

Supporting Information

Stereoselective Synthesis of Difunctionalized Succinimides from Aza-1,6-Enynes by Radical Cascade Reaction

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(1) General Information.

All reagents were purchased (unless specified) at highest commercial quality and used as received. Reaction mixtures were stirred magnetically. All required temperatures for reactions were achieved using a IKA heating plate and oil bath.

Rf: LC analysis was performed on commercially prepared 60 F₂₅₄ silica gel plates and visualized by either UV irradiation or by staining with I₂. Column chromatography was performed using 100- 200 mesh silica gel.

Melting Point: Melting points were measured on a Kofler hot-stage melting point apparatus and are uncorrected.

¹H NMR: Spectra were recorded on JEOL ECS (400 MHz) instruments. Chemical shifts (δ H) are quoted in parts per million (ppm) was used. Spin-spin coupling constants (*J*) are reported in Hertz (Hz).

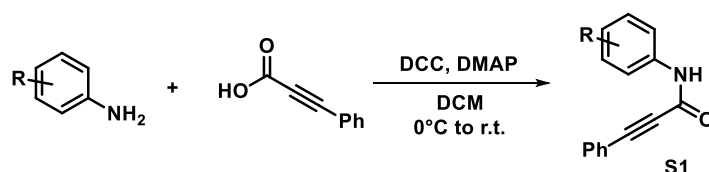
¹³C NMR: Spectra were recorded on JEOL ECS (100 MHz) instruments. Chemical shifts (δ C) are quoted in parts per million (ppm) and referenced to the appropriate solvent peak(s). Spin-spin coupling constants (*J*) are reported in Hertz (Hz).

HRMS: High resolution mass spectra were recorded on an Agilent 6500 series B5125 mass spectrometer (ESI-TOF).

(2) Synthesis of Substrates 1:

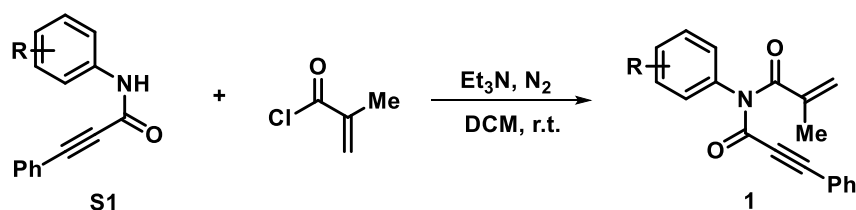
Substrates **1(1a-1k)** were prepared following the reported procedure.¹

(i) Amide coupling for the synthesis of N-arylpropiolamides (S1):

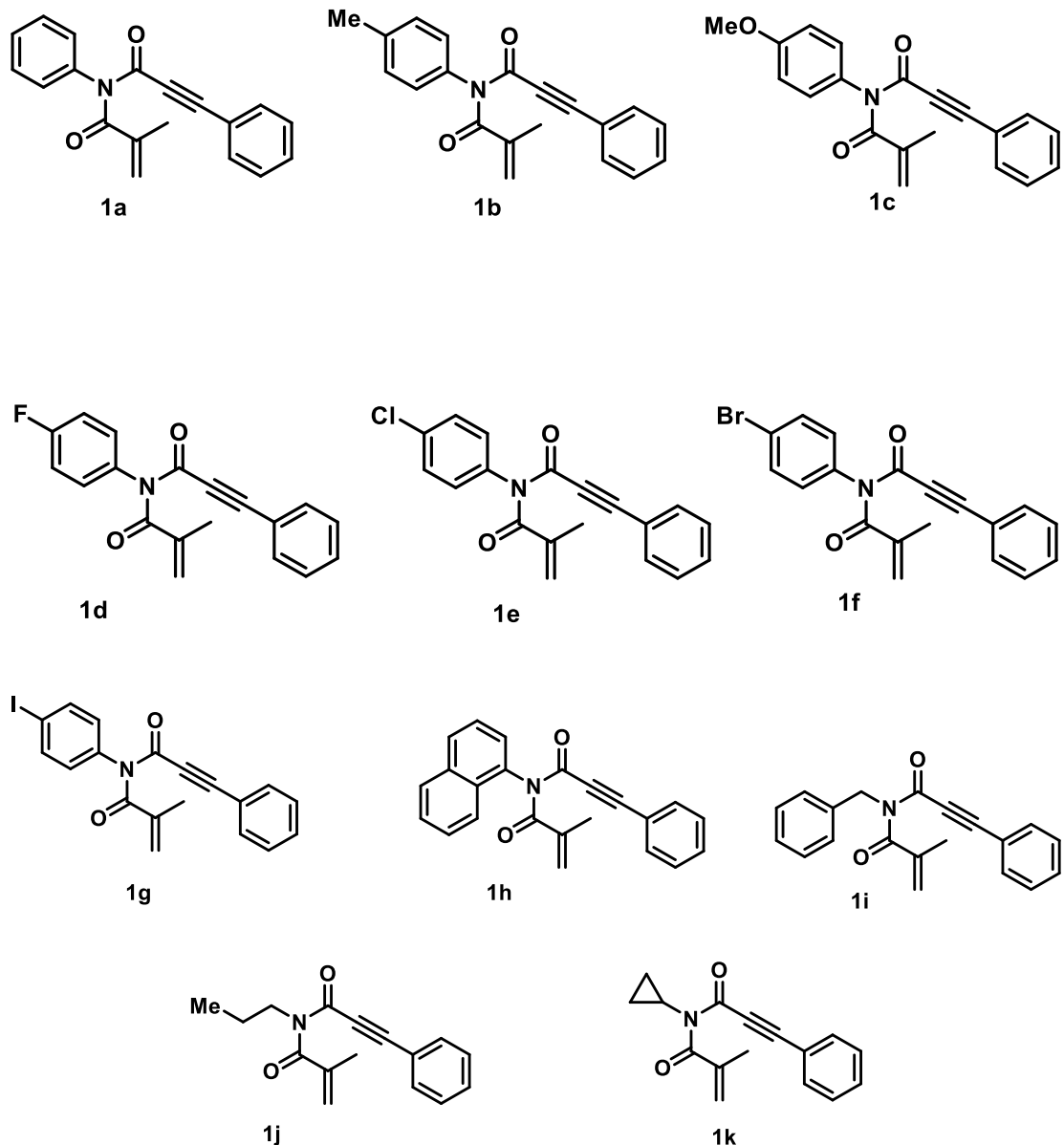


Phenylpropionic acid (1 equiv) and DMAP (10 mol%) were charged into an oven-dried round-bottom flask, which was then purged with nitrogen gas for 10 minutes. After dissolving the mixture in DCM, amine (1.1 equiv) was added. The mixture was cooled to 0°C and a saturated solution of DCC (1.0 equiv) in DCM was added dropwise. After addition the reaction mixture was warmed to the room temperature and stirred for approximately 12 hours (overnight). The contents of the flask were then filtered using a plug of Celite. The filtrate obtained was then concentrated under reduced pressure while adsorbing onto silica gel. The obtained adsorbed silica plug was then purified using silica gel column chromatography (PE:EA=19:1) to afford pure product **S1**.

(ii) Methallylation of S1



An oven-dried round-bottom flask equipped with a magnetic stir bar was charged with **S1** (1.0 equiv) then sealed with septum and purged with nitrogen gas for 10 minutes. Afterwards DCM were added. Then, Methacryloyl chloride (1.5 equiv) and Et_3N (2.0 equiv) were added successively in dropwise manner while stirring the reaction mixture. The reaction mixture was then stirred at room temperature for 6 h until **S1** was consumed completely. The solvent was removed under reduced pressure while adsorbing the filtrate onto silica gel. The crude residue was purified by silica gel column chromatography (PE:EA=0.5:9.5) to afford pure product **1**. The prepared substrates (**1a-1k**) are as follows:



(3) General procedure for the synthesis of sulfonothioates:

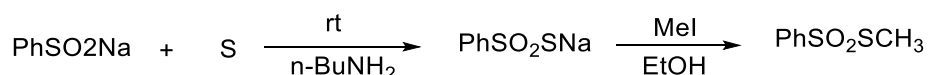
Sulfonothioates were prepared following the reported procedure.^{2,3}

(i) Synthesis of S-phenyl arene/heteroarenesulfonothioates S-Aryl arenesulfonothioates:

p-methyl benzenesulfinate salt (1.0 g, 6.4 mmol) was mixed with diphenyl disulfide (0.437 g, 2.0 mmol) in CH₂Cl₂ (10 mL), I₂ (1.015 g, 4.0 mmol) was added while mixing. The mixture was stirred until the disulfide was consumed completely (2 hours). Then aqueous Na₂S₂O₃

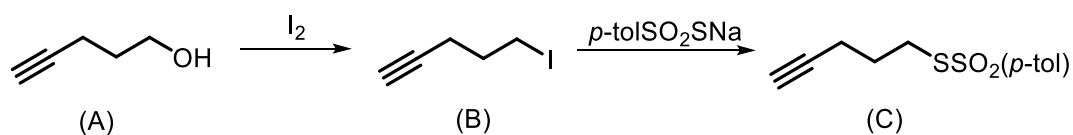
was added. The organic layer was concentrated under reduced pressure. The product was purified by column chromatography system using silica applying a PE: EtOAc gradient (95: 5). S-phenyl benzenethiosulfonate was obtained in 96% (0.966 g) yield. Yellow solid, m.p.: 45-47 °C.

(ii) Synthesis of S-alkyl arenesulfonothioates:



A mixture of PhSO₂Na (6.56 g, 40 mmol) and S (1.28 g, 40 mmol) in n-BuNH₂ (40 mL) was stirred at room temperature for 0.5 h, after removal of the solvent under reduced pressure, the residue was washed by Et₂O to obtain a white solid PhSO₂SNa. Then PhSO₂SNa was dissolved in EtOH (40 mL), then CH₃I (11.36 g, 80 mmol) was added to the solution. The reaction mixture was stirred at 40-45 °C for 24 h. After removal of the solvent under reduced pressure, the reaction mixture was poured on a solution of Na₂S₂O₃ and CH₂Cl₂ (30 mL). The precipitate was filtered and dried by anhydrous Na₂SO₄, the residue was purified through column chromatography (PE:EA = 20:1) afforded the desired product 3a (3.1 g, 40% yield) as a yellow oil.

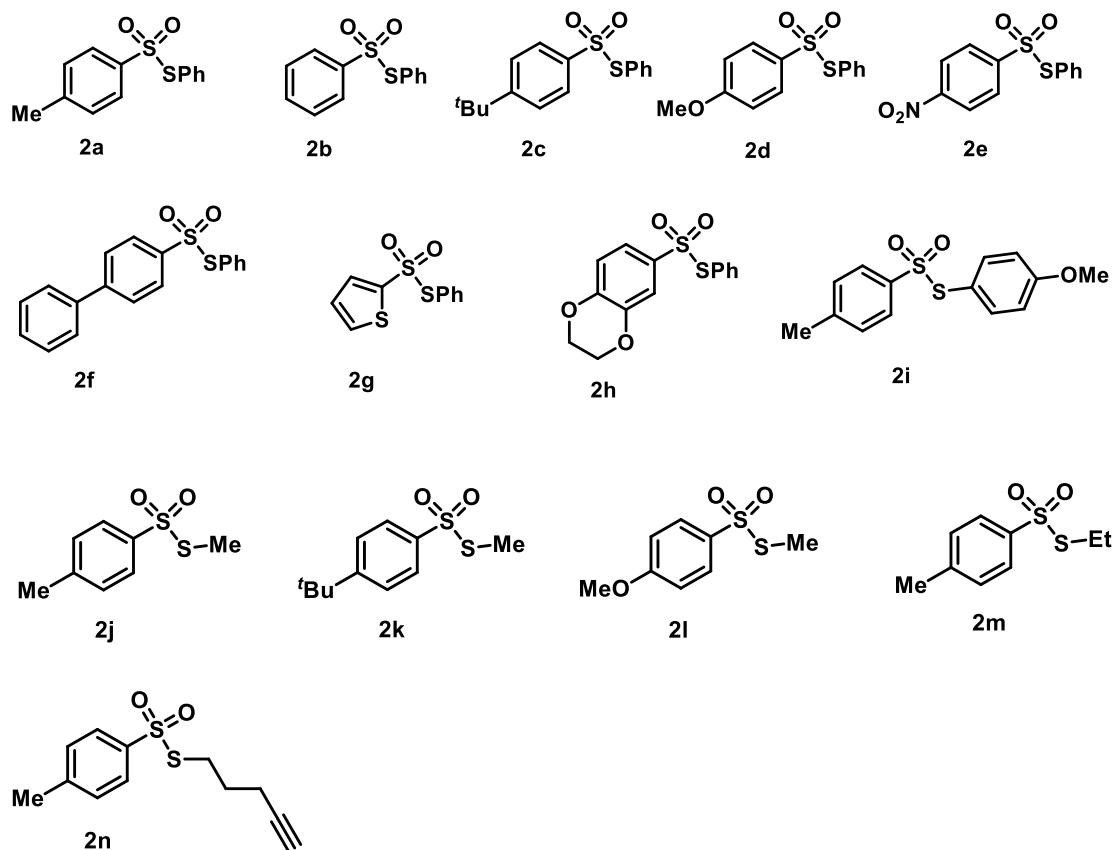
(iii) S-(pent-4-yn-1-yl) 4-methylbenzenesulfonothioate:



To a solution of imidazole (1.64 g, 24 mmol), PPh₃ (6.3 g, 24 mmol) and **A** (1.4 g, 20 mmol) in dry DCM (30 mL) was added I₂ (6.1 g, 24 mmol) slowly at 0 °C and stirred for 1 h at RT. The reaction mixture was quenched with saturated aqueous Na₂S₂O₃, diluted with EtOAc, washed with water and brine, dried over Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by silica column chromatography to afford compound **B**. Then PhSO₂SNa (20 mmol) was dissolved in EtOH (40 mL), **B** was added to the solution. The reaction mixture was stirred at 40-45 °C overnight. After removal of the solvent under

reduced pressure, the reaction mixture was quenched with saturated aqueous $\text{Na}_2\text{S}_2\text{O}_3$, diluted with DCM, dried over Na_2SO_4 and the residue was purified through column chromatography (PE:EA = 30:1) afforded the desired product **C** (1.4 g, 30% yield) as a yellow oil.

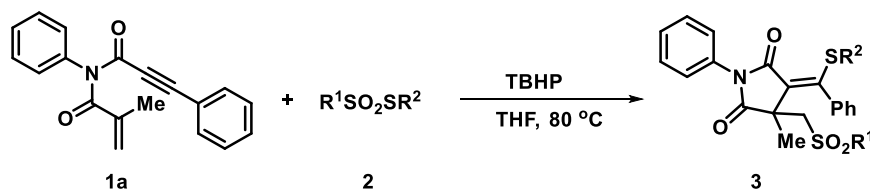
The prepared sulfonylthioates (**2a-2n**) are as follows:



(4) General procedure for the synthesis of Sulfonylthioates:

Sulfonylthioates were prepared following the reported procedure.⁴ A mixture of sulfinic acid sodium salt (4.0 mmol), diselenide (1.0 mmol), and NBS (2.0 mmol, 356 mg) in MeCN was stirred at room temperature. After the completion of the reaction, as monitored by TLC, the reaction mixture was washed with water and extracted with ethyl acetate. The organic phase was separated, dried over anhydrous Na_2SO_4 , and then filtered. The filtrate was concentrated under reduced pressure and the resulting residue was purified by column chromatography to provide **4** in 90% yield as a white solid.

(5) General procedure for the Radical cascade sulfonation and thiolation:



An oven-dried seal tube equipped with a magnetic stir bar was charged with **1a** (100 mg, 0.346 mmol) and **2** (0.692 mmol), then THF (10 mL) was added before adding 70% TBHP in water (133 μ L, 1.038 mmol). The reaction mixture was then stirred at 80 °C oil bath for 3hrs (monitored reactions by TLC). Afterwards the solvent was removed under reduced pressure and the resulting residue was purified by silica gel column chromatography to afford pure product **3**.

(6) Standardization of reaction conditions

We initiated our investigation using *N*-phenyl-*N*-(3-phenylpropioloyl)acrylamide **1a** and *S*-phenyl 4-methylbenzenesulfonothioate **2a** as a model substrate (Table 1). In the reaction of **1a** with **2a** (3.0 equiv) using 3.0 equiv of TBHP in dioxane at 80 °C for 3 h, the desired product **3aa** was obtained in 76% yield (Table 1, entry 1). The reaction showed high diastereoselectivity as the sole *E*-isomer of **3aa** was formed. The structure of **3aa** was further confirmed by single-crystal XRD.

Table S1. Optimization of Reaction Conditions^a

Entry	TolSO ₂ SPh (x equiv)	Oxidant	Solvent	Yield ^b (%)
1	3	TBHP	Dioxane	76%
2	3	TBHP	ACN	62%
3	3	TBHP	EtOH	46%
4	3	TBHP	THF	87%
5	3	TBHP	DMF	traces
6	3	TBHP	DMSO	NR
7	3	TBHP	H ₂ O	45%

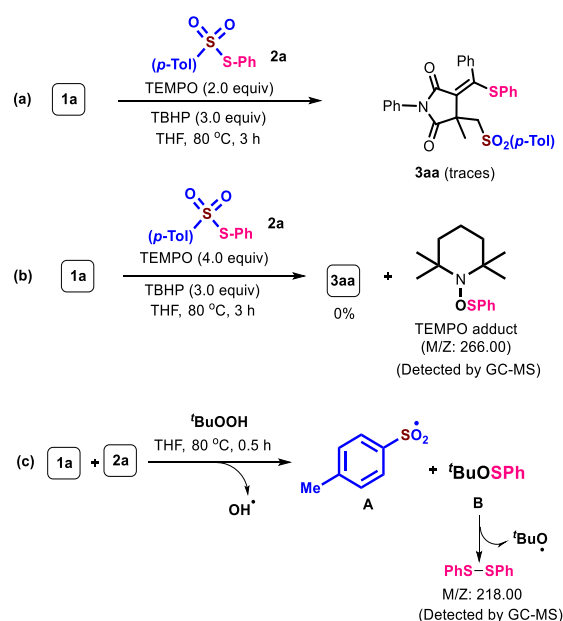
8	2	TBHP	THF	87%
9	1.5	TBHP	THF	75%
10	1.2	TBHP	THF	70%
11	2	TBHP	THF	58 ^c , 37 ^d , 82 ^e
12	2	TBHP	THF	67 ^f , 75 ^g
13	2	DTBP	THF	68
14	2	K ₂ S ₂ O ₈	THF	72
15	2	PIDA	THF	53
16	2	TBHP	THF	81 ^h
17	2	-	THF	NR
18	2	TBHP	THF	72 ⁱ , 54 ^j

^aReaction Conditions: **1a** (1.0 equiv), TolSO₂SPh (**2a**) and Oxidant in solvent at 80 °C for 3 h under air atmosphere. ^bIsolated yield of **3aa**, ^c60 °C, ^d40 °C, ^e100 °C, ^f2 h, ^g6 h, ^hN₂ atmosphere. ⁱ2 & ^j1 equiv. of TBHP used.

From entries 2-7 in table 1, it is apparent that the solvent has a substantial role in the success of the reaction. THF was found to be the most appropriate solvent for the reaction, as product **3aa** obtained in 87% yield (Table 1, entry 4). A highly polar solvent such as DMF and DMSO was found unsuitable for the reaction (Table 1, entries 5,6). Decreasing the amount of sulfonothioate **2a** from 3.0 equiv to 2.0 equiv did not affect the yield of the reaction and afforded product **3aa** in 87% yield (Table 1, entry 8). Furthermore, decreasing the amount of **2a** to 1.5 and 1.2 equivalents resulted in a decreased yield of the product i.e., 75% and 70% respectively (Table 1, entries 9,10). Lowering the temperature from 80°C to 60°C and 40°C led to incomplete conversion of substrates and provided the desired product **3aa** in 58% and 37% respectively however, elevation in temperature up to 100 °C gave the product in slightly lower amount (Table 1, entry 11). When the reaction was performed for 2 h, the formation of product **3aa** was observed in a lower yield (67%); while running the reaction for 6 h resulted the product in a 75% yield (Table 1, entry 12). Screening of other oxidants such as DTBP, K₂S₂O₈, and PIDA was found inferior for the reaction

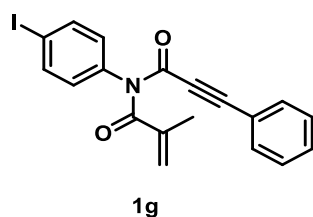
(Table 1, entries 13-15). Performing the reaction in an inert atmosphere (nitrogen atmosphere) did not affect the yield of product **3aa** (Table 1, entry 16). In the absence of an oxidant, no product was formed (Table 1, entry 17). Lowering the amount of TBHP to 2.0 equiv and 1.0 equiv yielded the product in lower yields, 72 % and 54 % respectively (Table 1, entry 18).

(7) Control Experiments:



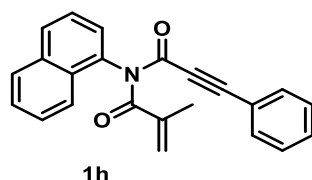
Scheme S1. Control Experiments

(8) Characterization Data for the Products 1,2,3,5:

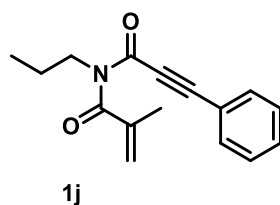


N-(4-iodophenyl)-N-(3-phenylpropioloyl)methacrylamide (1g): Purification by silica gel chromatography (PE:EA=95:5) afforded the desired **1g** as yellow solid in 60% yield (1.87 g), mp 90-92 °C; $^1\text{H-NMR}$ (100 MHz, CDCl_3) δ 7.98 (dd, $J = 8.0, 1.4$ Hz, 1H), 7.47 (td, $J = 7.6, 1.4$ Hz, 1H), 7.42-7.34 (m, 2H), 7.31-7.27 (m, 2H), 7.22-7.15 (m, 3H), 5.77 (s, 1H), 5.48 (d, $J = 2.1$ Hz, 1H), 2.14 (q, $J = 0.8$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 171.9, 154.0, 141.5,

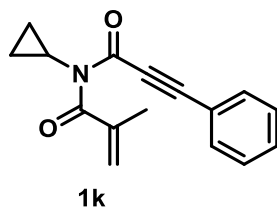
140.8, 140.1, 133.1, 131.1, 130.8, 129.5, 128.7, 121.2, 119.4, 100.4, 94.7, 82.8, 19.3; **MS** (ESI) m/z 416 $[M+H]^+$; HRMS Calculated for $C_{19}H_{15}INO_2^+$ 416.0142; Found: 416.0143. $[M+H]^+$.



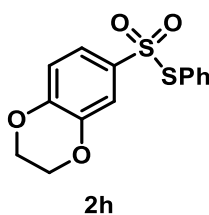
***N*-(naphthalen-1-yl)-*N*-(3-phenylpropioloyl)methacrylamide (1h):** Purification by silica gel chromatography (PE:EA=95:5) afforded the desired **1h** as yellow liquid in 70% yield (1.79 g); **¹H-NMR** (400 MHz, $CDCl_3$) δ 7.97-7.91 (m, 3H), 7.60-7.47 (m, 4H), 7.33-7.29 (m, 1H), 7.21-7.17 (m, 2H), 7.01-6.99 (m, 2H), 5.78 (s, 1H), 5.50 (d, $J = 1.5$ Hz, 1H), 2.12-2.16 (3H); **¹³C-NMR** (100 MHz, $CDCl_3$) δ 173.2, 155.2, 141.5, 134.6, 132.9, 131.3, 130.9, 130.0, 128.7, 128.5, 127.7, 127.6, 126.8, 125.6, 122.4, 121.4, 119.4, 94.3, 83.0, 19.3; **MS** (ESI) m/z 340 $[M+H]^+$; HRMS Calculated for $C_{23}H_{18}NO_2^+$ 340.1332; Found: 340.1332. $[M+H]^+$.



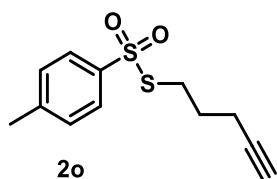
***N*-(3-phenylpropioloyl)-*N*-propylmethacrylamide (1j):** Purification by silica gel chromatography (PE:EA=98:2) afforded the desired **1j** as colourless oil in 85% yield (1.63 g); **¹H-NMR** (400 MHz, $CDCl_3$) δ 7.51-7.48 (m, 2H), 7.45-7.41 (m, 1H), 7.38-7.34 (m, 2H), 5.47-5.46 (m, 2H), 3.83-3.80 (m, 2H), 2.06 (t, $J = 1.2$ Hz, 3H), 1.72-1.62 (m, 2H), 0.94 (t, $J = 7.4$ Hz, 3H); **¹³C-NMR** (100 MHz, $CDCl_3$) δ 174.6, 155.2, 142.7, 132.5, 130.8, 128.8, 121.8, 93.7, 83.1, 46.8, 22.1, 19.0, 11.5; **MS** (ESI) m/z 256 $[M+H]^+$; HRMS Calculated for $C_{16}H_{18}NO_2^+$ 256.1332; Found: 256.1343. $[M+H]^+$.



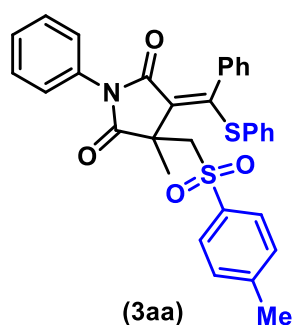
***N*-cyclopropyl-*N*-(3-phenylpropioloyl)methacrylamide (1k):** Purification by silica gel chromatography (PE:EA=98:2) afforded the desired **1k** as yellow semisolid in 80% yield (1.52 g); **¹H-NMR** (400 MHz, CDCl₃) δ 7.53-7.51 (m, 2H), 7.45-7.41 (m, 1H), 7.38-7.34 (m, 2H), 5.54-5.52 (m, 2H), 2.91-2.86 (m, 1H), 2.01 (s, 3H), 1.07 (q, J = 6.8 Hz, 2H), 0.75-0.71 (m, 2H); **¹³C-NMR** (100 MHz, CDCl₃) δ 175.3, 155.7, 142.4, 132.7, 130.8, 128.7, 123.2, 120.0, 93.3, 82.8, 28.1, 18.3, 9.2; **MS** (ESI) m/z 254 [M+H]⁺; HRMS Calculated for C₁₆H₁₆NO₂⁺ 254.1176; Found: 254.1197. [M+H]⁺.



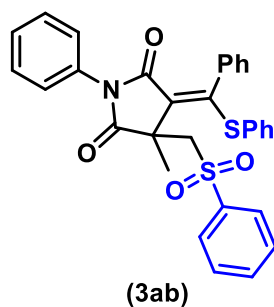
***S*-phenyl 2,3-dihydrobenzo[*b*][1,4]dioxine-6-sulfonothioate (2h):** Purification by silica gel chromatography (PE:EA=95:5) afforded the desired **2h** as white solid in 75% yield (1.48 g), mp 92-94 °C; **¹H-NMR** (400 MHz, CDCl₃) δ 7.50-7.45 (m, 1H), 7.41-7.33 (m, 4H), 7.12 (d, J = 2.2 Hz, 1H), 7.00 (dd, J = 8.6, 2.3 Hz, 1H), 6.82 (d, J = 8.7 Hz, 1H), 4.32-4.30 (m, 2H), 4.27-4.25 (m, 2H); **¹³C-NMR** (100 MHz, CDCl₃) δ 148.4, 143.3, 136.7, 135.6, 131.5, 129.5, 128.2, 121.6, 117.3, 117.3, 64.7, 64.2; **MS** (ESI) m/z 326 [M+NH₄]⁺; HRMS Calculated for C₁₄H₁₆NO₄S₂⁺ 326.0515; Found: 326.0528. [M + NH₄]⁺.



S-(pent-4-yn-1-yl) 4-methylbenzenesulfonothioate (2n): Purification by silica gel chromatography (PE:EA=95:5) afforded the desired **2o** as colourless oil in 70% yield (3.56 g); ¹H-NMR (400 MHz, CDCl₃) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 3.03 (t, *J* = 7.3 Hz, 2H), 2.37 (s, 3H), 2.17 (td, *J* = 6.8, 2.6 Hz, 2H), 1.92 (t, *J* = 2.7 Hz, 1H), 1.80-1.73 (m, 2H); ¹³C-NMR (101 MHz, CDCl₃) δ 145.0, 141.8, 130.0, 127.1, 82.4, 34.7, 27.5, 21.7, 17.3; MS (ESI) *m/z* 255 [M+H]⁺; HRMS Calculated for C₁₂H₁₅O₂S₂⁺ 255.0508; Found: 255.1176. [M+H]⁺.

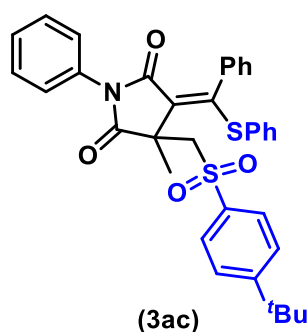


(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-tosylmethylpyrrolidine-2,5-dione (3aa): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3aa** as white solid in 87% yield (166.5 mg), mp 201-203 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 8.4 Hz, 2H), 7.43-7.38 (m, 8H), 7.36-7.31 (m, 2H), 7.23 (s, 1H), 7.15-7.08 (m, 6H), 4.84 (d, *J* = 13.9 Hz, 1H), 3.93 (d, *J* = 14.0 Hz, 1H), 2.46 (s, 3H), 1.84 (s, 3H); ¹³C-NMR (125 MHz, CDCl₃) δ 177.5, 165.1, 157.4, 145.0, .1378, 135.4, 135.2, 132.2, 130.1, 129.2, 128.9, 128.8, 128.7, 128.5, 128.4, 127.9, 127.4, 127.0, 123.1, 57.8, 46.5, 24.3, 21.7. MS (ESI) *m/z* 554 [M+H]⁺; HRMS Calculated for C₃₂H₂₈NO₄S₂⁺ 554.1454; Found: 554.1454. [M+H]⁺.



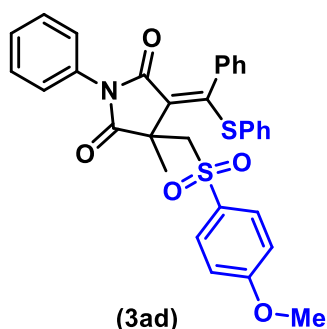
(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-

((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3ab): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ab** as white solid in 84% yield (157 mg), mp 198-200 °C; ¹H-NMR (400 MHz, CDCl₃) δ 8.01 (d, *J* = 8.0 Hz, 2H), 7.70-7.66 (m, 1H), 7.61-7.57 (m, 2H), 7.44-7.40 (m, 6H), 7.36-7.32 (m, 1H), 7.23-7.11 (m, 8H), 4.87 (d, *J* = 14 Hz, 1H), 3.95 (d, *J* = 14 Hz, 1H), 1.85 (s, 3H). ¹³C-NMR (100 MHz, CDCl₃) δ 177.5, 165.1, 157.5, 140.7, 135.3, 135.2, 133.9, 132.2, 129.5, 129.1, 128.9, 128.8, 128.7, 128.5, 128.4, 127.8, 127.5, 127.0, 123.1, 57.7, 46.5, 24.3. MS (ESI) *m/z* 540 [M+H]⁺; HRMS Calculated for C₃₁H₂₆NO₄S₂⁺ 540.1303; Found: 540.1298. [M+H]⁺.



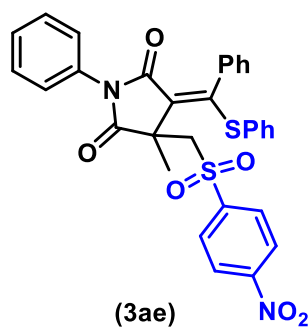
(E)-3-(((4-(tert-butyl)phenyl)sulfonyl)methyl)-3-methyl-1-phenyl-4-

(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione (3ac): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ac** as white solid in 82% yield (169 mg), mp 200-202 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.91 (d, *J* = 6.7 Hz, 2H), 7.58 (d, *J* = 8.7 Hz, 2H), 7.41-7.30 (m, 8H), 7.23 (d, *J* = 15.1 Hz, 1H), 7.16-7.06 (m, 6H), 4.85 (d, *J* = 14.0 Hz, 1H), 3.94 (d, *J* = 14.2 Hz, 1H), 1.84 (s, 3H), 1.35 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 177.6, 165.2, 157.9, 157.4, 137.7, 135.4, 135.2, 132.3, 129.2, 128.9, 128.9, 128.7, 128.6, 128.5, 127.8, 127.5, 127.1, 126.5, 123.2, 57.8, 46.5, 35.4, 31.2, 24.4. MS (ESI) *m/z* 596 [M+H]⁺; HRMS Calculated for C₃₅H₃₄NO₄S₂⁺ 596.1924; Found: 596.1910. [M+H]⁺.



(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-1-phenyl-4-

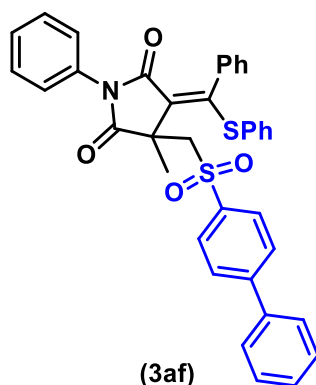
(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione (3ad): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ad** as yellow solid in 87% yield (171 mg), mp 168-170 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.93-7.89 (m, 2H), 7.43-7.38 (m, 7H), 7.34-7.30 (m, 1H), 7.23 (s, 1H), 7.14-7.07 (m, 6H), 7.02 (dd, *J* = 6.9, 2.1 Hz, 2H), 4.83 (d, *J* = 14.0 Hz, 1H), 3.92 (d, *J* = 14.0 Hz, 1H), 3.86 (s, 3H), 1.84 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.6, 165.2, 164.0, 157.5, 135.5, 135.2, 132.3, 130.1, 129.3, 129.1, 128.9, 128.9, 128.8, 128.6, 128.5, 127.5, 127.0, 123.2, 114.7, 58.1, 55.8, 46.6, 24.4. MS (ESI) *m/z* 570 [M+H]⁺; HRMS Calculated for C₃₂H₂₈NO₅S₂⁺ 570.1403; Found: 570.1392. [M+H]⁺.



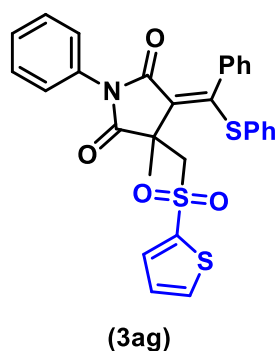
(E)-3-methyl-3-(((4-nitrophenyl)sulfonyl)methyl)-1-phenyl-4-

(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione (3ae): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ae** as white solid in 81% yield (164 mg), mp 213-215 °C; ¹H-NMR (400 MHz, CDCl₃) δ 8.42 (d, *J* = 8.8 Hz, 2H), 8.19 (d, *J* = 8.8 Hz, 2H), 7.44-7.32 (m, 8H), 7.19-7.17 (m, 1H), 7.16-7.08 (m, 6H), 4.97 (d, *J* = 14.0 Hz, 1H), 3.97 (d, *J* = 14.0 Hz, 1H), 1.86 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.3, 164.8, 157.9, 151.0, 146.0, 135.1, 132.1, 129.5, 129.4, 129.2, 129.0, 128.9, 128.8, 128.7, 128.6, 127.5,

126.8, 124.7, 122.8, 57.8, 46.6, 24.2. MS (ESI) m/z 585 $[M+H]^+$; HRMS Calculated for $C_{31}H_{25}N_2O_6S_2^+$ 585.1149; Found: 585.1141. $[M+H]^+$.

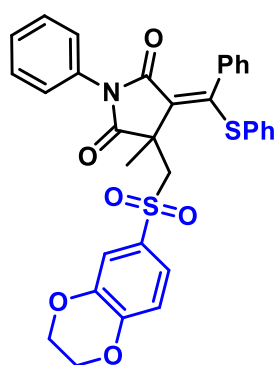


(E)-3-(((1,1'-biphenyl)-4-ylsulfonyl)methyl)-3-methyl-4-phenyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione (3af): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3af** as white solid in 86% yield (183 mg), mp 130-132 °C; 1H -NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 8.5 Hz, 2H), 7.78 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.52-7.39 (m, 10H), 7.35-7.32 (m, 1H), 7.22 (s, 1H), 7.15-7.08 (m, 6H), 4.91 (d, J = 14.0 Hz, 1H), 4.00 (d, J = 14.0 Hz, 1H), 1.87 (s, 3H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ 177.4, 165.0, 157.5, 147.0, 139.2, 136.5, 135.3, 135.2, 132.2, 130.0, 129.1, 128.87, 128.83, 128.74, 128.68, 128.5, 128.4, 128.1, 127.5, 127.0, 123.1, 57.9, 46.5, 24.3. MS (ESI) m/z 616 $[M+H]^+$; HRMS Calculated for $C_{37}H_{30}NO_4S_2^+$ 616.1611; Found: 616.1600. $[M+H]^+$.



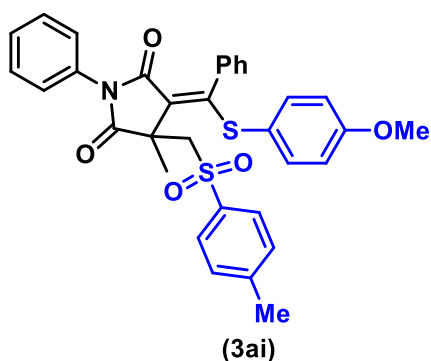
(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-((thiophen-2-ylsulfonyl)methyl)pyrrolidine-2,5-dione (3ag) : Purification by silica gel chromatography

(PE:EA=88:12) afforded the desired **3ag** as white solid in 78% yield (147 mg), mp 210-212 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.78-7.73 (m, 2H), 7.43-7.31 (m, 8H), 7.17 (dd, *J* = 4.9, 3.8 Hz, 2H), 7.15-7.08 (m, 6H), 5.00 (d, *J* = 13.9 Hz, 1H), 4.10 (d, *J* = 14.0 Hz, 1H), 1.87 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.2, 165.0, 157.8, 141.8, 135.4, 135.2, 134.4, 134.2, 132.2, 129.6, 129.1, 128.9, 128.8, 128.6, 128.5, 128.2, 127.5, 127.0, 122.9, 59.2, 46.6, 24.4. **MS** (ESI) *m/z* 546 [M+H]⁺; HRMS Calculated for C₂₉H₂₄NO₄S₃⁺ 546.0862; Found: 546.0879 [M+H]⁺.



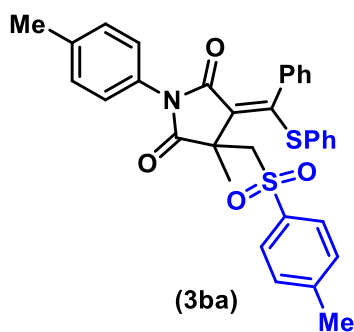
(3ah)

(E)-3-(((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)sulfonyl)methyl) 3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione (3ah): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ah** as white solid in 82% yield (169 mg), mp 209-211 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.48-7.39 (m, 2H), 7.36-7.23 (m, 8H), 7.19-7.15 (m, 1H), 7.09-7.01 (m, 6H), 6.94 (d, *J* = 8.4 Hz, 1H), 4.75 (d, *J* = 14.0 Hz, 1H), 4.28-4.21 (m, 4H), 3.84 (d, *J* = 14.0 Hz, 1H), 1.76 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.4, 165.1, 157.4, 148.5, 143.8, 135.4, 135.2, 133.1, 132.2, 129.2, 128.83, 128.8, 128.7, 128.5, 128.4, 127.4, 127.0, 123.1, 121.5, 118.2, 117.5, 64.6, 64.1, 57.8, 46.4, 24.3. **MS** (ESI) *m/z* 598 [M+H]⁺; HRMS Calculated for C₃₃H₂₈NO₆S₂⁺ 598.1353; Found: 598.1340 [M+H]⁺.



(E)-4-(((4-methoxyphenyl)thio)(phenyl)methylene)-3-methyl-1-phenyl-3-

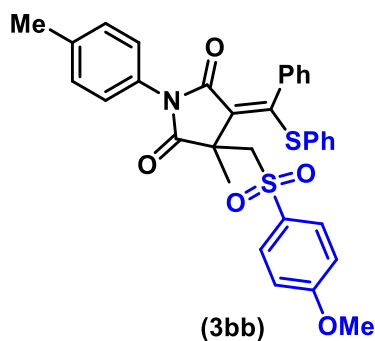
(tosylmethyl)pyrrolidine-2,5-dione (3ai): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ai** as white solid in 87% yield (176 mg), mp 192-194 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.42-7.29 (m, 10H), 7.17 (s, 1H), 7.09 (d, *J* = 5.2 Hz, 4H), 6.64-6.60 (m, 2H), 4.86 (d, *J* = 14.0 Hz, 1H), 3.91 (d, *J* = 14.0 Hz, 1H), 3.69 (s, 3H), 2.45 (s, 3H), 1.82 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.7, 165.1, 160.3, 158.6, 145.0, 137.9, 137.1, 135.6, 132.3, 130.1, 128.9, 128.4, 127.9, 127.6, 127.0, 122.5, 119.6, 114.3, 57.7, 55.3, 46.5, 24.3, 21.8. MS (ESI) *m/z* 584 [M+H]⁺; HRMS Calculated for C₃₃H₂₈NO₆S₂⁺ 584.1560; Found: 584.1546. [M+H]⁺.



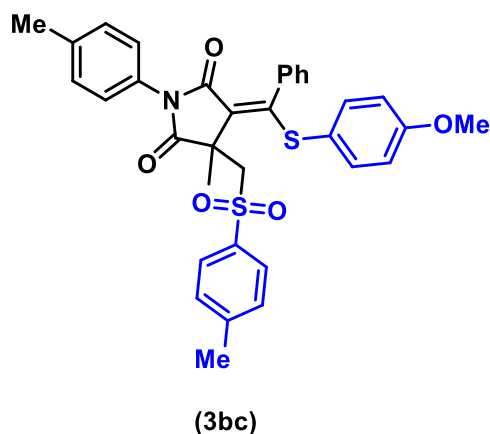
(E)-3-methyl-4-(phenyl(phenylthio)methylene)-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-

2,5-dione (3ba): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ba** as yellow solid in 84% yield (165 mg), mp 208-210 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.39-7.34 (m, 4H), 7.26-7.18 (m, 6H), 7.13-7.06 (m, 6H), 4.82 (d, *J* = 14.0 Hz, 1H), 3.91 (d, *J* = 14.0 Hz, 1H), 2.44 (s, 3H), 2.32 (s, 3H), 1.81 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.6, 165.2, 157.1, 144.9, 138.3, 137.8, 135.4, 135.1, 130.0,

129.6, 129.5, 129.3, 128.8, 128.6, 128.4, 127.8, 127.4, 126.7, 123.3, 57.8, 46.5, 24.3, 21.7, 21.2. **MS** (ESI) m/z 568 [M+H]⁺; HRMS Calculated for C₃₃H₃₀NO₄S₂⁺ 568.1611; Found: 568.1597 [M+H]⁺.

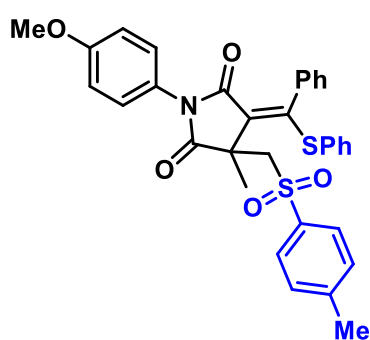


(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-4-(phenyl(phenylthio)methylene)-1-(p-tolyl)pyrrolidine-2,5-dione (3bb): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bb** as yellow solid in 87% yield (176 mg), mp 202-204 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.90 (dd, J = 6.9, 2.0 Hz, 2H), 7.40-7.38 (m, 2H), 7.28-7.19 (m, 6H), 7.14-7.07 (m, 6H), 7.03-6.99 (m, 2H), 4.82 (d, J = 14.2 Hz, 1H), 3.92 (d, J = 14.2 Hz, 1H), 3.87 (s, 3H), 2.33 (s, 3H), 1.83 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.7, 165.3, 164.0, 157.1, 138.4, 135.5, 135.2, 132.4, 130.1, 129.7, 129.6, 129.4, 128.8, 128.7, 128.5, 127.5, 126.8, 123.4, 114.7, 58.1, 55.8, 46.6, 24.4, 21.3. **MS** (ESI) m/z 584 [M+H]⁺; HRMS Calculated for C₃₃H₃₀NO₅S₂⁺ 584.1560; Found: 584.1544 [M+H]⁺.



(E)-4-(((4-methoxyphenyl)thio)(phenyl)methylene)-3-methyl-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione (3bc): Purification by silica gel chromatography

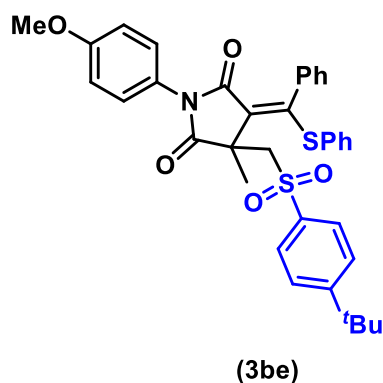
(PE:EA=88:12) afforded the desired **3bc** as white solid in 86% yield (178 mg), mp 226-228 °C; **¹H-NMR** (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.32-7.28 (m, 2H), 7.24 (d, *J* = 6.6 Hz, 3H), 7.19 (d, *J* = 8.4 Hz, 3H), 7.10-7.05 (m, 3H), 6.62 (d, *J* = 8.8 Hz, 2H), 4.85 (d, *J* = 14.0 Hz, 1H), 3.90 (d, *J* = 14.0 Hz, 1H), 3.68 (d, *J* = 8.7 Hz, 3H), 2.45 (s, 3H), 2.32 (s, 3H), 1.81 (s, 3H); **¹³C-NMR** (100 MHz, CDCl₃) δ 177.7, 165.2, 160.2, 158.1, 144.9, 138.3, 137.9, 137.0, 135.6, 130.0, 129.6, 129.5, 128.3, 127.8, 127.5, 126.7, 122.6, 119.6, 114.2, 57.7, 55.2, 46.4, 24.2, 21.7, 21.2; **MS** (ESI) *m/z* 598 [M+H]⁺; HRMS Calculated for C₃₄H₃₂NO₅S₂⁺ 598.1716; Found: 598.1703 [M+H]⁺.



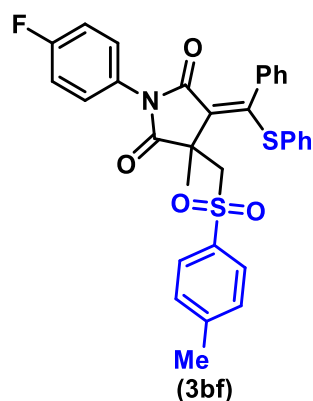
(**3bd**)

(E)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (3bd): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bd** as white solid in 87% yield (176 mg), mp 185-187 °C; **¹H-NMR** (400 MHz, CDCl₃) δ 7.89-7.85 (m, 2H), 7.41-7.35 (m, 4H), 7.33-7.29 (m, 2H), 7.22 (s, 1H), 7.16-7.04 (m, 7H), 6.94-6.90 (m, 2H), 4.82 (d, *J* = 14.0 Hz, 1H), 3.91 (d, *J* = 14.0 Hz, 1H), 3.77 (s, 3H), 2.45 (s, 3H), 1.82 (s, 3H); **¹³C-NMR** (100 MHz, CDCl₃) δ 177.8, 165.4, 159.5, 157.2, 145.0, 137.9, 135.5, 135.2, 130.1, 129.3, 128.9, 128.7, 128.5, 128.2, 127.9, 127.5, 125.0, 123.3, 114.3, 57.9, 55.6, 46.5, 24.4, 21.8. **MS** (ESI) *m/z* 584 [M+H]⁺; HRMS Calculated for C₃₃H₃₀NO₅S₂⁺ 584.1560; Found: 584.1543 [M+H]⁺.

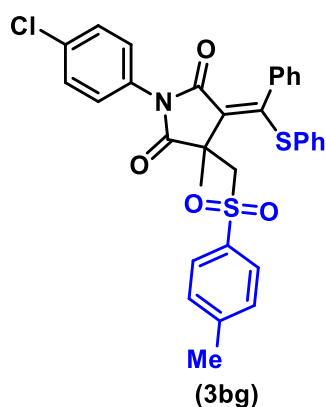


(E)-3-(((4-(tert-butyl)phenyl)sulfonyl)methyl)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione (3be): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3be** as white solid in 84% yield (182 mg), mp 262-264 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8H, 2H), 7.39 (d, *J* = 4.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.21-7.08 (m, 8H), 6.93 (d, *J* = 8.0 Hz, 2H), 4.84 (d, *J* = 16 Hz, 1H), 3.94 (d, *J* = 16 Hz, 1H), 3.79 (s, 3H), 1.84 (s, 3H), 1.36 (s, 9H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.7, 165.3, 159.4, 157.9, 157.0, 137.7, 135.4, 135.1, 129.2, 128.8, 128.7, 128.4, 128.2, 127.7, 127.4, 126.5, 125.0, 123.3, 114.2, 57.9, 55.5, 46.4, 35.3, 31.1, 24.2; **MS** (ESI) *m/z* 626 [M+H]⁺; HRMS Calculated for C₃₆H₃₆NO₅S₂⁺ 626.2029; Found: 626.2023 [M+H]⁺.



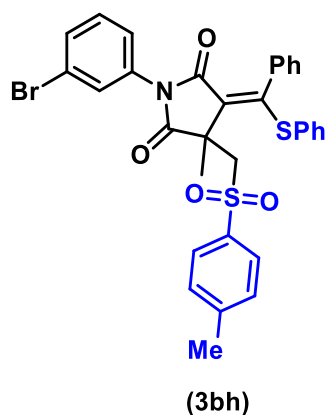
(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione (3bf): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bf** as white solid in 80% yield (158 mg), mp 150-152 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 8.2 Hz, 2H), 7.41-7.37 (m, 6H), 7.22 (s, 1H),

7.16-7.08 (m, 9H), 4.84 (d, $J = 14.0$ Hz, 1H), 3.91 (d, $J = 14.0$ Hz, 1H), 2.47 (s, 3H), 1.84 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 177.6, 165.1, 162.3 (d, $J = 247.3$ Hz), 158.0, 145.2, 137.7, 135.4, 135.3, 130.2, 129.1, 129.0, 128.97 (d, $J = 8.7$ Hz), 128.8, 128.6, 128.21 ($J = 1.9$ Hz), 127.9, 127.6, 122.9, 115.9 ($J = 23.0$ Hz), 57.8, 46.5, 24.3, 21.8; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -112.9 (s, 1F); **MS** (ESI) m/z 572 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{32}\text{H}_{27}\text{NO}_4\text{FS}_2^+$ 572.1360; Found: 572.1351 $[\text{M}+\text{H}]^+$.



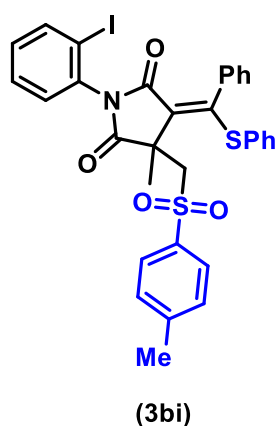
(E)-1-(4-chlorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (3bg): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bg** as white solid in 85% yield (173 mg), mp 192-194 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.87 (d, $J = 8.2$ Hz, 2H), 7.57 (t, $J = 1.8$ Hz, 1H), 7.48-7.46 (m, 1H), 7.41-7.38 (m, 5H), 7.29 (t, $J = 8.0$ Hz, 1H), 7.23 (s, 1H), 7.17-7.10 (m, 7H), 4.85 (d, $J = 14.0$ Hz, 1H), 3.91 (d, $J = 14.0$ Hz, 1H), 2.47 (s, 3H), 1.84 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 177.3, 164.7, 158.4, 145.2, 137.7, 135.3, 133.5, 131.6, 130.2, 130.1, 129.1, 129.0, 128.8, 128.7, 127.9, 127.6, 125.8, 122.6, 122.2, 57.7, 46.5, 24.4, 21.8. **MS** (ESI) m/z 588 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{32}\text{H}_{27}\text{NO}_4\text{ClS}_2^+$ 588.1065; Found: 588.1048 $[\text{M}+\text{H}]^+$.



(E)-1-(3-bromophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-

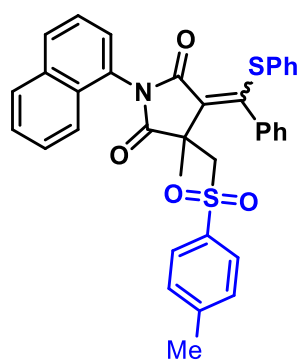
(tosylmethyl)pyrrolidine-2,5-dione (3bh): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bh** as white solid in 83% yield (181 mg), mp 246-248 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.41-7.34 (m, 8H), 7.26 (s, 1H), 7.17-7.08 (m, 7H), 4.84 (d, *J* = 13.9 Hz, 1H), 3.90 (d, *J* = 14.0 Hz, 1H), 2.46 (s, 3H), 1.83 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.4, 164.9, 158.3, 145.2, 137.7, 135.3, 135.2, 134.2, 130.8, 130.2, 129.1, 129.0, 128.8, 128.7, 128.4, 127.9, 127.6, 122.7, 57.8, 46.5, 24.3, 21.8. **MS** (ESI) *m/z* 632 [M+H]⁺; HRMS Calculated for C₃₂H₂₇NO₄BrS₂⁺ 632.0559; Found: 632.0545 [M+H]⁺.



(E)-1-(2-iodophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (3bi): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bi** as white solid in 77% yield (181 mg), mp 236-238

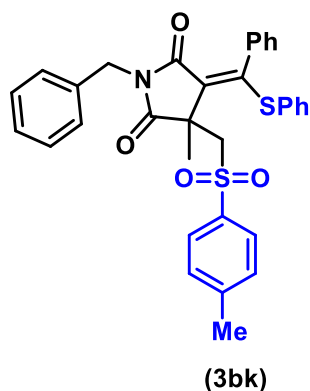
°C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.85 (d, $J = 8.0$ Hz, 3H), 7.51 (d, $J = 7.8$ Hz, 1H), 7.43 (t, $J = 7.6$ Hz, 1H), 7.37 (t, $J = 5.9$ Hz, 4H), 7.21 (s, 1H), 7.14-7.07 (m, 8H), 4.81 (d, $J = 14.0$ Hz, 1H), 3.95 (d, $J = 14.3$ Hz, 1H), 2.46 (s, 3H), 1.94 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 176.6, 164.3, 157.7, 145.0, 139.2, 138.0, 135.6, 135.2, 135.2, 130.8, 130.1, 130.0, 129.6, 129.3, 128.9, 128.7, 128.6, 127.9, 127.5, 123.4, 98.0, 58.3, 47.1, 23.7, 21.8. **MS** (ESI) m/z 680 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{32}\text{H}_{27}\text{NO}_4\text{BrS}_2^+$ 680.0421; Found: 680.0425 $[\text{M}+\text{H}]^+$.



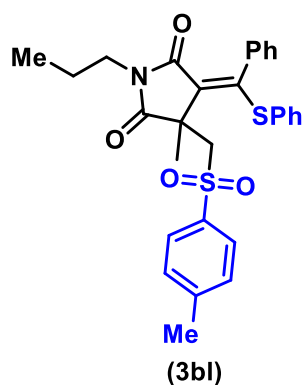
(3bj)

(Z)/(E)-3-methyl-1-(naphthalen-1-yl)-4-(phenyl(phenylthio)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (3bj): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bj** as white solid in 87% yield (182 mg), mp 188-190 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.418-8.397 (d, $J = 8.4, 0.51$), 7.92-7.85 (m, 6H), 7.59-7.52 (m, 2H), 7.50-7.44 (m, 5H), 7.36 (dd, $J = 12.1, 8.1$ Hz, 2H), 7.16-7.13 (m, 3H), 7.07 (d, $J = 7.8$ Hz, 3H), 4.97 (d, 0.29H), 4.91 (d, $J = 14.2$ Hz, 1H), 4.05 (d, $J = 14.2$ Hz, 0.48H), 4.01 (d, $J = 13.9$ Hz, 1H), 2.46 (s, 3H), 2.44 (s, 1.12H), 2.01 (s, 3H), 1.90 (s, 1.21H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 178.1, 178.0, 171.3, 165.7, 165.6, 157.6, 157.3, 145.1, 138.2, 138.0, 135.5, 135.3, 135.2, 135.2, 134.5, 134.3, 130.5, 130.2, 130.0, 129.9, 129.6, 129.4, 129.3, 129.1, 128.9, 128.8, 128.7, 128.6, 128.0, 127.9, 127.9, 127.6, 127.5, 127.4, 127.0, 126.8, 126.7, 126.3, 126.1, 125.8, 125.0, 124.1, 123.7, 123.5, 122.0, 60.5, 58.1, 57.5, 47.5, 47.1, 25.2, 24.7, 21.8, 21.2, 14.3; **MS** (ESI) m/z 604 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{36}\text{H}_{30}\text{NO}_4\text{S}_2^+$ 604.1611; Found: 604.1623 $[\text{M}+\text{H}]^+$.

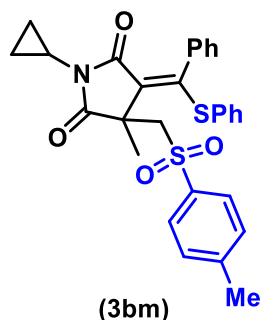


(E)-1-benzyl-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione (3bk): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bk** as white solid in 86% yield (169 mg), mp 175-177 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.30-7.27 (m, 6H), 7.21-7.15 (m, 5H), 7.04 - 6.99 (m, 6H), 4.70 (d, *J* = 12 Hz, 1H), 4.61-4.53 (m, 2H), 3.78 (d, *J* = 12 Hz, 1H), 2.38 (s, 3H), 1.58 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.7, 165.5, 156.1, 144.9, 137.7, 136.0, 135.4, 135.0, 130.0, 129.4, 129.0, 128.7, 128.63, 128.61, 128.6, 128.5, 127.9, 127.6, 127.4, 123.6, 57.4, 46.5, 42.6, 30.9, 30.9, 24.4, 21.7; MS (ESI) *m/z* 568 [M+H]⁺; HRMS Calculated for C₃₃H₃₀NO₄S₂⁺ 568.1611; Found: 568.1614 [M+H]⁺.



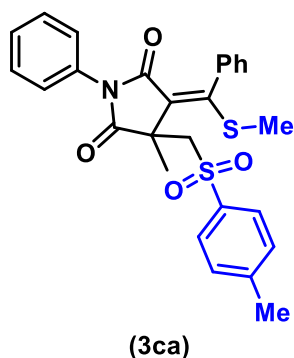
(E)-3-methyl-4-(phenyl(phenylthio)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione (3bl): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bl** as white solid in 88% yield (158 mg), mp 285-287 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.84 (d, *J* = 8.0 Hz, 2H), 7.40-7.38 (m, 4H), 7.23-7.16 (m, 8H), 4.75 (d, *J* = 14.0 Hz, 1H), 3.86 (d, *J* = 14.0 Hz, 1H), 3.51-3.44 (m, 2H), 2.45 (s, 3H), 1.73 (s, 3H), 1.69-1.64 (m, 2H),

0.91 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 178.0, 166.0, 156.0, 144.9, 137.8, 135.5, 135.1, 130.0, 129.3, 128.7, 128.6, 128.5, 127.8, 127.4, 123.8, 57.5, 46.3, 40.7, 24.4, 21.7, 20.8, 11.4. **MS** (ESI) m/z 520 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{29}\text{H}_{30}\text{NO}_4\text{S}_2^+$ 520.1611; Found: 520.1624 $[\text{M}+\text{H}]^+$.



(E)-1-cyclopropyl-3-methyl-4-(phenyl(phenylthio)methylene)-3-

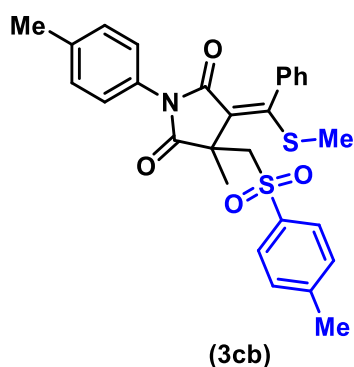
(tosylmethyl)pyrrolidine-2,5-dione (3bm): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3bm** as yellow solid in 89% yield (159 mg), mp 178-180 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.74 (d, $J = 8.0$ Hz, 2H), 7.28 (t, $J = 8$ Hz, 4H), 7.10-7.00 (m, 8H), 4.62 (d, $J = 14$ Hz, 1H), 3.72 (d, $J = 14$ Hz, 1H), 2.515 (q, $J = 4$ Hz, 1H), 2.4 (s, 3H), 1.6 (s, 3H), 1.03-0.99 (m, 1H), 0.83 (t, $J = 4$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 178.5, 166.5, 155.7, 144.9, 137.8, 135.4, 135.1, 130.0, 129.3, 128.7, 128.6, 128.4, 127.8, 127.4, 123.4, 57.8, 45.9, 24.1, 22.4, 21.7, 5.3, 5.0; **MS** (ESI) m/z 518 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{29}\text{H}_{28}\text{NO}_4\text{S}_2^+$ 518.1454; Found: 518.1461 $[\text{M}+\text{H}]^+$.



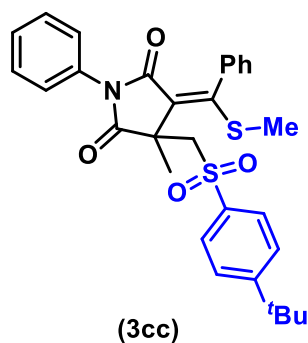
(E)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenyl-3-(tosylmethyl)pyrrolidine-

2,5-dione (3ca): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired

3ca as white solid in 85% yield (144 mg), mp 282-284 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.82 (d, $J = 8.0$ Hz, 2H), 7.42-7.30 (m, 12H), 4.74 (d, $J = 16$ Hz, 1H), 3.84 (d, $J = 16$ Hz, 1H), 2.44 (s, 3H), 1.96 (s, 3H), 1.73 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 177.6, 165.0, 157.8, 144.9, 137.9, 135.9, 132.2, 130.0, 128.9, 128.8, 128.4, 128.3, 127.8, 126.9, 123.7, 57.4, 46.4, 23.9, 21.7, 15.2; **MS** (ESI) m/z 492 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{27}\text{H}_{26}\text{NO}_4\text{S}_2^+$ 492.1298; Found: 492.1316 $[\text{M}+\text{H}]^+$.

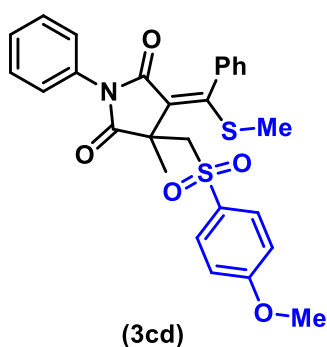


(E)-3-methyl-4-((methylthio)(phenyl)methylene)-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione (3cb): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired **3cb** as white solid in 83% yield (145 mg), mp 234-236 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.81 (d, $J = 8.0$ Hz, 2H), 7.40-7.33 (m, 7H), 7.24-7.18 (m, 4H), 4.74 (d, $J = 12.0$ Hz, 1H), 3.86 (d, $J = 12.0$ Hz, 1H), 2.44 (s, 3H), 2.33 (s, 3H), 1.95 (s, 3H), 1.72 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 177.7, 165.2, 157.5, 144.8, 138.3, 137.9, 135.9, 130.0, 129.6, 129.5, 128.8, 128.4, 127.8, 126.7, 123.9, 57.4, 46.4, 23.9, 21.7, 21.2, 15.2. **MS** (ESI) m/z 506 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{28}\text{H}_{28}\text{NO}_4\text{S}_2^+$ 506.1454; Found: 506.1440 $[\text{M}+\text{H}]^+$.

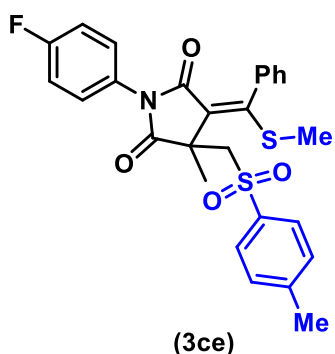


(E)-3-(((4-(tert-butyl)phenyl)sulfonyl)methyl)-3-methyl-4-

((methylthio)(phenyl)methylene)-1-phenylpyrrolidine-2,5-dione (3cc): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired **3cc** as white solid in 82% yield (151 mg), mp 238-240 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.8, 2.1 Hz, 2H), 7.56 (d, *J* = 8.8, 2.0 Hz, 2H), 7.44-7.30 (m, 10H), 4.76 (d, *J* = 14.0 Hz, 1H), 3.88 (d, *J* = 14.2 Hz, 1H), 1.95 (s, 3H), 1.73 (s, 3H), 1.34 (s, 9H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.7, 165.1, 157.8, 137.8, 135.9, 132.3, 128.9, 128.5, 128.4, 127.7, 127.0, 126.5, 123.7, 57.3, 46.4, 35.4, 31.1, 23.9, 15.3. MS (ESI) *m/z* 534 [M+H]⁺; HRMS Calculated for C₃₀H₃₂NO₄S₂⁺ 534.1767; Found: 534.1760 [M+H]⁺.

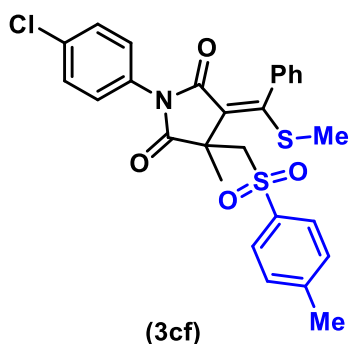


(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenylpyrrolidine-2,5-dione (3cd): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired **3cd** as brown solid in 88% yield (154 mg), mp 238-240 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.0 Hz, 2H), 7.41-7.29 (m, 10H), 7.00 (d, *J* = 8.0 Hz, 2H), 4.73 (d, *J* = 12.0 Hz, 1H), 3.86 (s, 3H), 3.85 (d, *J* = 12.0 Hz, 1H), 1.96 (s, 3H), 1.73 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.7, 165.1, 163.9, 157.8, 135.9, 132.4, 132.2, 130.0, 128.9, 128.8, 128.4, 128.3, 126.9, 123.7, 114.5, 57.6, 55.7, 46.4, 23.8, 15.23. MS (ESI) *m/z* 508 [M+H]⁺; HRMS Calculated for C₂₇H₂₆NO₅S₂⁺ 508.1247; Found: 508.1234 [M+H]⁺.



(E)-1-(4-fluorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (3ce): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired **3ce** as pale yellow solid in 81% yield (143 mg), mp 218-220 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 8.4 Hz, 2H), 7.46-7.30 (m, 9H), 7.10-7.04 (m, 2H), 4.72 (d, *J* = 14.0 Hz, 1H), 3.83 (d, *J* = 14.0 Hz, 1H), 2.44 (s, 3H), 1.95 (s, 3H), 1.72 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.8, 165.1, 162.3 (*J* = 246.3), 158.4, 145.0, 137.8, 135.8, 130.1, 129.0, 128.9 (*J* = 8.7 Hz), 128.6, 128.2 (*J* = 2.3 Hz) 127.8, 123.4, 115.9, (*J* = 22 Hz), 57.4, 46.4, 23.8, 21.8, 15.3; ¹⁹F NMR (376 MHz, CDCl₃) δ -112.9 (s, 1F); MS (ESI) *m/z* 510 [M+H]⁺; HRMS Calculated for C₂₇H₂₅FNO₄S₂⁺ 510.1204; Found: 510.1222 [M+H]⁺.

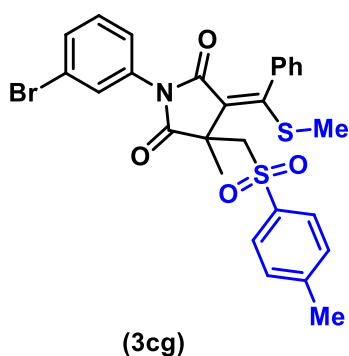


(E)-1-(4-chlorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (3cf): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired **3cf** as pale yellow solid in 84% yield (153 mg), mp 219-221 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.83 (d, *J* = 8.0 Hz, 2H), 7.40 (m, 11H), 4.76 (d, *J* = 12 Hz, 1H), 3.86 (d, *J* = 16 Hz, 1H), 2.47 (s, 3H), 1.98 (s, 3H), 1.75 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.4, 165.7, 158.5, 145.0, 137.8, 135.8, 134.1, 130.8, 130.3, 130.0, 129.0,

128.5, 128.2, 127.8, 123.3, 57.4, 46.3, 23.8, 21.7, 15.2; **MS** (ESI) m/z 526 $[M+H]^+$; HRMS

Calculated for $C_{27}H_{25}ClNO_4S_2^+$ 526.0908; Found: 526.0921 $[M+H]^+$.



(E)-1-(3-bromophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (3cg): Purification by silica gel chromatography

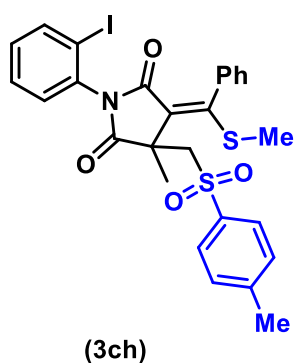
(PE:EA=93:7) afforded the desired **3cg** as white solid in 85% yield (167 mg), mp 212-214 °C;

¹H-NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H), 7.45 (t, J = 1.9 Hz, 1H), 7.40-7.25 (m, 8H), 7.25-7.18 (m, 2H), 4.66 (d, J = 14.0 Hz, 1H), 3.77 (d, J = 14.0 Hz, 1H), 2.38 (s, 3H),

1.90 (s, 3H), 1.66 (s, 3H); **¹³C-NMR** (100 MHz, $CDCl_3$) δ 177.3, 164.6, 158.6, 145.0, 137.7, 135.8, 133.4, 131.5, 130.0, 130.0, 129.0, 128.5, 127.8, 125.7, 123.2, 122.1, 57.3, 46.4, 23.8,

21.7, 15.3. **MS** (ESI) m/z 570 $[M+H]^+$; HRMS Calculated for $C_{27}H_{25}BrNO_4S_2^+$ 570.0403;

Found: 570.0414 $[M+H]^+$.



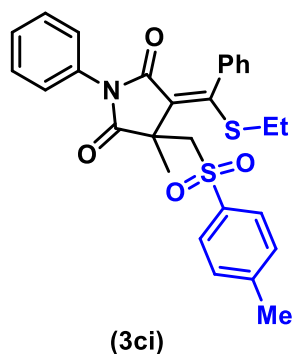
(E)-1-(2-iodophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (3ch): Purification by silica gel chromatography

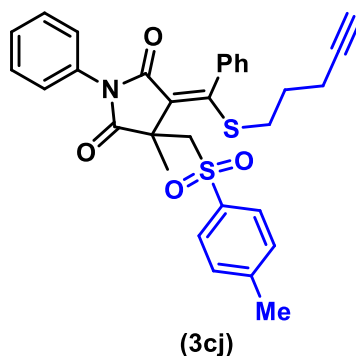
(PE:EA=93:7) afforded the desired **3ch** as white solid in 80% yield (171 mg), mp 265-267 °C;

¹H-NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, J = 13.5, 8.0 Hz, 3H), 7.48-7.35 (m, 9H), 7.09 (t, J =

6.9 Hz, 1H), 4.73 (d, $J = 14.0$ Hz, 1H), 3.89 (d, $J = 14.0$ Hz, 1H), 2.46 (s, 3H), 1.97 (s, 3H), 1.84 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 176.6, 164.1, 158.0, 144.8, 139.1, 138.0, 135.7, 135.6, 130.6, 130.0, 129.9, 129.5, 128.9, 128.4, 127.7, 123.9, 97.9, 57.8, 46.9, 23.3, 21.7, 15.2; **MS** (ESI) m/z 618 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{27}\text{H}_{25}\text{INO}_4\text{S}_2^+$ 618.0264; Found: 618.0282 $[\text{M}+\text{H}]^+$.

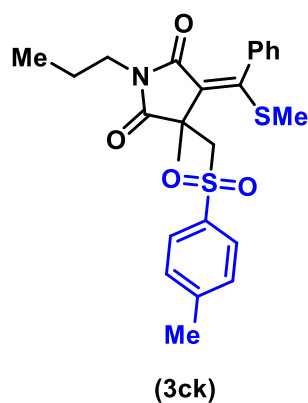


(E)-4-((ethylthio)(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione (3ci): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired **3ci** as brown solid in 85% yield (149 mg), mp 190-192 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.82 (d, $J = 8.0$ Hz, 2H), 7.42-7.30 (m, 12H), 4.735 (d, $J = 12$ Hz, 1H), 3.835 (d, $J = 12$ Hz, 1H), 2.51-2.45 (m, 1H), 2.45 (s, 3H), 2.40-2.34 (m, 1H), 1.75 (s, 3H), 1.17 (t, $J = 8.0$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 177.6, 166.1, 157.7, 144.9, 137.9, 136.2, 132.3, 130.1, 129.0, 128.9, 128.4, 128.3, 127.9, 127.0, 123.5, 57.7, 46.4, 27.0, 23.9, 21.7, 14.7; **MS** (ESI) m/z 506 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{28}\text{H}_{28}\text{NO}_4\text{S}_2^+$ 506.1454; Found: 506.1460 $[\text{M}+\text{H}]^+$.



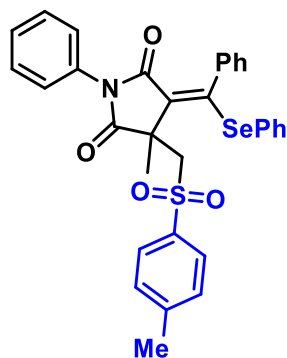
(E)-3-methyl-4-((pent-4-yn-1-ylthio)(phenyl)methylene)-1-phenyl-3-

(tosylmethyl)pyrrolidine-2,5-dione (3cj): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired **3cj** as brown solid in 85% yield (160 mg), mp 158-160 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.41-7.29 (m, 12H), 4.69 (d, *J* = 14.0 Hz, 1H), 3.82 (d, *J* = 13.9 Hz, 1H), 2.61-2.49 (m, 2H), 2.44 (s, 3H), 2.26-2.15 (m, 2H), 1.91 (t, *J* = 2.6 Hz, 1H), 1.73 (s, 3H), 1.69 (qd, *J* = 7.0, 2.5 Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.5, 165.0, 157.1, 144.9, 137.8, 135.7, 132.2, 130.0, 129.2, 129.0, 128.8, 128.4, 127.8, 127.0, 123.8, 82.8, 69.3, 57.6, 46.3, 31.3, 28.3, 23.9, 21.7, 17.4; **MS** (ESI) *m/z* 544 [M+H]⁺; HRMS Calculated for C₂₉H₂₈NO₄S₂⁺ 544.1611; Found: 544.1620 [M+H]⁺.



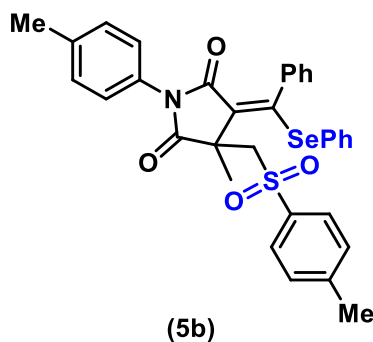
(E)-3-methyl-4-((methylthio)(phenyl)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-

2,5-dione (3ck): Purification by silica gel chromatography (PE:EA=93:7) afforded the desired **3ck** as pale yellow solid in 80% yield (127 mg), mp 153-155 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.79 (d, *J* = 8.0 Hz, 2H), 7.46-7.44 (m, 3H), 7.37 (d, *J* = 7.6 Hz, 4H), 4.66 (d, *J* = 14.0 Hz, 1H), 3.80 (d, *J* = 14.0 Hz, 1H), 3.49-3.37 (m, 2H), 2.47 (s, 3H), 1.95 (s, 3H), 1.66-1.59 (m, 2H), 0.89 (t, *J* = 7.2 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 178.2, 165.9, 155.9, 144.8, 137.9, 136.0, 129.9, 128.9, 128.3, 127.8, 124.3, 57.02, 46.2, 40.6, 24.01, 21.6, 20.7, 15.1, 11.3; **MS** (ESI) *m/z* 458 [M+H]⁺; HRMS Calculated for C₂₉H₂₈NO₄S₂⁺ 458.1454; Found: 458.1471 [M+H]⁺.



