Supporting Information

Visible Light Promoted Metal and Oxidant-Free Stereoselective Synthesis of Functionalized Succinimides from Aza-1,6-Enynes.

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(1) General Information.

All reagents were purchased (unless specified) at highest commercial quality from Chemscene India and used as received. Reaction mixtures were stirred magnetically. All require temperature for reactions were achieved using an IKA heating plate and oil bath.

Rf: LC analysis was performed on commercially prepared 60 F_{254} silica gel plates and visualized by either UV irradiation or by staining with I_2. 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.

^{1}H 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).

^{13}C 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) X-Ray Crystallographic Data of 3n.

Data Collection and Refinement Single-crystal X-ray data of compounds was collected on Bruker SMART CCD Diffractometer using graphite monochromated MoKα radiation (λ = 0.71073 Å). 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.[11] 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. 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 S2, S3 and S4. Further information on the crystal structure determination (excluding structure factors) has been given as table S1 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.

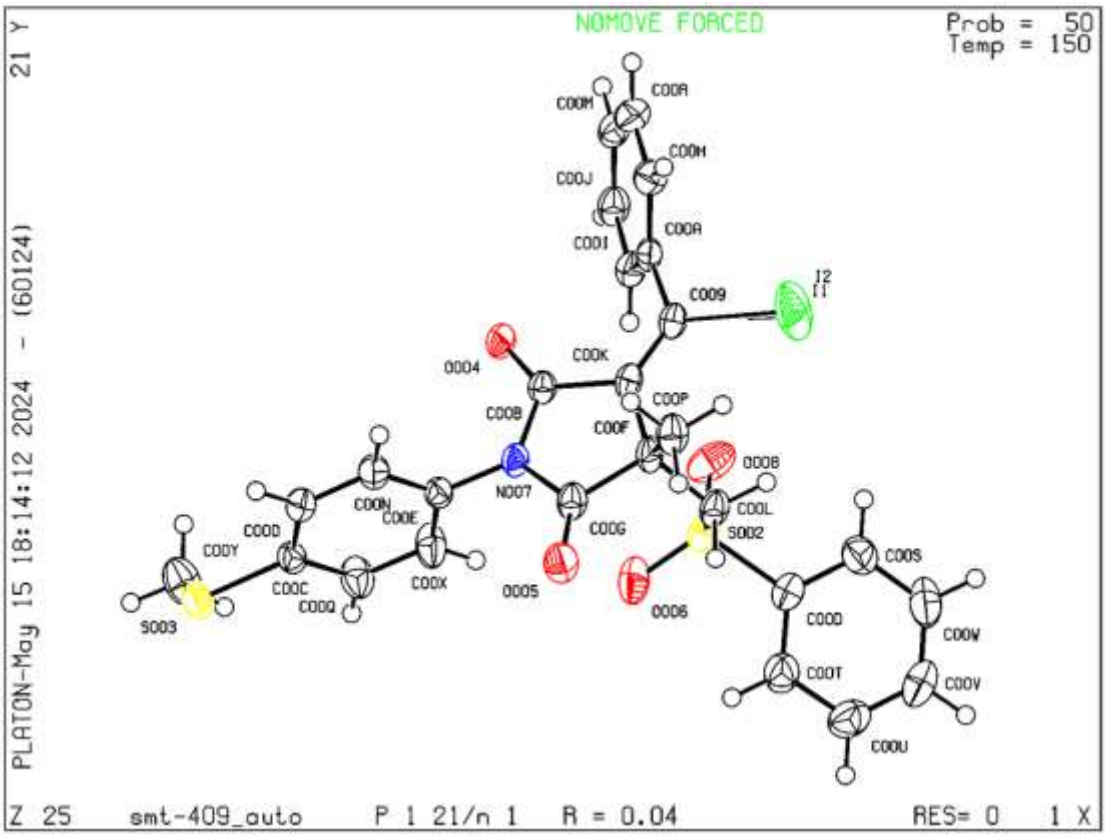


Figure S2: Ellipsoid plot

Table S1: Crystallographic description of (E)-4-(iodo(phenyl)methylene)-3-methyl-1-(4-(methylthio)phenyl)-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3m):

Identification code	SMT-409_auto	
Empirical formula	C26H22INO4S2	
Formula weight	603.46	
Temperature/K	149.99(10)	
Wavelength	0.71073	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.6157(2) Å	a= 90°.
	b = 12.7786(4)Å	b= 91.946(3)°.
	c = 24.7893(9) Å	g = 90°.
Volume	2411.05(13) $Å^3$	
Z	4	
Density (calculated)	1.662 Mg/m^3	
Absorption coefficient	1.536 mm^{-1}	
F(000)	1208.0	
Crystal size	0.20 x 0.24 x 0.18 mm^3	
2Theta range for data collection	6.23 to 52.744°.	
Index ranges	-8 ≤ h ≤ 9, -15 ≤ k ≤ 15, -30 ≤ l ≤ 30	
Reflections collected	24651	
Independent reflections	4923 [Rint = 0.0521, Rsigma = 0.0375]	
Completeness to theta = 27.71°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4923/0/318	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0366, wR2 = 0.0863	
R indices (all data)	R1 = 0.0483, wR2 = 0.0922	
Largest diff. peak and hole	0.74 and -0.60 $e.Å^{-3}$	
CCDC	2356138	

(3) Experimental Setup

1. **Instrument Name:** Aldrich Micro Photochemical Reactor (ALDKIT001)

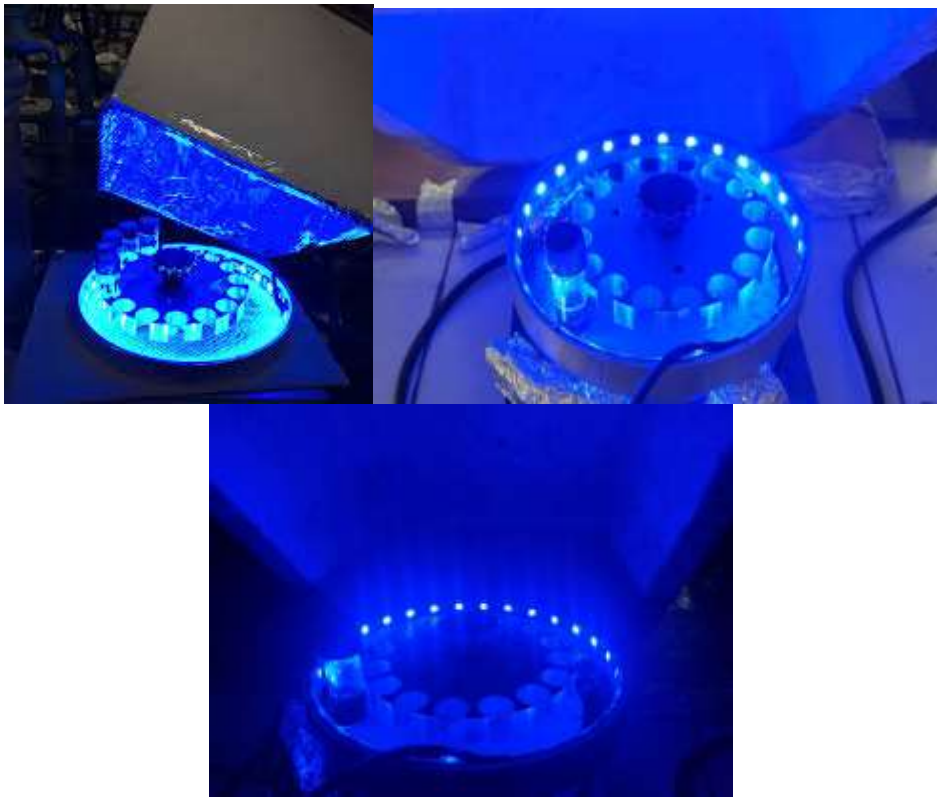
2. **Technical Specifications**

   i) Power Supply: 500 mA 5-6 watts

   ii) Input Voltage: 100-240 VAC

   iii) Wavelength: 435-445 nm

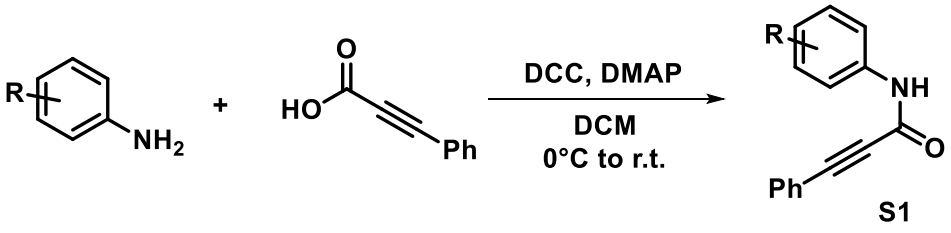
3. **Reaction Setup**



(4) Synthesis of Substrate 1:

