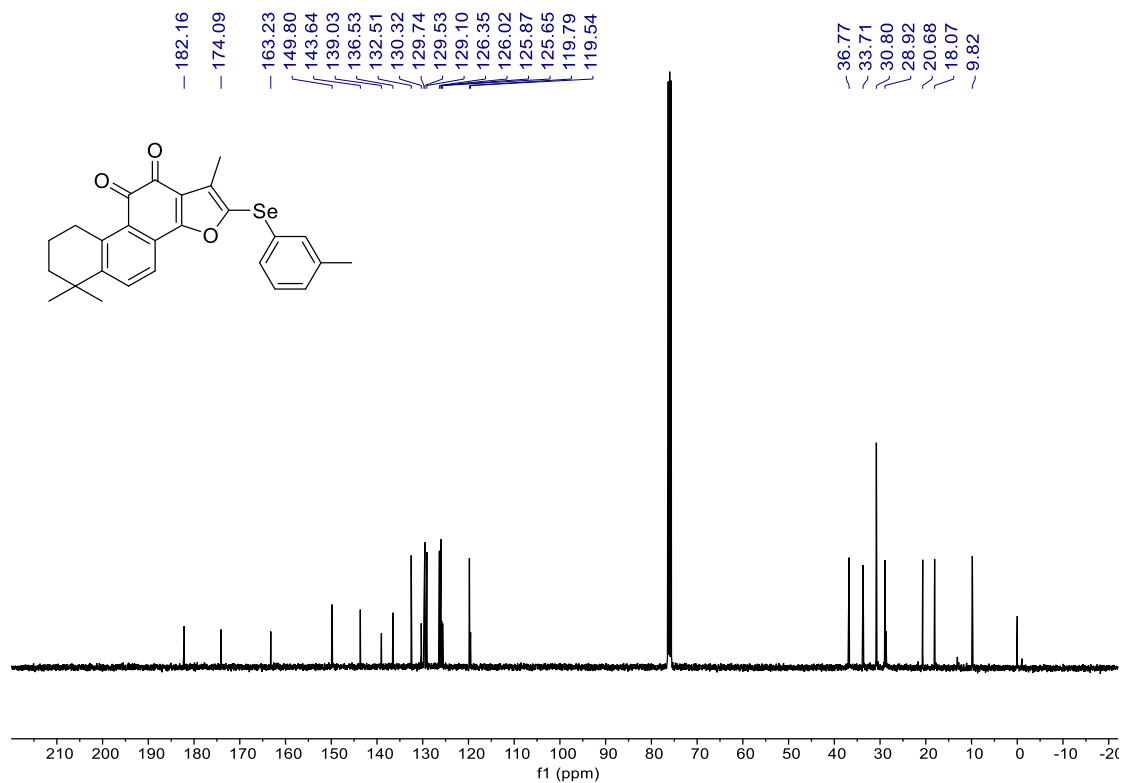
HRMS(ESI) of compound **2h**



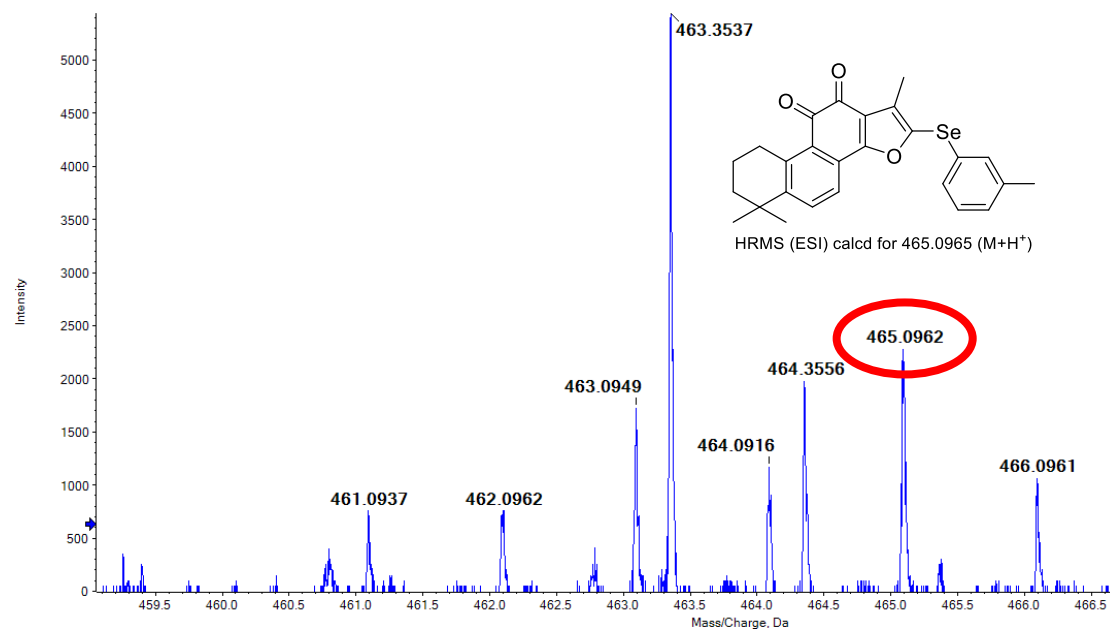
^1H NMR (400 MHz, CDCl_3) of compound **2i**



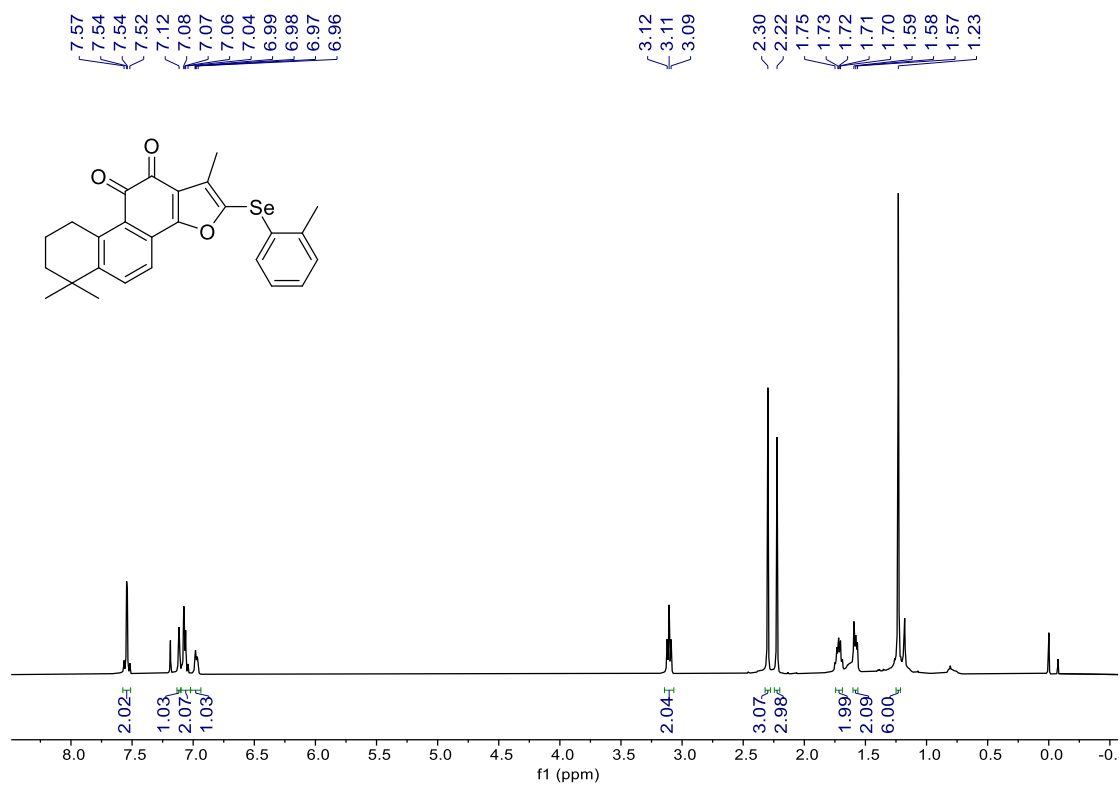
^{13}C NMR (101 MHz, CDCl_3) of compound **2i**



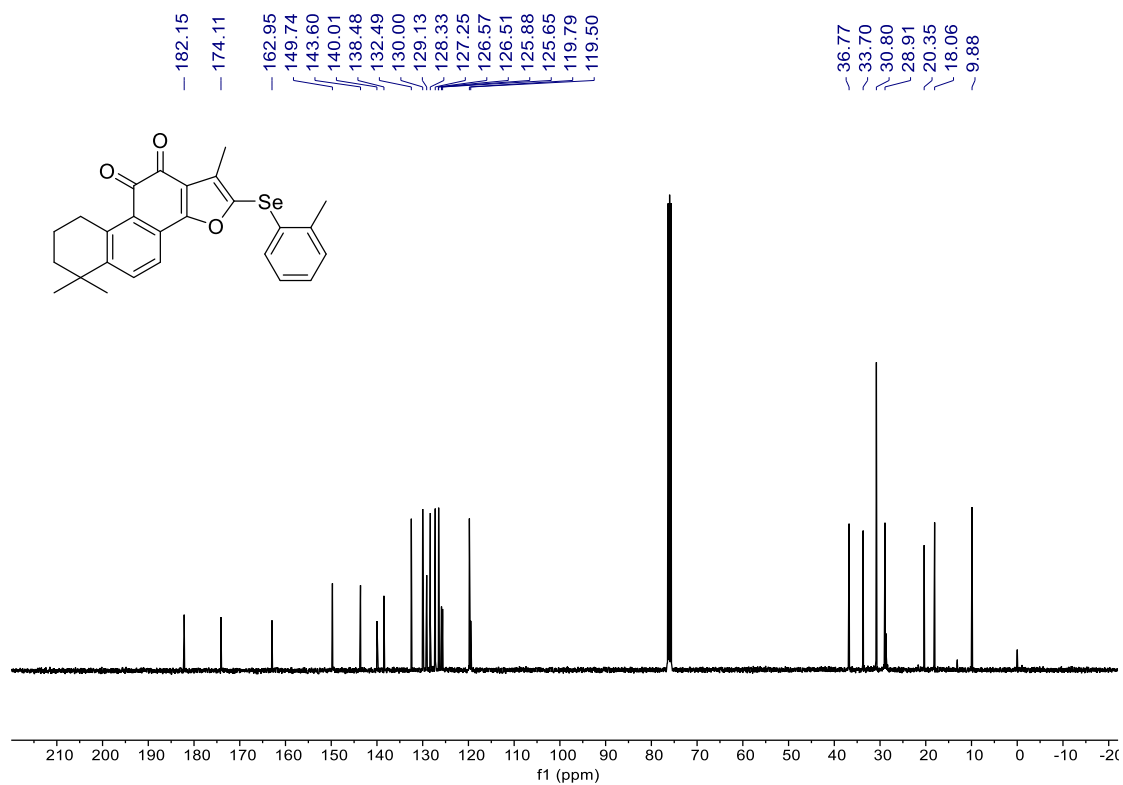
HRMS(ESI) of compound **2i**



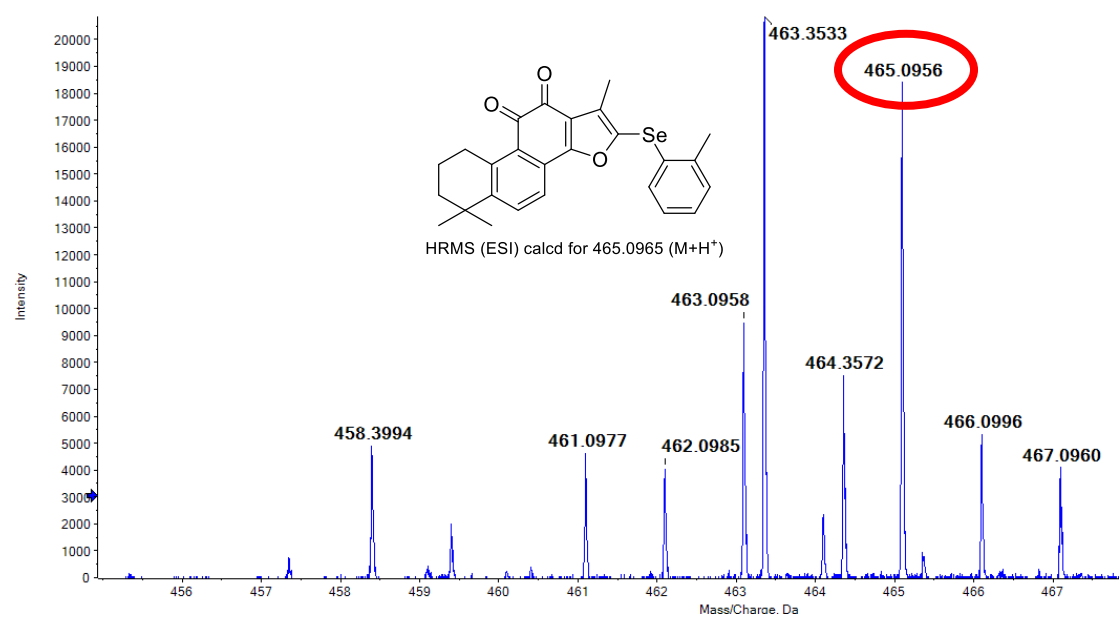
^1H NMR (400 MHz, CDCl_3) of compound **2j**



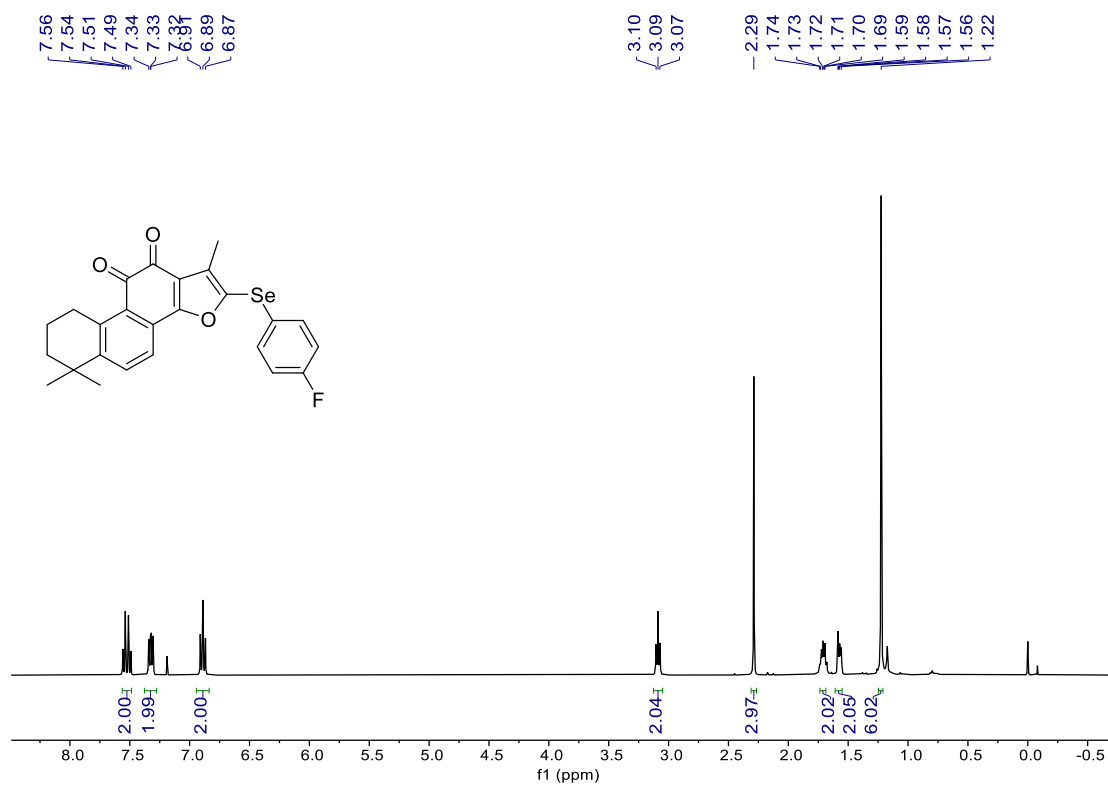
^{13}C NMR (101 MHz, CDCl_3) of compound **2j**



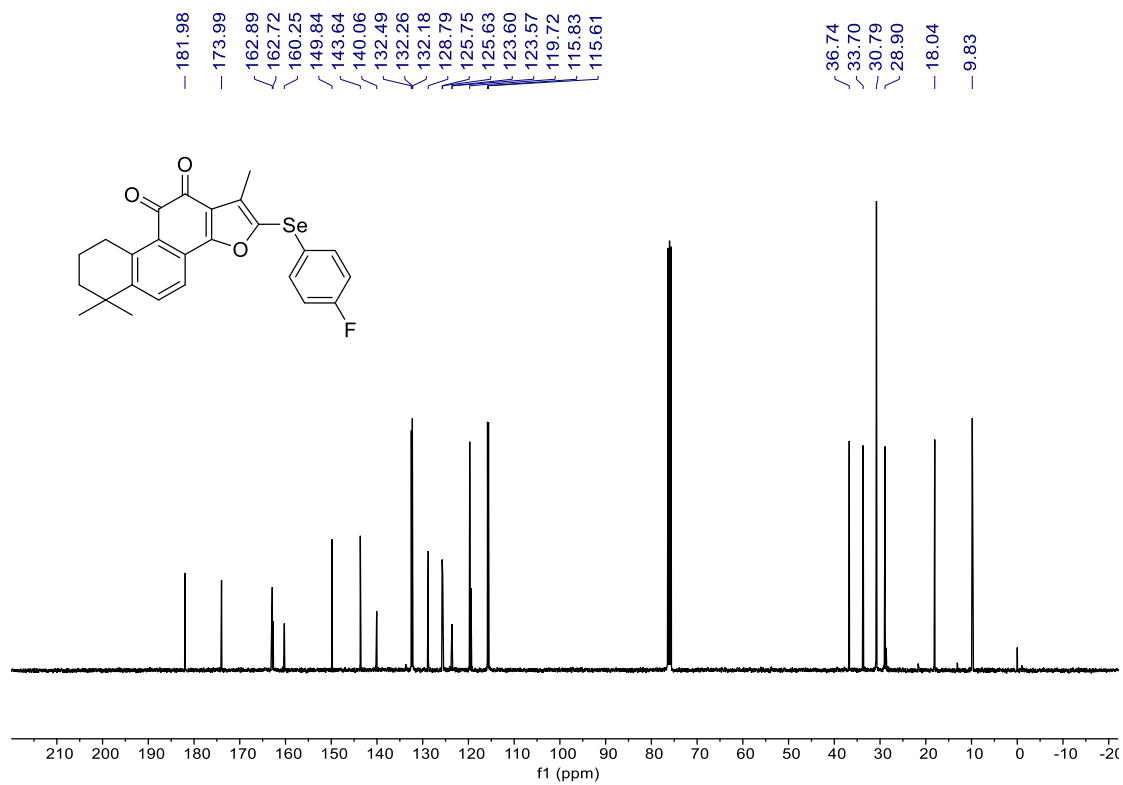
HRMS(ESI) of compound **2j**



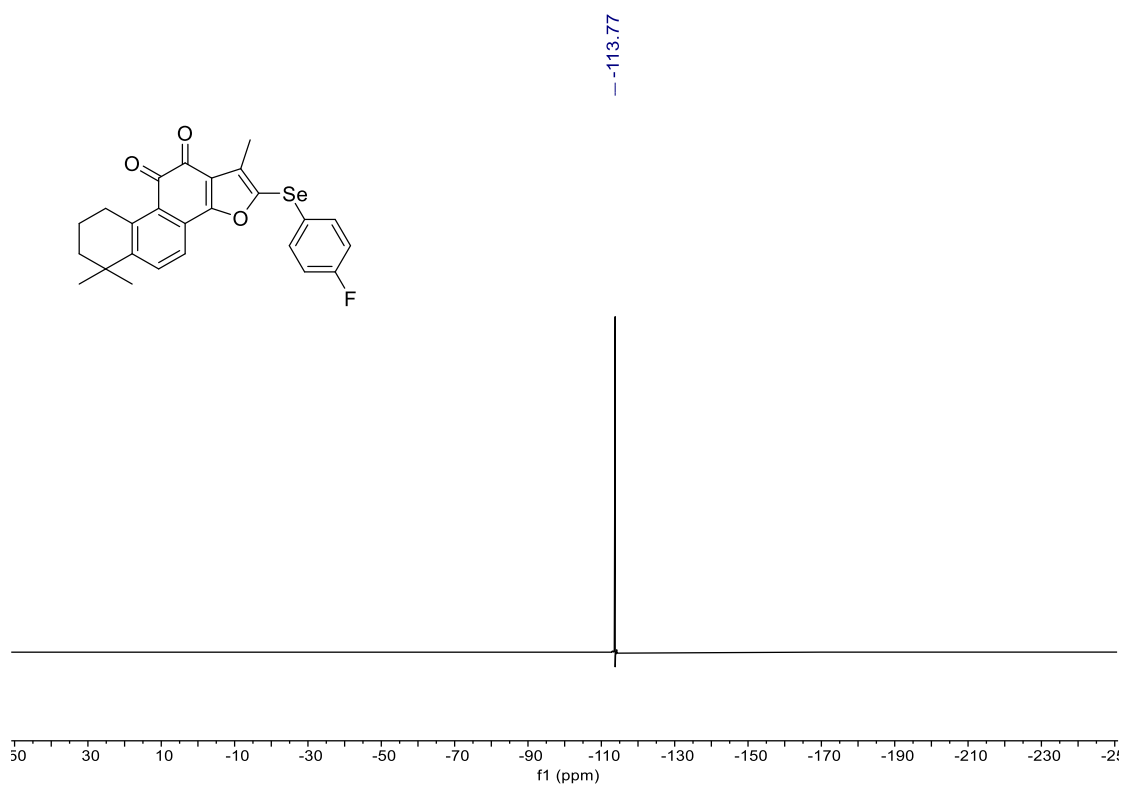
^1H NMR (400 MHz, CDCl_3) of compound **2k**