(5a)

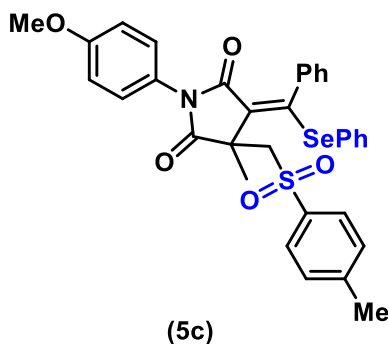
(E)-3-methyl-1-phenyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione (5a): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **5a** as white solid in 80% yield (166 mg), mp 238-240 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.90 (d, *J* = 8.0 Hz, 2H), 7.43-7.33 (m, 10H), 7.17 (t, *J* = 7.2 Hz, 2H), 7.08 (t, *J* = 7.4 Hz, 5H), 4.92 (d, *J* = 14.0 Hz, 1H), 3.91 (d, *J* = 14.2 Hz, 1H), 2.46 (s, 3H), 1.84 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.6, 164.7, 157.5, 145.2, 137.9, 137.5, 136.6, 132.3, 130.2, 129.0, 128.9, 128.5, 128.2, 127.9, 127.4, 127.1, 126.8, 125.7, 57.7, 47.1, 24.8, 21.8; MS (ESI) *m/z* 602 [M+H]⁺; HRMS Calculated for C₃₂H₂₈NO₄SSe⁺ 602.0899; Found: 602.0893 [M+H]⁺.



(5b)

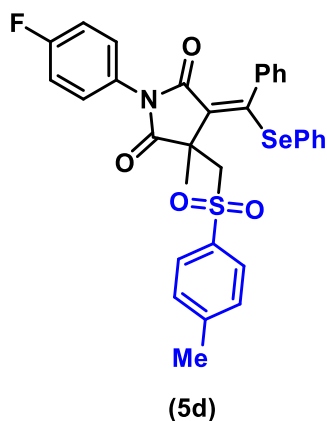
(E)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione (5b): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **5b** as brown solid in 83% yield (177 mg), mp 238-240 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.1 Hz, 2H), 7.40-7.35 (m, 4H), 7.24 (d, *J* = 3.8 Hz, 2H), 7.20-7.13 (m, 5H), 7.08-6.99 (m, 5H), 4.88 (d, *J* = 14.2 Hz, 1H), 3.88 (d, *J* = 14.0 Hz, 1H), 2.45 (s, 3H),

2.32 (s, 3H), 1.80 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 177.7, 164.8, 157.2, 145.1, 138.5, 137.9, 137.5, 136.5, 130.1, 129.9, 129.6, 129.3, 128.8, 128.2, 128.1, 127.9, 127.4, 126.8, 125.8, 57.6, 47.1, 24.8, 21.8, 21.3 **MS** (ESI) m/z 616 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{33}\text{H}_{30}\text{NO}_4\text{SSe}^+$ 616.1055; Found: 616.1060 $[\text{M}+\text{H}]^+$.



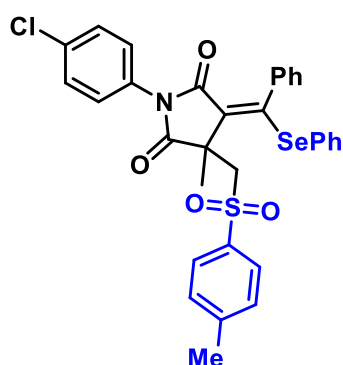
(E)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (5c): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **5c** as pale yellow solid in 88% yield (192 mg), mp 236-238 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.86 (d, $J = 8.4$ Hz, 2H), 7.37 (t, $J = 8.2$ Hz, 5H), 7.29 (dd, $J = 6.9, 2.2$ Hz, 2H), 7.17-7.12 (m, 2H), 7.07-6.99 (m, 5H), 6.91 (dd, $J = 6.9, 2.2$ Hz, 2H), 4.88 (d, $J = 14.0$ Hz, 1H), 3.87 (d, $J = 14.6$ Hz, 1H), 3.77 (s, 3H), 2.45 (s, 3H), 1.80 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 177.8, 164.9, 159.5, 157.0, 145.0, 137.9, 137.8, 137.5, 136.5, 130.1, 128.8, 128.5, 128.2, 127.9, 127.4, 126.8, 125.8, 125.0, 114.3, 57.7, 55.6, 47.0, 24.7, 21.8. **MS** (ESI) m/z 632 $[\text{M}+\text{H}]^+$; HRMS Calculated for $\text{C}_{33}\text{H}_{30}\text{NO}_5\text{SSe}^+$ 632.1004; Found: 632.1019 $[\text{M}+\text{H}]^+$.



(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-

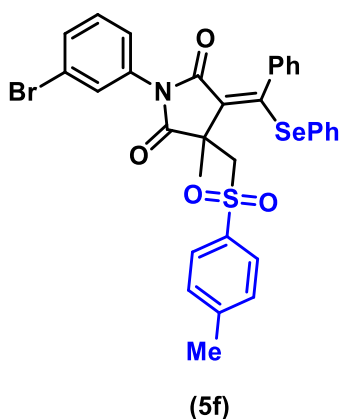
(tosylmethyl)pyrrolidine-2,5-dione(5d): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **5d** as white solid in 85% yield (182 mg), mp 204-206 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.1 Hz, 2H), 7.39-7.37 (m, 6H), 7.17-7.04 (m, 10H), 4.89 (d, *J* = 14.0 Hz, 1H), 3.86 (d, *J* = 14.0 Hz, 1H), 2.46 (s, 3H), 1.81 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.6, 164.6, 162.3 (d, *J* = 246.3Hz), 158.0, 145.2, 137.7, 137.4, 136.6, 130.2, 129.0, 128.9, 128.7, 128.2, 128.1, 127.9, 127.4, 126.6, 125.4, 115.9 (d, *J* = 23.0 Hz), 57.6, 47.0, 24.7, 21.8; 19F NMR (376 MHz, CDCl₃) δ -112.9 (s, 1F); MS (ESI) *m/z* 620 [M+H]⁺; HRMS Calculated for C₃₂H₂₈NO₄S⁺ 620.0805; Found: 620.0824 [M+H]⁺.



(5e)

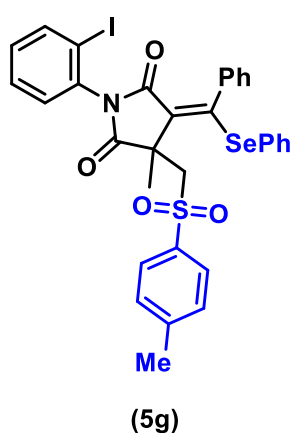
(E)-1-(4-chlorophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (5e): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3l** as pale yellow solid in 84% yield (185 mg), mp 201-203 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 8.3 Hz, 2H), 7.40-7.35 (m, 9H), 7.17 (t, *J* = 7.4 Hz, 2H), 7.07 (t, *J* = 7.4 Hz, 5H), 4.91 (d, *J* = 14.0 Hz, 1H), 3.87 (d, *J* = 13.9 Hz, 1H), 2.47 (s, 3H), 1.82 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.3, 164.3, 158.1, 145.1, 137.7, 137.3, 136.5, 134.2, 130.7, 130.1, 129.0, 128.8, 128.3, 128.2, 127.8, 127.4, 126.6, 125.2, 121.8, 57.5, 47.0, 24.6, 21.7 MS (ESI) *m/z* 636 [M+H]⁺; HRMS Calculated for C₃₂H₂₈NO₄S⁺ 636.0509; Found: 636.0513 [M+H]⁺.



(E)-1-(3-bromophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-

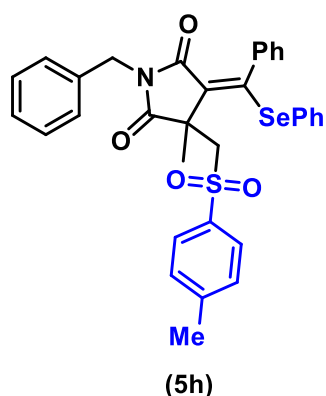
(tosylmethyl)pyrrolidine-2,5-dione (5f): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **5f** as white solid in 85% yield (199 mg), mp 232-235 °C; ¹H-NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 8.1 Hz, 2H), 7.55 (s, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.40-7.37 (m, 6H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.12 (*dt*, *J* = 36.7, 7.4 Hz, 7H), 4.90 (d, *J* = 14.0 Hz, 1H), 3.87 (*d*, *J* = 14.0 Hz, 1H), 2.47 (s, 3H), 1.82 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 177.3, 164.2, 158.5, 145.2, 137.8, 137.7, 137.4, 136.6, 133.4, 131.6, 130.2, 130.0, 128.9, 128.3, 128.2, 127.9, 127.5, 126.6, 125.8, 125.1, 122.2, 57.5, 47.1, 24.7, 21.8 **MS** (ESI) *m/z* 680 [M+H]⁺; HRMS Calculated for C₃₂H₂₇NO₄BrSSe⁺ 680.0004; Found: 680.0020 [M+H]⁺.



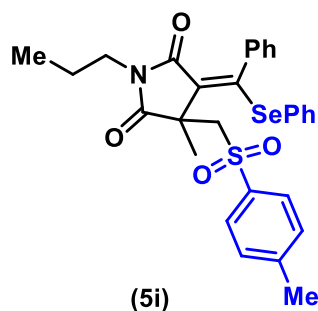
(E)-1-(2-iodophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-

(tosylmethyl)pyrrolidine-2,5-dione (5g): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **5g** as white solid in 80% yield (201 mg), mp 232-234 °C;

¹H-NMR (400 MHz, CDCl₃) δ 7.87-7.83 (m, 3H), 7.49 (dd, J = 7.9, 1.6 Hz, 1H), 7.44-7.36 (m, 5H), 7.19-6.99 (m, 9H), 4.86 (d, J = 14.0 Hz, 1H), 3.91 (d, J = 14.0 Hz, 1H), 2.46 (s, 3H), 1.92 (s, 3H) **¹³C-NMR** (100 MHz, CDCl₃) δ 176.6, 163.8, 157.6, 145.1, 139.2, 138.0, 137.3, 136.5, 135.6, 130.8, 130.1, 129.9, 129.6, 128.9, 128.2, 127.9, 127.4, 126.7, 125.9, 97.9, 58.2, 47.6, 24.1, 21.8; **MS** (ESI) m/z 727 [M+H]⁺; **HRMS** Calculated for C₃₂H₂₇NO₄ISse⁺ 727.9865; Found: 727.9844 [M+H]⁺.



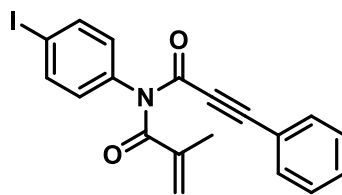
(E)-1-benzyl-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione (5i): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3i** as white solid in 86% yield (183 mg), mp 165-167 °C; **¹H-NMR** (400 MHz, CDCl₃) δ 7.77 (d, J = 8.2 Hz, 2H), 7.37-7.32 (m, 6H), 7.28-7.20 (m, 4H), 7.17-7.11 (m, 2H), 7.10-7.02 (m, 5H), 4.83 (d, J = 14.2 Hz, 1H), 4.63 (dd, J = 15.9, 14.5 Hz, 2H), 3.81 (d, J = 14.3 Hz, 1H), 2.45 (s, 3H), 1.64 (s, 3H); **¹³C-NMR** (100 MHz, CDCl₃) δ 177.8, 165.1, 156.0, 145.0, 137.8, 137.5, 136.5, 136.0, 130.0, 129.1, 128.8, 128.7, 128.5, 128.2, 128.0, 127.7, 127.4, 126.8, 126.0, 57.3, 47.1, 42.7, 24.8, 21.8. **MS** (ESI) m/z 616 [M+H]⁺; **HRMS** Calculated for C₃₃H₃₀NO₄Sse⁺ 616.1055; Found: 616.1063 [M+H]⁺.



(E)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione (5i): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **5j** as yellow solid in 80% yield (157 mg), mp 170-172 °C; **¹H-NMR** (400 MHz, CDCl₃) δ 7.74 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 7.6 Hz, 4H), 7.09-6.98 (m, 8H), 4.71 (d, J = 14.4 Hz, 1H), 3.73 (d, J = 14.0 Hz, 1H), 3.40-3.31 (m, 2H), 2.39 (s, 3H), 1.61 (s, 3H), 1.59-1.53 (m, 2H), 0.80 (t, J = 7.2 Hz, 3H); **¹³C-NMR** (100 MHz, CDCl₃) δ 178.1, 165.5, 155.3, 145.0, 137.8, 137.6, 136.5, 130.1, 128.8, 128.7, 128.1, 127.9, 127.3, 126.7, 126.3, 57.4, 46.9, 40.8, 24.8, 21.8, 20.8, 11.4; **MS** (ESI) m/z 568 [M+H]⁺; HRMS Calculated for C₂₉H₃₀NO₄SSe⁺ 568.1055; Found: 568.1071 [M+H]⁺.

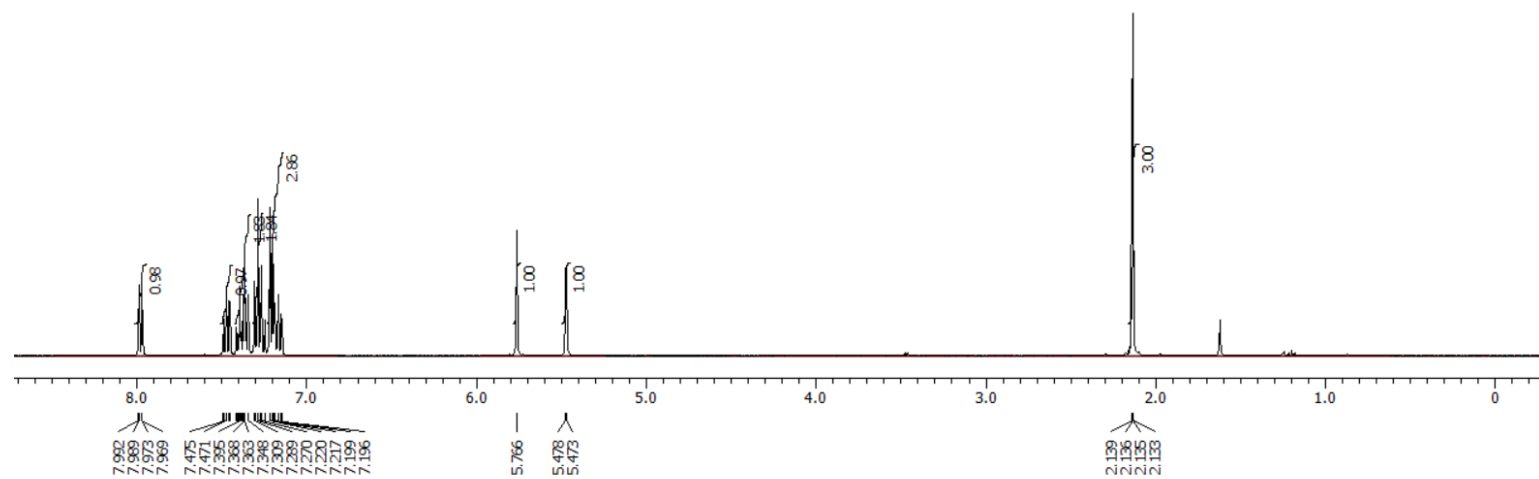
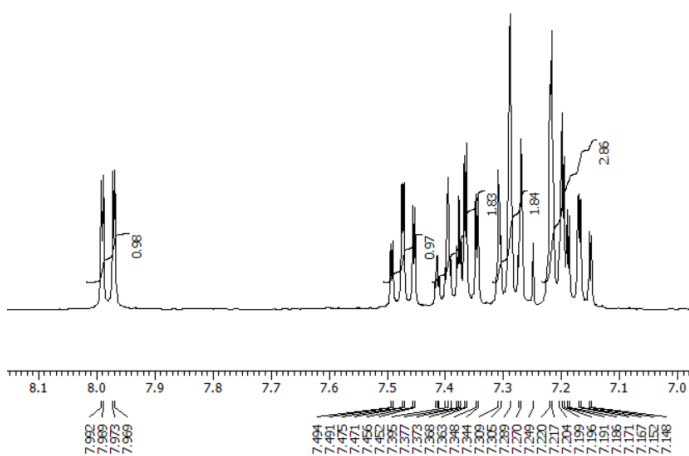
(8) Copies of ^1H NMR, ^{13}C NMR, ^{19}F NMR and Mass Spectra

¹H NMR spectrum of 1g (400 MHz, CDCl₃)

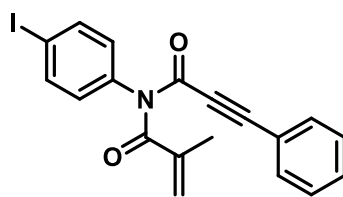


1g

N-(4-iodophenyl)-*N*-(3-phenylpropioyl)methacrylamide (1g)

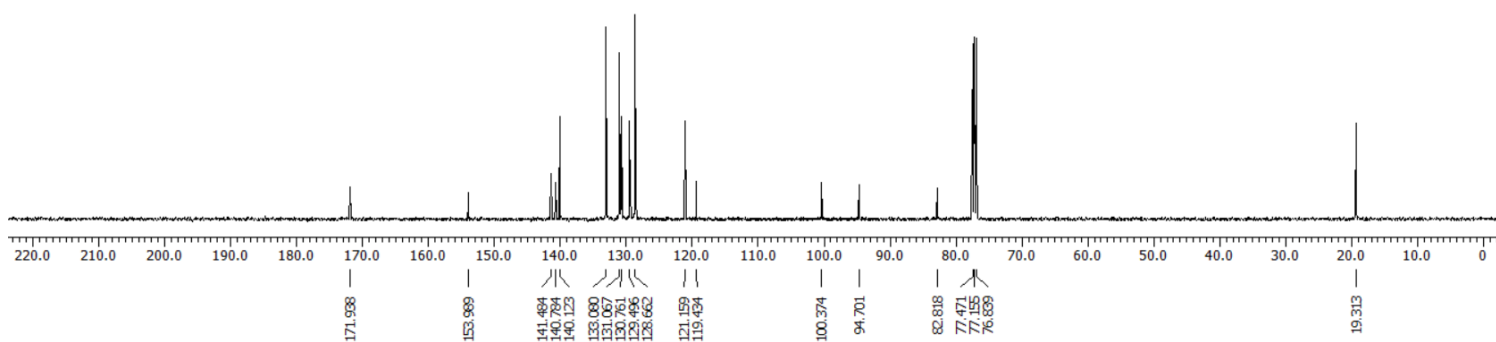
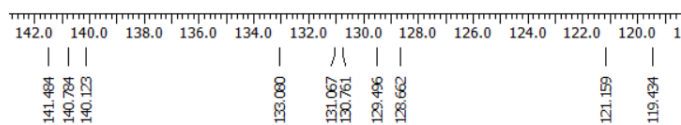
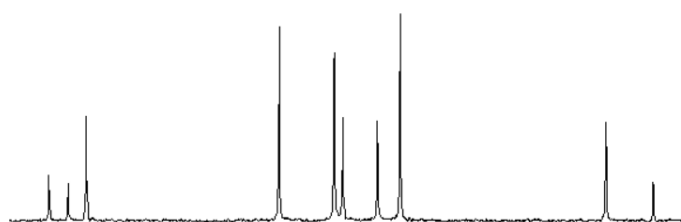


¹³C NMR spectrum of 1g (100 MHz, CDCl₃)

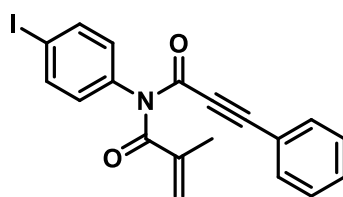


1g

N-(4-iodophenyl)-*N*-(3-phenylpropioloyl)methacrylamide (1g)



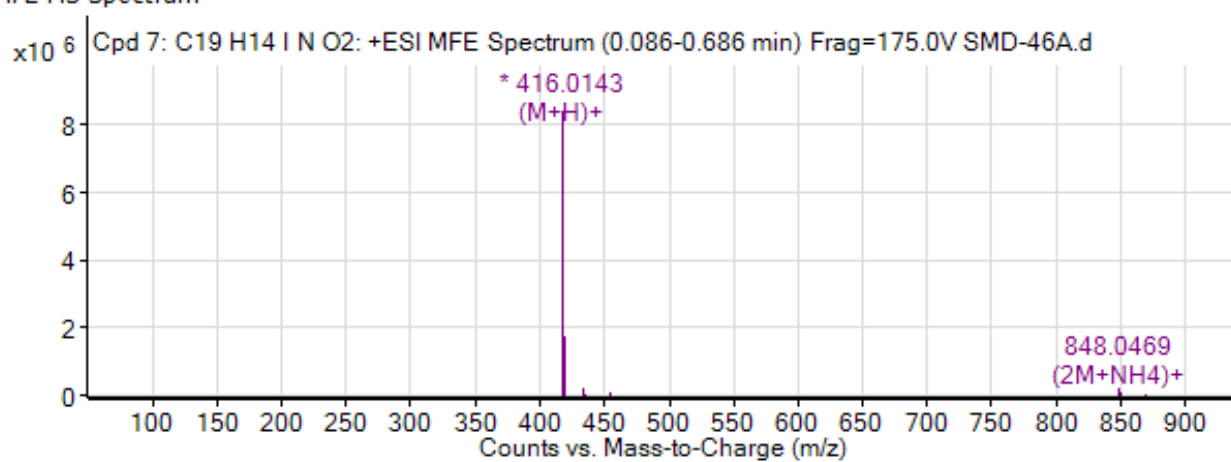
Mass spectrum of 1g



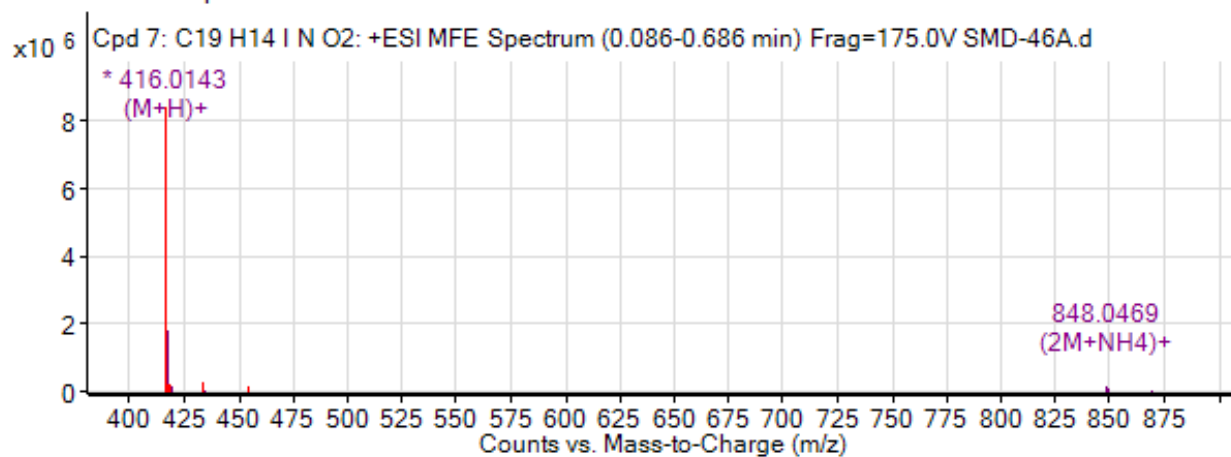
1g

N-(4-iodophenyl)-*N*-(3-phenylpropioloyl)methacrylamide (1g)

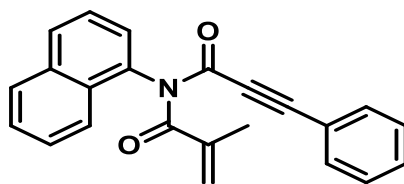
MFE MS Spectrum



MFE MS Zoomed Spectrum

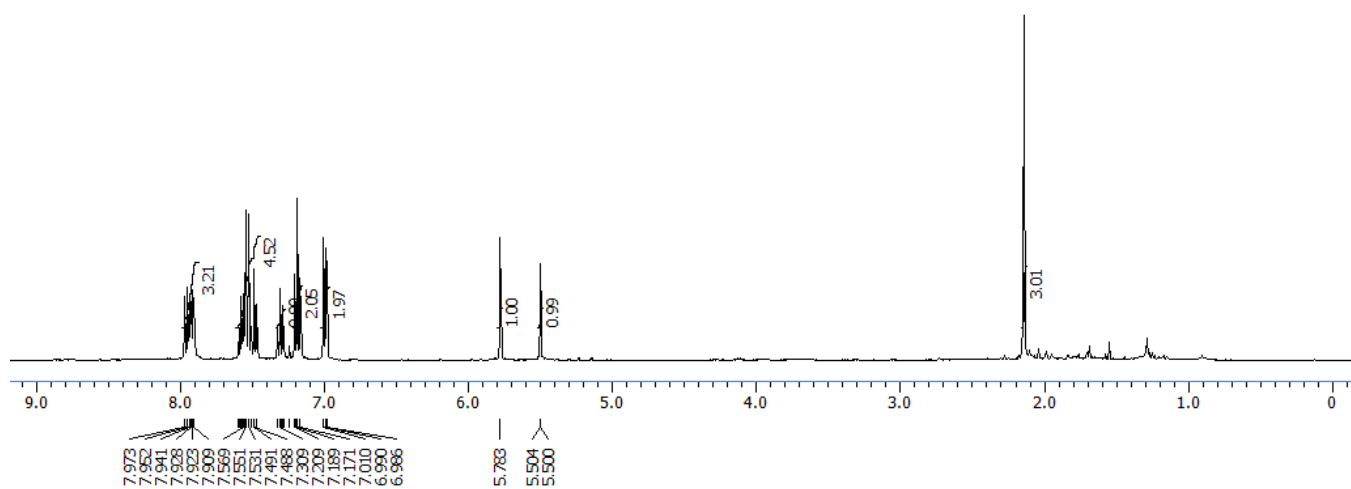
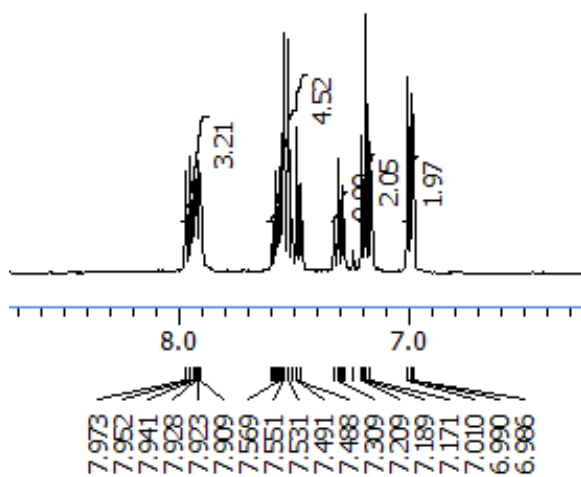


¹H NMR spectrum of 1h (400 MHz, CDCl₃)

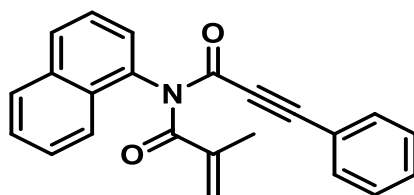


1h

O-(naphthalen-1-yl)-*N*-(3-phenylpropioloyl)methacrylamide (1h)

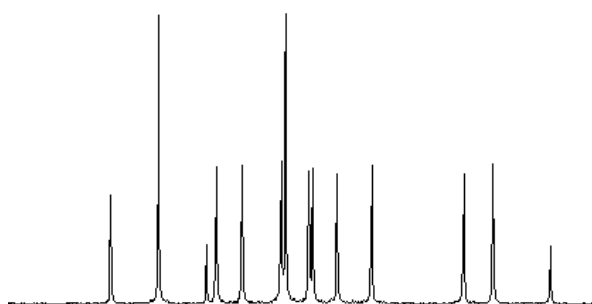


¹³C NMR spectrum of 1h (100 MHz, CDCl₃)



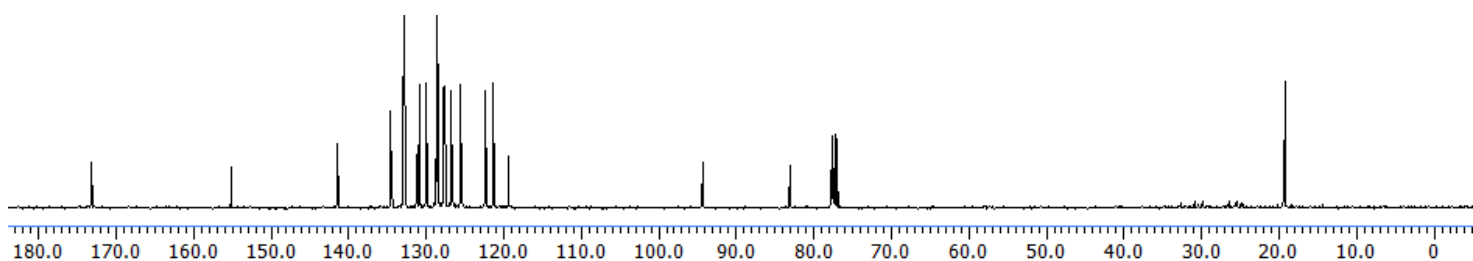
1h

N-(naphthalen-1-yl)-*N*-(3-phenylpropioloyl)methacrylamide (1h)



137.0 135.0 133.0 131.0 129.0 127.0 125.0 123.0 121.0 119.0

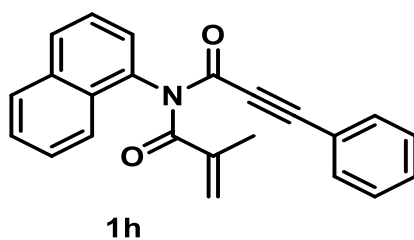
134.555
132.917
131.259
130.923
130.023
128.691
128.547
127.732
127.608
126.765
125.567
122.404
121.389
119.405



173.183
155.158
141.464
134.555
132.917
131.259
130.923
130.023
128.691
128.547
127.732
127.608
126.765
125.567
122.404
121.389
119.405

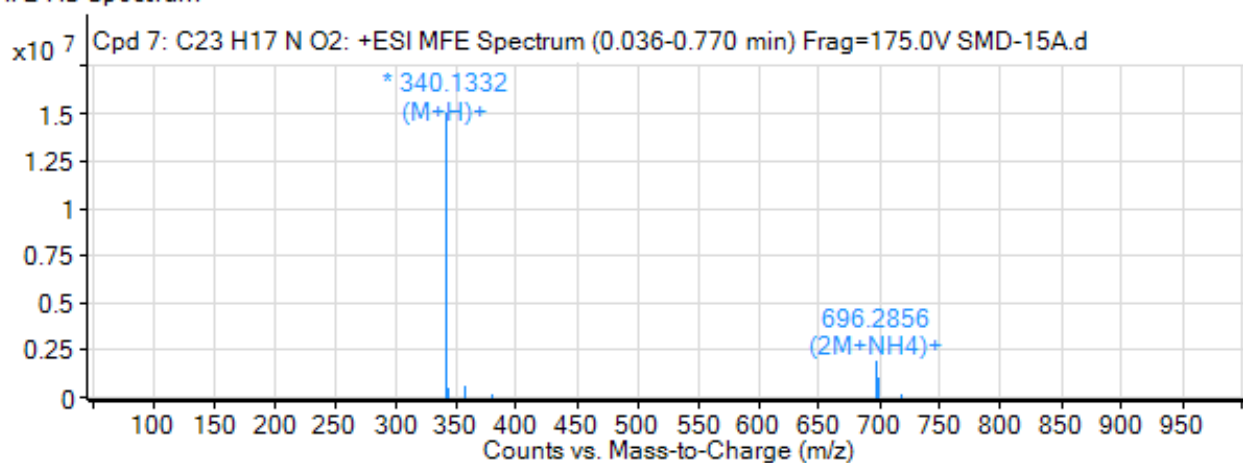
94.279
88.010
77.586
77.270
76.954
19.265

Mass spectrum of 1h

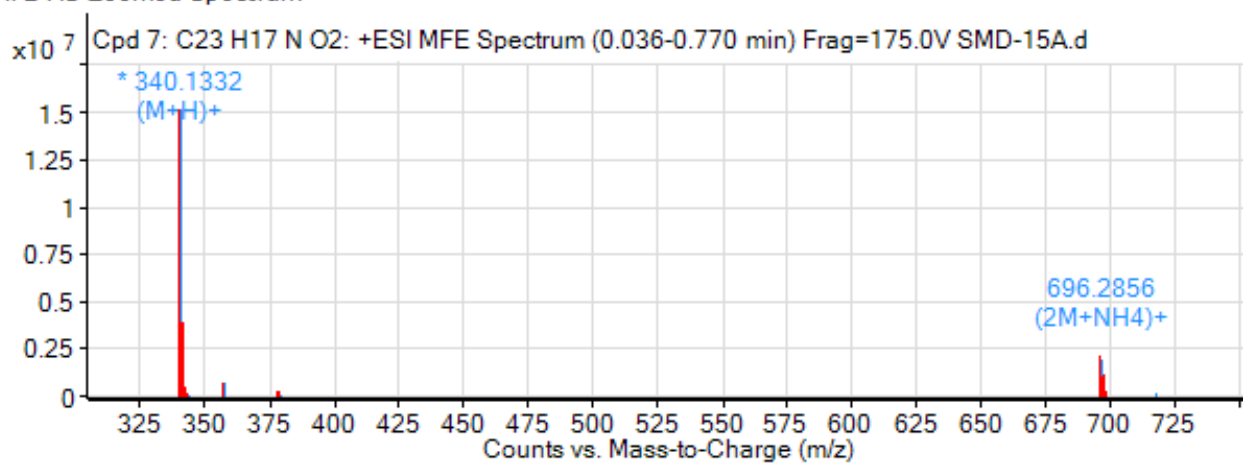


N-(naphthalen-1-yl)-*N*-(3-phenylpropioloyl)methacrylamide (1h)

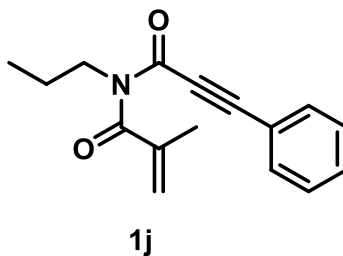
MFE MS Spectrum



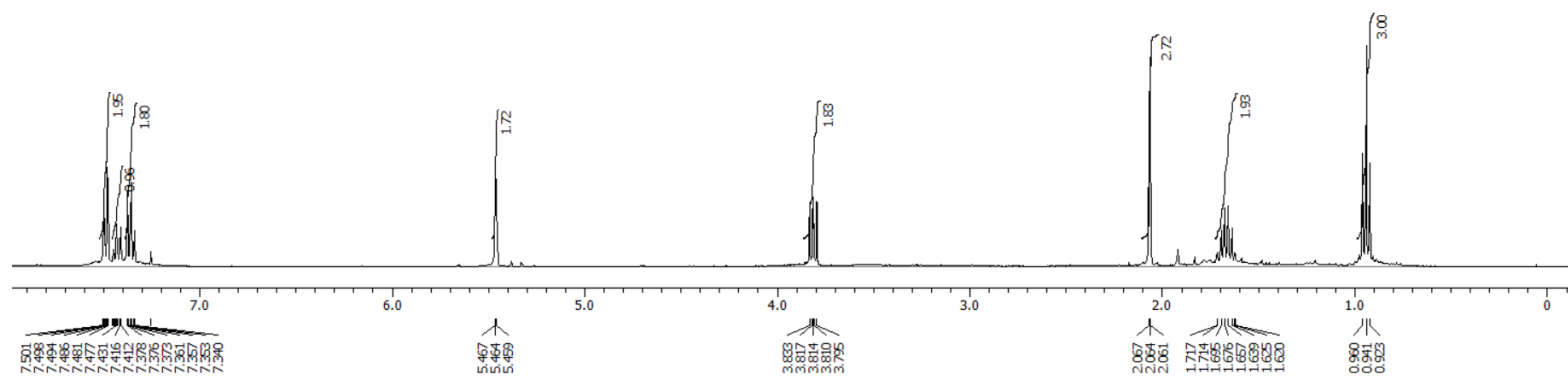
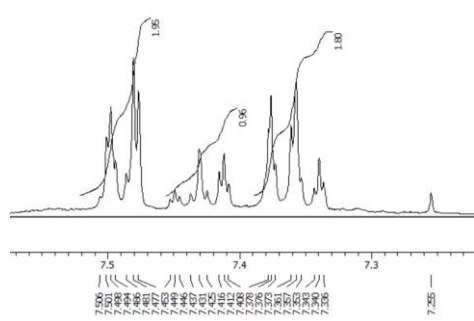
MFE MS Zoomed Spectrum



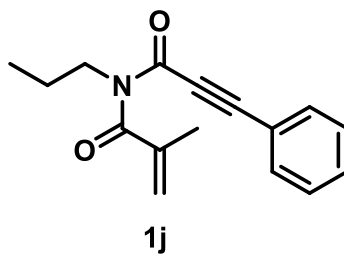
¹H NMR spectrum of 1j (400 MHz, CDCl₃)



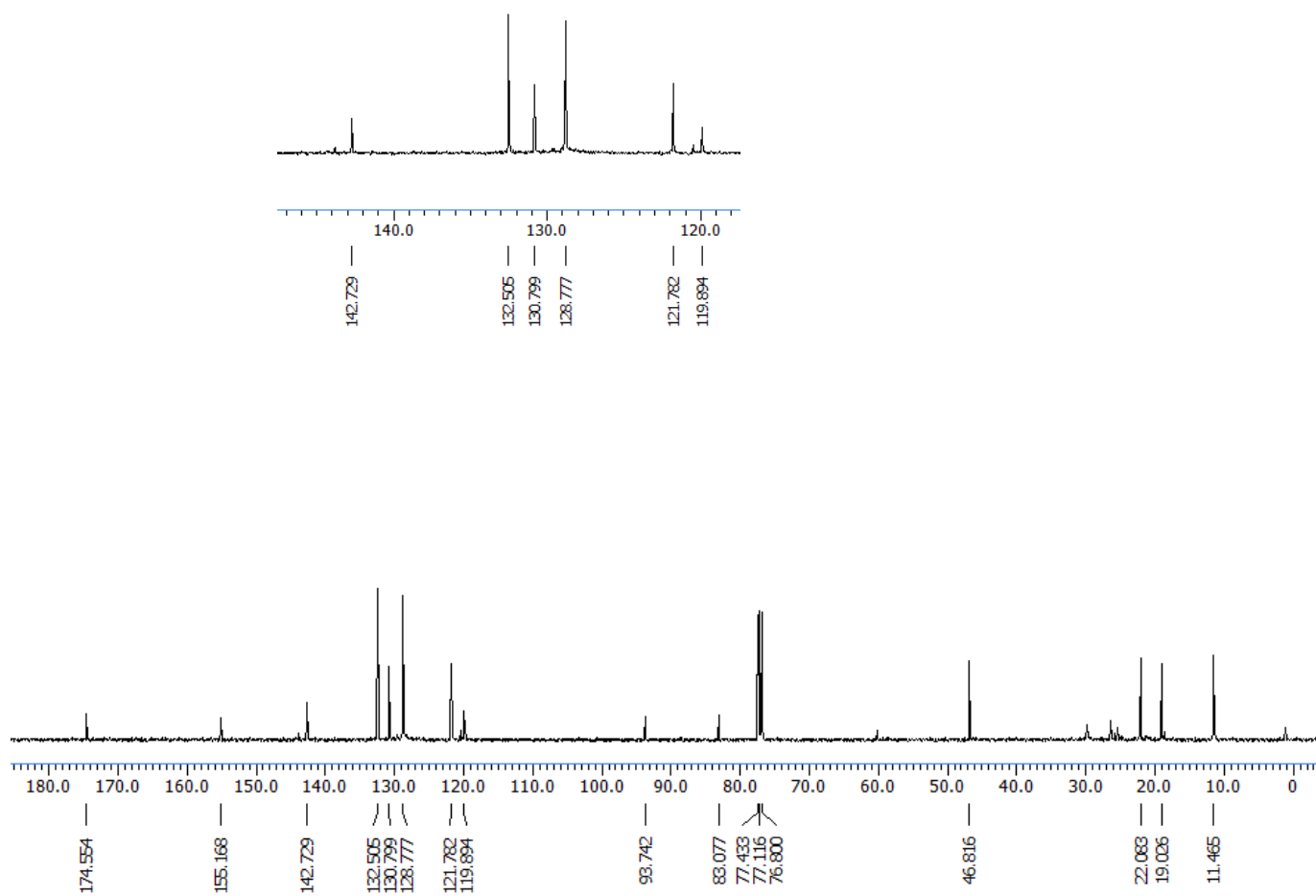
N-(3-phenylprop-1-yn-1-yl)-*N*-propylmethacrylamide (1j)



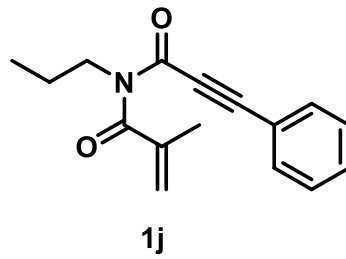
¹³C NMR spectrum of 1j (100 MHz, CDCl₃)



N-(3-phenylpropioloyl)-*N*-propylmethacrylamide (1j)

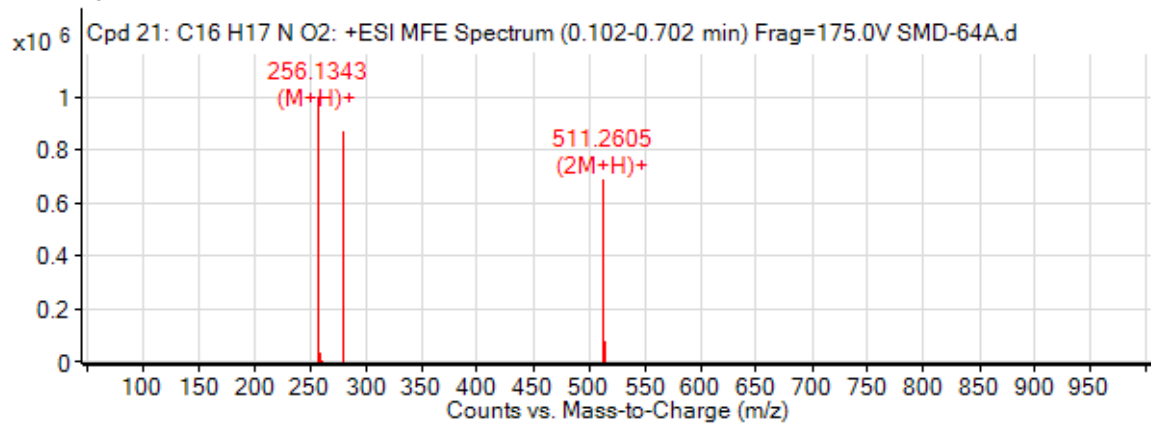


Mass spectrum of 1j

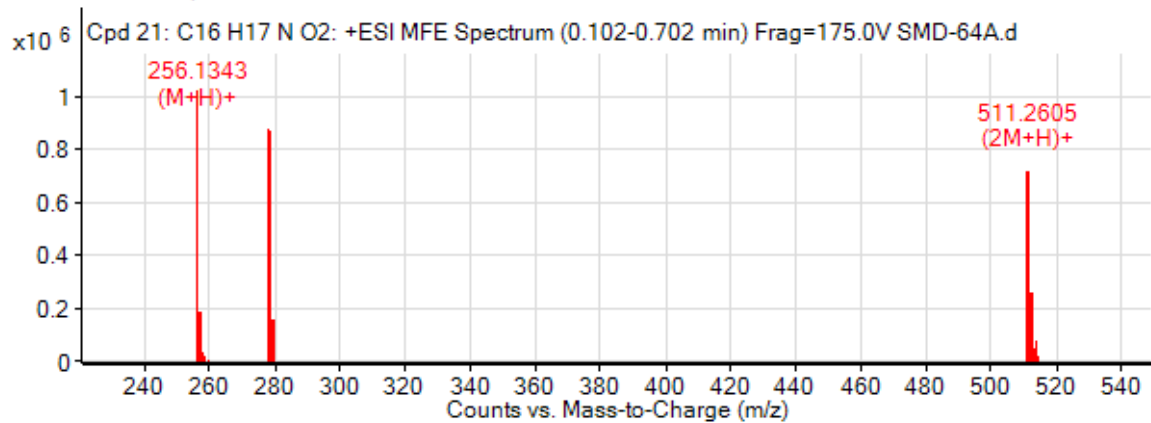


N-(3-phenylpropioloyl)-*N*-propylmethacrylamide (1j)

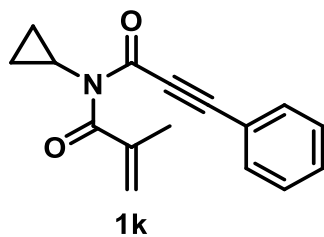
MFE MS Spectrum



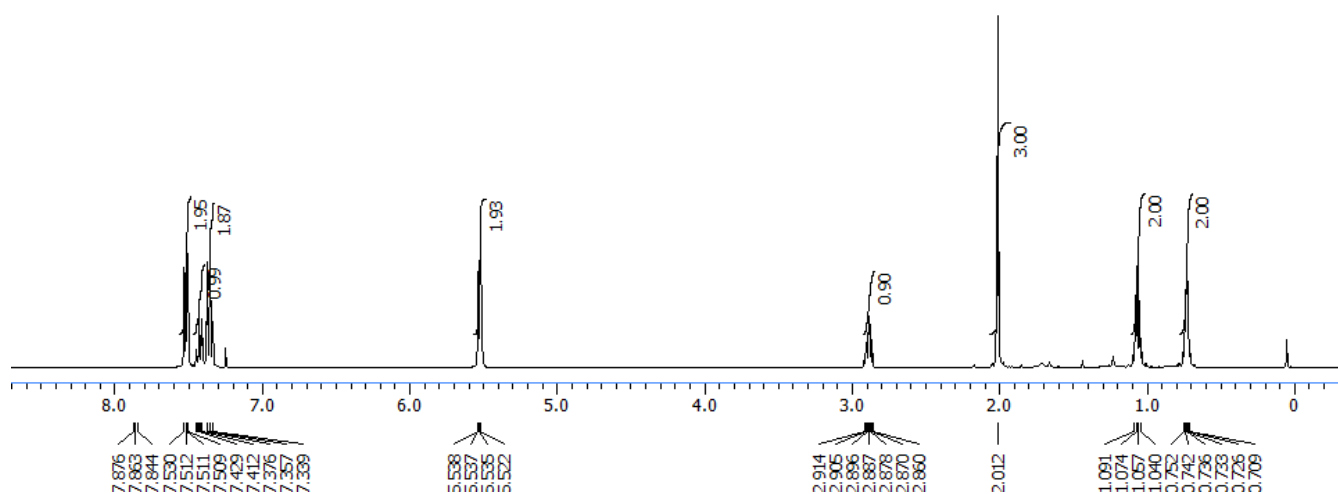
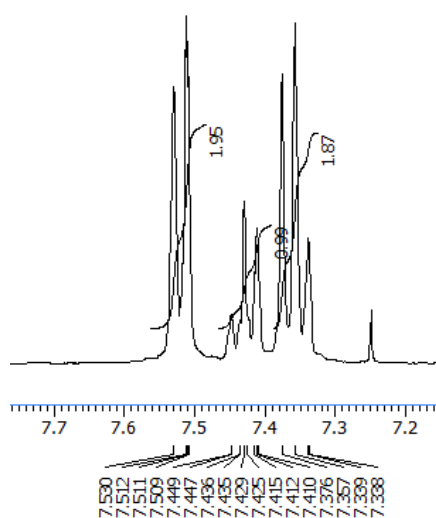
MFE MS Zoomed Spectrum



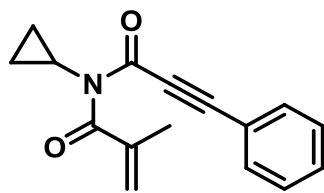
¹H NMR spectrum of 1k (400 MHz, CDCl₃)



N-cyclopropyl-*N*-(3-phenylpropioloyl)methacrylamide (1k)

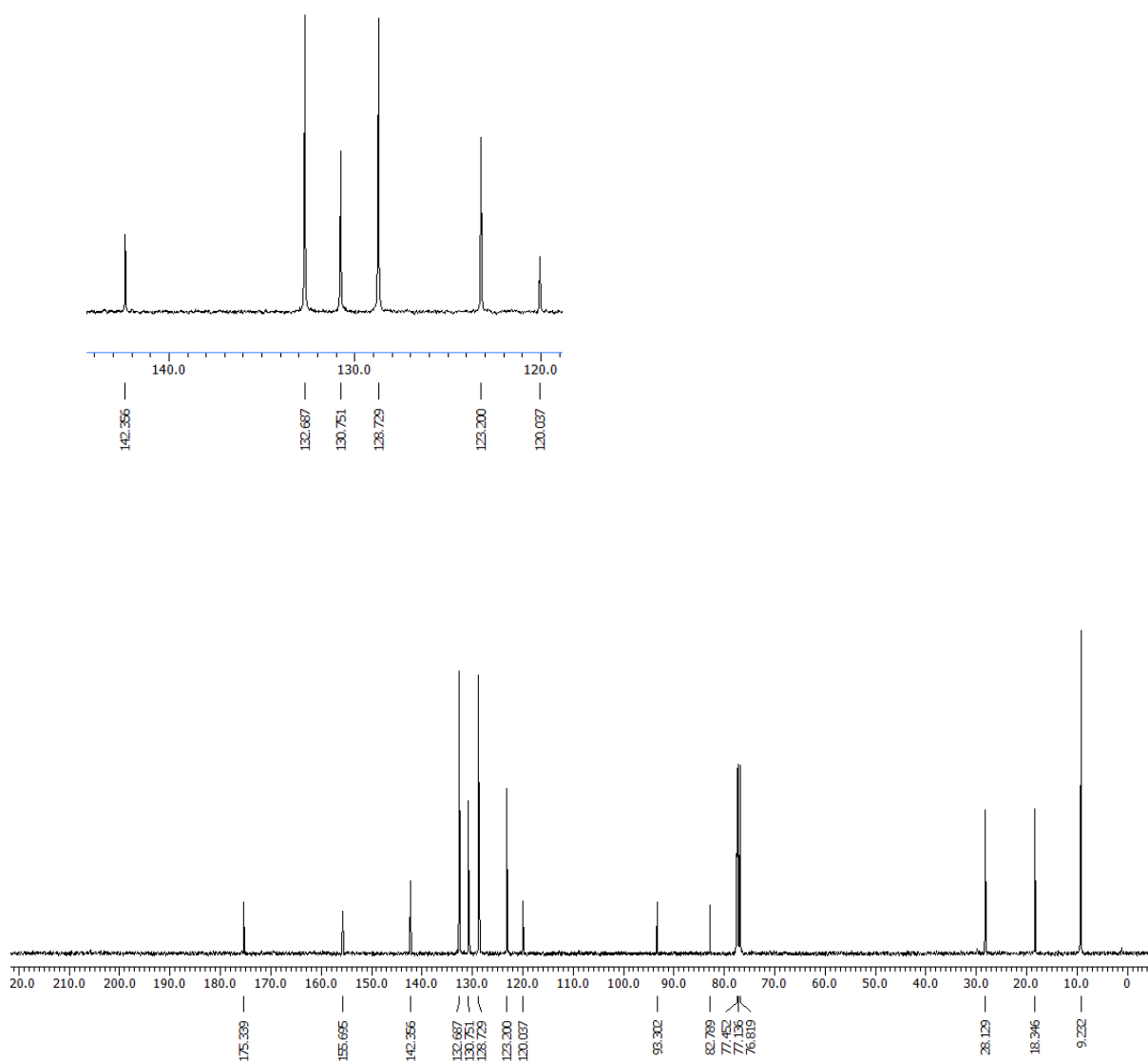


¹³C NMR spectrum of 1k (100 MHz, CDCl₃)

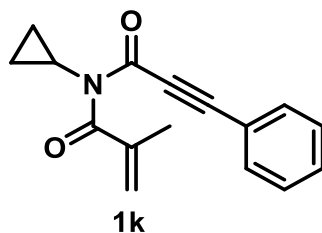


1k

N-cyclopropyl-*N*-(3-phenylpropioloyl)methacrylamide (1k)

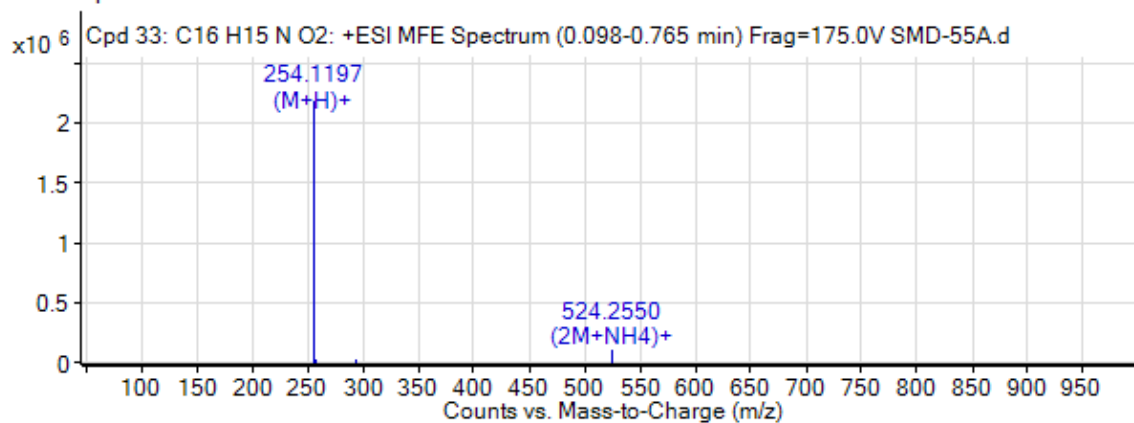


Mass Spectrum of 1k

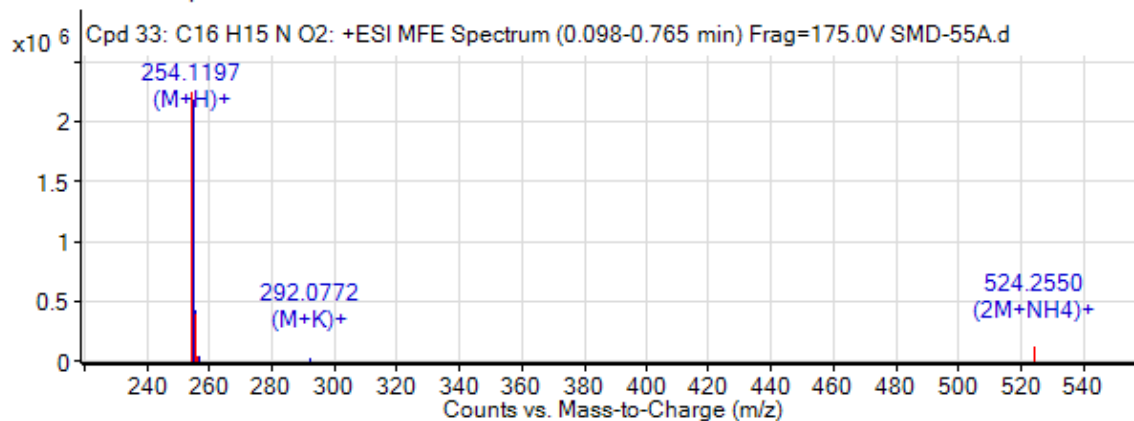


N-cyclopropyl-*N*-(3-phenylpropioloyl)methacrylamide (1k)

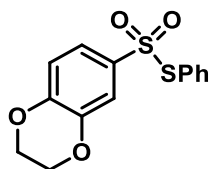
MFE MS Spectrum



MFE MS Zoomed Spectrum

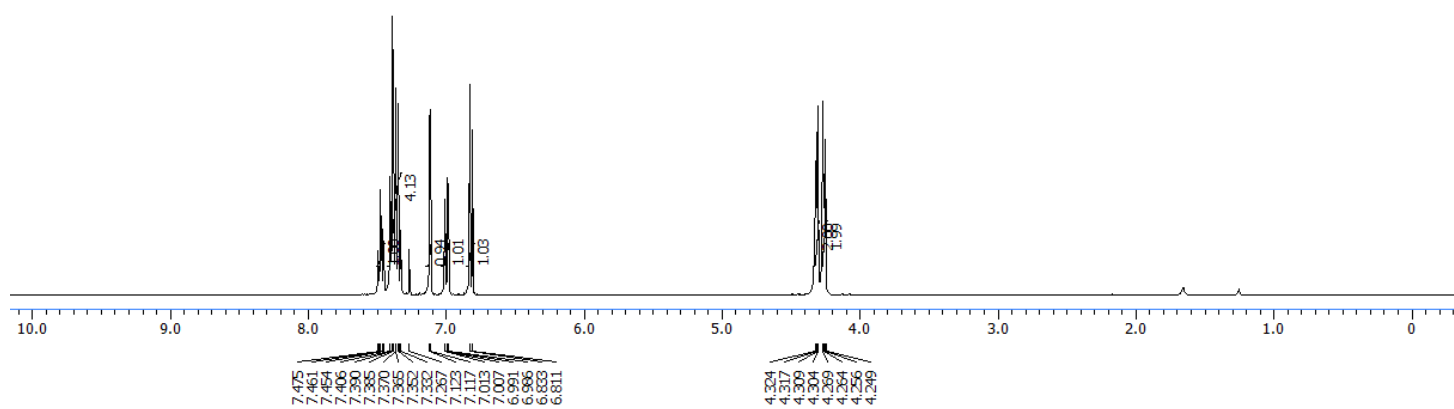
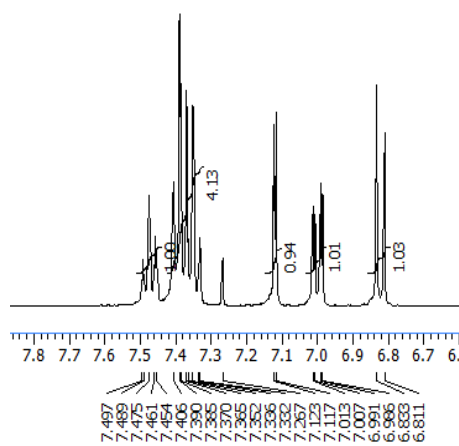


¹H NMR spectrum of 2h (400 MHz, CDCl₃)

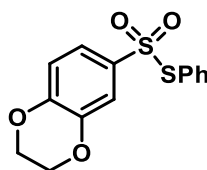


2h

S-phenyl 2,3-dihydrobenzo[*b*][1,4]dioxine-6-sulfonothioate (2h)

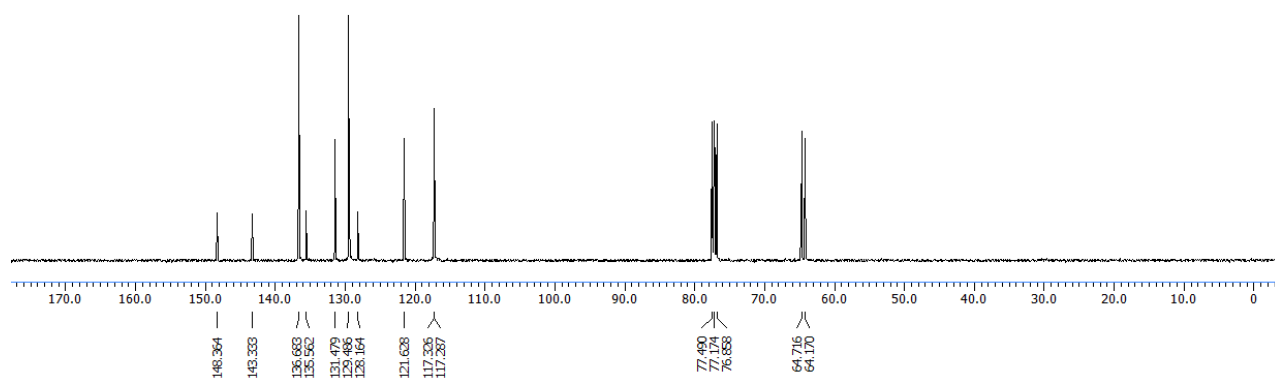
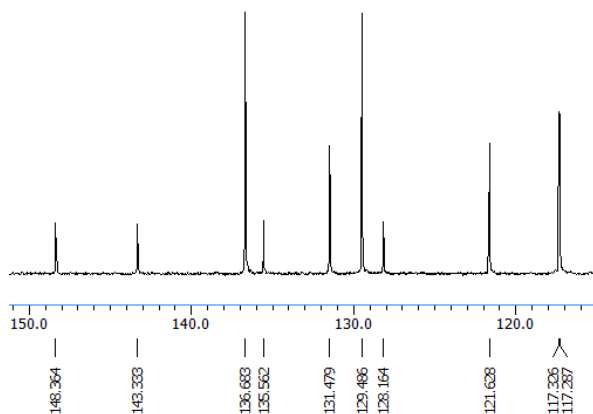


¹³C NMR spectrum of 2h (100 MHz, CDCl₃)

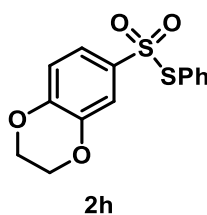


2h

S-phenyl 2,3-dihydrobenzo[*b*][1,4]dioxine-6-sulfonothioate (2h)

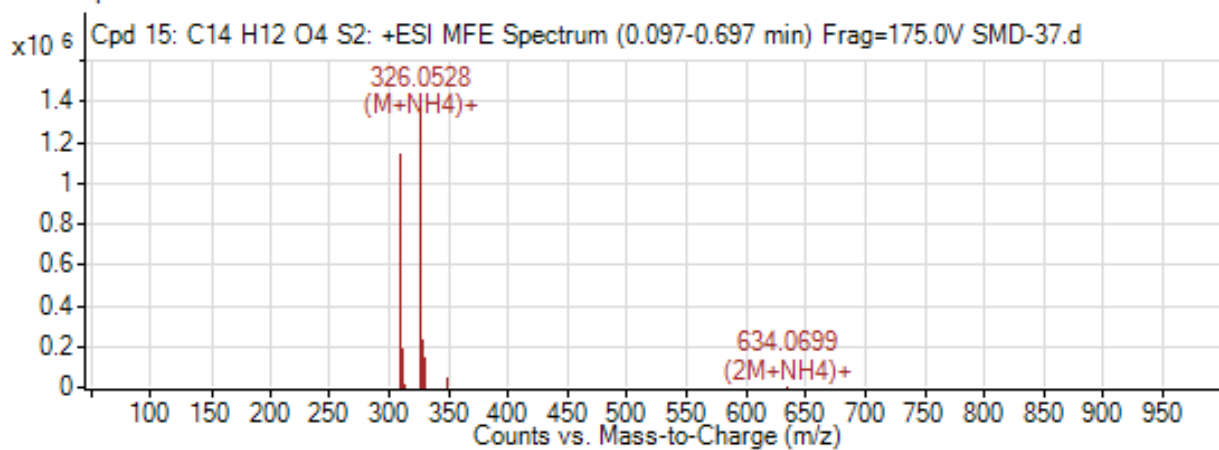


Mass spectrum of 2h

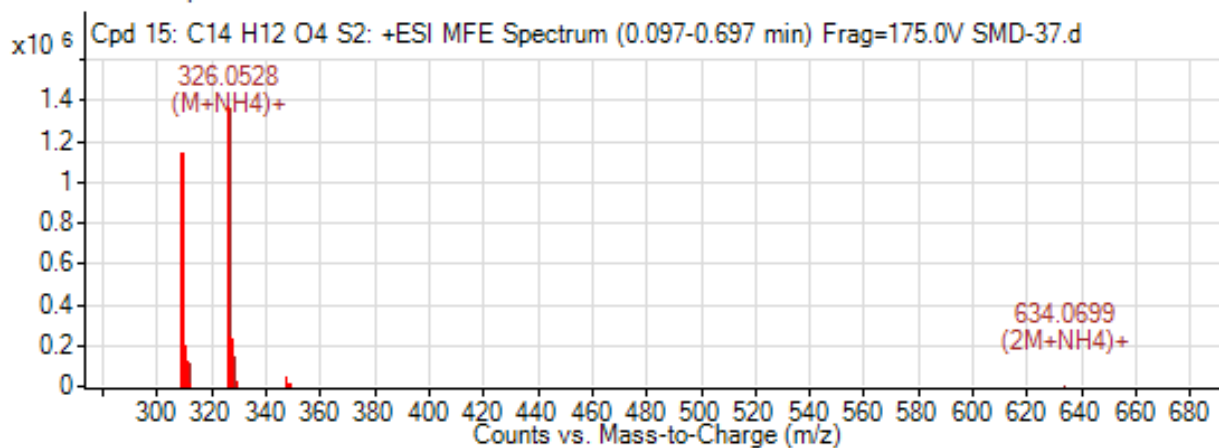


S-phenyl 2,3-dihydrobenzo[b][1,4]dioxine-6-sulfonothioate (2h)

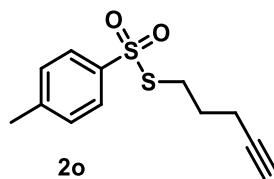
MFE MS Spectrum



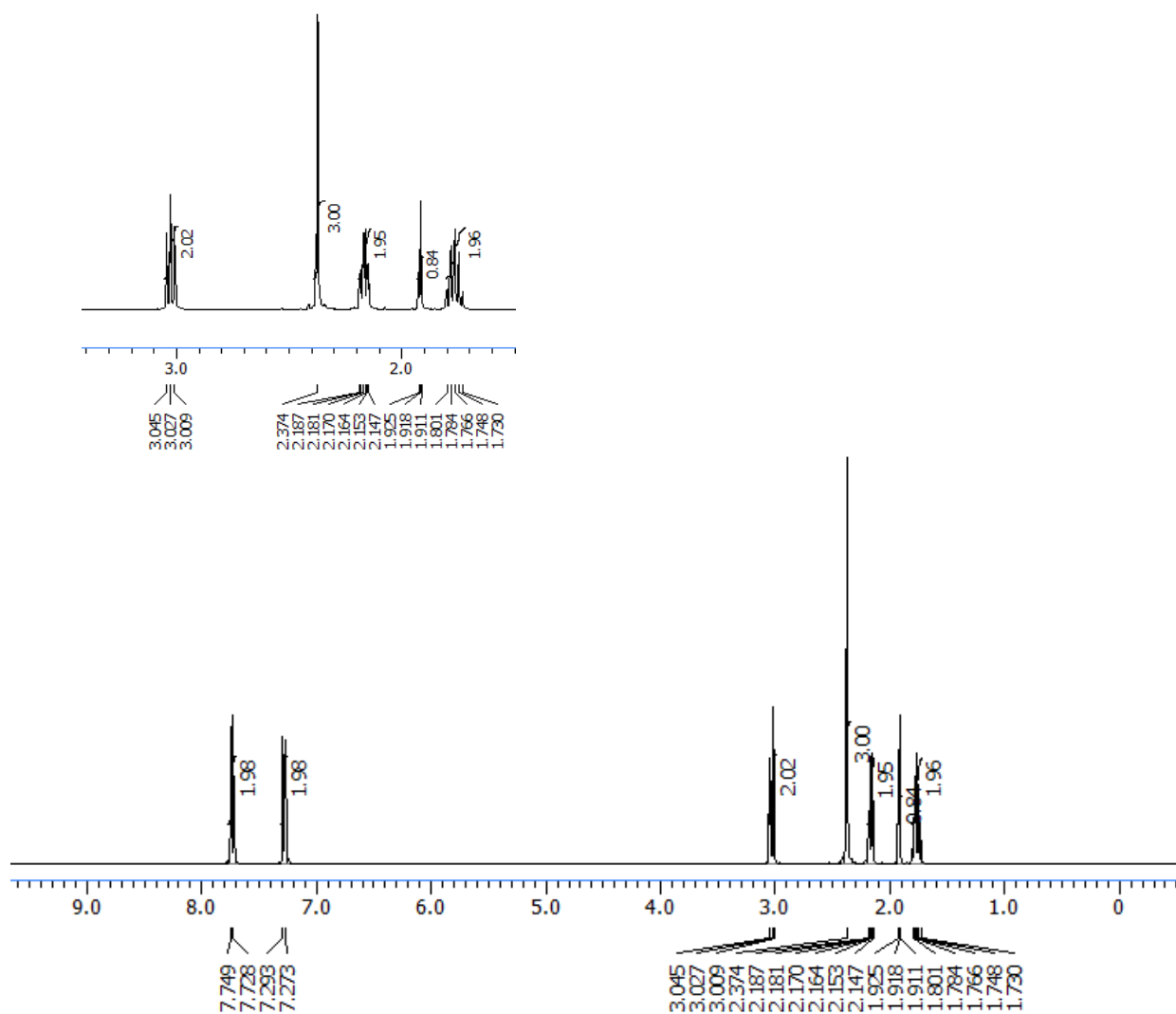
MFE MS Zoomed Spectrum



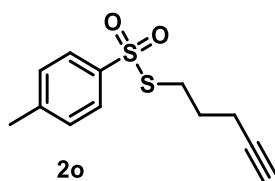
¹H NMR spectrum of 2n (400 MHz, CDCl₃)



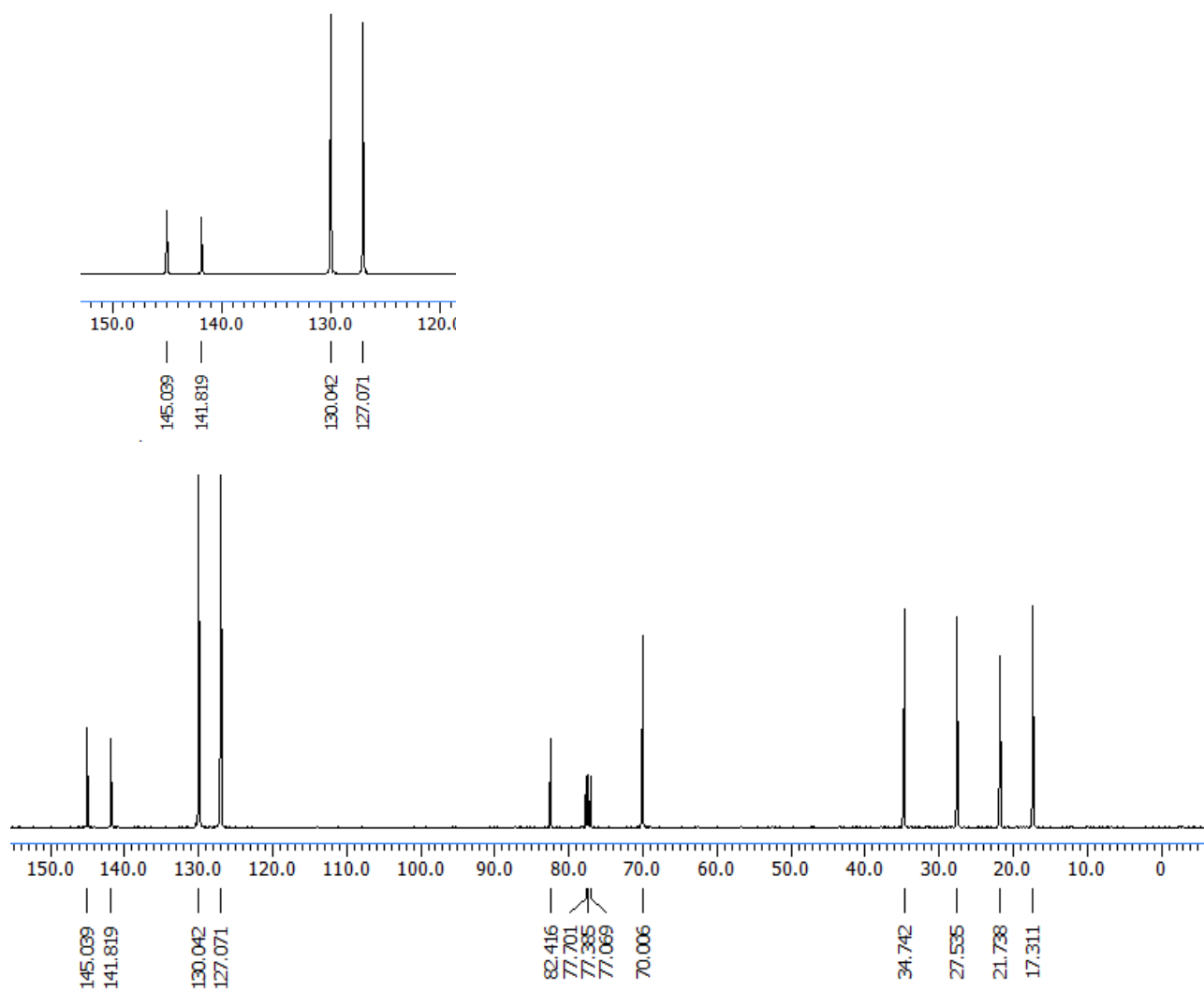
S-(pent-4-yn-1-yl) 4-methylbenzenesulfonothioate (2o)



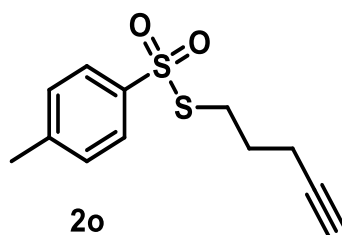
¹³C NMR spectrum of 2n (100 MHz, CDCl₃)



S-(pent-4-yn-1-yl) 4-methylbenzenesulfonothioate (2o)

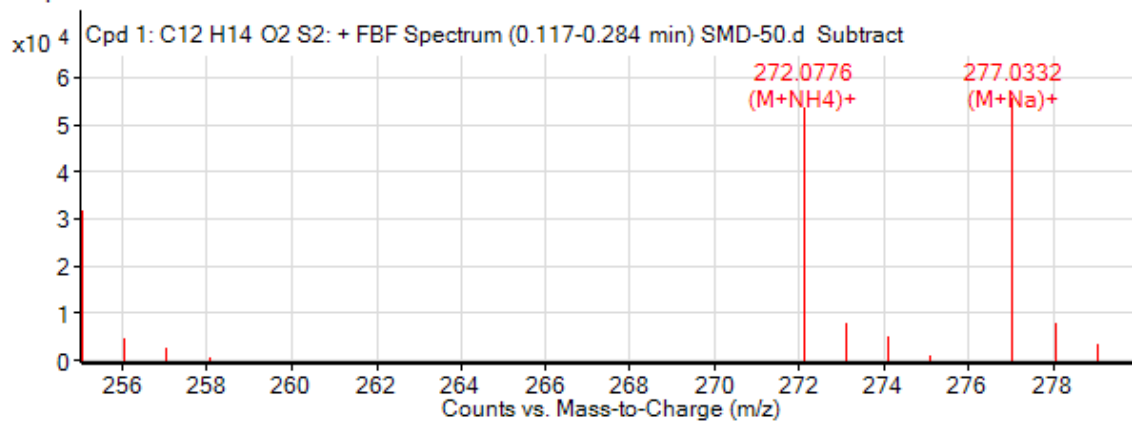


Mass spectrum of 2n

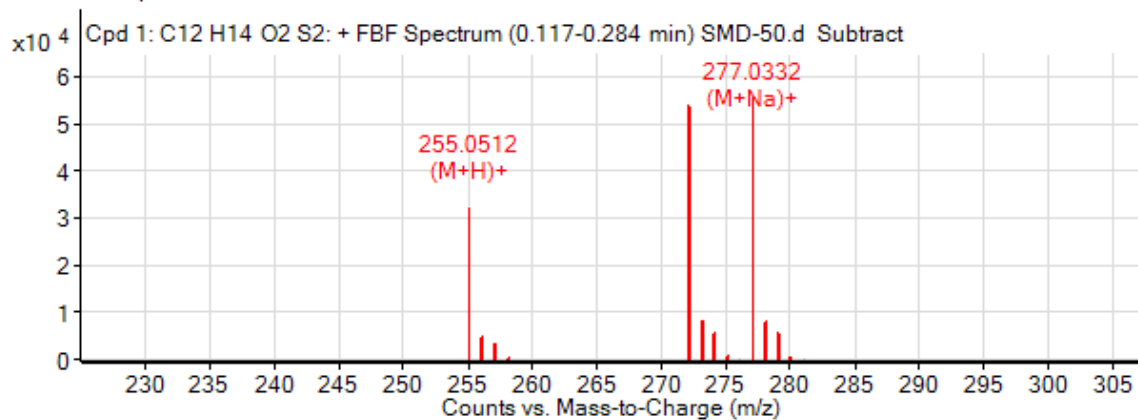


S-(pent-4-yn-1-yl) 4-methylbenzenesulfonothioate (2o)