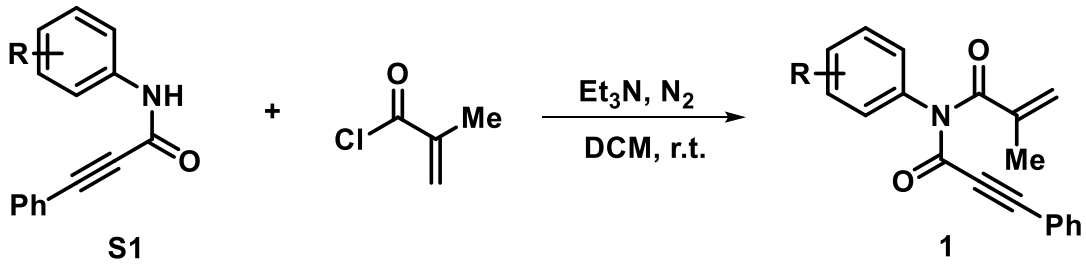
Substrate **1** were prepared following the reported procedure.[1]

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

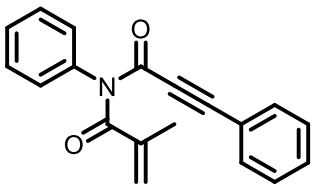


Phenylpropiolic acid (1 equiv) and DMAP (10 mol%) were charged into an oven-dried round-bottom flask, which was then purged with nitrogen gas for 10 minutes. After dissolving the mixture in DCM, amine (1.1 equiv) was added. The mixture was cooled to 0°C and a saturated solution of DCC (1.0 equiv) in 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 comlumn chromatography (PE:EA=0.5:9.5) to afford pure product **1**. The prepared substrates (**1a-1k**) are as follows: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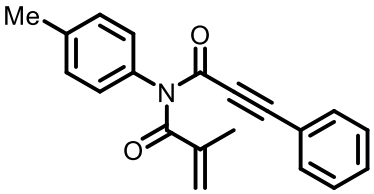
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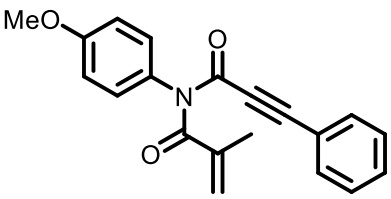
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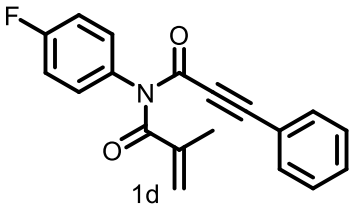
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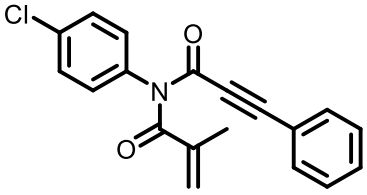
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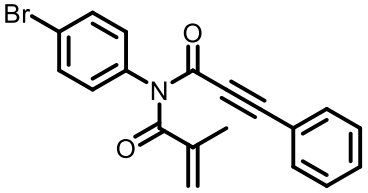
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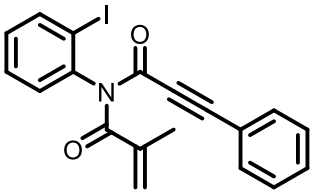
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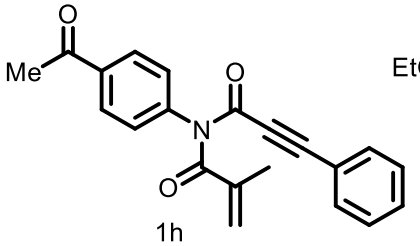
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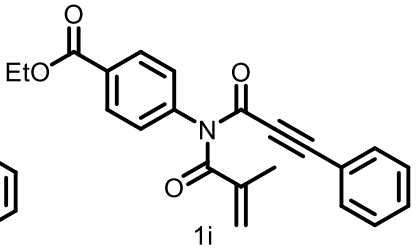
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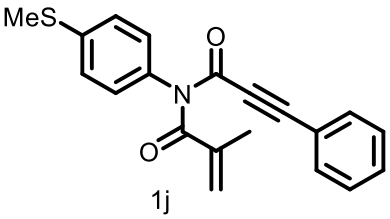
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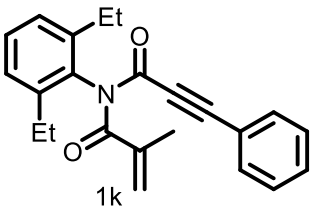
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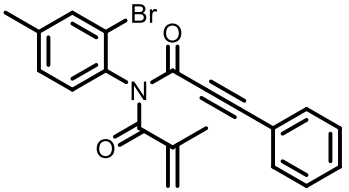
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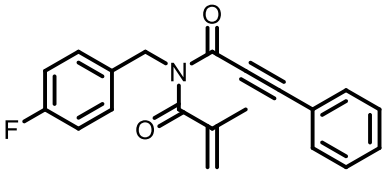
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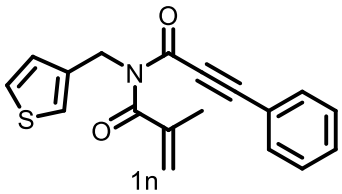
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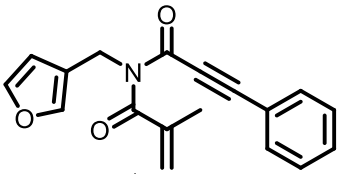
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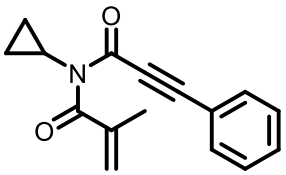
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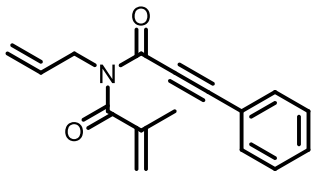
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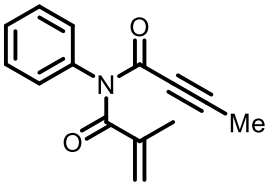
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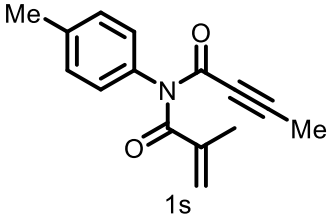
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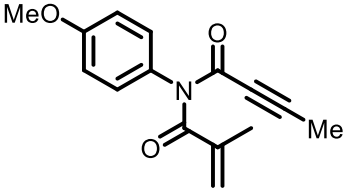
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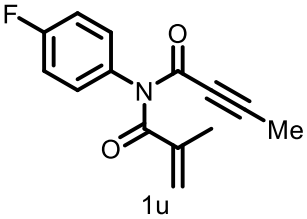
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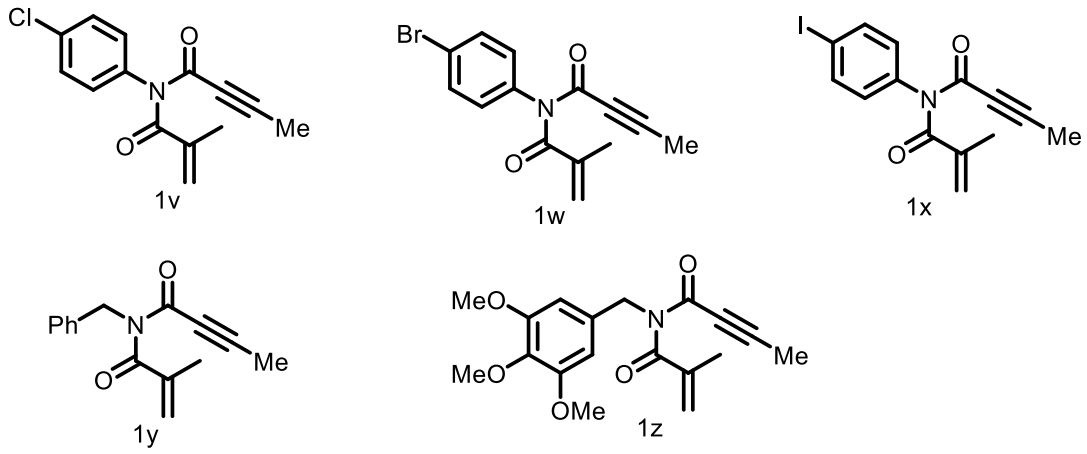
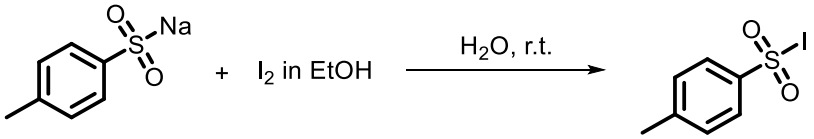
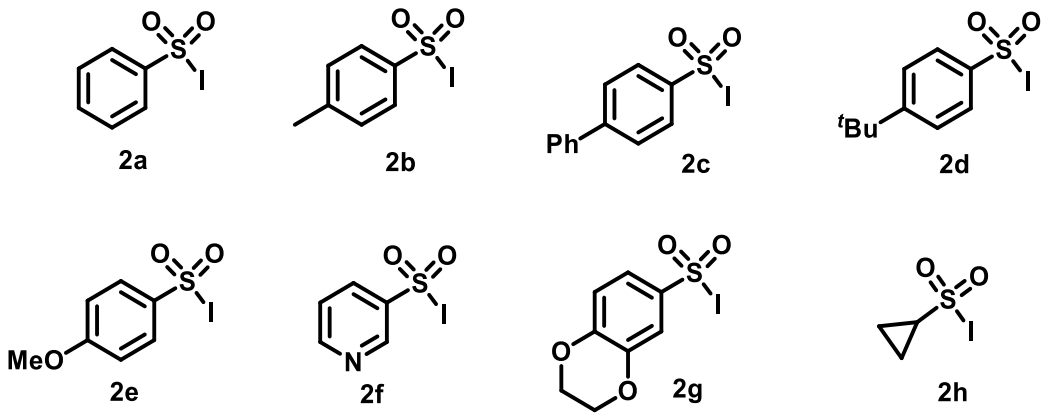