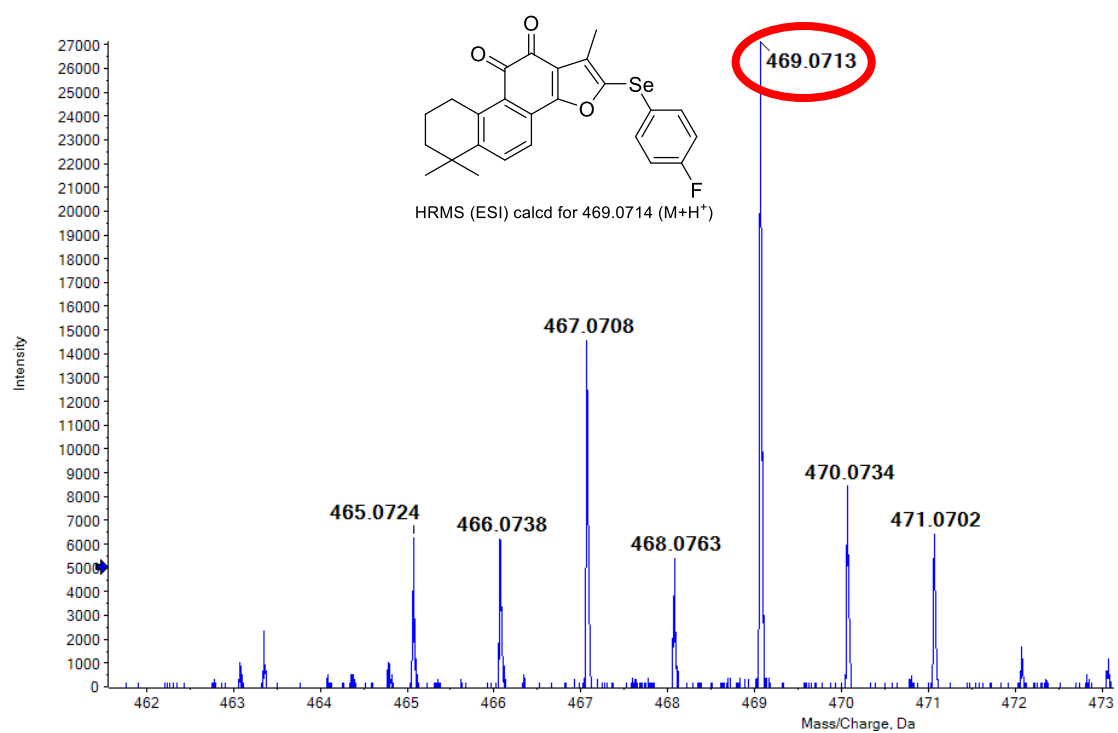
^{13}C NMR (101 MHz, CDCl_3) of compound **2k**



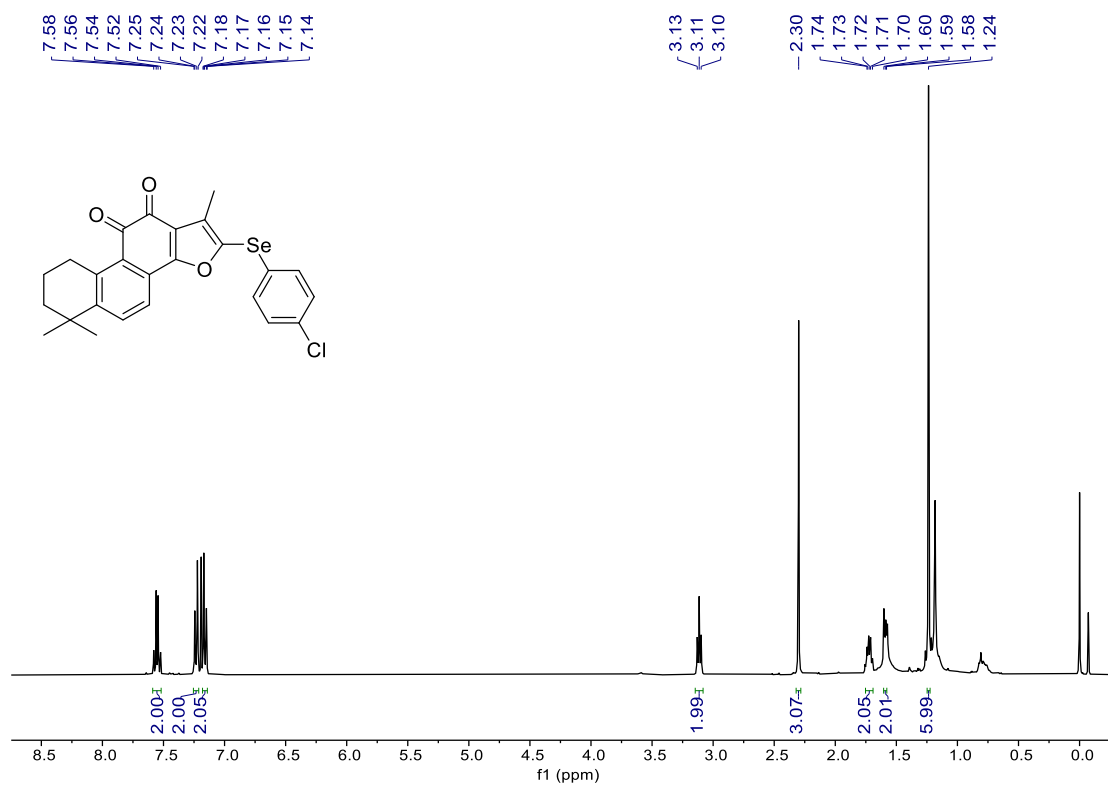
^{19}F NMR (376 MHz, CDCl_3) of compound **2k**



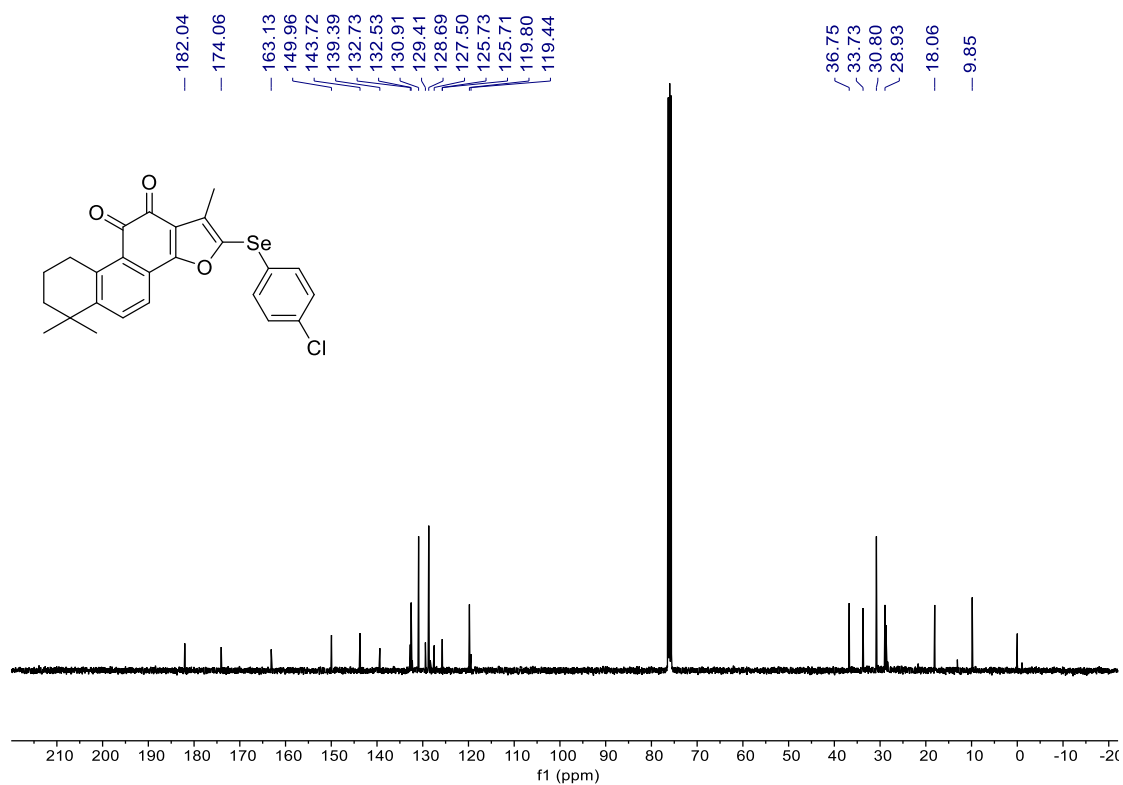
HRMS(ESI) of compound **2k**



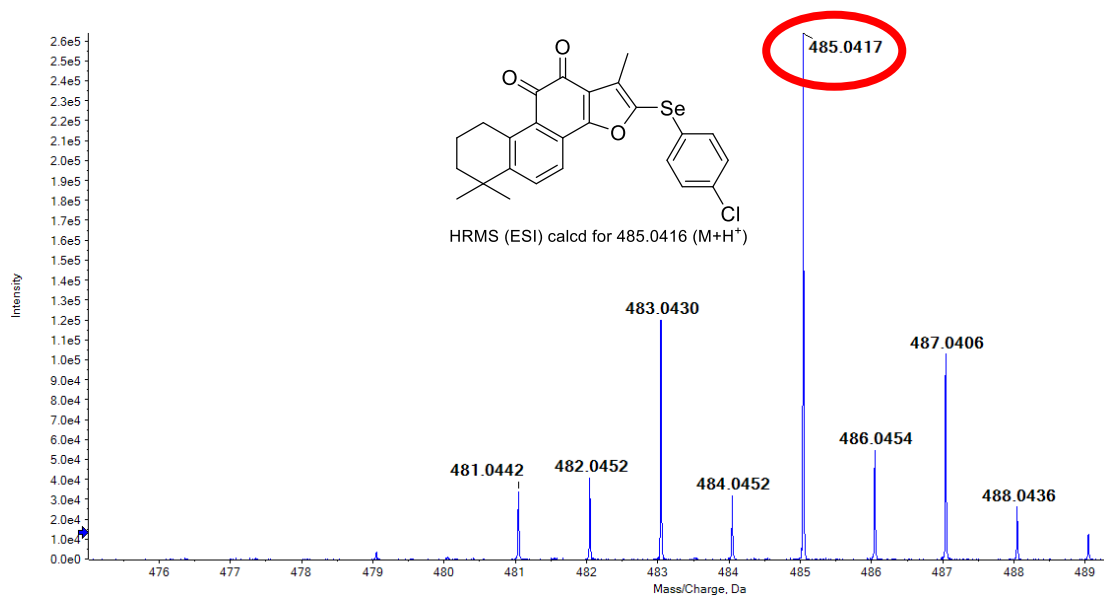
^1H NMR (400 MHz, CDCl_3) of compound **21**



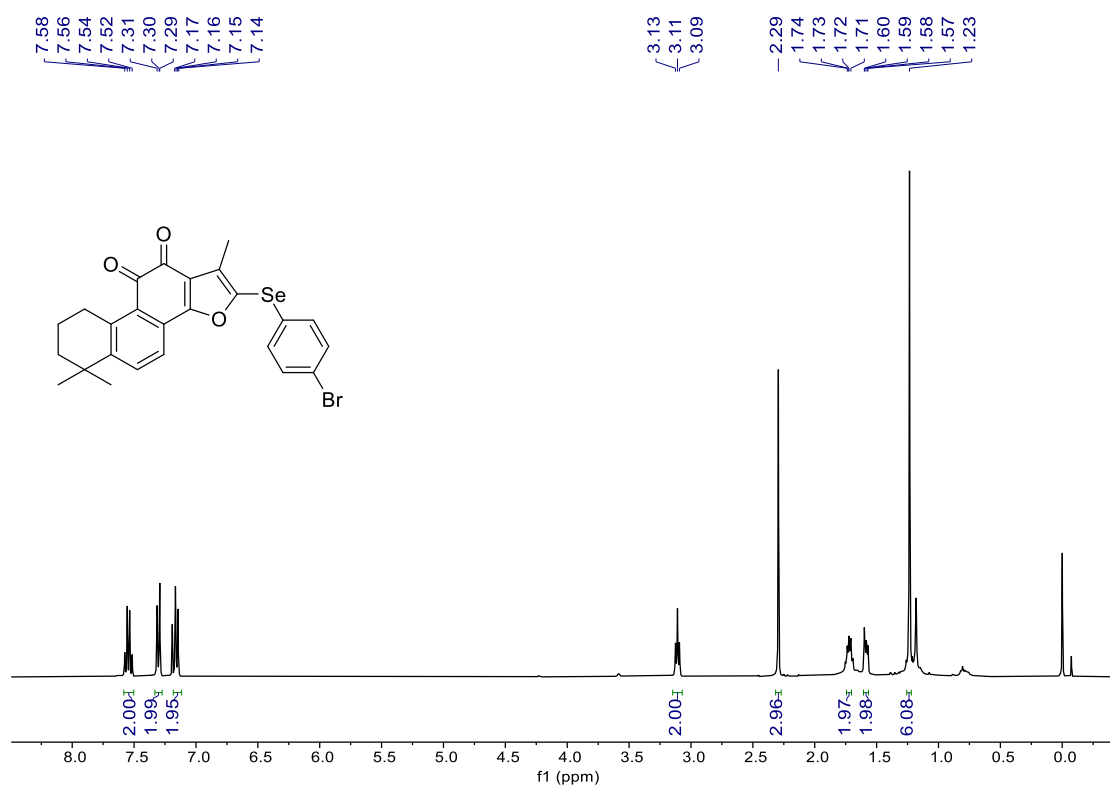
^{13}C NMR (101 MHz, CDCl_3) of compound **21**



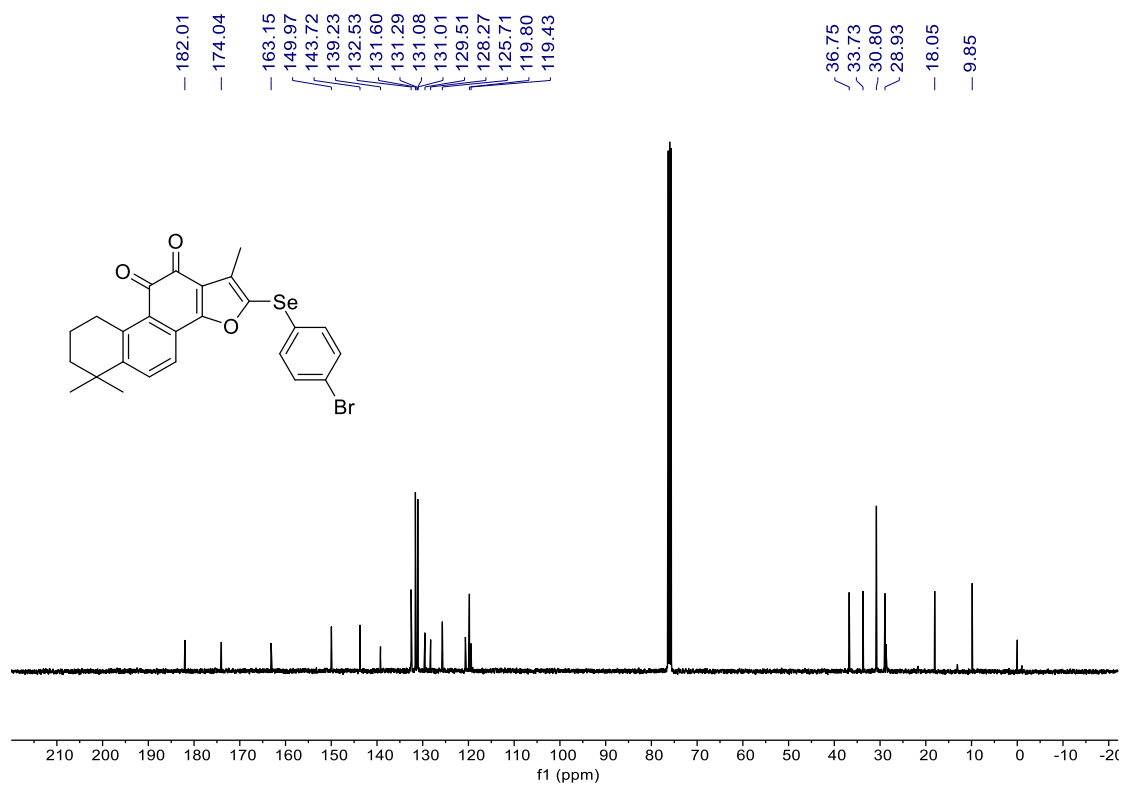
HRMS(ESI) of compound **2l**



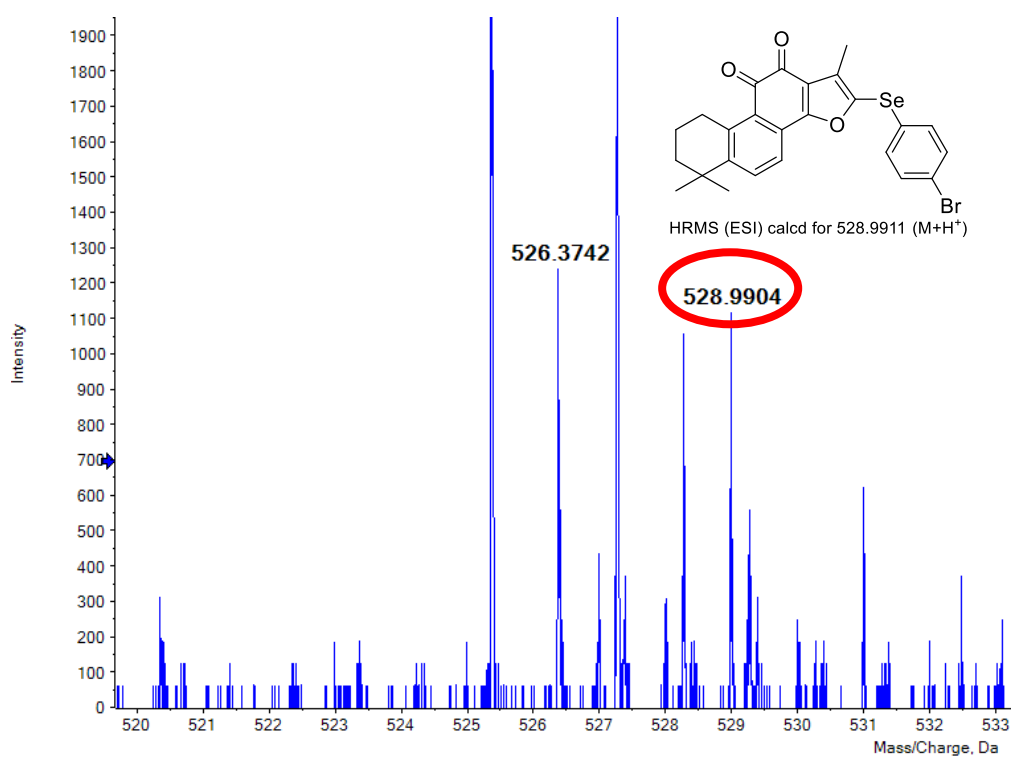
1H NMR (400 MHz, $CDCl_3$) of compound **2m**