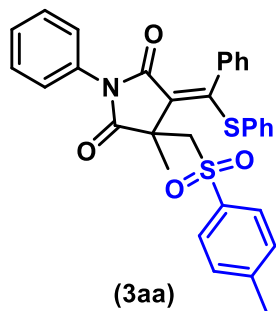
MS Spectrum



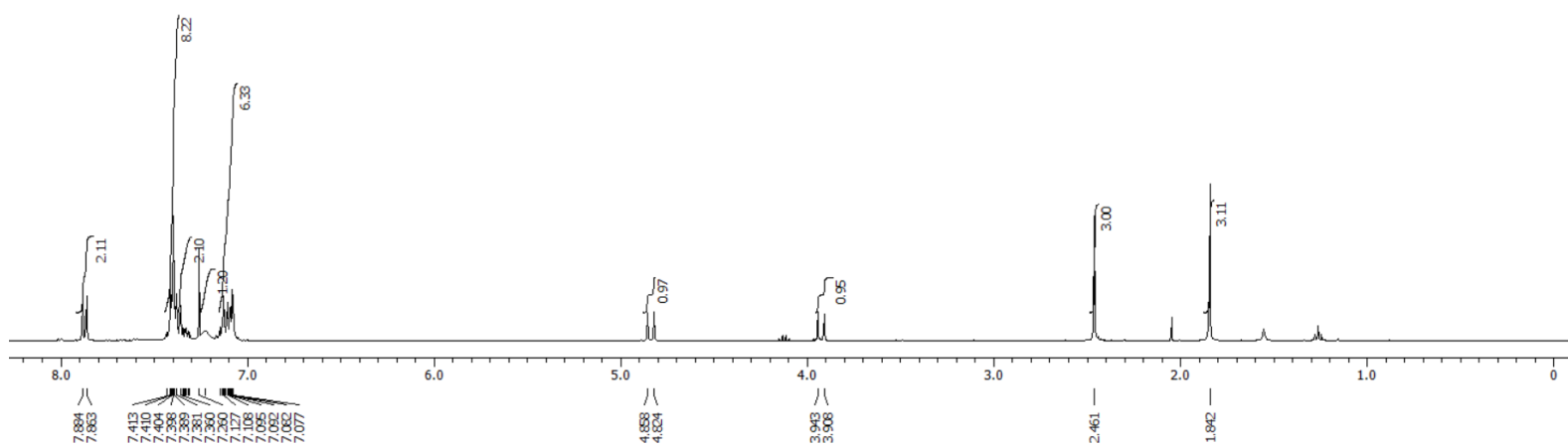
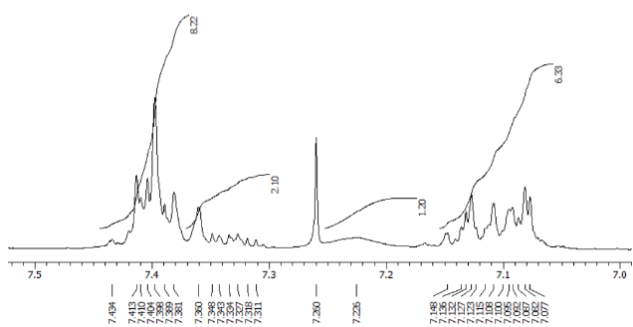
MS Zoomed Spectrum



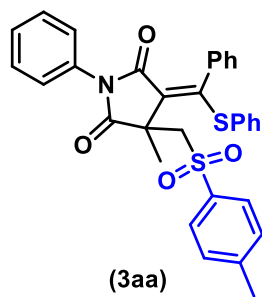
¹H NMR spectrum of 3aa (400 MHz, CDCl₃)



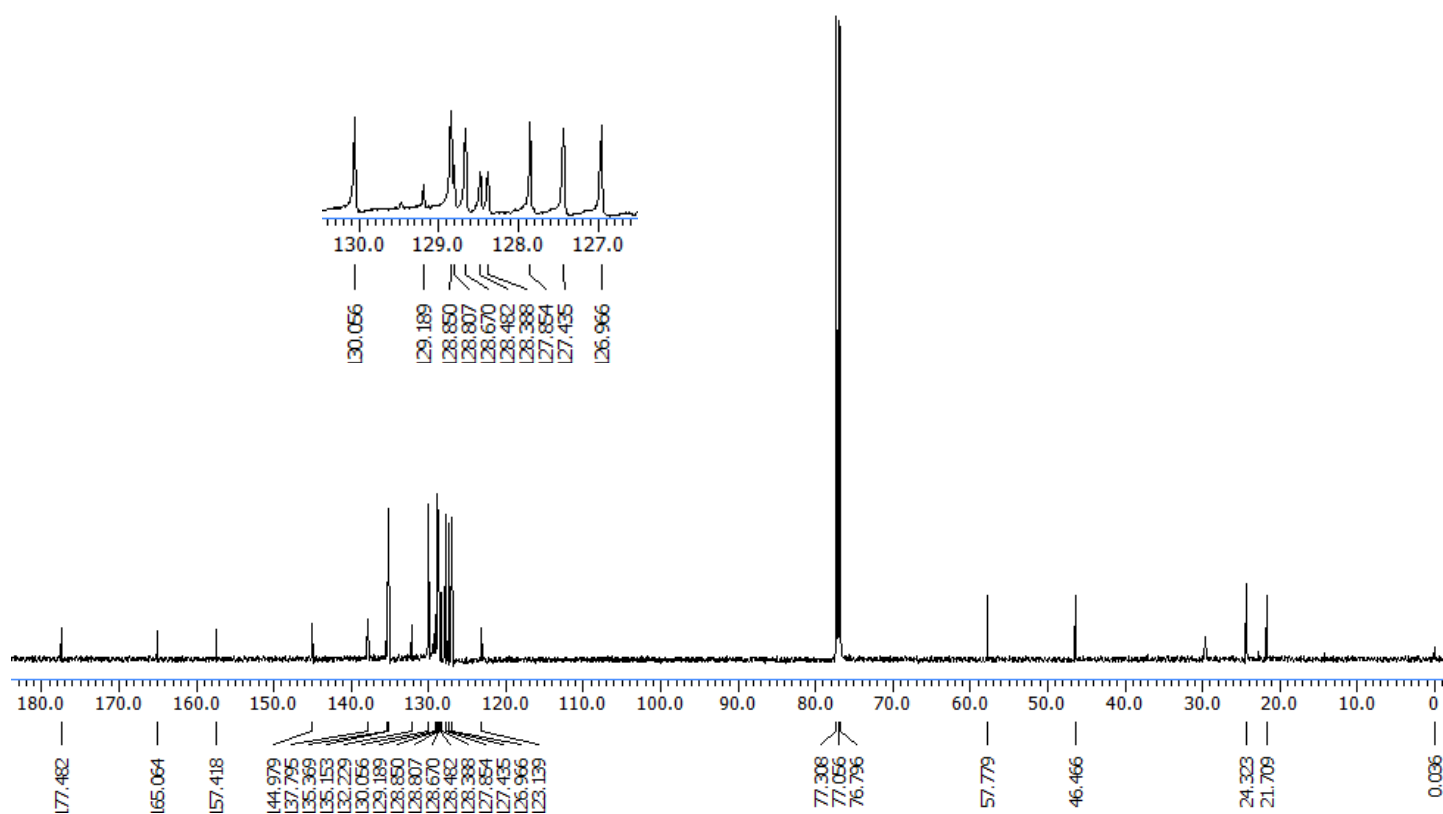
(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



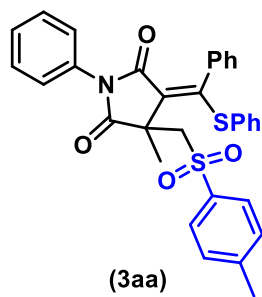
¹³C NMR spectrum of 3aa (100 MHz, CDCl₃)



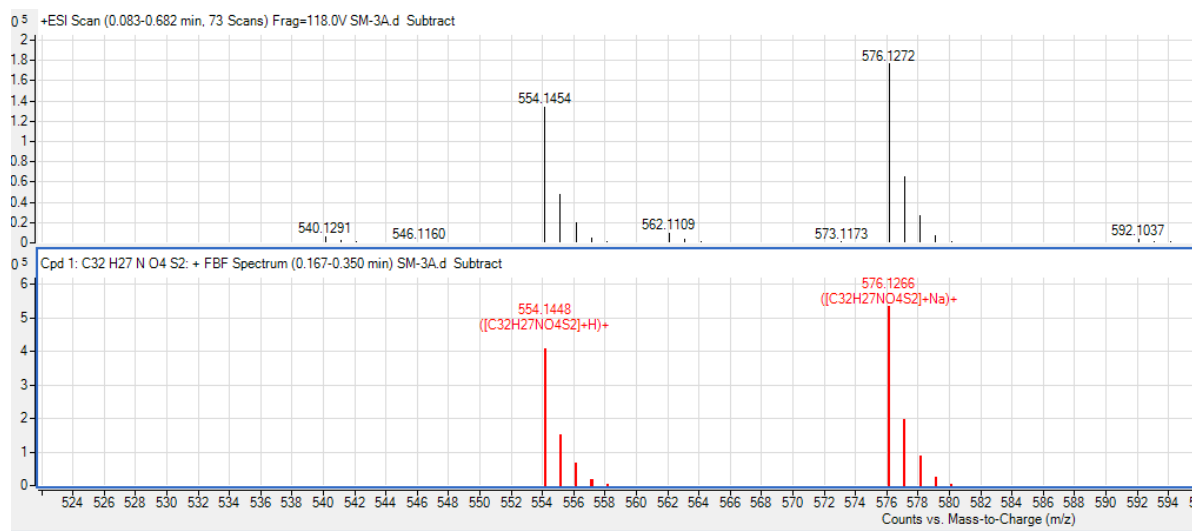
(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



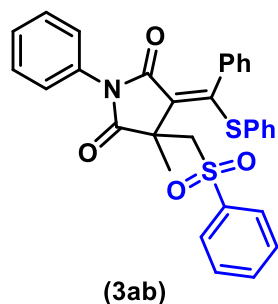
HRMS Spectrum of 3aa



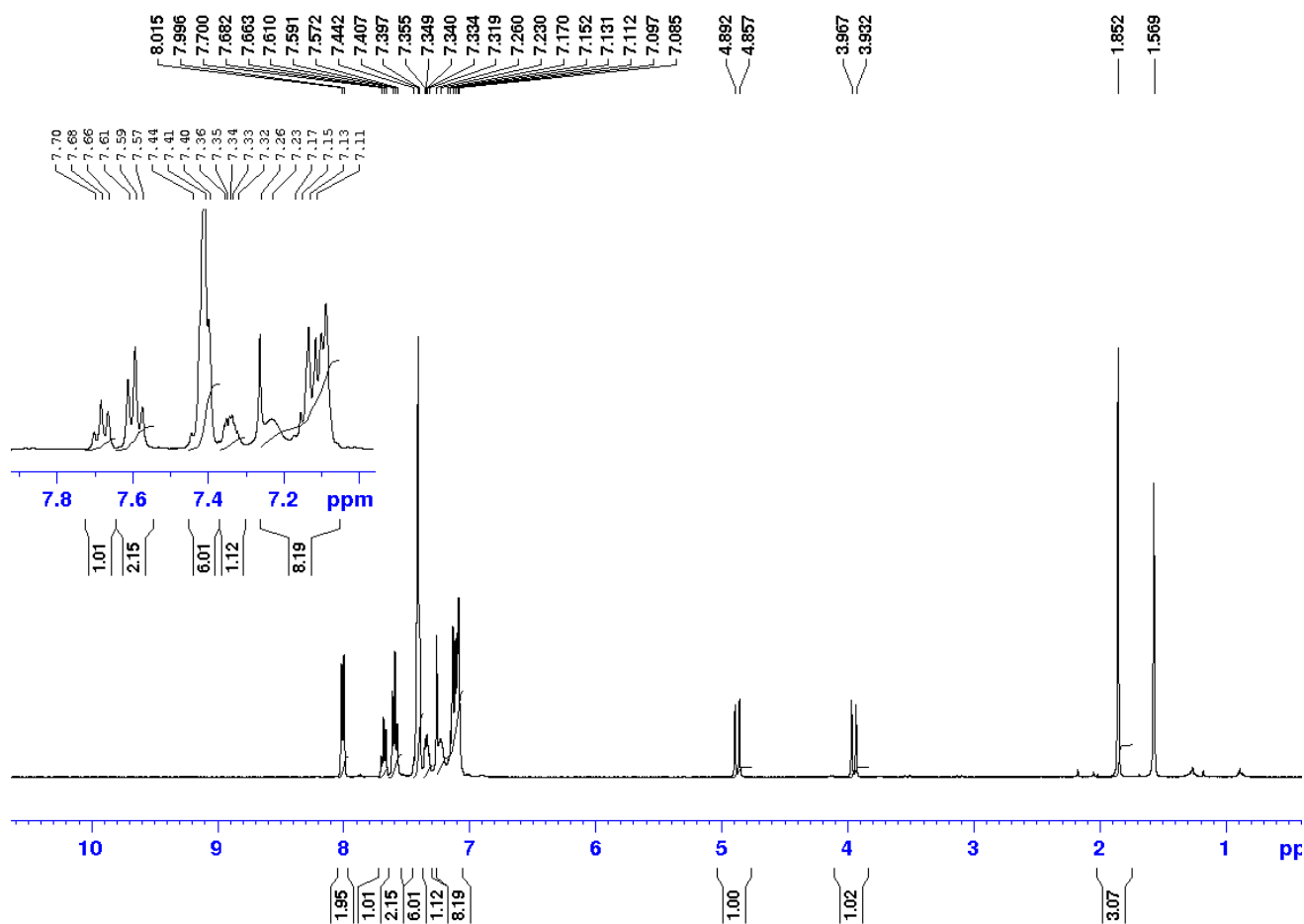
(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



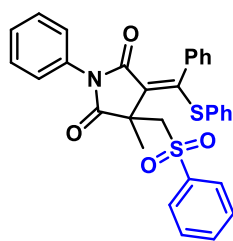
¹H NMR spectrum of 3ab (400 MHz, CDCl₃)



(*E*)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione

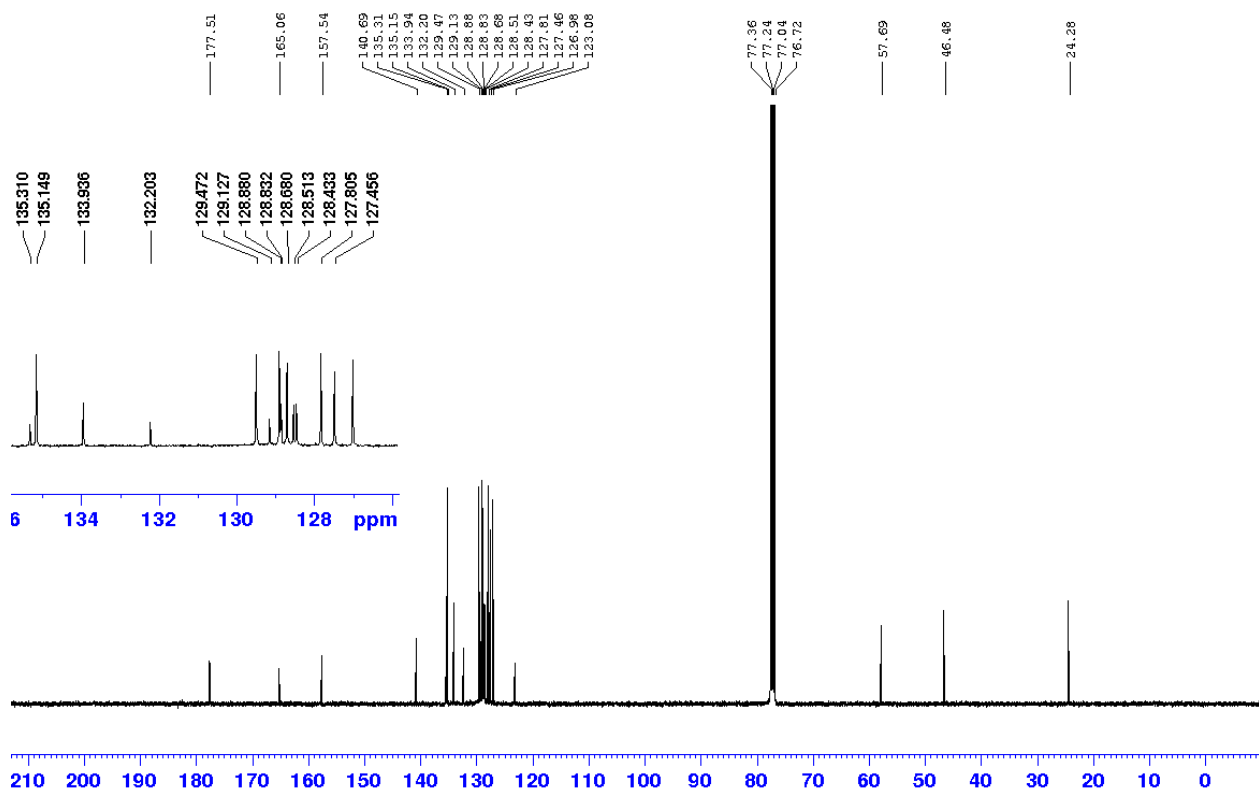


¹³C NMR spectrum of 3ab (100 MHz, CDCl₃)

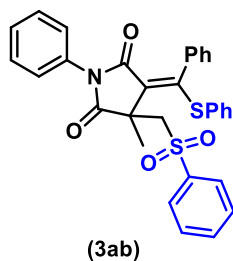


(3ab)

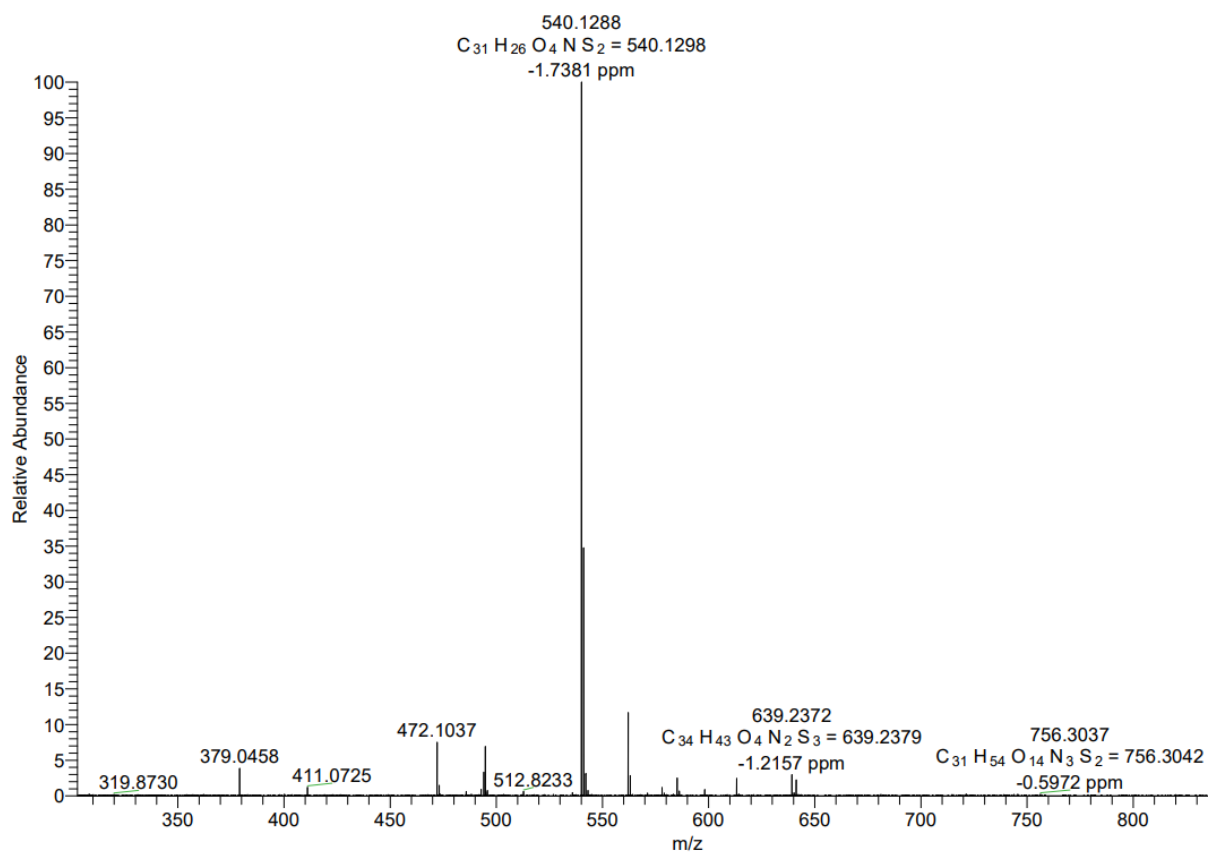
(*E*)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



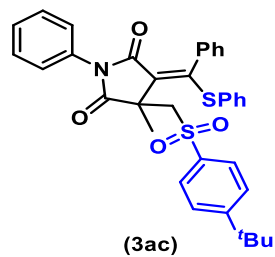
HRMS Spectrum of 3ab



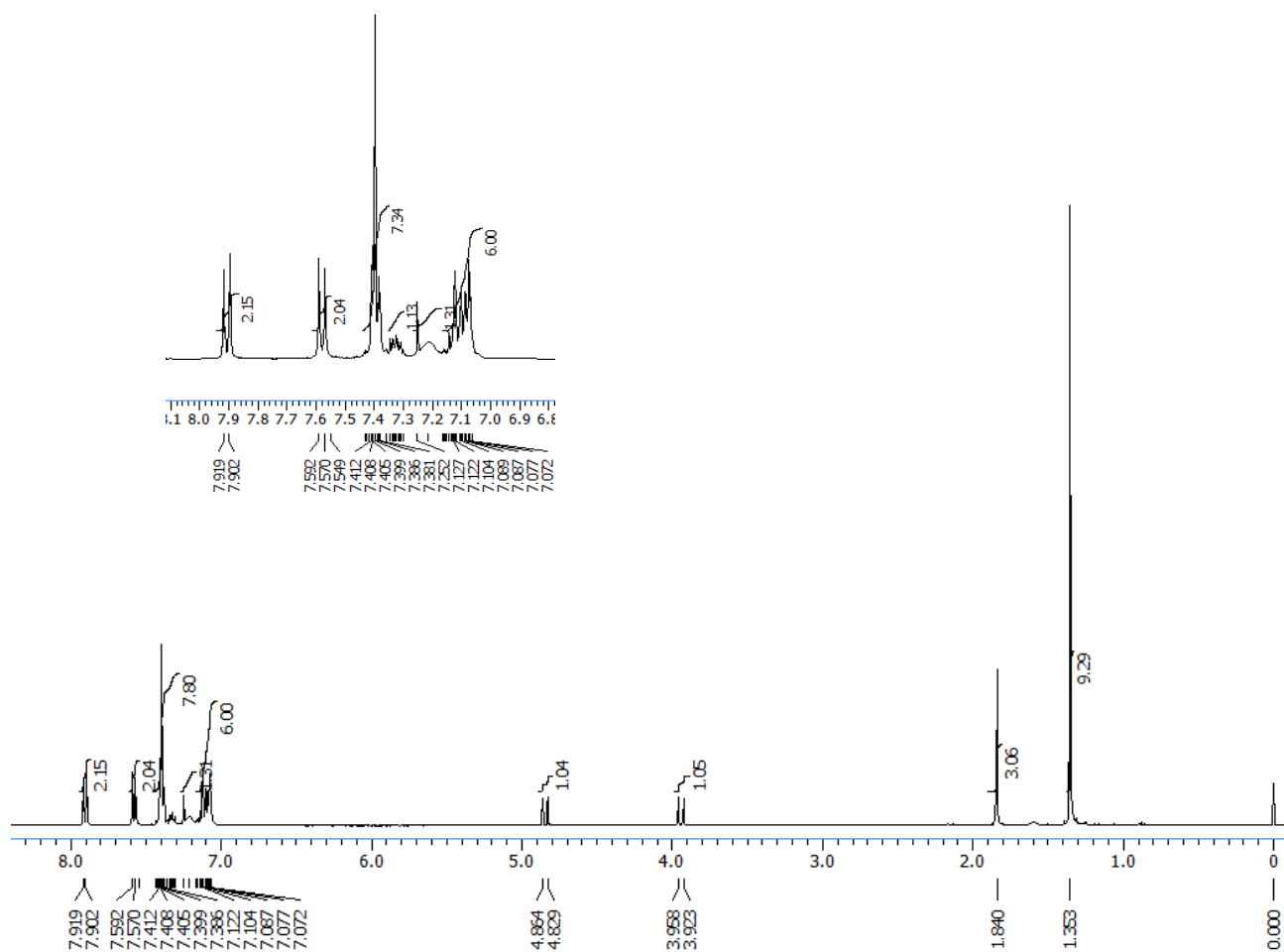
(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



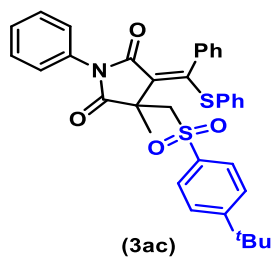
¹H NMR spectrum of 3ac (400 MHz, CDCl₃)



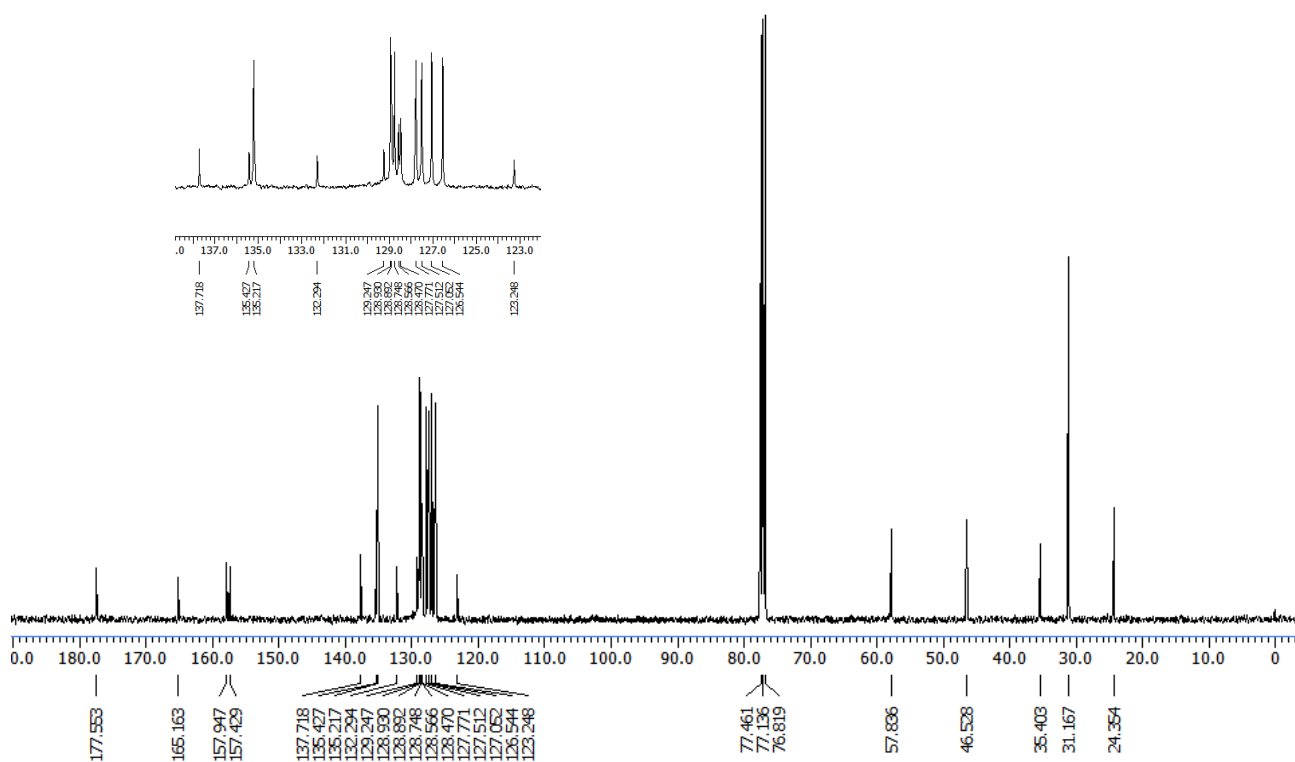
(E)-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



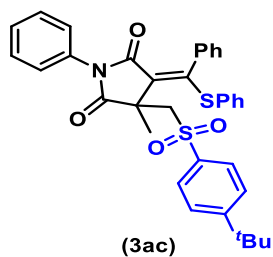
^{13}C NMR spectrum of 3ac (100 MHz, CDCl_3)



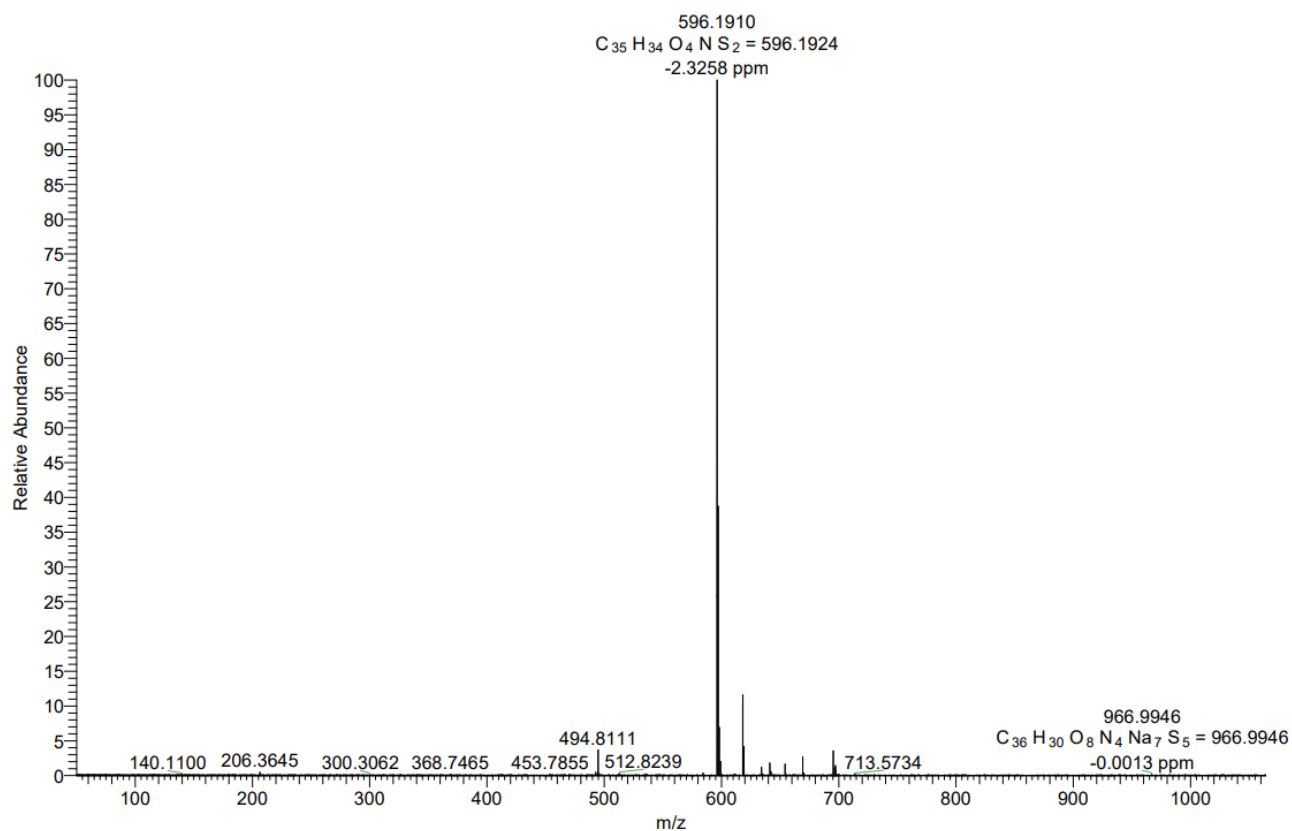
(E)-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



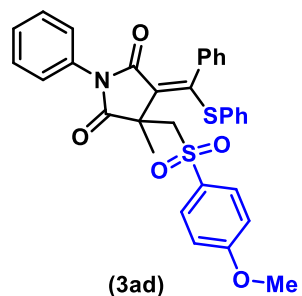
HRMS Spectrum of 3ac



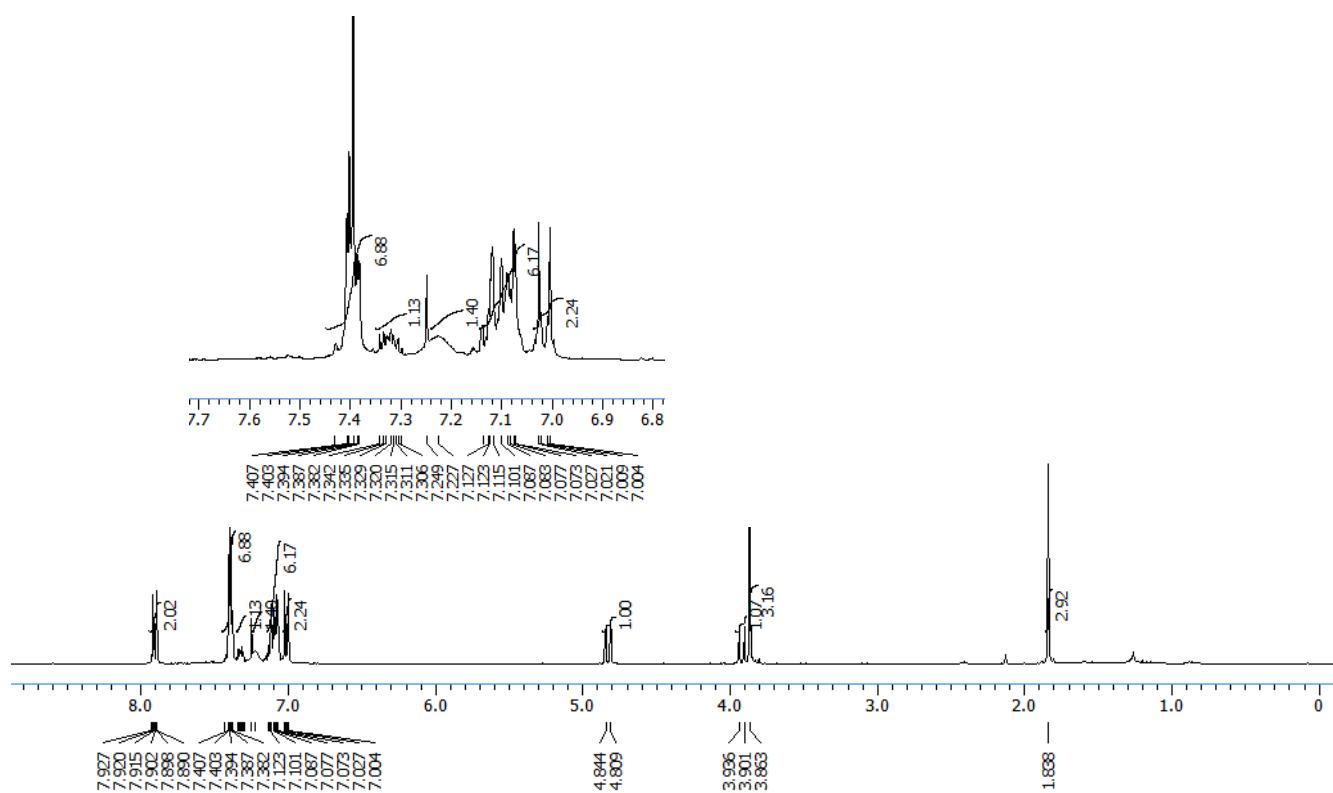
(E)-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



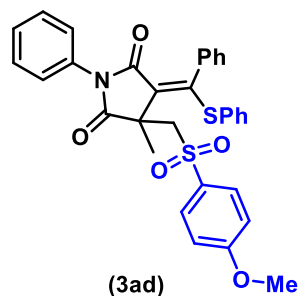
¹H NMR spectrum of 3ad (400 MHz, CDCl₃)



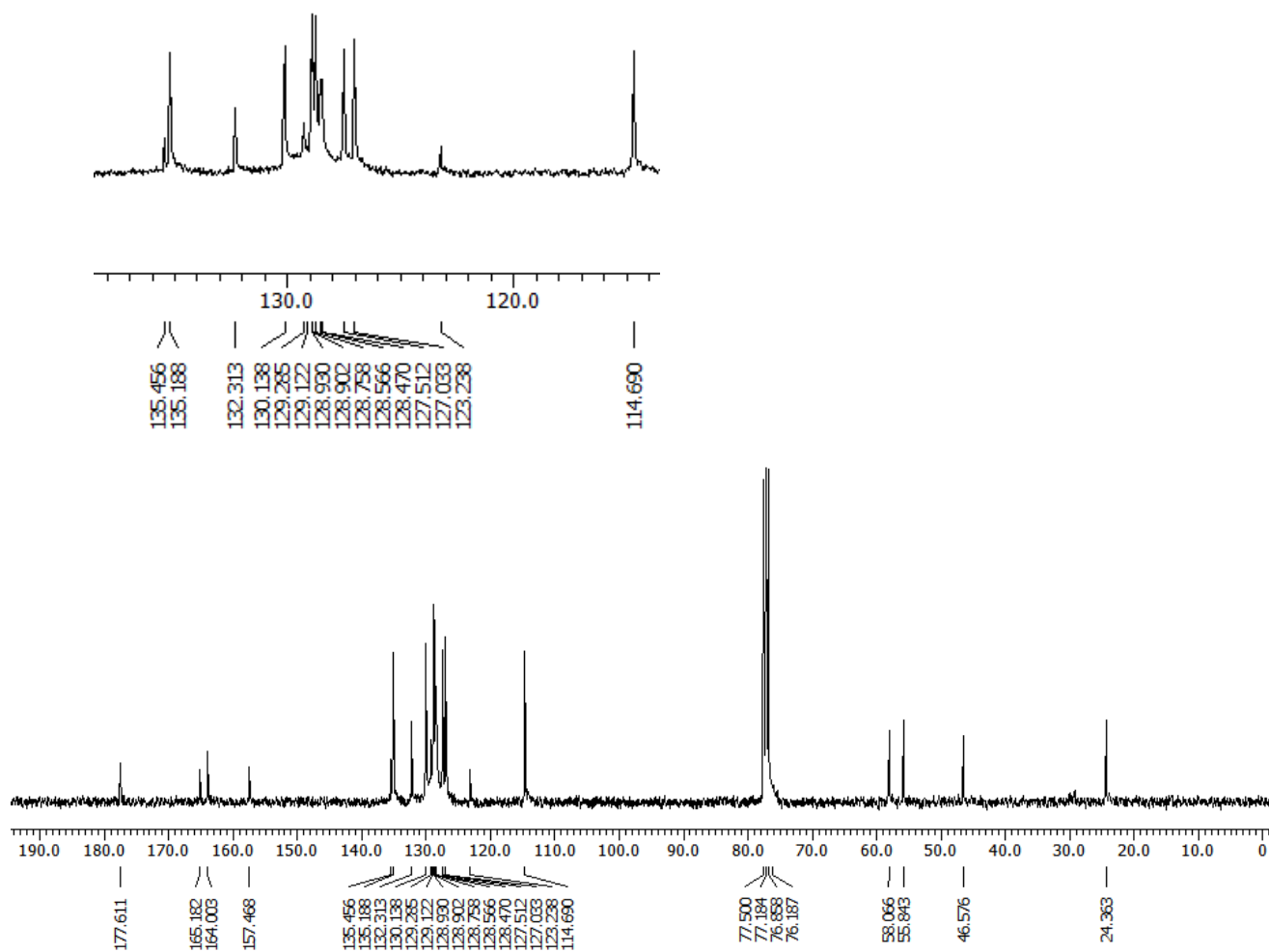
(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



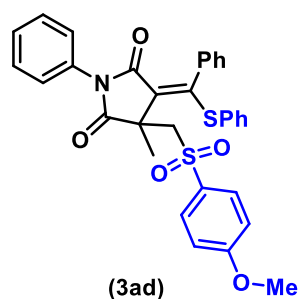
¹³C NMR spectrum of 3ad (100 MHz, CDCl₃)



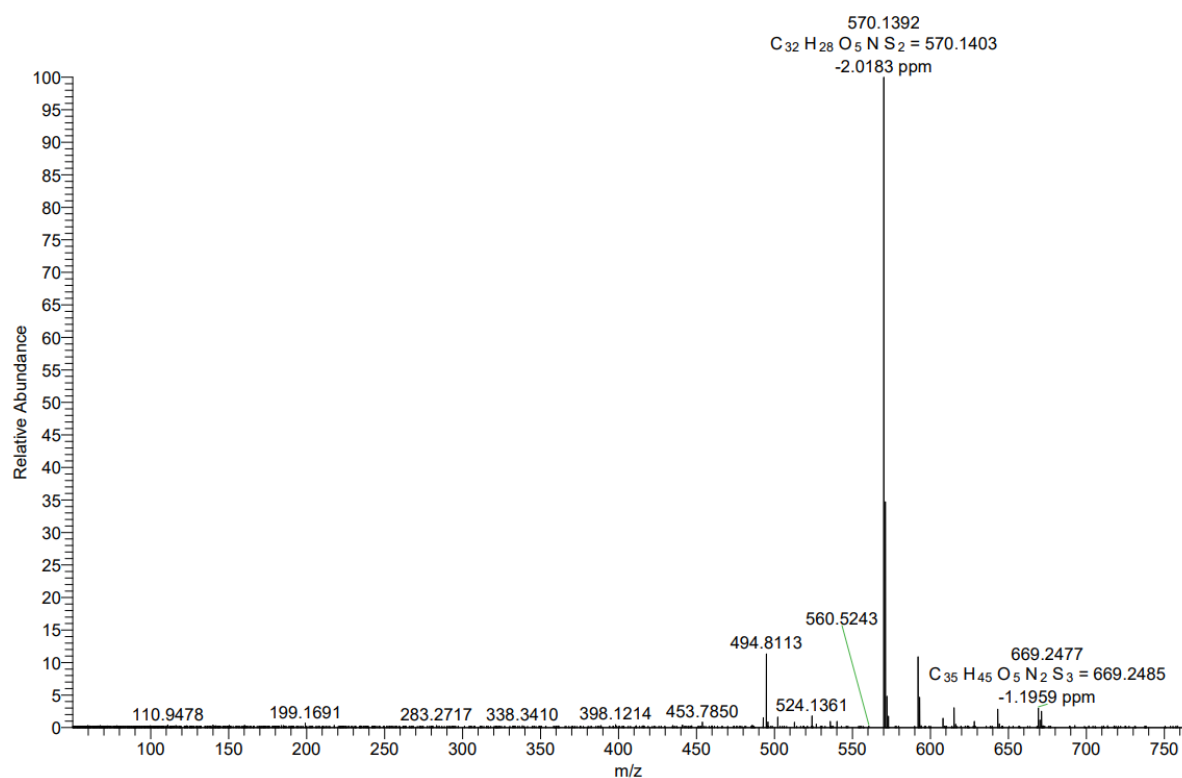
(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



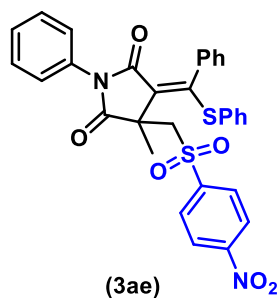
HRMS Spectrum of 3ad



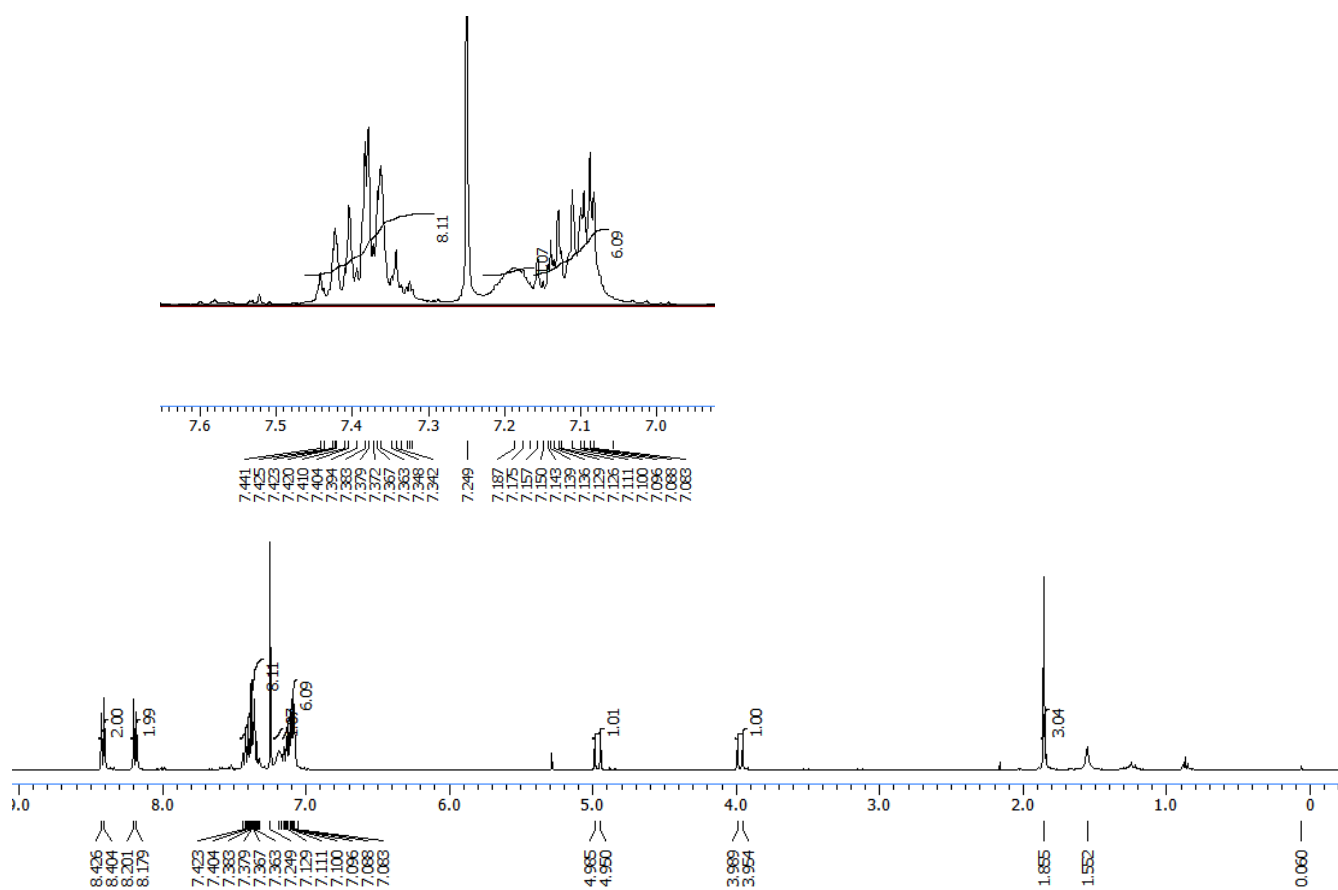
(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



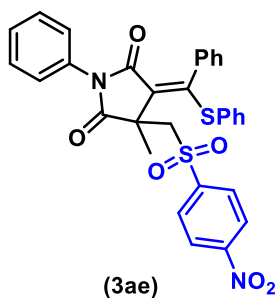
¹H NMR spectrum of 3ae (400 MHz, CDCl₃)



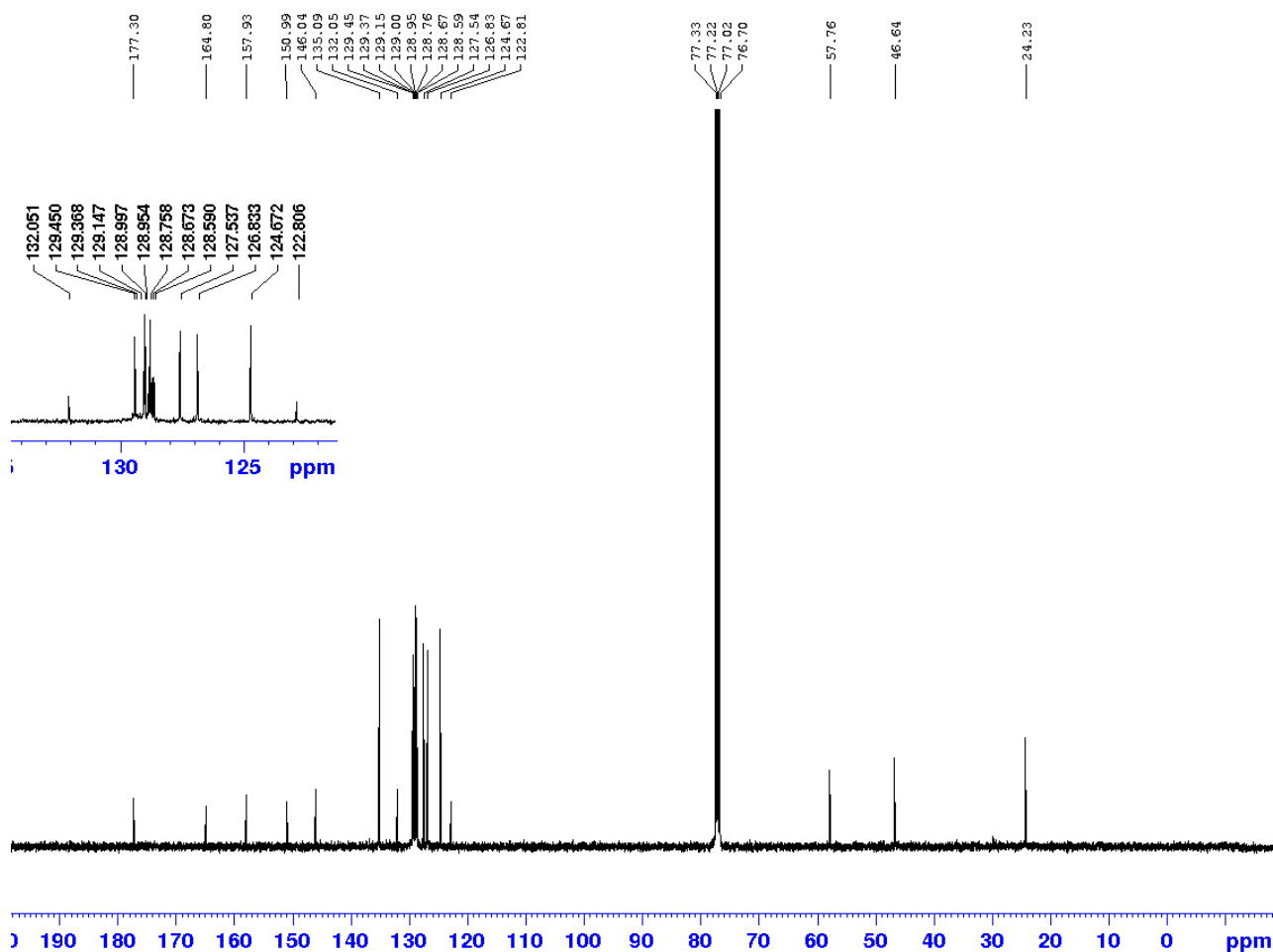
(E)-3-methyl-3-(((4-nitrophenyl)sulfonyl)methyl)-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



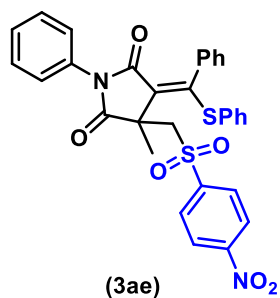
¹³C NMR spectrum of 3ae (100 MHz, CDCl₃)



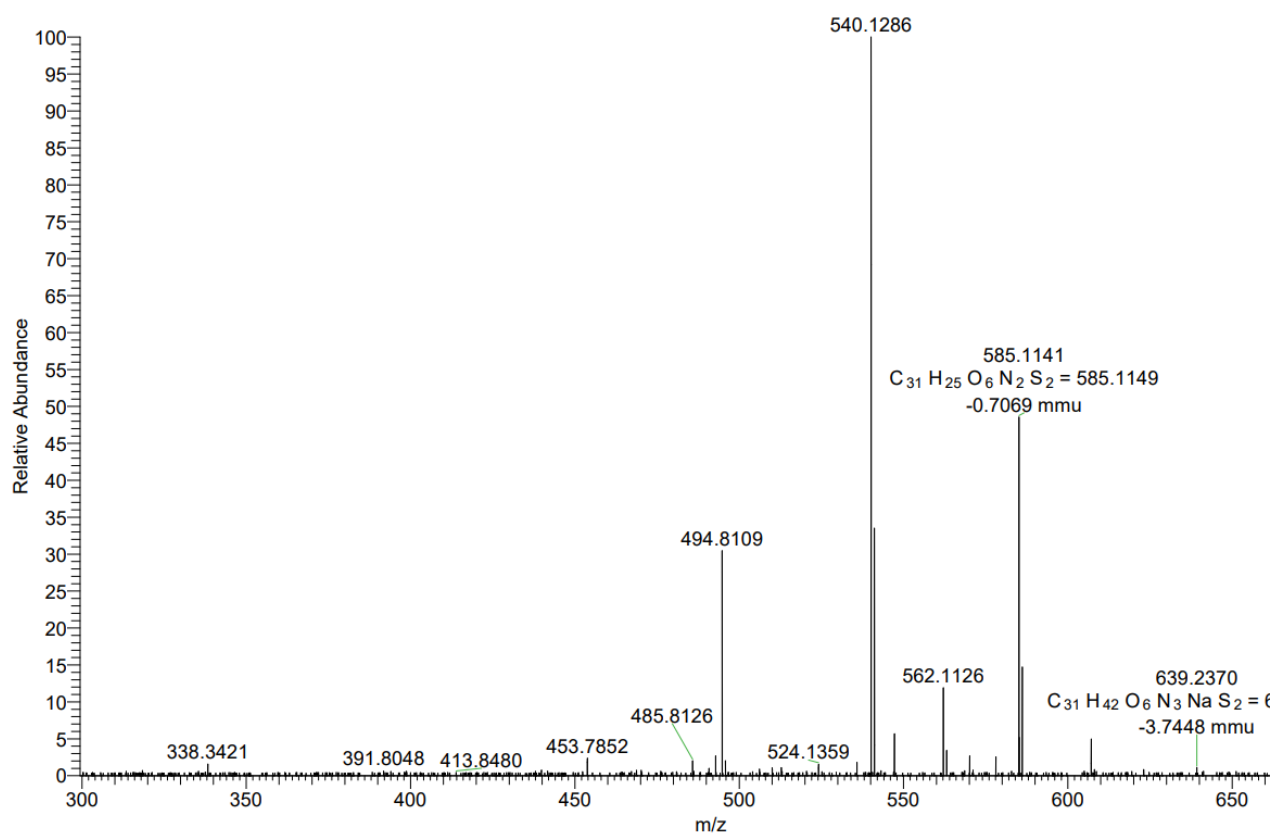
(E)-3-methyl-3-(((4-nitrophenyl)sulfonyl)methyl)-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



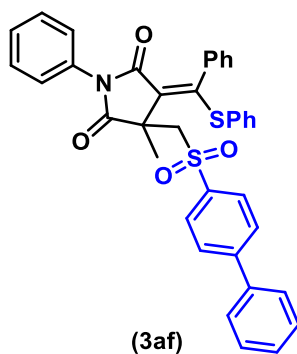
HRMS Spectrum of 3ae



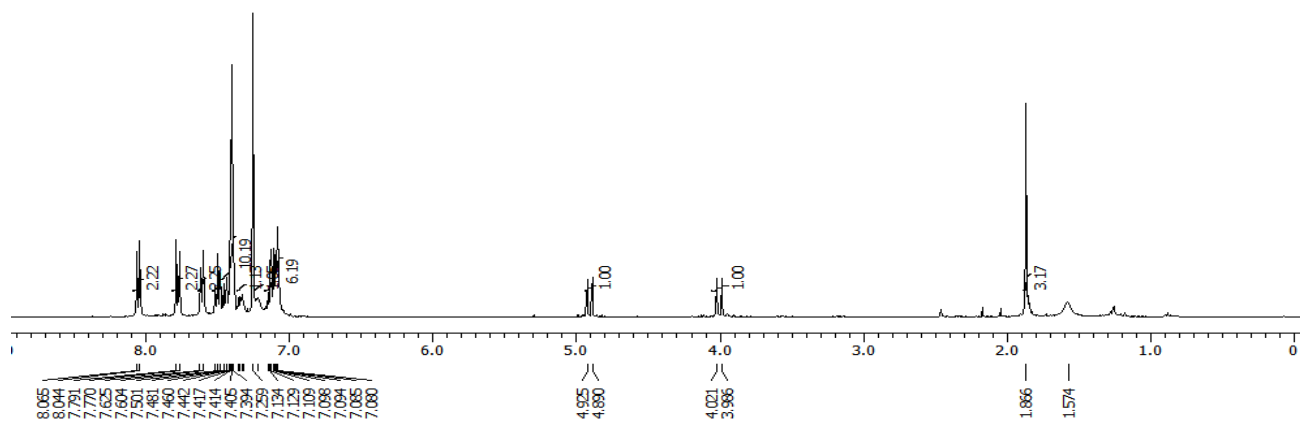
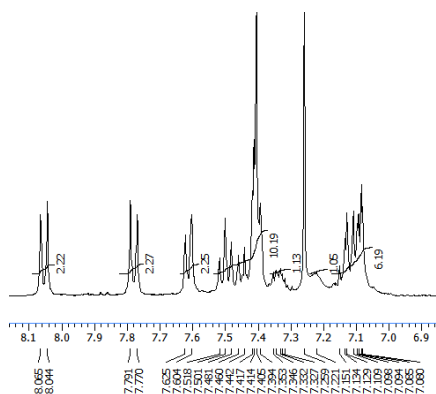
(E)-3-methyl-3-(((4-nitrophenyl)sulfonyl)methyl)-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



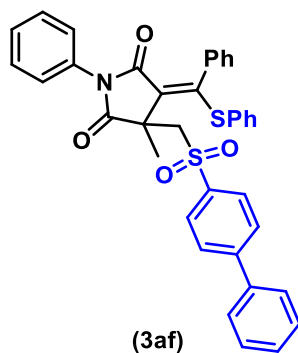
¹H NMR spectrum of 3af (400 MHz, CDCl₃)



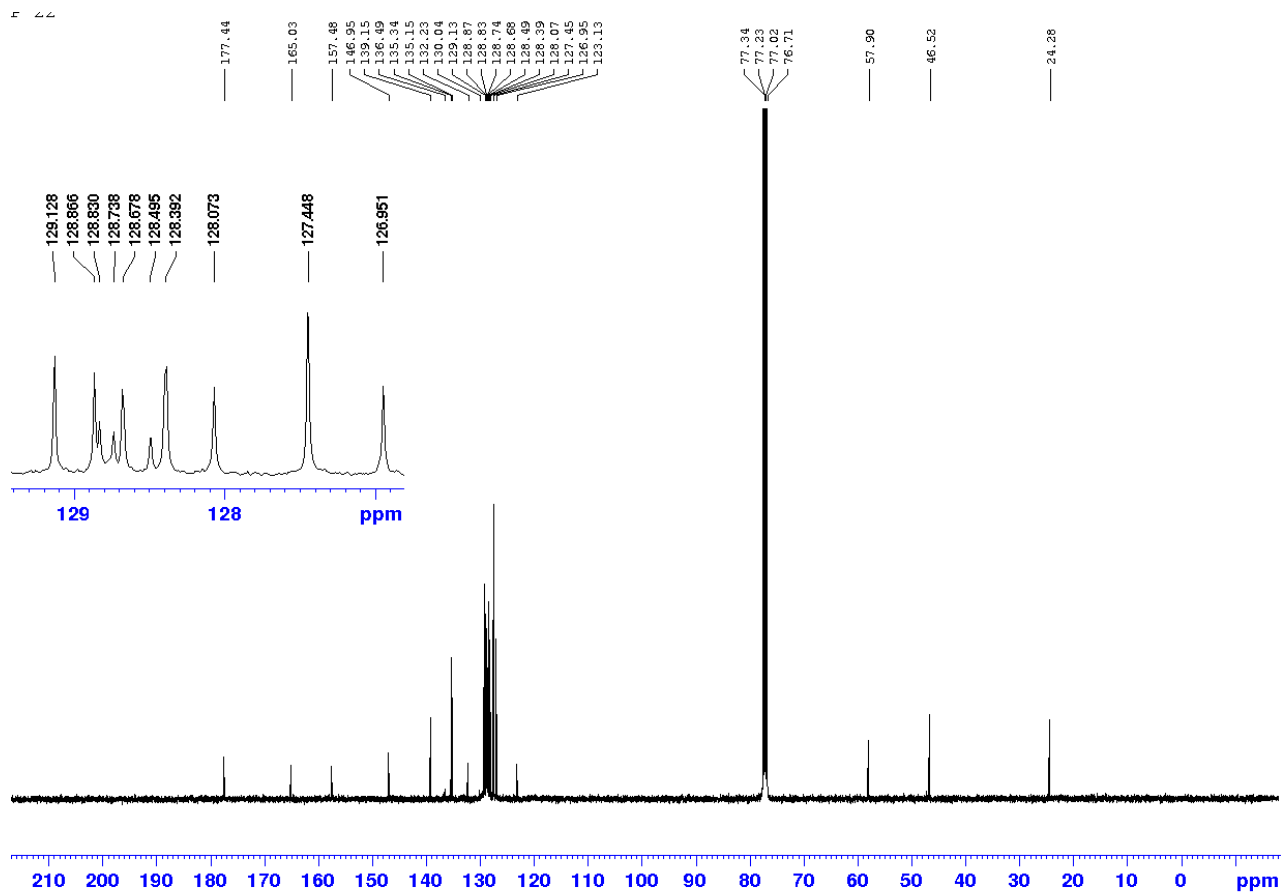
(E)-3-(((1,1'-biphenyl)-4-ylsulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



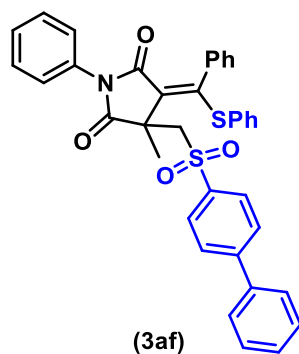
¹³C NMR spectrum of 3af (100 MHz, CDCl₃)



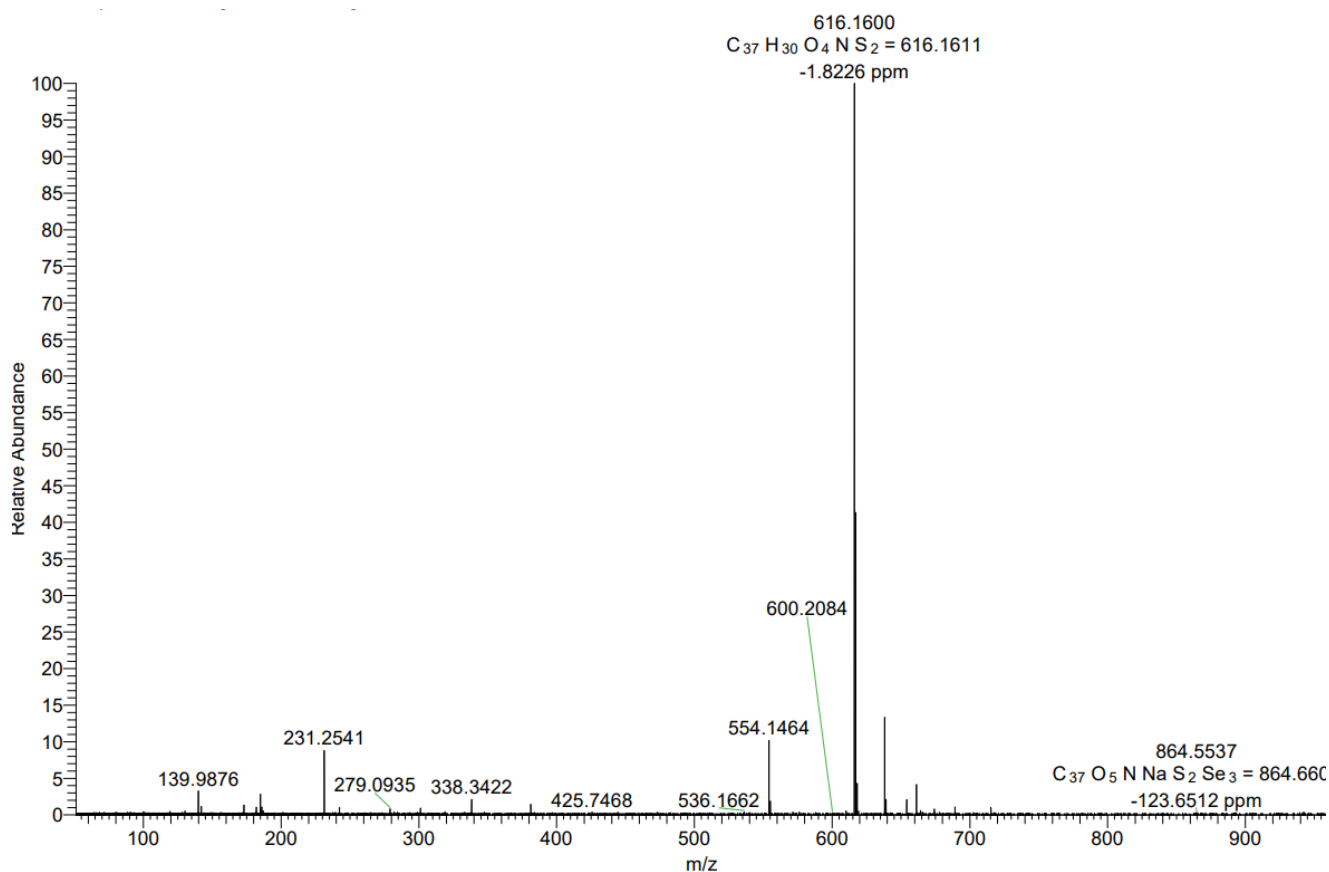
(E)-3-(((1,1'-biphenyl]-4-ylsulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



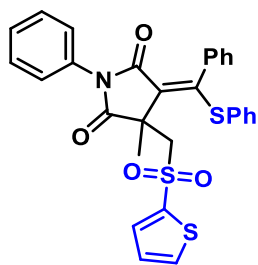
HRMS Spectrum of 3af



(E)-3-((1,1'-biphenyl]-4-ylsulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione

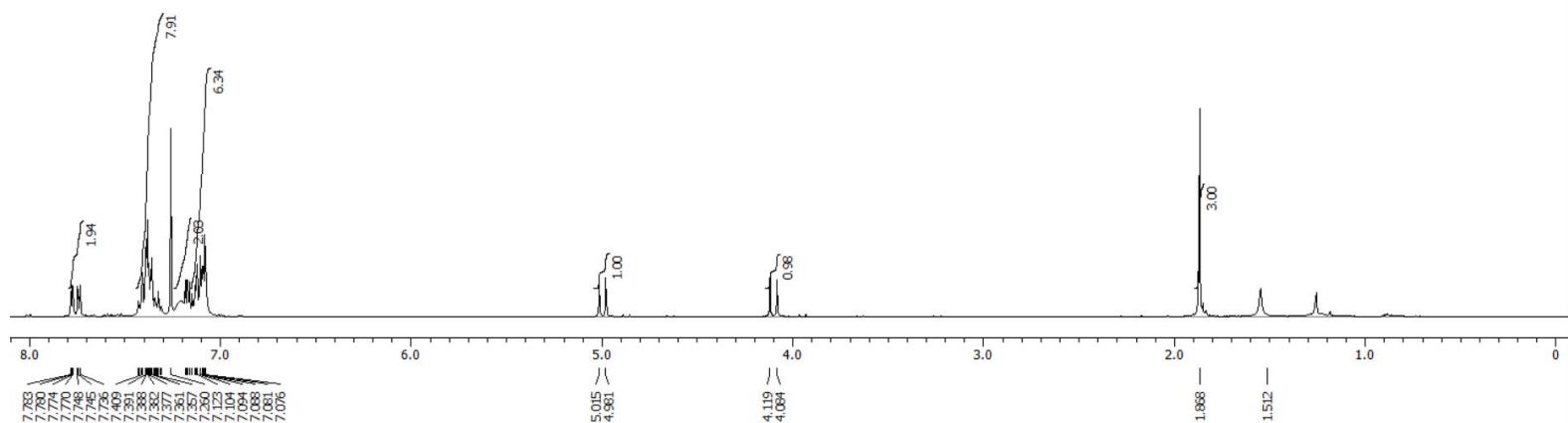
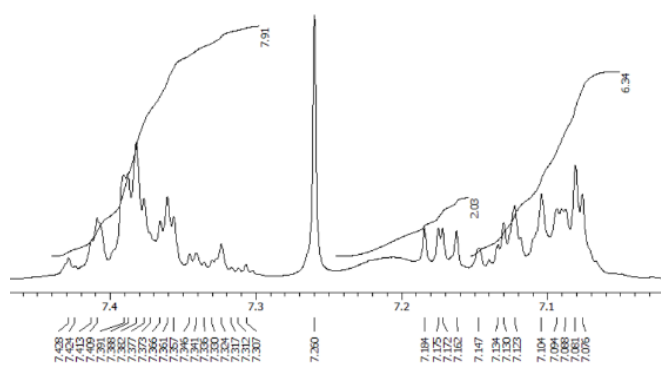


¹H NMR spectrum of 3ag (400 MHz, CDCl₃)

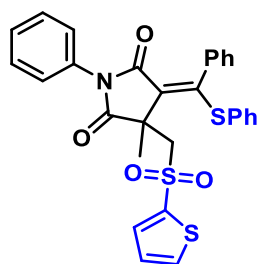


(3ag)

(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-((thiophen-2-ylsulfonyl)methyl)pyrrolidine-2,5-dione

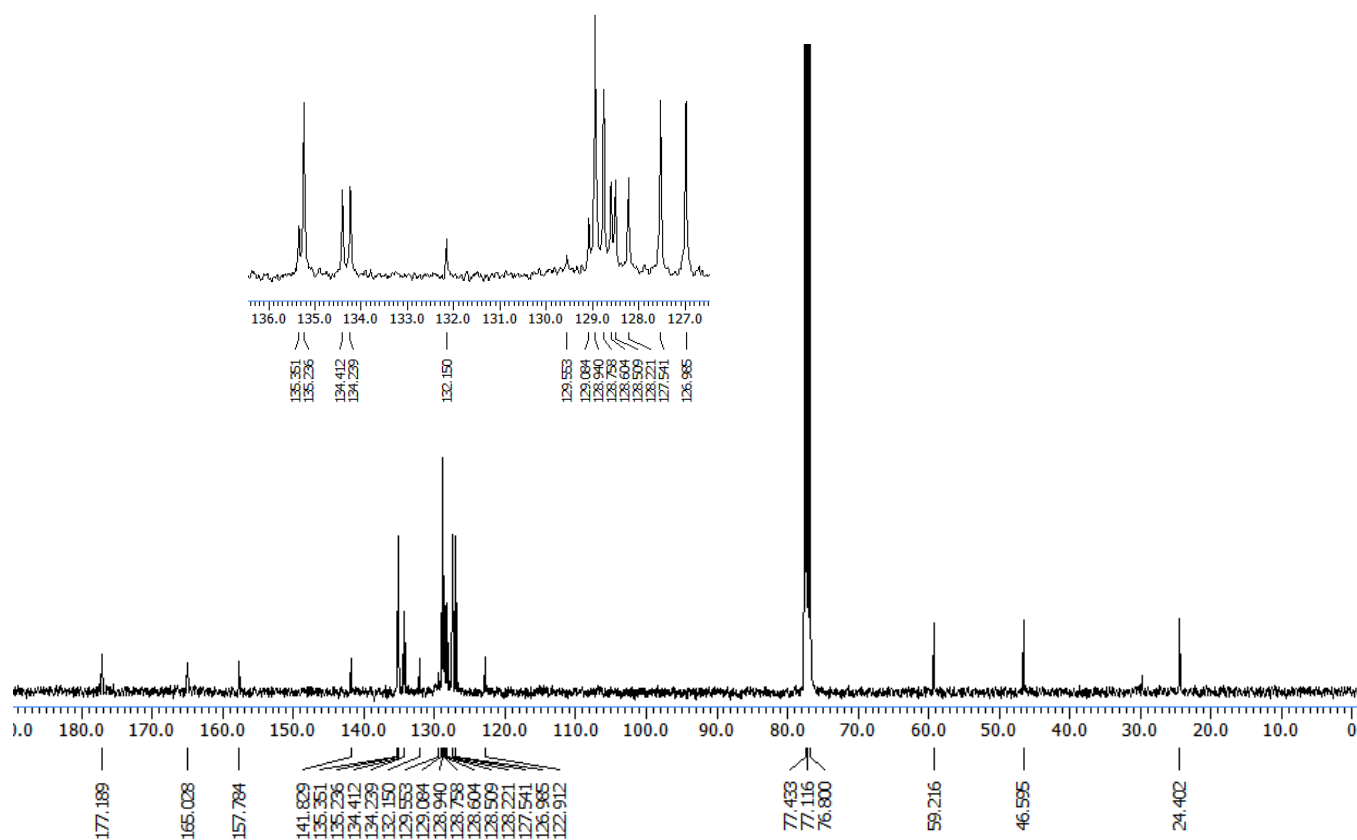


¹³C NMR spectrum of 3ag (100 MHz, CDCl₃)

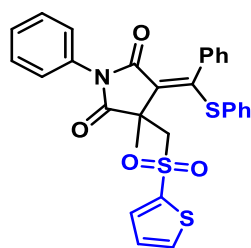


(3ag)

(*E*)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-((thiophen-2-ylsulfonyl)methyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3ag



(3ag)

(E)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-((thiophen-2-ylsulfonyl)methyl)pyrrolidine-2,5-dione

Qualitative Compound Report

Data File	SMP-25.d	Sample Name	SMP-25
Sample Type	Sample	Position	P1-A9
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	21-05-2022 12:28:47
IRM Calibration Status	Success	DA Method	Default.m
Comment			

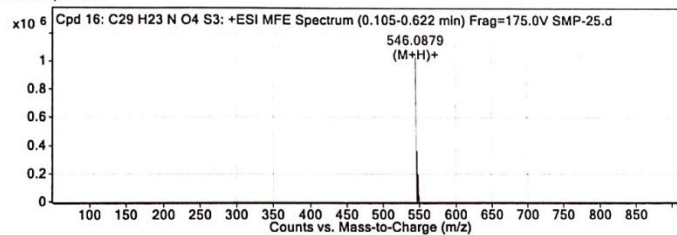
Sample Group	Info.	3
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

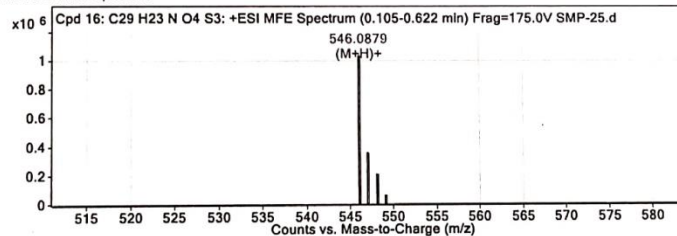
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C ₂₉ H ₂₃ N O ₄ S ₃	0.185	545.0804	C ₂₉ H ₂₃ N O ₄ S ₃	C ₂₉ H ₂₃ N O ₄ S ₃	-2.8	C ₂₉ H ₂₃ N O ₄ S ₃

Compound Label	m/z	RT	Algorithm	Mass
Cpd 16: C ₂₉ H ₂₃ N O ₄ S ₃	546.0879	0.185	Find by Molecular Feature	545.0804

MFE MS Spectrum



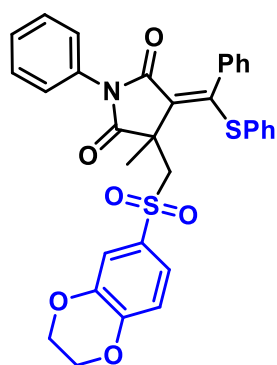
MFE MS Zoomed Spectrum



MS Spectrum Peak List

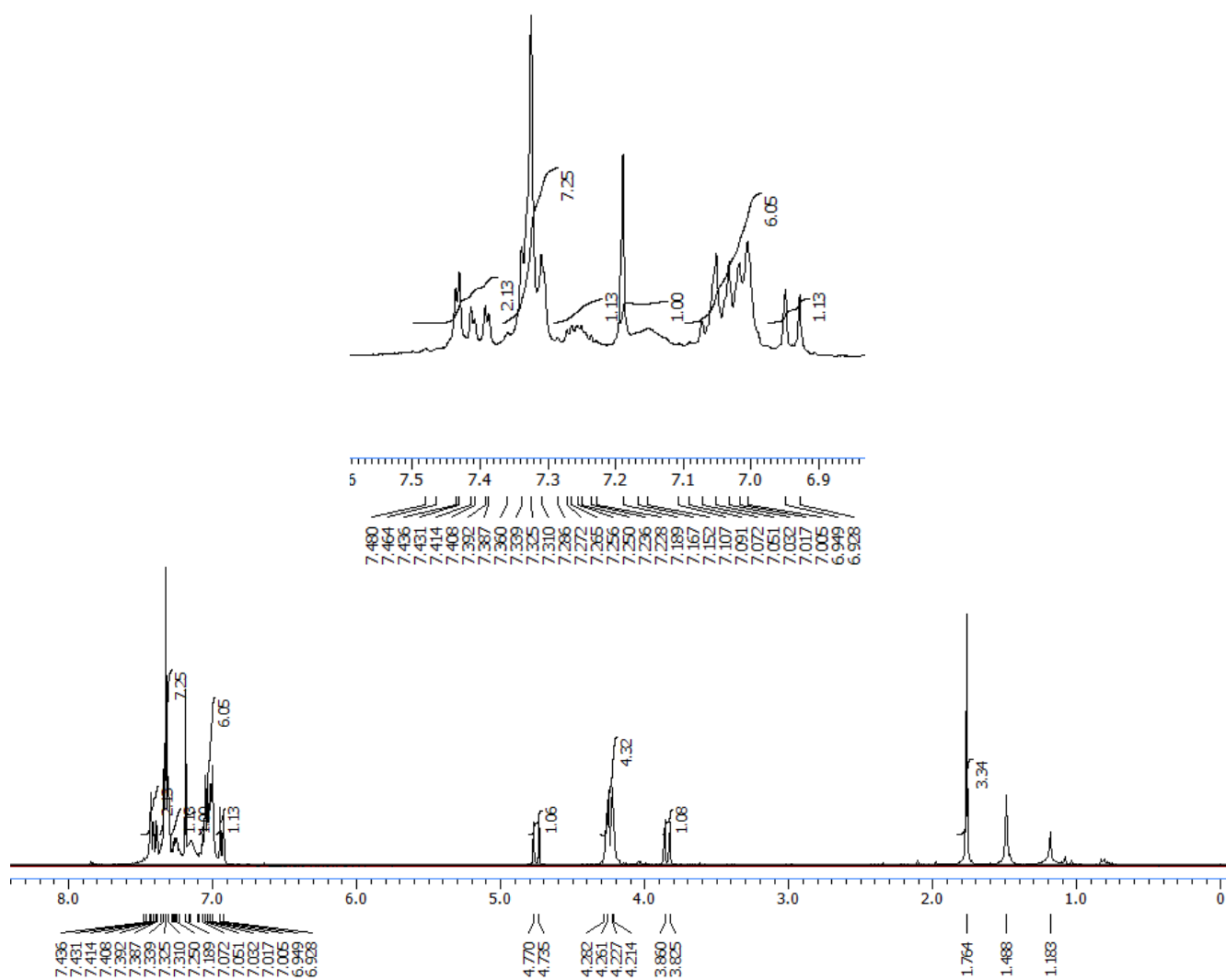
m/z	z	Abund	Formula	Ion
546.0879	1	1044326.25	C ₂₉ H ₂₄ N O ₄ S ₃	(M+H) ⁺
547.0905	1	361133.85	C ₂₉ H ₂₄ N O ₄ S ₃	(M+H) ⁺
548.0866	1	196223.48	C ₂₉ H ₂₄ N O ₄ S ₃	(M+H) ⁺
549.0876	1	48562.02	C ₂₉ H ₂₄ N O ₄ S ₃	(M+H) ⁺