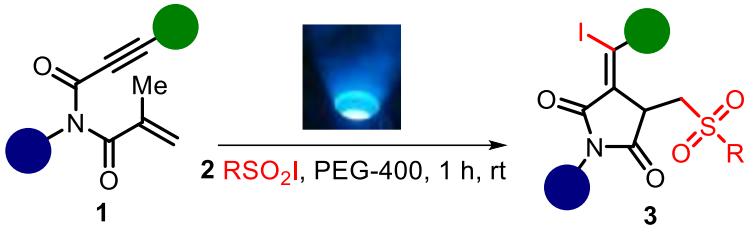
(5) General procedure for the synthesis of 4-methylbenzenesulfonyliodide (2):



To a round-bottom flask (50 mL) was added sodium *p*-toluenesulfinate salt (0.56 mmol, 1 equiv) in distilled water at room temperature. A saturated solution of iodine (0.56 mmol, 1 equiv) in ethanol (1-2 mL) was prepared and added gradually to the above sodium *p*-toluenesulfinate solution. While addition, yellow precipitate was formed gradually. The precipitate was filtered, washed with cold water, and dried carefully at room temperature to give *p*-toluenesulfonyl iodide as a yellow solid. The synthesized 4-methyl benzenesulfonyl iodide was immediately used for next step because of spontaneous decomposition of sulfonyl iodides. Other sulfonyl iodides were obtained in a similar protocol.



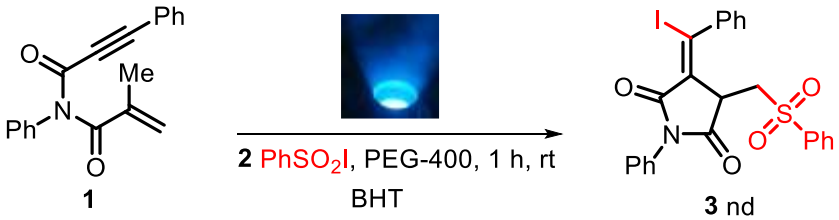
(6) General procedure for radical cascade synthesis of iodosulfonylated succinimides (3):



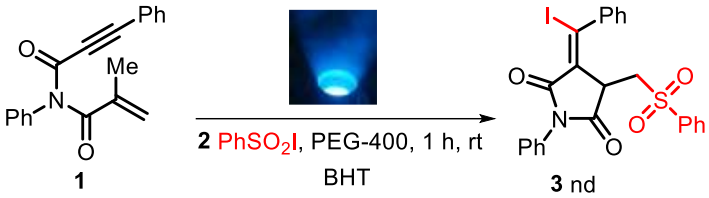
To a reaction vial (50 mL) was added aza-1,6-enyne **1** (0.346 mmol, 1equiv) and benzenesulfonyliodide **2** (0.415 mmol, 1.2 equiv) in 2mL PEG-400. The resulting mixture was placed under blue LED irradiation and stirred at room temperature for 1 h. After that, the crude reaction mixture was diluted with water and extracted with ethyl acetate. The organic layer was dried over Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography using hexane: ethyl acetate as the eluent to give the desired product **3**.

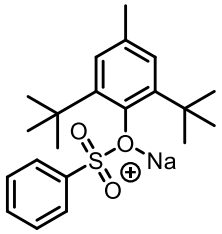
(7) Control Experiment and general procedure for post functionalization of products

(7.1) Radical trapping experiment



To a reaction vial (50 mL) was added aza-1,6-enyne **1** (0.346 mmol, 1equiv) and benzenesulfonyliodide **2** (0.415 mmol, 1.2 equiv) in 2mL PEG-400. To this reaction mixture, BHT (3.0 equiv) was added. The resulting mixture was placed under blue LED irradiation and stirred at room temperature for 1 h. After that After that, the crude reaction mixture was diluted with water and extracted with ethyl acetate. The organic layer was dried over Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography using hexane: ethyl acetate as the eluent gave the desired product **3**.





Detected *via* HRMS
$[M+Na]^+$ 384.1730

Qualitative Compound Report

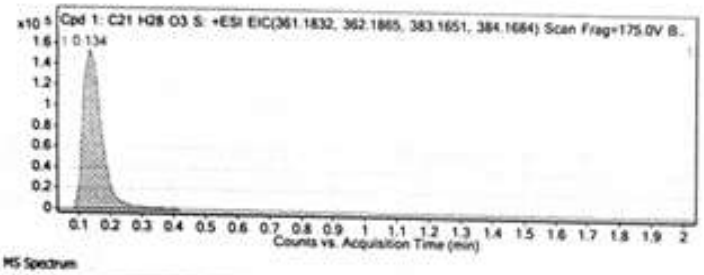
Data File	BHT-TEMPO.d	Sample Name	BHT-TEMPO
Sample Type	Sample	Position	P1-B8
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	13-06-2024 13:55:22
IRM Calibration Status	Success	DA Method	Default.m
Comment			

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

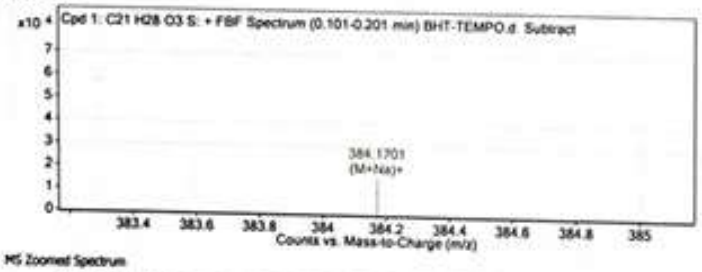
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C21 H28 O3 S	0.134	360.1778	67658	C21 H28 O3 S	360.1759	5.27	C21 H28 O3 S	C21 H28 O3 S

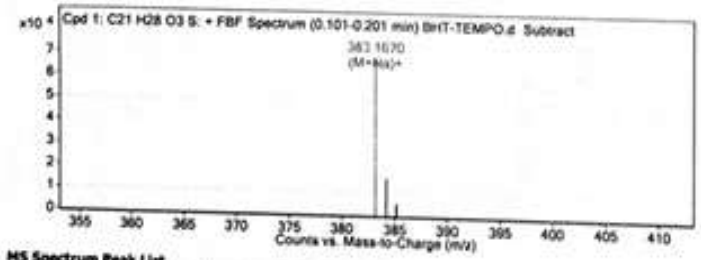
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C21 H28 O3 S	383.167	0.134	Find By Formula	360.1778