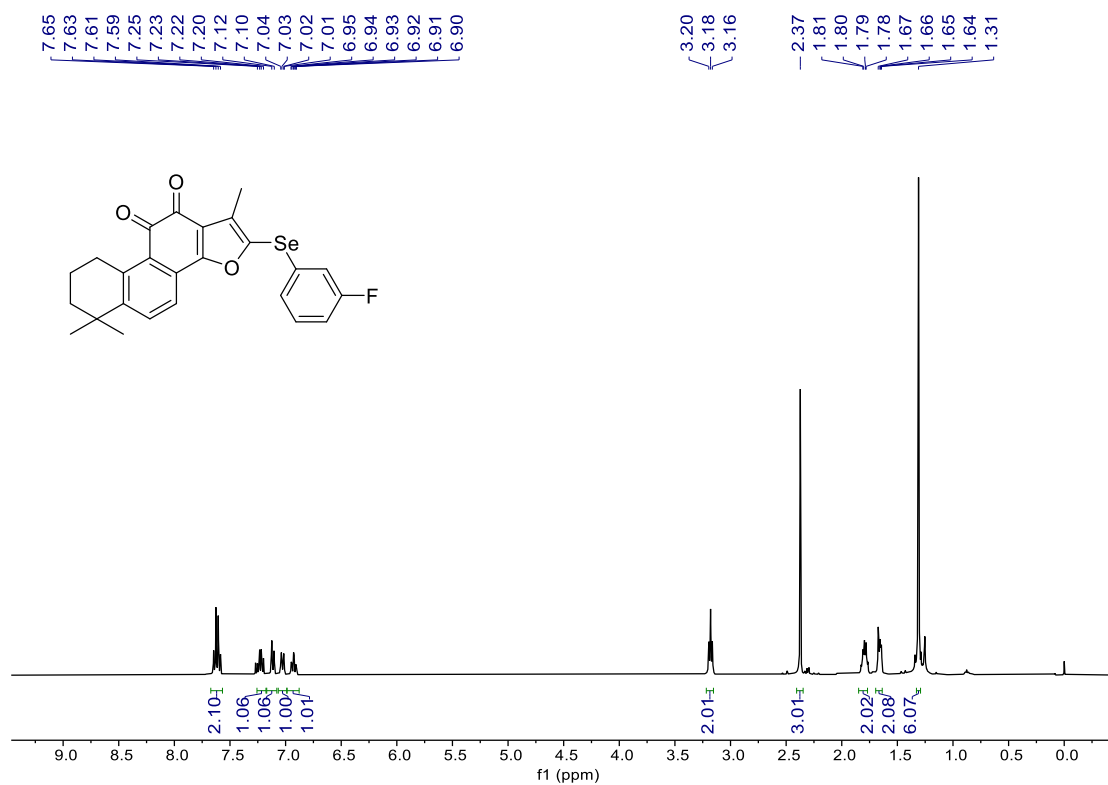
^{13}C NMR (101 MHz, CDCl_3) of compound **2m**



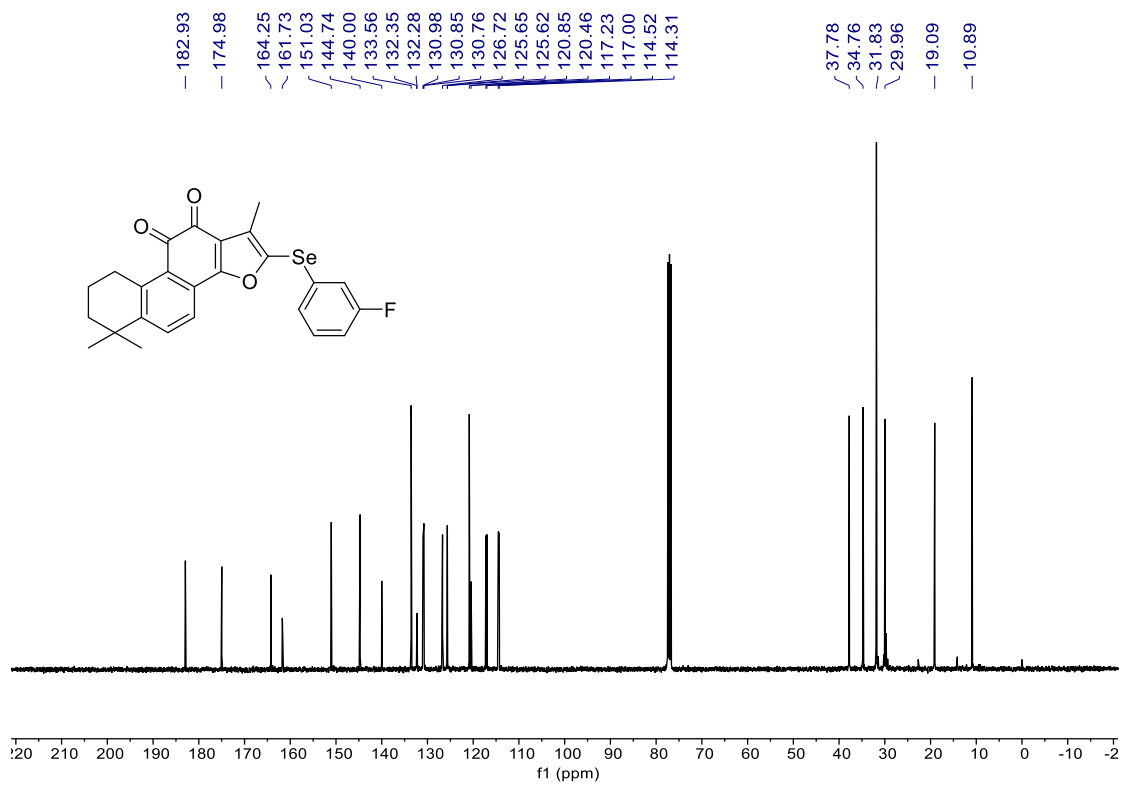
HRMS(ESI) of compound **2m**



^1H NMR (400 MHz, CDCl_3) of compound **2n**



^{13}C NMR (101 MHz, CDCl_3) of compound **2n**



Chemical structure of the compound is shown above the spectrum. The structure is a complex molecule featuring a central benzene ring substituted with a cyclohexyl group, a carbonyl group, and a furan ring. The furan ring is further substituted with a methyl group and a phenyl group. The phenyl group is substituted with a fluorine atom.

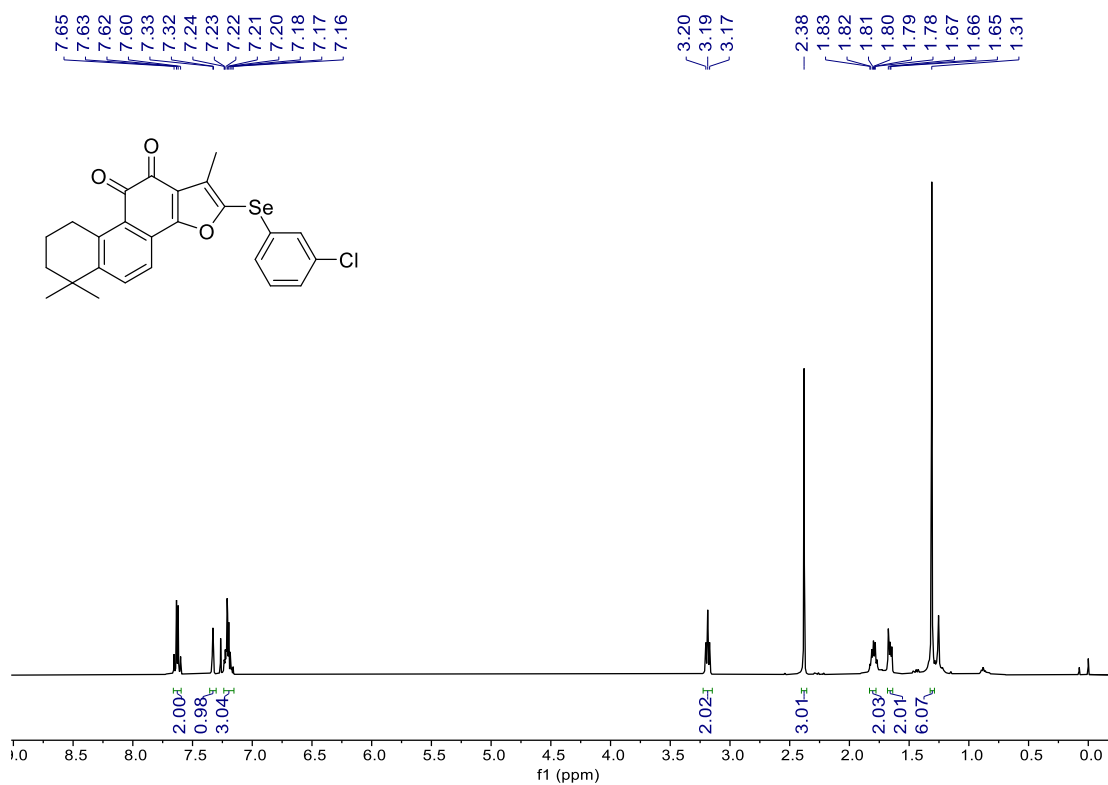
The spectrum shows a single sharp peak at approximately 110.8 ppm, labeled as δ 110.80. The x-axis is labeled "f1 (ppm)" and ranges from 50 to -250 ppm.

Chemical structure of compound 10 is shown above the mass spectrum. The structure is a complex polycyclic molecule featuring a benzene ring fused to a cyclohexane ring, which is further fused to a pyrone ring. A selenophene ring is attached to the pyrone ring, and a fluorophenyl group is attached to the selenophene ring.

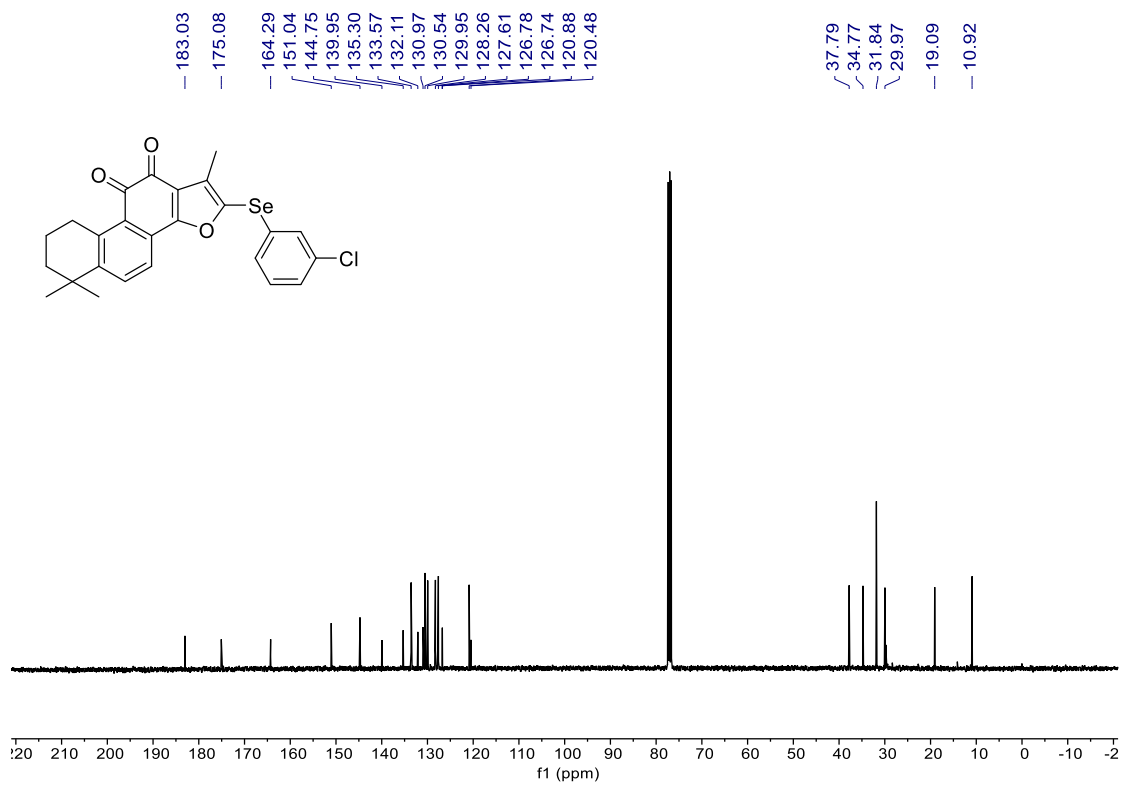
Mass spectrum data (m/z vs. Intensity):

m/z	Relative Intensity (%)
465.0624	~550
467.0668	~1150
469.0710	100 (Base Peak)
470.0747	~550

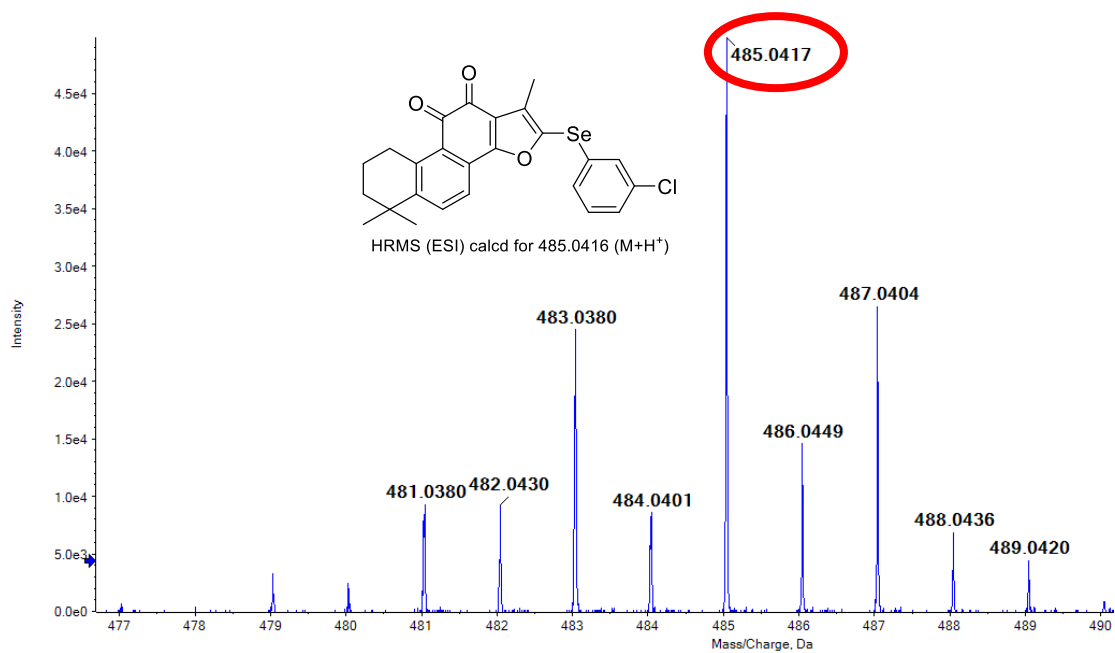
^1H NMR (400 MHz, CDCl_3) of compound **2o**



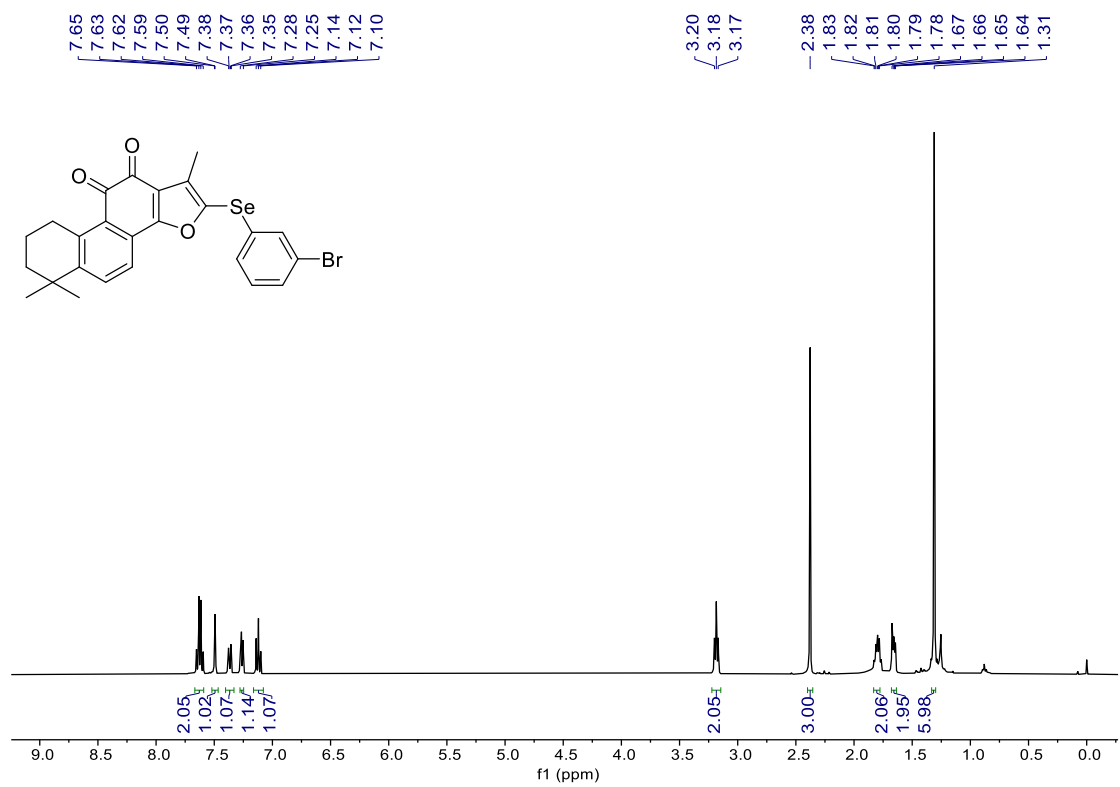
^{13}C NMR (101 MHz, CDCl_3) of compound **2o**



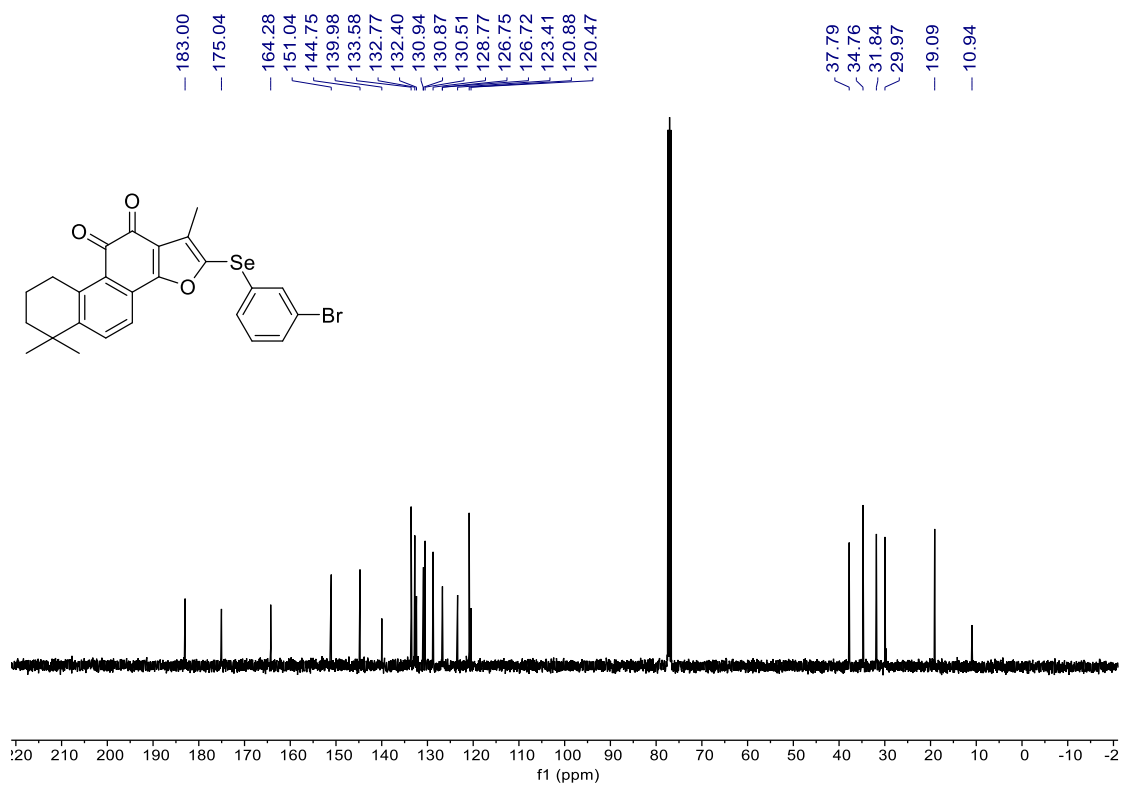
HRMS(ESI) of compound **2o**



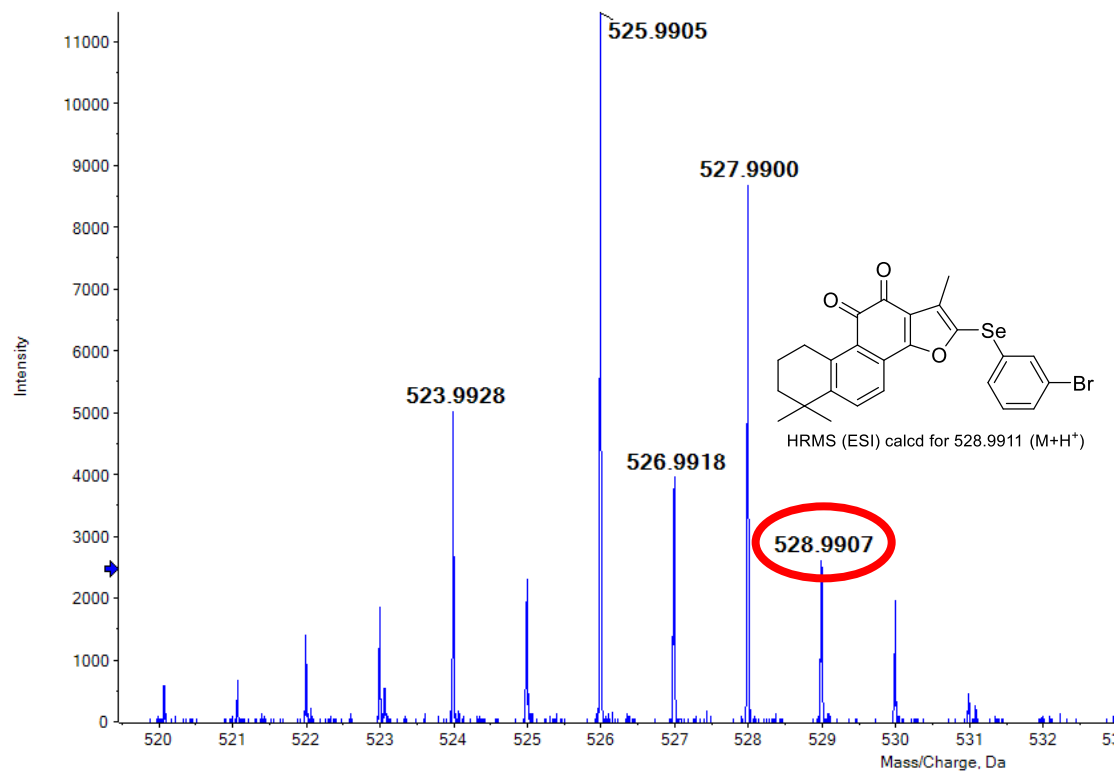
^1H NMR (400 MHz, CDCl_3) of compound **2p**