¹H NMR spectrum of 3ah (400 MHz, CDCl₃)

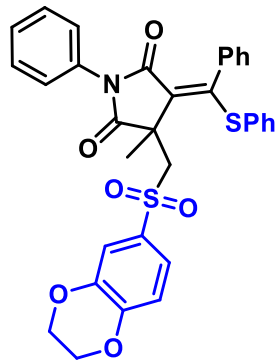


(3ah)

(E)-3-(((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)sulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione

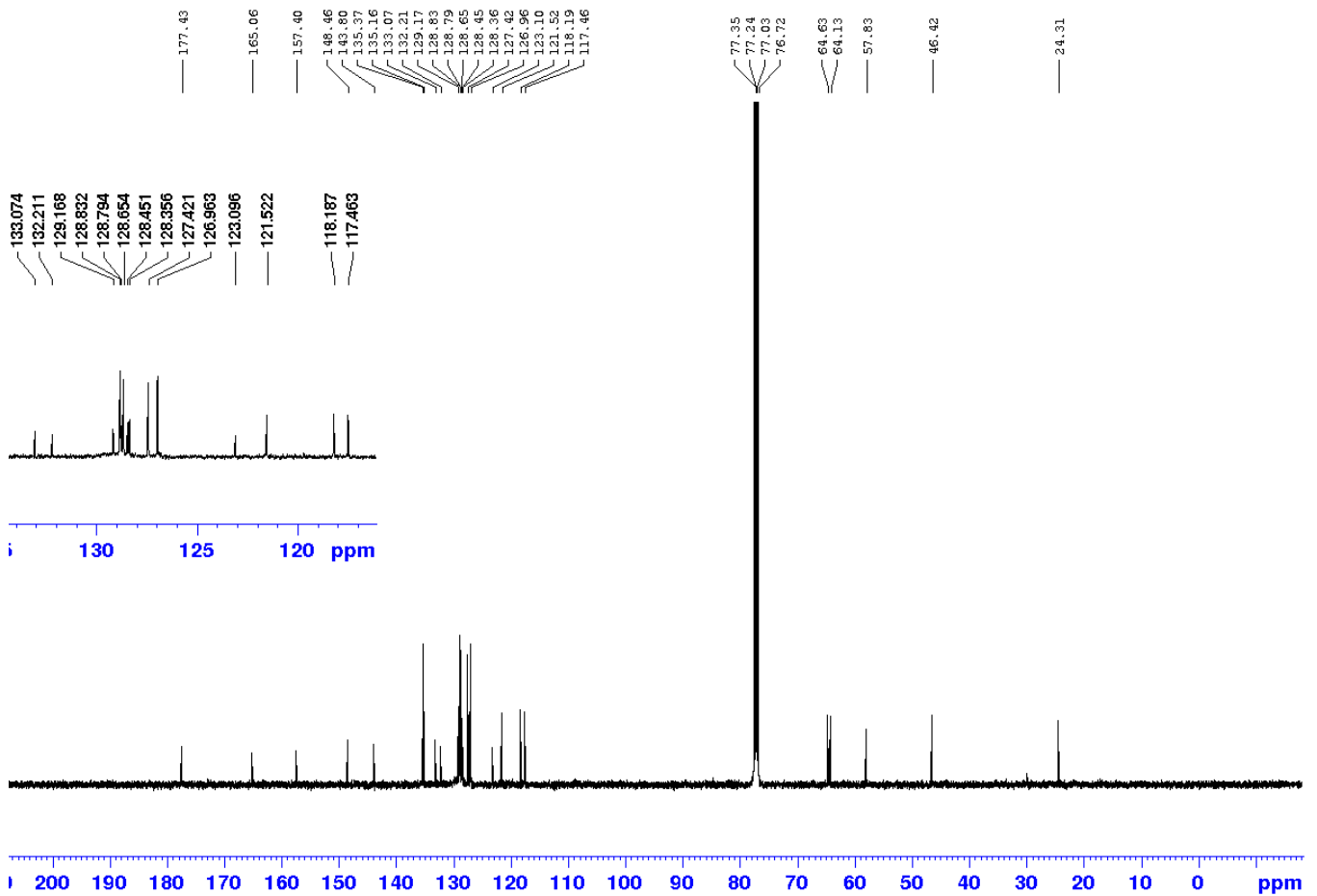


¹³C NMR spectrum of 3ah (100 MHz, CDCl₃)

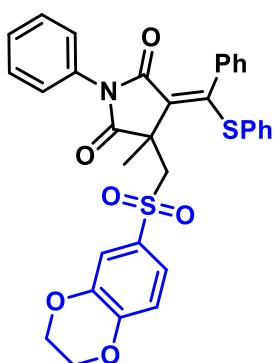


(3ah)

(*E*)-3-(((2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)sulfonyl)methyl)-3-methyl-1-phenyl-4-phenylthio)methylene)pyrrolidine-2,5-dione

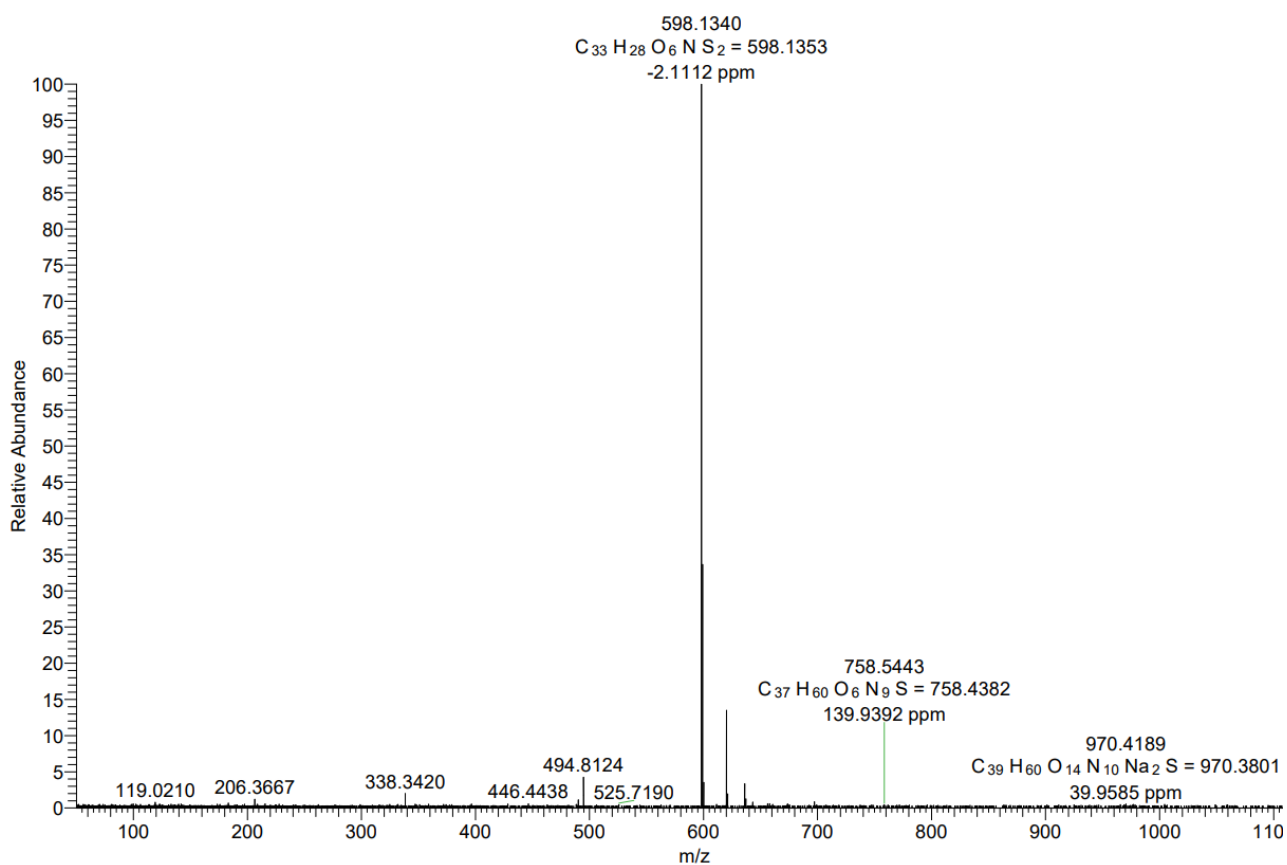


HRMS Spectrum of 3ah

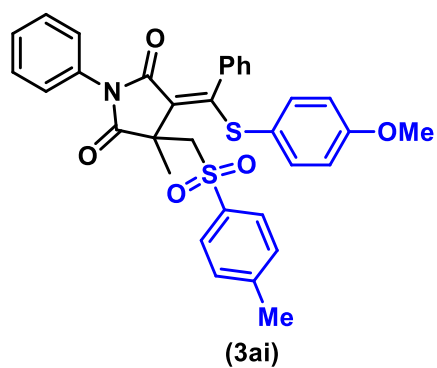


(3ah)

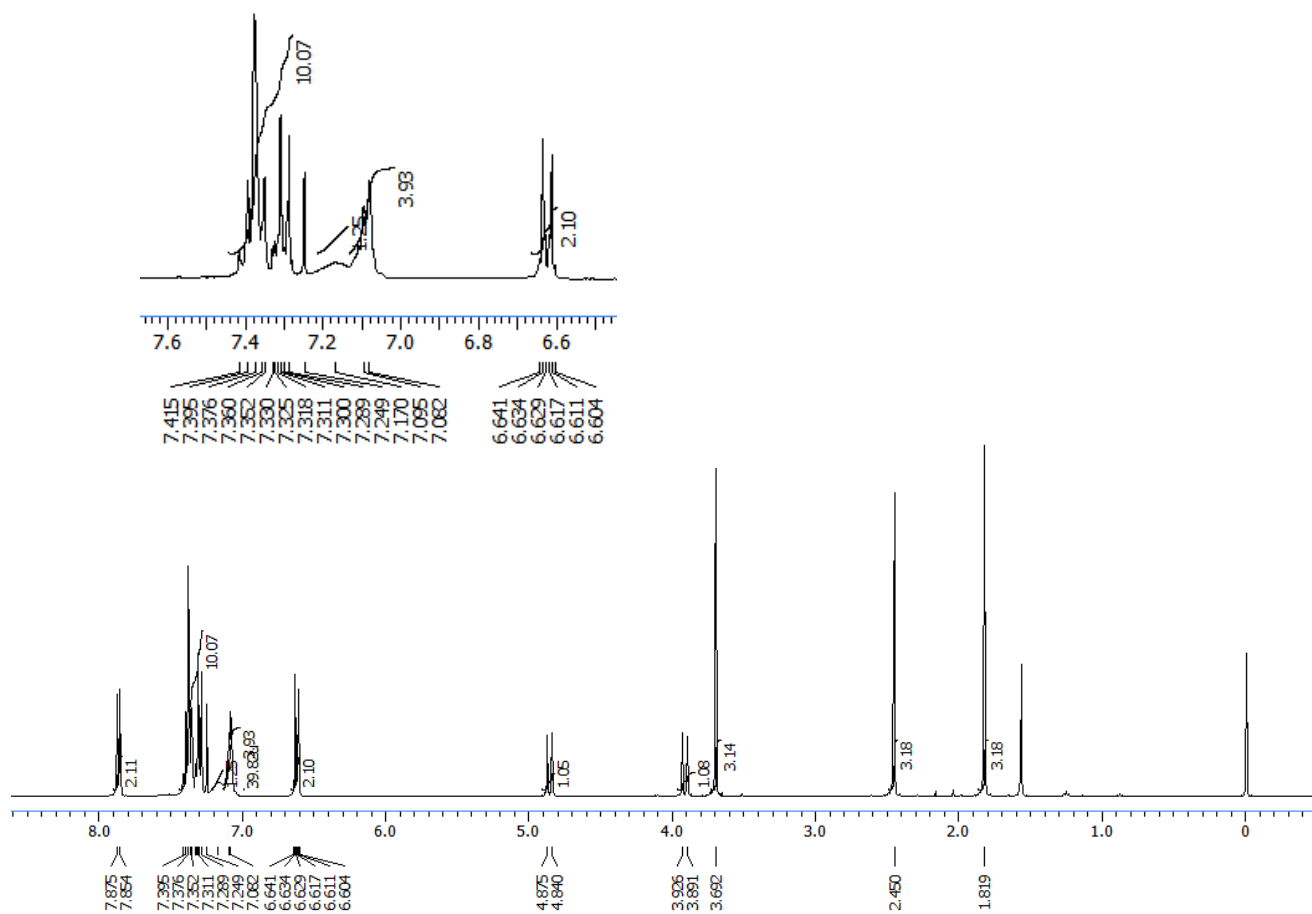
(E)-3-(((2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)sulfonyl)methyl)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



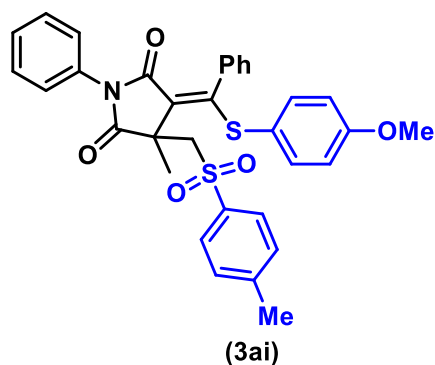
¹H NMR spectrum of 3ai (400 MHz, CDCl₃)



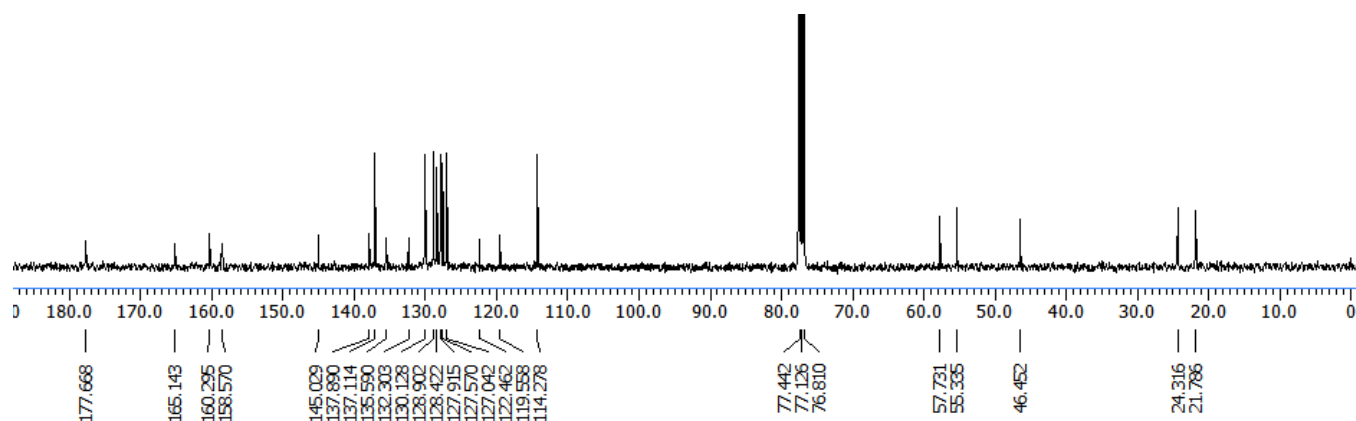
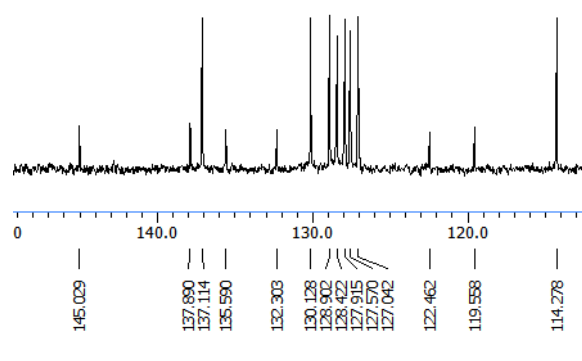
(E)-4-(((4-methoxyphenyl)thio)(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione



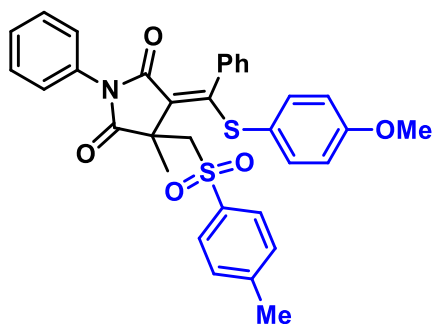
¹³C NMR spectrum of 3i (100 MHz, CDCl₃)



(*E*)-4-(((4-methoxyphenyl)thio)(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione

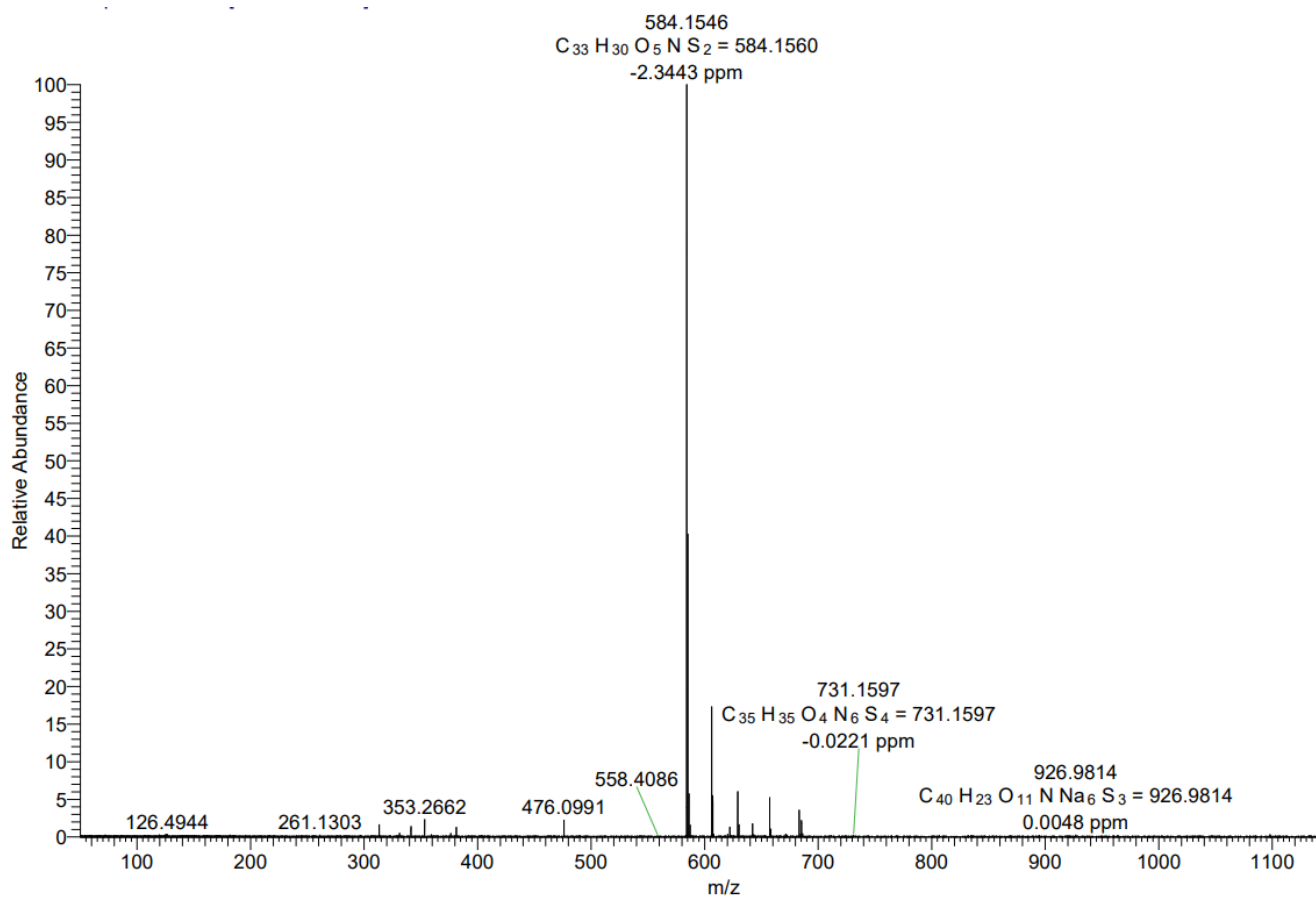


HRMS Spectrum of 3i

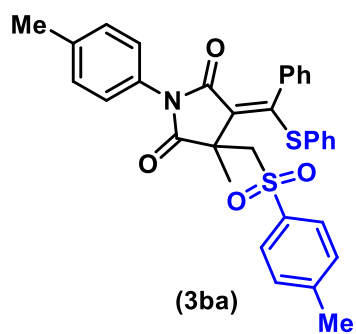


(3ai)

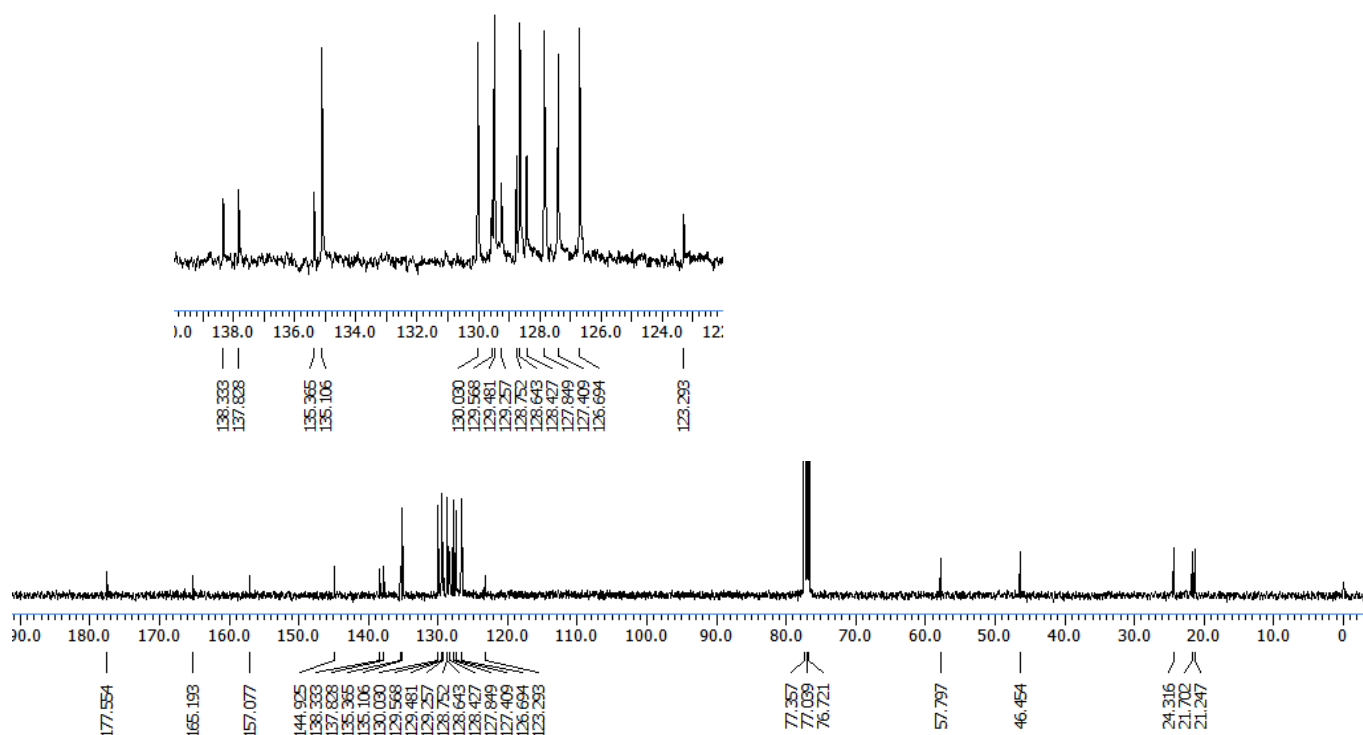
(*E*)-4-(((4-methoxyphenyl)thio)(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione



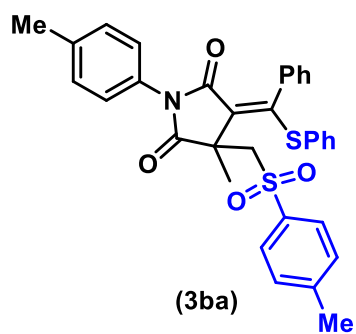
¹³C NMR spectrum of 3ba (100 MHz, CDCl₃)



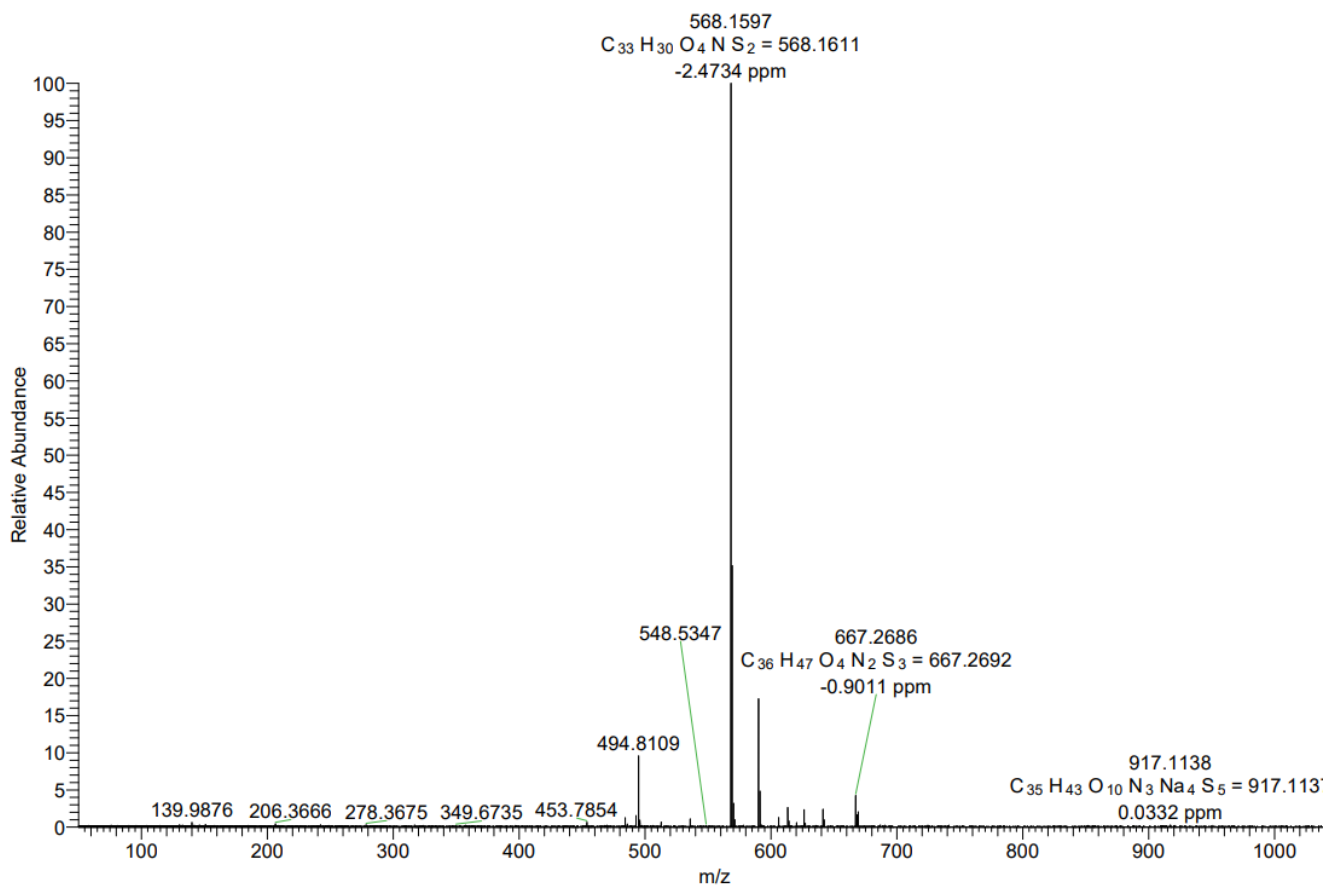
(E)-3-methyl-4-(phenyl(phenylthio)methylene)-1-(*p*-tolyl)-3-(tosylmethyl)pyrrolidine-2,5 dione



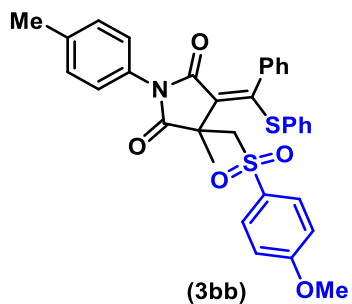
HRMS Spectrum of 3ba



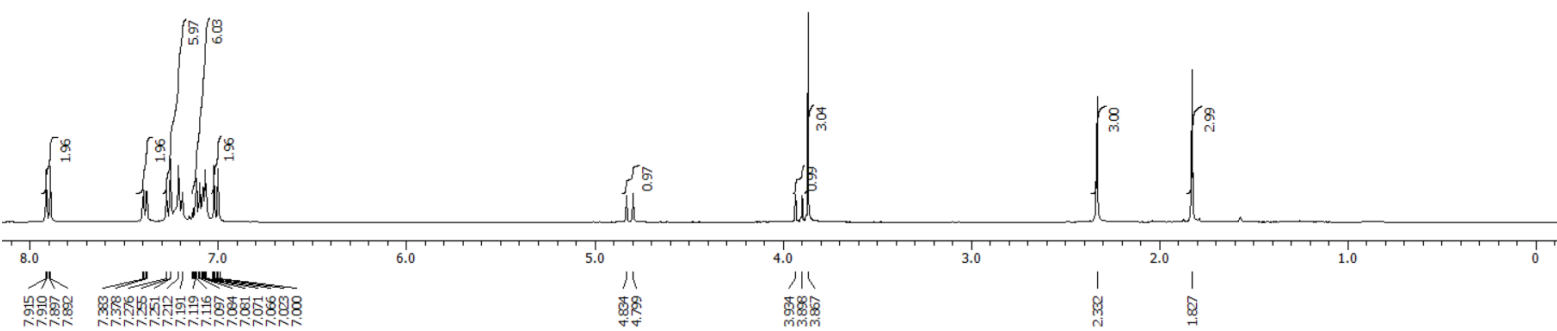
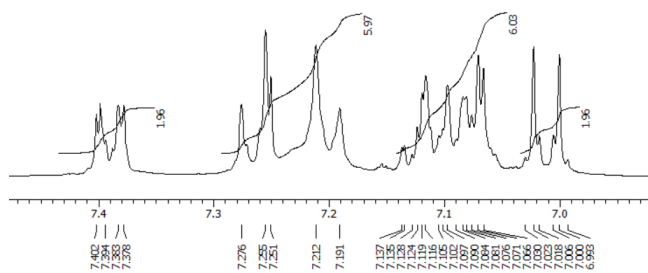
(E)-3-methyl-4-(phenyl(phenylthio)methylene)-1-(*p*-tolyl)-3-(tosylmethyl)pyrrolidine-2,5 dione



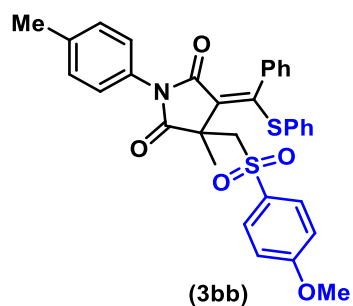
¹H NMR spectrum of 3bb (400 MHz, CDCl₃)



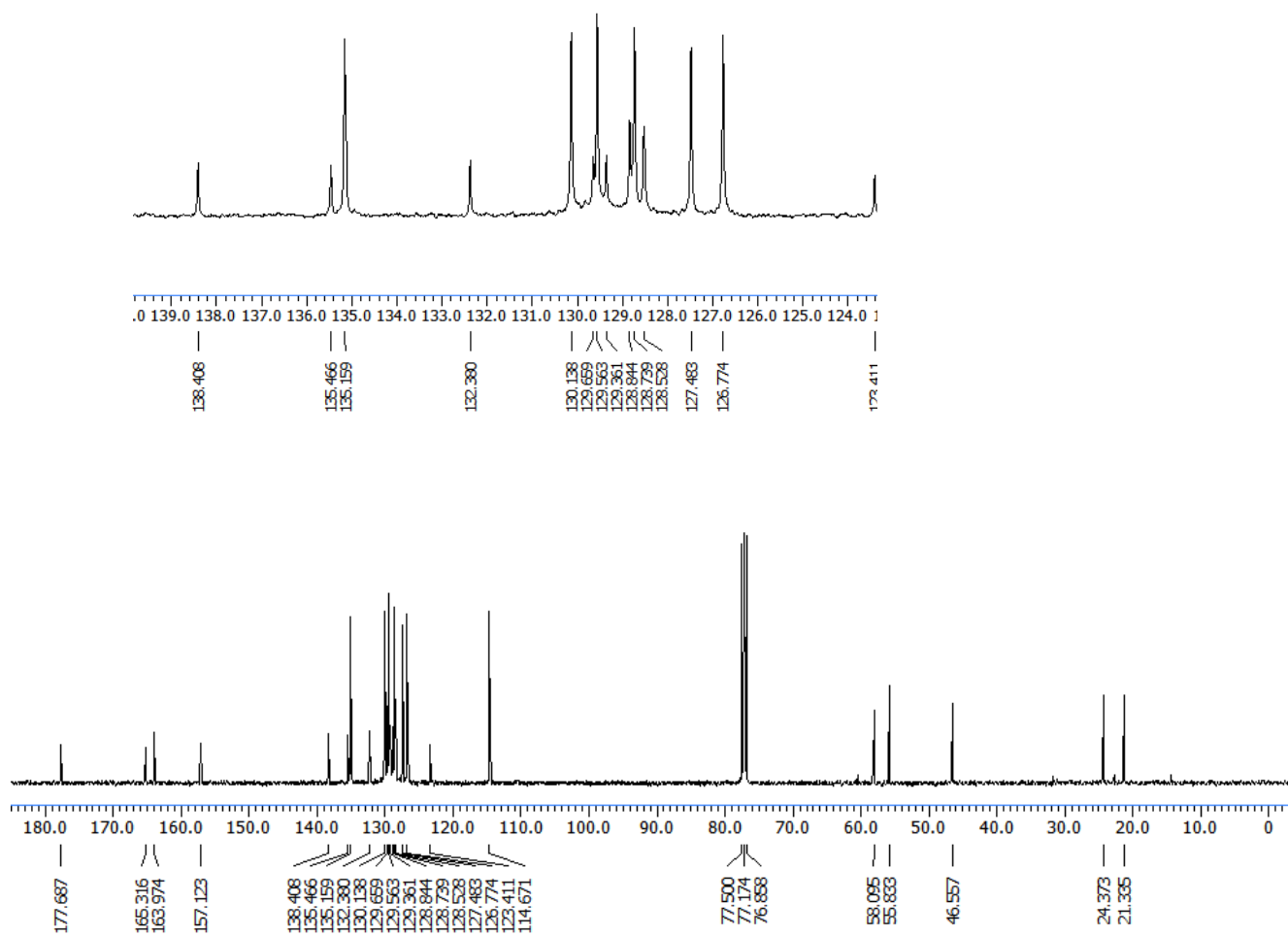
(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-4-(phenyl(phenylthio)methylene)-1-(*p*-tolyl)pyrrolidine-2,5-dione



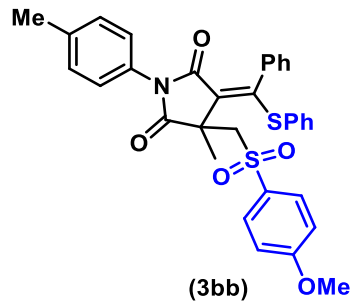
¹³C NMR spectrum of 3bb (100 MHz, CDCl₃)



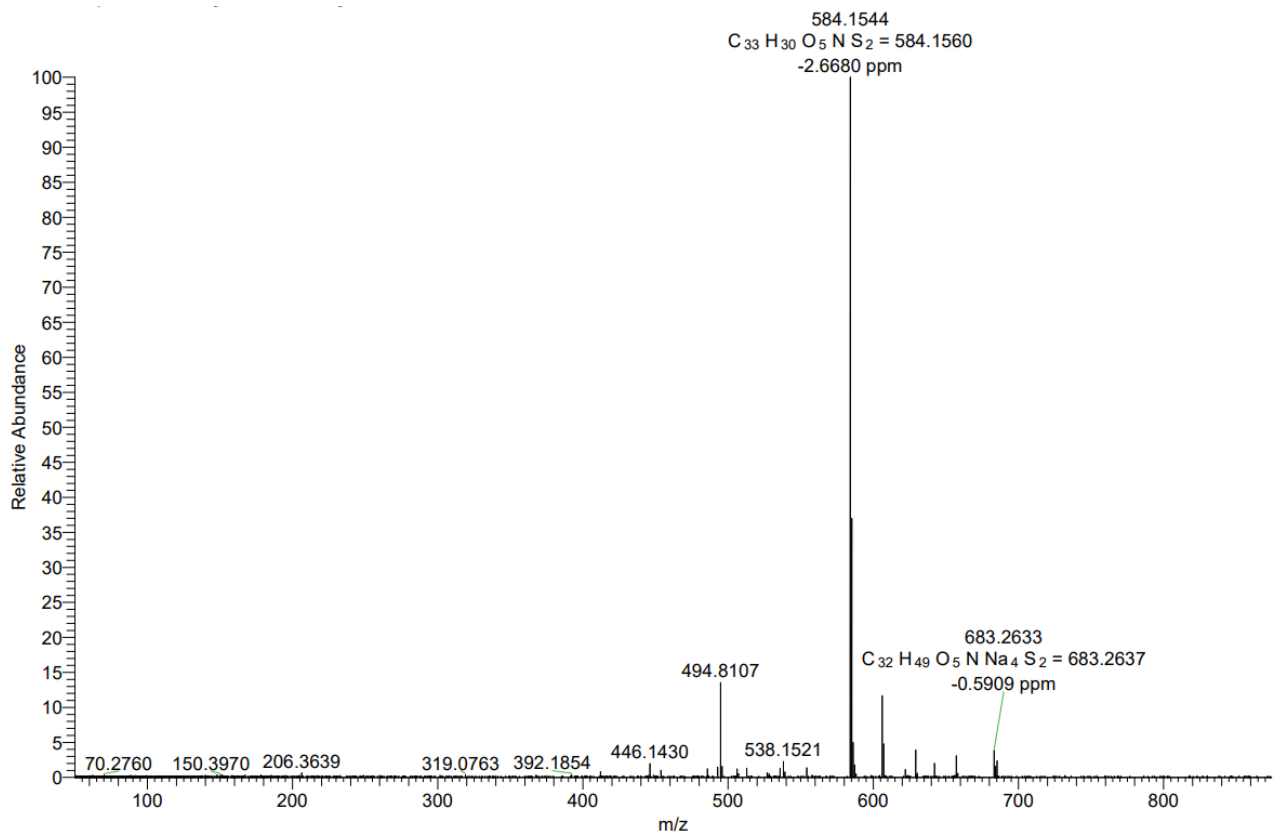
(*E*)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-4-(phenyl(phenylthio)methylene)-1-(*p*-tolyl)pyrrolidine-2,5-dione



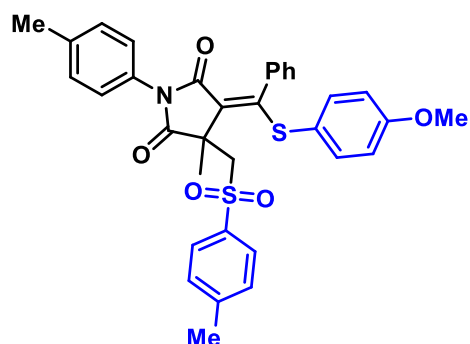
HRMS spectrum of 3bb



(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-4-(phenyl(phenylthio)methylene)-1-(p-tolyl)pyrrolidine-2,5-dione

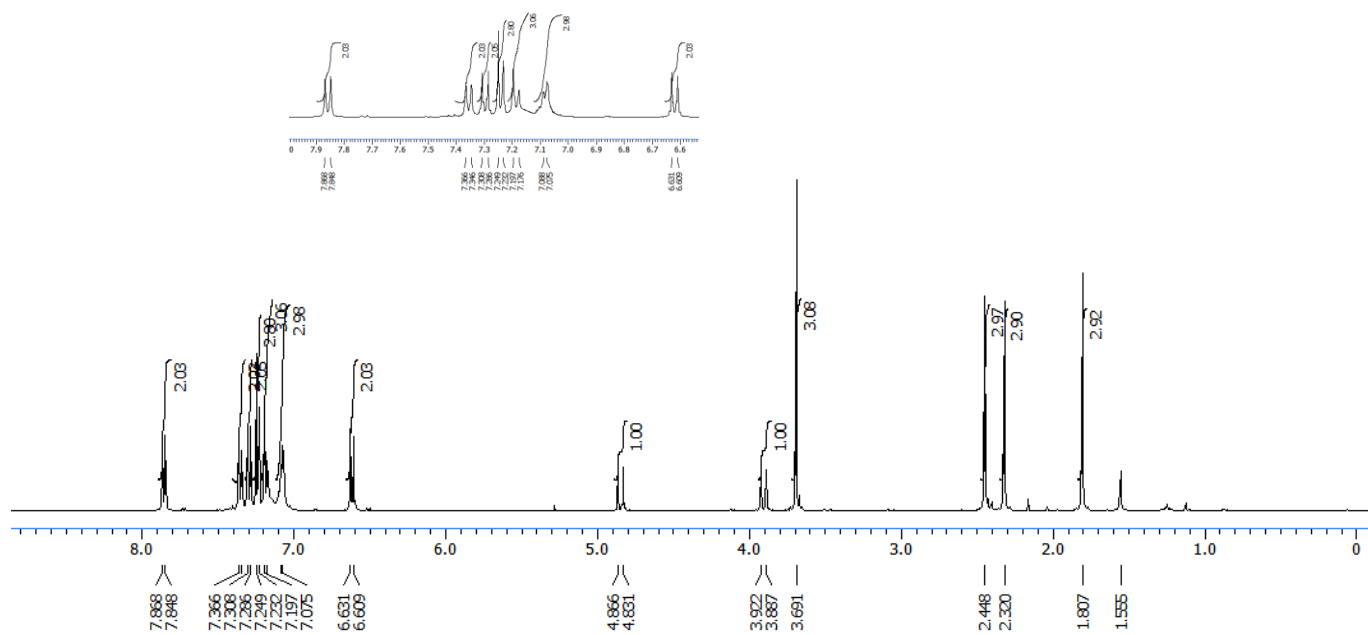


¹H NMR spectrum of 3bc (400 MHz, CDCl₃)

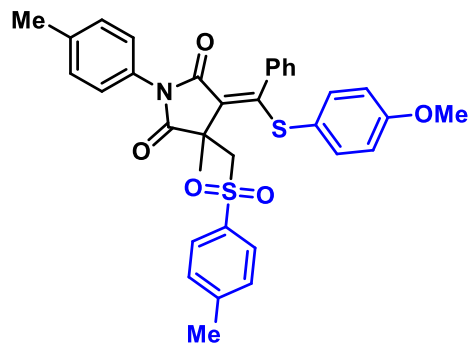


(3bc)

(*E*)-4-(((4-methoxyphenyl)thio)(phenyl)methylene)-3-methyl-1-(*p*-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione



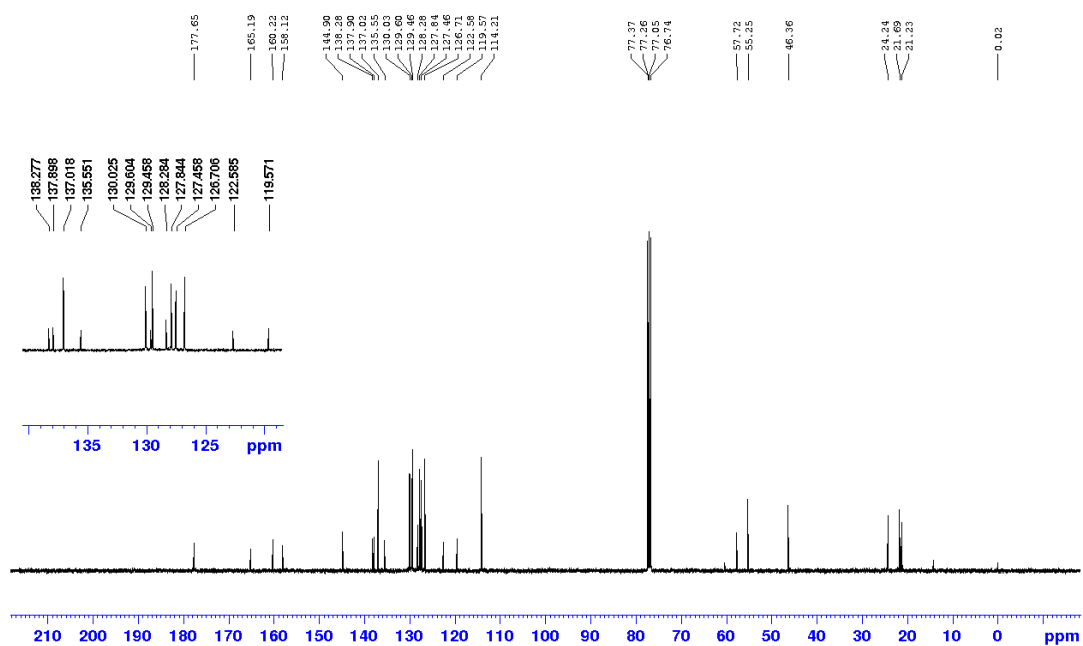
¹³CNMR spectrum of 3bc (100 MHz, CDCl₃)



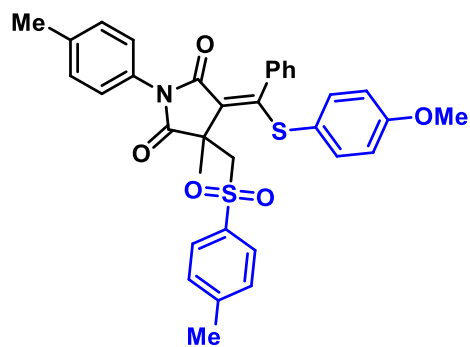
(3bc)

(E)-4-(((4-methoxyphenyl)thio)(phenyl)methylene)-3-methyl-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione

SMP-17

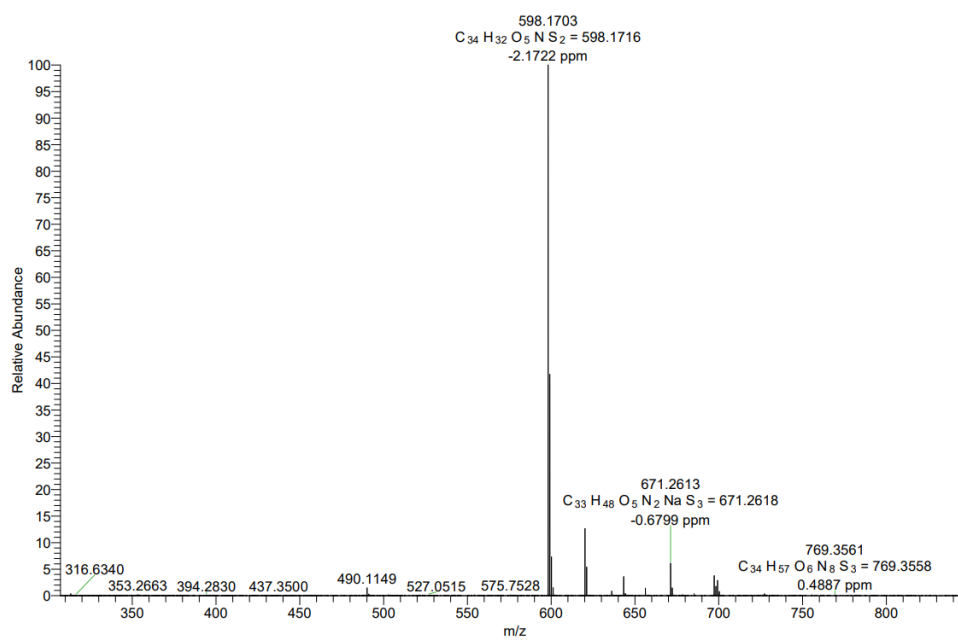


HRMS spectrum of 3bc

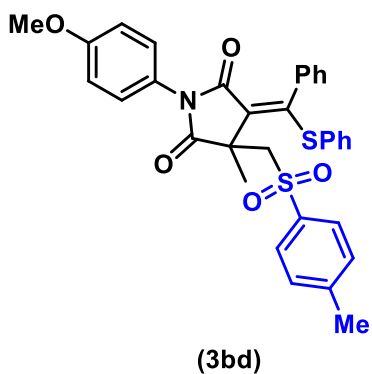


(3bc)

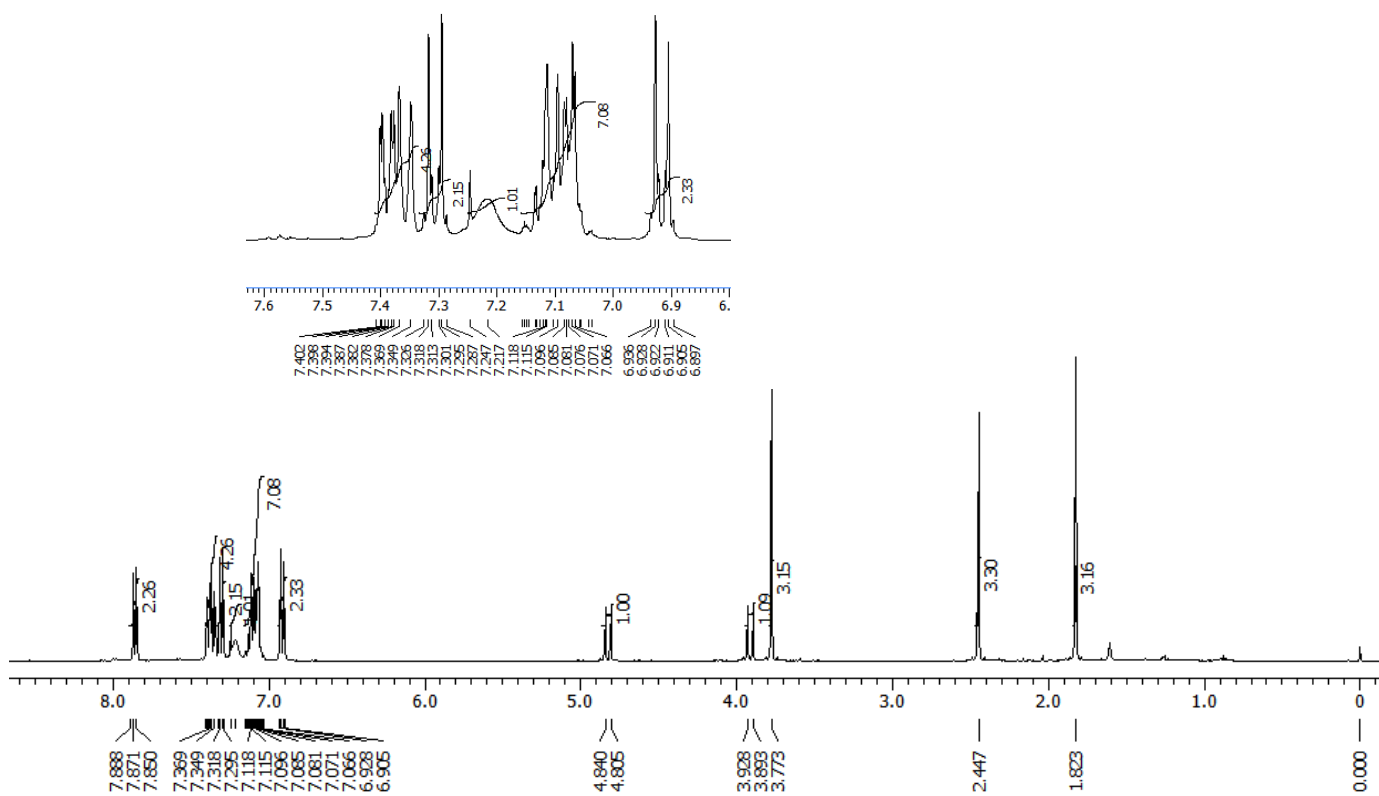
(E)-4-(((4-methoxyphenyl)thio)(phenyl)methylene)-3-methyl-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione



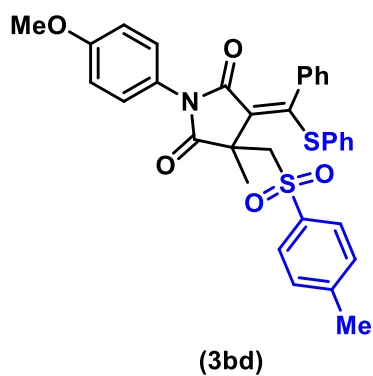
¹H NMR spectrum of 3bd (400 MHz, CDCl₃)



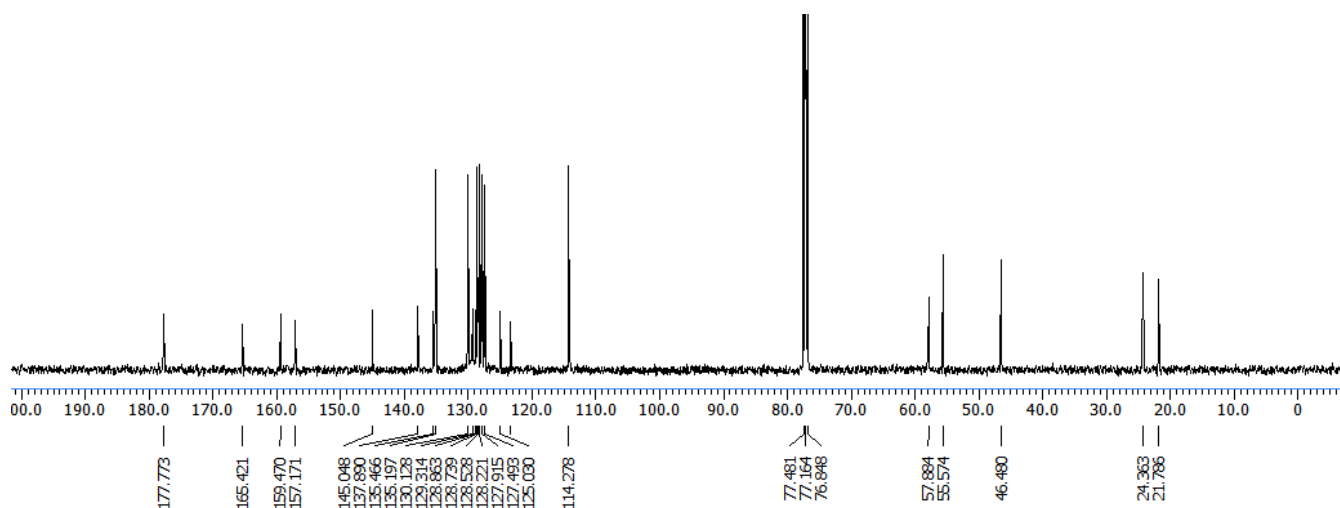
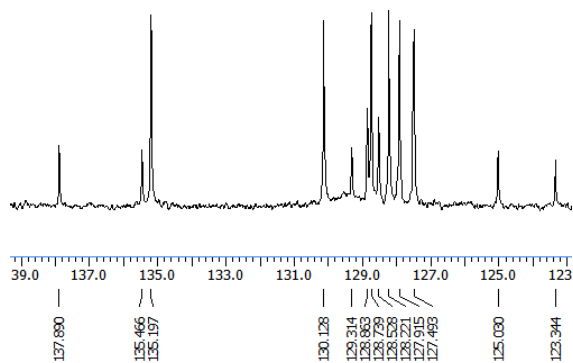
(*E*)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



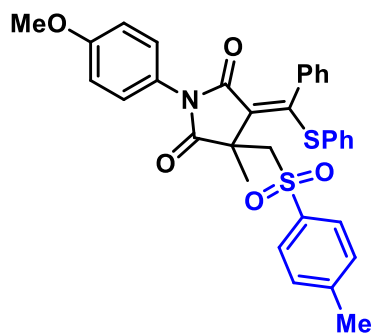
¹³C NMR spectrum of 3bd (100 MHz, CDCl₃)



(E)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

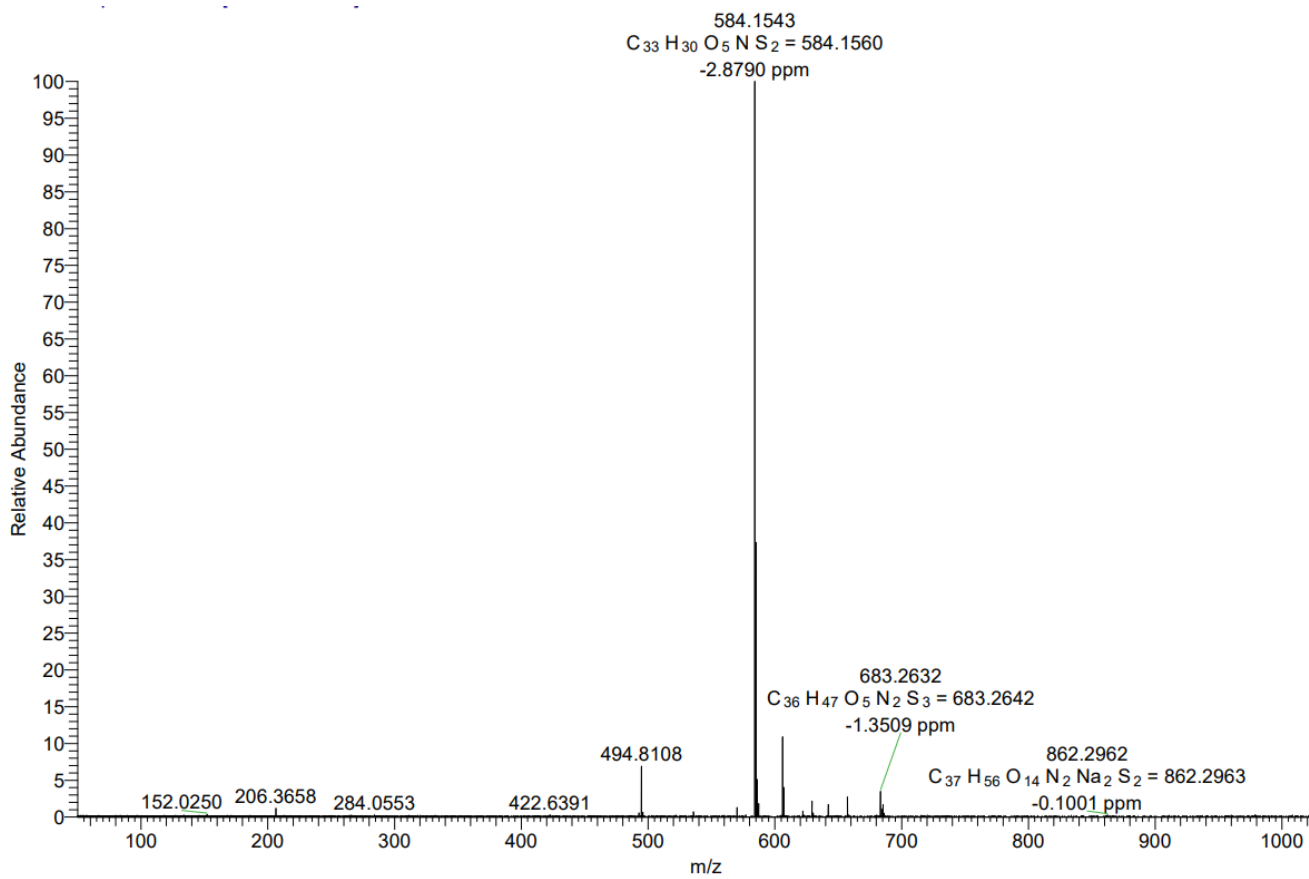


HRMS spectrum of 3bd

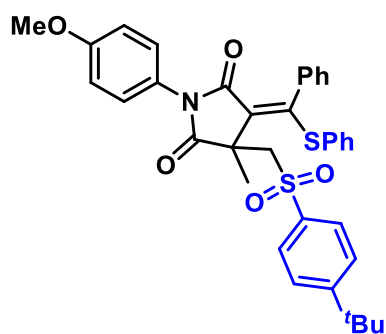


(3bd)

(E)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

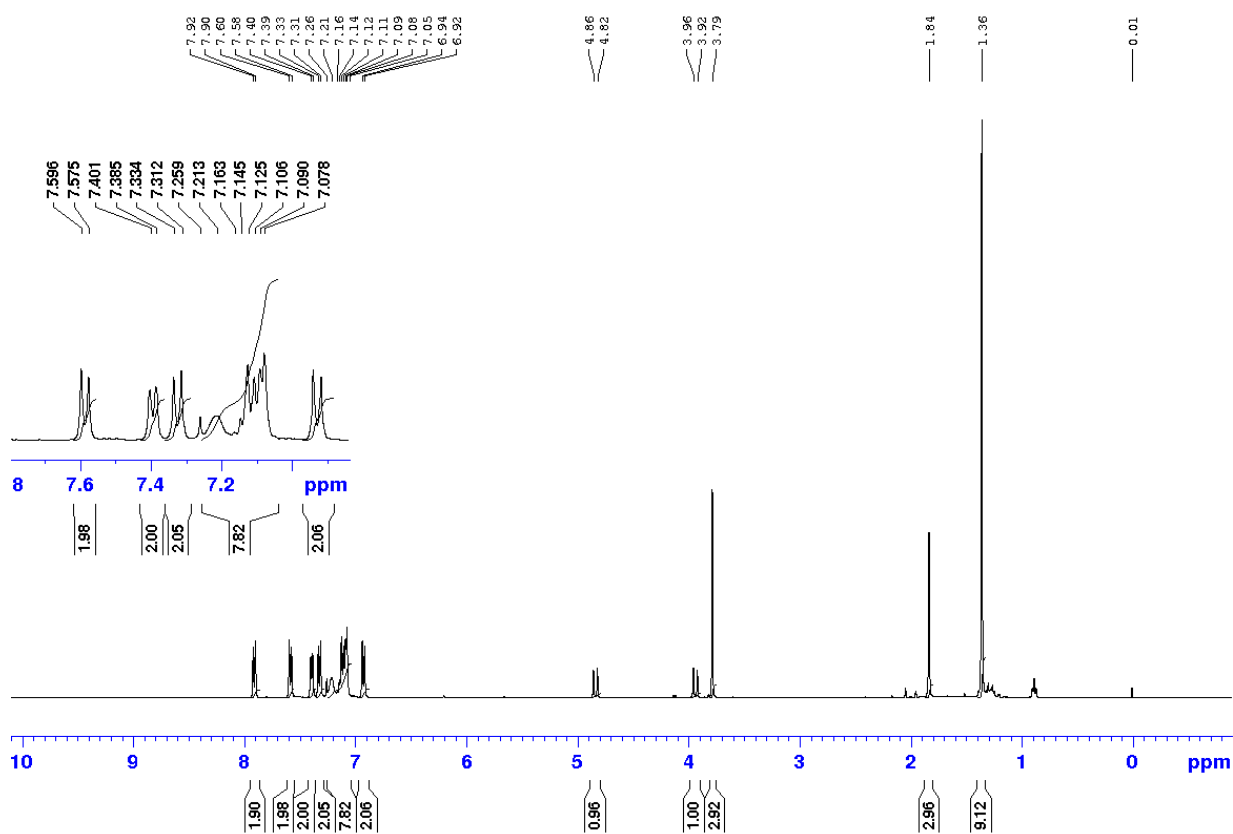


¹H NMR spectrum of 3be (400 MHz, CDCl₃)

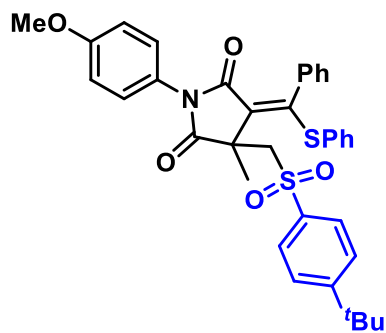


(3be)

(*E*)-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione

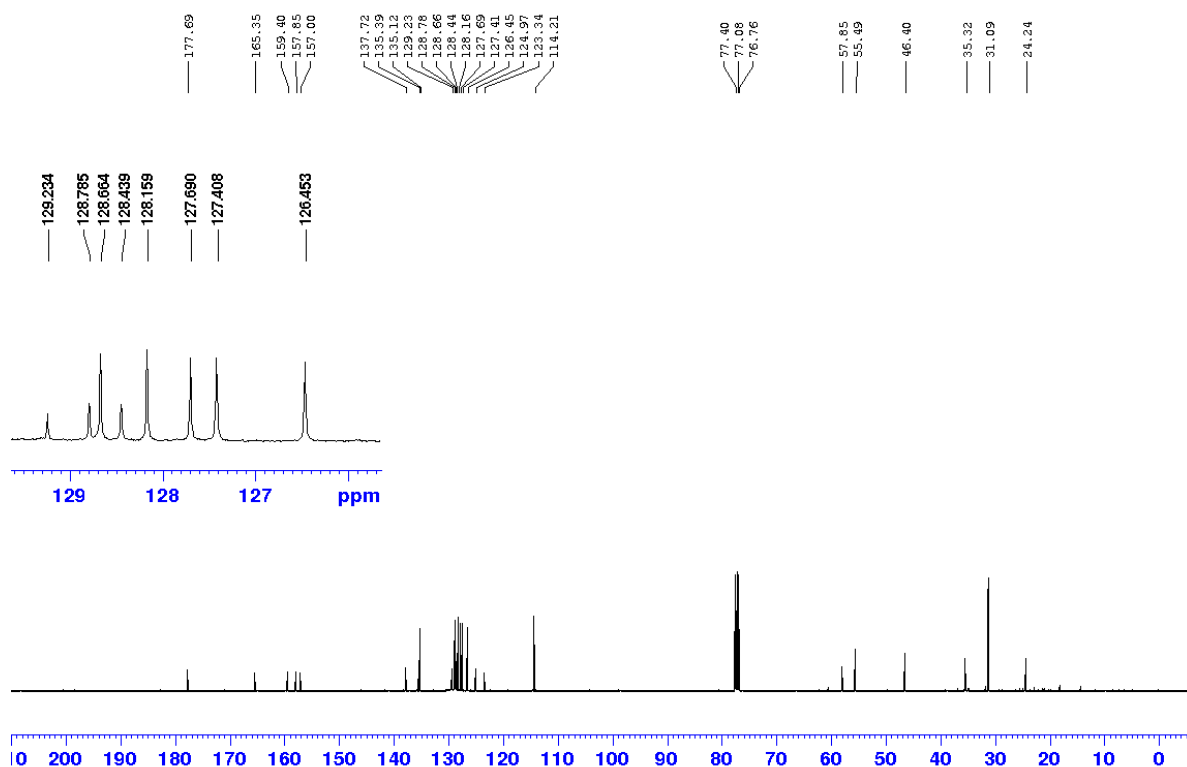


¹³C NMR spectrum of 3be (100 MHz, CDCl₃)

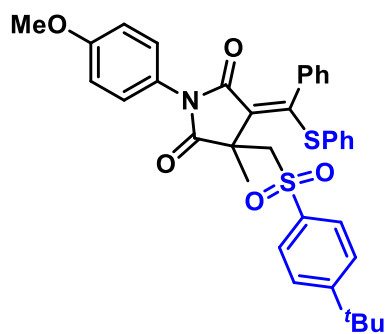


(3be)

(E)-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylthio)methylene)pyrrolidine-2,5-dione

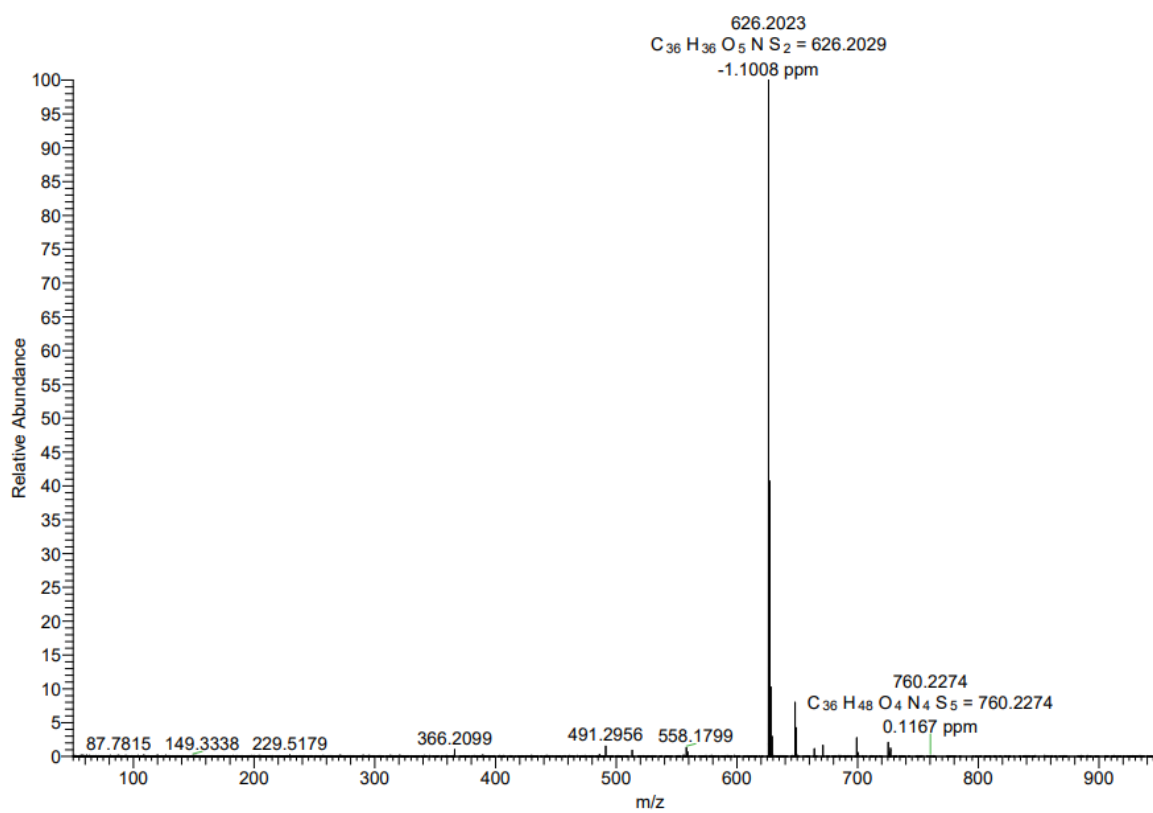


HRMS spectrum of 3be

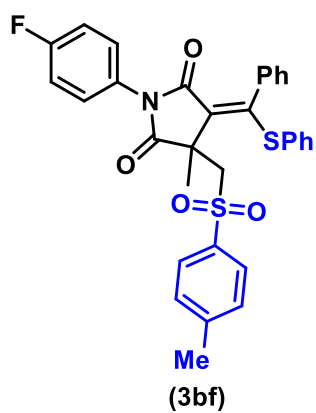


(3be)

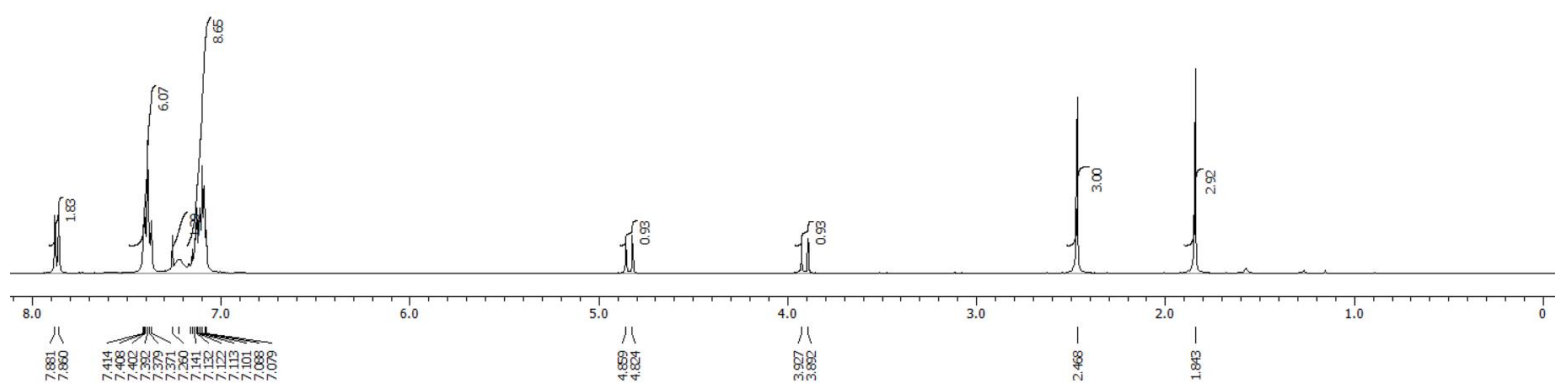
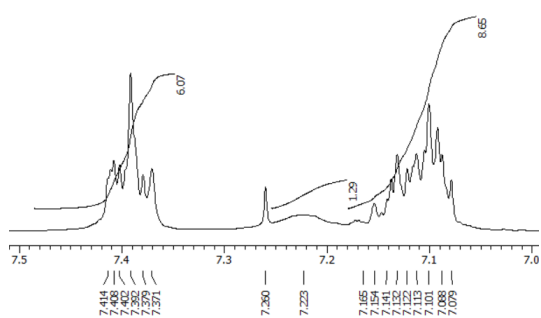
(*E*)-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-1-(4-methoxyphenyl)-3-methyl-4-phenyl(phenylthio)methylene)pyrrolidine-2,5-dione



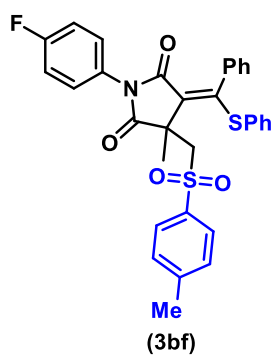
¹H NMR spectrum of 3bf (400 MHz, CDCl₃)