MS Spectrum



MS Zoomed Spectrum

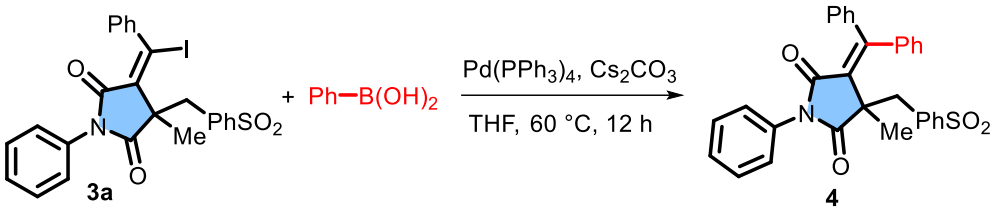


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
383.167	1	67657.61	C21H28NaO3S	(M+Na)+
384.1701	1	16368.35	C21H28NaO3S	(M+Na)+
385.1684	1	5417.13	C21H28NaO3S	(M+Na)+

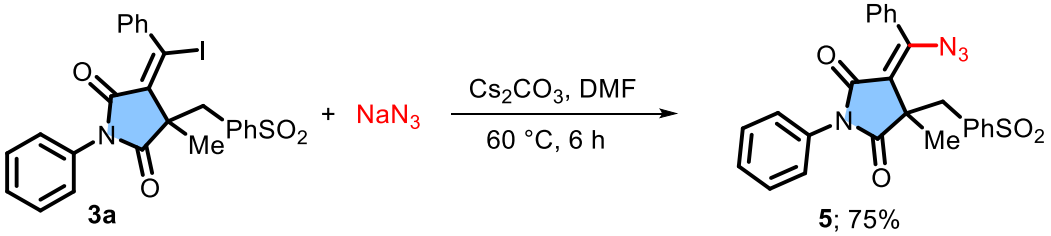
--- End Of Report ---

(7.2) Suzuki- Miyaura Coupling



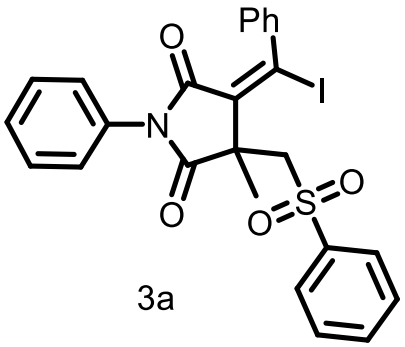
To a solution of compound **3a** (1 equiv, 0.274 mmol), tetrakis (0.1 equiv, 0.02 mmol) in THF (4 mL) phenylboronic acid (2 equiv, 0.4 mmol) and Cs_2CO_3 (2 equiv, 0.4 mmol) and the mixture was stirred under reflux at 85°C. The reaction progress was monitored by TLC. After completion of the reaction, the reaction mixture was washed with brine, and the aqueous phase was re-extracted with ethyl acetate. The combined organic extracts were dried over Na_2SO_4, concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane: ethyl acetate) to afford the desired product **4**.

(7.3) Azidation reaction



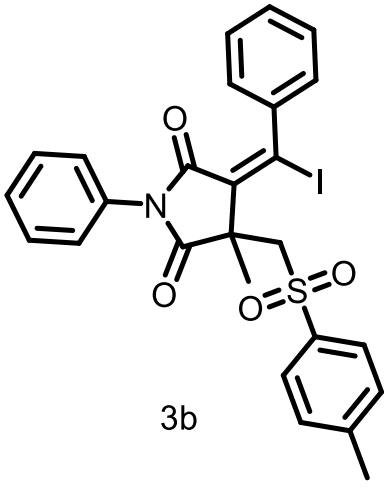
An oven-dried vial was charged with the obtained product **3a** (0.10mmol, 1.0 equiv), NaN_3 (0.25 mmol, 2.5 equiv.), Cs_2CO_3 (0.25 mmol, 2.5 equiv.) in 2 mL DMF. Then the reaction mixture was stirred at 60 ^oC for 4 h. When the reaction was completed, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate. Then organic layer was washed with aqueous saturated brine solution and dried over Na_2SO_4 and concentrated under reduced pressure. The crude material obtained was purified by column chromatography to afford the desired product **5**.

(8) Characterization Data for the Products:



3a

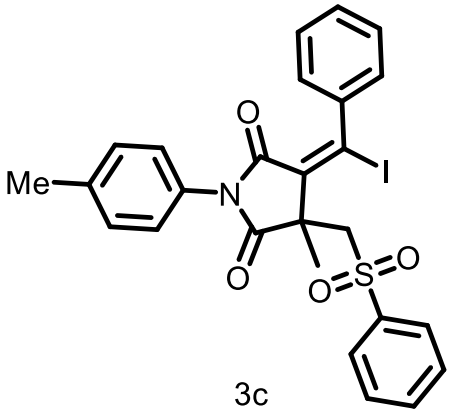
***(E)*-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3a):** Purification by silica gel chromatography (PE:EA= 88:12) afforded the desired **3a** as white solid in 85% yield (1634 mg), mp 201-203 ^{o}C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.99-7.96 (m, 2H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 2H), 7.46-7.27 (m, 10H), 4.68 (d, *J* = 14.0 Hz, 1H), 3.79 (d, *J* = 14.3 Hz, 1H), 1.81 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.1, 163.7, 144.7, 140.3, 134.2, 134.1, 131.6, 129.6, 129.2, 129.0, 128.8, 128.1, 127.9, 126.9, 126.7, 119.5, 58.1, 48.0, 22.4. **MS (ESI)** *m/z* 558 $[M+H]^+$; HRMS Calculated for $C_{25}H_{21}INO_4S^+$ 558.0231; Found: 558.0198. $[M+H]^+$.



3b

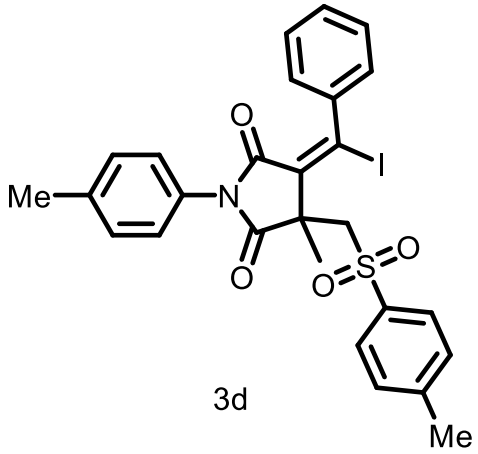
***(E)*-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione (3b):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3b** as

white solid in 72% yield (139 mg), mp 198-200 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.45-7.40 (m, 4H), 7.38-7.29 (m, 8H), 4.65 (d, *J* = 14.2 Hz, 1H), 3.76 (d, *J* = 14.3 Hz, 1H), 2.46 (s, 3H), 1.80 (s, 3H). **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.2, 163.8, 145.3, 144.9, 137.5, 134.3, 131.7, 130.2, 129.2, 129.1, 128.9, 128.2, 128.0, 127.0, 126.8, 119.5, 58.2, 48.0, 22.5, 21.8. **MS (ESI)** *m/z* 572 $[M+H]^+$; HRMS Calculated for $C_{26}H_{23}INO_4S^+$ 572.0387; Found: 572.0388. $[M+H]^+$.