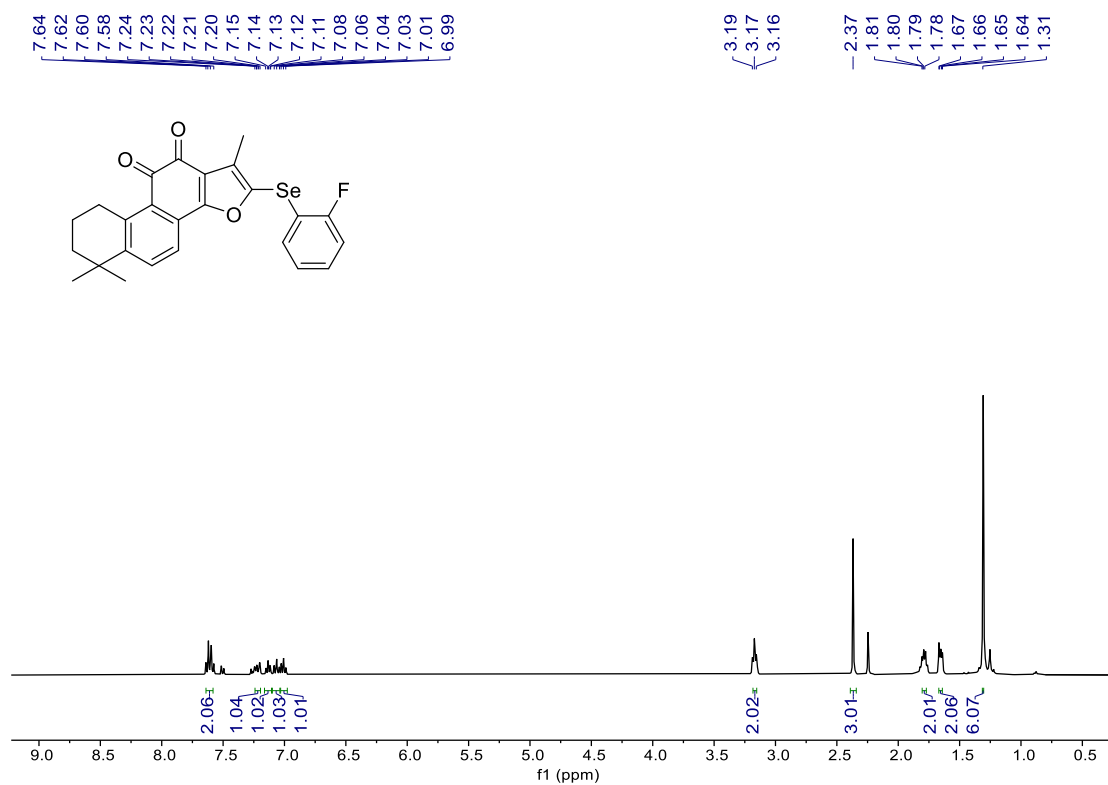
^{13}C NMR (101 MHz, CDCl_3) of compound **2p**



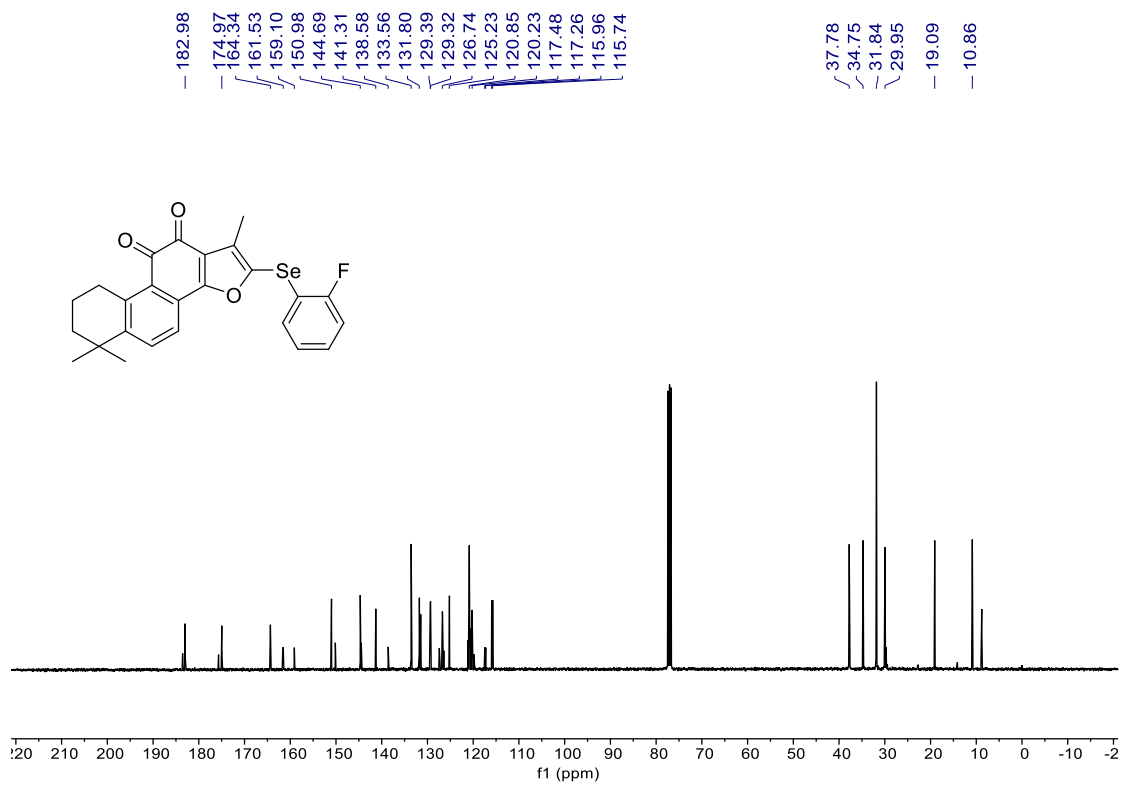
HRMS(ESI) of compound **2p**



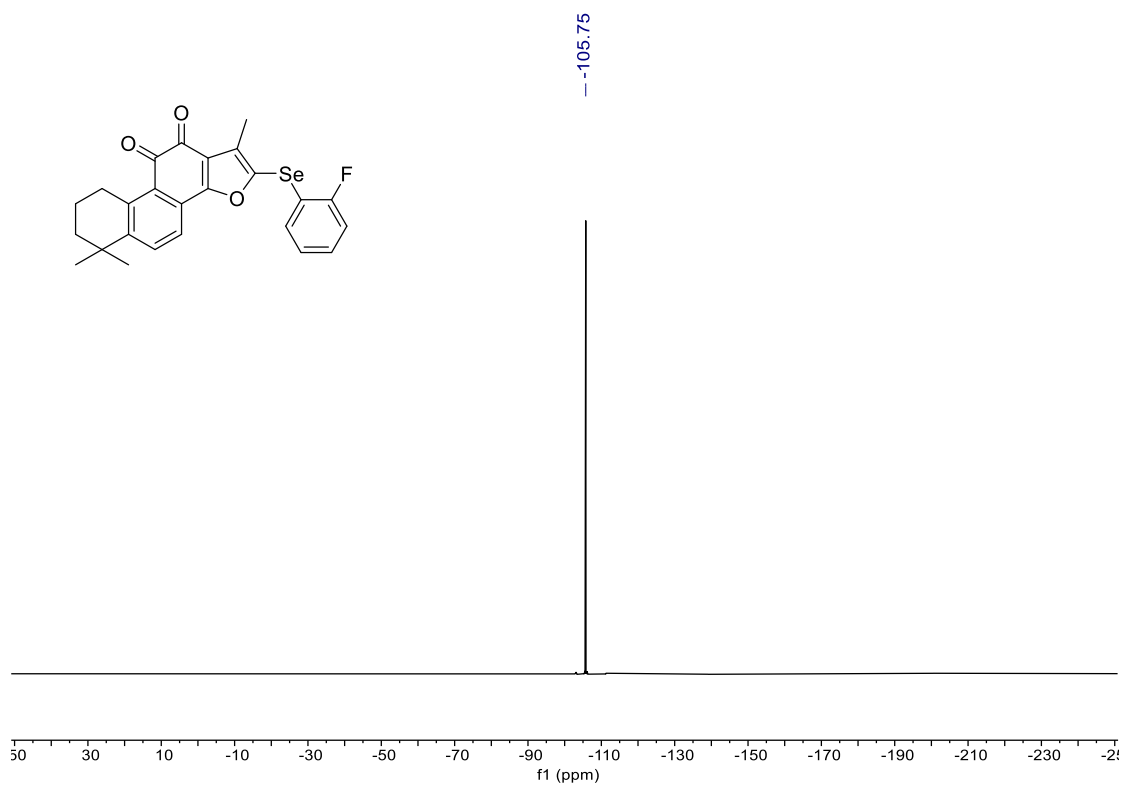
^1H NMR (400 MHz, CDCl_3) of compound **2q**



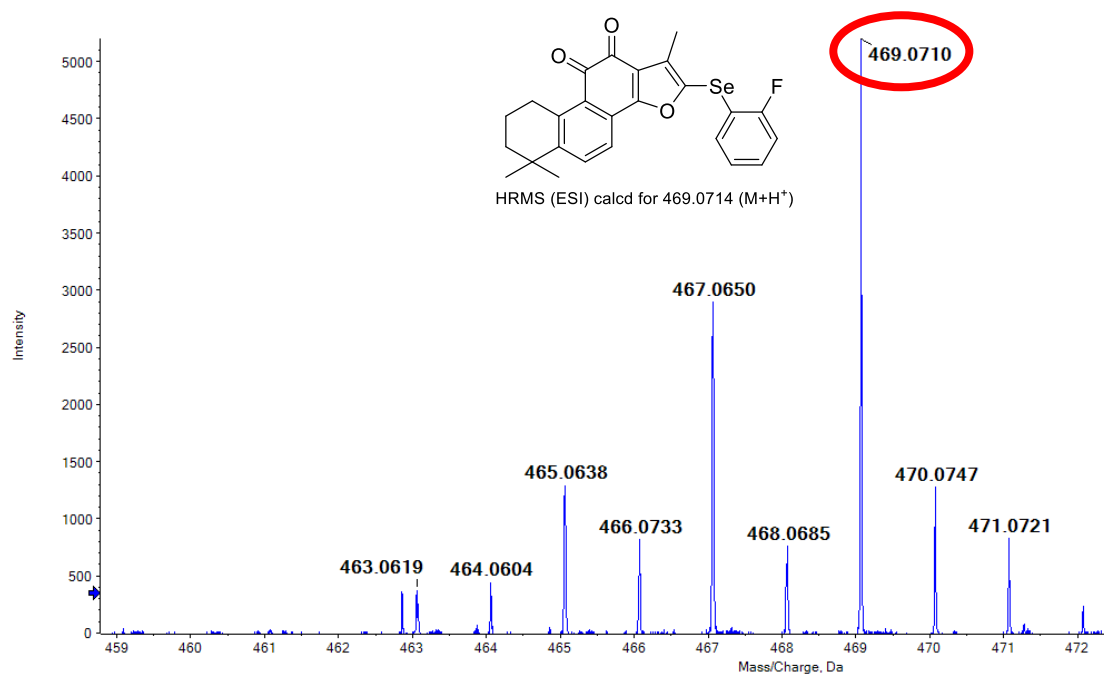
^{13}C NMR (101 MHz, CDCl_3) of compound **2q**



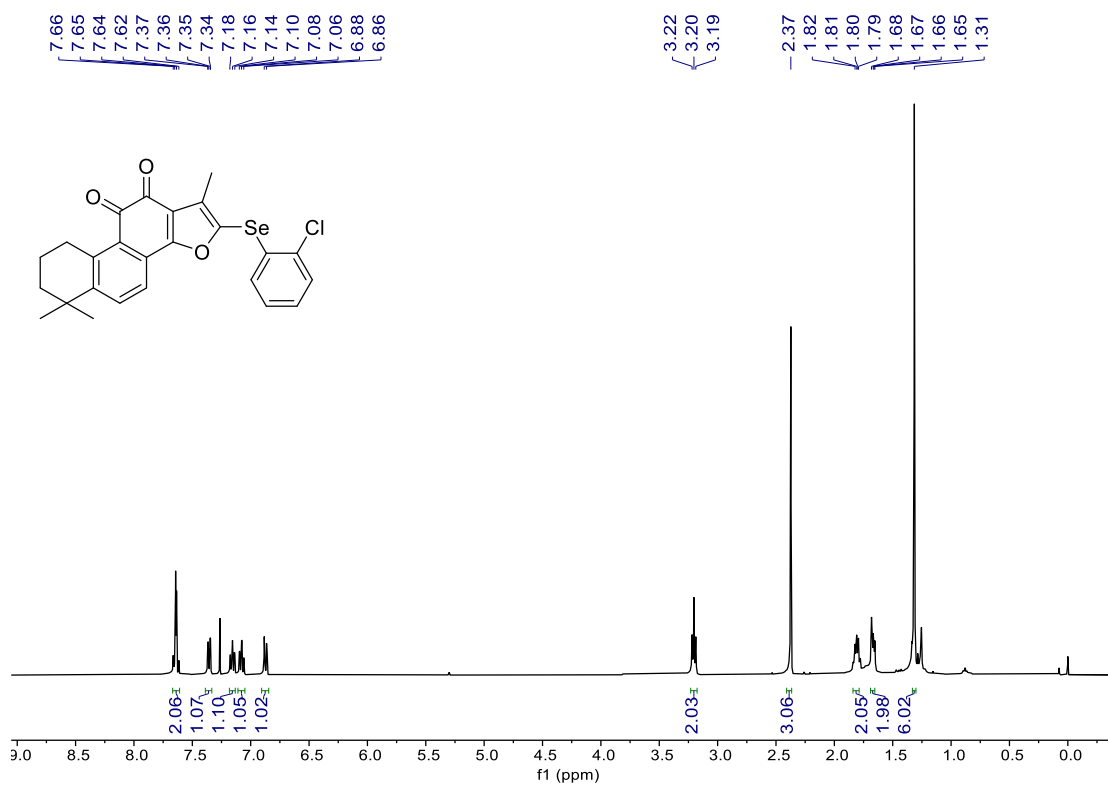
^{19}F NMR (376 MHz, CDCl_3) of compound **2q**



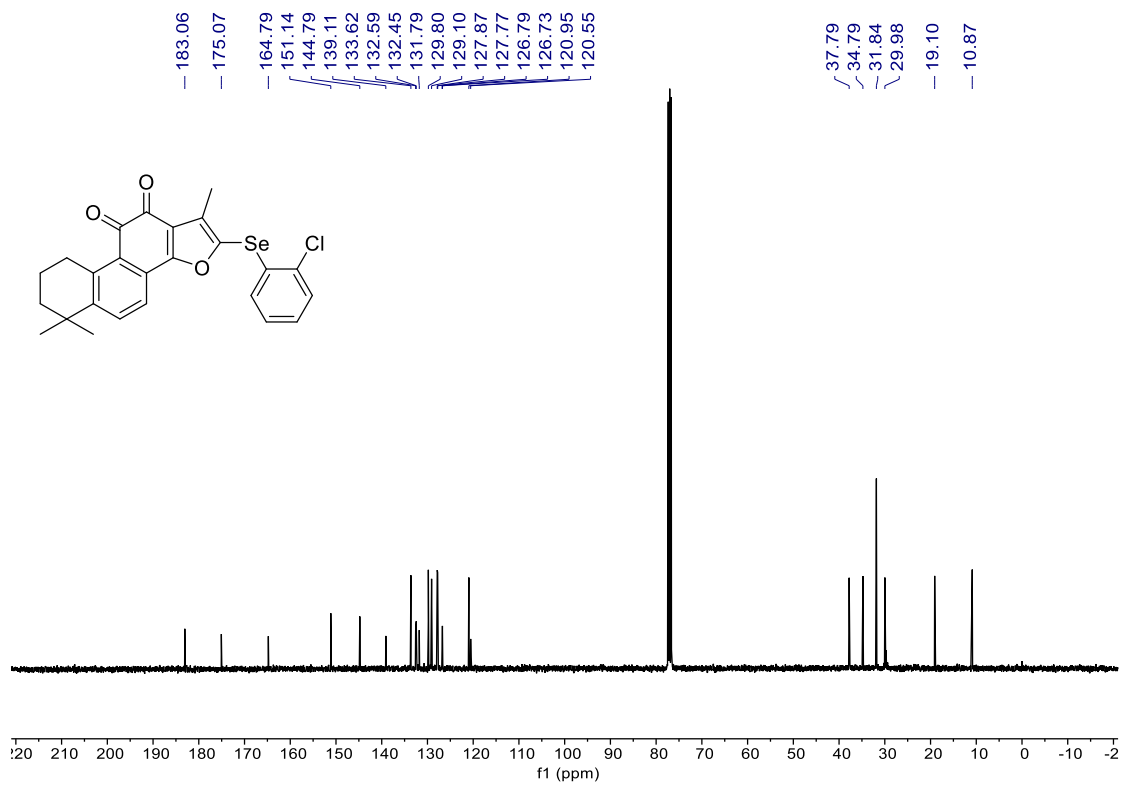
HRMS(ESI) of compound **2q**



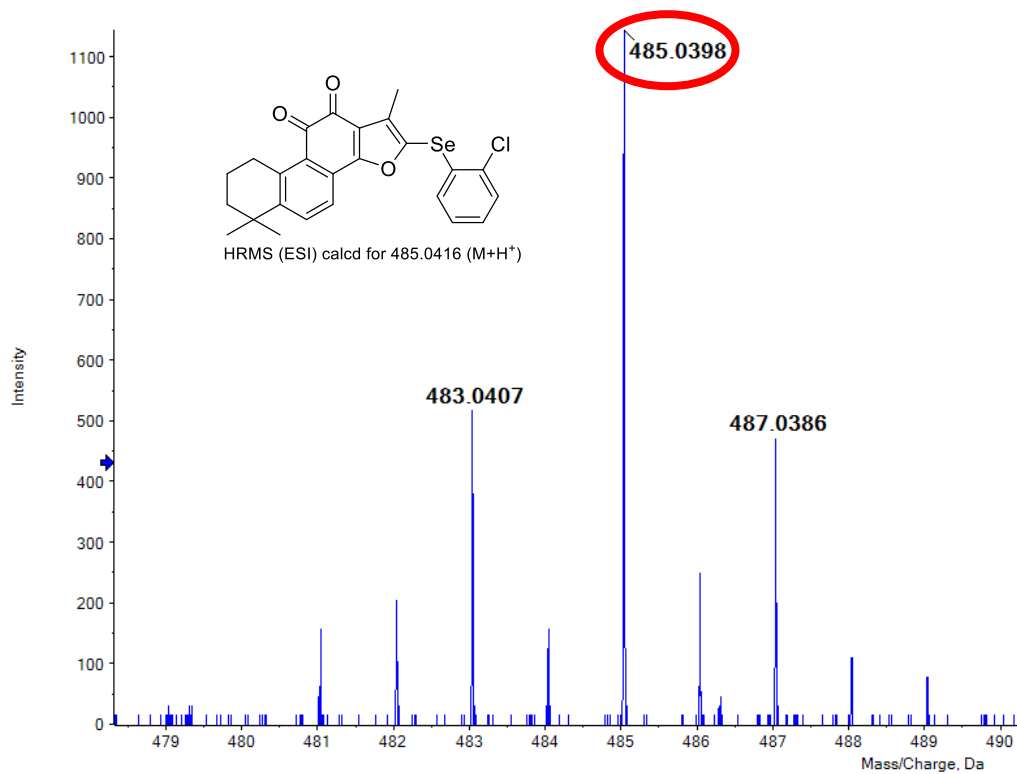
^1H NMR (400 MHz, CDCl_3) of compound **2r**