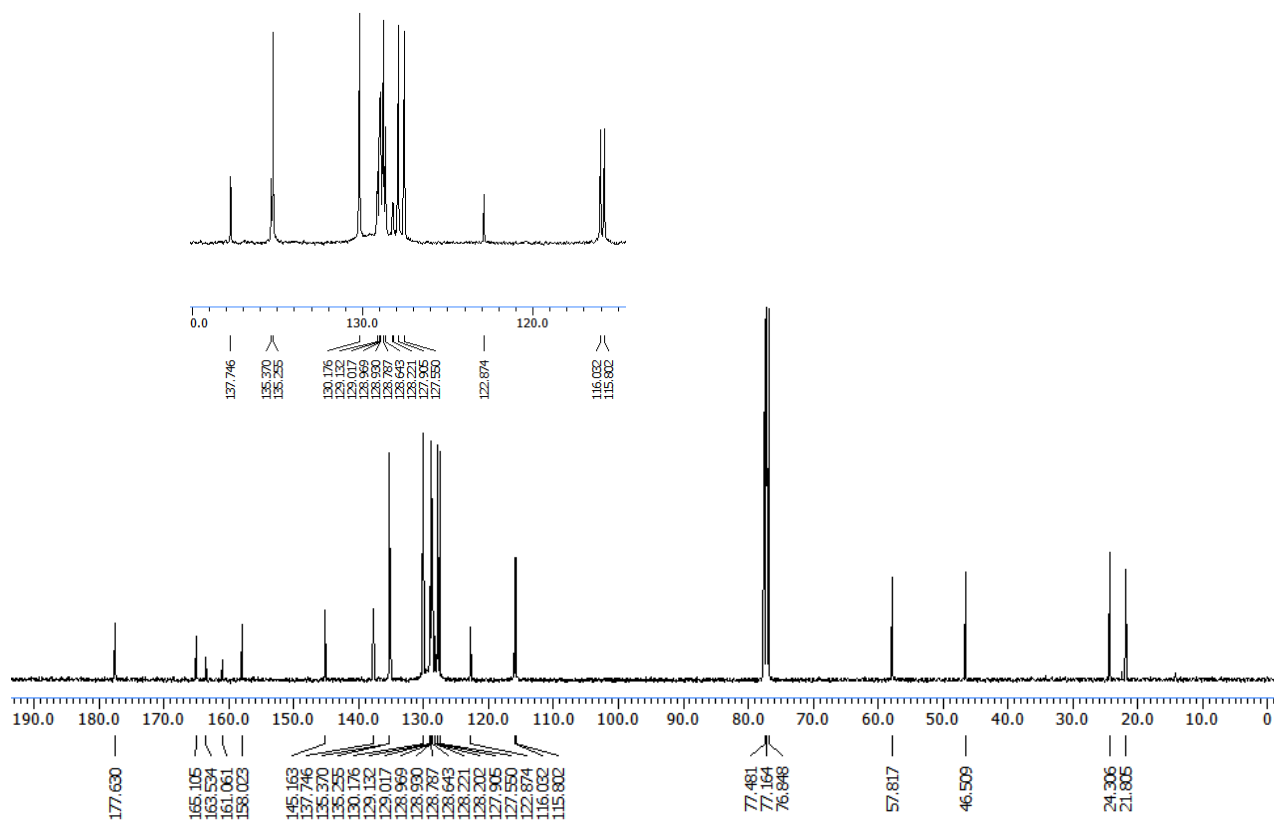
(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



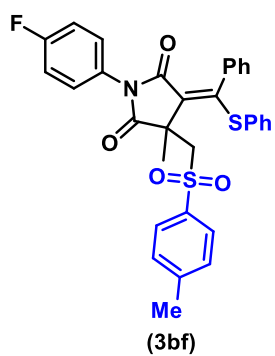
¹³C NMR spectrum of 3bf (100 MHz, CDCl₃)



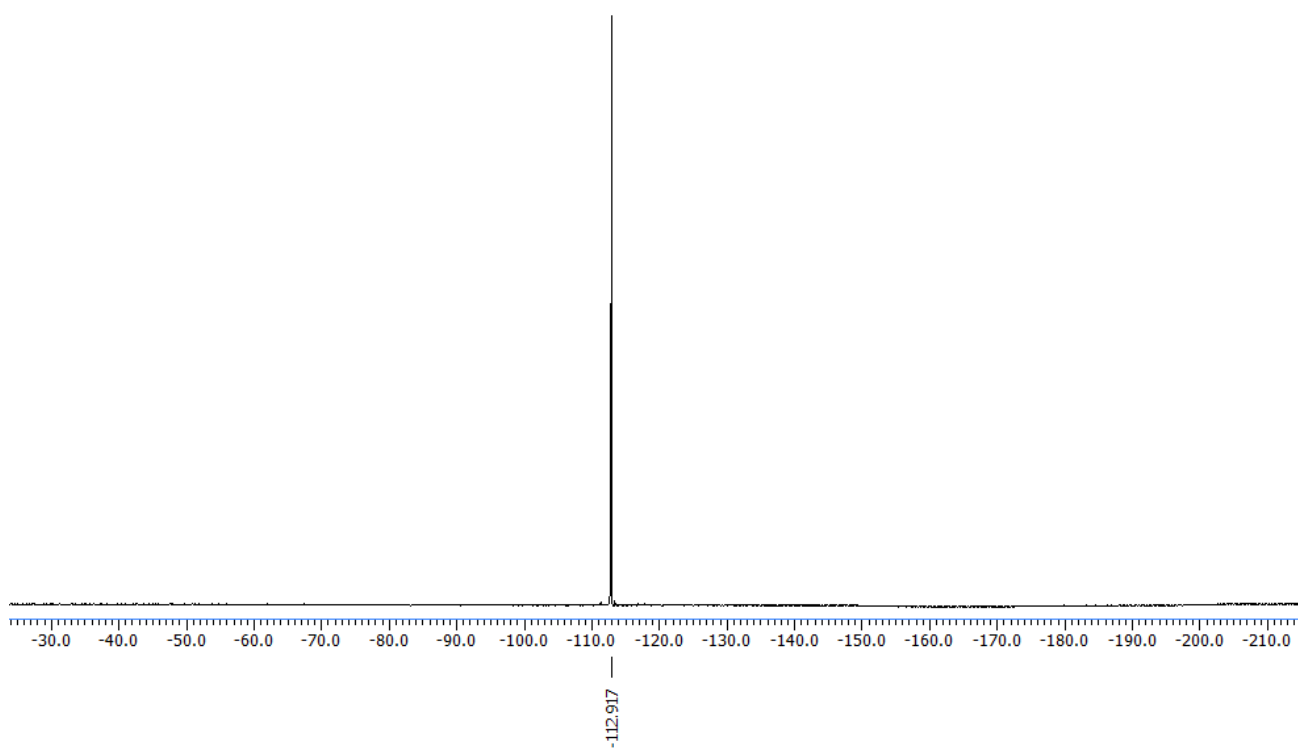
(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



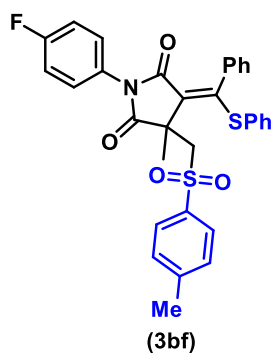
¹³C NMR spectrum of 3bf (376 MHz, CDCl₃)



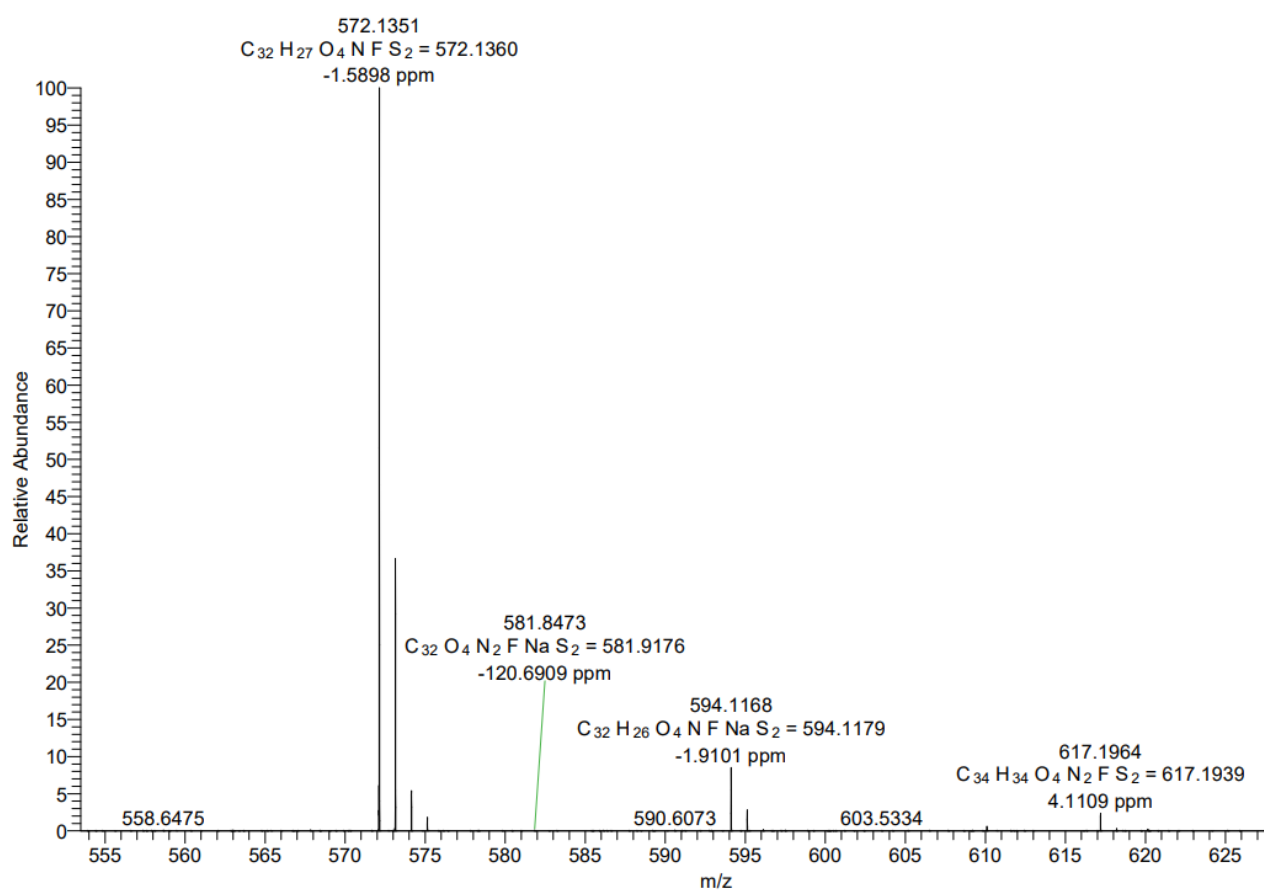
(*E*)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



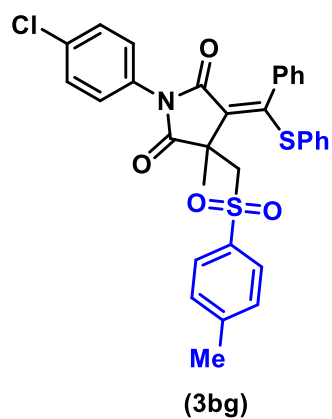
HRMS spectrum of 3bf



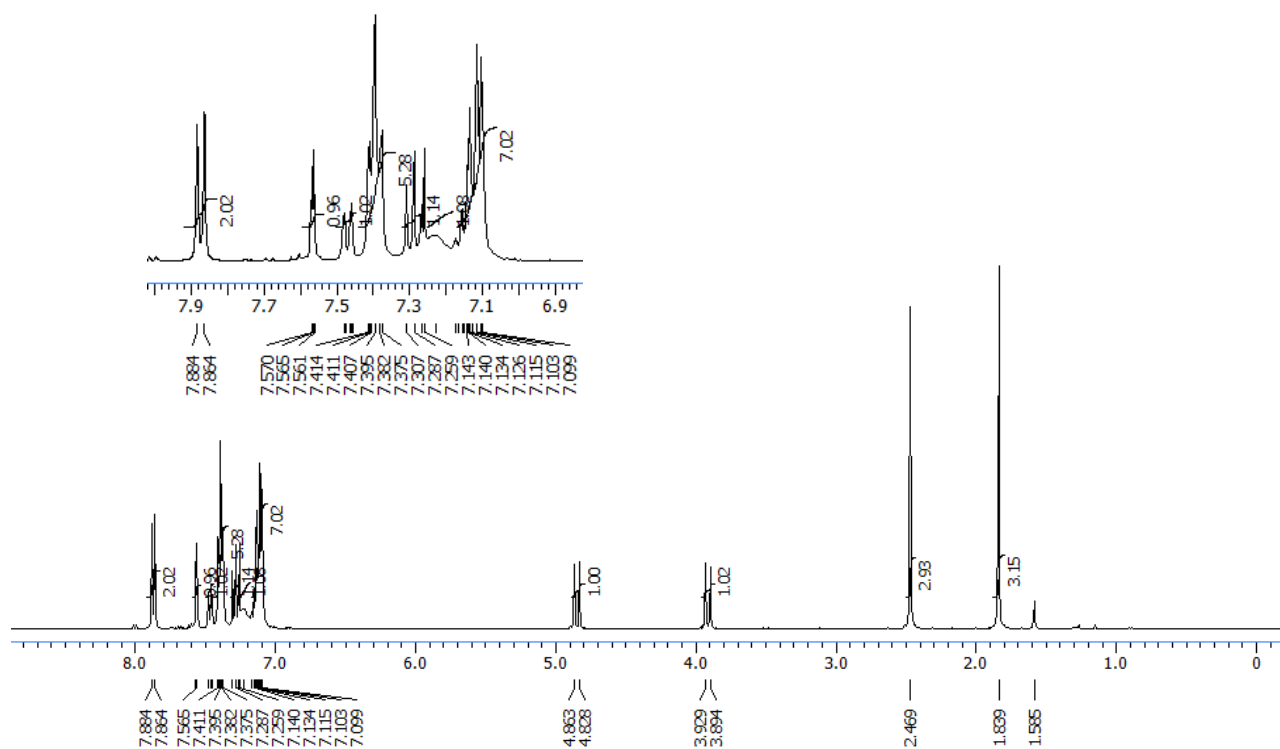
(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



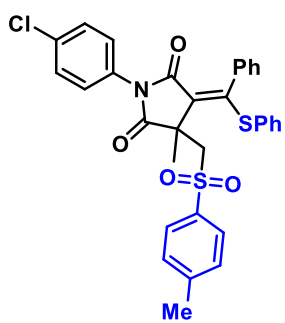
¹H NMR spectrum of 3bg (400 MHz, CDCl₃)



(E)-1-(4-chlorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

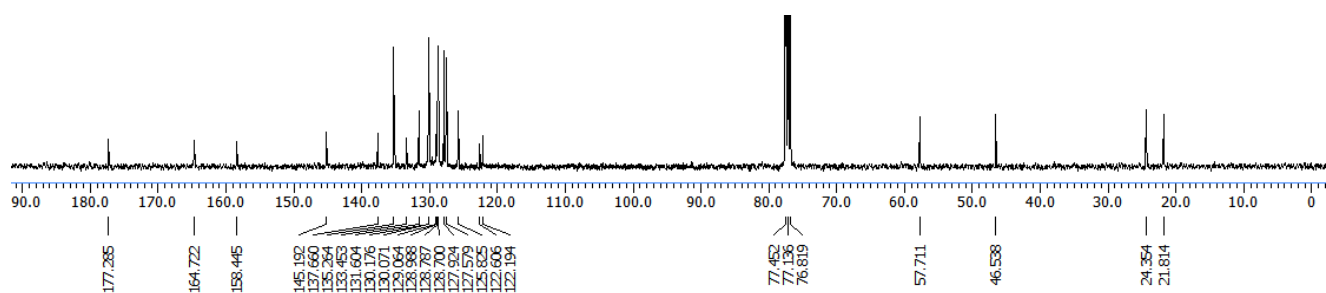
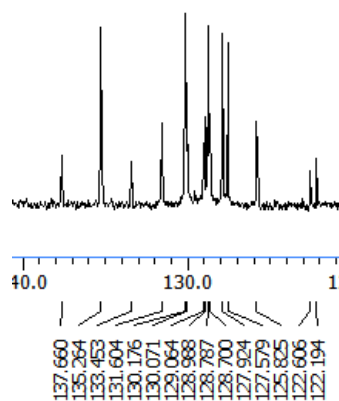


¹³C NMR spectrum of 3bg (100 MHz, CDCl₃)

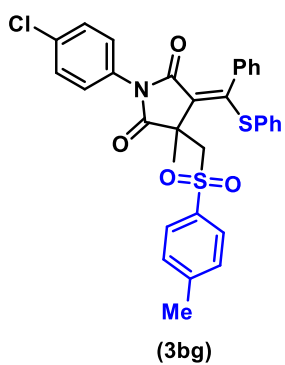


(3bg)

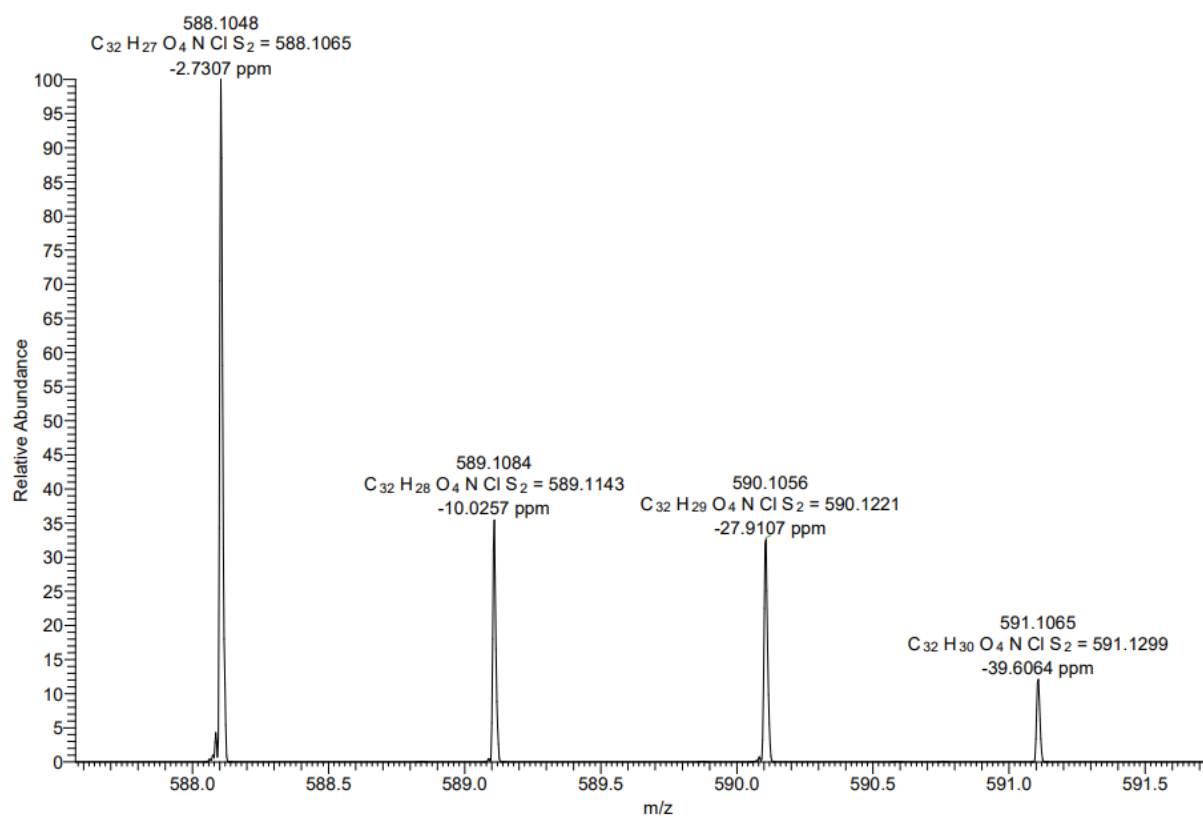
(E)-1-(4-chlorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



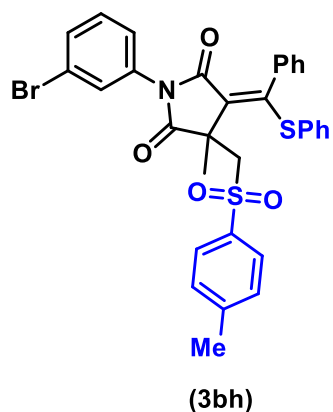
HRMS spectrum of 3bg



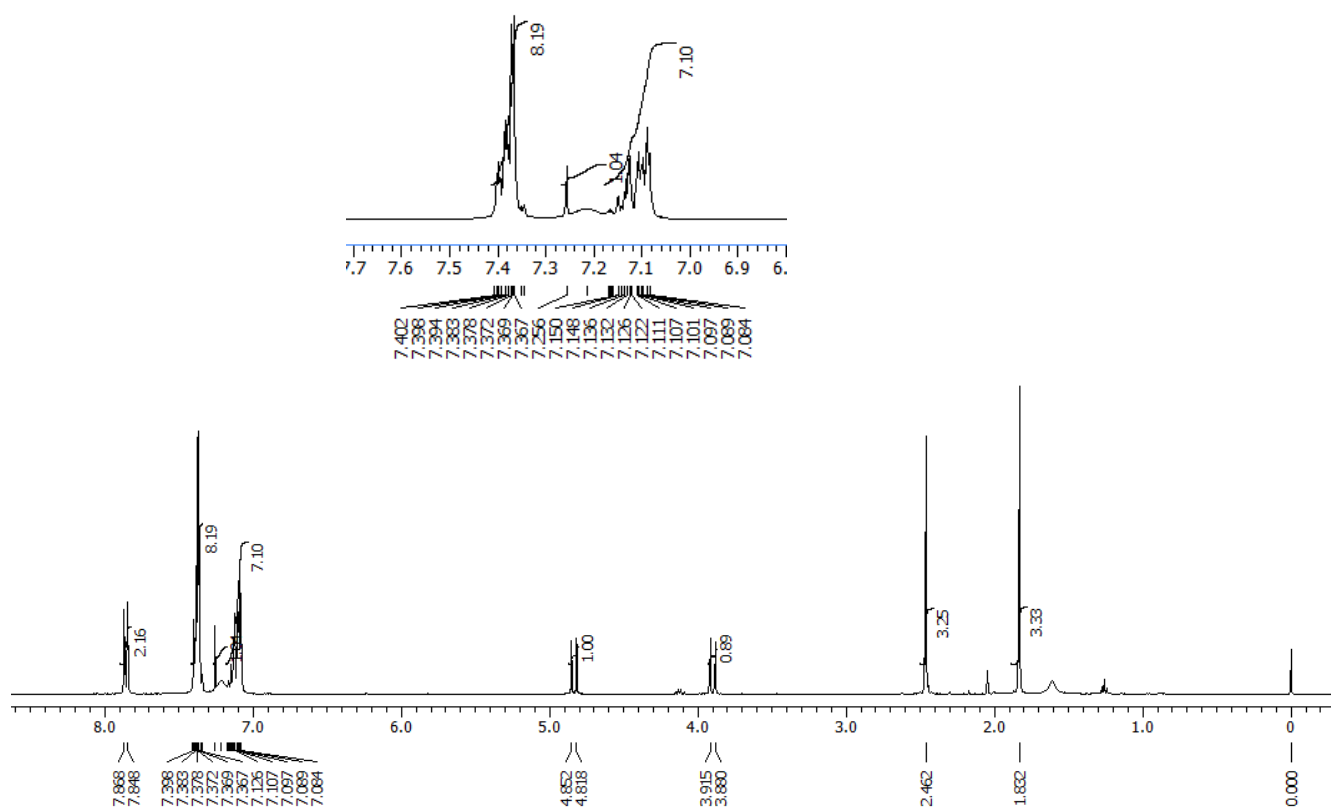
(E)-1-(4-chlorophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



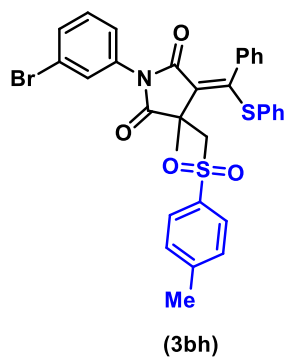
¹H NMR spectrum of 3bh (400 MHz, CDCl₃)



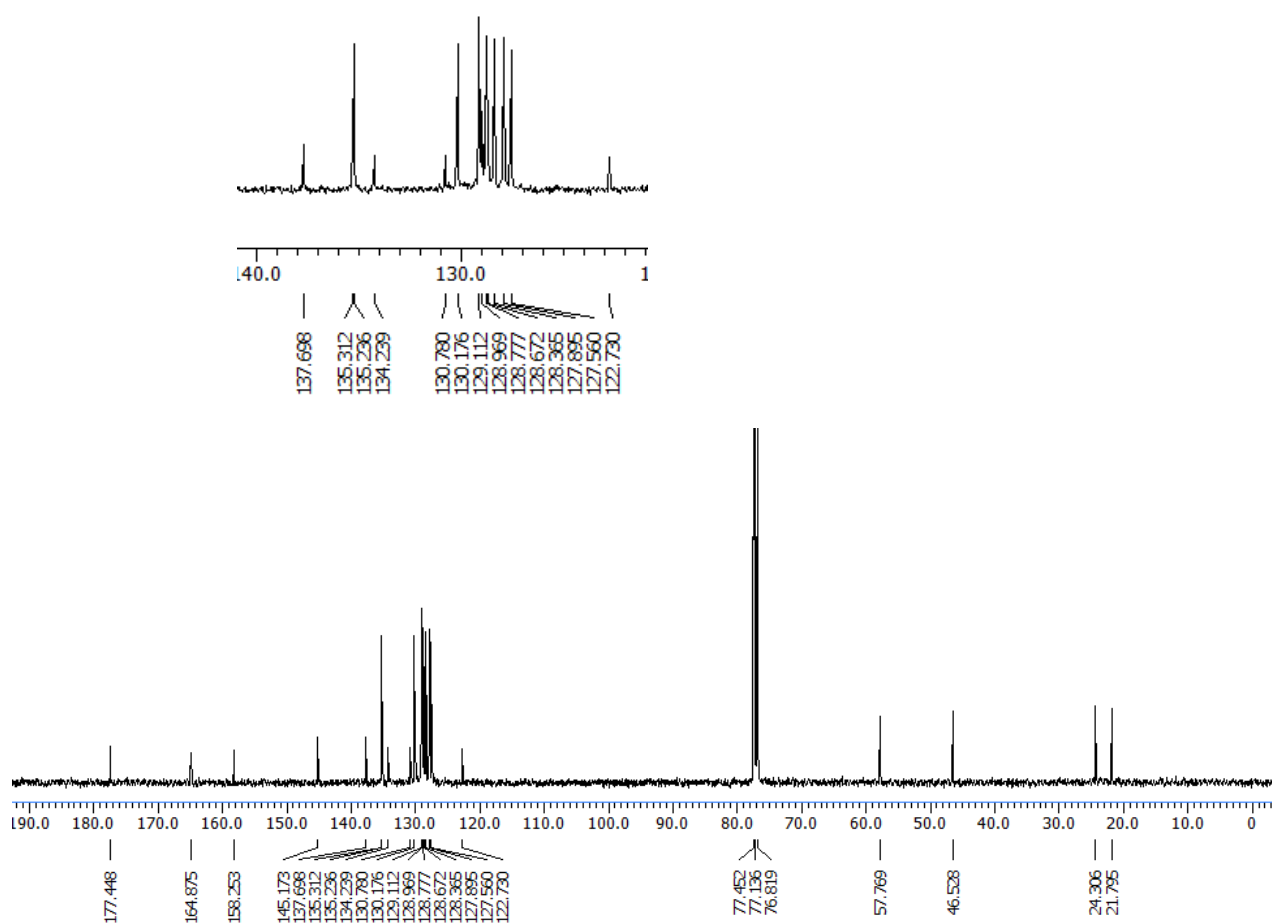
(*E*)-1-(3-bromophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



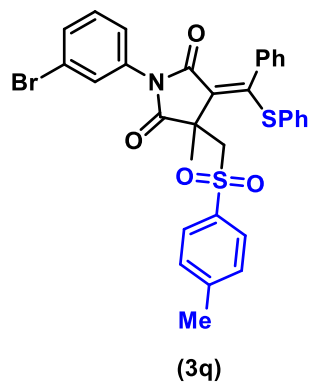
¹³C NMR spectrum of 3bh (100 MHz, CDCl₃)



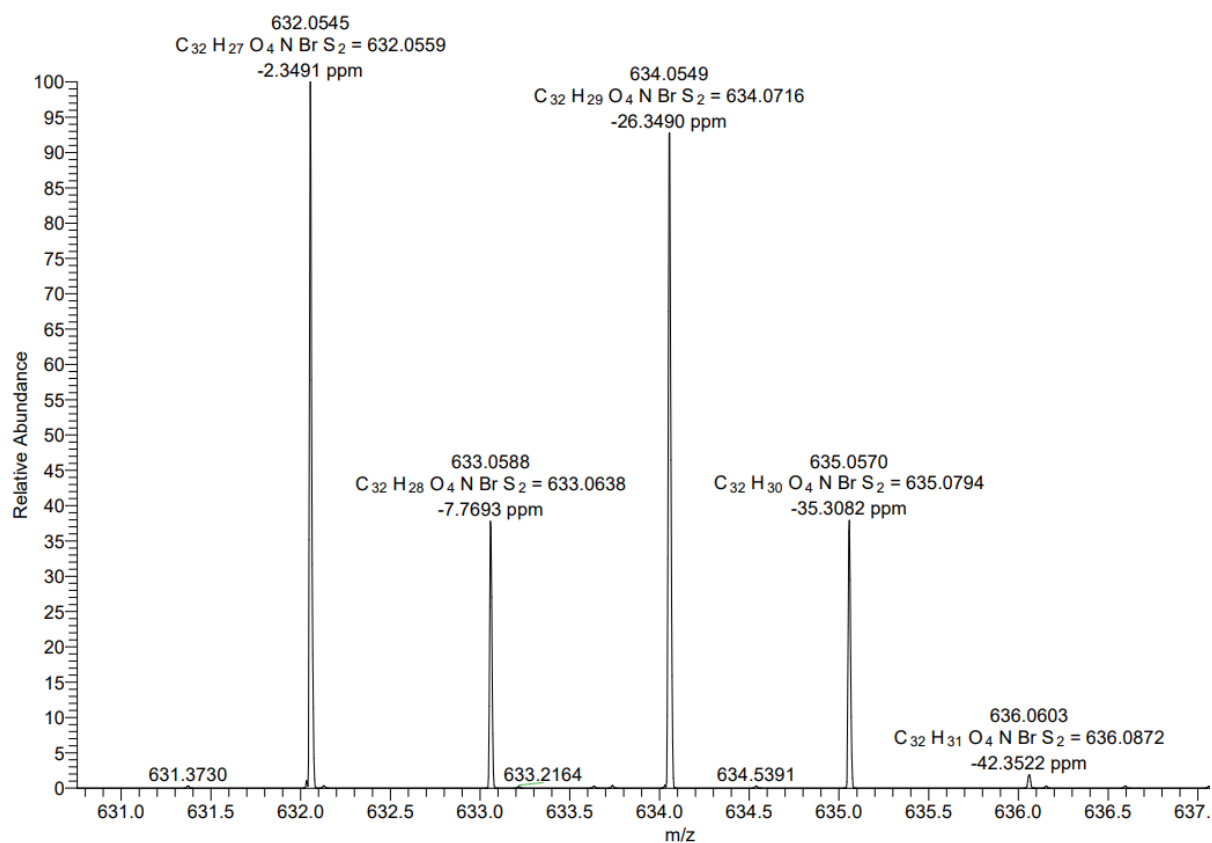
(E)-1-(3-bromophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



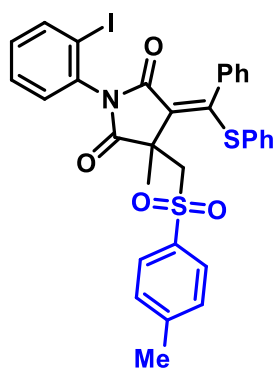
HRMS spectrum of 3bh



(E)-1-(3-bromophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

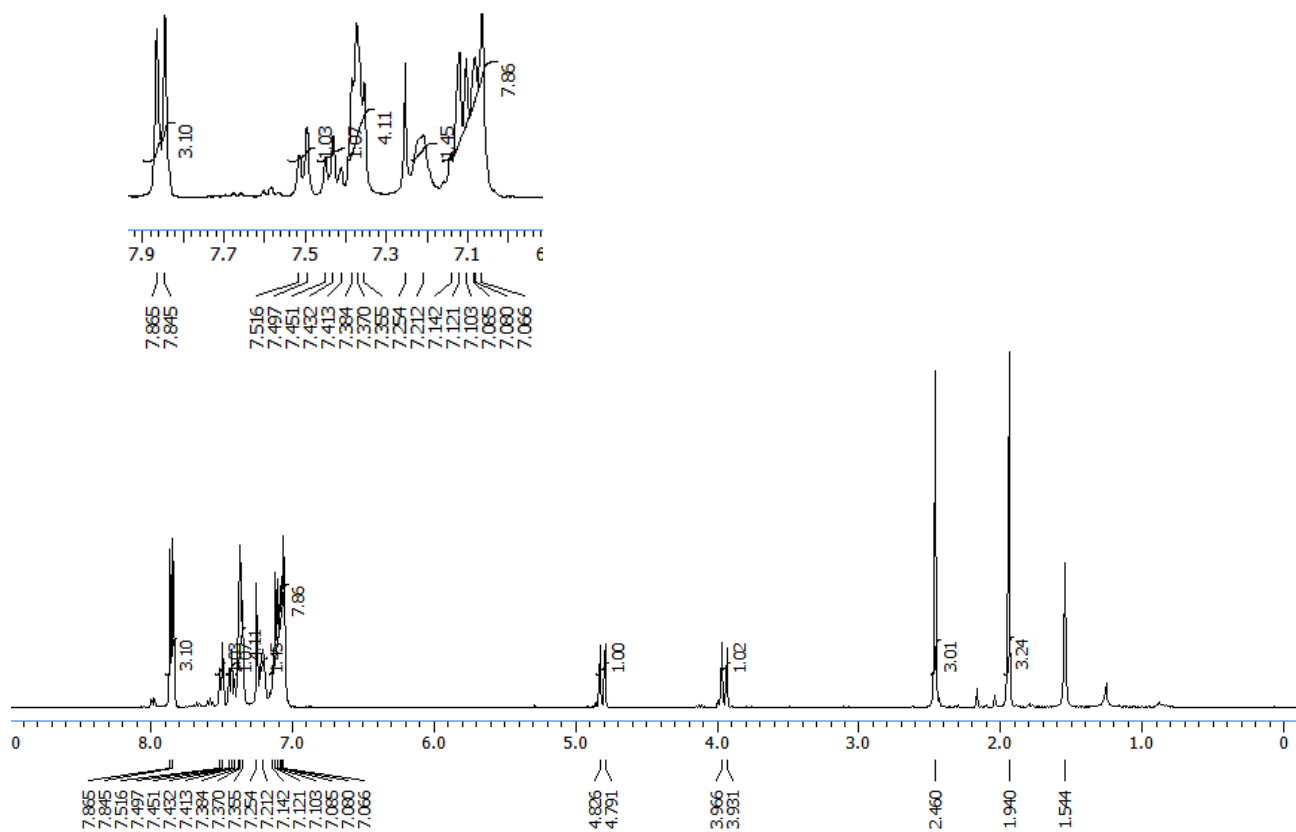


¹H NMR spectrum of 3bi (400 MHz, CDCl₃)

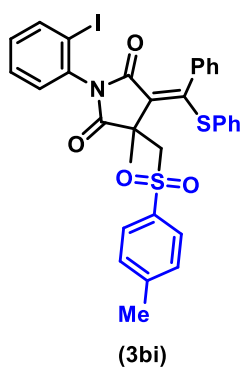


(3bi)

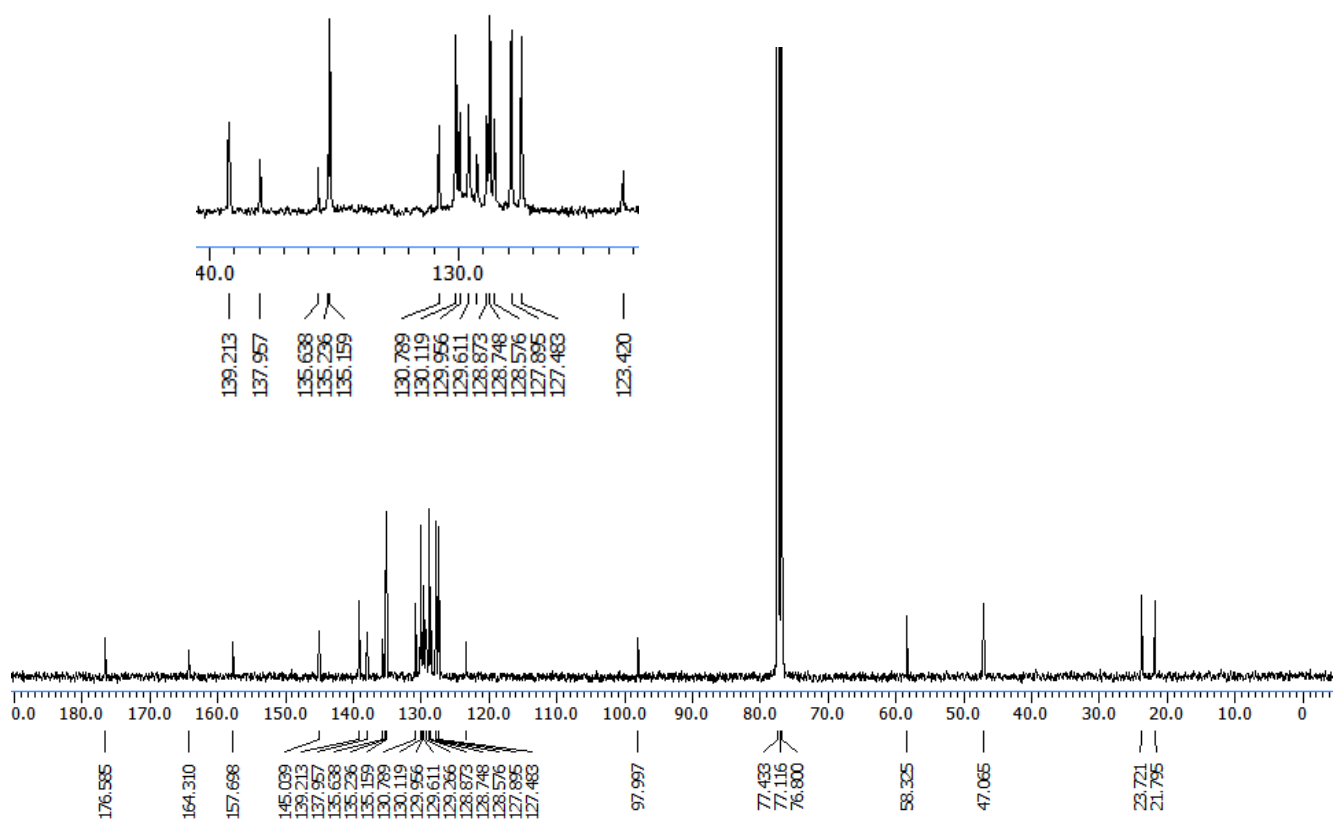
(E)-1-(2-iodophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



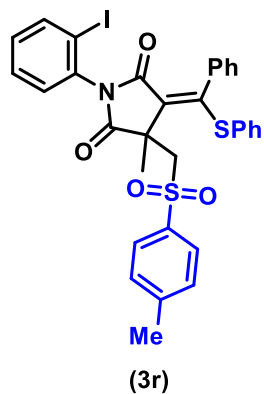
¹³C NMR spectrum of 3bi (100 MHz, CDCl₃)



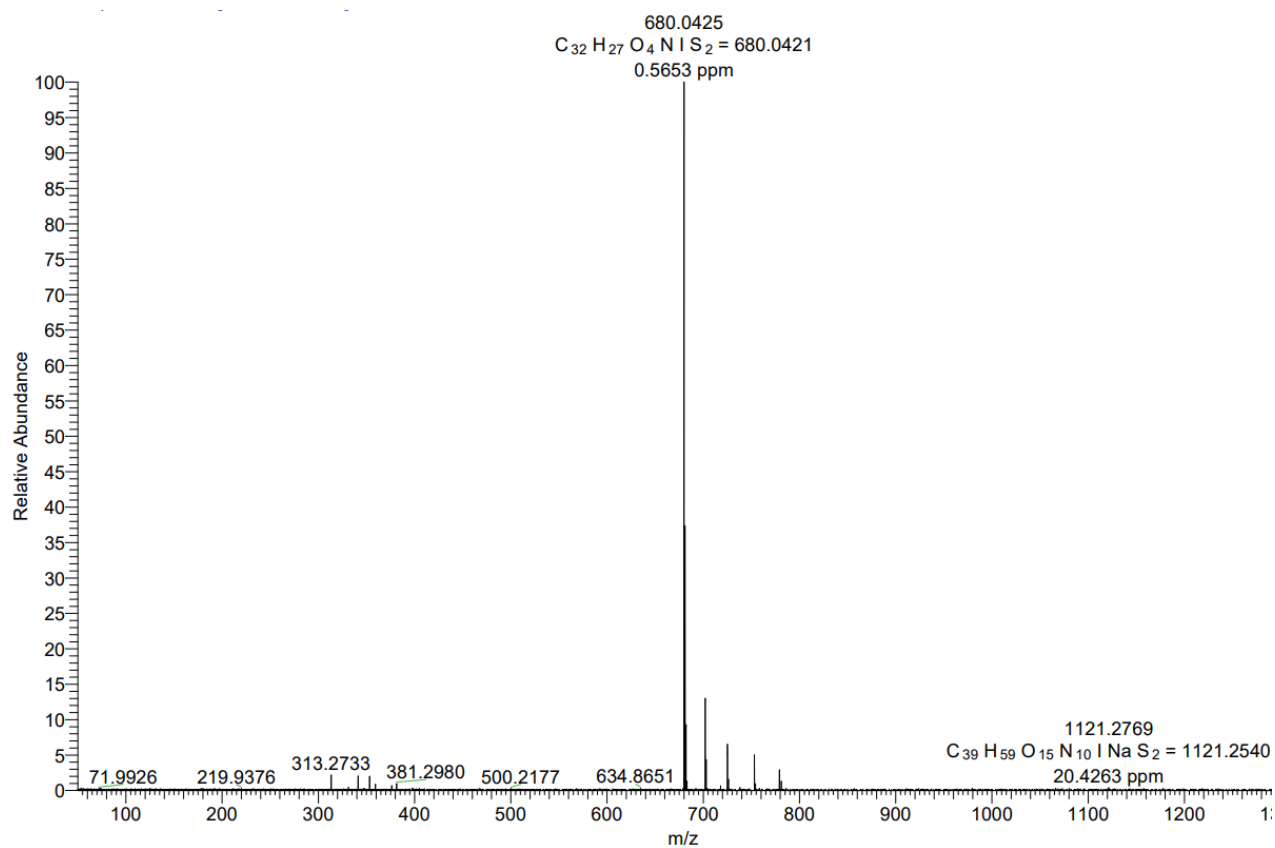
(*E*)-1-(2-iodophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



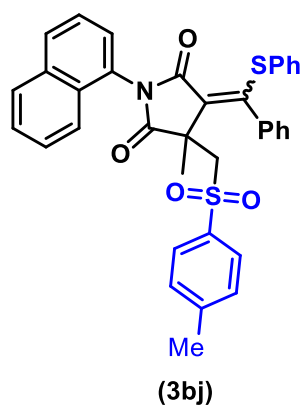
HRMS spectrum of 3bi



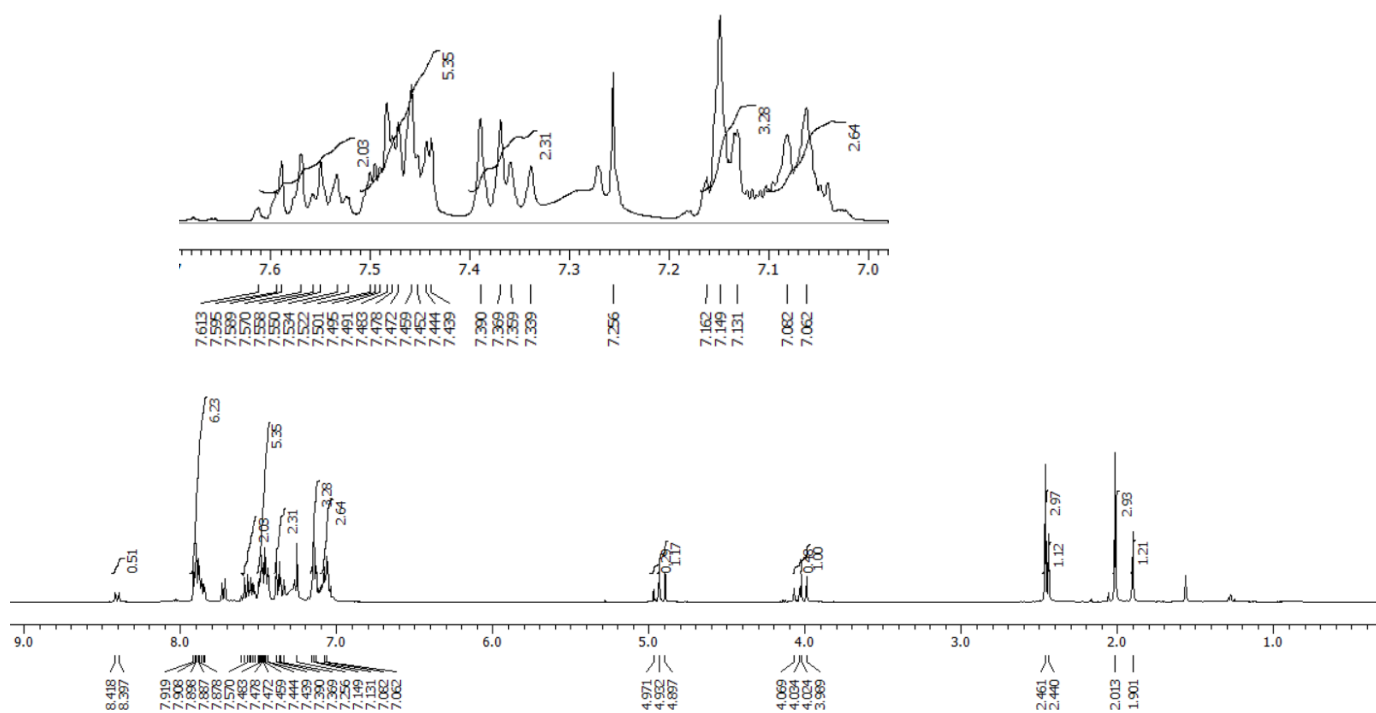
(E)-1-(2-iodophenyl)-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



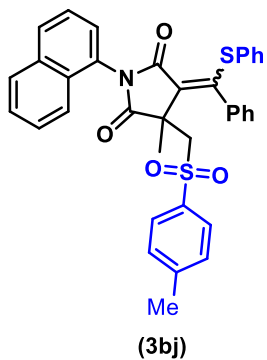
¹H NMR spectrum of 3bj (400 MHz, CDCl₃)



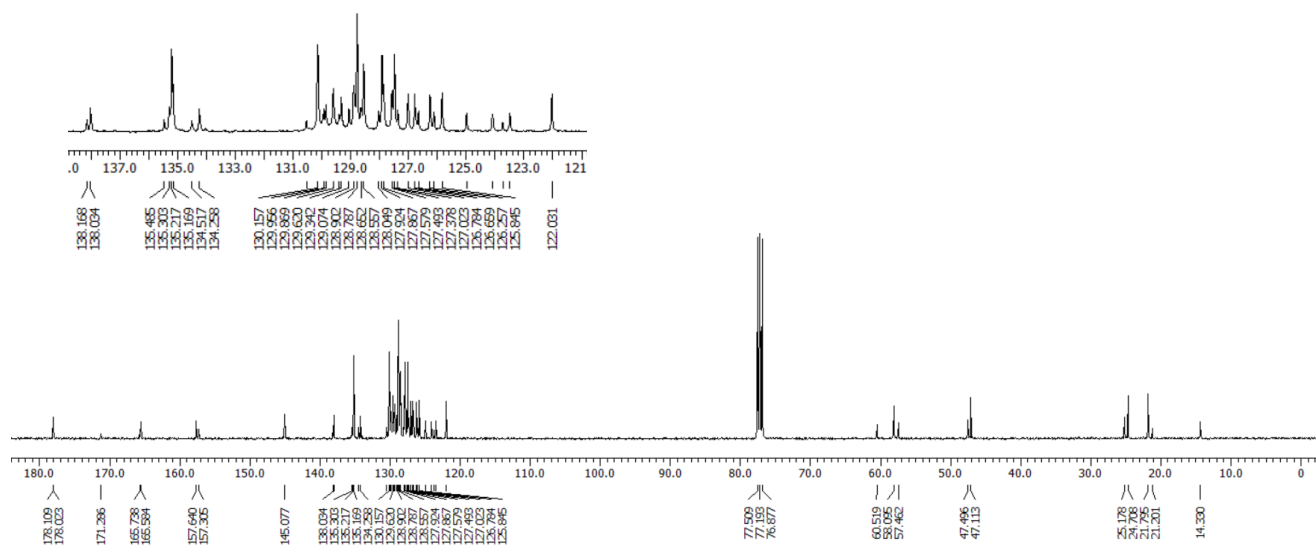
3-methyl-1-(naphthalen-1-yl)-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



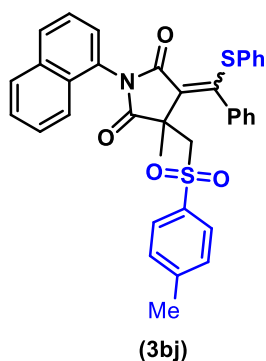
¹³C NMR spectrum of 3bj (100 MHz, CDCl₃)



3-methyl-1-(naphthalen-1-yl)-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS spectrum of 3bj



3-methyl-1-(naphthalen-1-yl)-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

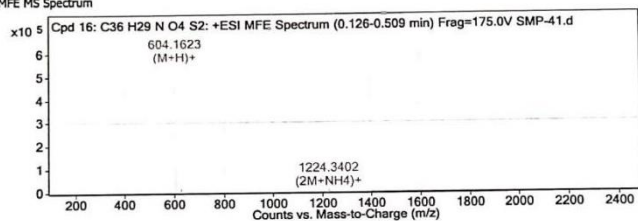
Data File	SMP-41.d	Sample Name	SMP-41
Sample Type	Sample	Position	P1-A6
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	28-04-2022 10:51:11
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125)		

Compound Table

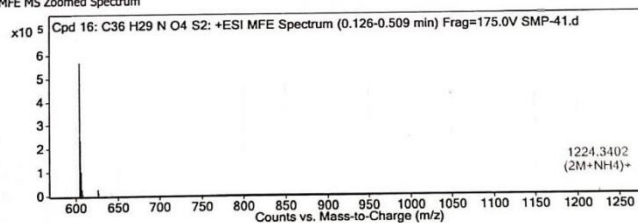
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C ₃₆ H ₂₉ N O ₄ S ₂	0.197	603.155	C ₃₆ H ₂₉ N O ₄ S ₂	C ₃₆ H ₂₉ N O ₄ S ₂	-2.05	C ₃₆ H ₂₉ N O ₄ S ₂

Compound Label	m/z	RT	Algorithm	Mass
Cpd 16: C ₃₆ H ₂₉ N O ₄ S ₂	604.1623	0.197	Find by Molecular Feature	603.155

MFE MS Spectrum



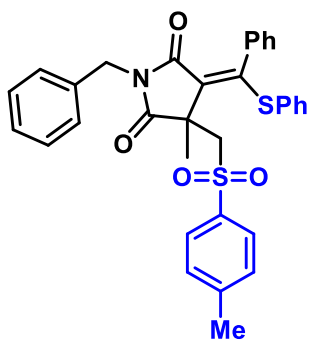
MFE MS Zoomed Spectrum



MS Spectrum Peak List

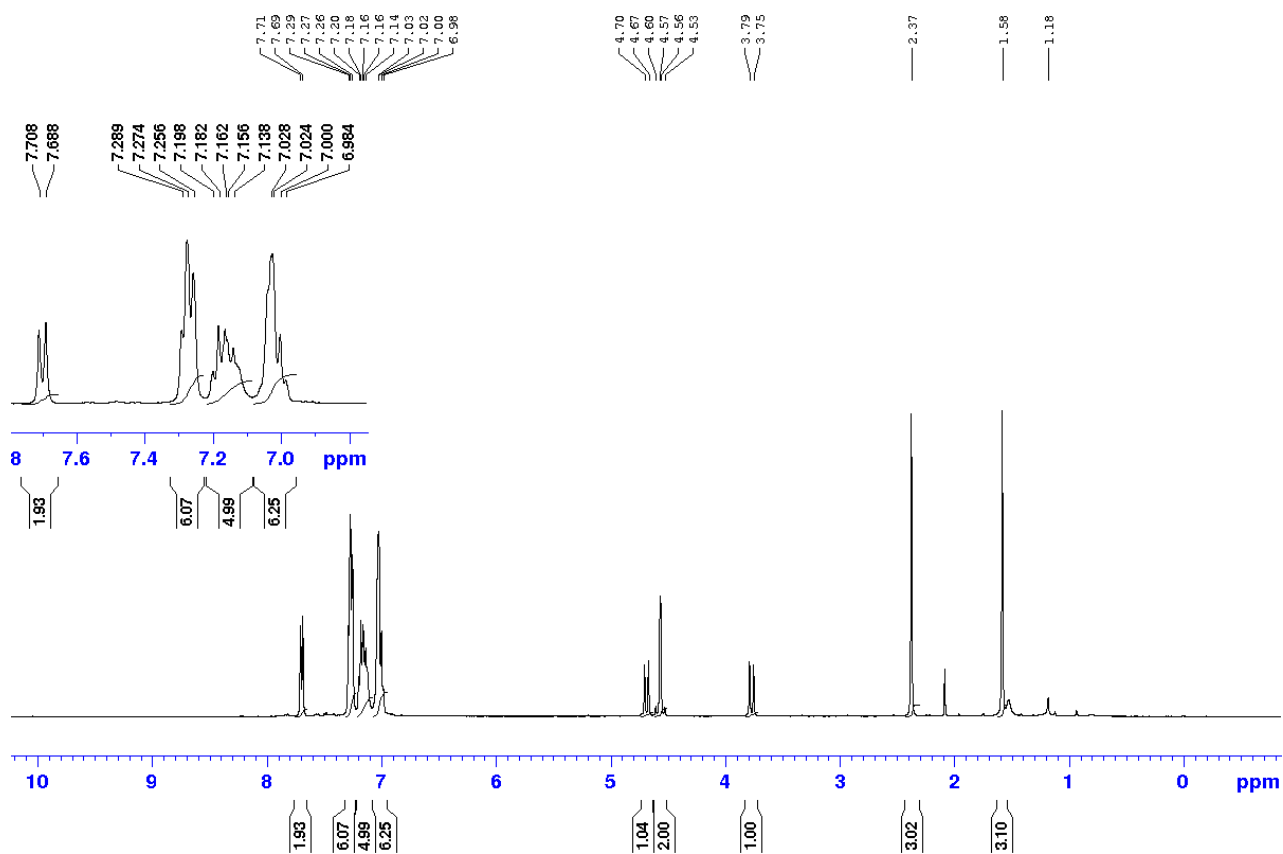
m/z	z	Abund	Formula	Ion
604.1623	1	579030.63	C ₃₆ H ₃₀ N O ₄ S ₂	(M+H)+
605.1652	1	232107.23	C ₃₆ H ₃₀ N O ₄ S ₂	(M+H)+
606.1638	1	96581.18	C ₃₆ H ₃₀ N O ₄ S ₂	(M+H)+
607.1653	1	27481.75	C ₃₆ H ₃₀ N O ₄ S ₂	(M+H)+
608.1664	1	6773.76	C ₃₆ H ₃₀ N O ₄ S ₂	(M+H)+
626.144	1	27243.95	C ₃₆ H ₂₉ N Na O ₄ S ₂	(M+Na)+
627.1469	1	12238.35	C ₃₆ H ₂₉ N Na O ₄ S ₂	(M+Na)+
642.1206	1	9460.14		(M+K)+
1224.3402	1	11070.97		(2M+NH ₄)+
1225.3437	1	8821.13		(2M+NH ₄)+

¹H NMR spectrum of 3bk (400 MHz, CDCl₃)

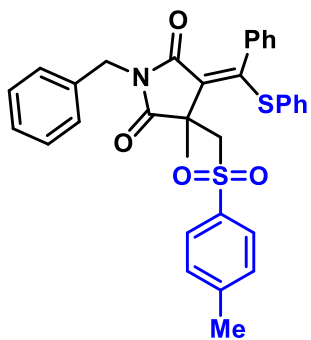


(3bk)

(E)-1-benzyl-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

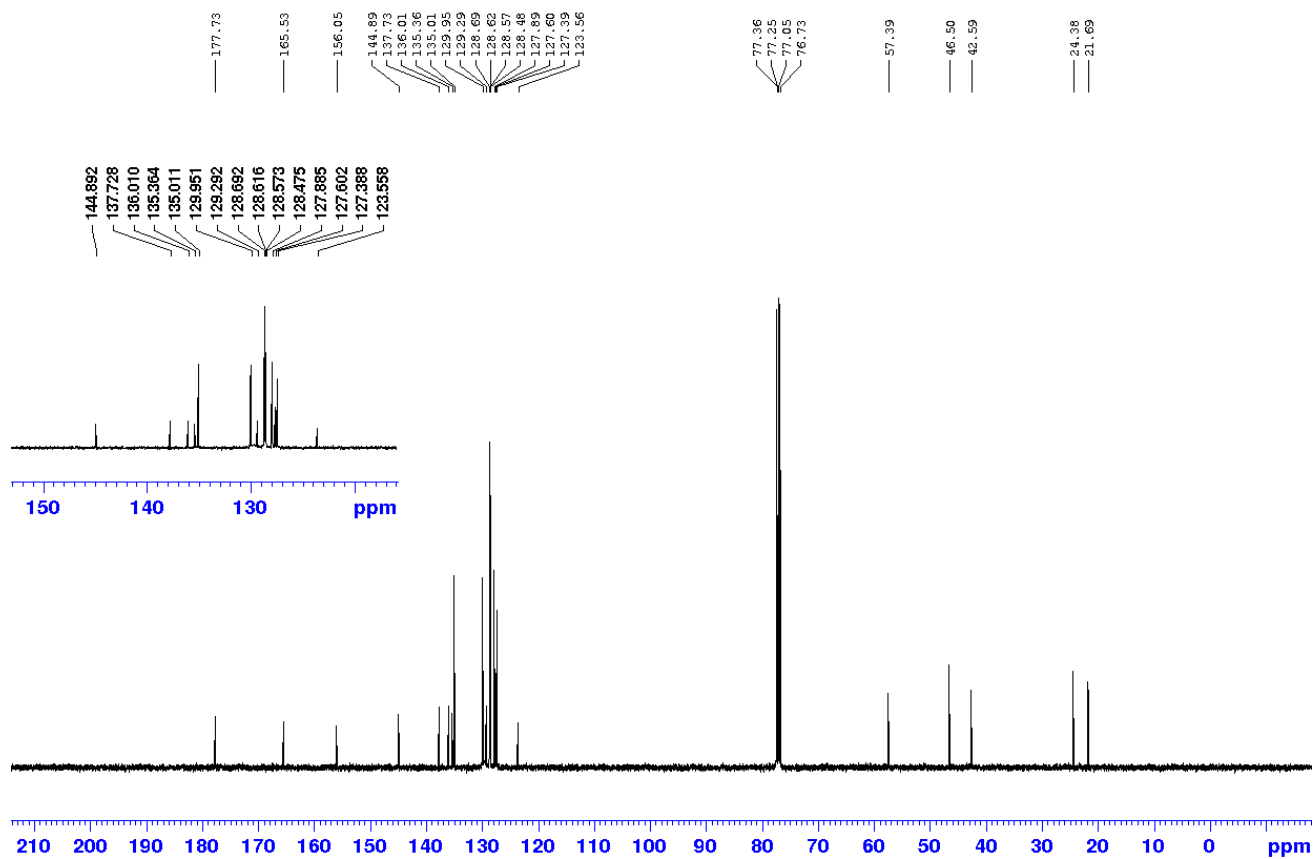


^{13}C NMR spectrum of 3bk (100 MHz, CDCl_3)

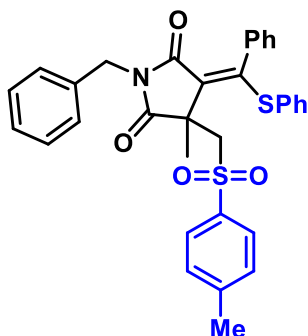


(3bk)

(*E*)-1-benzyl-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS spectrum of 3bk



(3bk)

(E)-1-benzyl-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

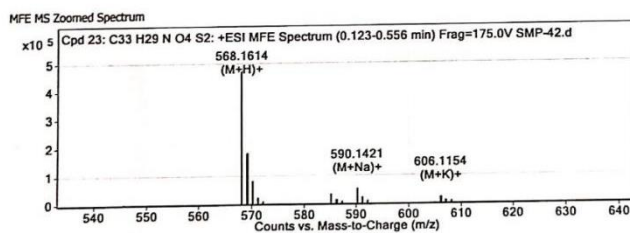
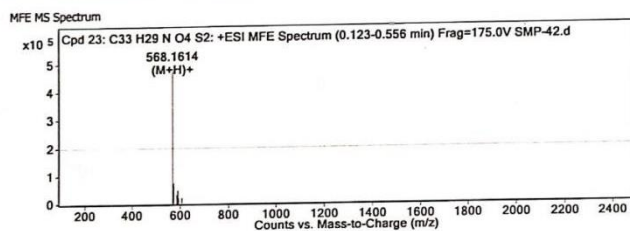
Qualitative Compound Report

Data File SMP-42.d Sample Name SMP-42
 Sample Type Sample Position P1-A5
 Instrument Name Instrument 1 User Name
 Acq Method MS Scan.m Acquired Time 02-05-2022 11:39:06
 IRM Calibration Status Success DA Method Default.m
 Comment

Sample Group Info. 3
 Acquisition SW 6200 series TOF/6500 series
 Version Q-TOF B.05.01 (B5125)

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 23: C33 H29 N O4 S2	0.204	567.1538	C33 H29 N O4 S2	C33 H29 N O4 S2	-0.05	C33 H29 N O4 S2

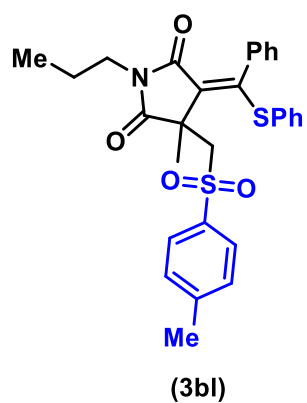
Compound Label	m/z	RT	Algorithm	Mass
Cpd 23: C33 H29 N O4 S2	568.1614	0.204	Find by Molecular Feature	567.1538



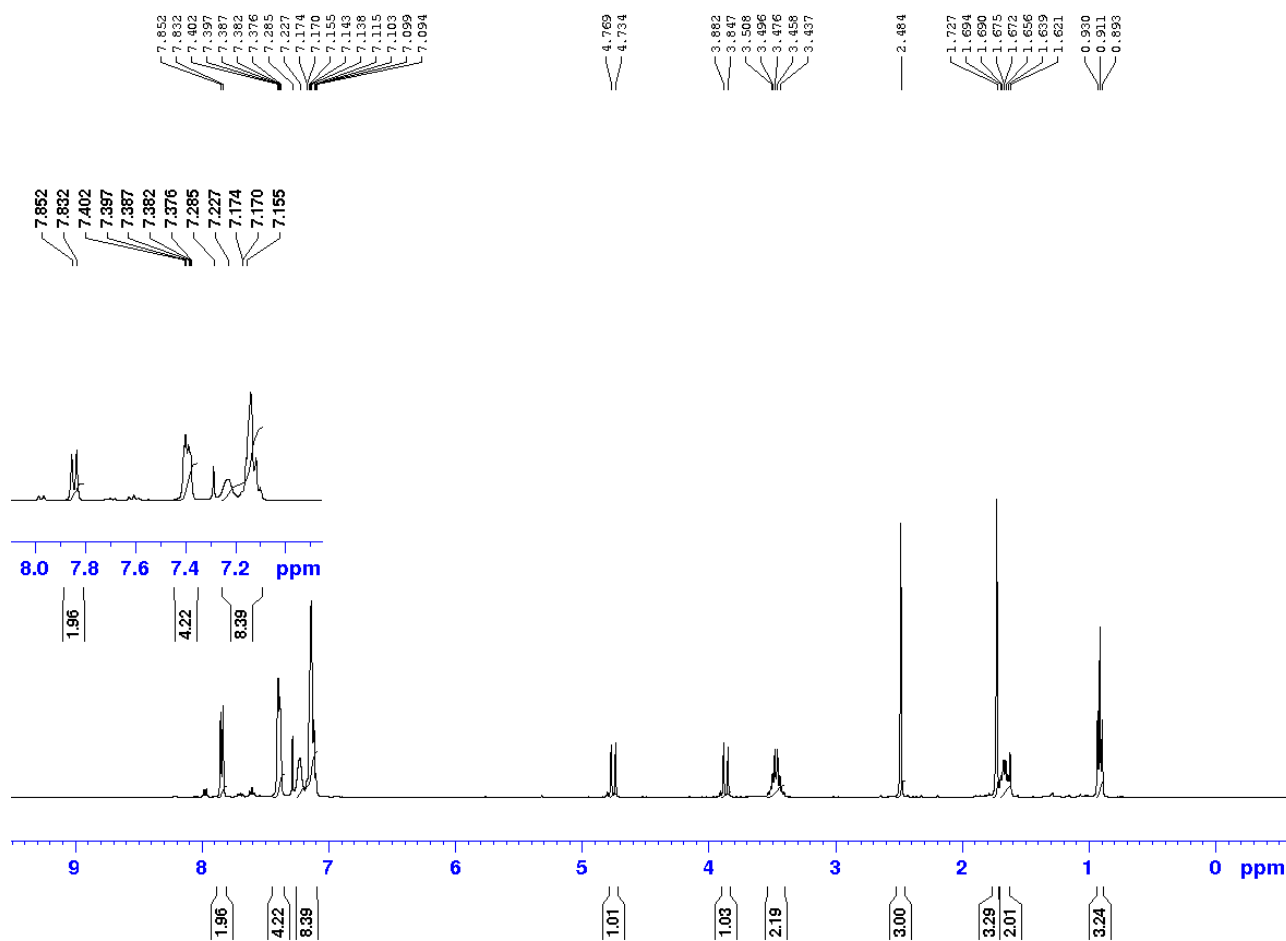
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
568.1614	1	475761.41	C33 H30 N O4 S2	(M+H)+
569.1641	1	175481.3	C33 H30 N O4 S2	(M+H)+
570.1611	1	74361.71	C33 H30 N O4 S2	(M+H)+
571.1611	1	21925.35	C33 H30 N O4 S2	(M+H)+
585.1861	1	30009.82	C33 H33 N2 O4 S2	(M+NH4)+
586.1899	1	12226.39	C33 H33 N2 O4 S2	(M+NH4)+
590.1421	1	49186.74	C33 H29 N Na O4 S2	(M+Na)+
591.1455	1	19545.25	C33 H29 N Na O4 S2	(M+Na)+
592.1395	1	9372.95	C33 H29 N Na O4 S2	(M+Na)+
606.1154	1	19620.28	C33 H29 K N O4 S2	(M+K)+

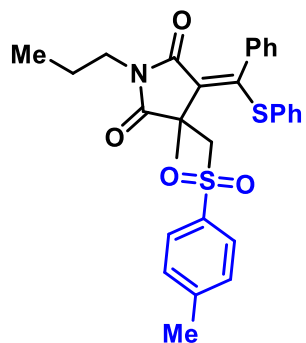
¹H NMR spectrum of 3bl (400 MHz, CDCl₃)



(E)-3-methyl-4-(phenyl(phenylthio)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione

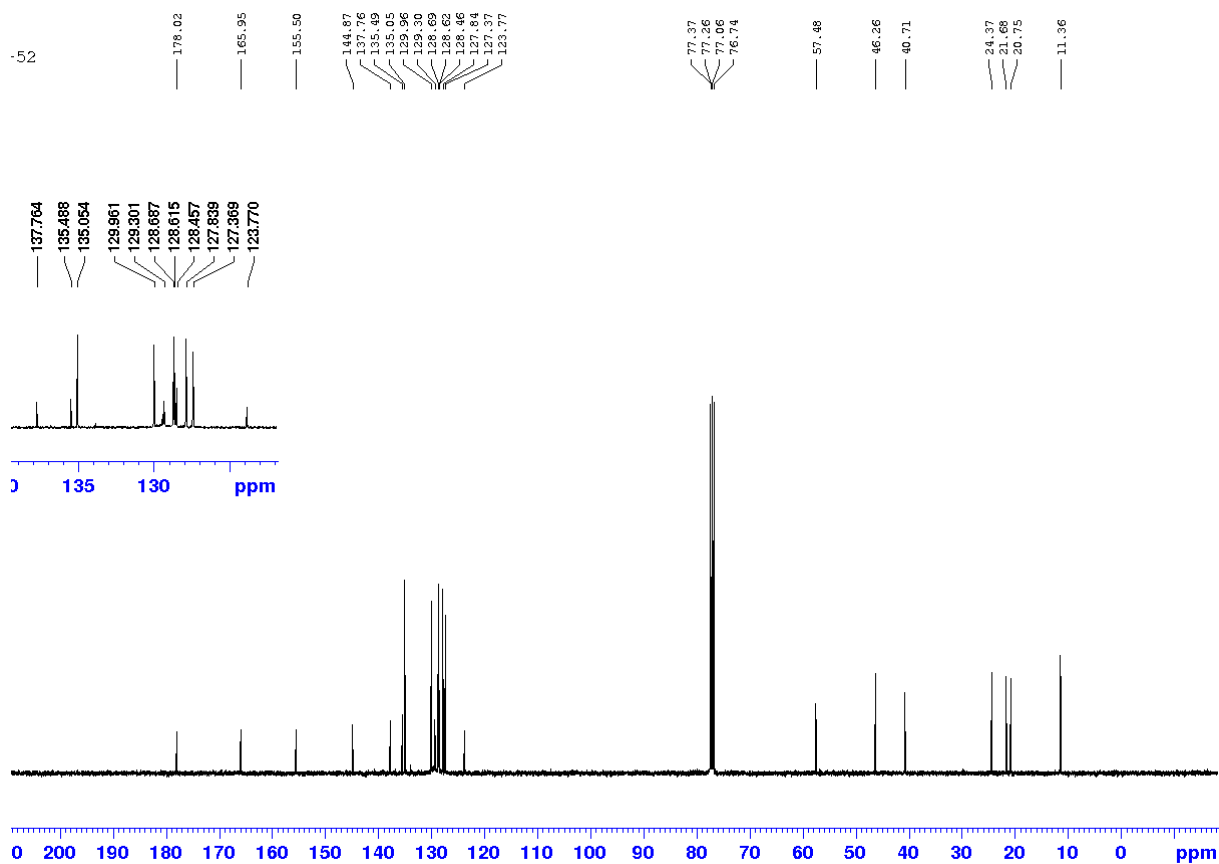


¹³C NMR spectrum of 3bl (100 MHz, CDCl₃)

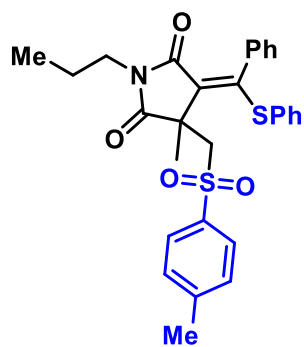


(3bl)

(*E*)-3-methyl-4-(phenyl(phenylthio)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS spectrum of 3bl



(3bl)

(E)-3-methyl-4-(phenyl(phenylthio)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

Data File	SMP-52.d	Sample Name	SMP-52
Sample Type	Sample	Position	PI-B1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	21-05-2022 12:30:30
IRM Calibration Status	Success	DA Method	Default.m
Comment			

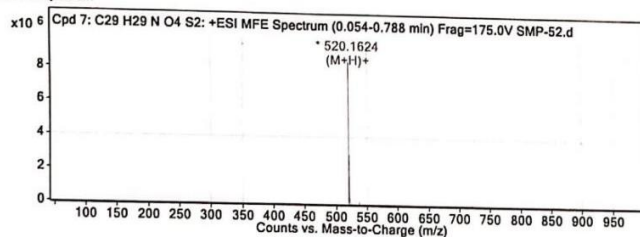
Sample Group	Info.	3
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

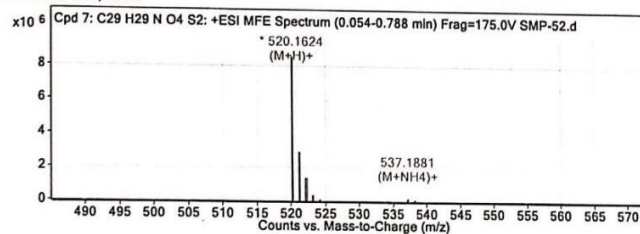
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C ₂₉ H ₂₉ N O ₄ S ₂	0.185	519.1553	C ₂₉ H ₂₉ N O ₄ S ₂	C ₂₉ H ₂₉ N O ₄ S ₂	-2.86	C ₂₉ H ₂₉ N O ₄ S ₂

Compound Label	m/z	RT	Algorithm	Mass
Cpd 7: C ₂₉ H ₂₉ N O ₄ S ₂	520.1624	0.185	Find by Molecular Feature	519.1553

MFE MS Spectrum



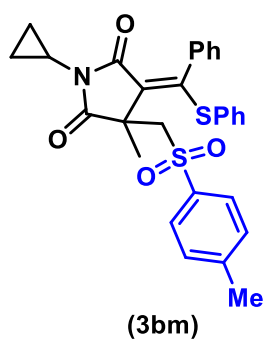
MFE MS Zoomed Spectrum



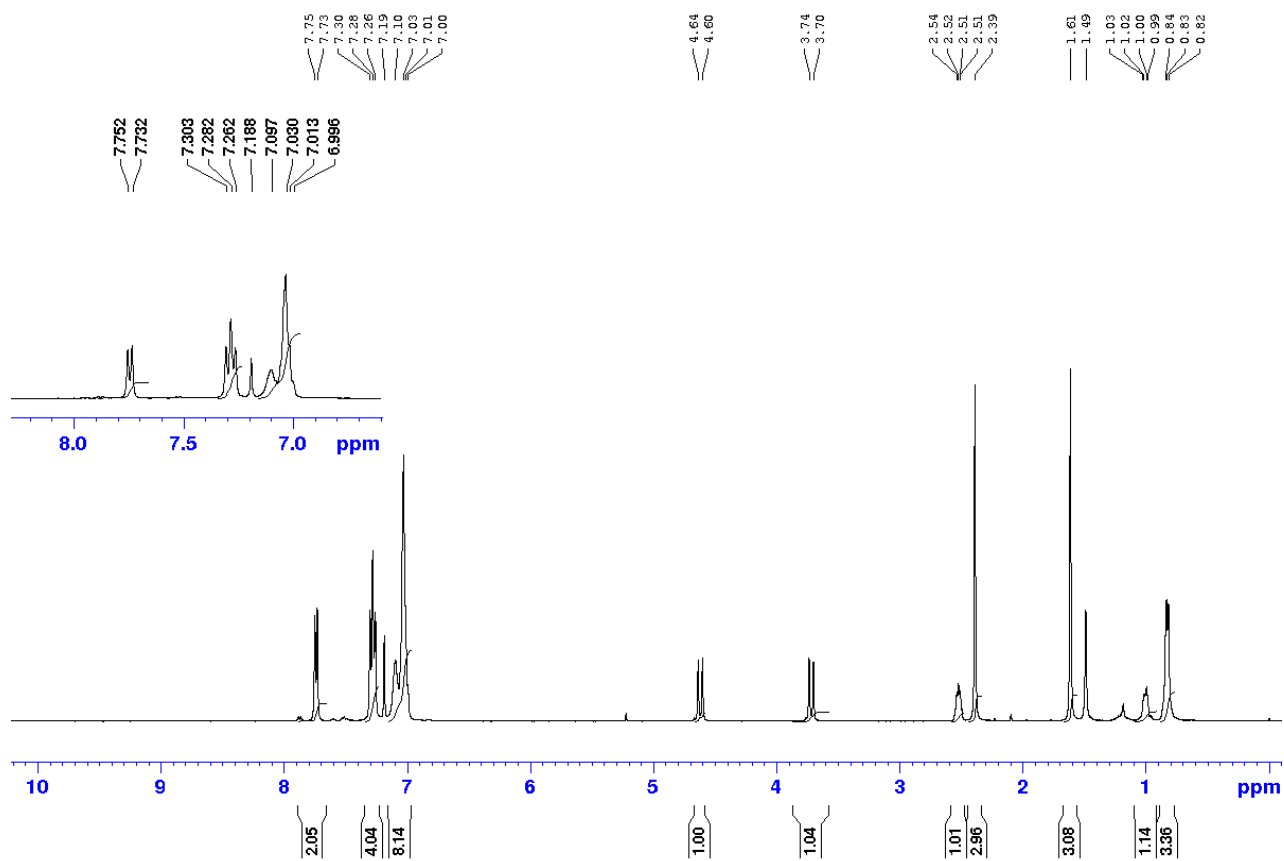
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
520.1624	1	8535982	C ₂₉ H ₃₀ N O ₄ S ₂	(M+H)+
521.1657	1	2929043.6	C ₂₉ H ₃₀ N O ₄ S ₂	(M+H)+
522.1635	1	1270176.8	C ₂₉ H ₃₀ N O ₄ S ₂	(M+H)+
523.1641	1	303783.66	C ₂₉ H ₃₀ N O ₄ S ₂	(M+H)+
524.1627	1	64535.73	C ₂₉ H ₃₀ N O ₄ S ₂	(M+H)+
525.1617	1	10146.59	C ₂₉ H ₃₀ N O ₄ S ₂	(M+H)+
526.163	1	2280.58	C ₂₉ H ₃₀ N O ₄ S ₂	(M+H)+
537.1881	1	111329.6	C ₂₉ H ₃₃ N ₂ O ₄ S ₂	(M+NH ₄)+
538.1908	1	34077.82	C ₂₉ H ₃₃ N ₂ O ₄ S ₂	(M+NH ₄)+