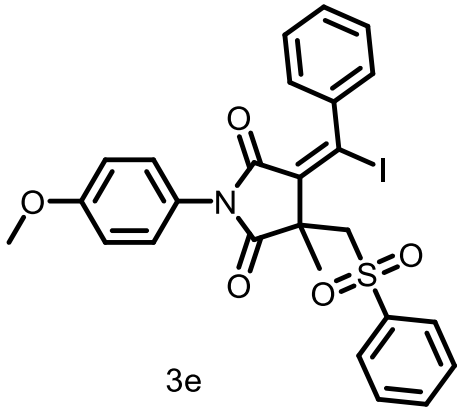
3c

***(E)*-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)-1-(*p*-tolyl)pyrrolidine-2,5-dione (3c):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3c** as white solid in 80% yield (164 mg), mp 200-202 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 (d, *J* = 7.4 Hz, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.59-7.56 (m, 2H), 7.35 (d, *J* = 4.4 Hz, 4H), 7.30-7.20 (m, 5H), 4.65 (d, *J* = 14.2 Hz, 1H), 3.77 (d, *J* = 14.3 Hz, 1H), 2.34 (s, 3H), 1.79 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 177.1, 163.7, 144.6, 140.3, 138.7, 134.2, 134.0, 129.6, 129.4, 129.0, 128.9, 128.0, 127.8, 126.6, 119.1, 60.4, 58.0, 47.8, 22.3, 21.2, 21.0, 14.2. **MS (ESI)** *m/z* 572 $[M+H]^+$; HRMS Calculated for $C_{26}H_{23}INO_4S^+$ 572.0387; Found: 572.0376. $[M+H]^+$.



3d

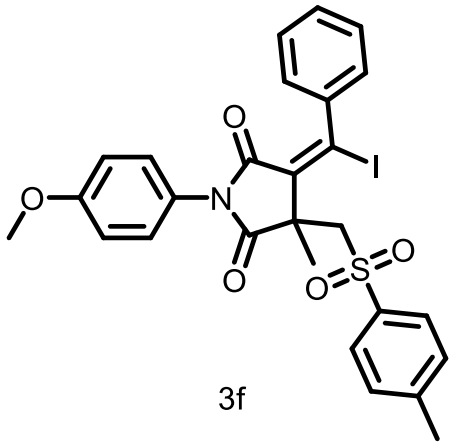
***(E)*-4-(iodo(phenyl)methylene)-3-methyl-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione (3d):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3d** as yellow solid in 75% yield (154 mg), mp 188-190 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.83 (d, *J* = 7.8 Hz, 2H), 7.36 (d, *J* = 7.4 Hz, 6H), 7.28-7.20 (m, 6H), 4.63 (d, *J* = 14.2 Hz, 1H), 3.75 (d, *J* = 14.2 Hz, 1H), 2.45 (s, 3H), 2.34 (s, 3H), 1.78 (s, 3H)**; ^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.3, 163.9, 145.3, 144.8, 138.9, 137.5, 134.4, 130.2, 129.7, 129.2, 129.0, 128.2, 128.0, 126.8, 126.7, 119.2, 58.2, 48.0, 22.5, 21.8, 21.4. **MS (ESI)** *m/z* 586 $[M+H]^+$; HRMS Calculated for $C_{27}H_{25}INO_4S^+$ 586.0543; Found: 586.0566. $[M+H]^+$.



3e

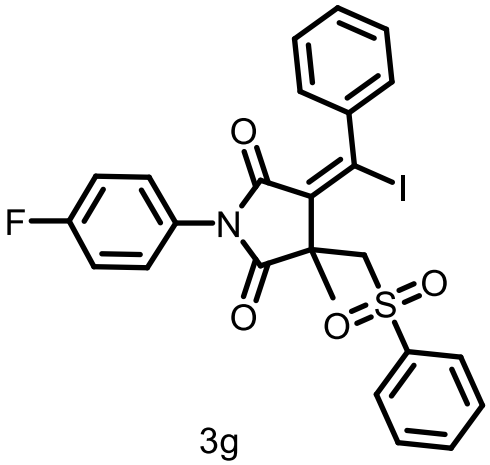
***(E)*-4-(iodo(phenyl)methylene)-1-(4-methoxyphenyl)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3e):** Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **3e** as white solid in 74% yield (150 mg), mp 213-215 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.97 (d, *J* = 7.3 Hz, 2H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.37 (d, *J* = 4.5 Hz, 4H), 7.32-7.26 (m, 3H), 6.94 (d, *J* = 9.0 Hz,

2H), 4.67 (d, *J* = 14.3 Hz, 1H), 3.78 (d, *J* = 11.3 Hz, 4H), 1.80 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.3, 164.0, 159.7, 144.7, 140.3, 134.2, 134.1, 129.5, 129.1, 128.1, 127.9, 126.7, 124.2, 119.2, 114.5, 114.3, 58.1, 55.5, 47.9, 22.4. **MS** (ESI) *m/z* 588 $[M+H]^+$; HRMS Calculated for $C_{26}H_{23}INO_5S^+$ 588.0336; Found: 588.0361. $[M+H]^+$.



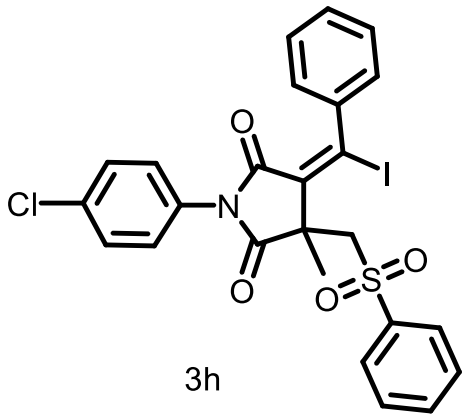
3f

***(E)*-4-(iodo(phenyl)methylene)-1-(4-methoxyphenyl)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (3f):** Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **3f** as white solid in 70% yield (142 mg), mp 213-215 ºC; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.37-7.34 (m, 6H), 7.30-7.25 (m, 3H), 6.92 (d, *J* = 9.1 Hz, 2H), 4.62 (d, *J* = 14.2 Hz, 1H), 3.78 (s, 3H), 3.74 (d, *J* = 14.2 Hz, 1H), 2.45 (s, 3H), 1.78 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.4, 164.0, 159.7, 145.3, 144.8, 137.5, 134.3, 130.2, 129.2, 128.1, 128.0, 126.8, 124.3, 119.2, 114.4, 58.2, 55.6, 47.9, 22.5, 21.8. **MS (ESI)** *m/z* 602 $[M+H]^+$; HRMS Calculated for $C_{27}H_{25}INO_5S^+$ 602.0493; Found: 602.0537. $[M+H]^+$.



3g

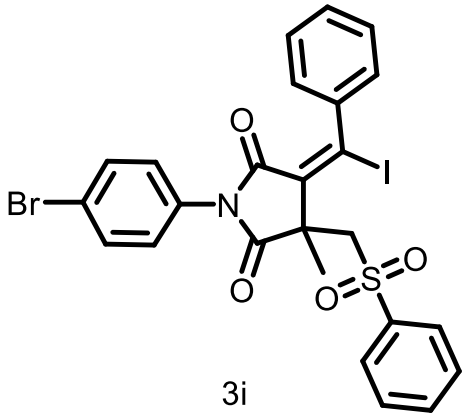
***(E)*-1-(4-fluorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3g)**: Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **3g** as white solid in 66% yield (131 mg), mp 209-211 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.96 (d, *J* = 11.5 Hz, 2H), 7.71-7.68 (m, 1H), 7.60 (t, *J* = 7.6 Hz, 2H), 7.39-7.28 (m, 7H), 7.14-7.09 (m, 2H), 4.67 (d, *J* = 14.2 Hz, 1H), 3.77 (d, *J* = 14.3 Hz, 1H), 1.80 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.1, 162.40 (d, J_{C-F} = 243.3 Hz, 1C), 144.7, 140.2, 134.2, 134.0, 129.6, 129.2, 128.84 (d, J_{C-F} = 8.7 Hz, 1C), 128.1, 127.9, 127.48 (d, J_{C-F} = 22.9 Hz, 1C), 126.6, 119.8, 116.1, 115.9, 77.4, 77.1, 76.7, 58.1, 47.9, 22.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ −112.2 (s, 1F); **MS (ESI)** *m/z* 576 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}FINO_4S^+$ 576.0136; Found: 576.0144 $[M+H]^+$.