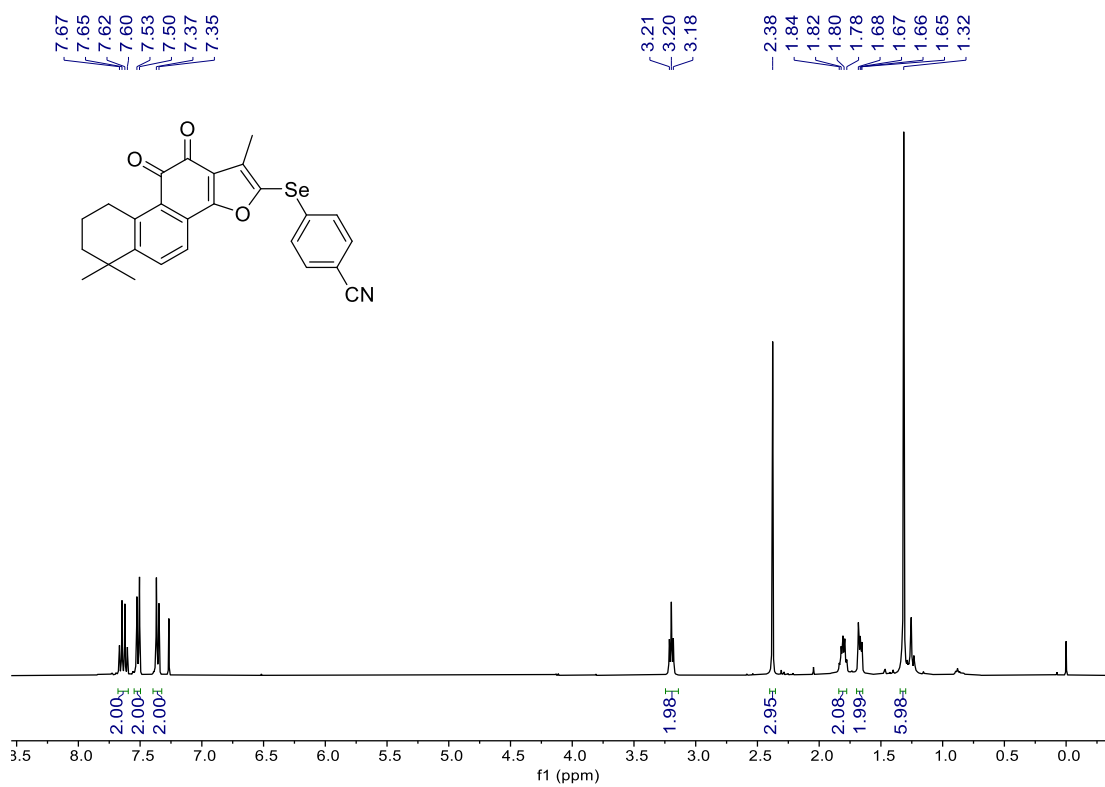
^{13}C NMR (101 MHz, CDCl_3) of compound **2r**



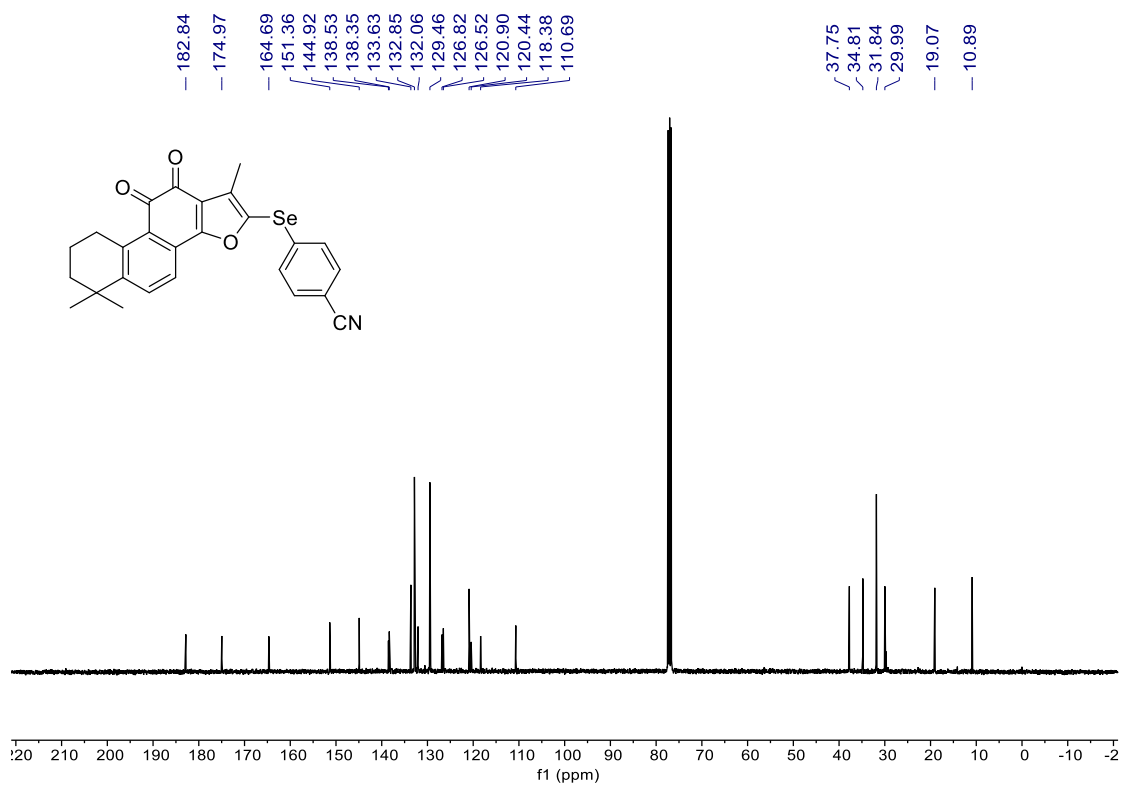
HRMS(ESI) of compound **2r**



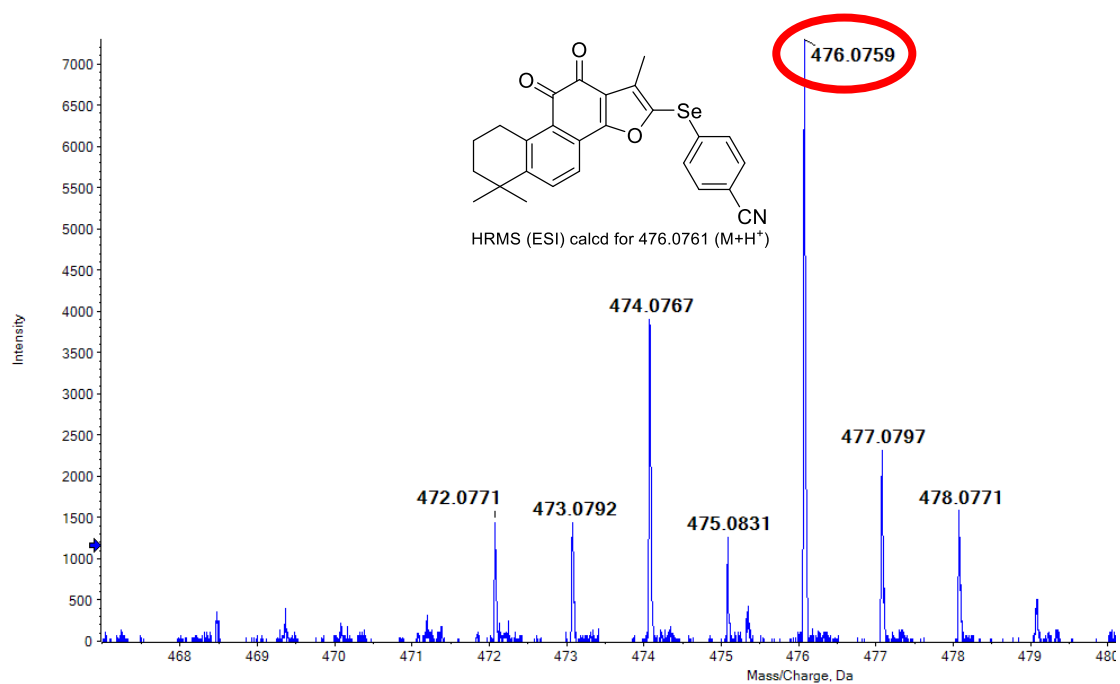
^1H NMR (400 MHz, CDCl_3) of compound **2s**



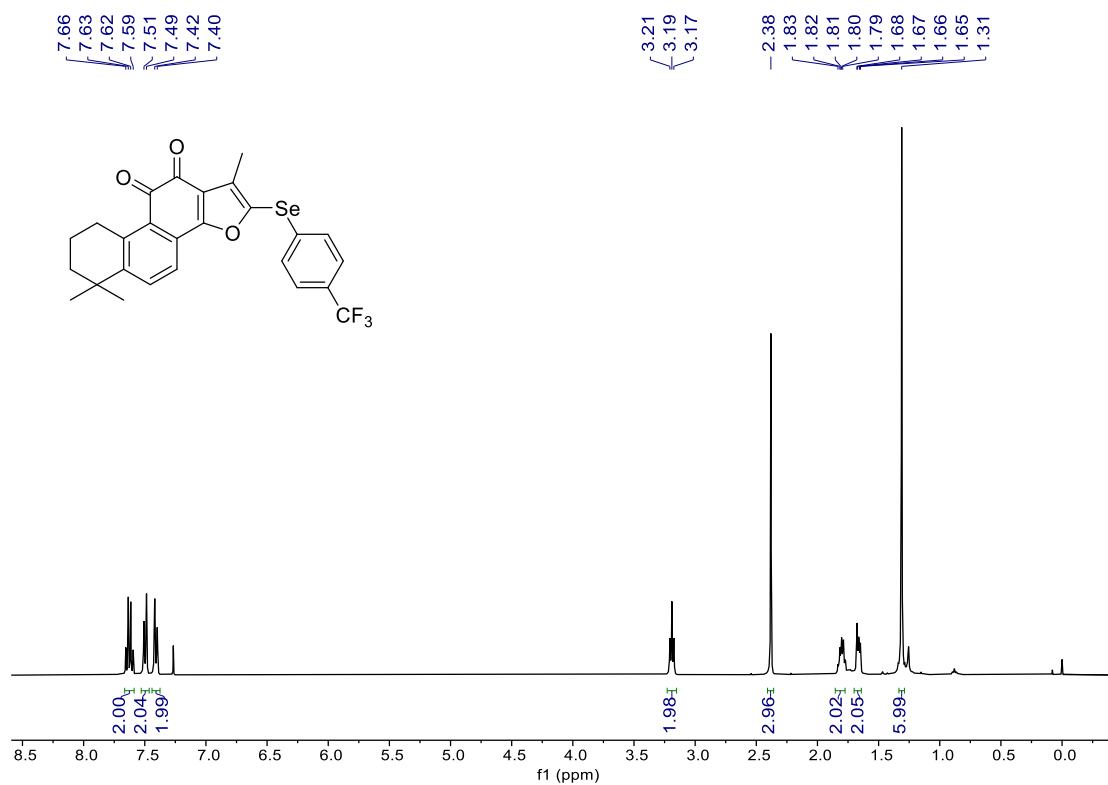
^{13}C NMR (101 MHz, CDCl_3) of compound **2s**



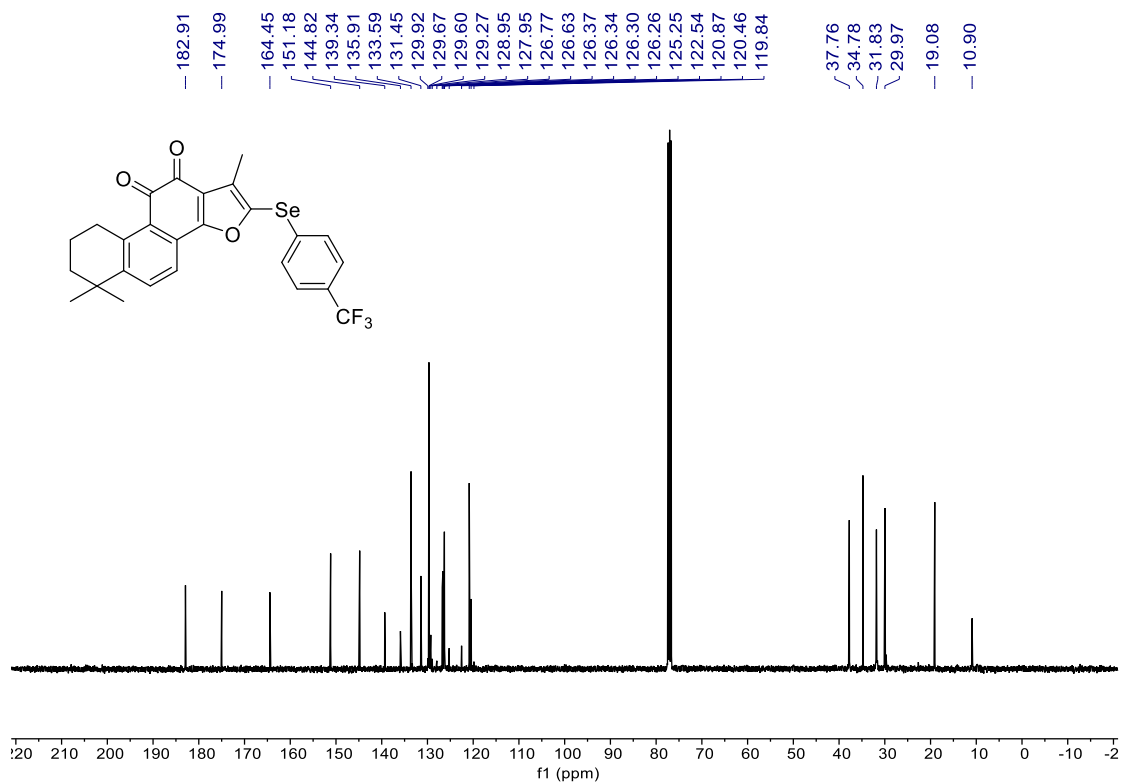
HRMS(ESI) of compound **2s**



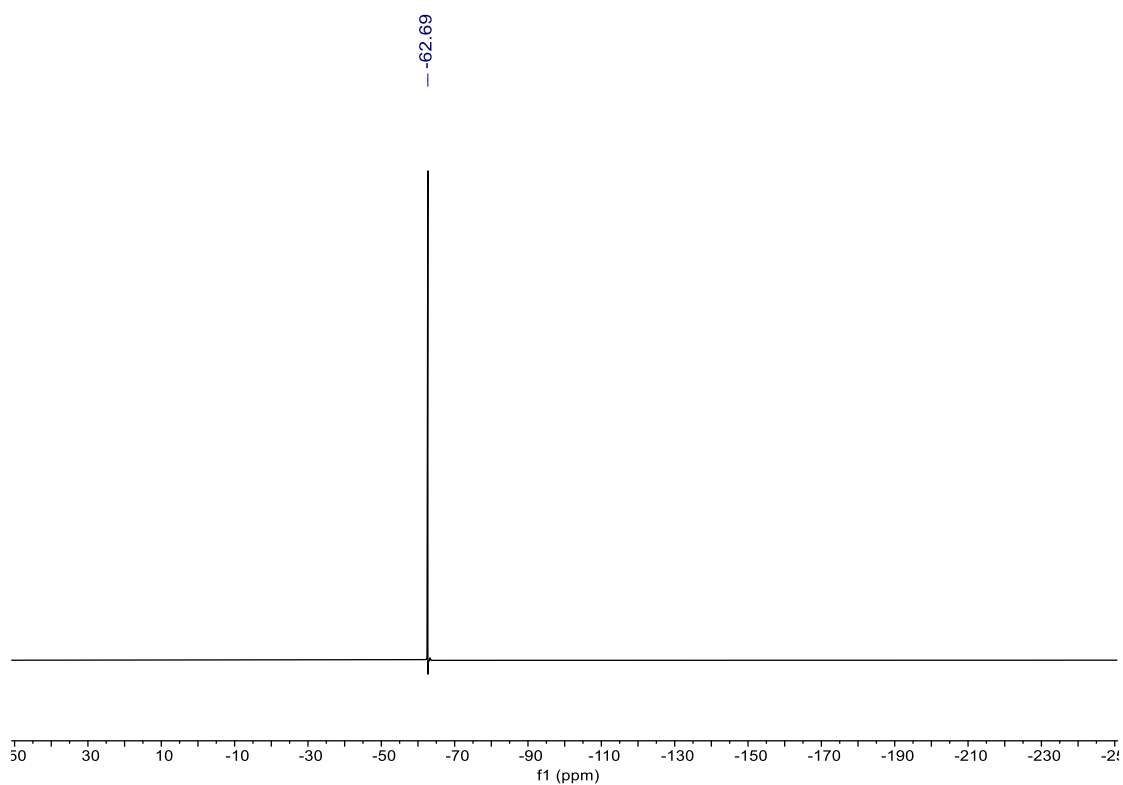
^1H NMR (400 MHz, CDCl_3) of compound **2t**



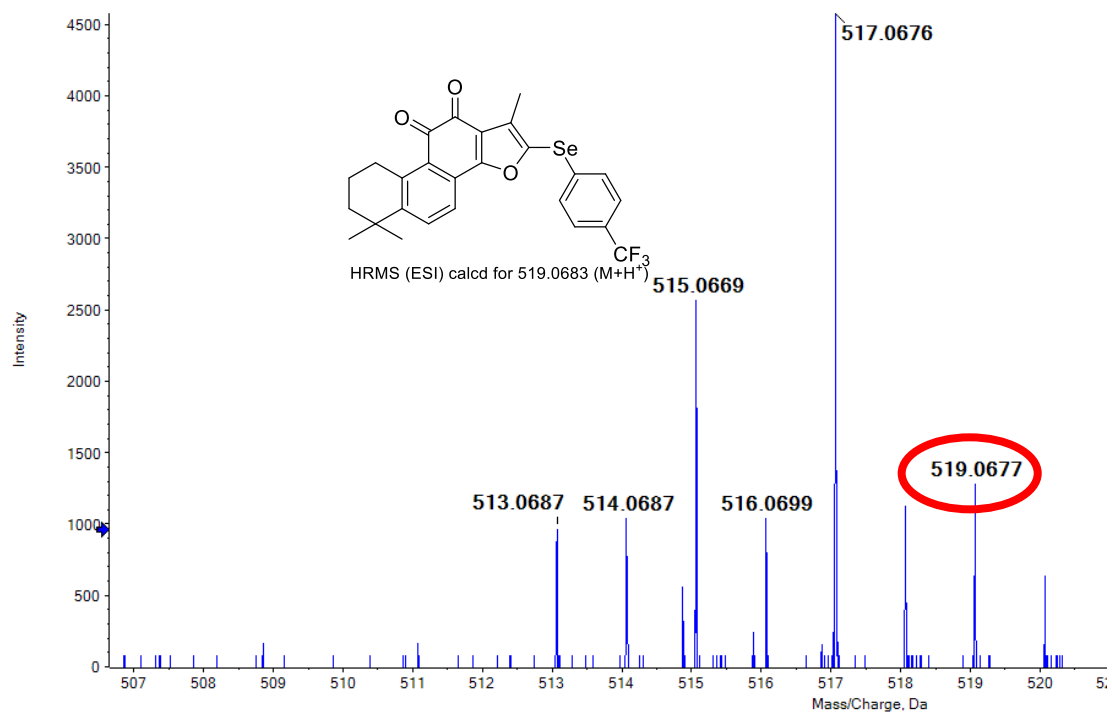
^{13}C NMR (101 MHz, CDCl_3) of compound **2t**