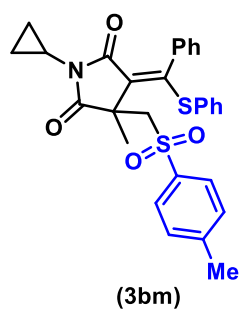
¹H NMR spectrum of 3bm (400 MHz, CDCl₃)



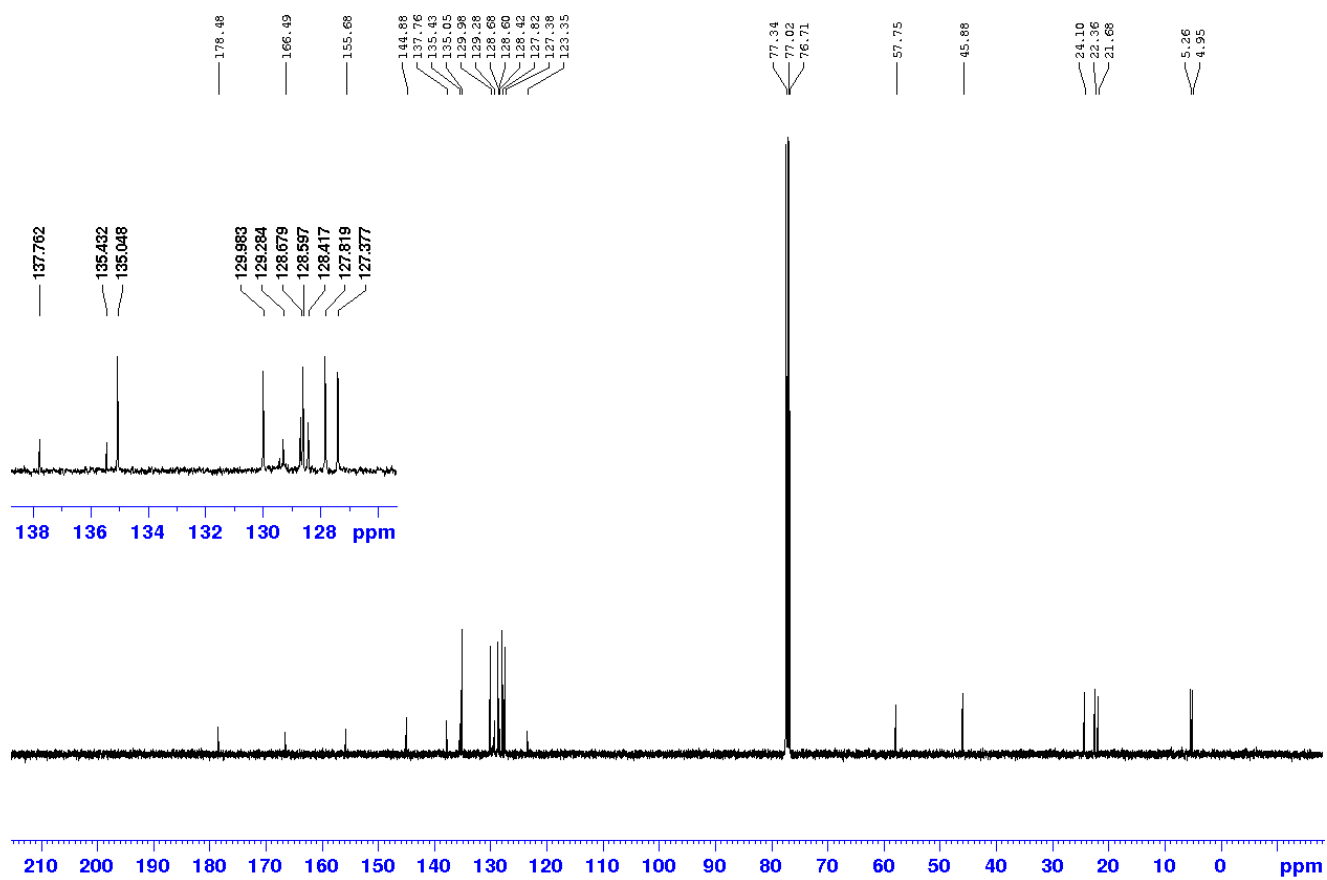
(E)-1-cyclopropyl-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



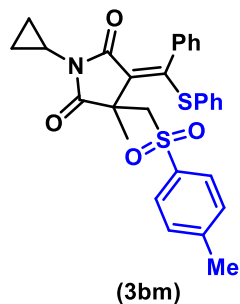
^{13}C NMR spectrum of 3bm (100 MHz, CDCl_3)



(E)-1-cyclopropyl-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3bm



(E)-1-cyclopropyl-3-methyl-4-(phenyl(phenylthio)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

Data File	SMP-47.d	Sample Name	SMP-47
Sample Type	Sample	Position	P1-A1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	02-05-2022 11:32:08
IRM Calibration Status	Success	DA Method	Default.m
Comment			

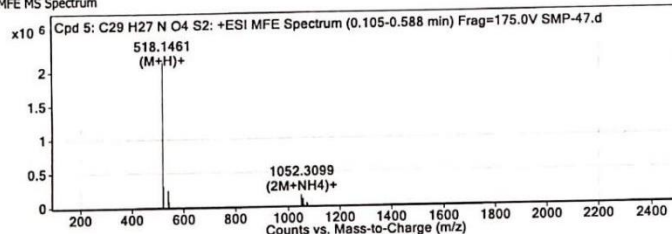
Sample Group	Info.	3
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

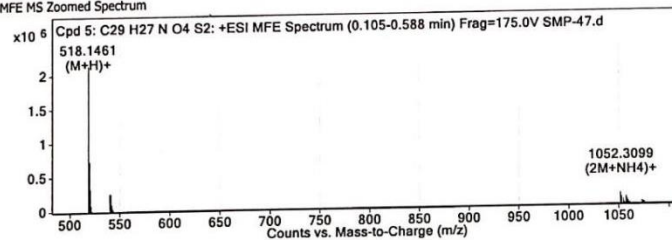
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C ₂₉ H ₂₇ N O ₄ S ₂	0.201	517.1388	C ₂₉ H ₂₇ N O ₄ S ₂	C ₂₉ H ₂₇ N O ₄ S ₂	-1.32	C ₂₉ H ₂₇ N O ₄ S ₂

Compound Label	m/z	RT	Algorithm	Mass
Cpd 5: C ₂₉ H ₂₇ N O ₄ S ₂	518.1461	0.201	Find by Molecular Feature	517.1388

MFE MS Spectrum



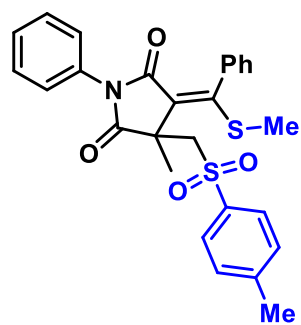
MFE MS Zoomed Spectrum



MS Spectrum Peak List

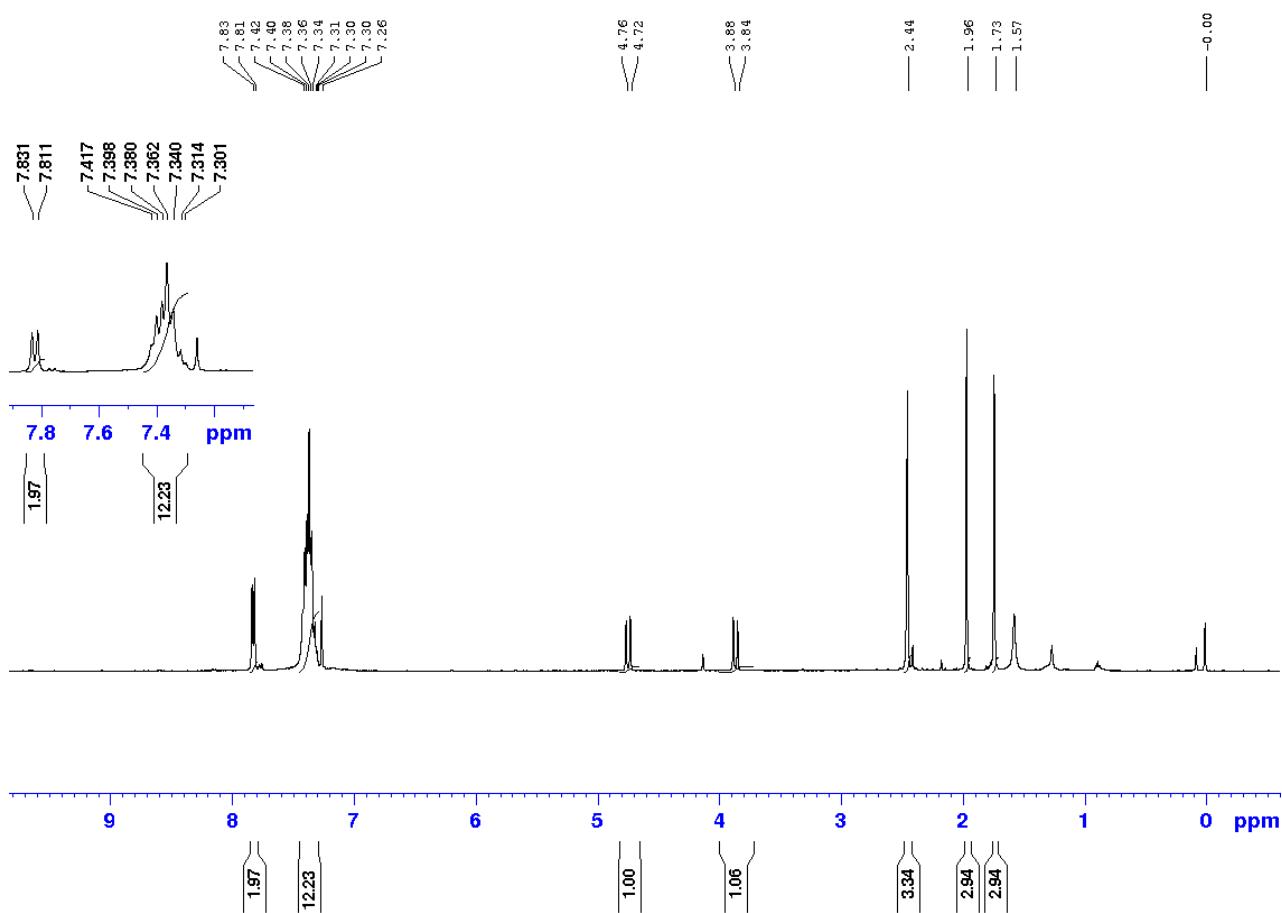
m/z	z	Abund	Formula	Ion
518.1461	1	2141317.75	C ₂₉ H ₂₈ N O ₄ S ₂	(M+H)+
519.1493	1	732881.95	C ₂₉ H ₂₈ N O ₄ S ₂	(M+H)+
520.1462	1	307246.26	C ₂₉ H ₂₈ N O ₄ S ₂	(M+H)+
521.147	1	74109.12	C ₂₉ H ₂₈ N O ₄ S ₂	(M+H)+
540.1278	1	249084.36	C ₂₉ H ₂₇ N Na O ₄ S ₂	(M+Na)+
541.1305	1	82245.06	C ₂₉ H ₂₇ N Na O ₄ S ₂	(M+Na)+
1052.3099	1	157159.11		(2M+NH ₄)+
1053.3126	1	106410.59		(2M+NH ₄)+
1057.2659	1	102381.66		(2M+Na)+
1058.2685	1	67179.77		(2M+Na)+

¹H NMR spectrum of 3ca (400 MHz, CDCl₃)

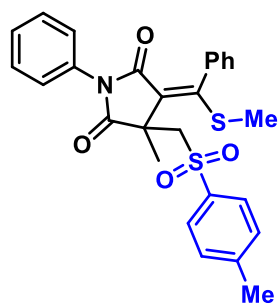


(3ca)

(*E*)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione

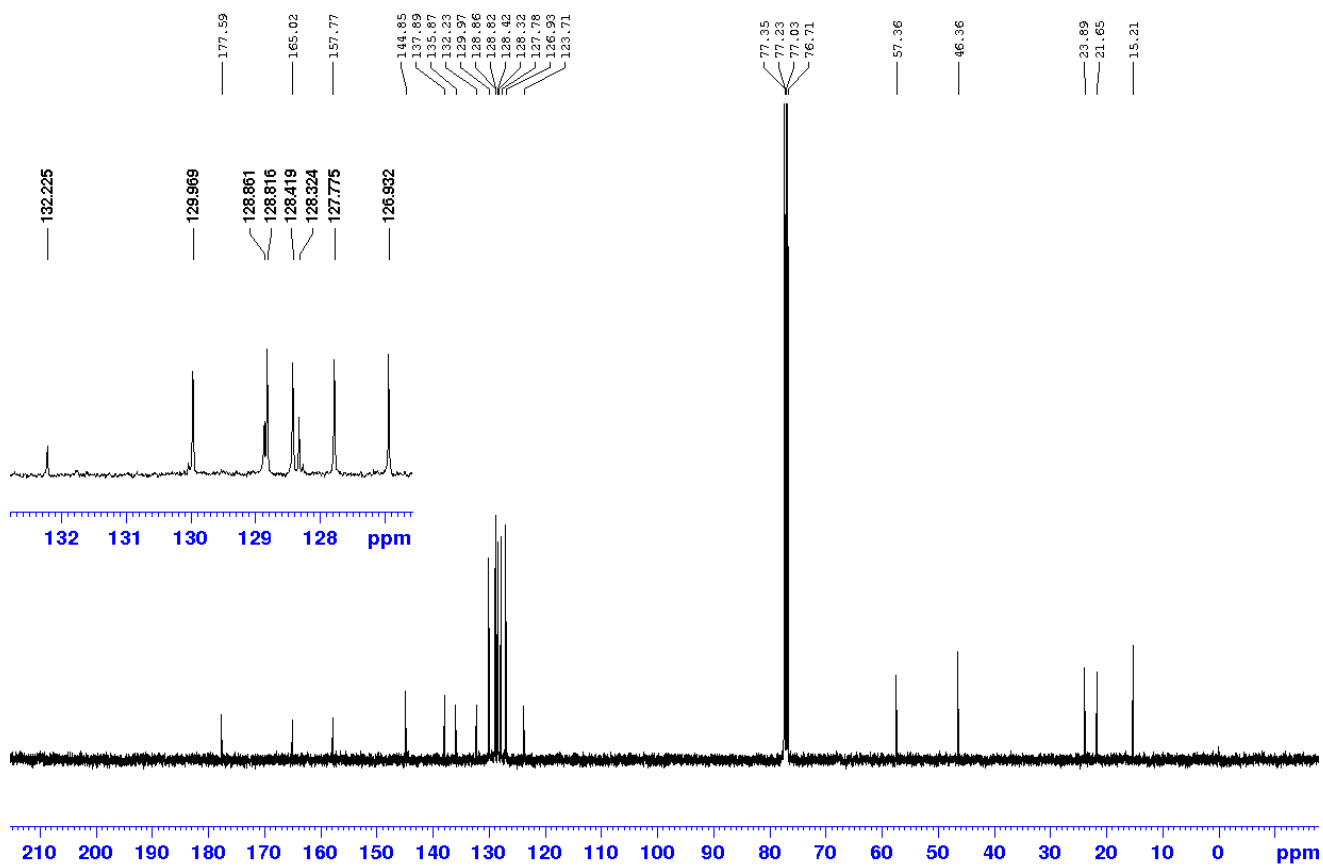


¹³C NMR spectrum of 3ca (100 MHz, CDCl₃)

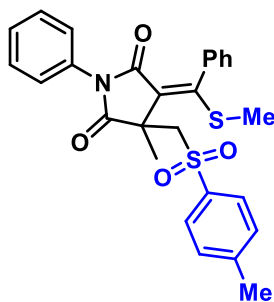


(3ca)

(E)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3ca



(3ca)

(E)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

Data File	SMD-6.d	Sample Name	SMD-6
Sample Type	Sample	Position	P1-C1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	26-05-2022 14:52:09
IRM Calibration Status	Success	DA Method	Default.m
Comment			

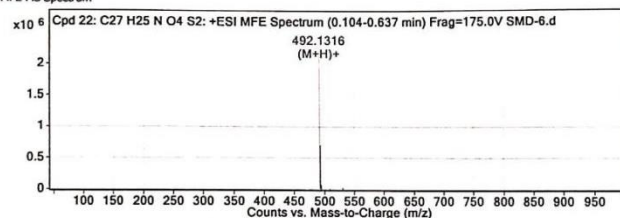
Sample Group		Info.	3
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (85125)		

Compound Table

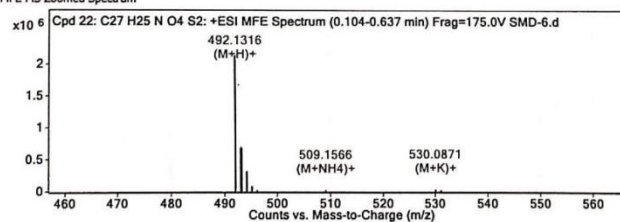
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C27 H25 N O4 S2	0.175	491.1243	C27 H25 N O4 S2	C27 H25 N O4 S2	-3.7	C27 H25 N O4 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 22: C27 H25 N O4 S2	492.1316	0.175	Find by Molecular Feature	491.1243

MFE MS Spectrum



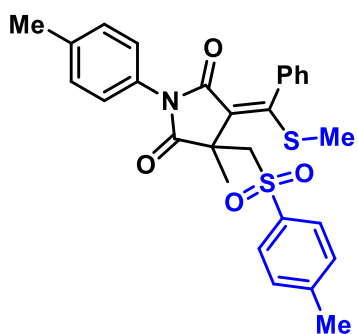
MFE MS Zoomed Spectrum



MS Spectrum Peak List

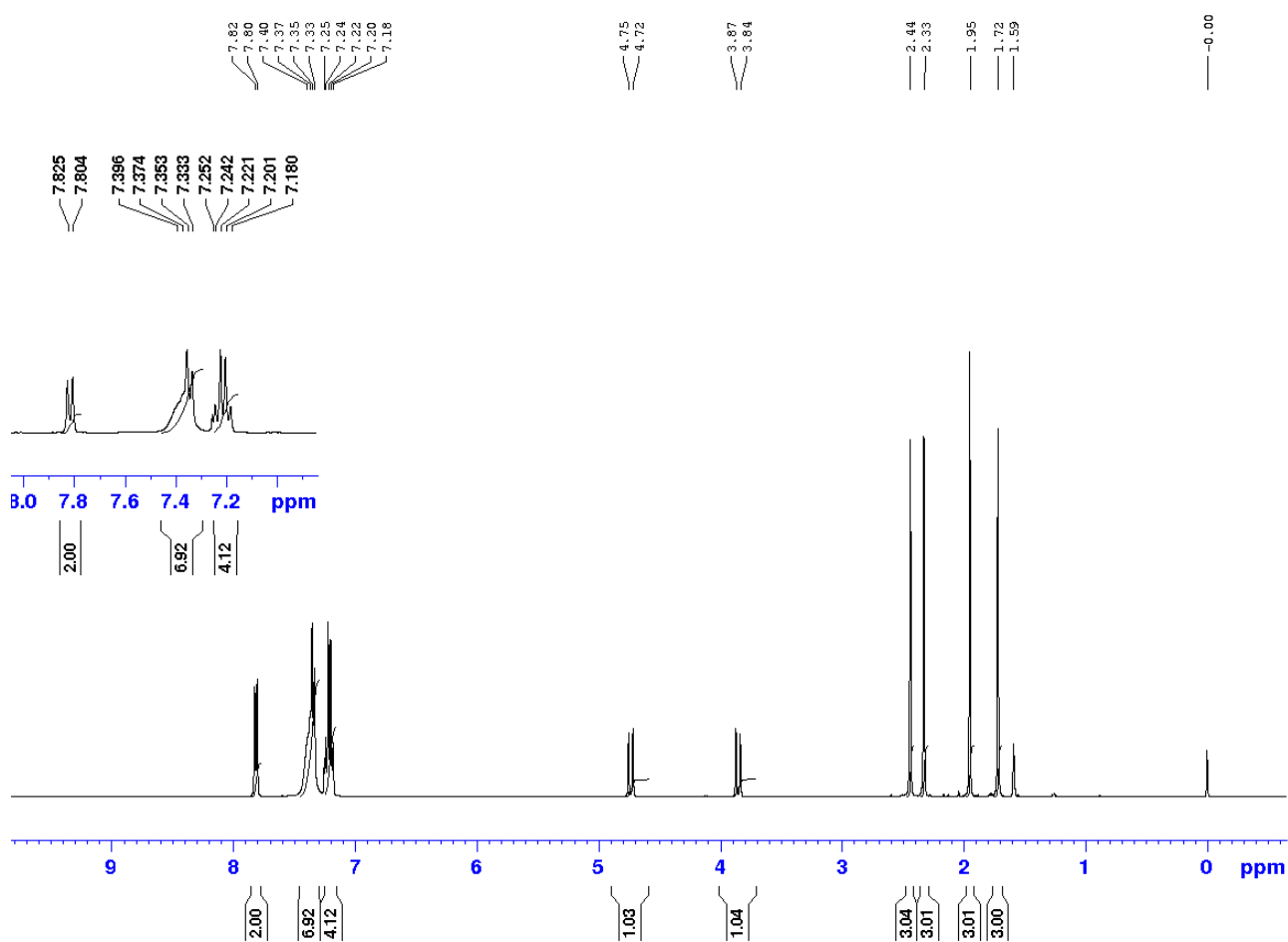
m/z	z	Abund	Formula	Ion
492.1316	1	2150319.5	C27 H26 N O4 S2	(M+H)+
493.1347	1	705296.08	C27 H26 N O4 S2	(M+H)+
494.1315	1	294695.24	C27 H26 N O4 S2	(M+H)+
495.1323	1	66303.24	C27 H26 N O4 S2	(M+H)+
496.1316	1	15138.21	C27 H26 N O4 S2	(M+H)+
509.1566	1	18154.05	C27 H29 N2 O4 S2	(M+NH4)+
510.1594	1	6097.5	C27 H29 N2 O4 S2	(M+NH4)+
530.0871	1	27806.61	C27 H25 K N O4 S2	(M+K)+
531.0906	1	9037.55	C27 H25 K N O4 S2	(M+K)+
532.0882	1	5841.85	C27 H25 K N O4 S2	(M+K)+

¹H NMR spectrum of 3cb (400 MHz, CDCl₃)

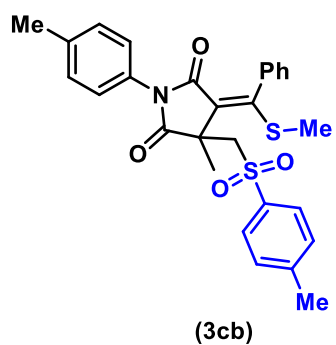


(3cb)

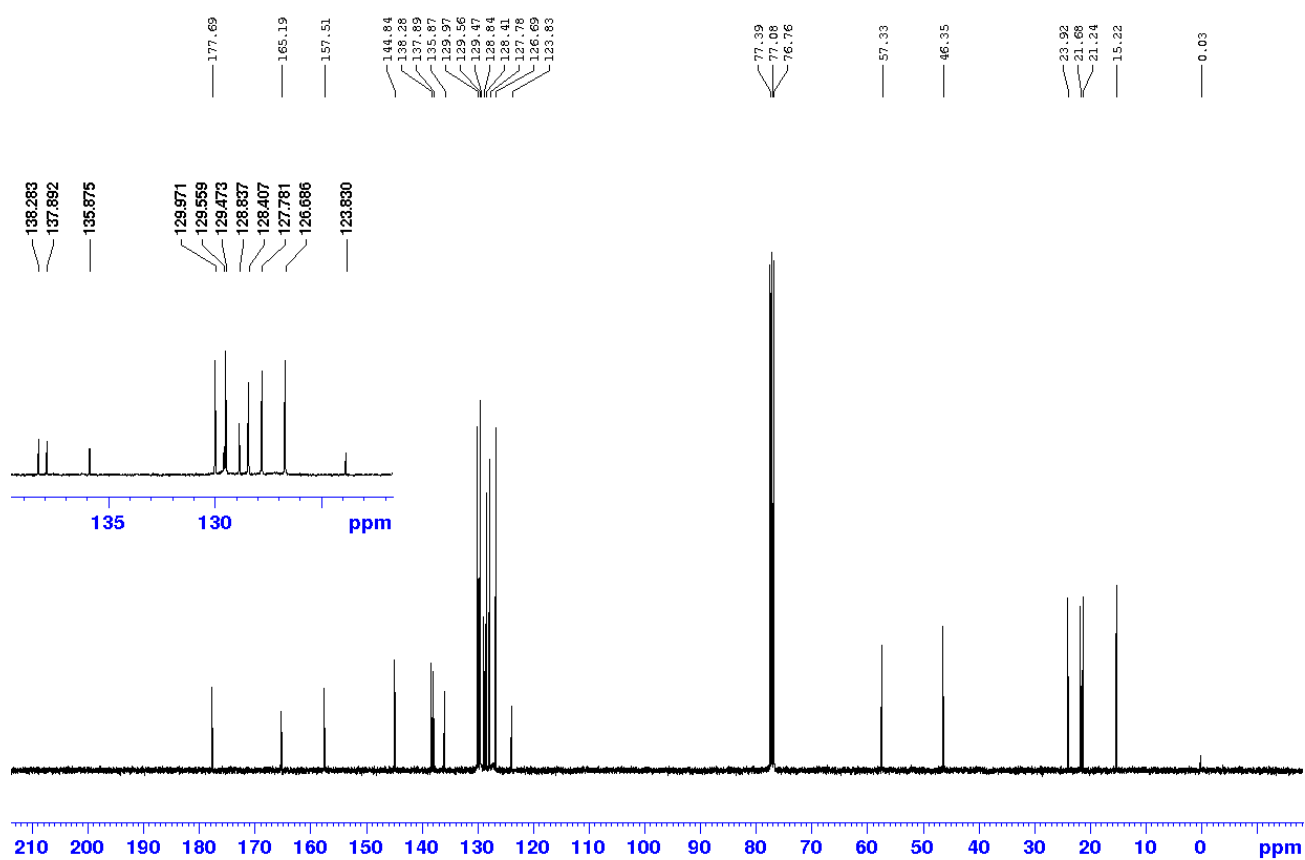
(*E*)-3-methyl-4-((methylthio)(phenyl)methylene)-1-(*p*-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione



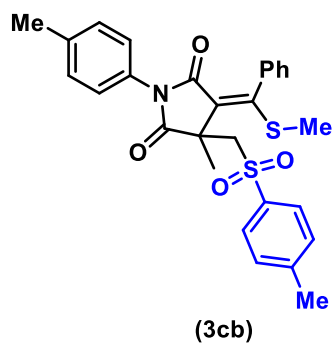
¹³C NMR spectrum of 3cb (100 MHz, CDCl₃)



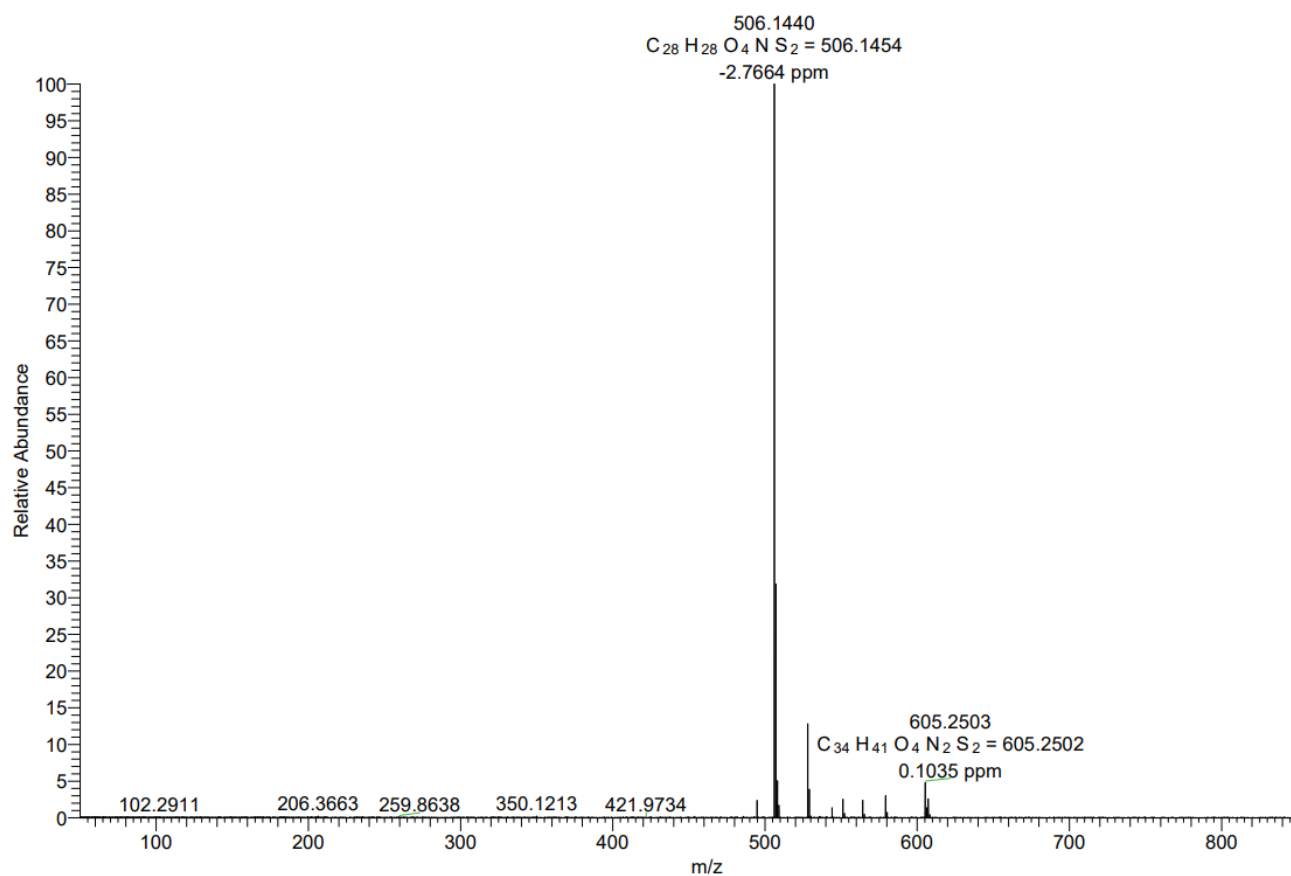
(E)-3-methyl-4-((methylthio)(phenyl)methylene)-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione



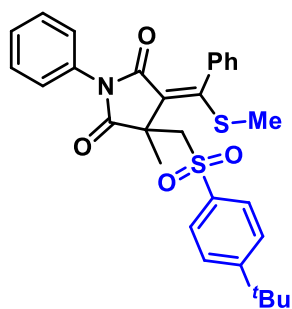
HRMS Spectrum of 3cb



(E)-3-methyl-4-((methylthio)(phenyl)methylene)-1-(*p*-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione

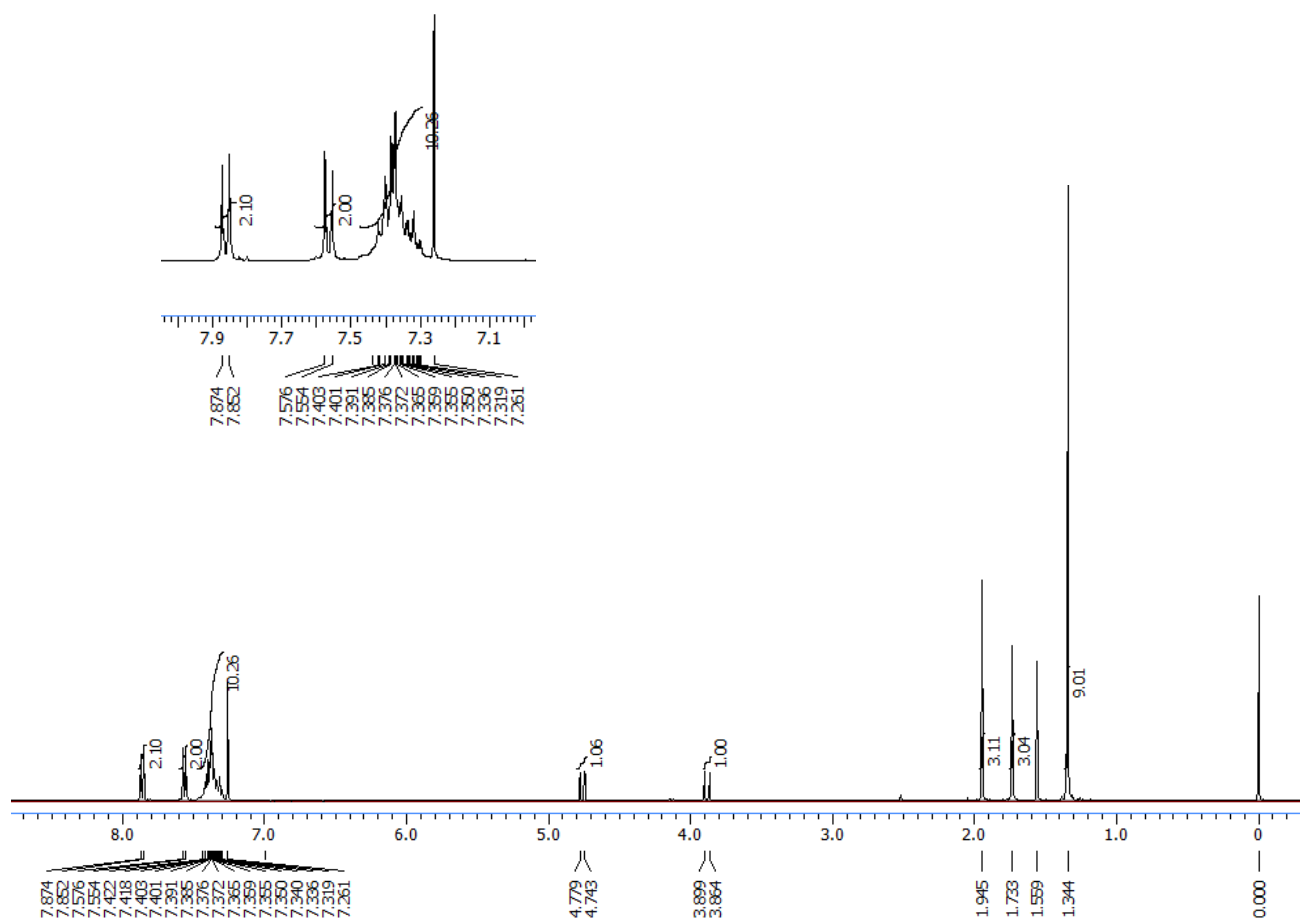


¹H NMR spectrum of 3cc (400 MHz, CDCl₃)

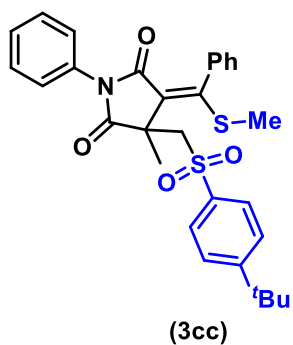


(3cc)

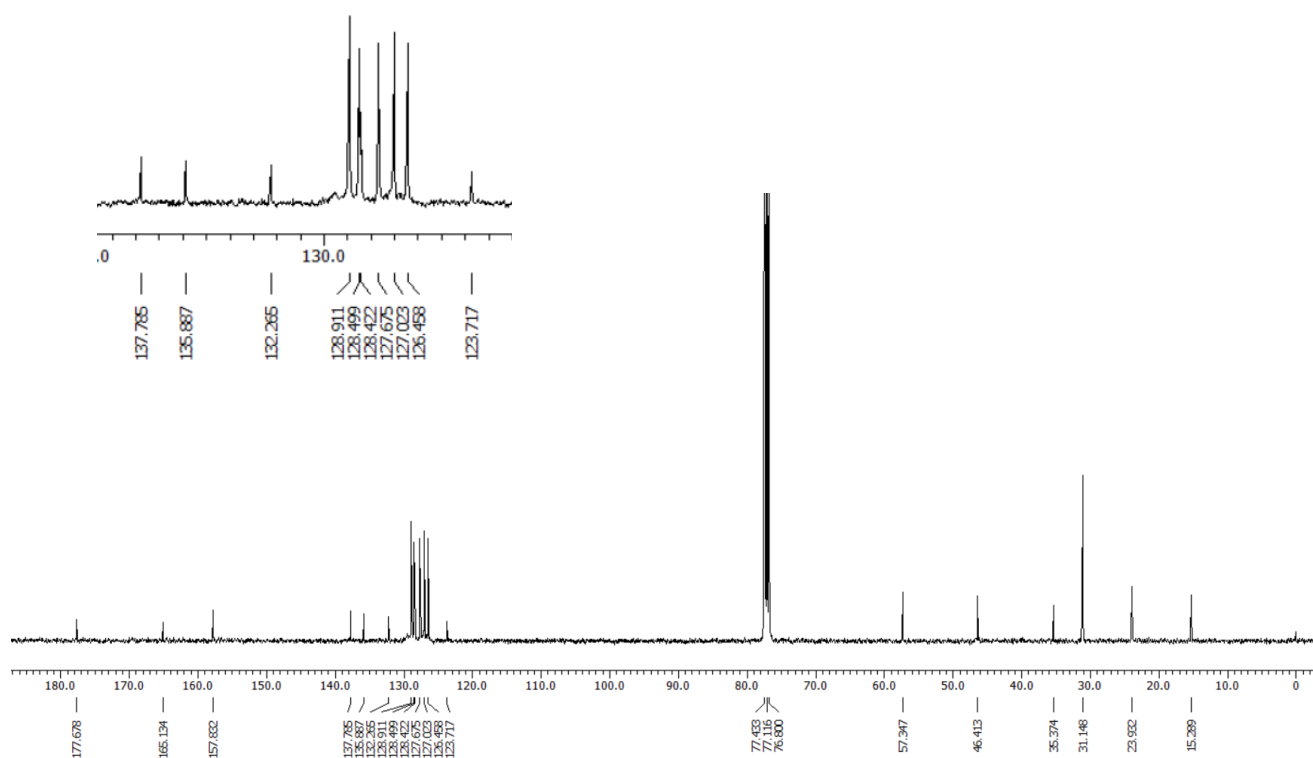
(E)-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenylpyrrolidine-2,5-dione



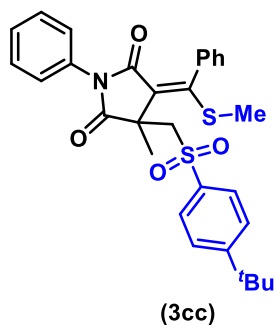
¹³C NMR spectrum of 3cc (100 MHz, CDCl₃)



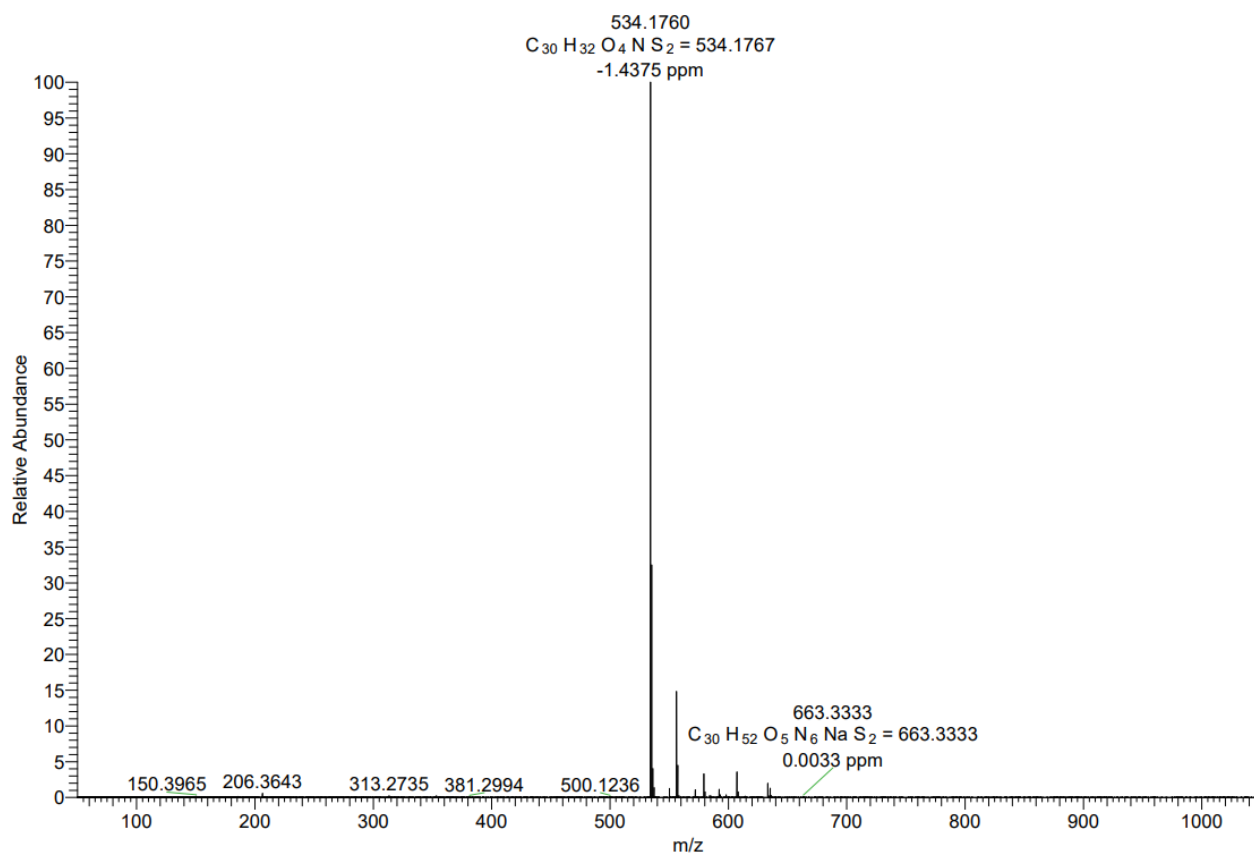
(E)-3-(((4-*tert*-butyl)phenyl)sulfonyl)methyl)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenylpyrrolidine-2,5-dione



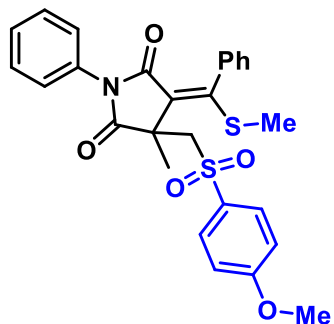
HRMS spectrum of 3cc



(E)-3-(((4-(tert-butyl)phenyl)sulfonyl)methyl)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenylpyrrolidine-2,5-dione

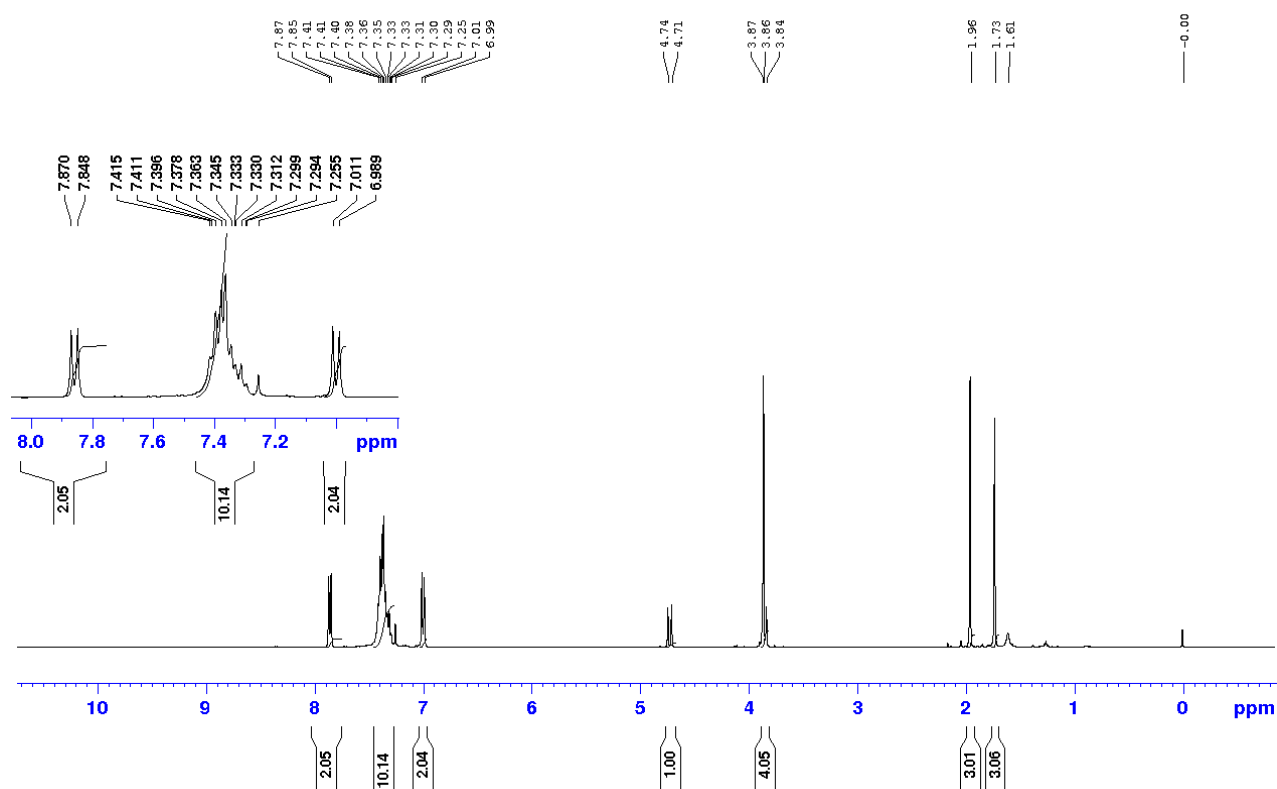


¹H NMR spectrum of 3cd (400 MHz, CDCl₃)

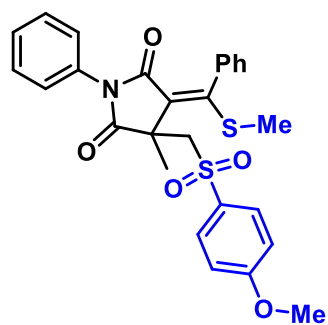


(3cd)

(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenylpyrrolidine-2,5-dione

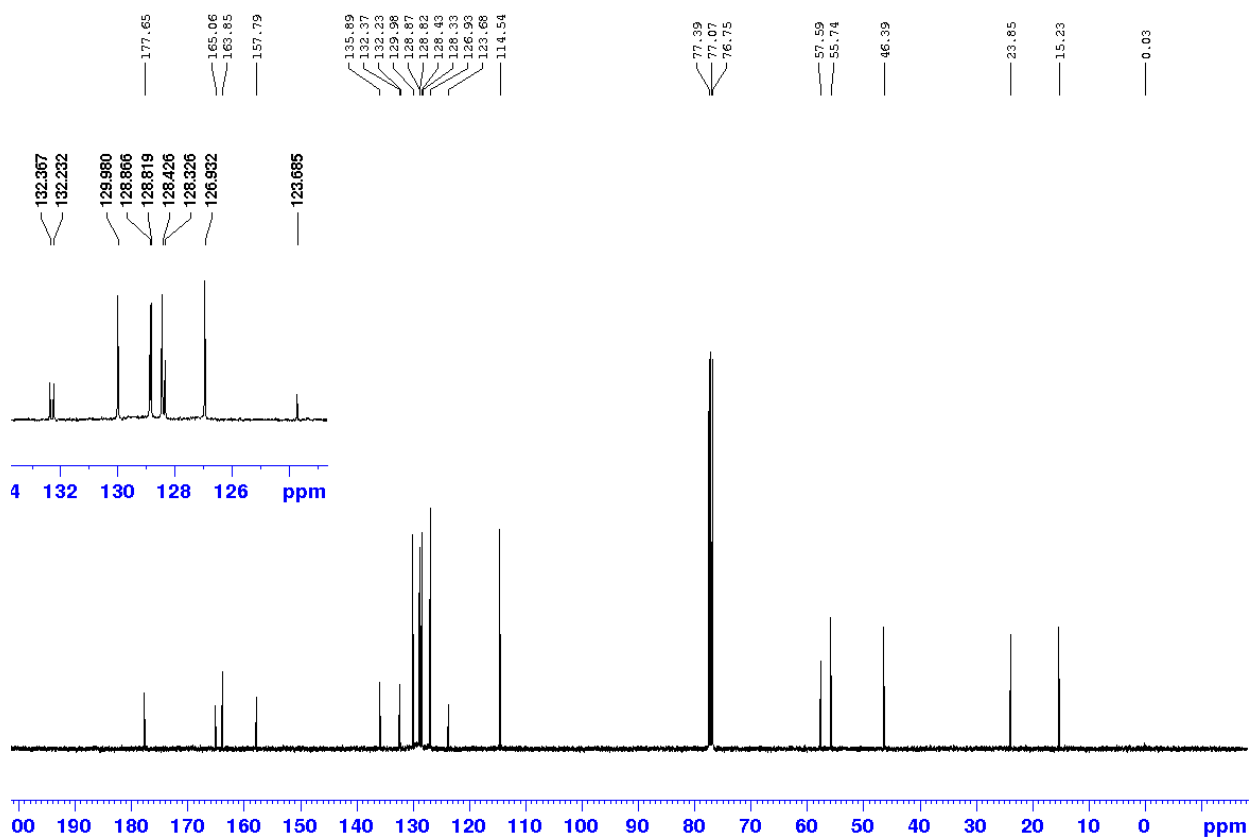


¹³C NMR spectrum of 3cd (100 MHz, CDCl₃)

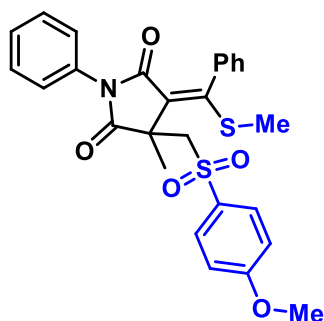


(3cd)

(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenylpyrrolidine-2,5-dione

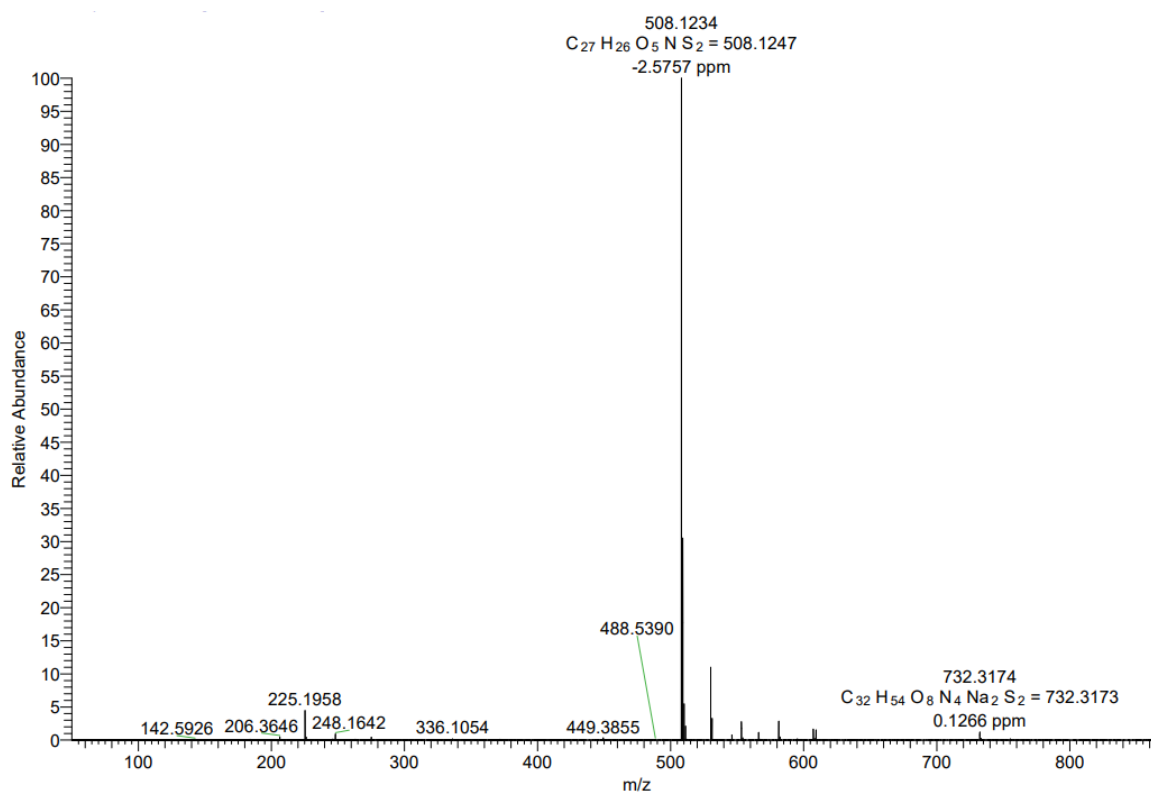


HRMS spectrum of 3cd

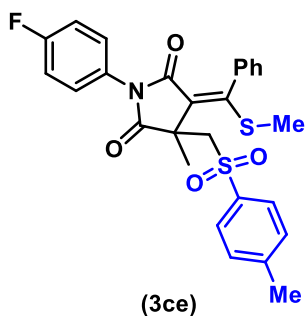


(3cd)

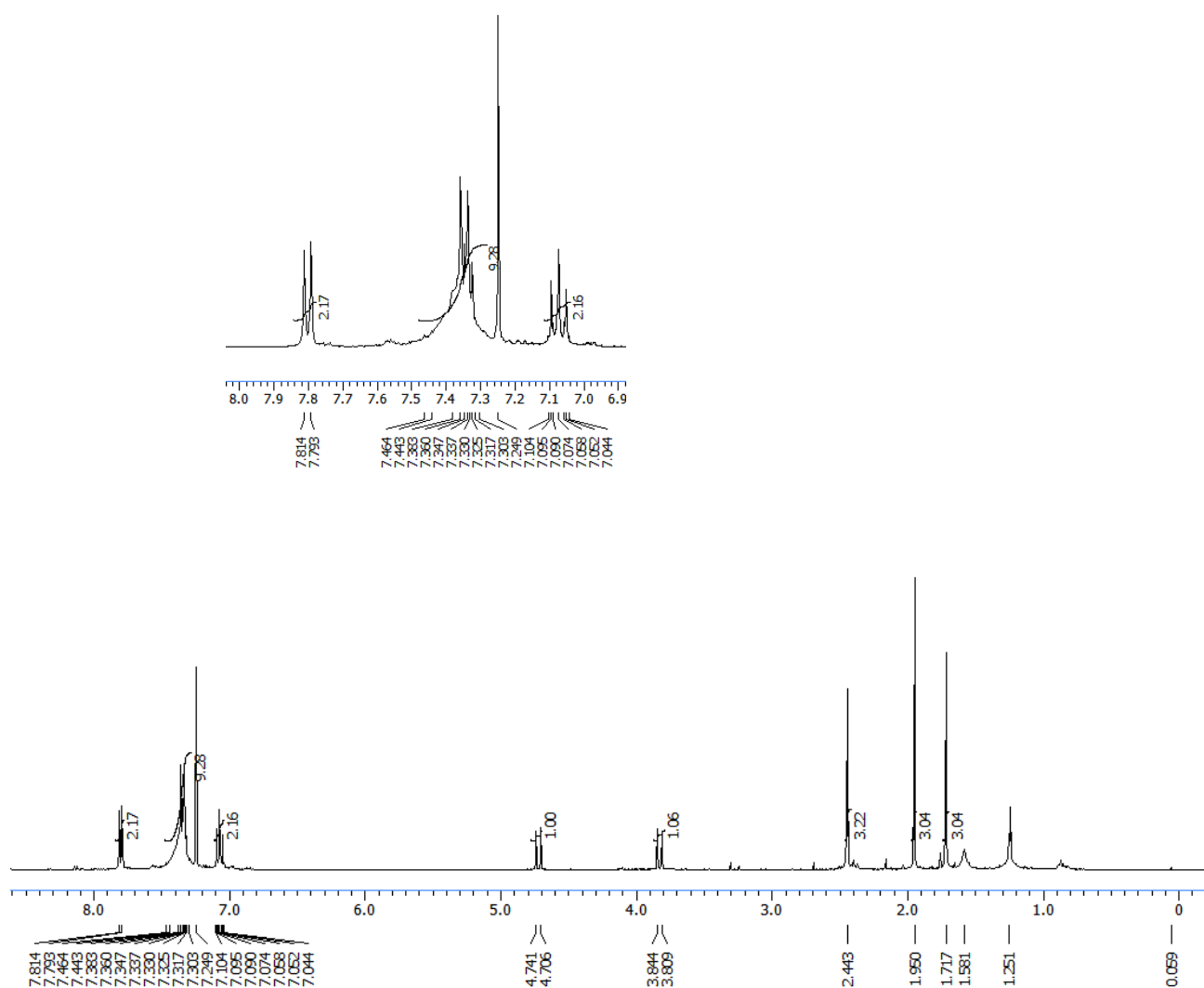
(E)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-4-((methylthio)(phenyl)methylene)-1-phenylpyrrolidine-2,5-dione



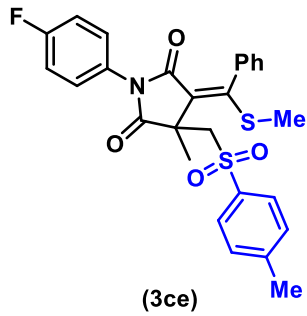
¹H NMR spectrum of 3ce (400 MHz, CDCl₃)



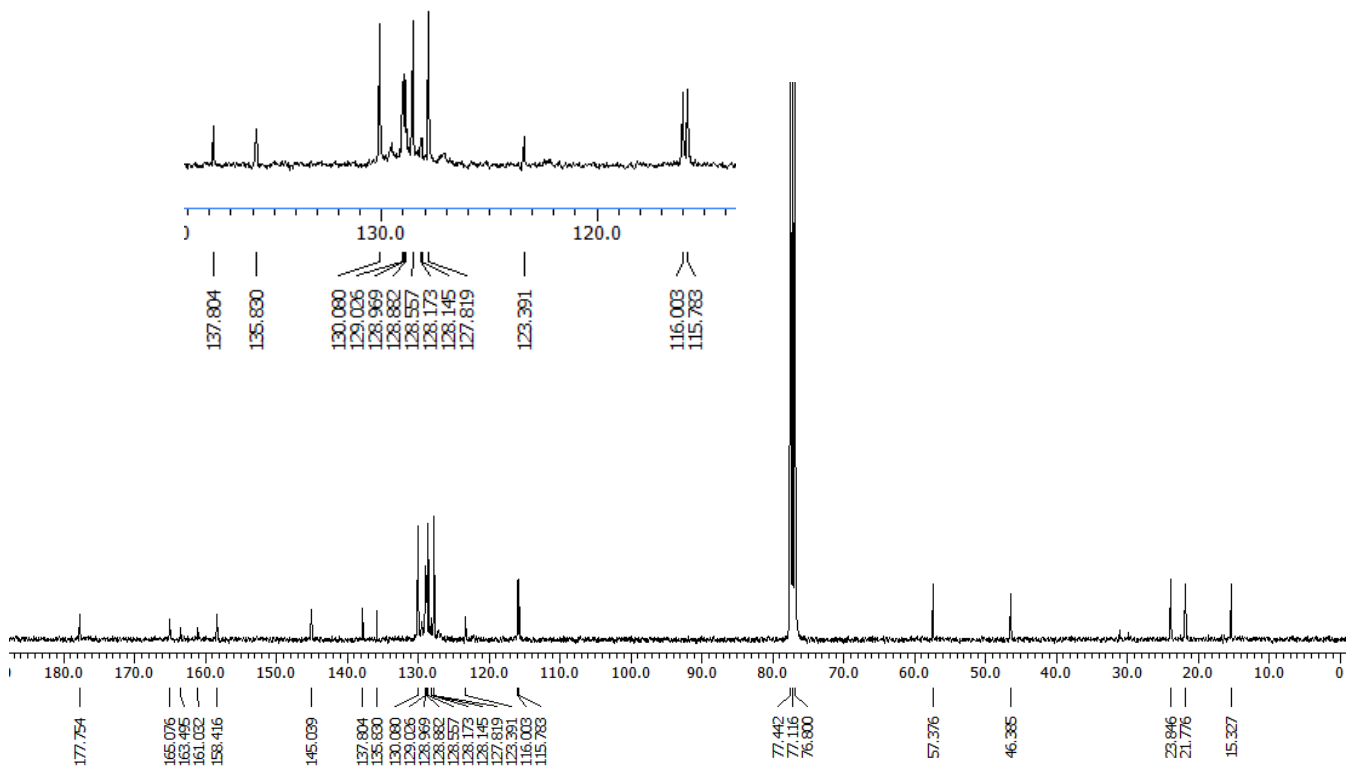
(E)-1-(4-fluorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



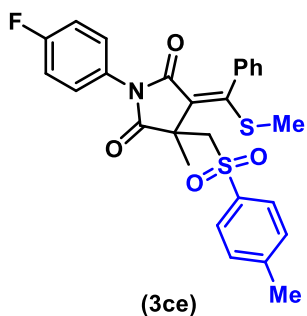
¹³C NMR spectrum of 3ce (100 MHz, CDCl₃)



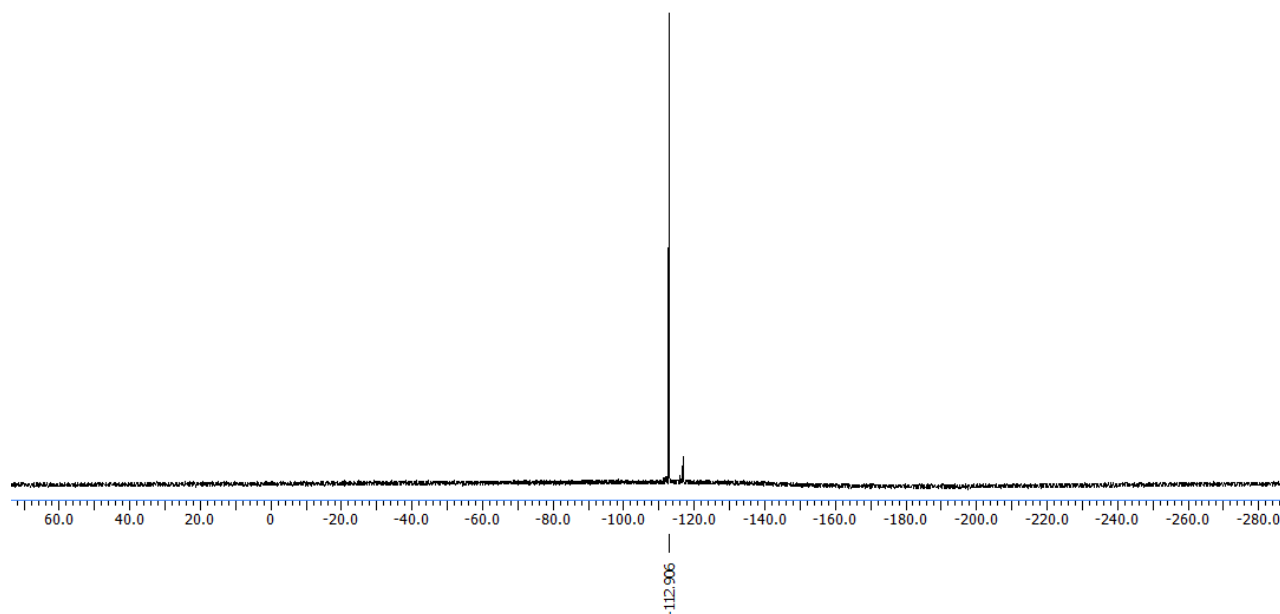
(E)-1-(4-fluorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



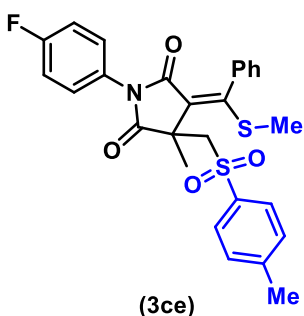
¹⁹F NMR spectrum of 3ce (376 MHz, CDCl₃)



(E)-1-(4-fluorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS spectrum of 3ce



(E)-1-(4-fluorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

Data File	SMP-35.d	Sample Name	SMP-35
Sample Type	Sample	Position	P1-B4
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	21-05-2022 12:34:45
IRM Calibration Status	Success	DA Method	Default.m
Comment			

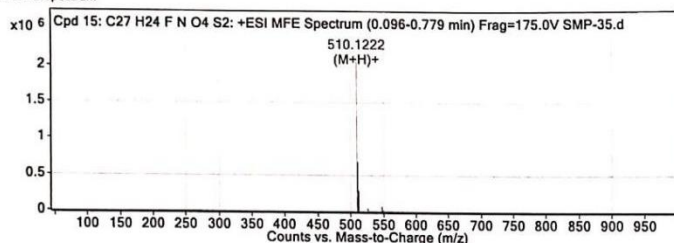
Sample Group		Info.	3
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125)		

Compound Table

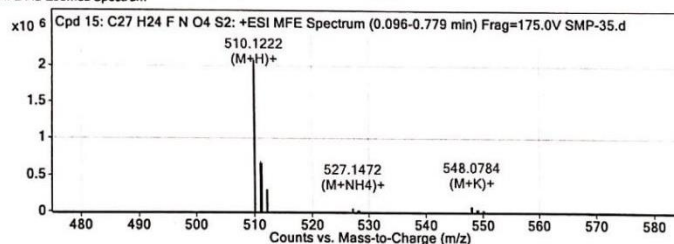
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 15: C27 H24 F N O4 S2	0.174	509.1149	C27 H24 F N O4 S2	C27 H24 F N O4 S2	-3.58	C27 H24 F N O4 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 15: C27 H24 F N O4 S2	510.1222	0.174	Find by Molecular Feature	509.1149

MFE MS Spectrum



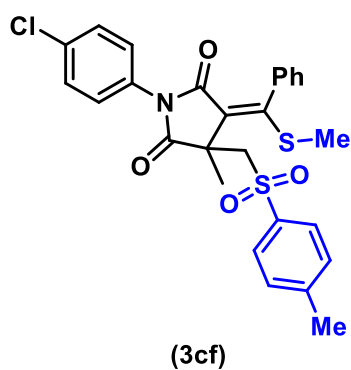
MFE MS Zoomed Spectrum



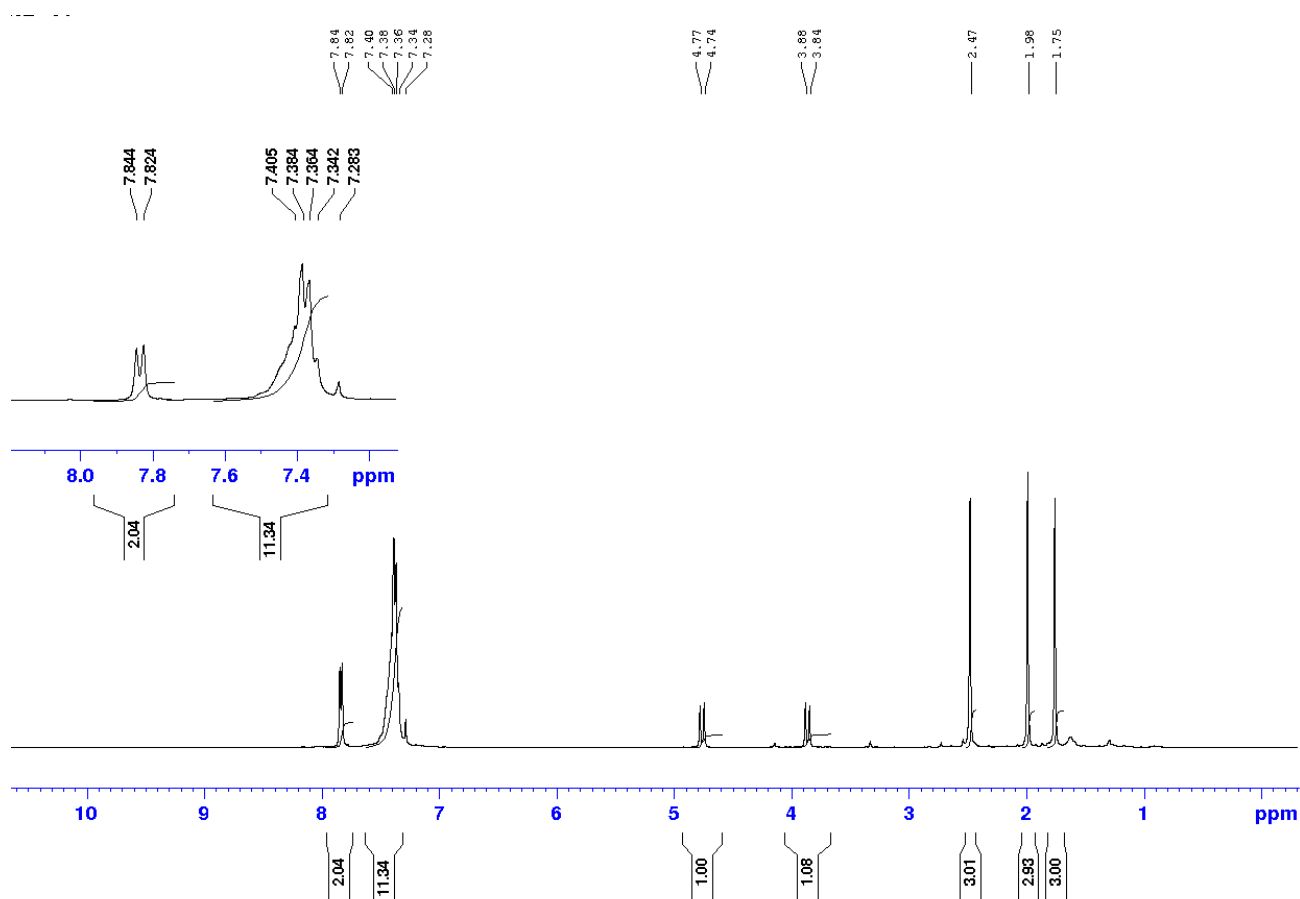
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
510.1222	1	2075499.5	C27 H25 F N O4 S2	(M+H)+
511.1253	1	676911.62	C27 H25 F N O4 S2	(M+H)+
512.122	1	281590.88	C27 H25 F N O4 S2	(M+H)+
527.1472	1	34260.25	C27 H28 F N2 O4 S2	(M+NH4)+
528.1503	1	11413.7	C27 H28 F N2 O4 S2	(M+NH4)+
529.1345	1	5845.99	C27 H28 F N2 O4 S2	(M+NH4)+
548.0784	1	64579.69	C27 H24 F K N O4 S2	(M+K)+
549.0816	1	20421.02	C27 H24 F K N O4 S2	(M+K)+
550.0775	1	13670.2	C27 H24 F K N O4 S2	(M+K)+

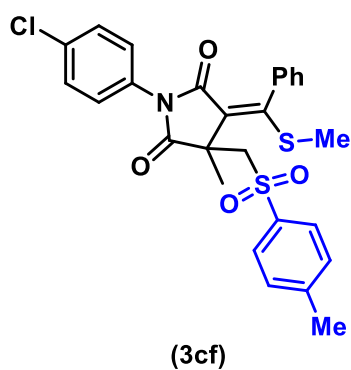
¹H NMR spectrum of 3cf (400 MHz, CDCl₃)



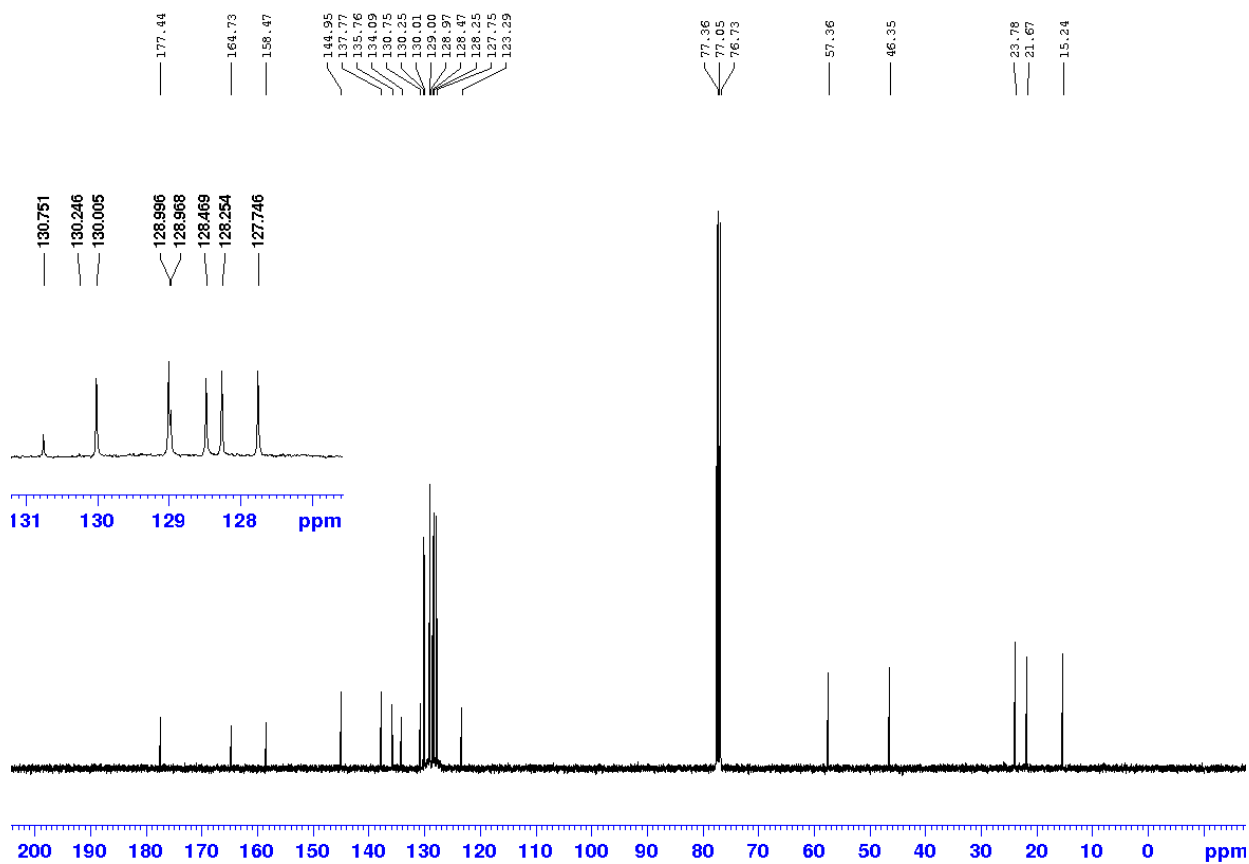
(E)-1-(4-chlorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



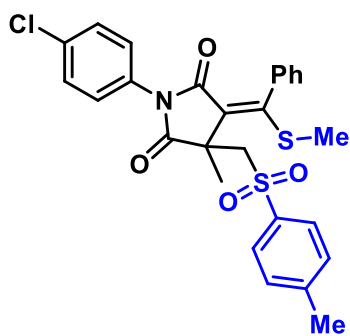
¹³C NMR spectrum of 3cf (100 MHz, CDCl₃)



(E)-1-(4-chlorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3cf



(3cf)

(E)-1-(4-chlorophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

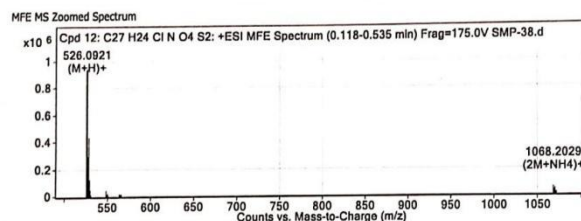
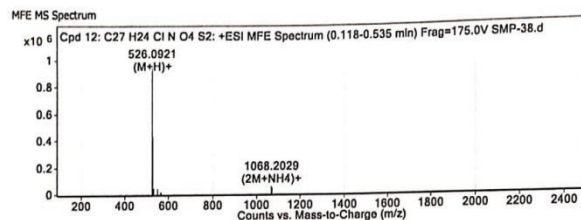
Qualitative Compound Report

Data File SMP-38.d Sample Name SMP-38
 Sample Type Sample Position P1-A2
 Instrument Name Instrument 1 User Name
 Acq Method MS Scan.m Acquired Time 02-05-2022 11:33:53
 IRM Calibration Status Success DA Method Default.m
 Comment

Sample Group Info. 3
 Acquisition SW 6200 series TOF/6500 series
 Version Q-TOF B.05.01 (B5125)

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 12: C27 H24 Cl N O4 S2	0.204	525.0844	C27 H24 Cl N O4 S2	C27 H24 Cl N O4 S2	-1.59	C27 H24 Cl N O4 S2