3h

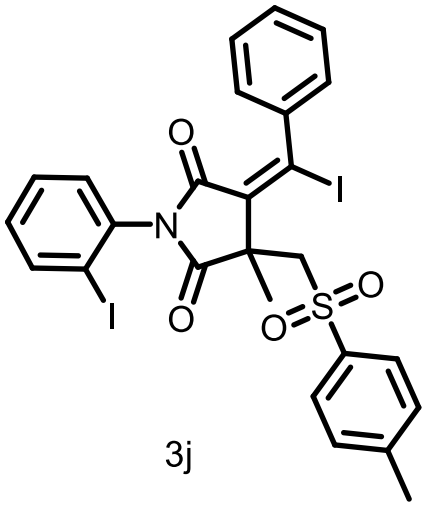
***(E)*-1-(4-chlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3h):** Purification by silica gel

chromatography (PE:EA=85:15) afforded the desired **3h** as white solid in 78% yield (159 mg), mp 192-194 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.89-7.87 (m, 2H), 7.64-7.60 (m, 1H), 7.54-7.50 (m, 2H), 7.34-7.26 (m, 9H), 4.59 (d, J = 14.2 Hz, 1H), 3.69 (d, J = 14.2 Hz, 1H), 1.73 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.9, 163.4, 144.6, 140.1, 134.6, 134.2, 133.8, 130.0, 129.5, 129.1, 128.2, 128.1, 127.8, 126.6, 119.9, 58.0, 47.9, 22.3. **MS (ESI)** *m/z* 591 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}ClINO_4S^+$ 591.9841; Found: 591.9851. $[M+H]^+$.



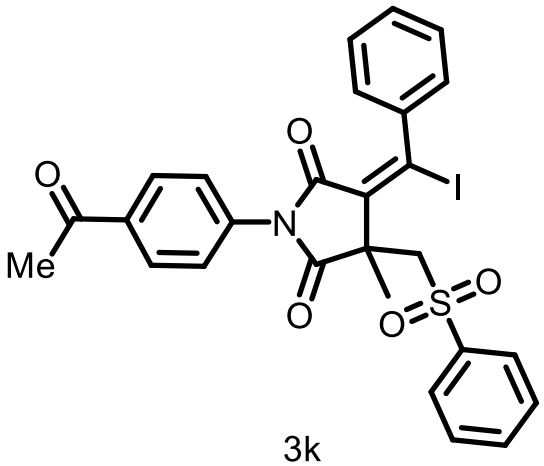
3i

***(E)*-1-(4-bromophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3i):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3i** as white solid in 70% yield (153 mg), mp 208-210 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.97-7.95 (m, 2H), 7.71-7.64 (m, 1H), 7.61-7.54 (m, 4H), 7.44-7.36 (m, 4H), 7.33-7.28 (m, 3H), 4.67 (d, J = 14.3 Hz, 1H), 3.77 (d, J = 14.3 Hz, 1H), 1.80 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.8, 163.3, 144.7, 140.2, 134.2, 133.9, 132.2, 130.6, 129.6, 129.3, 128.5, 128.2, 127.9, 126.6, 122.7, 120.0, 58.1, 48.0, 22.4. **MS (ESI)** *m/z* 635 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}BrINO_4S^+$ 635.9336; Found: 635.9329 $[M+H]^+$.



3j

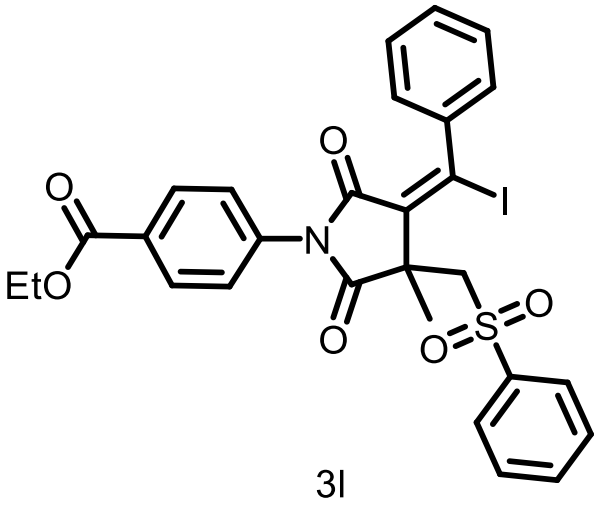
***(E)*-4-(iodo(phenyl)methylene)-1-(2-iodophenyl)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (3j):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3j** as yellow solid in 65% yield (93 mg), mp 202-204 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.84 (m, 3H), 7.48-7.41 (m, 2H), 7.37-7.34 (m, 5H), 7.29-7.25 (m, 2H), 7.13-7.08 (m, 1H), 4.64 (d, *J* = 14.2 Hz, 1H), 3.77 (d, *J* = 14.3 Hz, 1H), 2.46 (s, 3H), 1.88 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.0, 162.8, 145.2, 144.5, 139.2, 137.4, 134.9, 134.2, 131.0, 130.1, 129.7, 129.6, 129.1, 128.0, 127.9, 126.8, 119.7, 97.6, 58.3, 48.4, 29.7, 21.8, 21.7. **MS (ESI)** *m/z* 697 $[M+H]^+$; HRMS Calculated for $C_{26}H_{22}I_2NO_4S^+$ 697.9353; Found: 697.9342 $[M+H]^+$.



3k

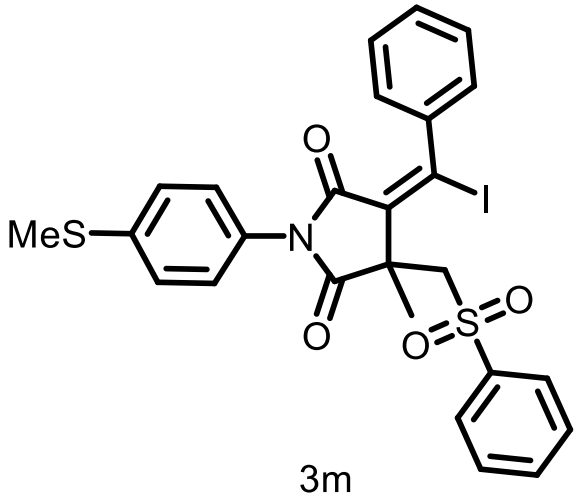
***(E)*-1-(4-acetylphenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3k):** Purification by silica gel

chromatography (PE:EA=83:17) afforded the desired **3k** as white solid in 72% yield (149 mg), mp 226-228 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 8.01 (m, 2H), 7.96 (d, *J* = 7.3 Hz, 2H), 7.71-7.67 (m, 1H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.53 (m, 2H), 7.36 (s, 4H), 7.27-7.33 (1H), 4.68 (d, *J* = 14.3 Hz, 1H), 3.78 (d, *J* = 14.3 Hz, 1H), 2.59 (s, 3H), 1.82 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 197.2, 176.8, 163.2, 144.6, 140.1, 136.8, 135.7, 134.2, 133.8, 129.6, 129.3, 129.0, 128.2, 127.9, 127.0, 126.6, 120.3, 58.1, 48.0, 26.8, 22.4; **MS (ESI)** *m/z* 600 $[M+H]^+$; HRMS Calculated for $C_{27}H_{23}INO_5S^+$ 600.0356; Found: 600.0385 $[M+H]^+$.



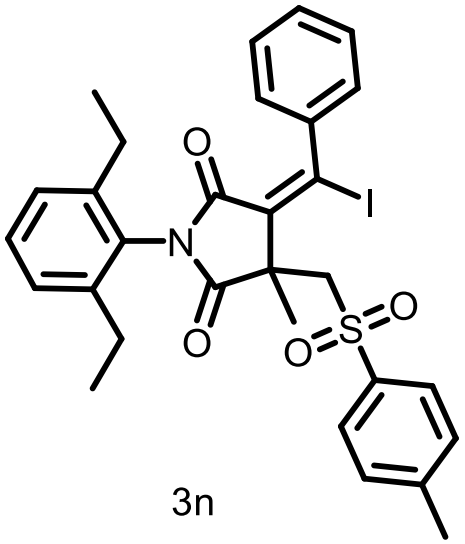
3l

ethyl *(E)*-4-(4-(iodo(phenyl)methylene)-3-methyl-2,5-dioxo-3-((phenylsulfonyl)methyl)pyrrolidin-1-yl)benzoate (3l): Purification by silica gel chromatography (PE:EA=83:17) afforded the desired **3l** as white solid in 76% yield (165 mg), mp 185-187 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 8.10 (m, 2H), 7.98-7.95 (m, 2H), 7.71-7.67 (m, 1H), 7.61-7.57 (m, 2H), 7.49 (m, 2H), 7.40-7.36 (m, 4H), 7.32-7.28 (m, 1H), 4.68 (d, *J* = 14.2 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.78 (d, *J* = 14.3 Hz, 1H), 1.81 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.7, 165.8, 163.1, 144.6, 140.2, 135.5, 134.1, 133.9, 130.5, 130.2, 129.5, 129.2, 128.1, 127.8, 126.7, 126.6, 120.1, 61.2, 58.1, 48.0, 22.4, 14.3. **MS (ESI)** *m/z* 630 $[M+H]^+$; HRMS Calculated for $C_{28}H_{25}INO_6S^+$ 630.0442; Found: 630.0441 $[M+H]^+$.