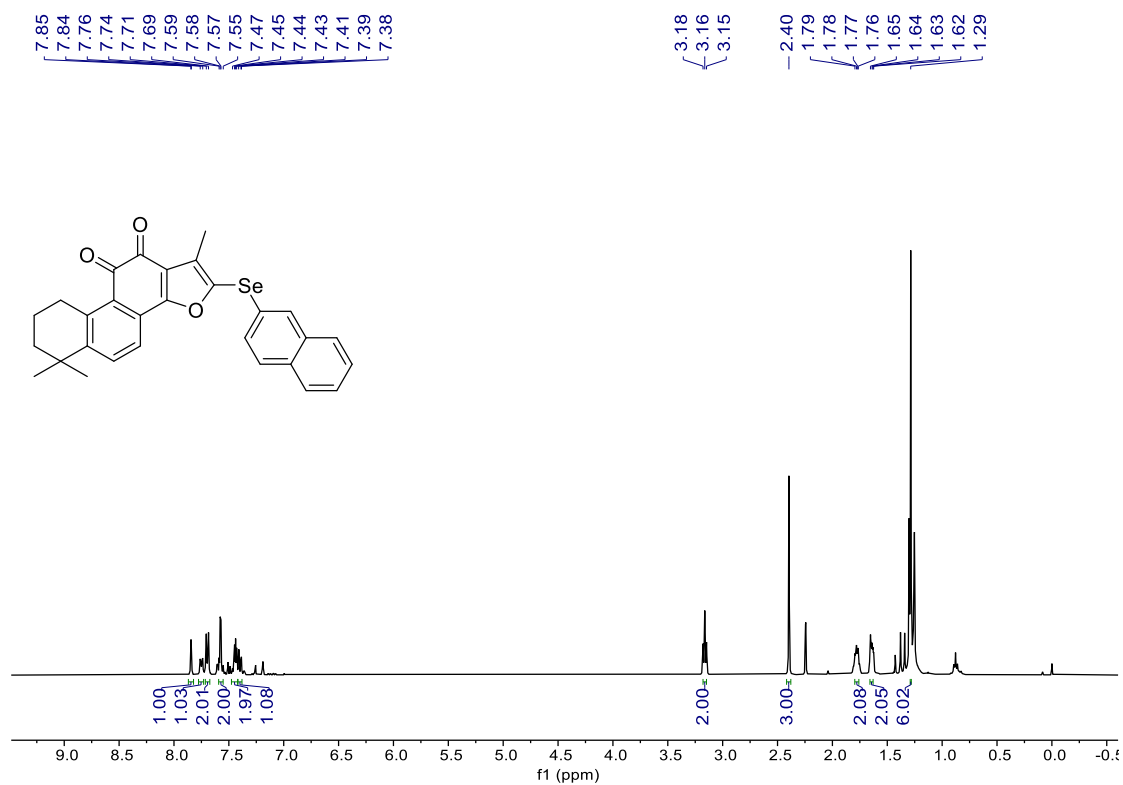
^{19}F NMR (376 MHz, CDCl_3) of compound **2t**



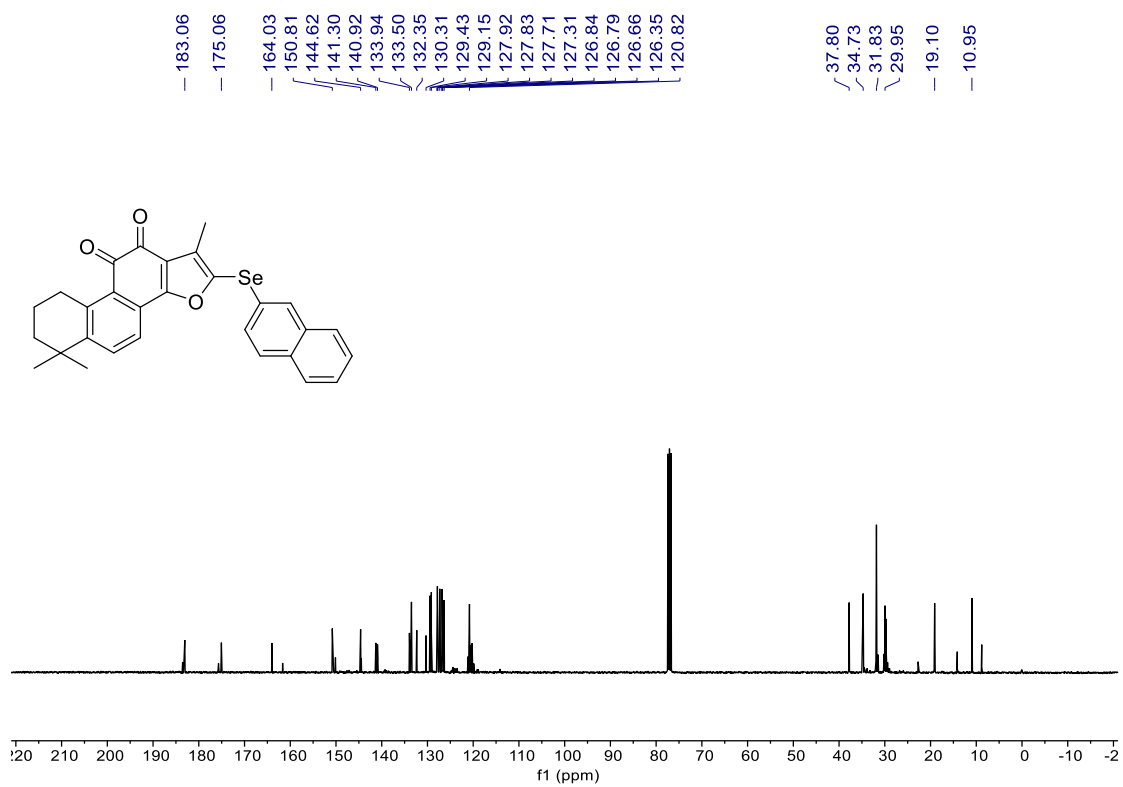
HRMS(ESI) of compound **2t**



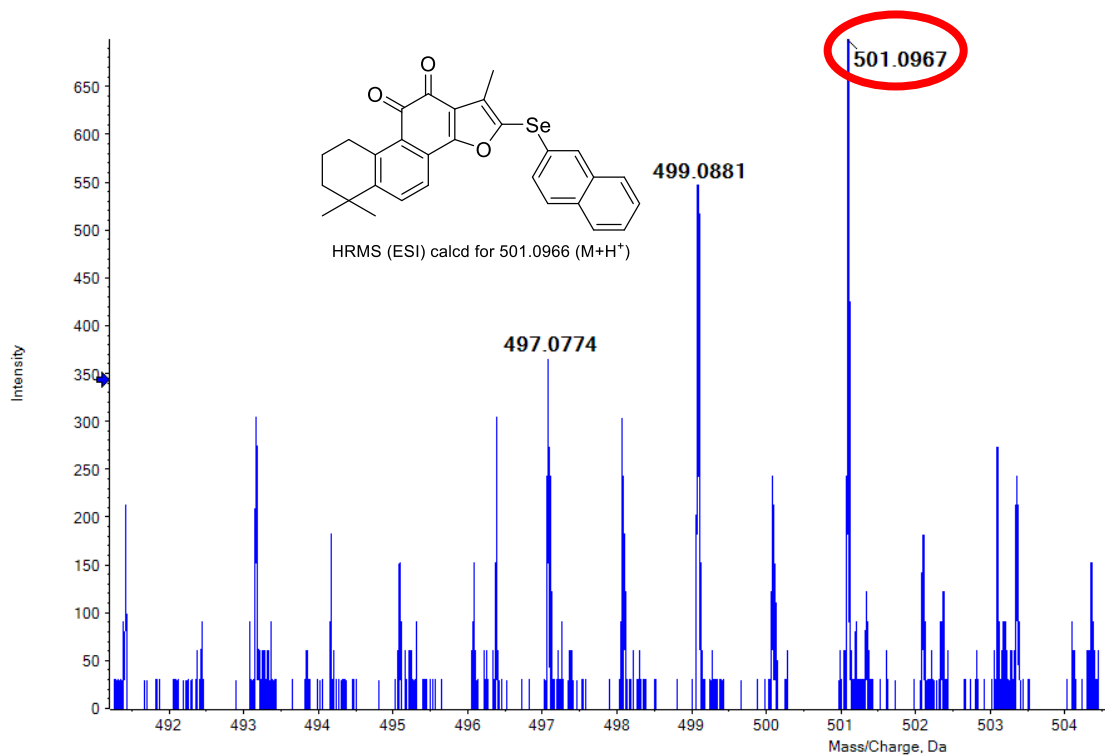
^1H NMR (400 MHz, CDCl_3) of compound **2u**



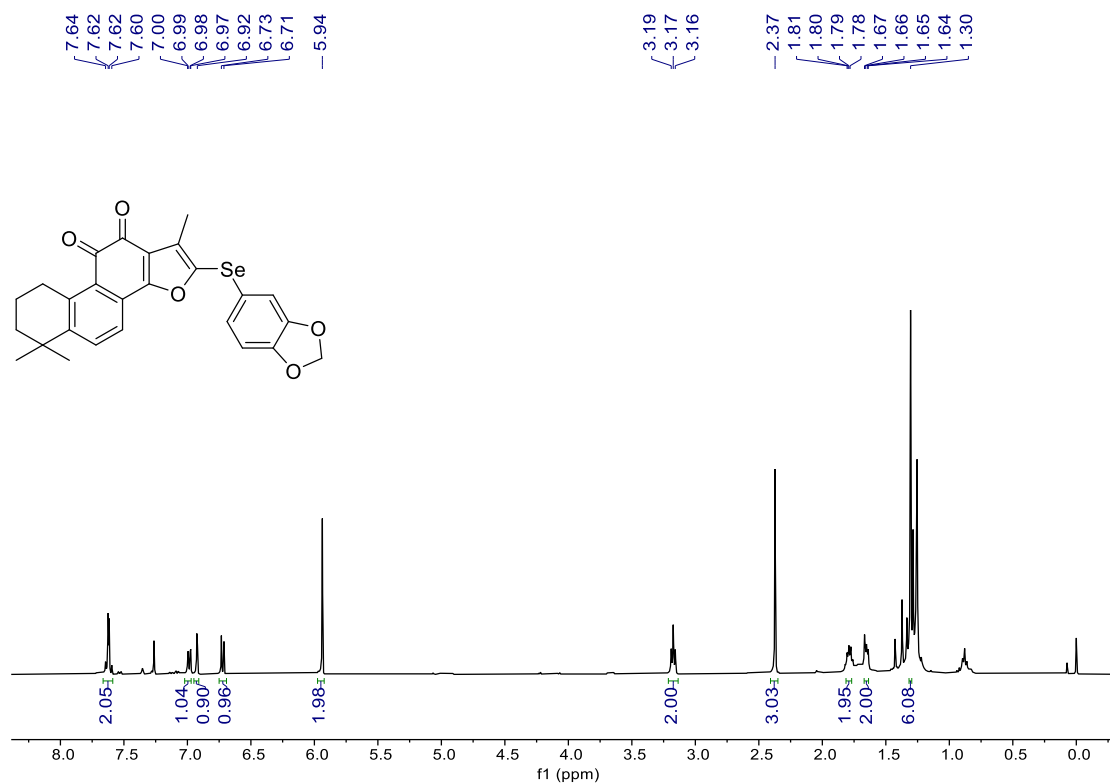
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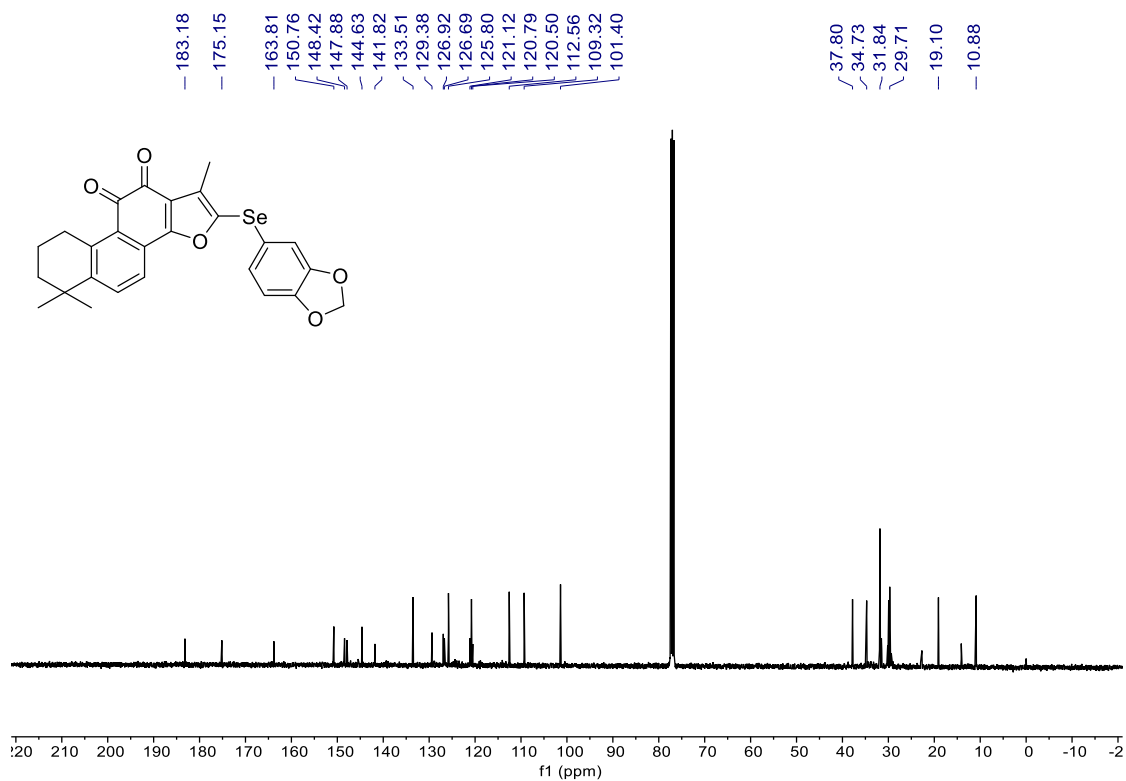
HRMS(ESI) of compound **2u**



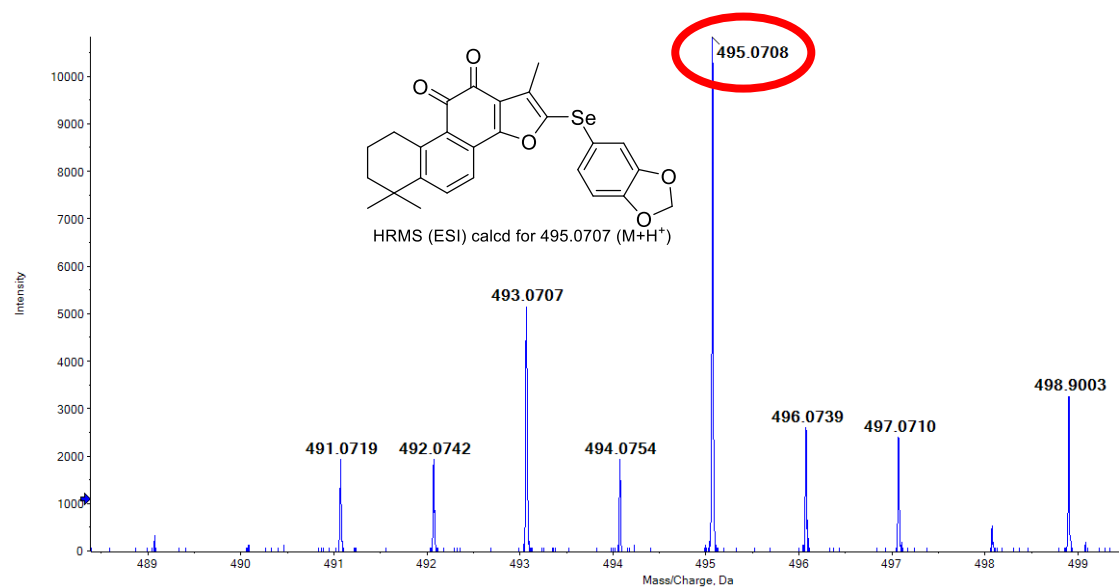
^1H NMR (400 MHz, CDCl_3) of compound **2v**



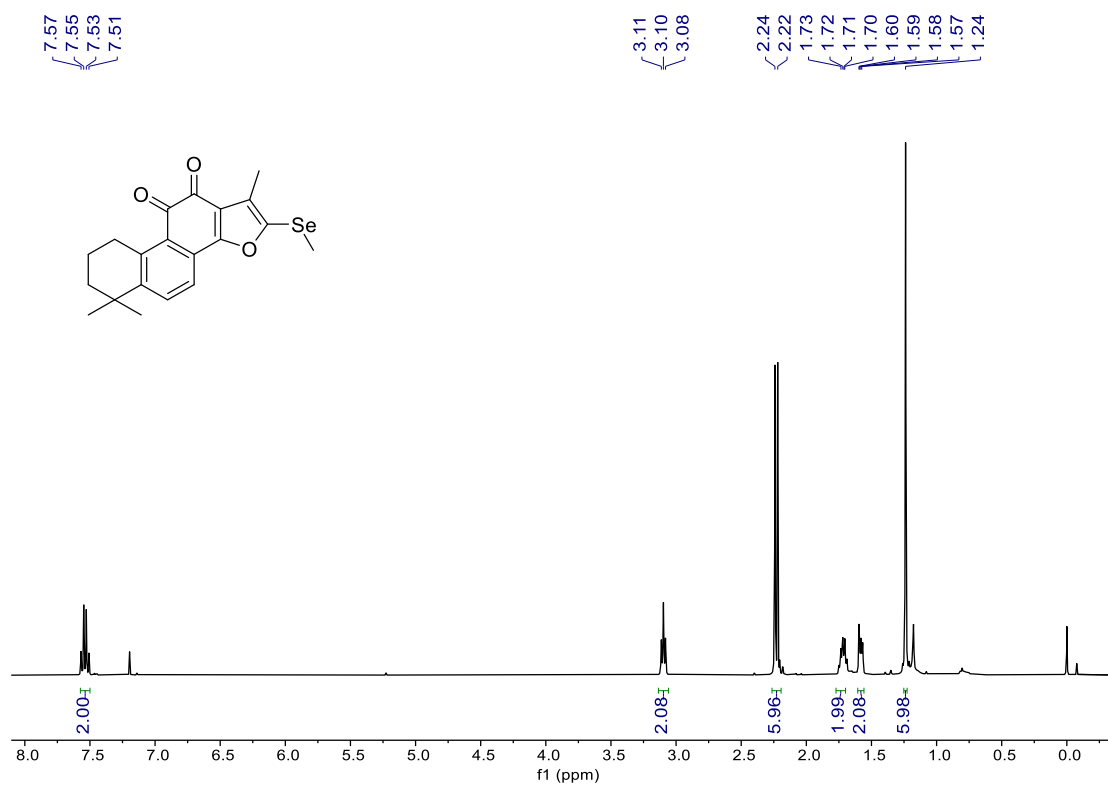
^{13}C NMR (101 MHz, CDCl_3) of compound **2v**



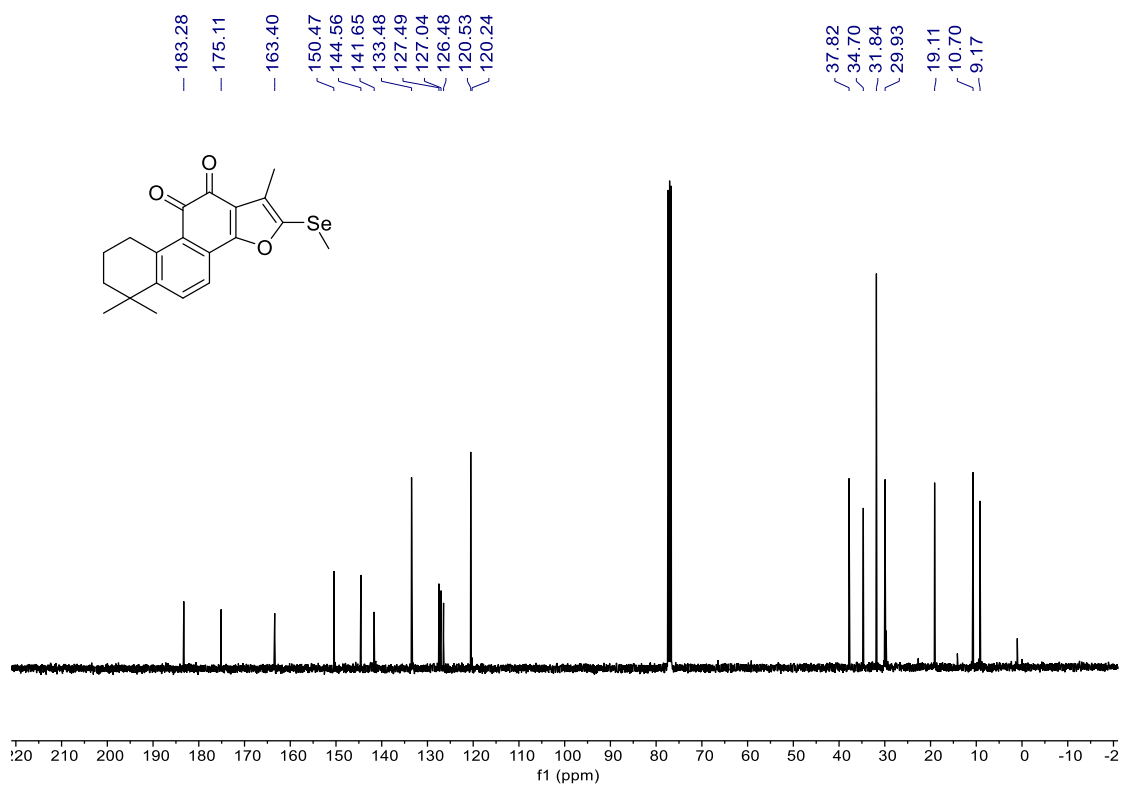
HRMS(ESI) of compound **2v**



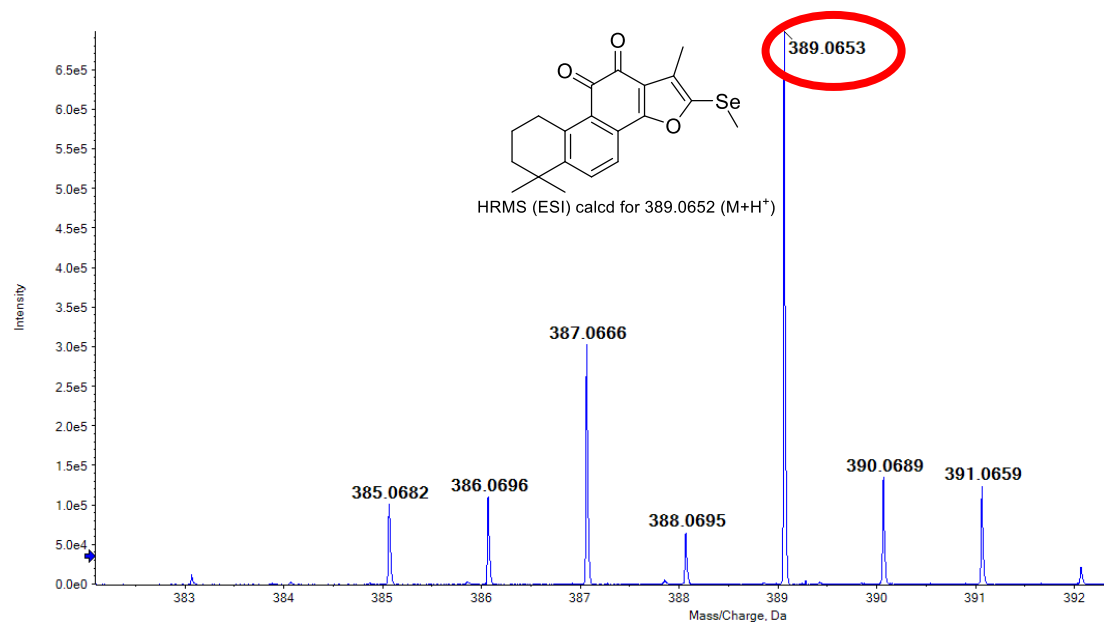
^1H NMR (400 MHz, CDCl_3) of compound **2w**