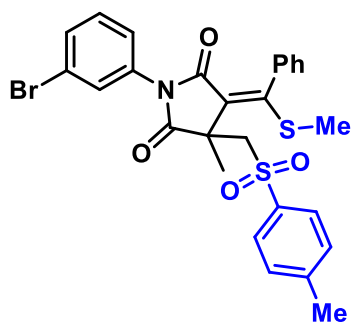
Compound Label	m/z	RT	Algorithm	Mass
Cpd 12: C27 H24 Cl N O4 S2	526.0921	0.204	Find by Molecular Feature	525.0844



MS Spectrum Peak List

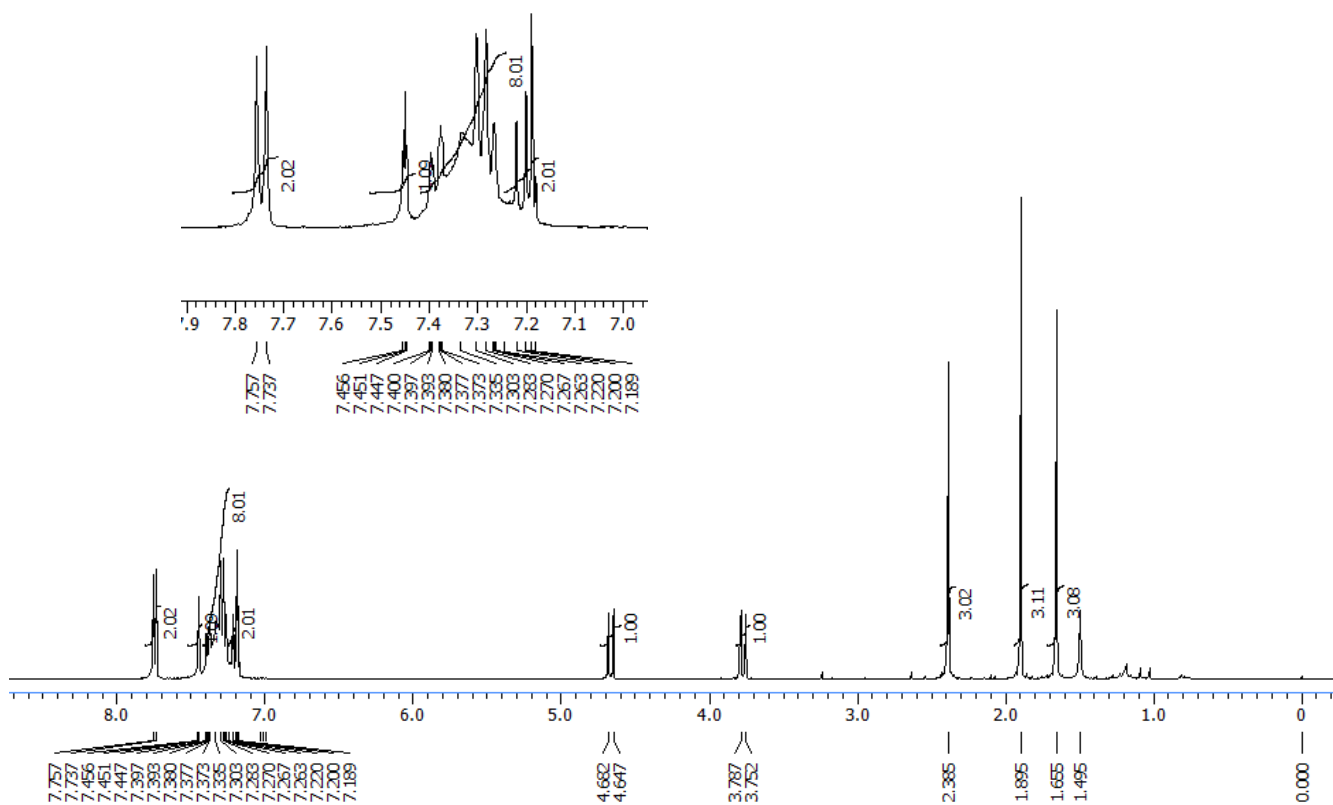
m/z	z	Abund	Formula	Ion
526.0921	1	945474	C27 H25 Cl N O4 S2	(M+H)+
527.0945	1	289422.15	C27 H25 Cl N O4 S2	(M+H)+
528.0891	1	435992.1	C27 H25 Cl N O4 S2	(M+H)+
529.0912	1	122322.96	C27 H25 Cl N O4 S2	(M+H)+
530.0872	1	46817.86	C27 H25 Cl N O4 S2	(M+H)+
548.0727	1	41863.77	C27 H24 Cl N Na O4 S2	(M+Na)+
1068.2029	1	55452.15		(2M+NH4)+
1069.2036	1	34503.22		(2M+NH4)+
1070.1992	1	45095.06		(2M+NH4)+
1071.2013	1	24920.92		(2M+NH4)+

¹H NMR spectrum of 3cg (400 MHz, CDCl₃)

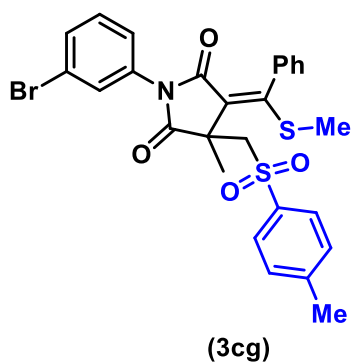


(3cg)

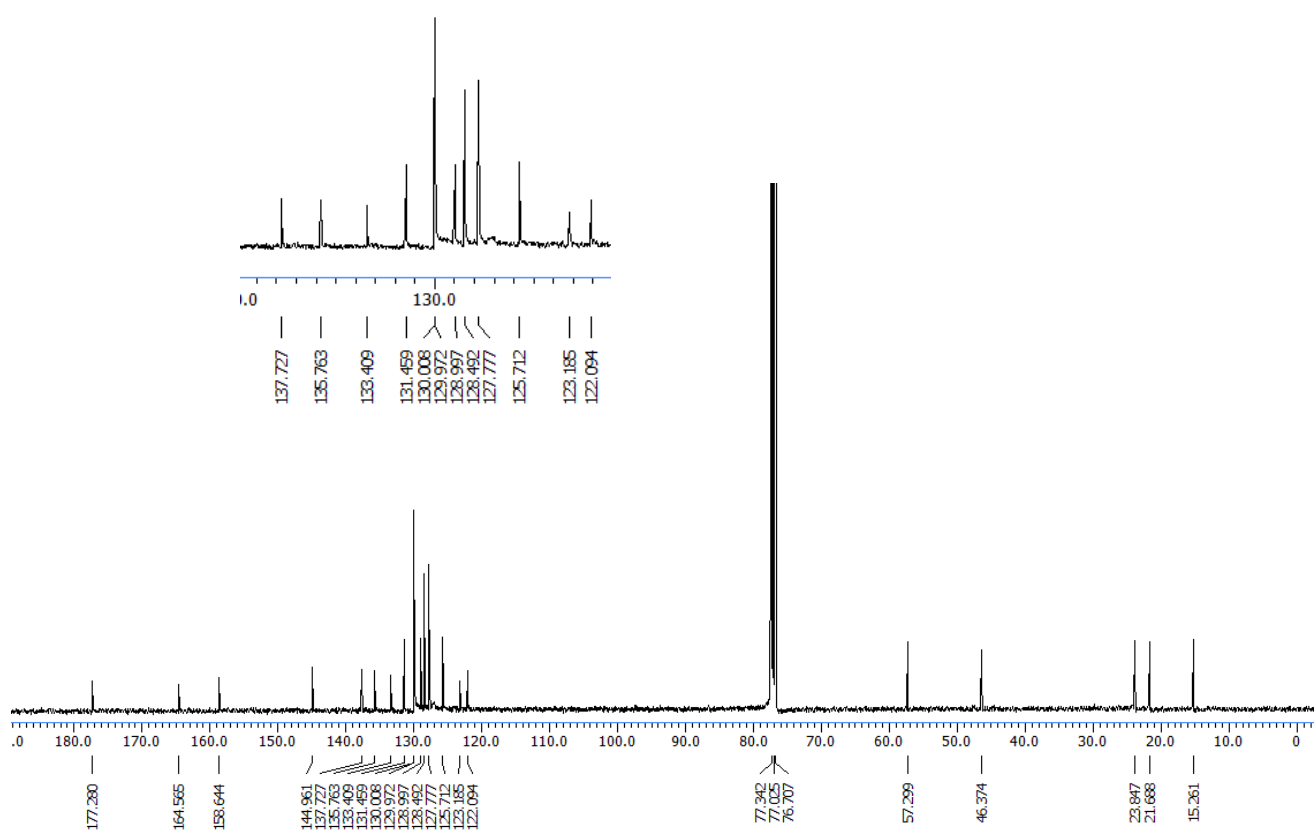
(E)-1-(3-bromophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



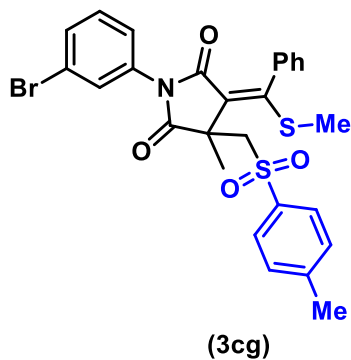
¹³C NMR spectrum of 3cg (100 MHz, CDCl₃)



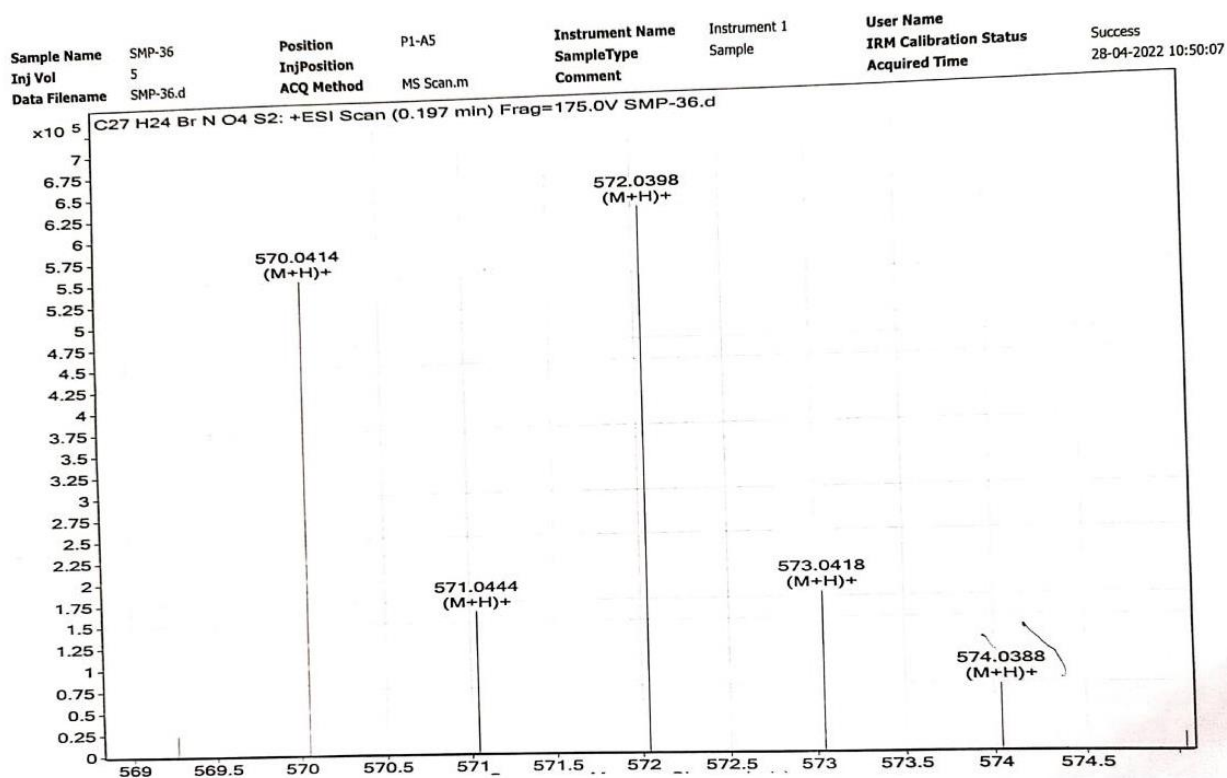
(E)-1-(3-bromophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



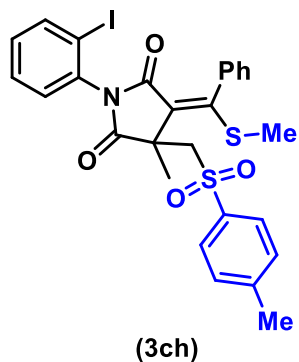
HRMS Spectrum of 3cg



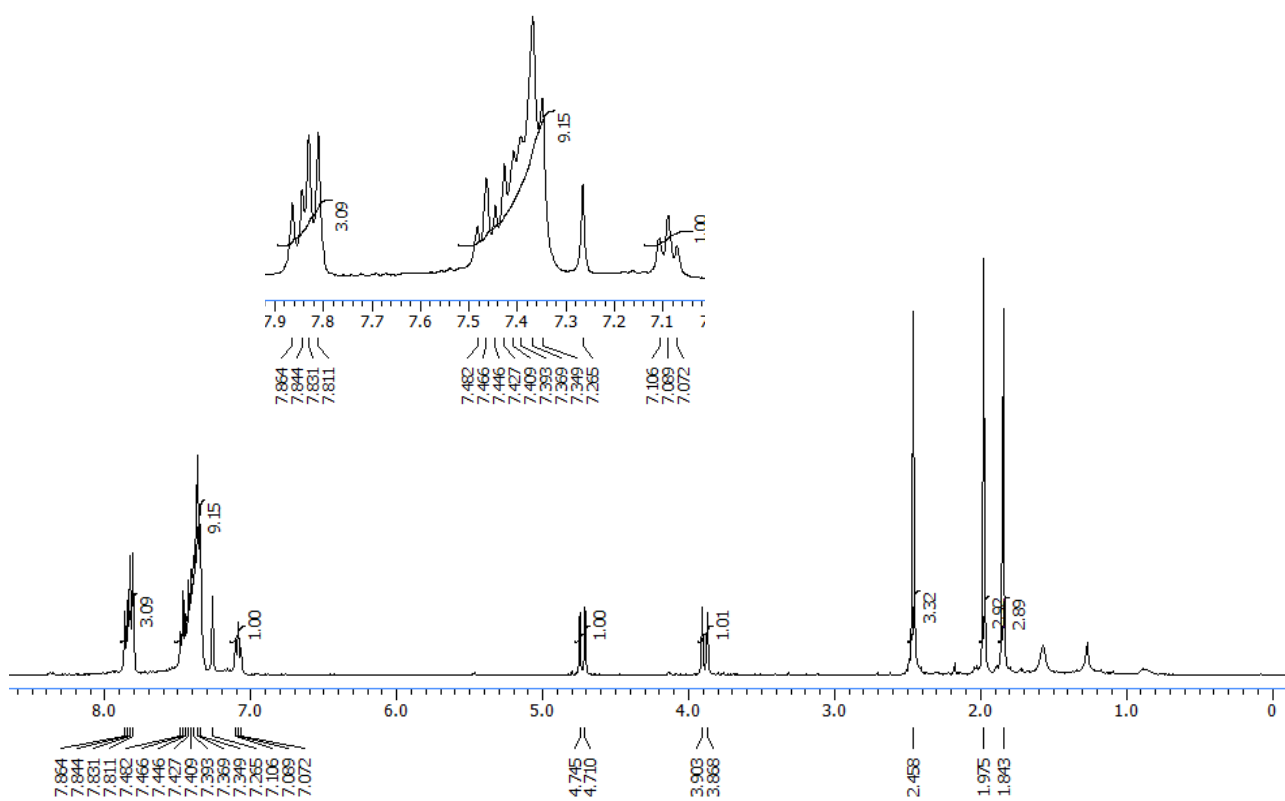
(E)-1-(3-bromophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



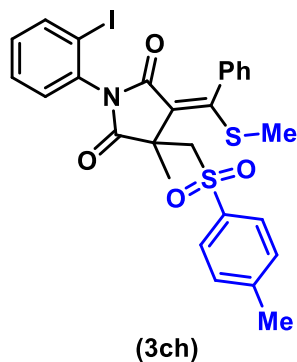
¹H NMR spectrum of 3ch (400 MHz, CDCl₃)



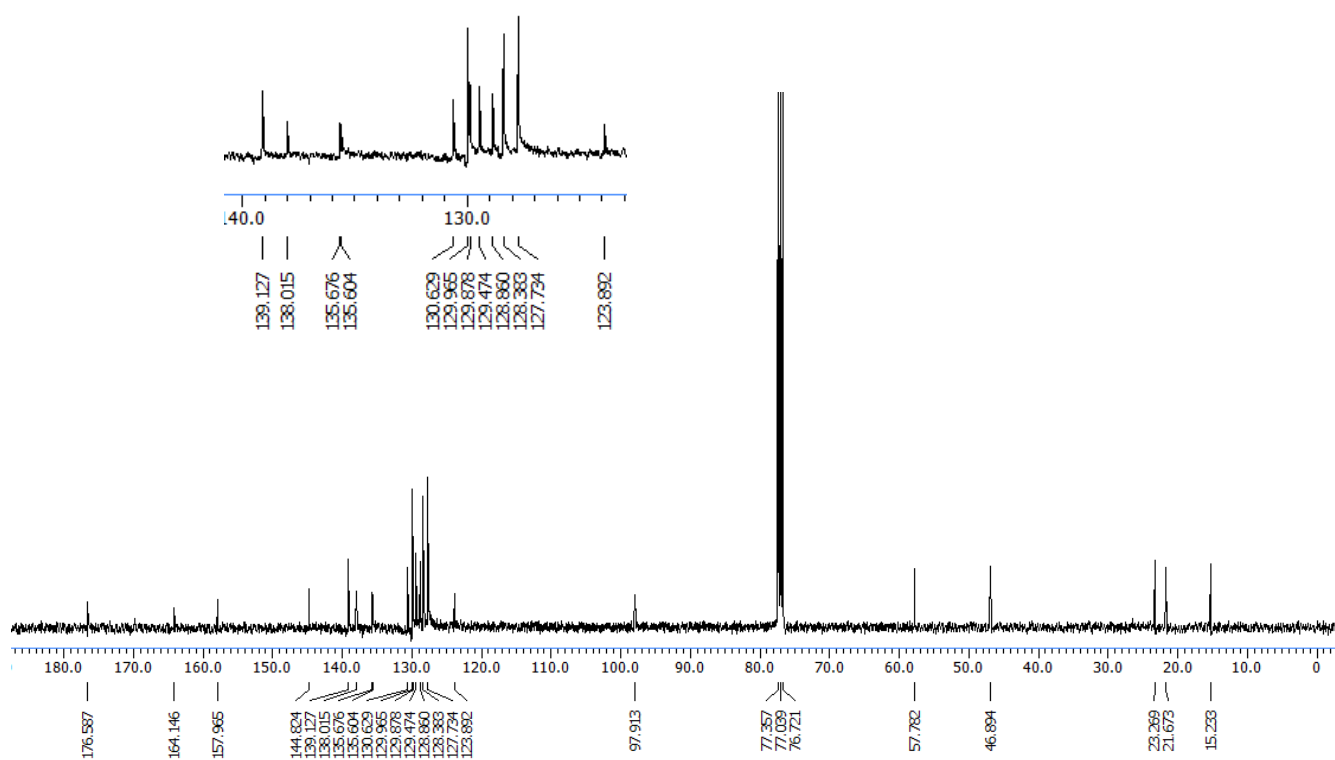
(E)-1-(2-iodophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



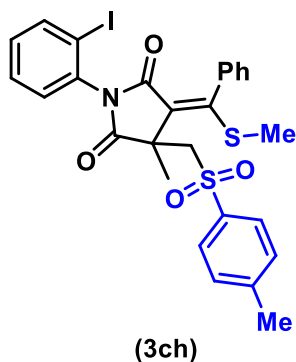
¹³C NMR spectrum of 3ch (100 MHz, CDCl₃)



(E)-1-(2-iodophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3ch



(E)-1-(2-iodophenyl)-3-methyl-4-((methylthio)(phenyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

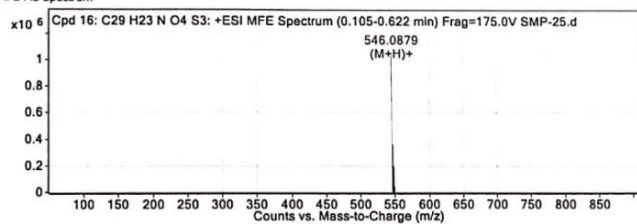
Data File	SMP-25.d	Sample Name	SMP-25
Sample Type	Sample	Position	P1-A9
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	21-05-2022 12:28:47
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125)		

Compound Table

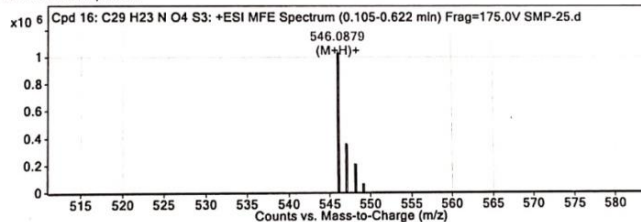
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C29 H23 N O4 S3	0.185	545.0804	C29 H23 N O4 S3	C29 H23 N O4 S3	-2.8	C29 H23 N O4 S3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 16: C29 H23 N O4 S3	546.0879	0.185	Find by Molecular Feature	545.0804

MFE MS Spectrum



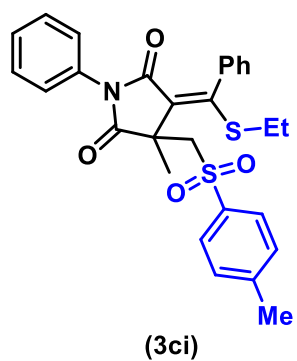
MFE MS Zoomed Spectrum



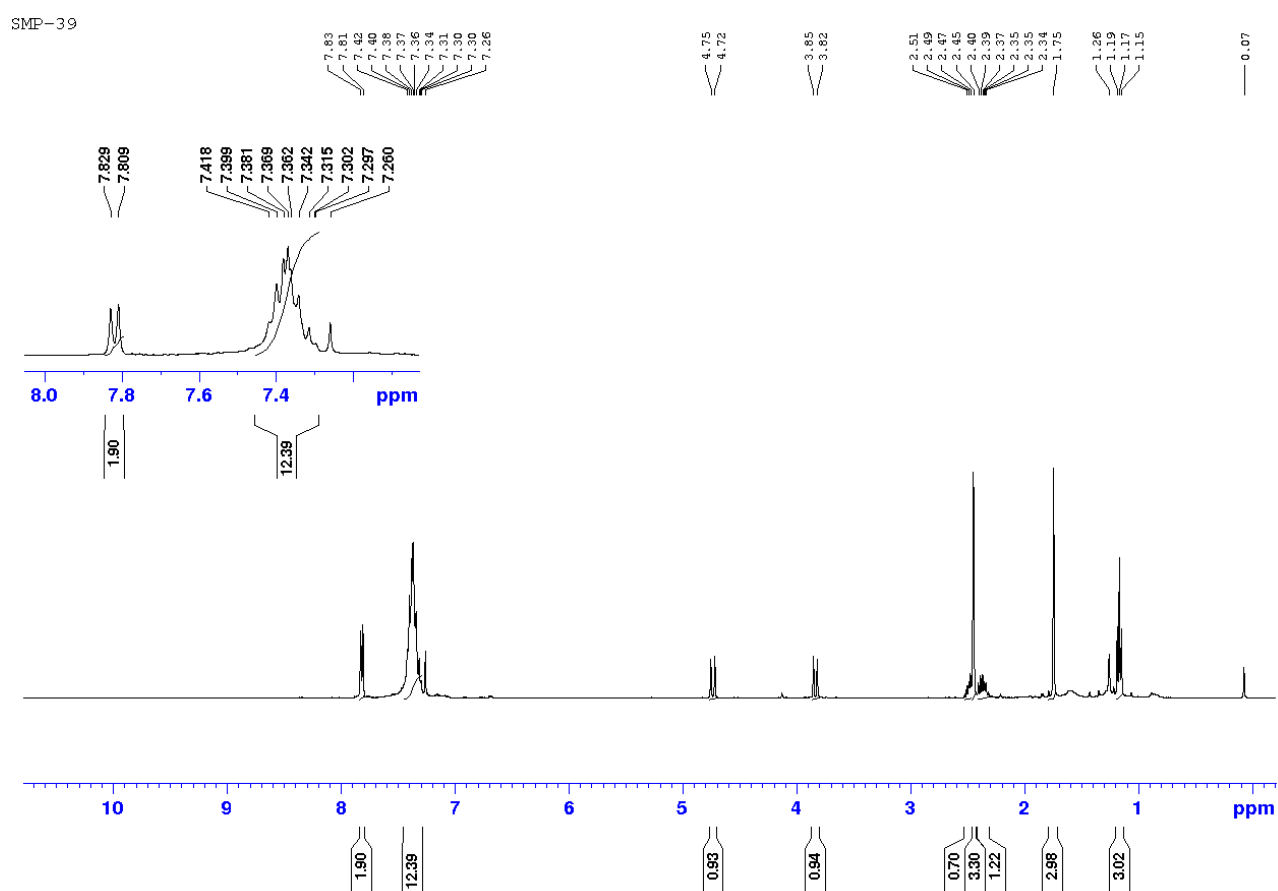
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
546.0879	1	1044326.25	C29 H24 N O4 S3	(M+H)+
547.0905	1	361133.85	C29 H24 N O4 S3	(M+H)+
548.0866	1	196223.48	C29 H24 N O4 S3	(M+H)+
549.0876	1	48562.02	C29 H24 N O4 S3	(M+H)+

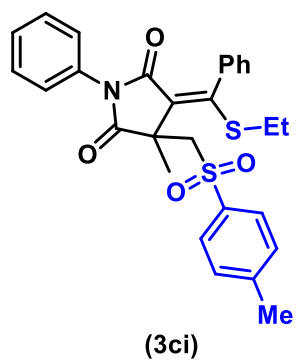
¹H NMR spectrum of 3ci (400 MHz, CDCl₃)



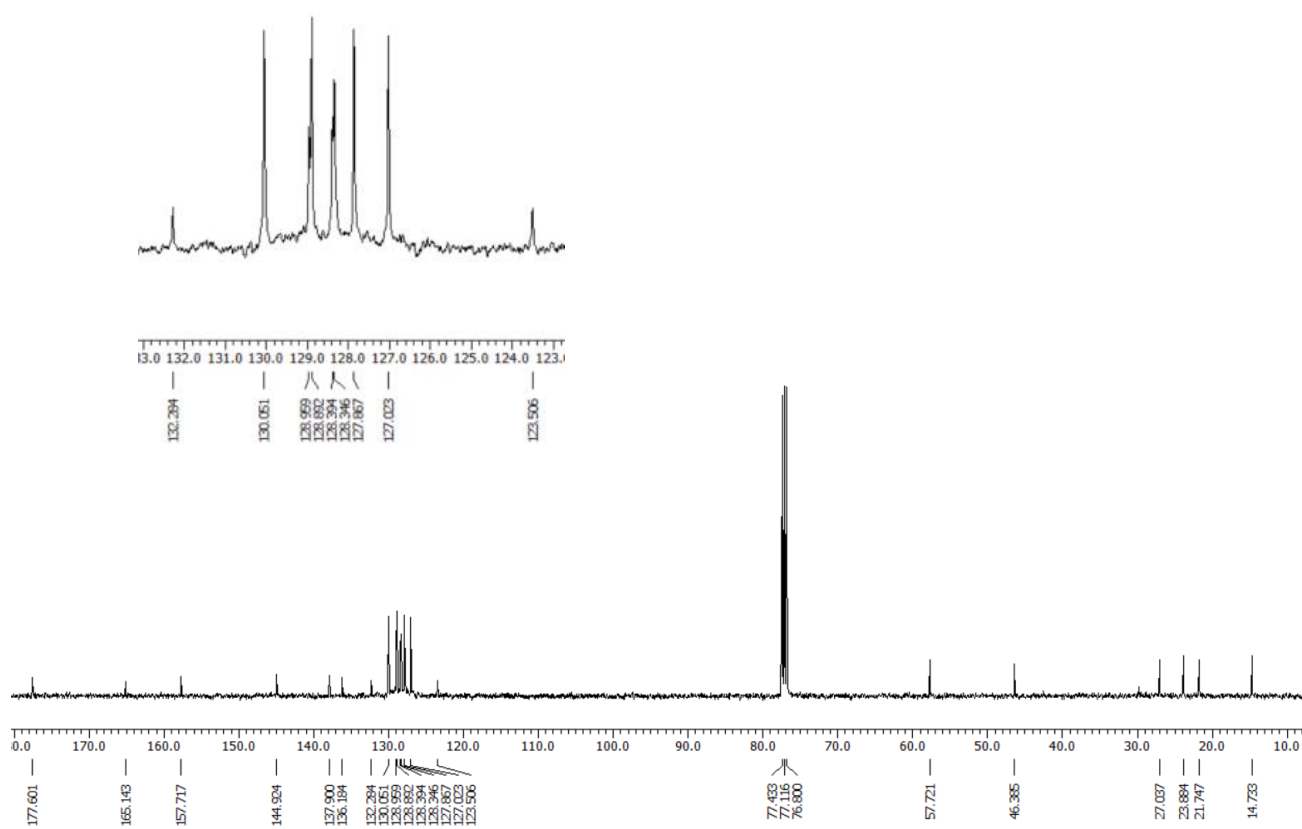
(E)-4-((ethylthio)(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione



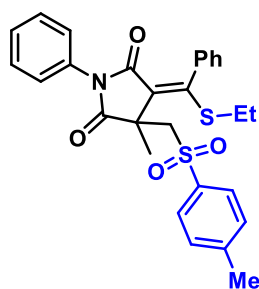
^{13}C NMR spectrum of 3ci (100 MHz, CDCl_3)



(E)-4-((ethylthio)(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3ci



(3ci)

(E)-4-((ethylthio)(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

Data File	SMP-39.d	Sample Name	SMP-39
Sample Type	Sample	Position	P1-B4
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	02-05-2022 11:52:57
IRM Calibration Status	Success	DA Method	Default.m
Comment			

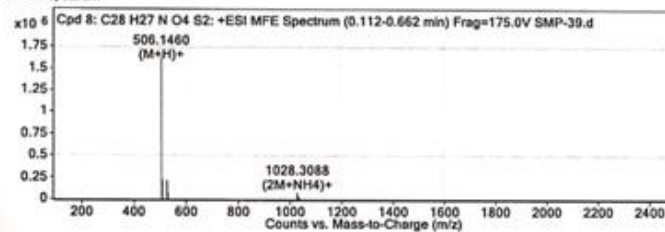
Sample Group		Info.	3
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF 8.05.01 (85125)		

Compound Table

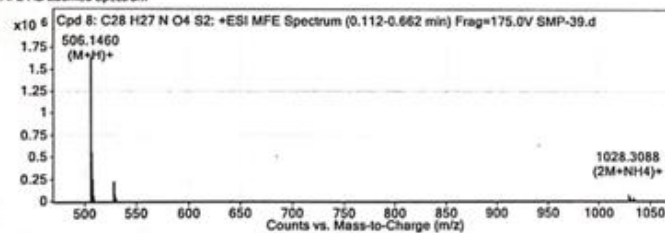
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C28 H27 N O4 S2	0.203	505.1386	C28 H27 N O4 S2	C28 H27 N O4 S2	-0.88	C28 H27 N O4 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 8: C28 H27 N O4 S2	506.146	0.203	Find by Molecular Feature	505.1386

MFE MS Spectrum



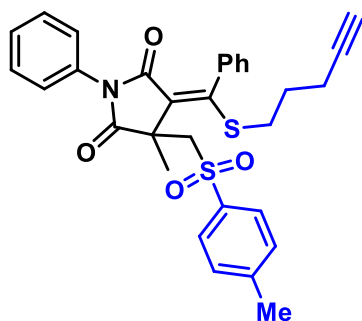
MFE MS Zoomed Spectrum



MS Spectrum Peak List

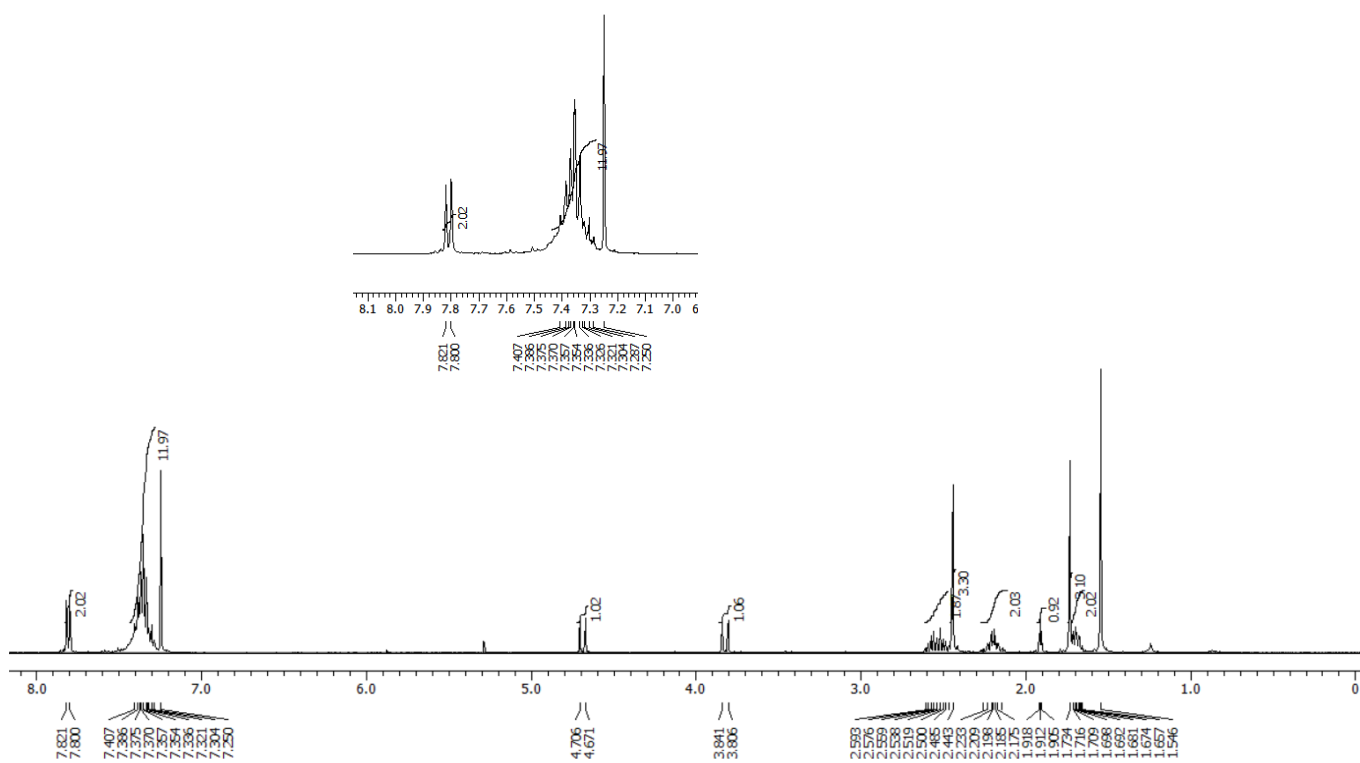
m/z	z	Abund	Formula	Ion
506.146	1	1647364.88	C28 H28 N O4 S2	(M+H)+
507.1489	1	552643.44	C28 H28 N O4 S2	(M+H)+
508.1456	1	229932.73	C28 H28 N O4 S2	(M+H)+
509.1464	1	54355.69	C28 H28 N O4 S2	(M+H)+
528.1275	1	219427.52	C28 H27 N Na O4 S2	(M+Na)+
529.1302	1	69987.47	C28 H27 N Na O4 S2	(M+Na)+
530.1267	1	31822.63	C28 H27 N Na O4 S2	(M+Na)+
1028.3088	1	67389.03		(2M+NH4)+
1029.3116	1	45486.52		(2M+NH4)+
1033.267	1	32111.34		(2M+Na)+

¹H NMR spectrum of 3cj (400 MHz, CDCl₃)

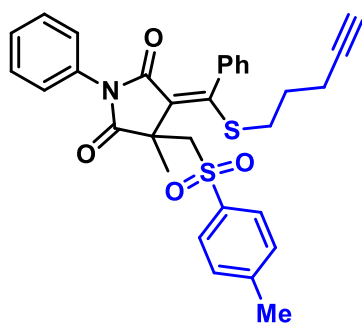


(3cj)

(*E*)-3-methyl-4-((pent-4-yn-1-ylthio)(phenyl)methylene)-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione

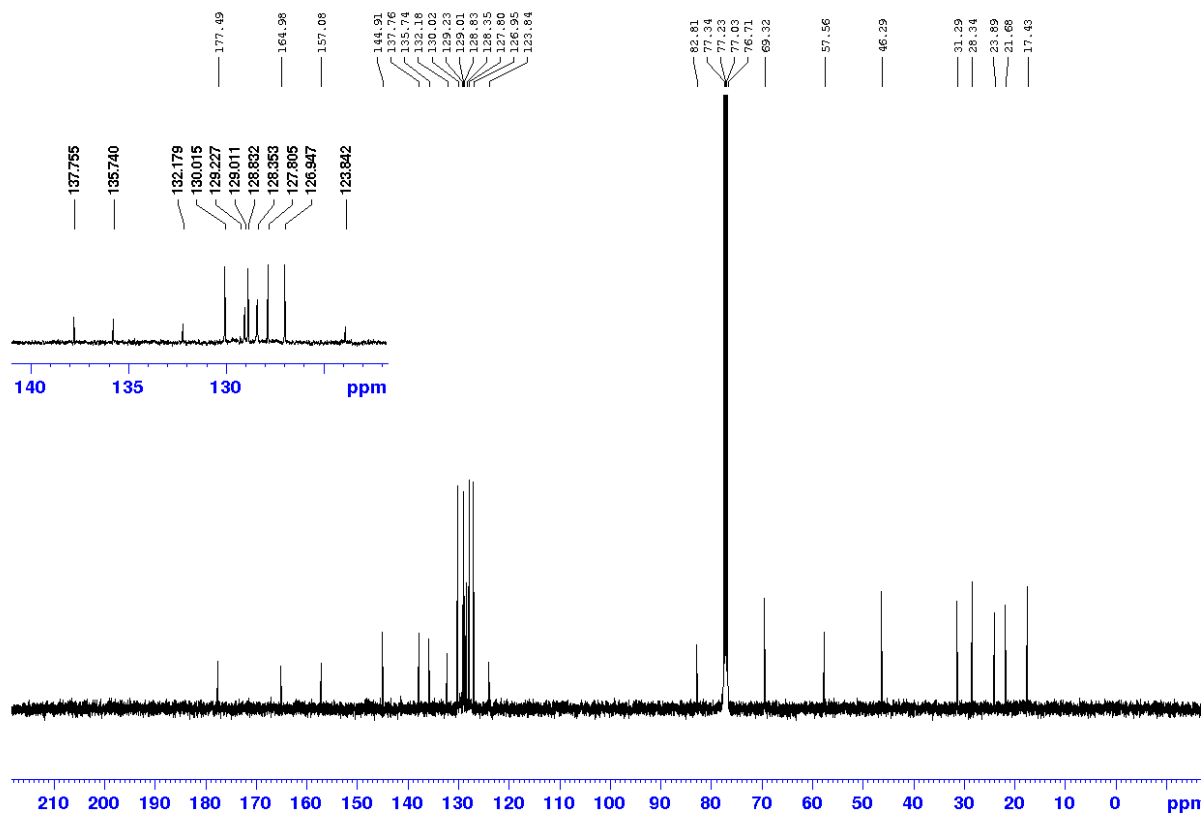


¹³C NMR spectrum of 3c (100 MHz, CDCl₃)

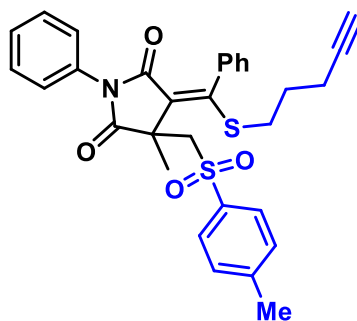


(3c)

(E)-3-methyl-4-((pent-4-yn-1-ylthio)(phenyl)methylene)-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione

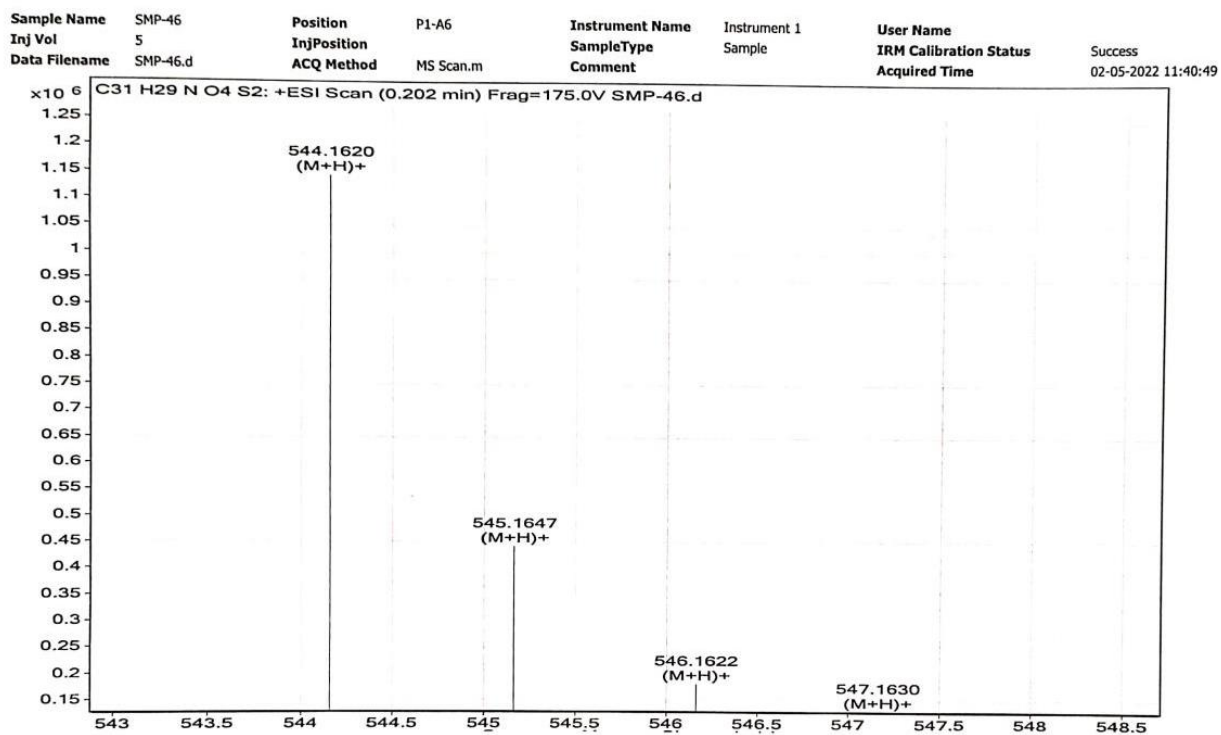


HRMS spectrum of 3cj

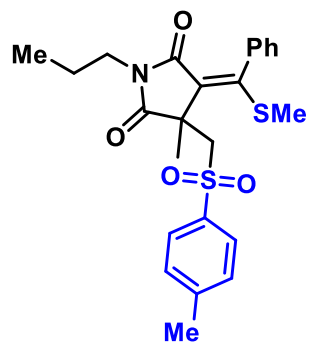


(3cj)

(E)-3-methyl-4-((pent-4-yn-1-ylthio)(phenyl)methylene)-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione

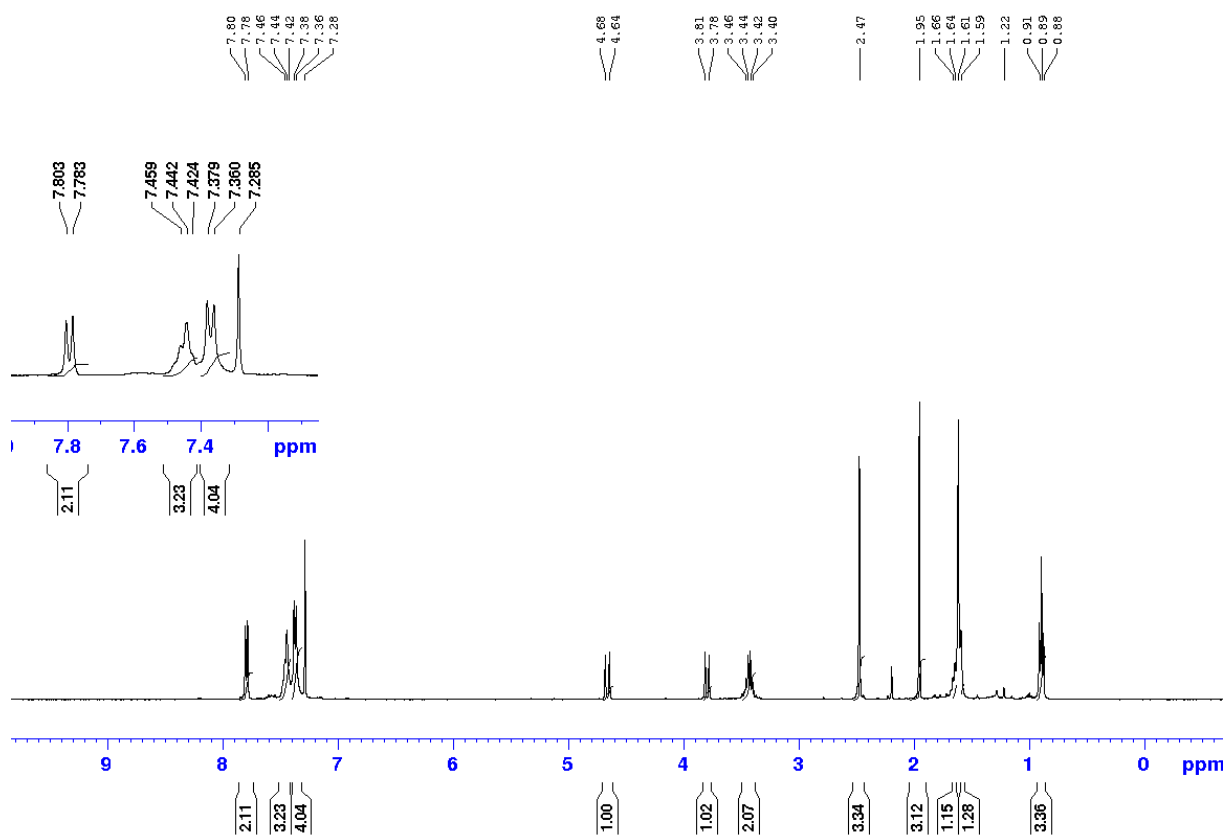


¹H NMR spectrum of 3ck (400 MHz, CDCl₃)

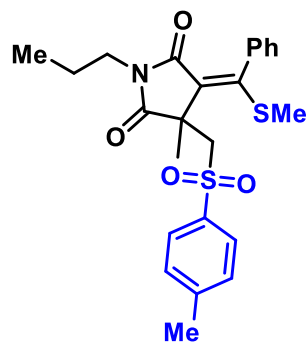


(3ck)

(*E*)-3-methyl-4-((methylthio)(phenyl)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione

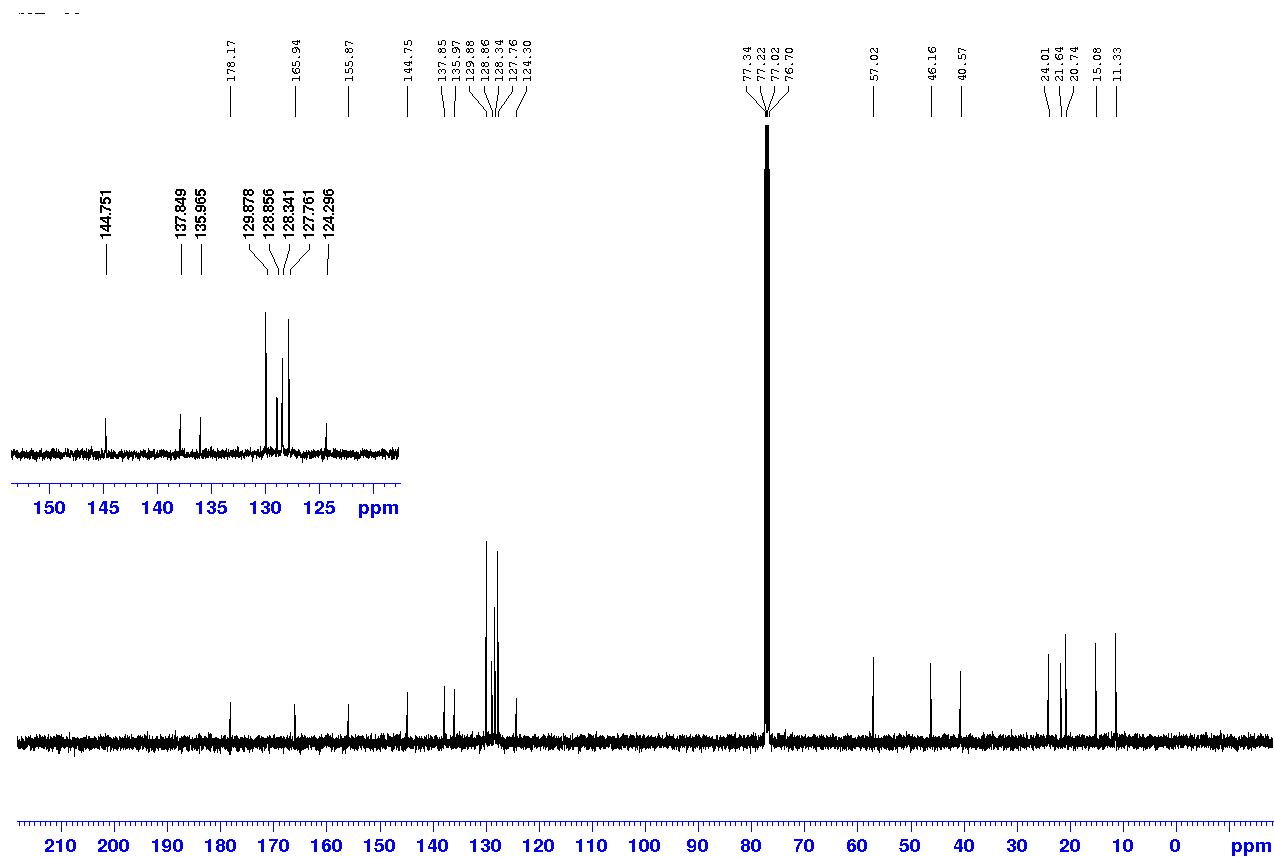


¹³C NMR spectrum of 3ck (100 MHz, CDCl₃)

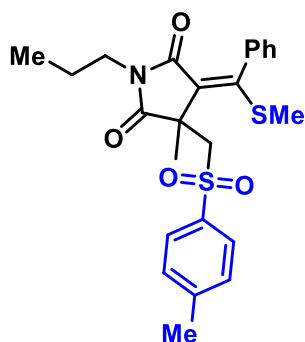


(3ck)

(*E*)-3-methyl-4-((methylthio)(phenyl)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3ck



(3ck)

(E)-3-methyl-4-((methylthio)(phenyl)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

Data File	SMP-53.d	Sample Name	SMP-53
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	21-05-2022 12:32:14
IRM Calibration Status	Success	DA Method	Default.m
Comment			

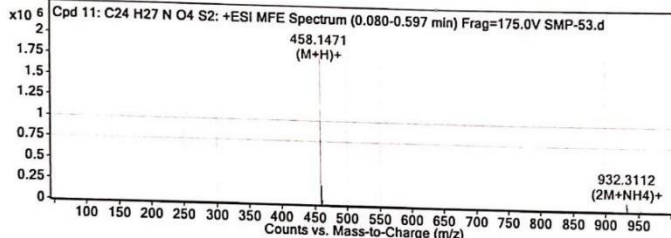
Sample Group	Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)	

Compound Table

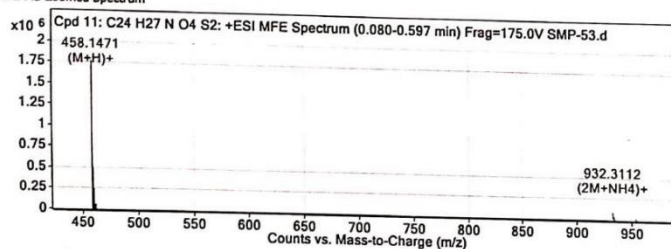
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C24 H27 N O4 S2	0.168	457.1398	C24 H27 N O4 S2	C24 H27 N O4 S2	-3.54	C24 H27 N O4 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 11: C24 H27 N O4 S2	458.1471	0.168	Find by Molecular Feature	457.1398

MFE MS Spectrum



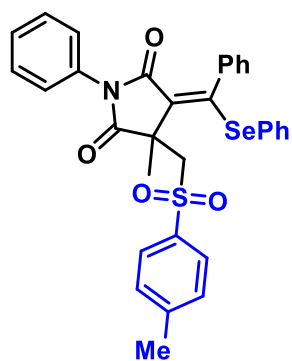
MFE MS Zoomed Spectrum



MS Spectrum Peak List

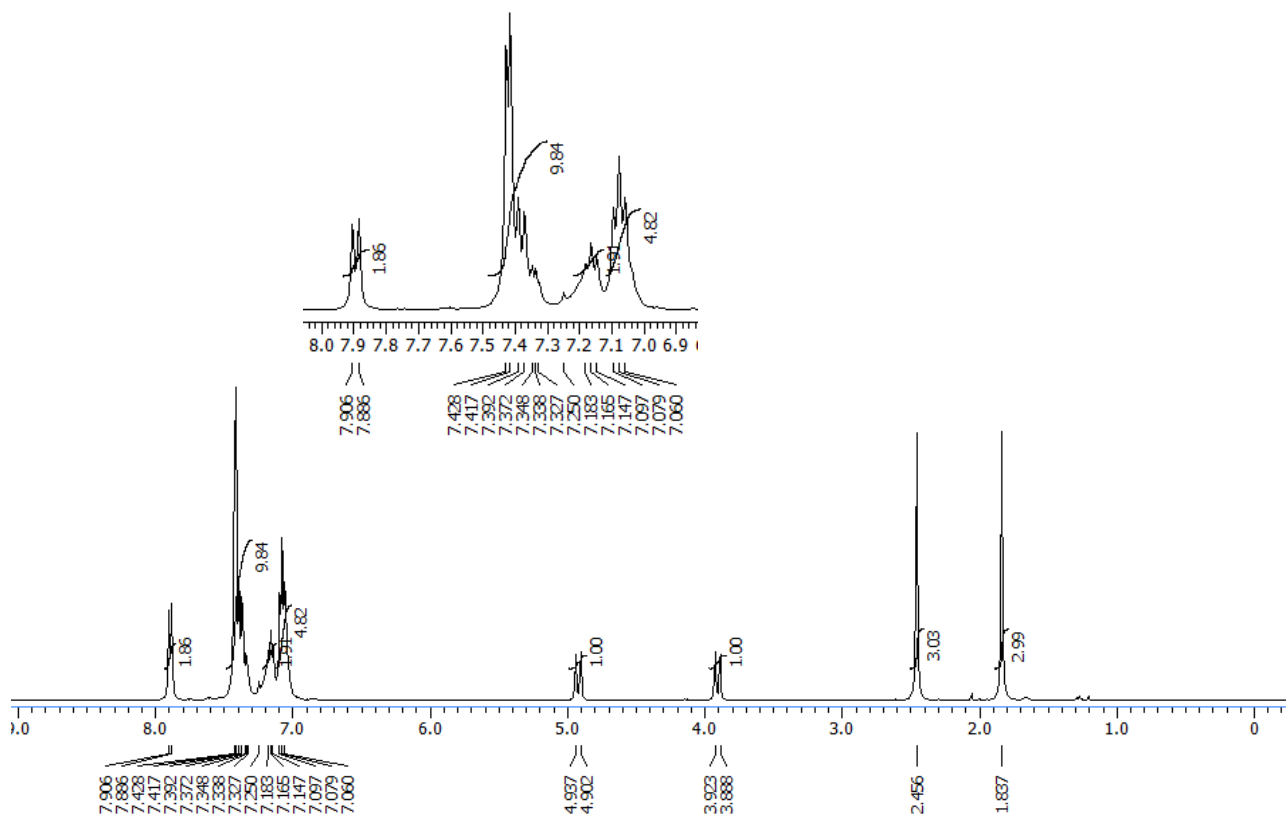
m/z	z	Abund	Formula	Ion
458.1471	1	1776080.38	C24 H28 N O4 S2	(M+H)+
459.1499	1	510288.45	C24 H28 N O4 S2	(M+H)+
460.1463	1	224335.98	C24 H28 N O4 S2	(M+H)+
461.1485	1	49149.96	C24 H28 N O4 S2	(M+H)+
932.3112	1	98226.48		(2M+NH4)+
933.3138	1	54833.99		(2M+NH4)+
934.3118	1	32858.77		(2M+NH4)+
935.3122	1	12767.99		(2M+NH4)+
953.2485	1	24509.31		(2M+K)+
954.2518	1	13705.86		(2M+K)+

¹H NMR spectrum of 5a (400 MHz, CDCl₃)

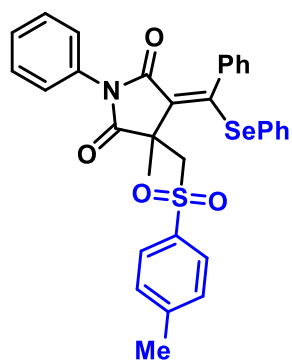


(5a)

(*E*)-3-methyl-1-phenyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

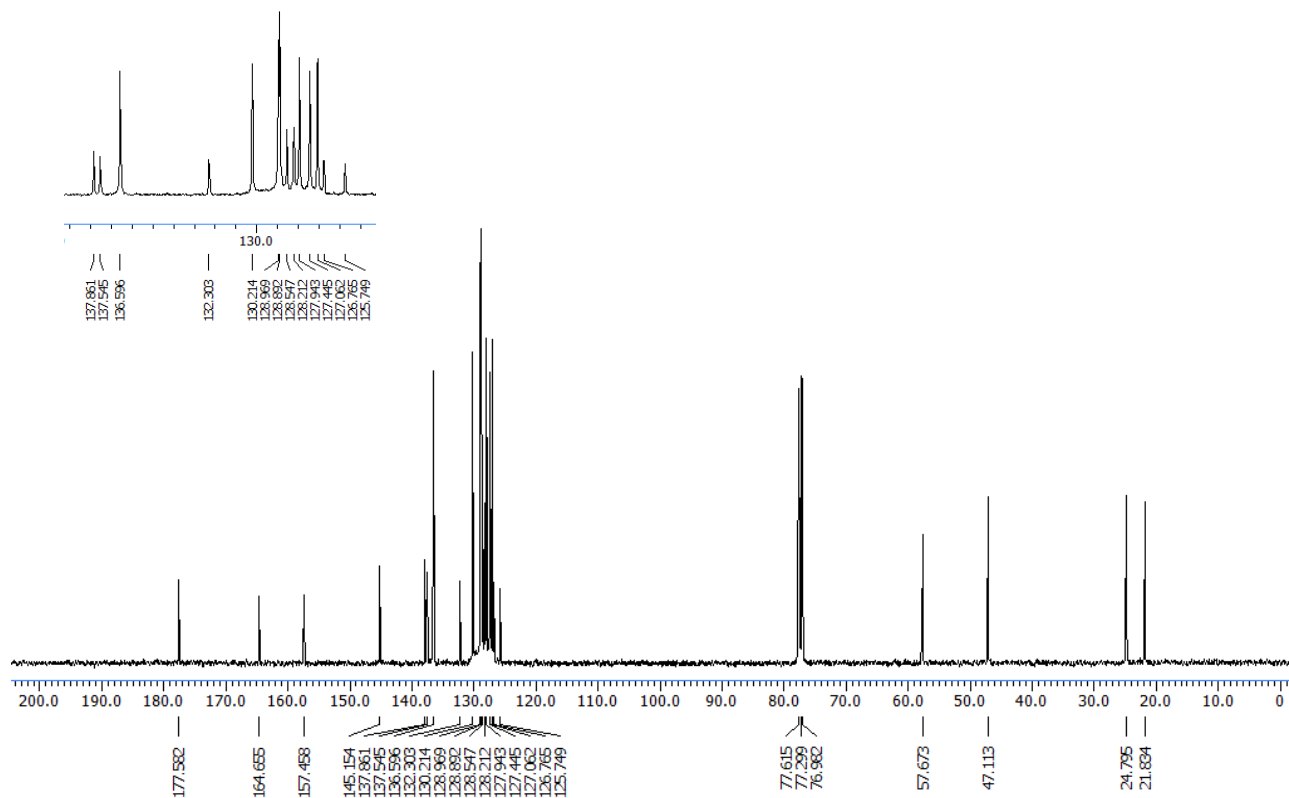


¹³C NMR spectrum of 5a (100 MHz, CDCl₃)

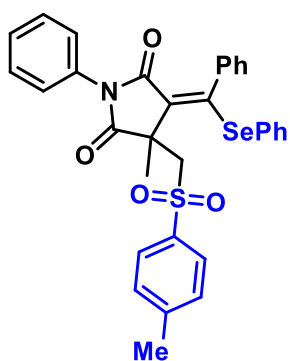


(5a)

(*E*)-3-methyl-1-phenyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

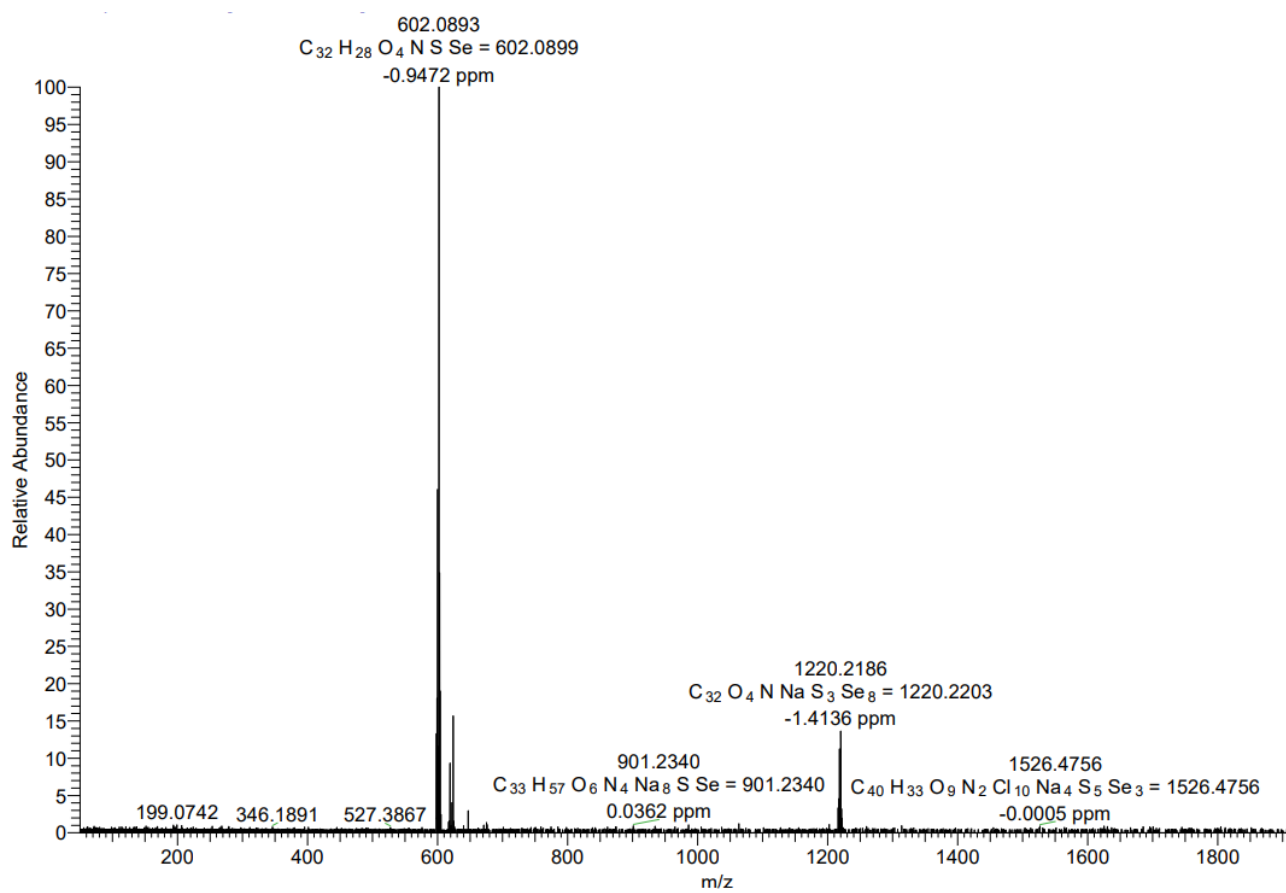


HRMS Spectrum of 5a

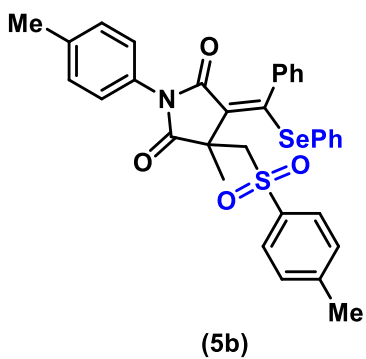


(5a)

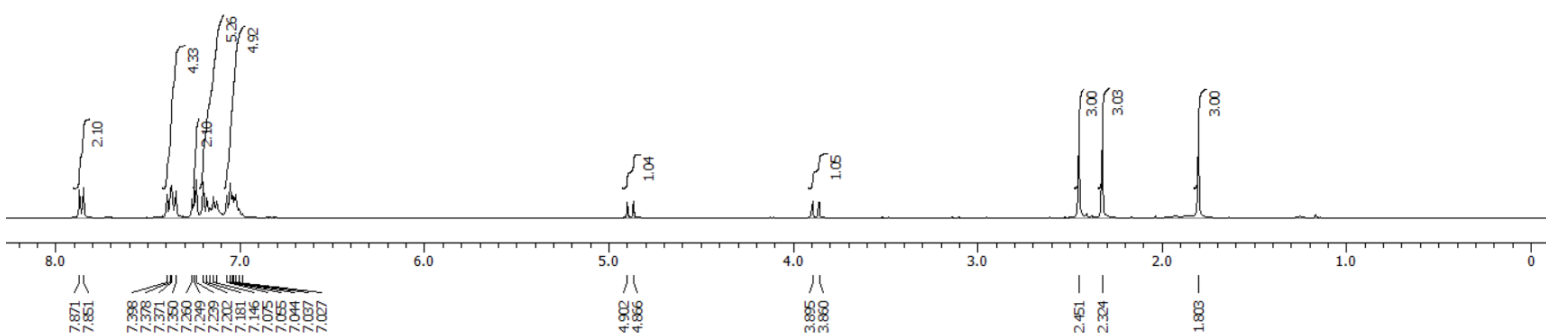
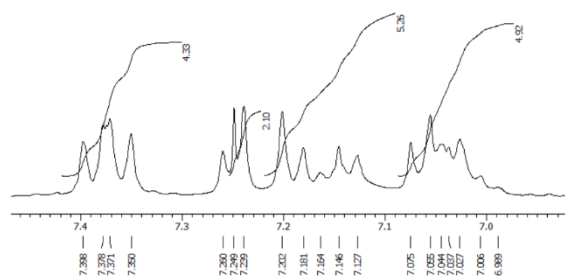
(E)-3-methyl-1-phenyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



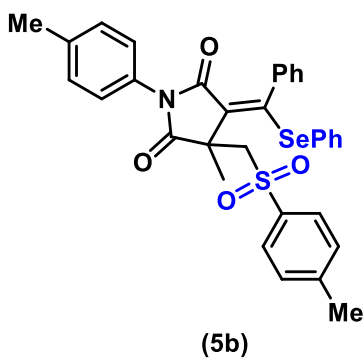
¹H NMR spectrum of 5b (400 MHz, CDCl₃)



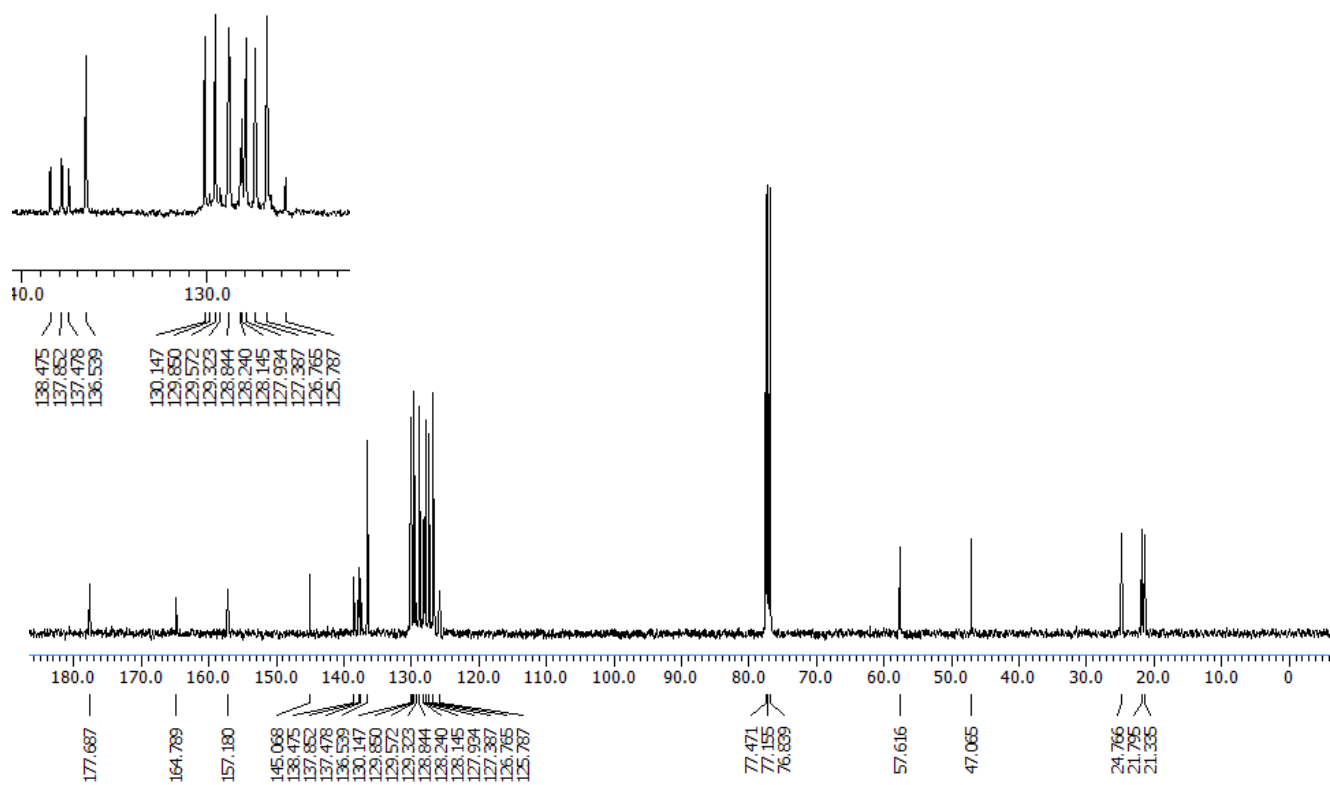
(E)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-(*p*-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione



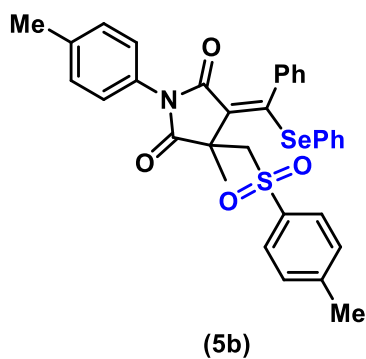
¹³C NMR spectrum of 5b (100 MHz, CDCl₃)



(E)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-(*p*-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione

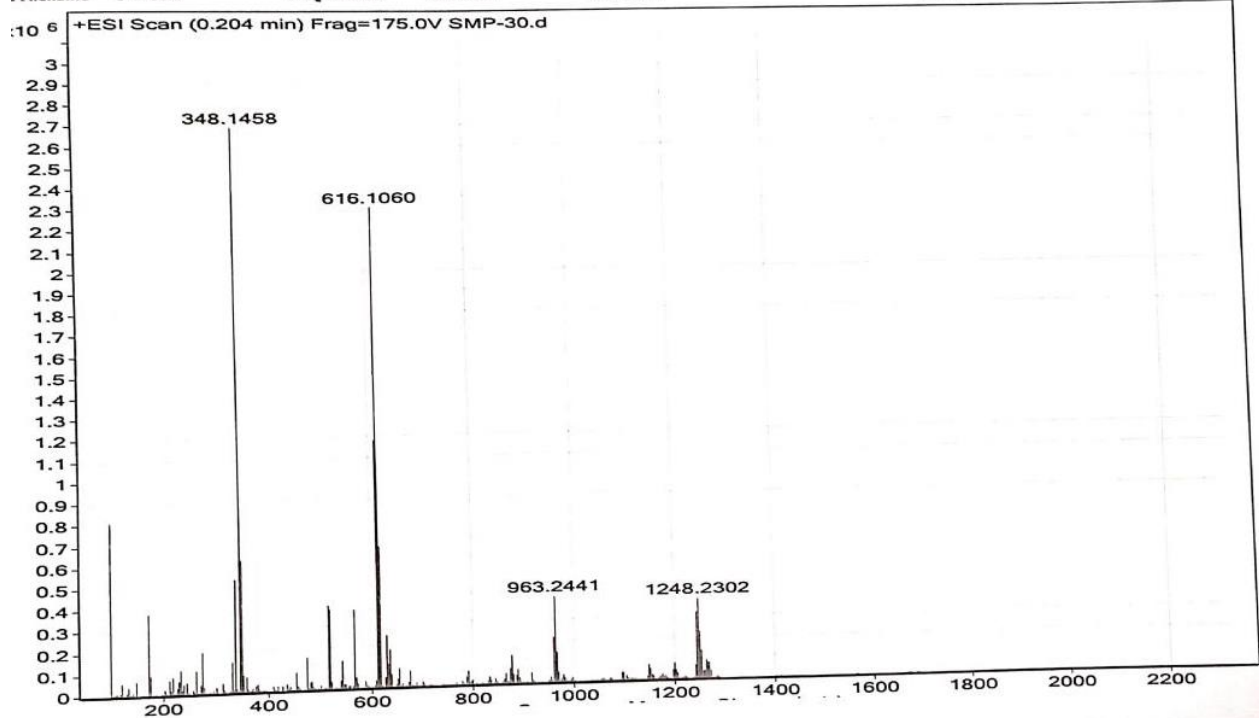


HRMS spectrum of 5b

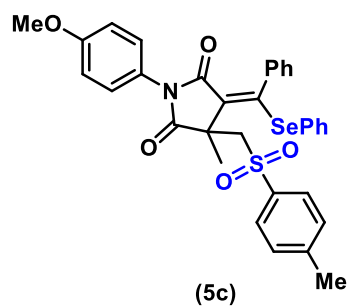


(E)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione

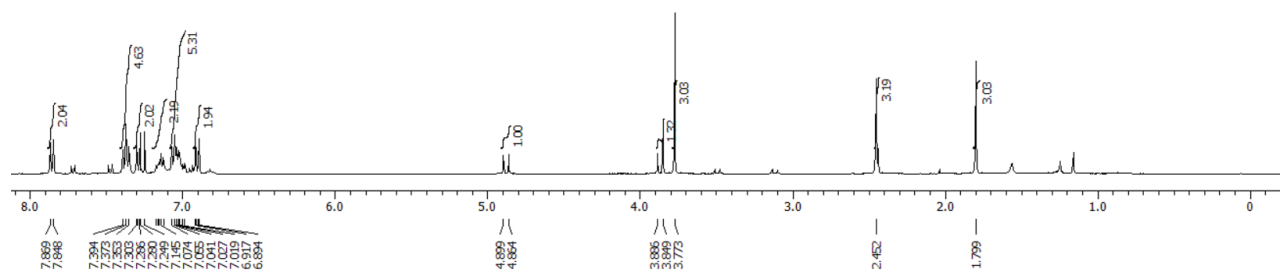
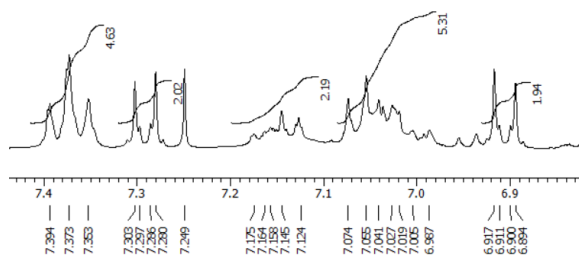
Sample Name	Position	Instrument Name	Instrument 1	User Name
SMP-30	P1-A9		Sample	
File Name	Injection Position	Sample Type	IRM Calibration Status	Success
SMP-30.d	MS Scan.m			02-05-2022 11:47:01
ACQ Method	Comment	Acquired Time		