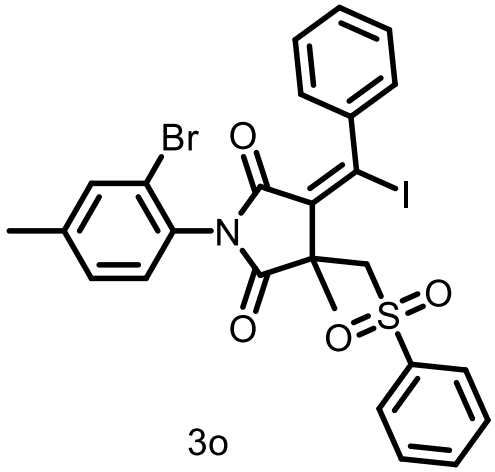
3m

***(E)*-4-(iodo(phenyl)methylene)-3-methyl-1-(4-(methylthio)phenyl)-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3m):** Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **3m** as white solid in 78% yield (163 mg), mp 262-264 ^{o}C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.98-7.95 (m, 2H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.37 (d, *J* = 4.5 Hz, 4H), 7.32-7.28 (m, 5H), 4.67 (d, *J* = 14.0 Hz, 1H), 3.78 (d, *J* = 14.3 Hz, 1H), 2.46 (s, 3H), 1.80 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.1, 163.7, 144.7, 140.3, 139.7, 134.2, 134.1, 129.6, 129.2, 128.5, 128.1, 127.9, 127.1, 126.8, 119.6, 58.1, 47.9, 22.4, 15.8; **MS (ESI)** *m/z* 604 $[M+H]^+$; HRMS Calculated for $C_{26}H_{23}INO_4S_2^+$ 604.0108; Found: 604.0155 $[M+H]^+$.



3n

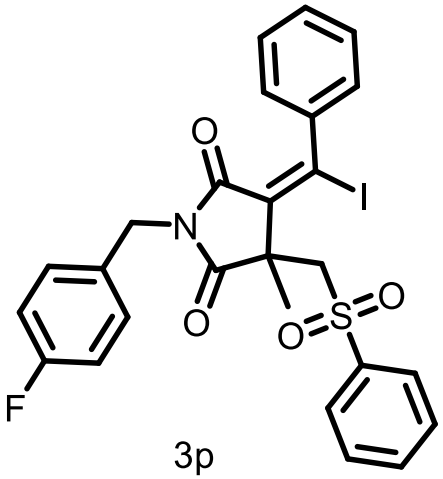
***(E)*-1-(2,6-diethylphenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (3n):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3n** as white solid in 65% yield (141 mg), mp 205-207 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 7.7 Hz, 2H), 7.30-7.24 (m, 4H), 7.22-7.18 (m, 2H), 7.11 (d, *J* = 6.6 Hz, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 4.56 (d, *J* = 14.4 Hz, 1H), 3.78 (d, *J* = 14.4 Hz, 1H), 2.74-2.57 (m, 2H), 2.38 (s, 3H), 2.28 (q, *J* = 7.6 Hz, 2H), 1.74 (s, 3H), 1.11 (t, *J* = 7.5 Hz, 3H), 1.04 (t, *J* = 7.6 Hz, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.1, 164.2, 145.0, 144.6, 143.6, 140.7, 137.8, 134.8, 130.1, 129.8, 129.3, 128.7, 128.1, 127.8, 127.3, 127.1, 126.1, 118.7, 57.5, 48.9, 31.0, 29.7, 24.6, 24.1, 23.3, 21.7, 15.1, 14.2; **MS (ESI)** *m/z* 628 $[M+H]^+$; HRMS Calculated for $C_{30}H_{31}INO_4S^+$ 628.1043; Found: 628.1068 $[M+H]^+$.



3o

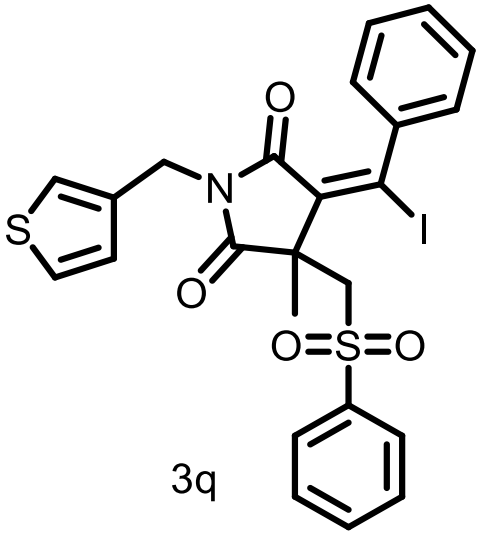
***(E)*-1-(2-bromo-4-methylphenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3o):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3o** as white solid in 72% yield (161 mg), mp 192-194 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.97-7.95 (m, 2H), 7.71-7.67 (m, 1H), 7.59 (t, *J* = 7.8 Hz, 2H), 7.46 (s, 1H), 7.38-7.35 (m, 4H), 7.30-7.26 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 1H), 4.68 (d, *J* = 14.3 Hz, 1H), 3.81 (d, *J* = 14.3 Hz, 1H), 2.34 (s, 3H), 1.85 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.2, 163.0, 144.5, 141.5, 140.5, 134.3, 134.1, 133.4, 129.8, 129.5, 129.4, 129.2, 128.6, 128.1, 127.9, 126.9, 121.8, 119.5, 58.2, 48.4, 22.0, 21.0. **MS** (ESI)

m/z 649 $[M+H]^+$; HRMS Calculated for $C_{26}H_{22}BrINO_4S^+$ 649.9492; Found: 649.9547 $[M+H]^+$.



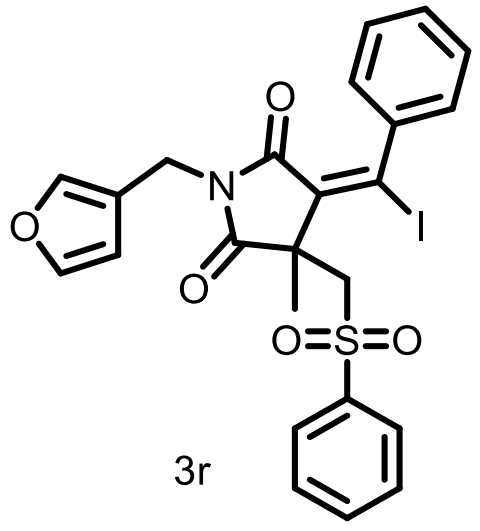
3p

***(E)*-1-(4-fluorobenzyl)-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3p):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3p** as white solid in 65% yield (132 mg), mp 206-208 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.89-7.87 (m, 2H), 7.70-7.64 (m, 1H), 7.58 (t, *J* = 7.8 Hz, 2H), 7.41-7.33 (m, 7H), 6.99-6.94 (m, 2H), 4.65 (s, 2H), 4.59 (d, *J* = 14.3 Hz, 1H), 3.70 (d, *J* = 14.3 Hz, 1H), 1.63 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.3, 164.8 (d, $J_{C\text{-}F}$ = 251.9 Hz, 1C), 144.6, 140.4, 134.3, 134.0, 131.2, 130.7 (d, $J_{C\text{-}F}$ = 8.3 Hz, 1C), 129.4, 129.3, 128.0, 127.8 (d, $J_{C\text{-}F}$ = 22.8 Hz, 1C), 126.9, 118.4, 115.5, 115.3, 57.6, 48.0, 42.0, 22.4; **^{19}F NMR (376 MHz, $CDCl_3$)** δ −112.2 (s, 1F); **MS (ESI)** *m/z* 590 $[M+H]^+$; HRMS Calculated for $C_{26}H_{22}FINO_4S^+$ 590.0293; Found: 590.0344 $[M+H]^+$.