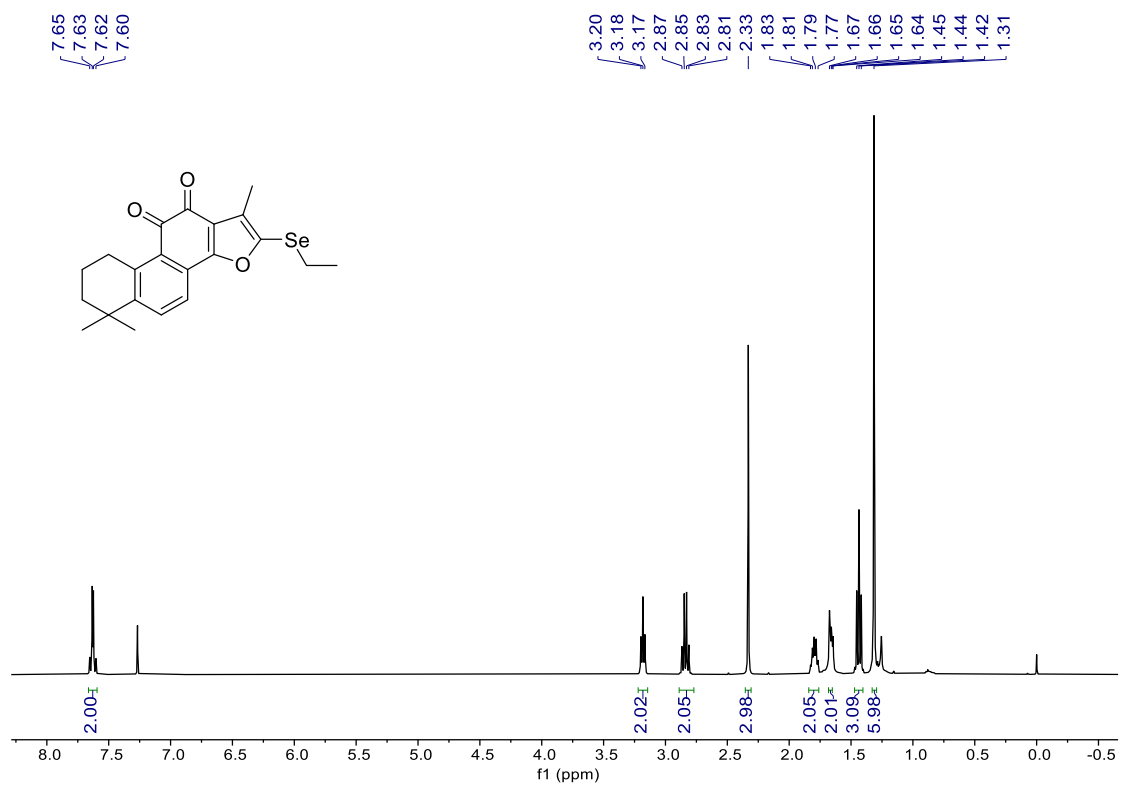
^{13}C NMR (101 MHz, CDCl_3) of compound **2w**



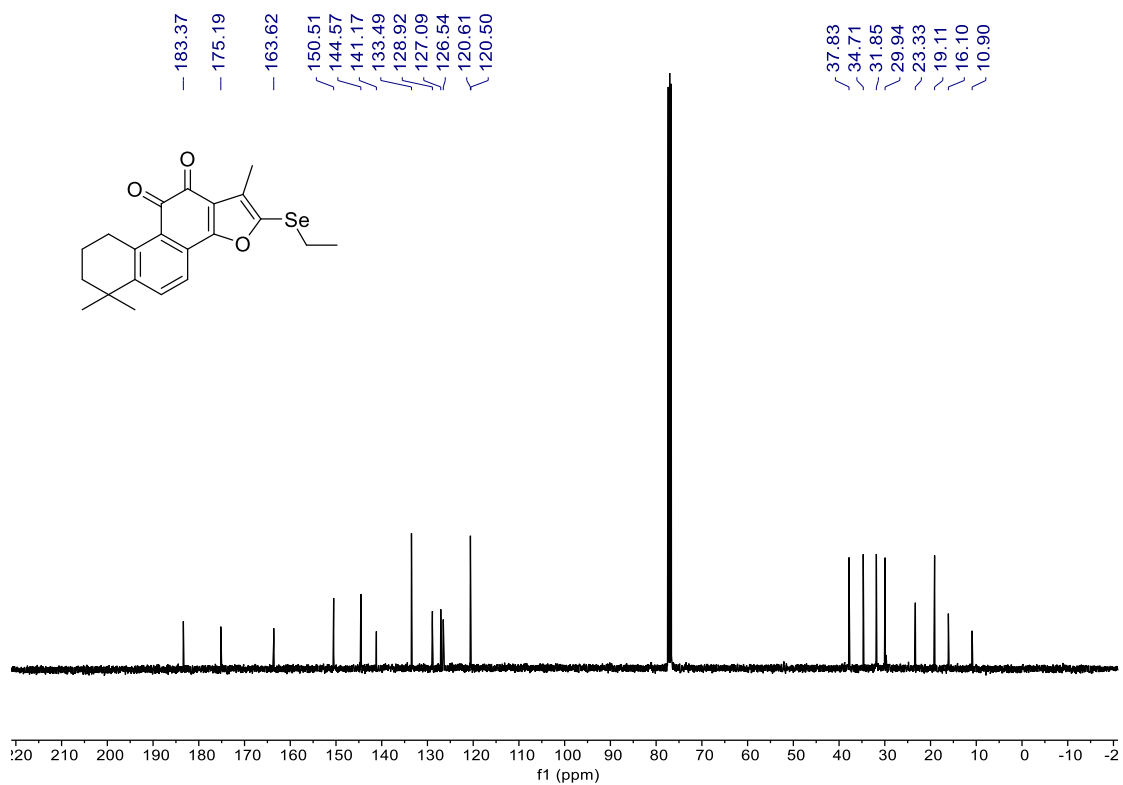
HRMS(ESI) of compound **2w**



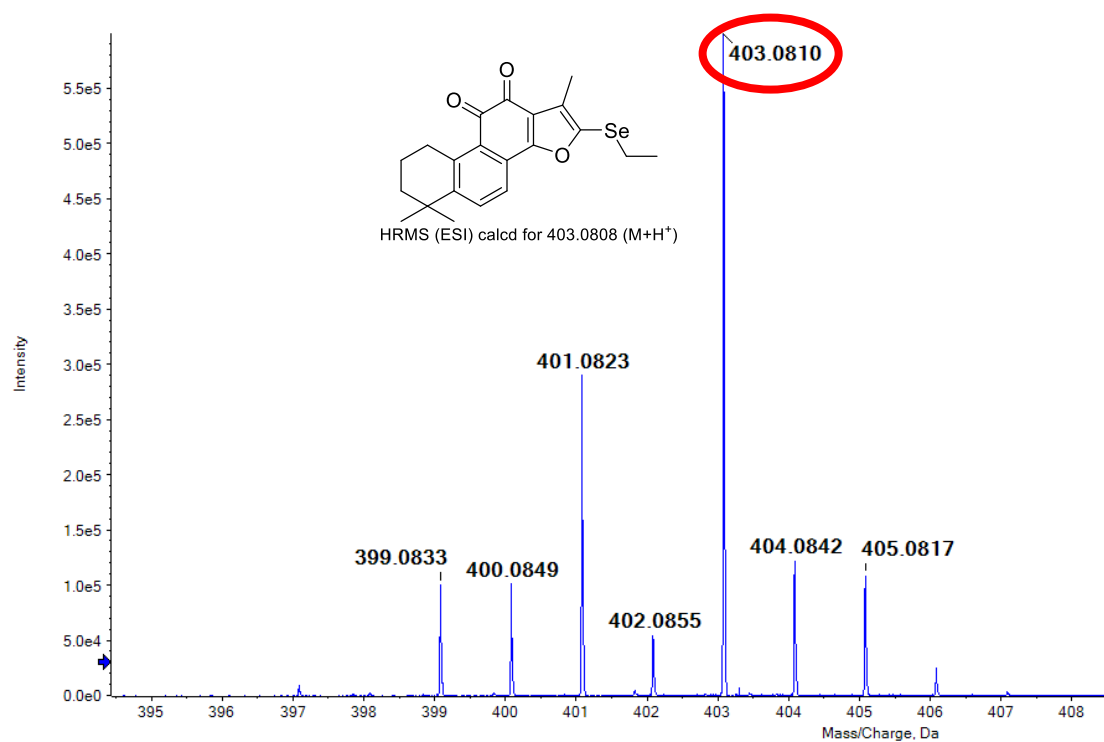
^1H NMR (400 MHz, CDCl_3) of compound **2x**



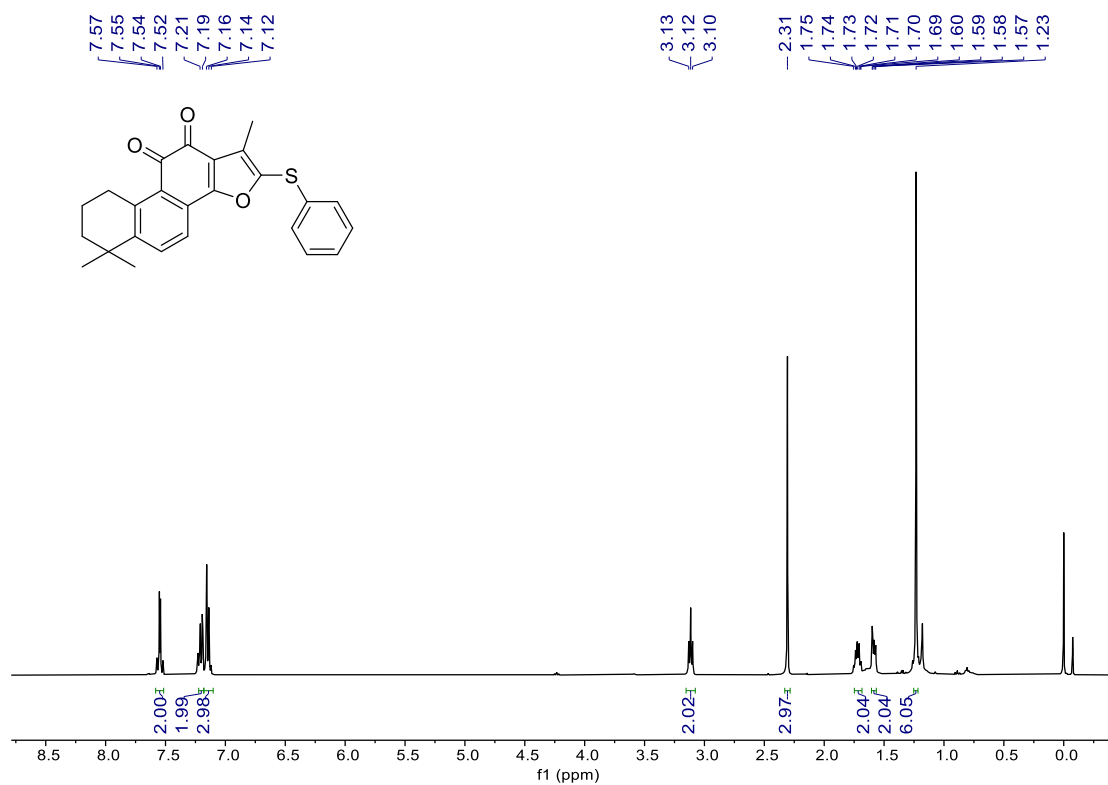
^{13}C NMR (101 MHz, CDCl_3) of compound **2x**



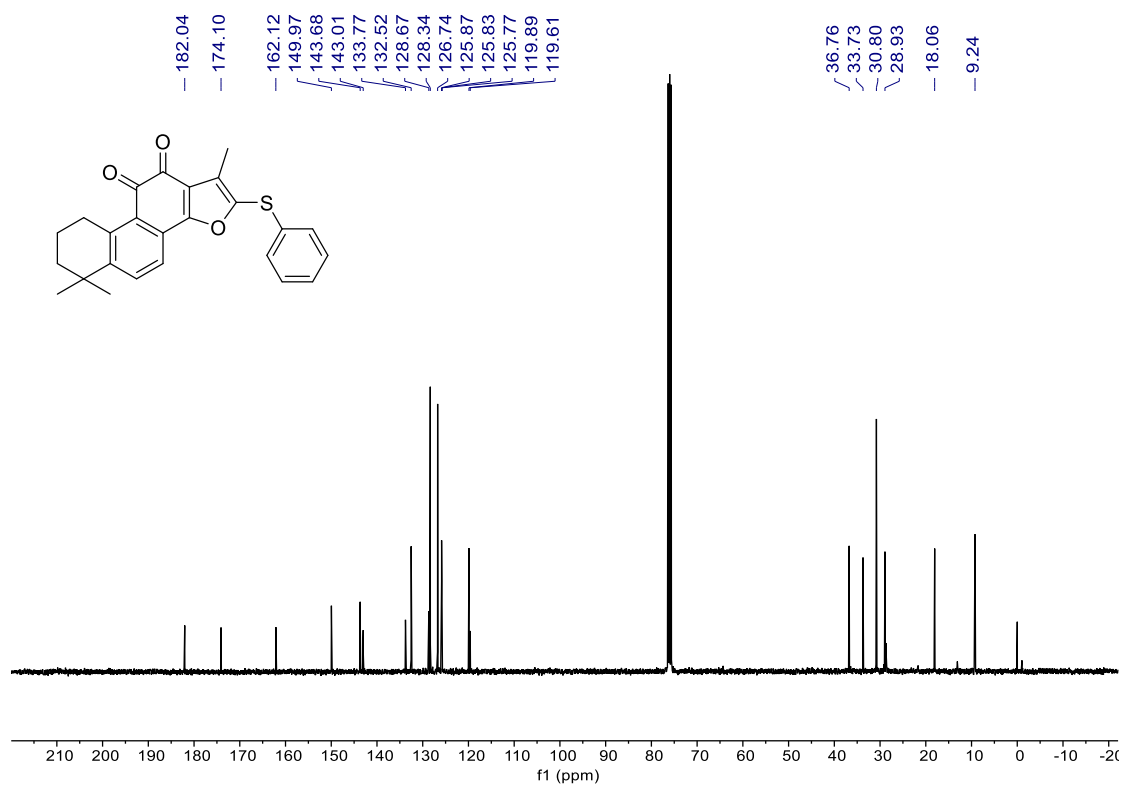
HRMS(ESI) of compound **2x**



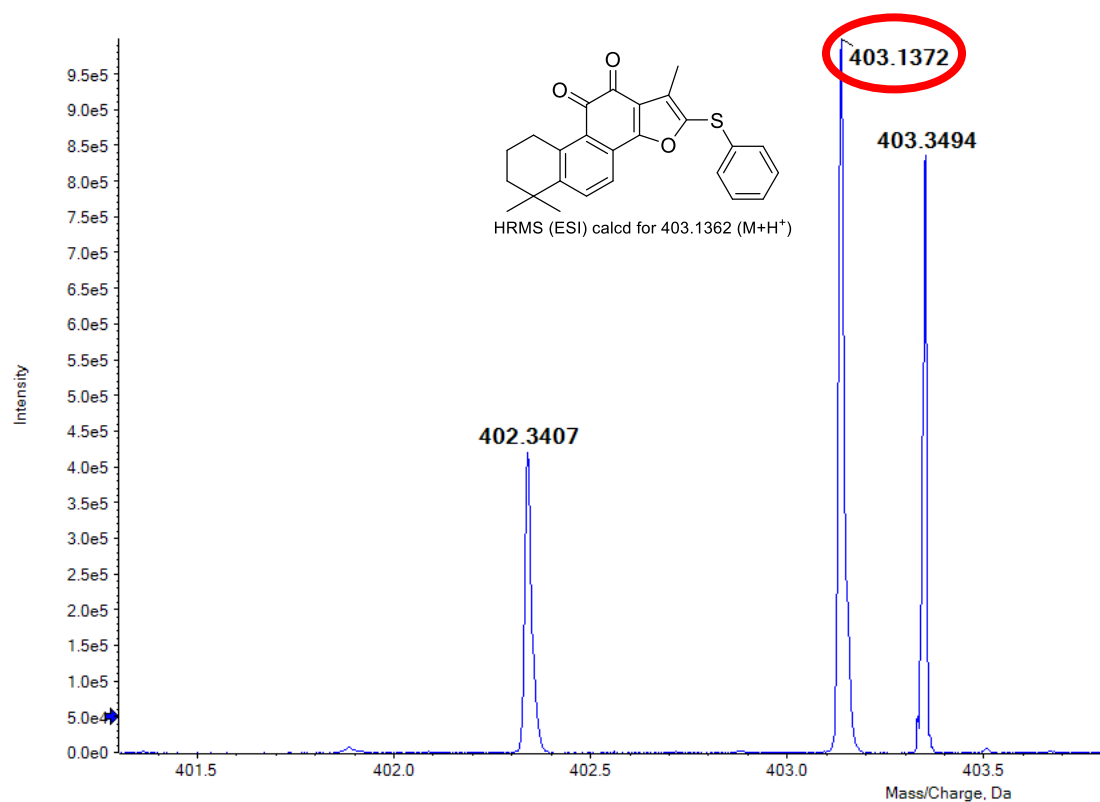
^1H NMR (400 MHz, CDCl_3) of compound **2y**



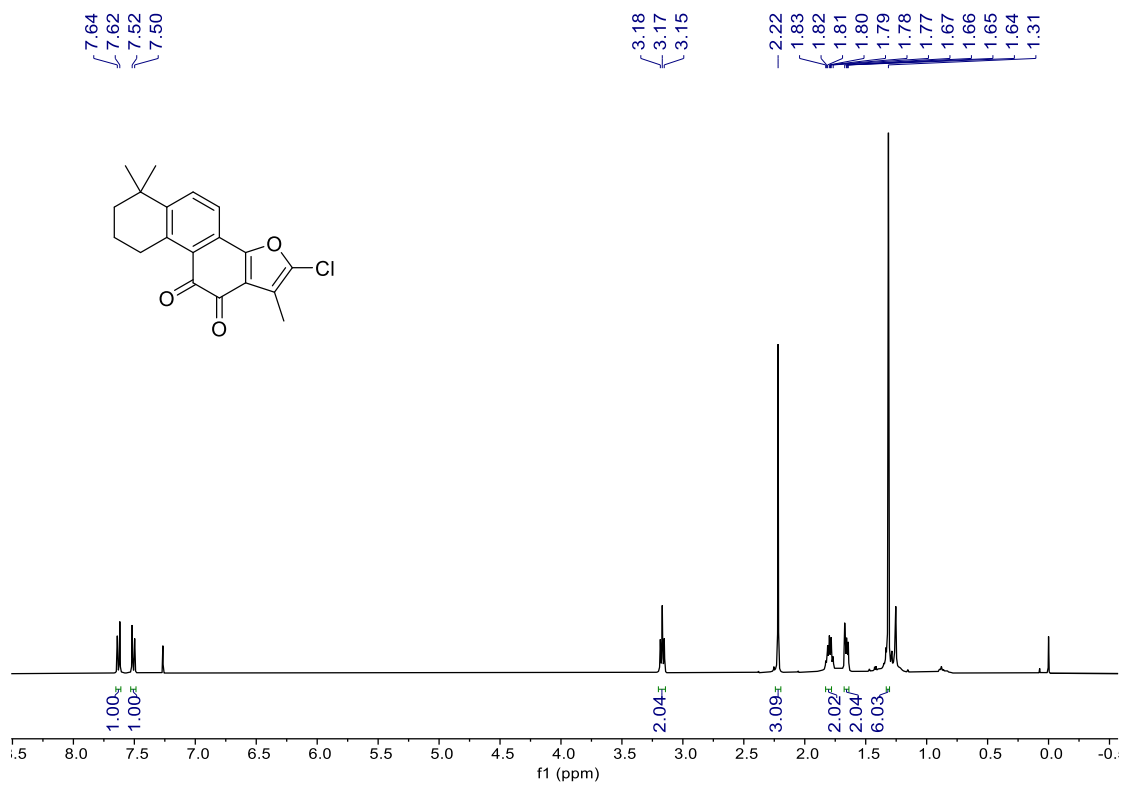
^{13}C NMR (101 MHz, CDCl_3) of compound **2y**