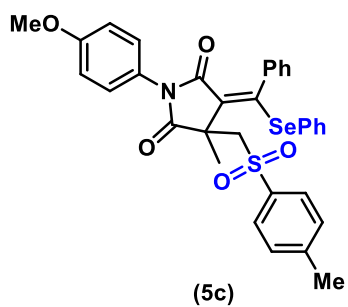
¹H NMR spectrum of 5c (400 MHz, CDCl₃)



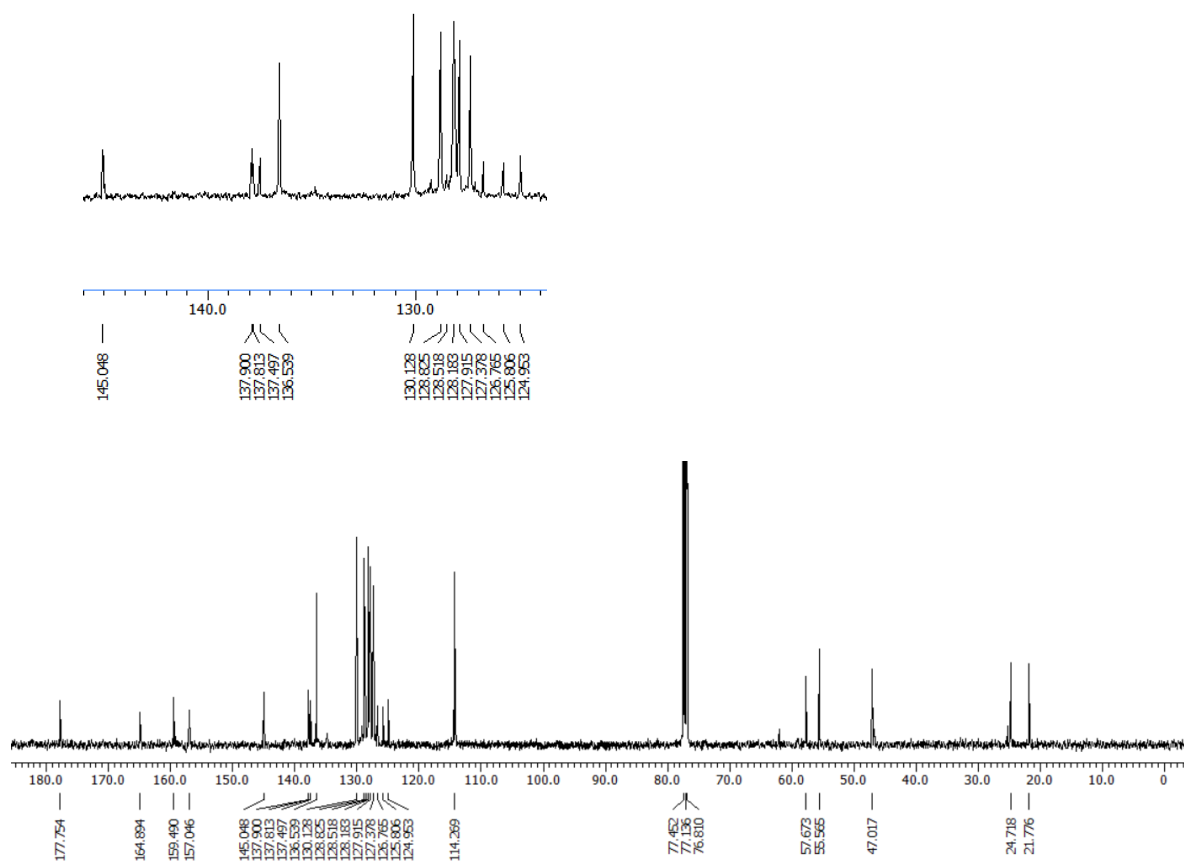
(E)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



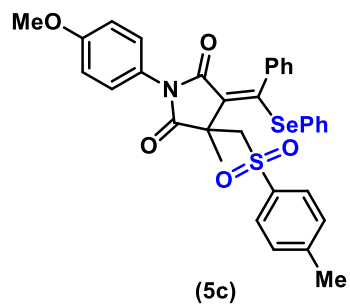
¹³C NMR spectrum of 5c (100 MHz, CDCl₃)



(E)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

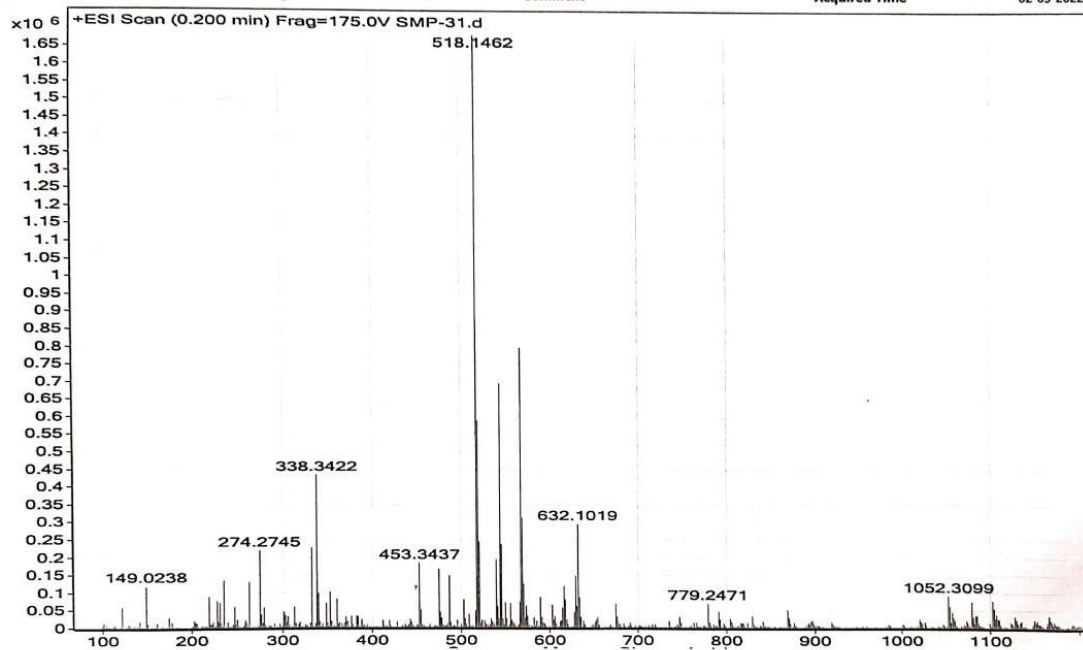


HRMS Spectrum of 5c

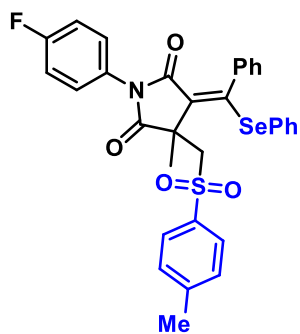


(E)-1-(4-methoxyphenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

Sample Name	SMP-31	Position	P1-A8	Instrument Name	Instrument 1	User Name	
Inj Vol	5	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SMP-31.d	ACQ Method	MS Scan.m	Comment		Acquired Time	02-05-2022 11:45:1

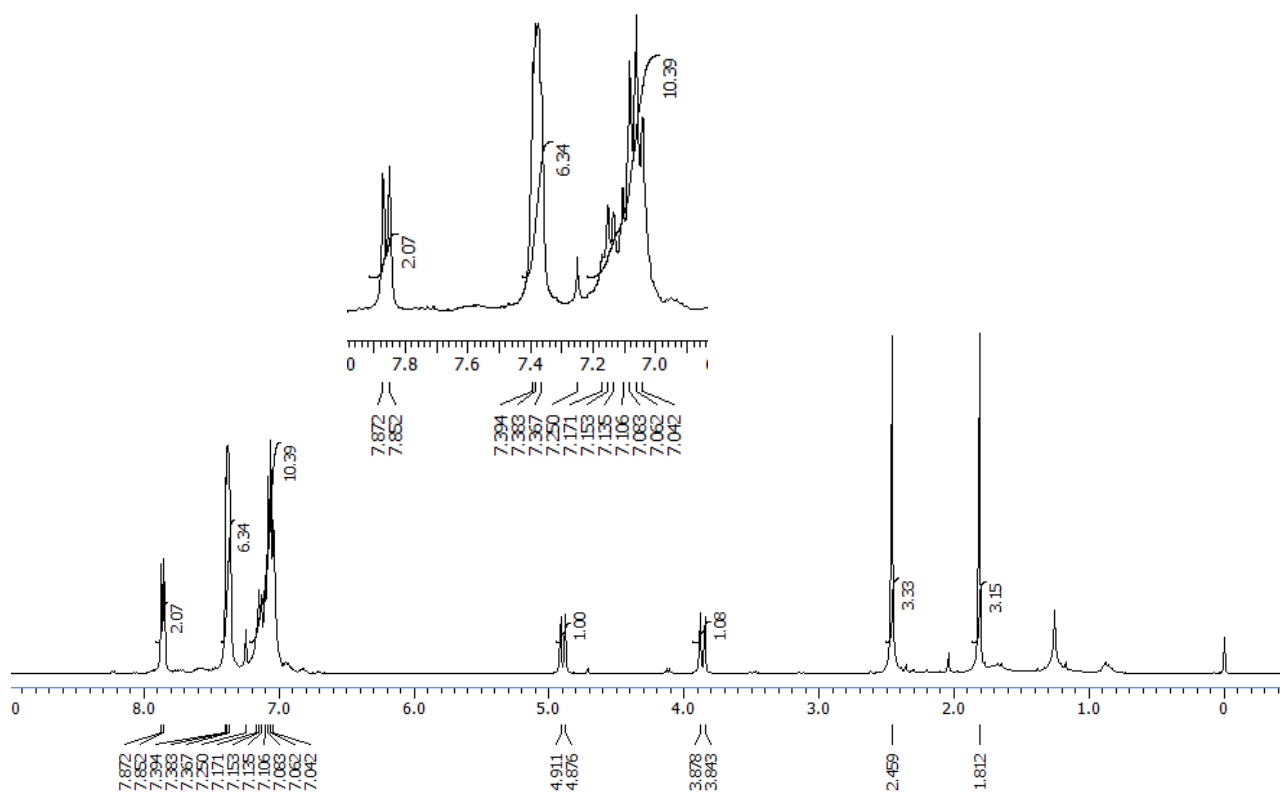


¹H NMR spectrum of 5d (400 MHz, CDCl₃)

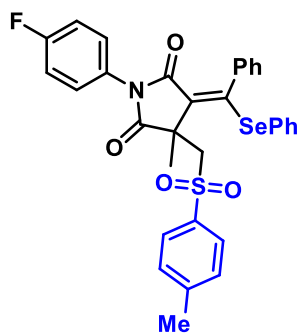


(5d)

(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

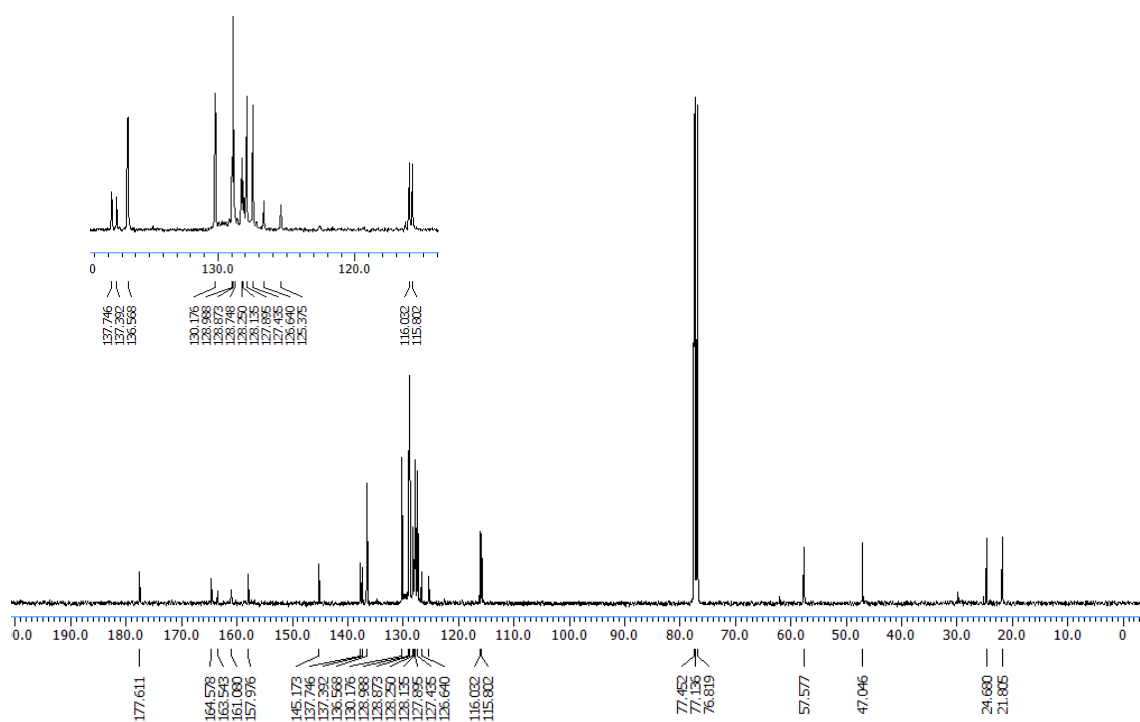


¹³C NMR spectrum of 5d (100 MHz, CDCl₃)

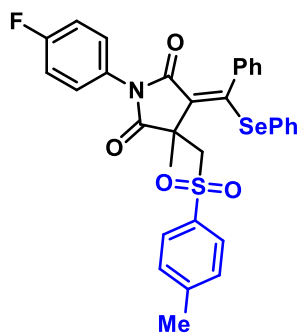


(5d)

(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

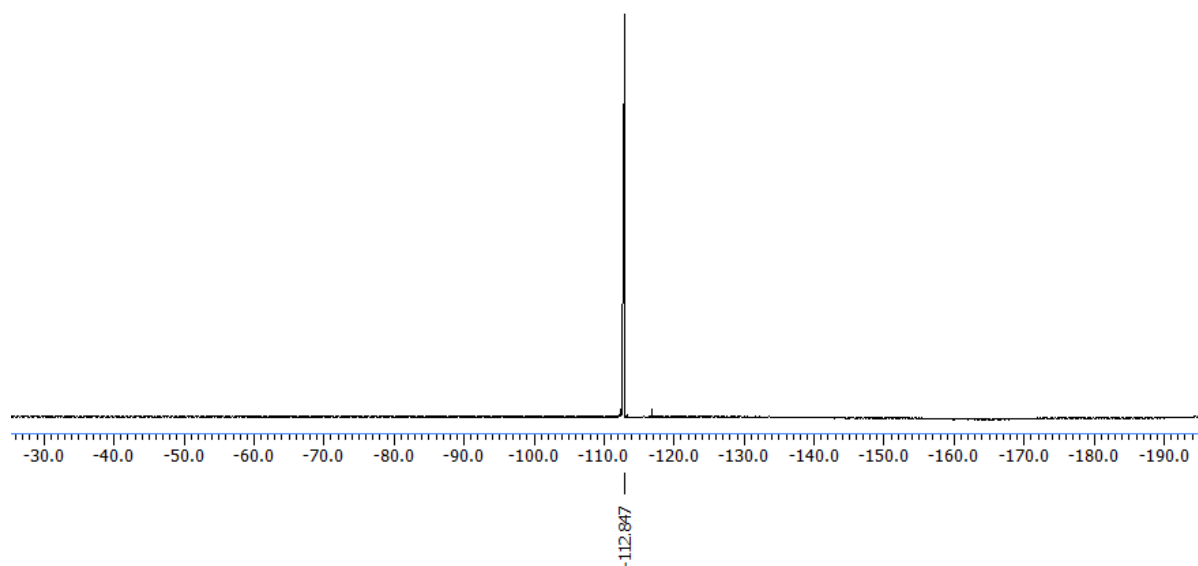


^{19}F Spectrum of 5d (376 MHz, CDCl_3)

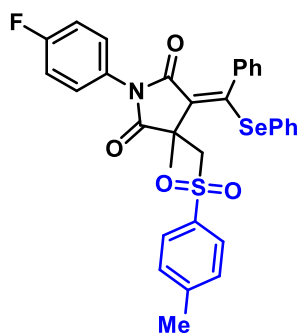


(5d)

(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS Spectrum of 5d



(5d)

(E)-1-(4-fluorophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

Qualitative Compound Report

Data File	SMP-26.d	Sample Name	SMP-26
Sample Type	Sample	Position	P1-A7
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	28-04-2022 10:57:44
IRM Calibration Status	Success	DA Method	Default.m
Comment			

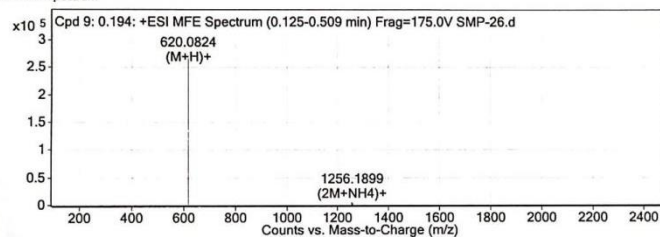
Sample Group	Info.	3
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

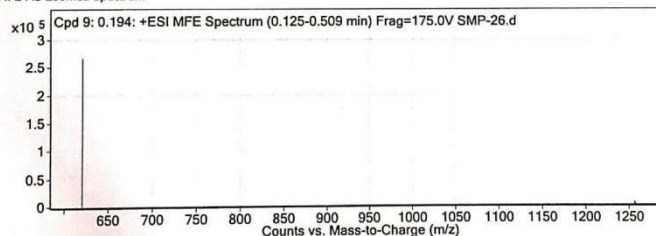
Compound Label	RT	Mass	MFG Formula
Cpd 9: 0.194	0.194	619.0752	<none>

Compound Label	m/z	RT	Algorithm	Mass
Cpd 9: 0.194	620.0824	0.194	Find by Molecular Feature	619.0752

MFE MS Spectrum



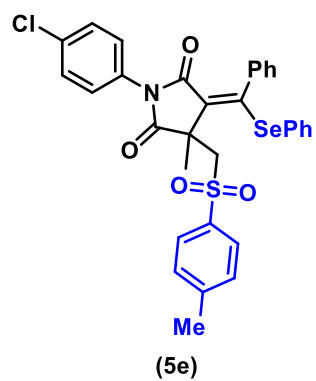
MFE MS Zoomed Spectrum



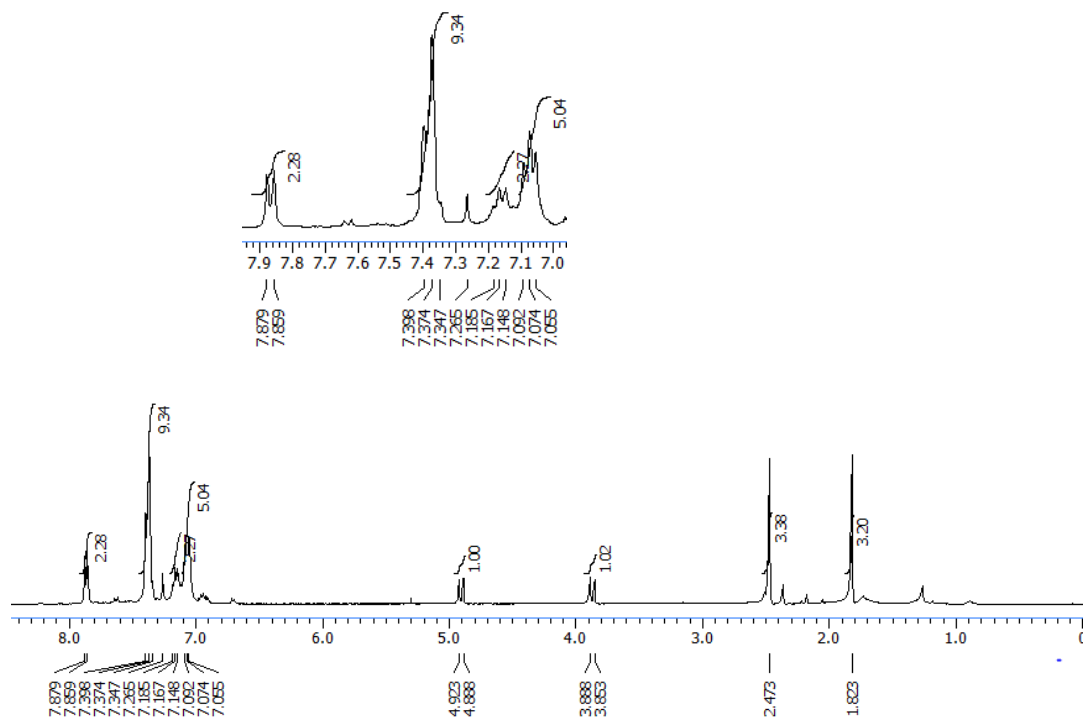
MS Spectrum Peak List

m/z	z	Abund	Ion
620.0824	1	267003.84	(M+H)+
1256.1899	1	4949.82	(2M+NH4)+
1257.1869	1	3838.71	(2M+NH4)+
1258.1891	1	3399.41	(2M+NH4)+

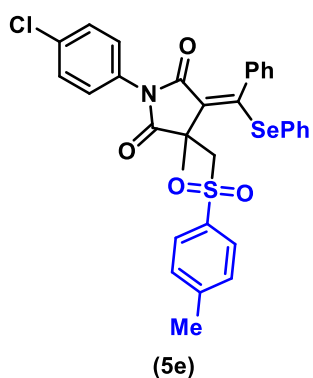
¹H NMR spectrum of 5e (400 MHz, CDCl₃)



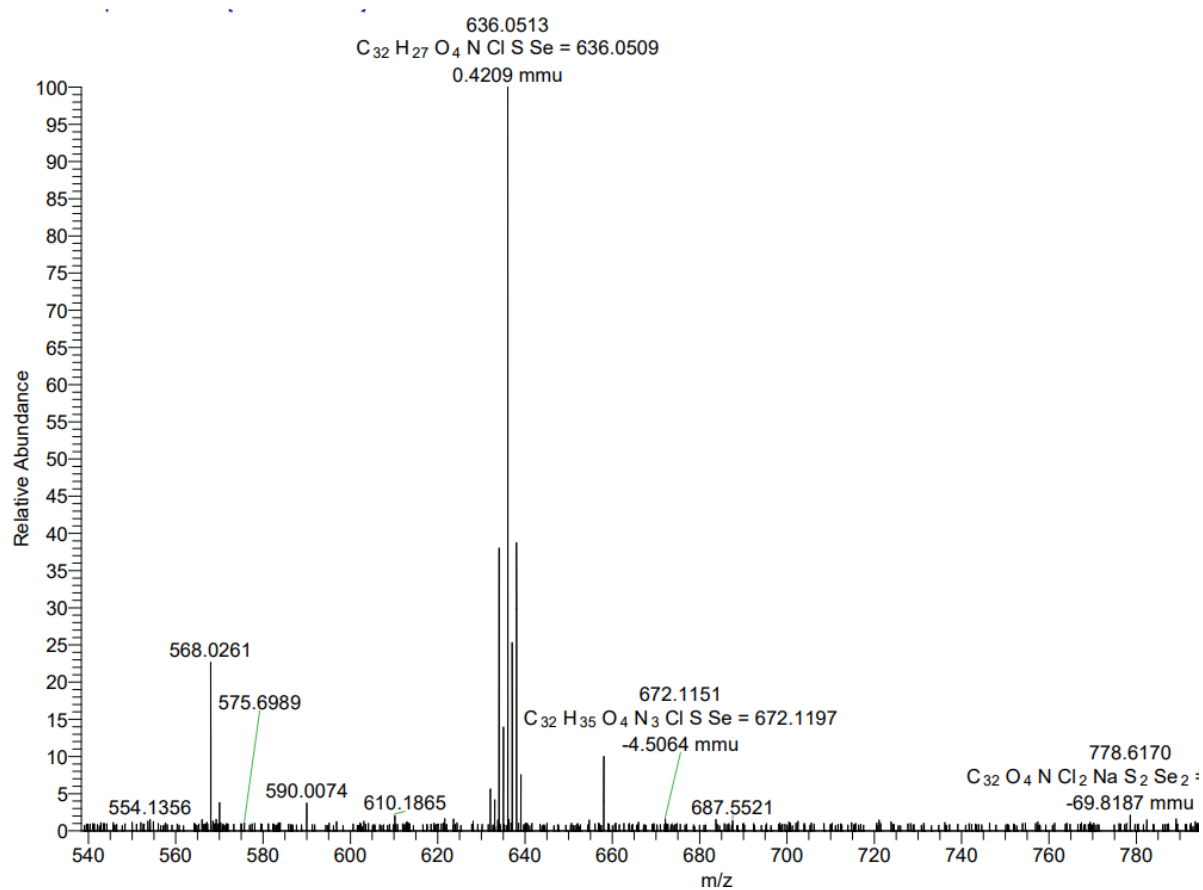
(E)-1-(4-chlorophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



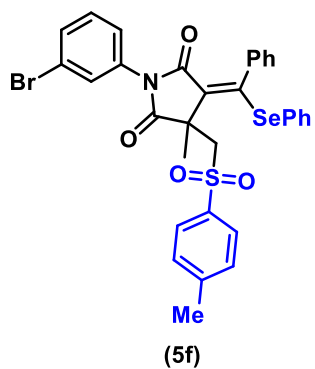
HRMS Spectrum of 5e



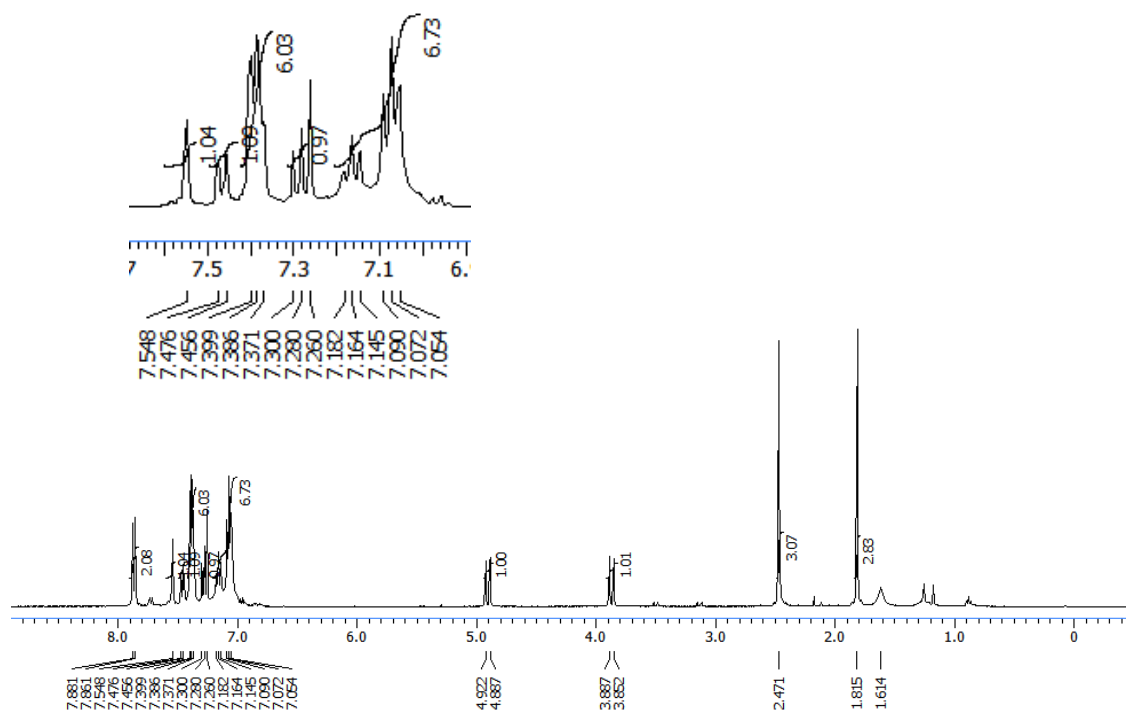
(E)-1-(4-chlorophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



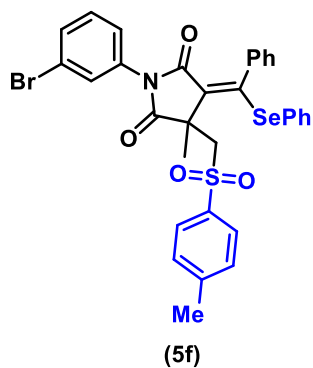
¹H NMR spectrum of 5f (400 MHz, CDCl₃)



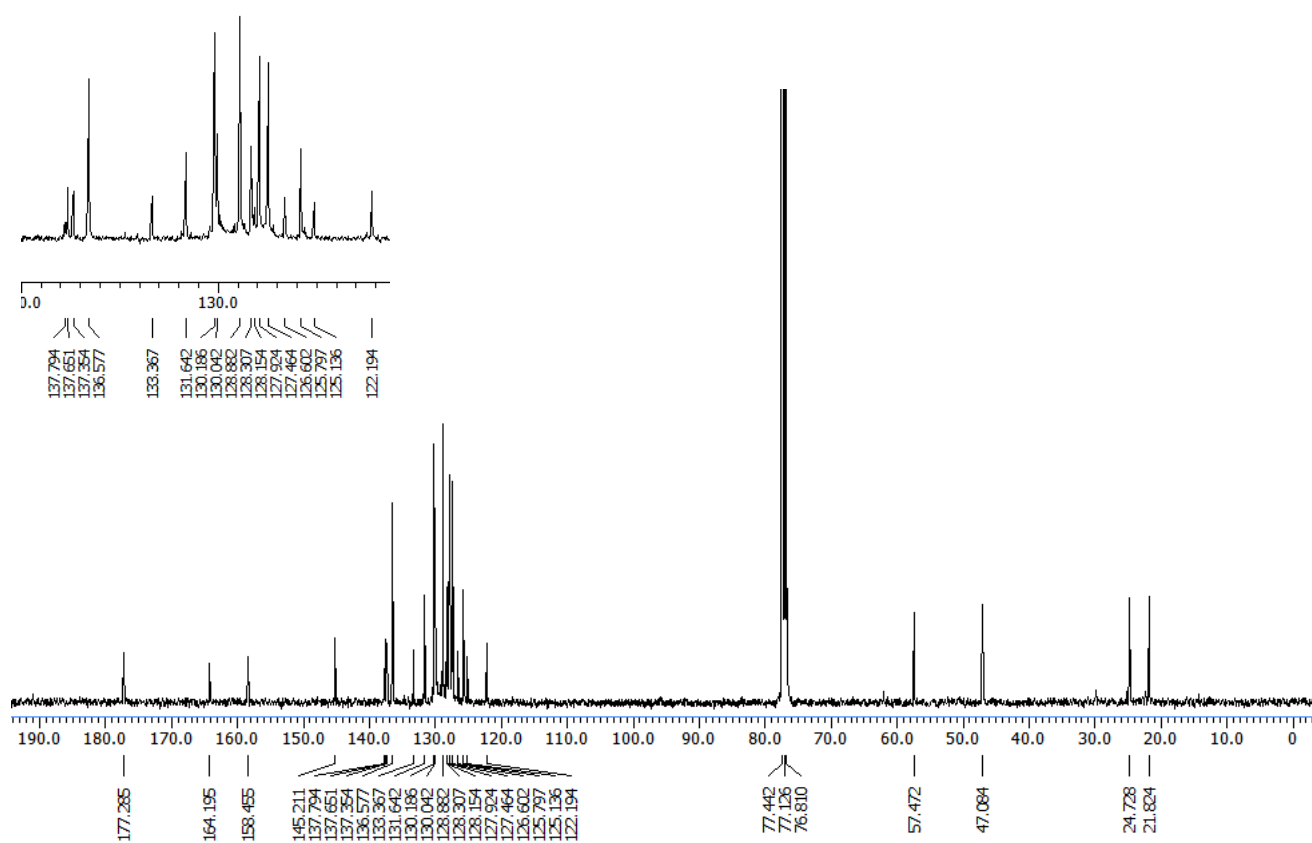
(E)-1-(3-bromophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



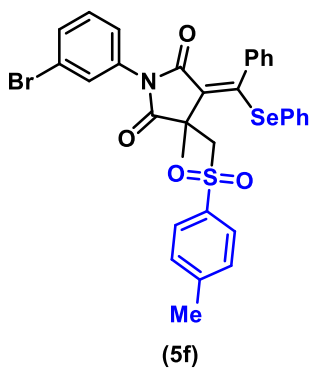
¹³C NMR spectrum of 5f (100 MHz, CDCl₃)



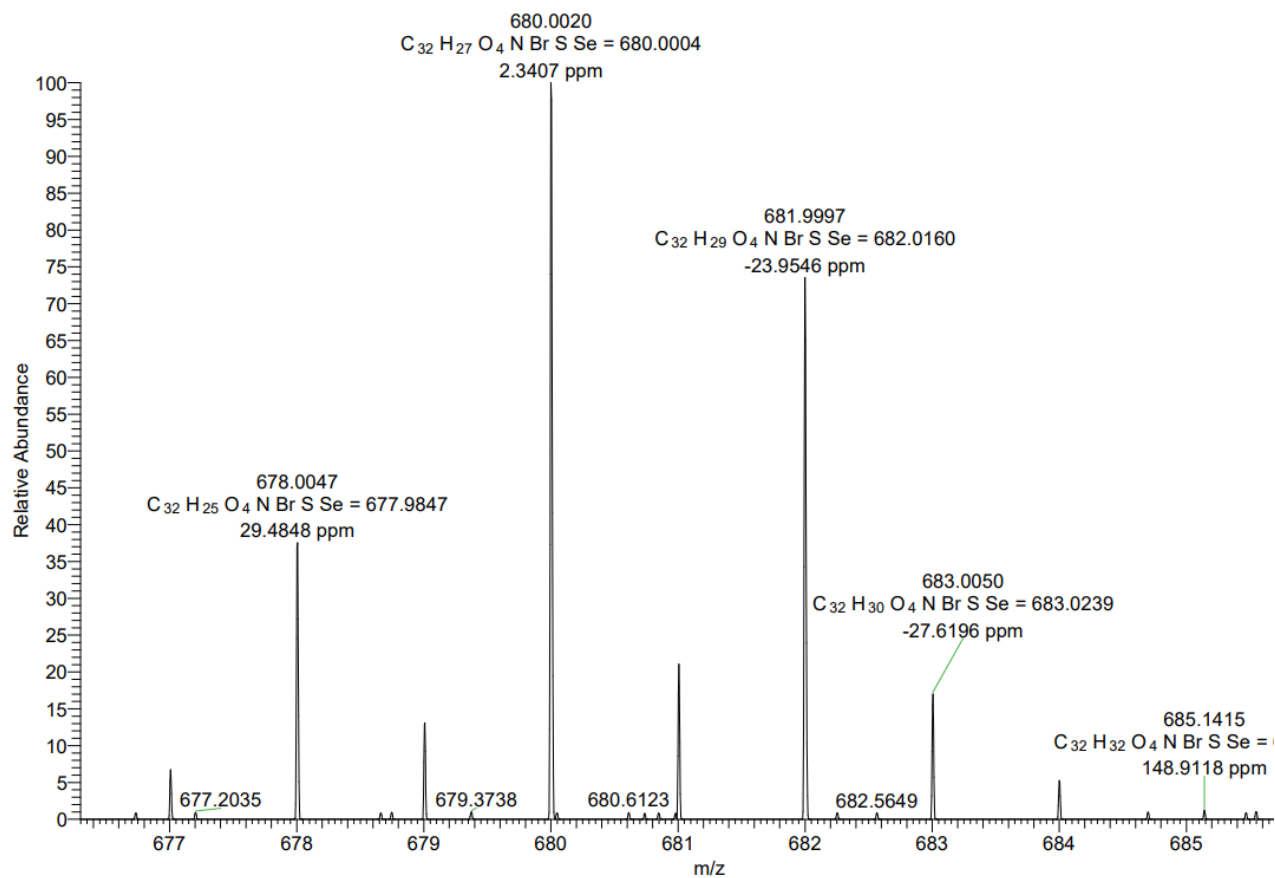
(E)-1-(3-bromophenyl)-3-methyl-4-(phenyl(phenylselenanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



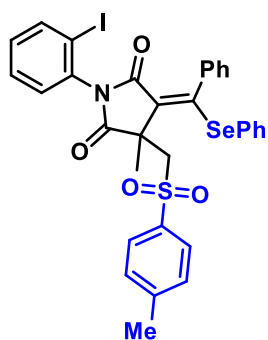
HRMS Spectrum of 5f



(E)-1-(3-bromophenyl)-3-methyl-4-(phenyl(phenylselenanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

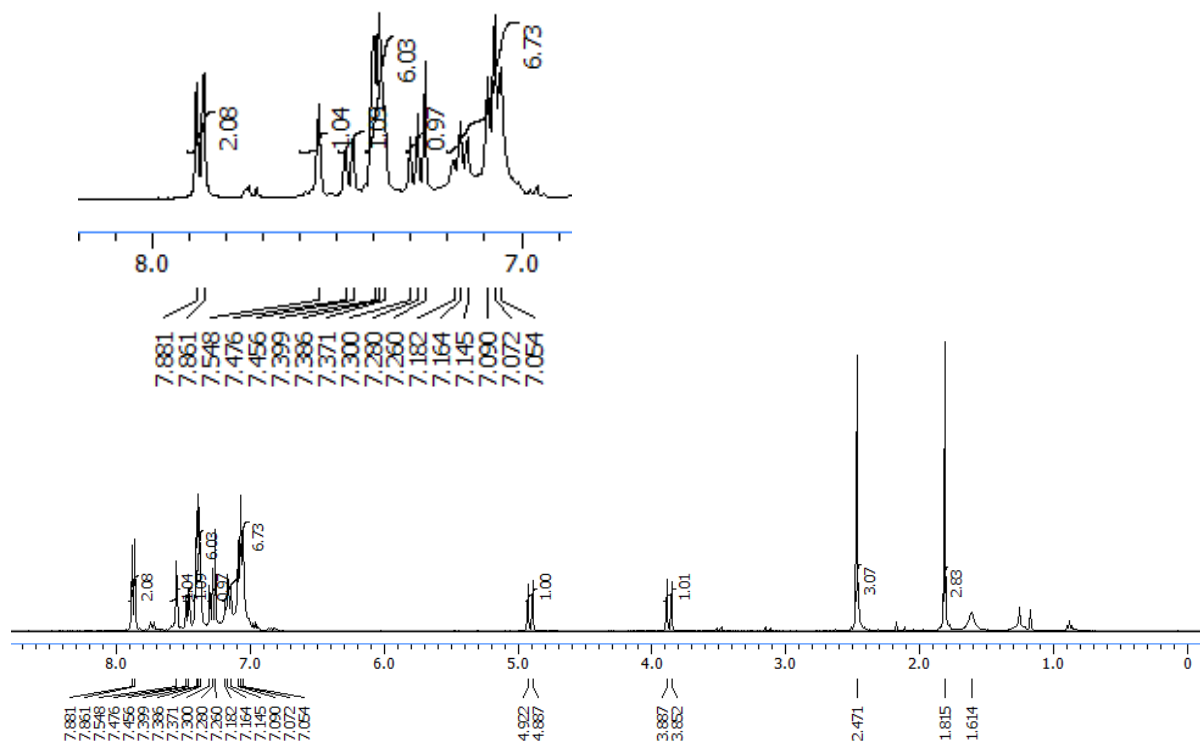


¹H NMR spectrum of 5g (400 MHz, CDCl₃)

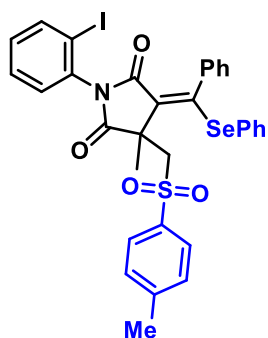


(5g)

(E)-1-(2-iodophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

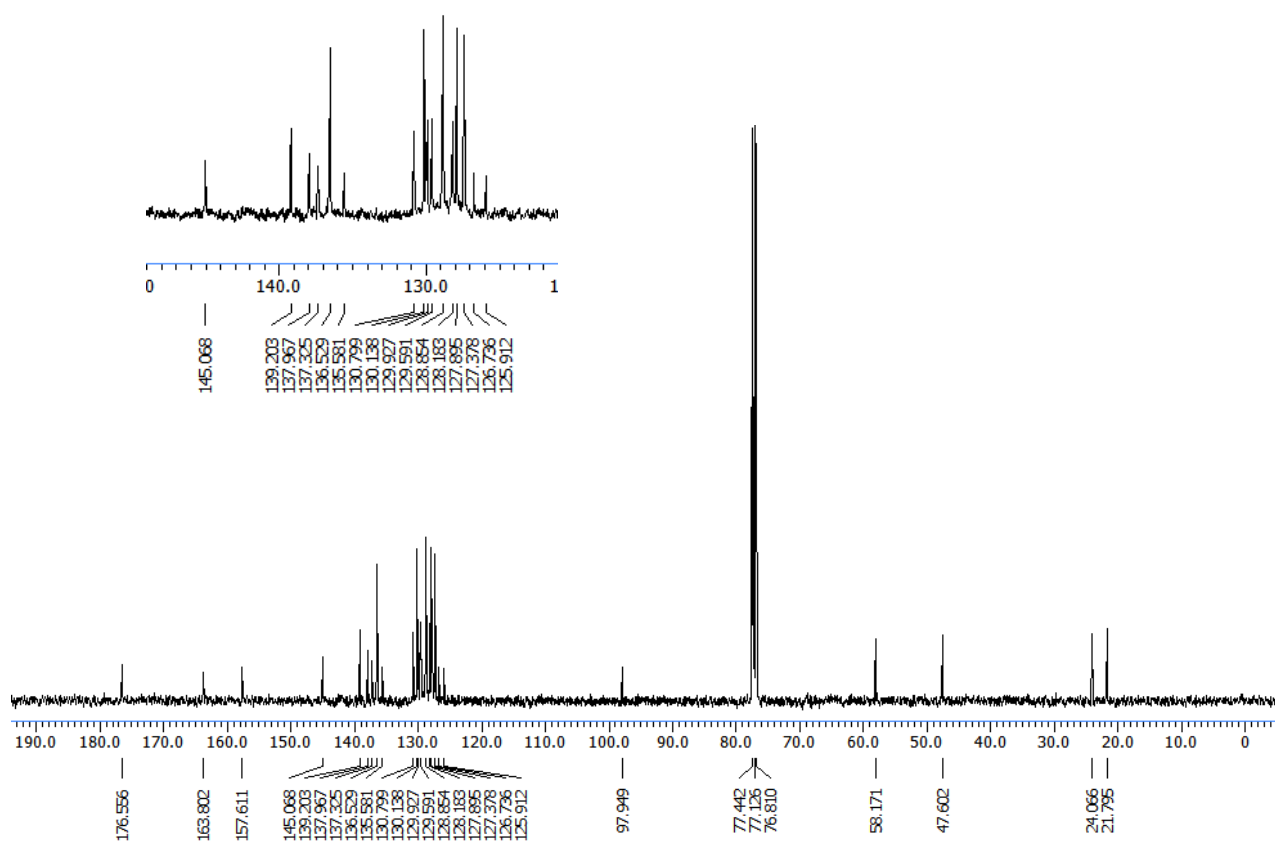


¹³CNMR spectrum of 5g (100 MHz, CDCl₃)

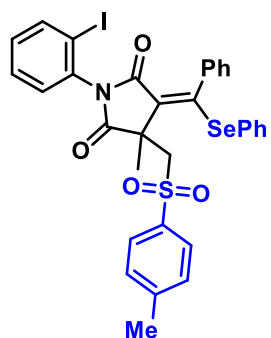


(5g)

(E)-1-(2-iodophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

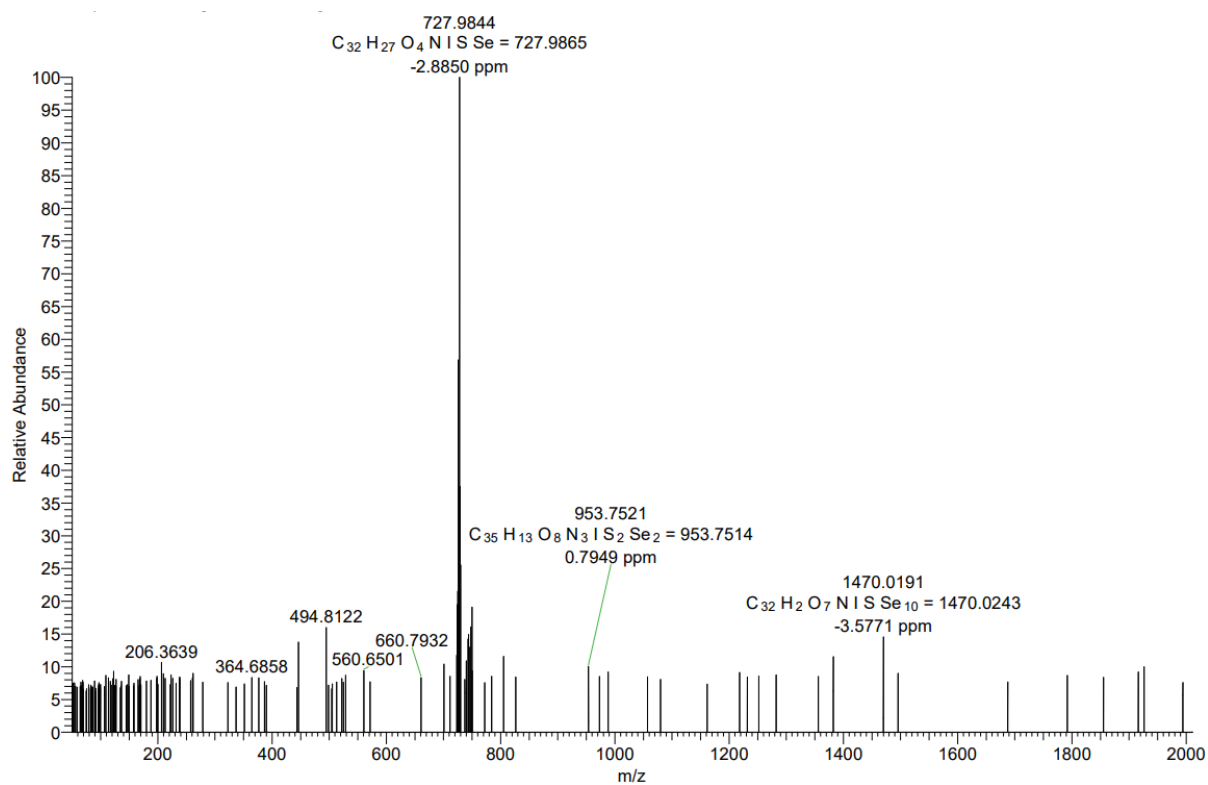


HRMS Spectrum of 5g

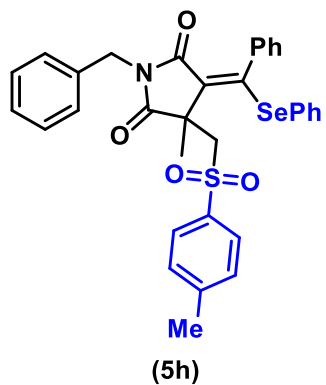


(5g)

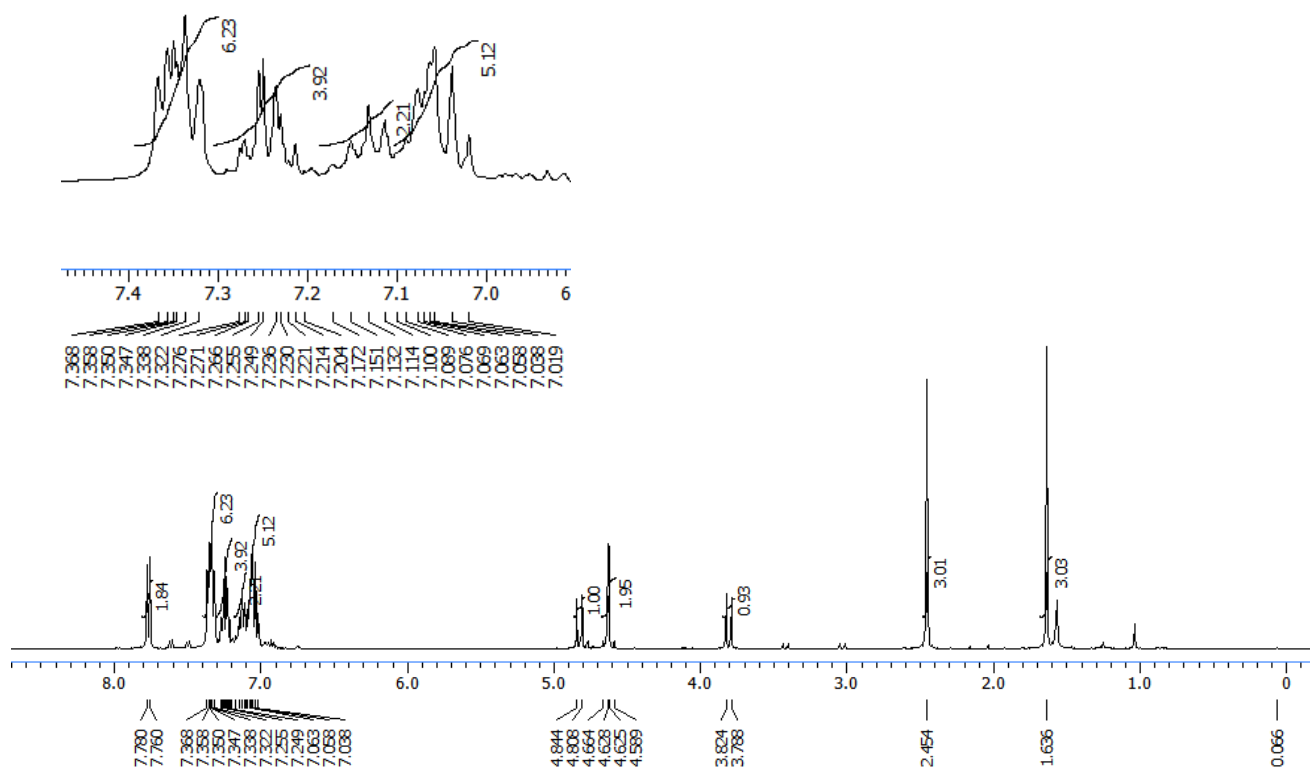
(E)-1-(2-iodophenyl)-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



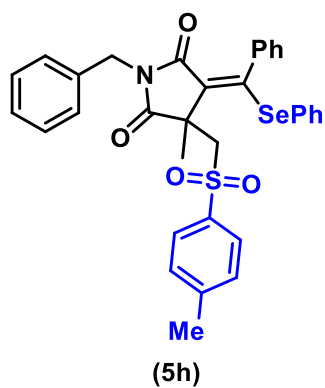
¹H NMR spectrum of 5h (400 MHz, CDCl₃)



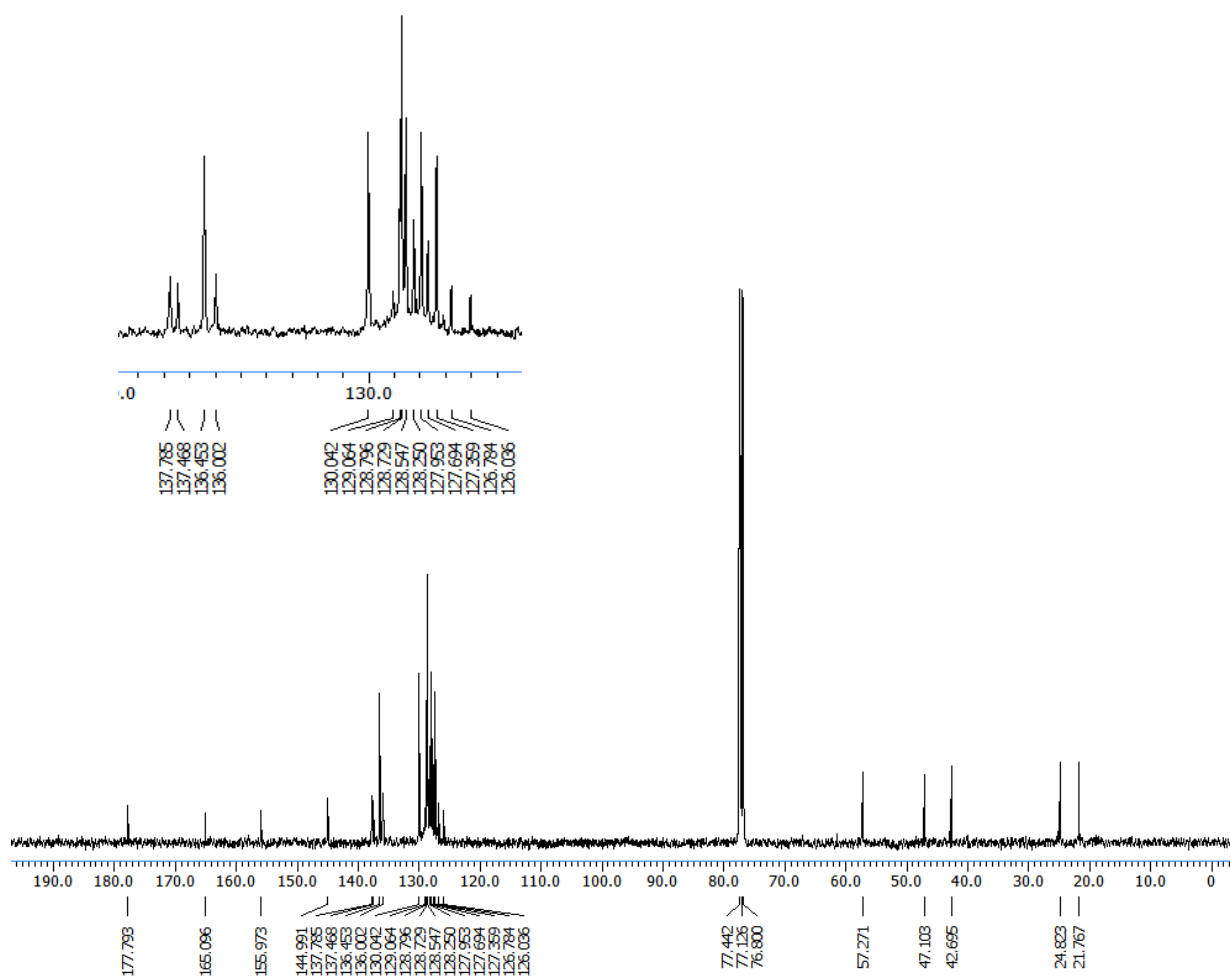
(*E*)-1-benzyl-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione



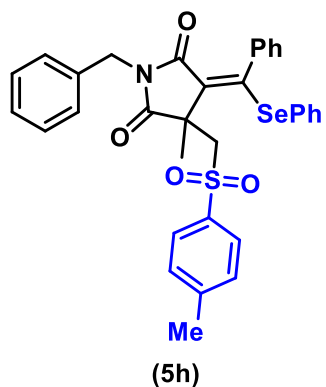
¹³C NMR spectrum of 5h (100 MHz, CDCl₃)



(*E*)-1-benzyl-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

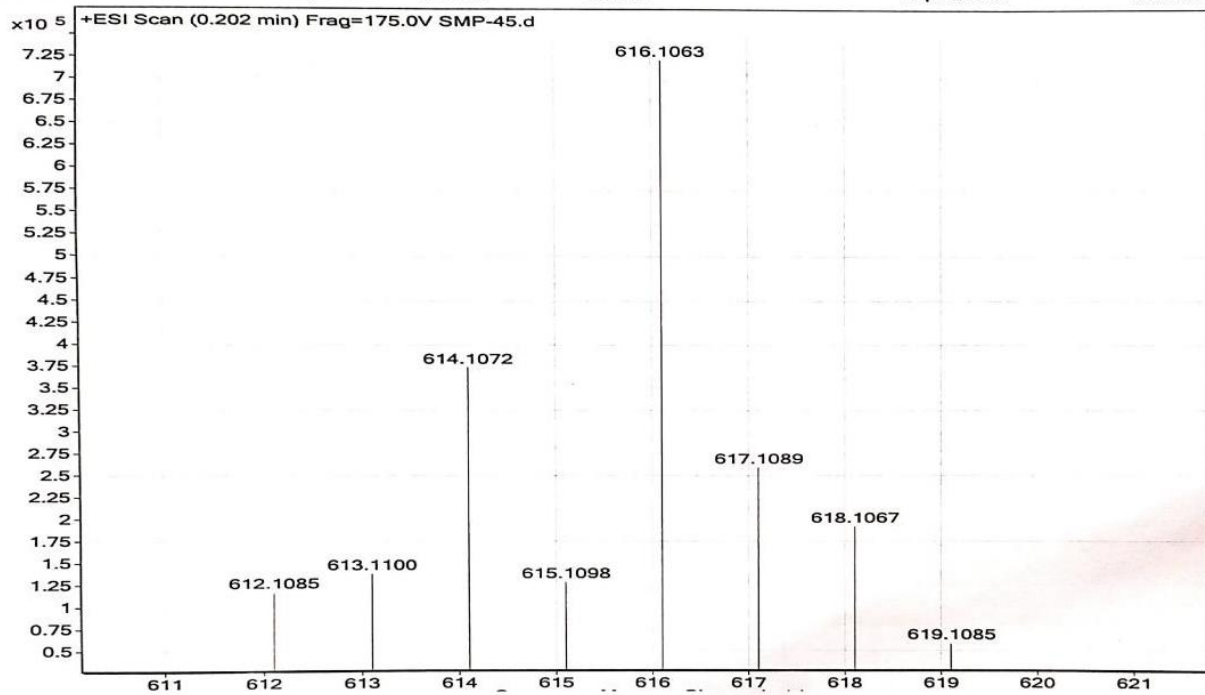


HRMS Spectrum of 5h

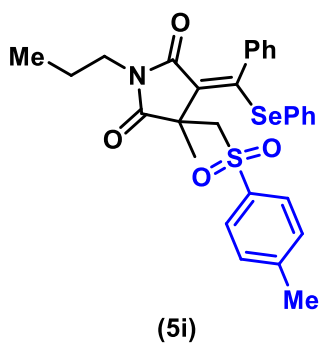


(E)-1-benzyl-3-methyl-4-(phenyl(phenylselanyl)methylene)-3-(tosylmethyl)pyrrolidine-2,5-dione

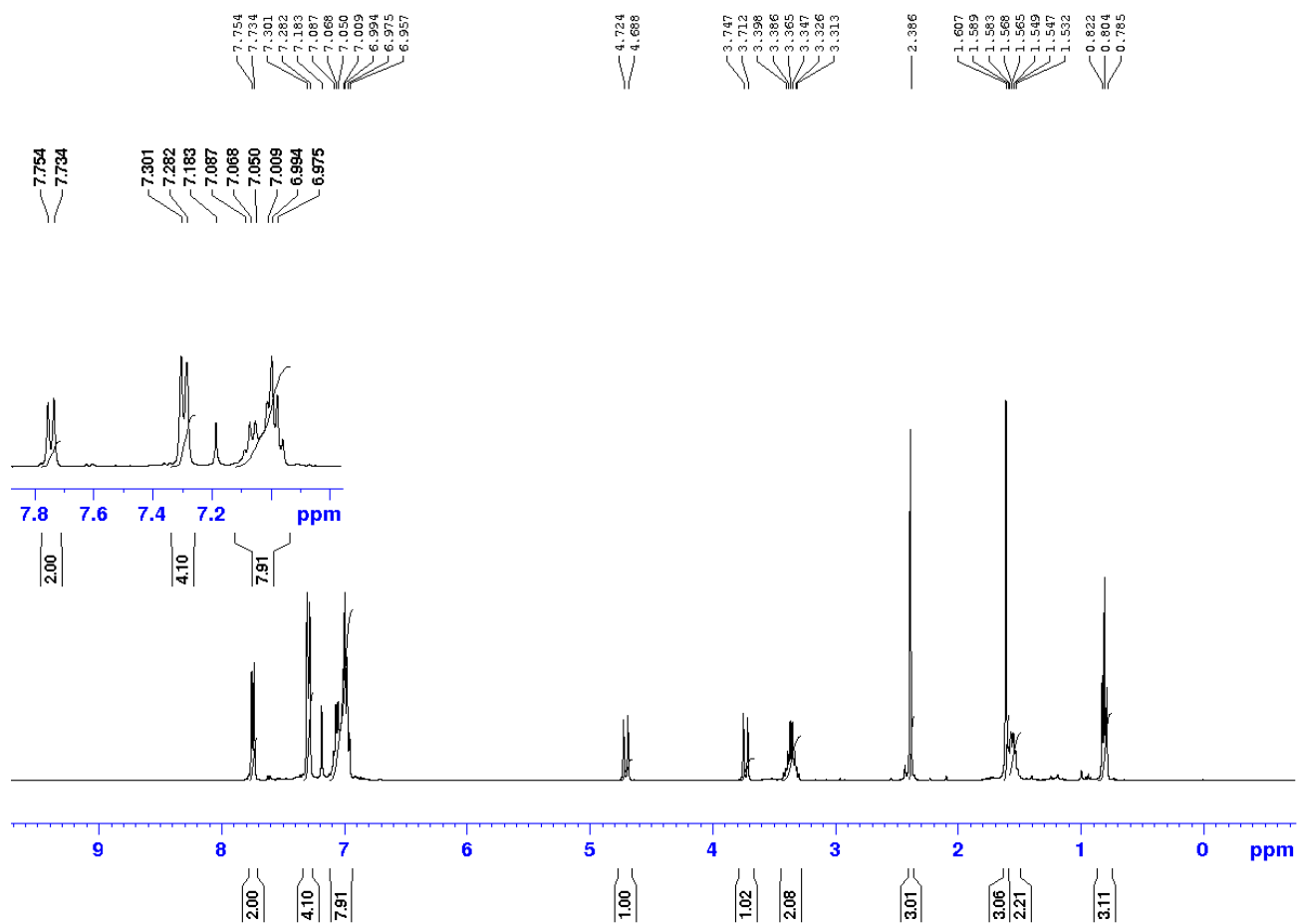
Sample Name	SMP-45	Position	P1-A3	Instrument Name	Instrument 1	User Name	
Inj Vol	5	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SMP-45.d	ACQ Method	MS Scan.m	Comment		Acquired Time	02-05-2022 11:35:38



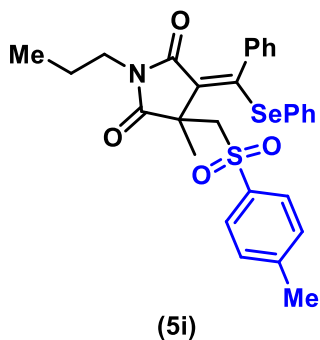
¹H NMR spectrum of 5i (400 MHz, CDCl₃)



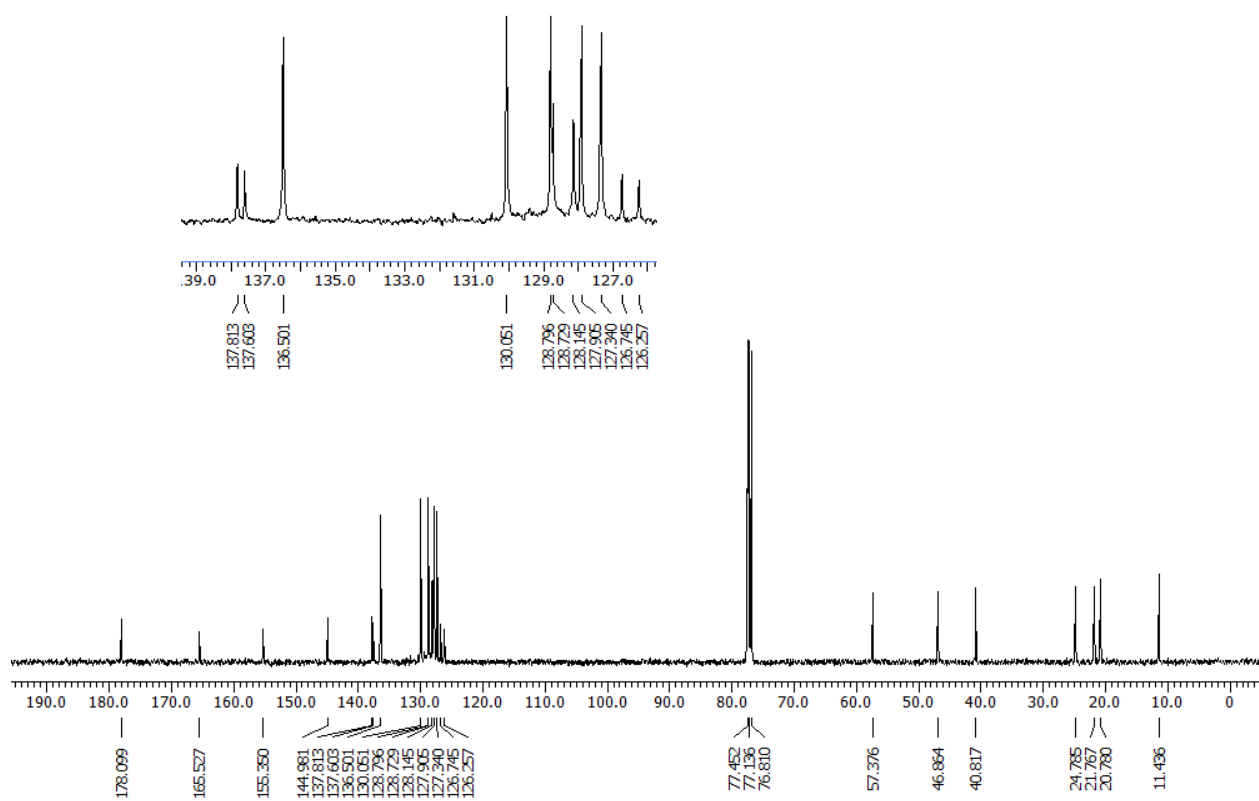
(E)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione



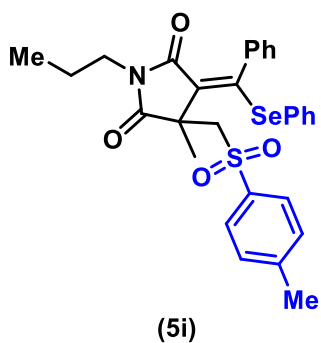
¹³C NMR spectrum of 5i (100 MHz, CDCl₃)



(E)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione

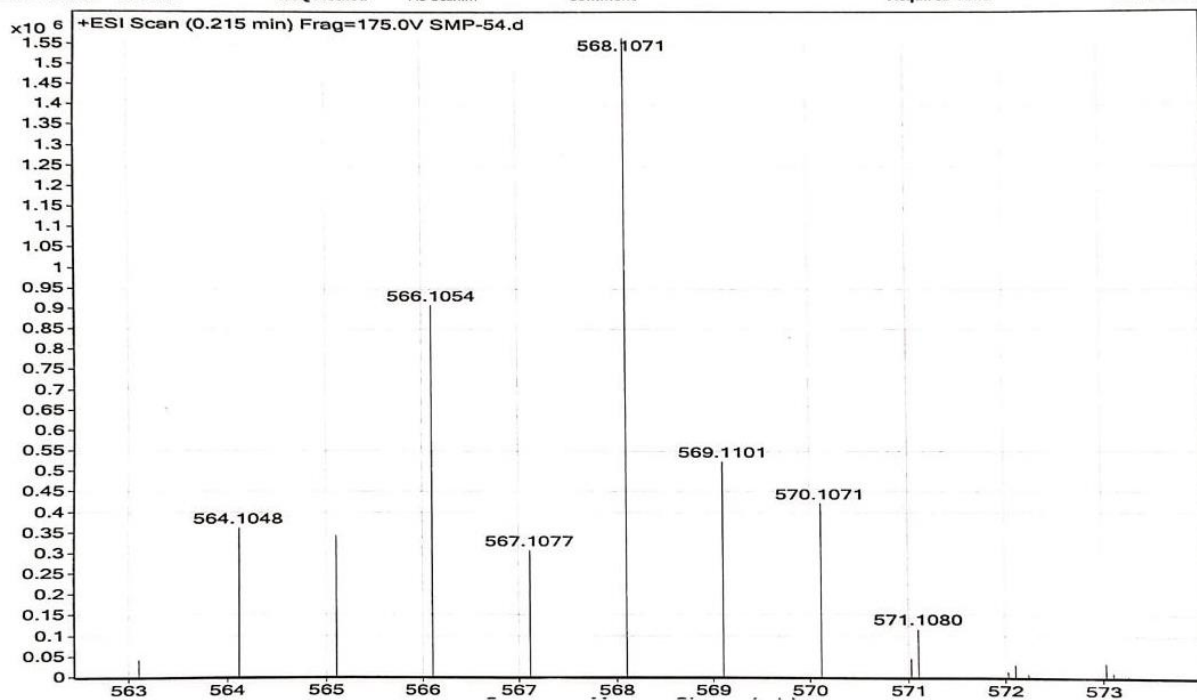


HRMS Spectrum of 5i



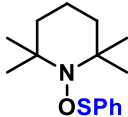
(*E*)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-propyl-3-(tosylmethyl)pyrrolidine-2,5-dione

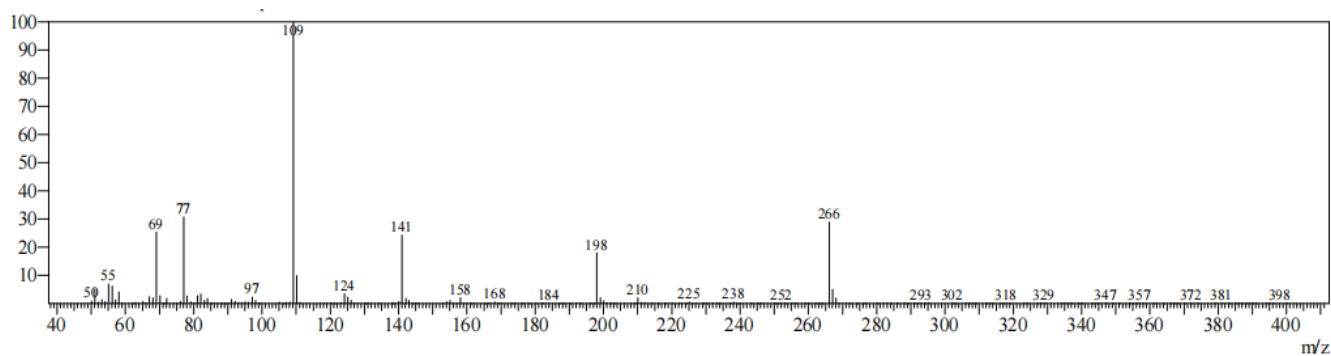
Sample Name	SMP-54	Position	P1-B2	Instrument Name	Instrument 1	User Name	
Inj Vol	5	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SMP-54.d	ACQ Method	MS Scan.m	Comment		Acquired Time	02-05-2022 11:50:29



(10) GCMS Data:

1) GCMS Data of TEMPO adduct:

Structure of TEMPO Adduct	Molecular Formula	Molecular weight	Molecular mass found
	C ₁₅ H ₂₃ NOS	265.42	266.0



2) GCMS Data of PhSSPh Intermediate:

Compound	Molecular Formula	Molecular weight	Molecular mass found
PhSSPh	C ₁₂ H ₁₀ S ₂	218.02	218.0

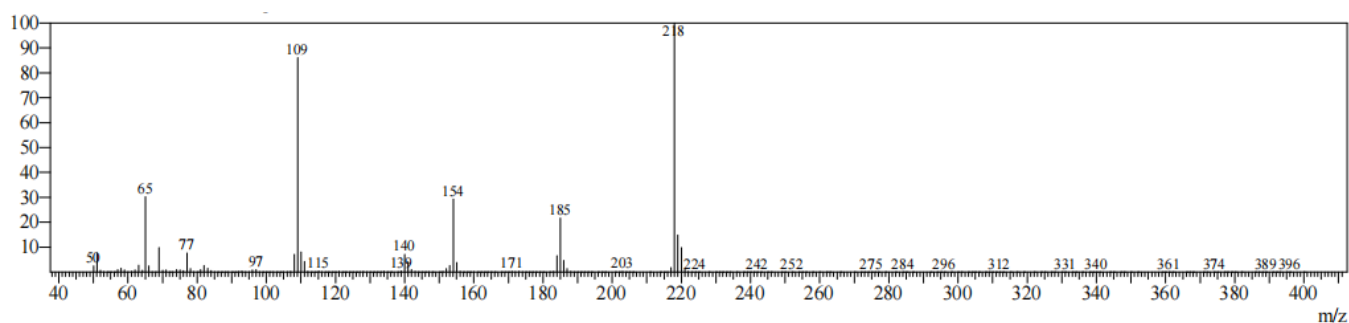


Figure S2: GC Mass Spectrum of PhSSPh

(11) X-Ray Crystallographic Data of 3aa and 5e:

Data Collection and Refinement Single-crystal X-ray data of compounds was collected on Bruker SMART CCD Diffractometer using graphite monochromated MoK α radiation ($\lambda = 0.71073 \text{ \AA}$). Frames were collected at T = 302 K by ω , ϕ , and 2θ -rotations with full quadrant data collection strategy (four domains each with 600 frames) at 10s per frame with SMART. The measured intensities were reduced to F^2 and corrected for absorption with SADABS. Structure solution, refinement, and data output were carried out with the SHELXTL package by direct methods. Non-hydrogen atoms were refined anisotropically using the WinGX (version 1.80.05) program package.¹³ All non-hydrogen atoms were refined anisotropically and hydrogen atoms were treated as riding atoms using SHELX default parameters. Molecular structures have drawn using ORTEP software shown in figure S1 and S2. Further information on the crystal structure determination (excluding structure factors) has been given as table S1 and S2 and also deposited in the Cambridge Crystallographic Data Centre as supplementary publications number 1587648. Copies of the data can be obtained free of charge upon application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033. e-mail: deposit@ccdc.cam.ac.uk) or via internet.

Table S2: Crystallographic description of (*E*)-3-methyl-1-phenyl-4-(phenyl(phenylthio)methylene)-3-tosylmethylpyrrolidine-2,5-dione (3aa):

Identification code	smt101_0ma_a	
Empirical formula	C ₃₂ H ₂₇ N O ₄ S ₂	
Formula weight	553.67	
Temperature	299 K	
Wavelength	0.71073	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 15.0121(19) Å	a = 90°.
	b = 13.2954(19) Å	b = 113.157(3)°.

	$c = 15.133(2) \text{ \AA}$	$g = 90^\circ$.
Volume	$2777.1(6) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.324 Mg/m^3	
Absorption coefficient	0.230 mm^{-1}	
F(000)	1160.0	
Crystal size	$0.20 \times 0.18 \times 0.16 \text{ mm}^3$	
Theta range for data collection	2.228 to 28.272°.	
Index ranges	-16<=h<=20, -12<=k<=17,- 20<=l<=20	
Reflections collected	4542	
Independent reflections	6739 [R(int) = 0.0366]	
Completeness to theta = 25.242°	100 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6739 / 0 / 354	
Goodness-of-fit on F ²	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0684, wR2 = 0.1389	
R indices (all data)	R1 = 0.1057, wR2 = 0.1591	
Largest diff. peak and hole	0.9325 and -0.7958 e.Å ⁻³	
CCDC	2145105	

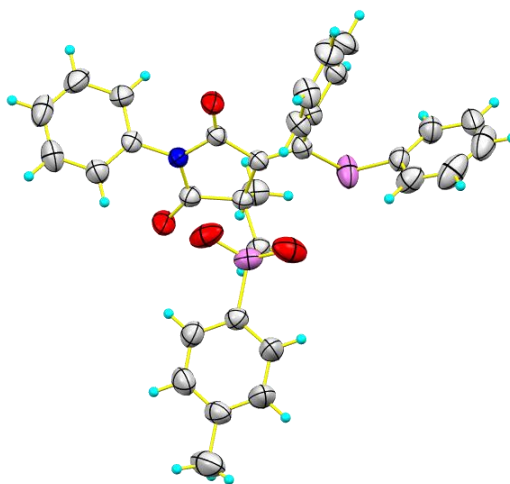


Figure S3: ORTEP diagram of **3aa**

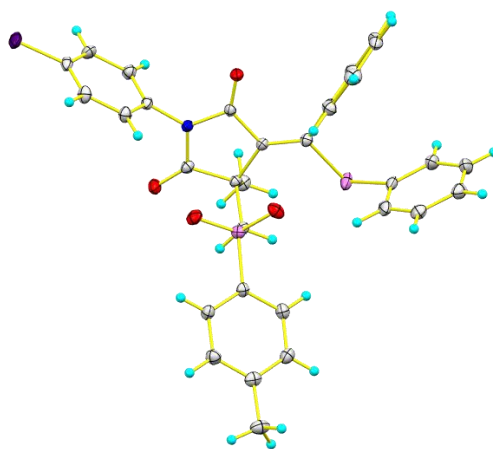


Figure S4: ORTEP diagram of **5e**

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- 4) Zhang, R; Xu, P; Wang, S.Y; Ji, S.J. *J. Org. Chem.* **2019**, *84*,12324.
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