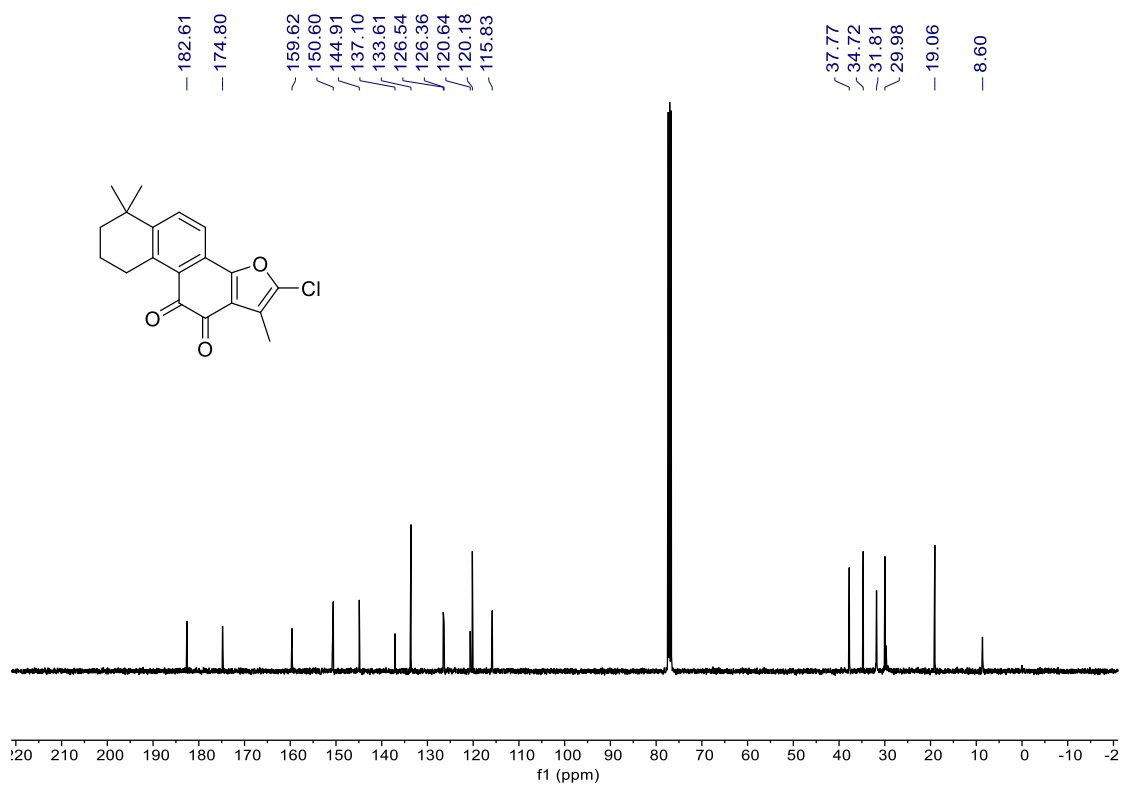
HRMS(ESI) of compound **2y**



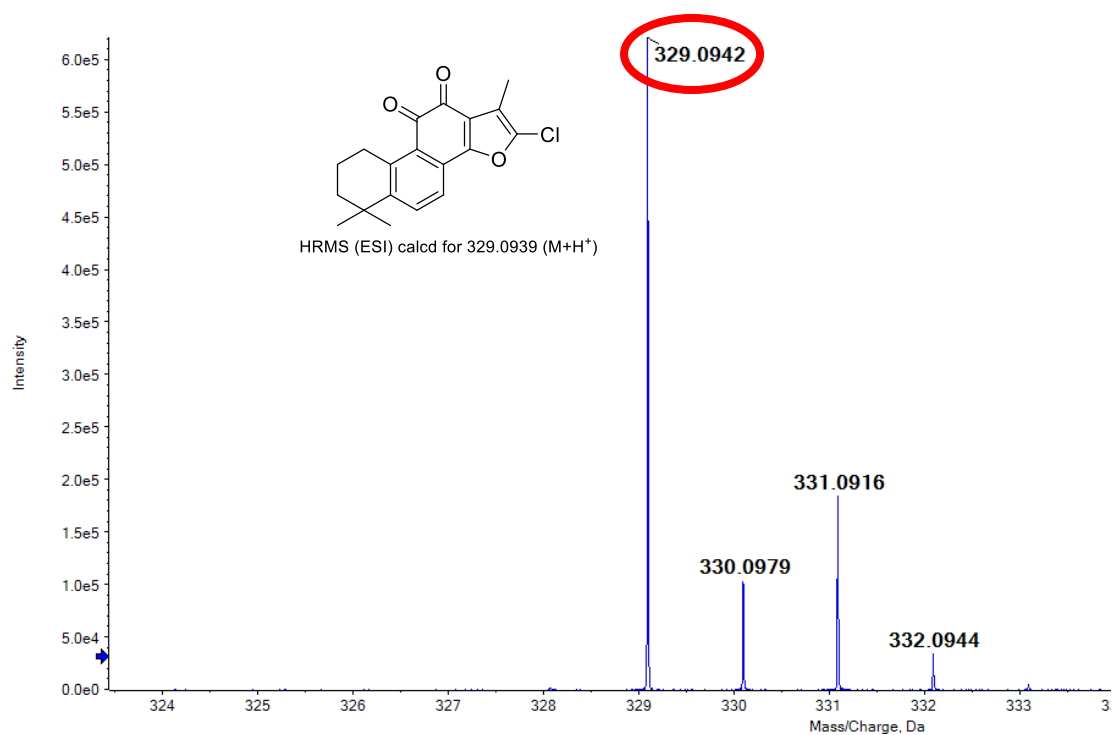
^1H NMR (400 MHz, CDCl_3) of compound **2z**



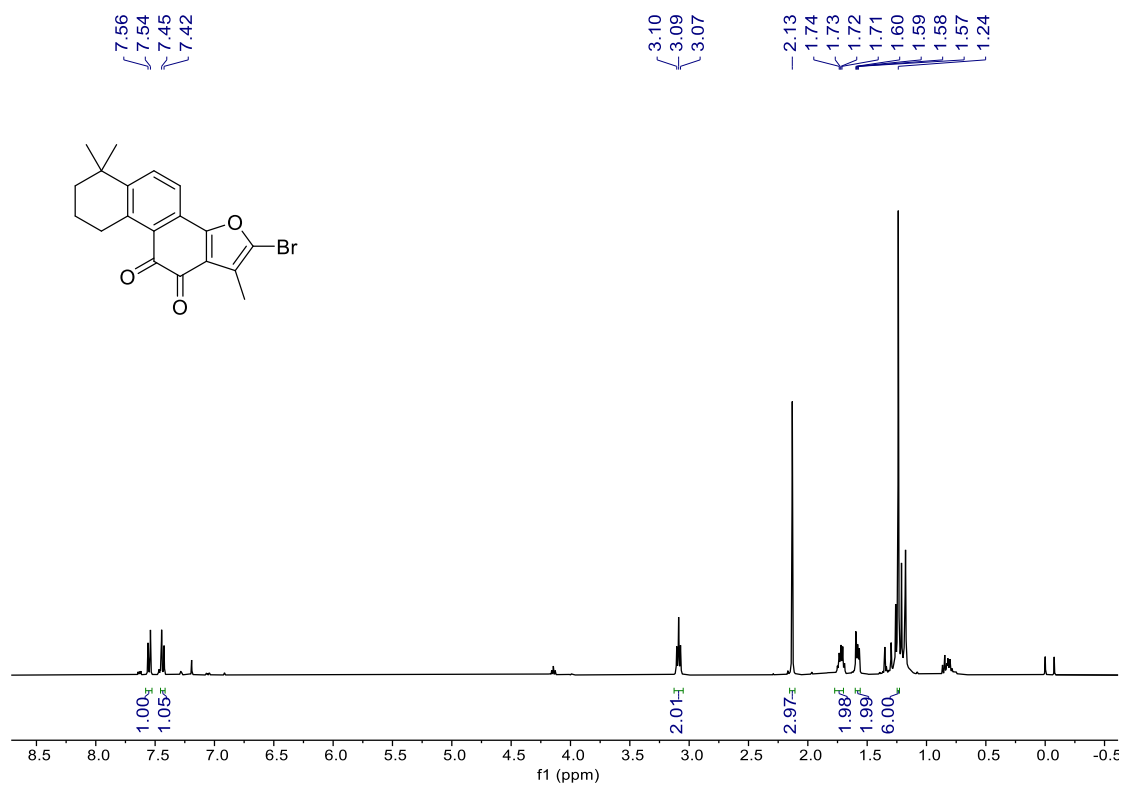
^{13}C NMR (101 MHz, CDCl_3) of compound **2z**



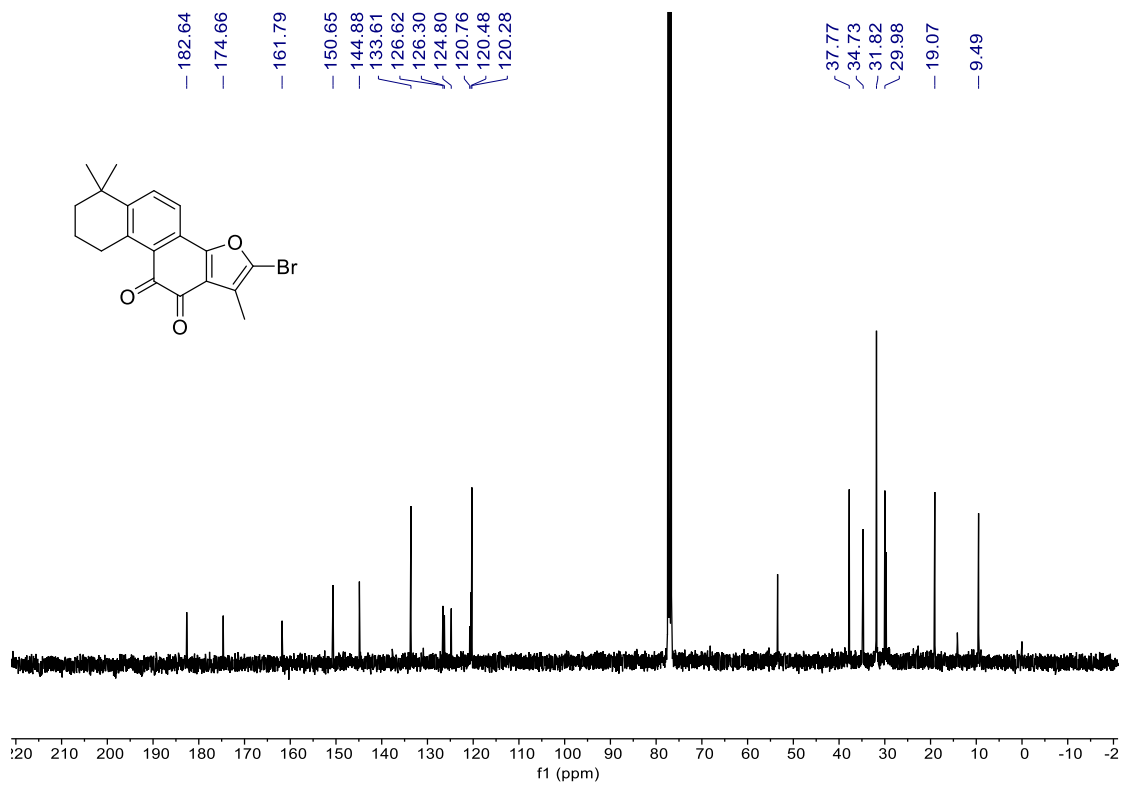
HRMS(ESI) of compound **2z**



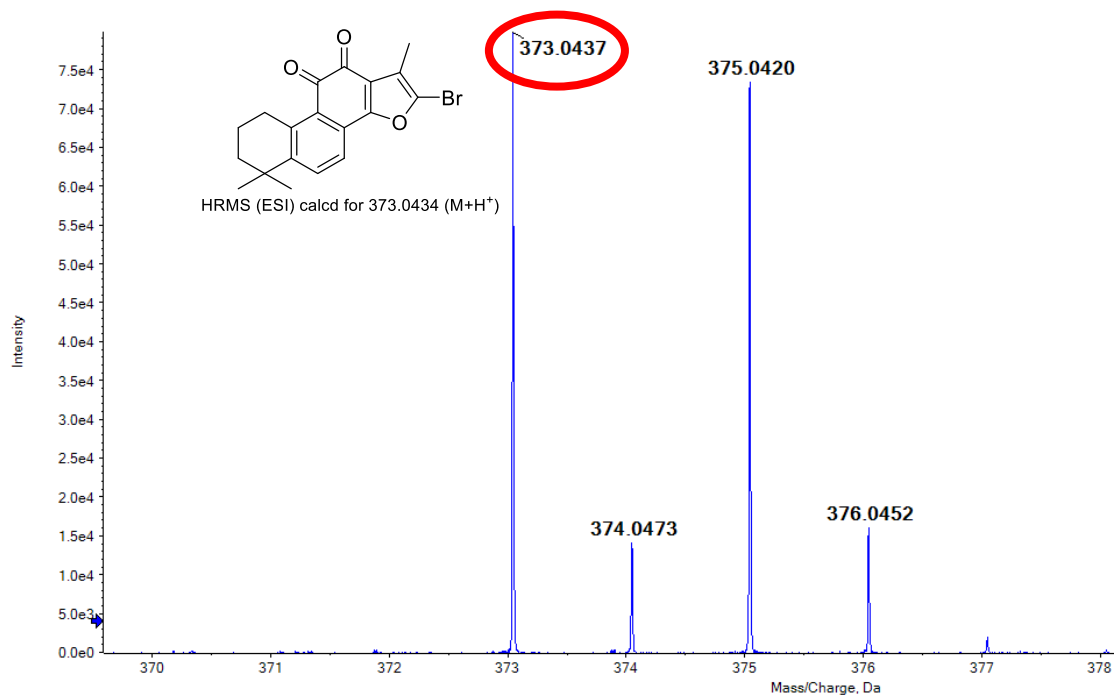
^1H NMR (400 MHz, CDCl_3) of compound **2za**



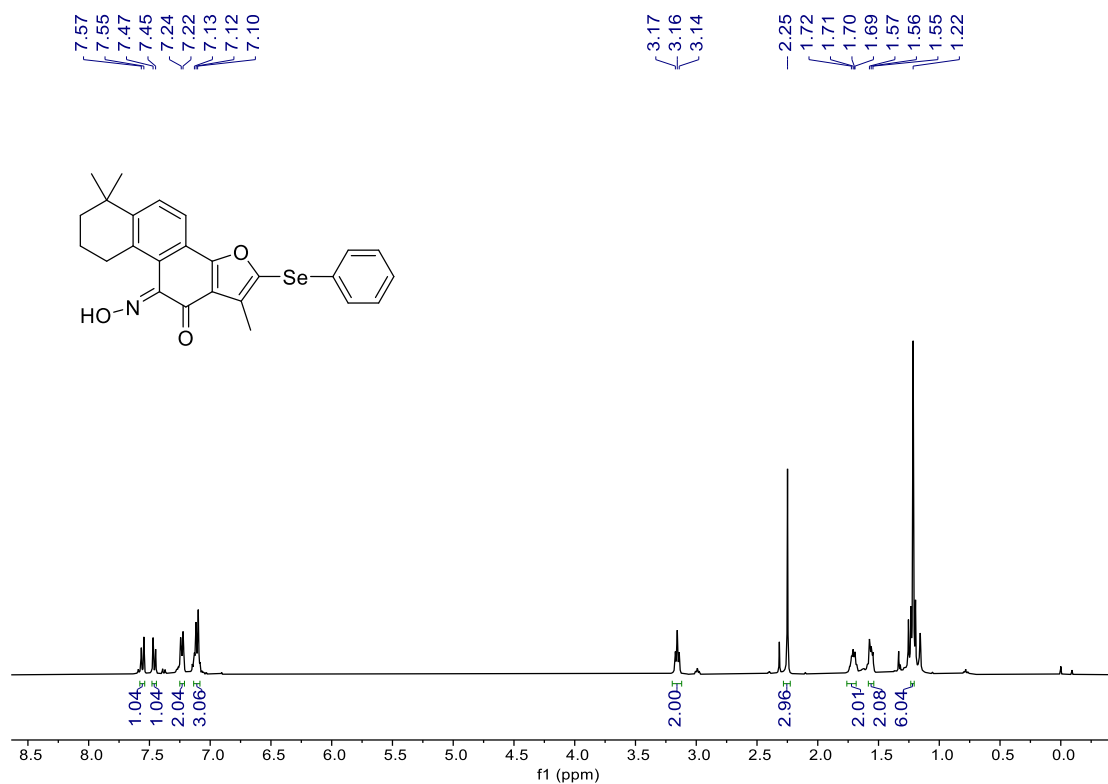
^{13}C NMR (101 MHz, CDCl_3) of compound **2za**



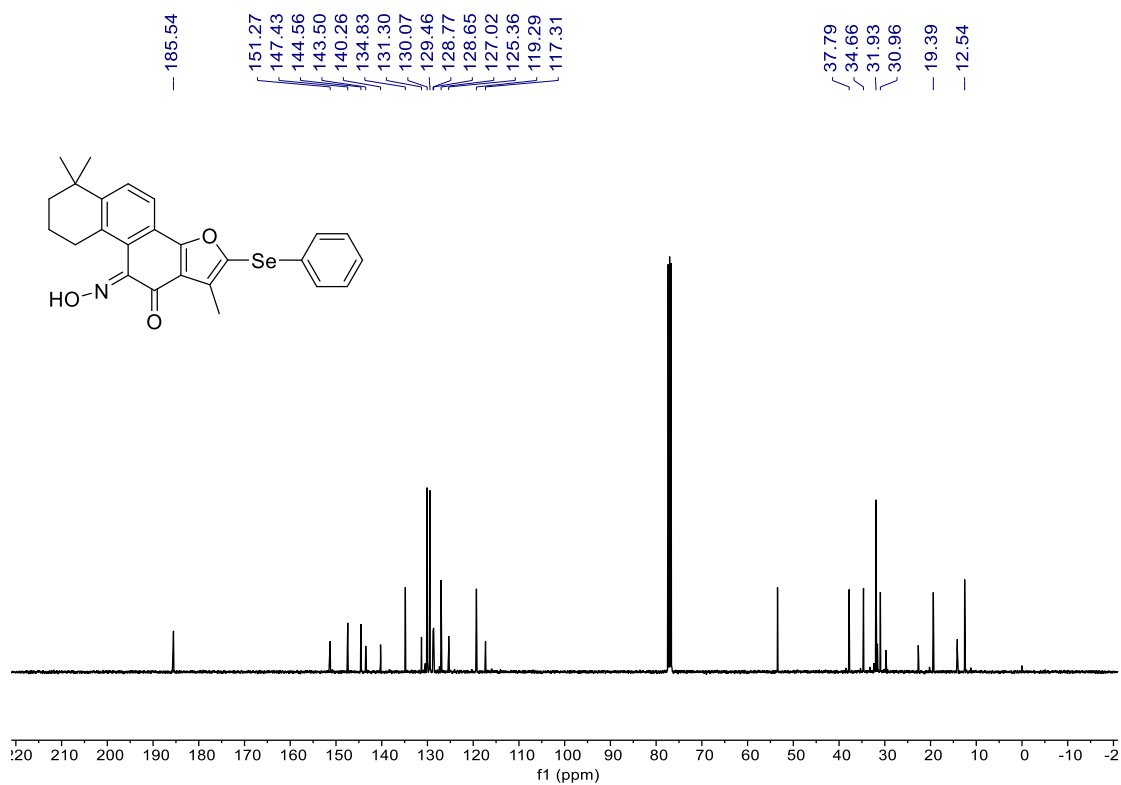
HRMS(ESI) of compound **2za**



^1H NMR (400 MHz, CDCl_3) of compound **3a**



^{13}C NMR (101 MHz, CDCl_3) of compound **3a**



HRMS(ESI) of compound **3a**