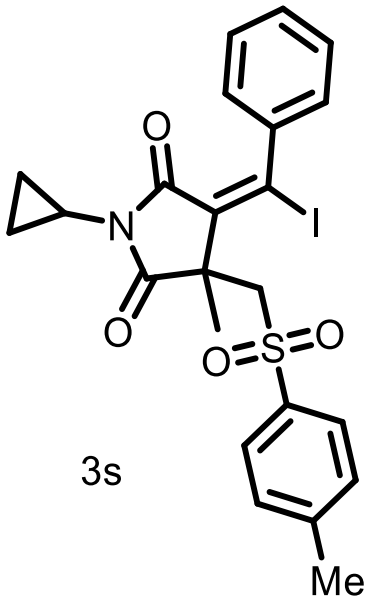
3q

***(E)*-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)-1-(thiophen-3-ylmethyl)pyrrolidine-2,5-dione (3q):** Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **3q** as white solid in 70% yield (139 mg), mp 186-188 ^{o}C; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.83-7.81 (m, 2H), 7.63-7.56 (m, 1H), 7.52-7.47 (m, 3H), 7.34-7.24 (m, 4H), 7.13-7.11 (m, 1H), 6.99 (d, *J* = 3.4 Hz, 1H), 6.83 (dd, *J* = 5.1, 3.4 Hz, 1H), 4.77 (d, *J* = 3.8 Hz, 2H), 4.51 (d, *J* = 14.4 Hz, 1H), 3.64 (d, *J* = 14.4 Hz, 1H), 1.55 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 176.9, 163.5, 144.4, 140.2, 136.8, 134.1, 134.0, 129.4, 129.2, 128.3, 128.0, 128.0, 127.8, 126.9, 126.7, 125.9, 118.5, 57.5, 47.9, 36.9, 22.1. **MS** (ESI) *m/z* 578 $[M+H]^+$; HRMS Calculated for $C_{24}H_{21}INO_4S_2^+$ 577.9961; Found: 578.0001 $[M+H]^+$.



3r

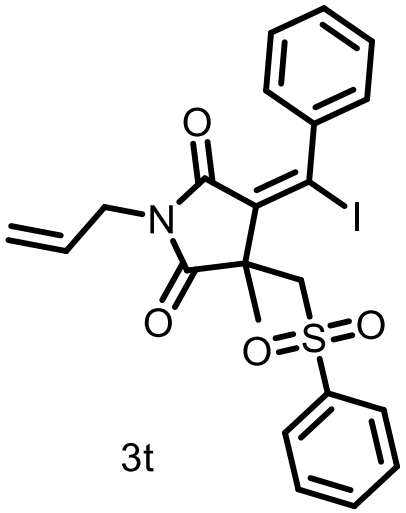
***(E)*-1-(furan-3-ylmethyl)-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3r):** Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **3r** as white solid in 75% yield (145 mg), mp 188-190 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.82 (m, 2H), 7.62-7.58 (m, 1H), 7.52-7.48 (m, 2H), 7.34-7.23 (m, 5H), 7.11 (m, 1H), 6.99-6.98 (m, 1H), 6.82 (dd, *J* = 5.1, 3.6 Hz, 1H), 4.77 (d, *J* = 3.7 Hz, 2H), 4.51 (d, *J* = 14.4 Hz, 1H), 3.64 (d, *J* = 14.4 Hz, 1H), 1.55 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.6, 164.2, 145.2, 140.9, 137.5, 134.9, 134.7, 130.1, 130.0, 129.0, 128.7, 128.7, 128.5, 127.6, 127.4, 126.6, 119.3, 58.2, 48.7, 37.6, 22.8; **MS (ESI)** *m/z* 562 $[M+H]^+$; HRMS Calculated for $C_{24}H_{21}INO_5S^+$ 562.0180; Found: 562.0190 $[M+H]^+$.



3s

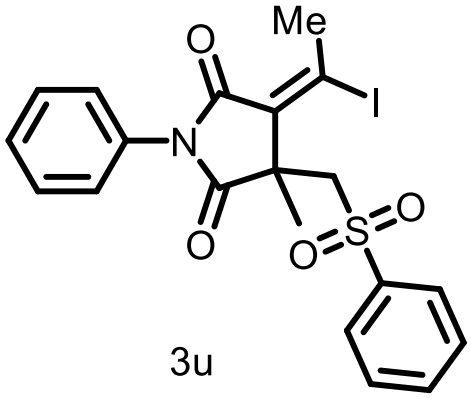
***(E)*-1-cyclopropyl-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (3s):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3s** as white solid in 78% yield (145 mg), mp 175-177 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 4H), 7.31 (t, *J* = 7.6 Hz, 3H), 4.51 (d, *J* = 14.3 Hz, 1H), 3.62 (d, *J* = 14.0 Hz, 1H), 2.62-2.56 (m, 1H), 2.47 (s, 3H), 1.65 (s, 3H), 1.12-1.08 (m, 1H), 0.92 (d, *J* = 6.3 Hz, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 178.0, 165.1, 145.1, 144.7, 137.4, 134.1, 130.1, 129.1, 128.1, 127.9, 126.7, 117.9, 57.9, 47.3, 22.4, 22.3, 21.7, 5.4, 5.0;

MS (ESI) *m/z* 536 $[M+H]^+$; HRMS Calculated for $C_{23}H_{23}INO_4S^+$ 536.0387; Found: 536.0394 $[M+H]^+$.



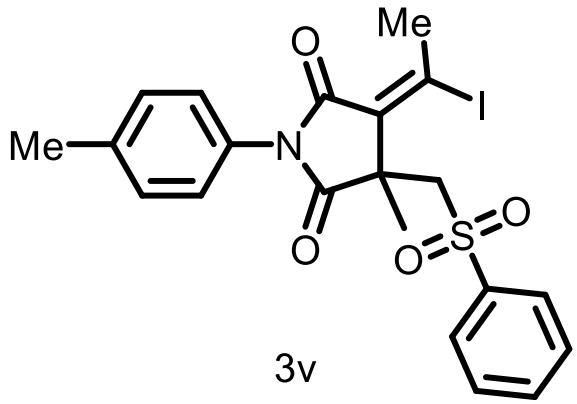
3t

***(E)*-1-allyl-4-(iodo(phenyl)methylene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3t):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3t** as white solid in 67% yield (121 mg), mp 185-187 ºC; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.86-7.83 (m, 2H), 7.63-7.58 (m, 1H), 7.52-7.49 (m, 2H), 7.33-7.22 (m, 5H), 5.90-5.68 (m, 1H), 5.21-5.09 (m, 2H), 4.50 (d, *J* = 14.3 Hz, 1H), 4.13-3.99 (m, 2H), 3.63 (d, *J* = 14.3 Hz, 1H), 1.60 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.1, 163.9, 144.5, 140.1, 134.2, 134.0, 130.3, 129.4, 129.1, 128.0, 127.8, 126.7, 118.6, 118.1, 57.5, 47.8, 41.3, 22.3. **MS (ESI)** *m/z* 522 $[M+H]^+$; HRMS Calculated for $C_{22}H_{21}INO_4S^+$ 522.0230; Found: 522.0263 $[M+H]^+$.



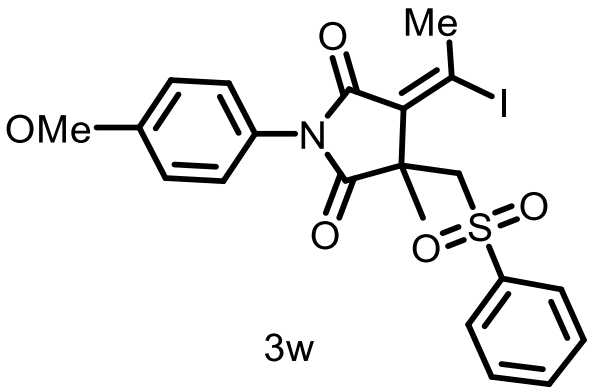
3u

***(E)*-4-(1-iodoethylidene)-3-methyl-1-phenyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3u):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3u** as white solid in 80% yield (174 mg), mp 192-194 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.87-7.85 (m, 2H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.58-7.53 (m, 2H), 7.52-7.49 (m, 2H), 7.46-7.42 (m, 3H), 4.56 (d, *J* = 14.8 Hz, 1H), 3.75 (d, *J* = 14.8 Hz, 1H), 3.23 (s, 3H), 1.66 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.9, 165.5, 140.1, 134.0, 132.0, 131.7, 129.4, 129.2, 129.0, 128.3, 127.0, 121.7, 58.3, 48.0, 34.7, 22.4; **MS (ESI)** *m/z* 496 $[M+H]^+$; HRMS Calculated for $C_{20}H_{19}INO_4S^+$ 496.0074; Found: 496.0089 $[M+H]^+$.



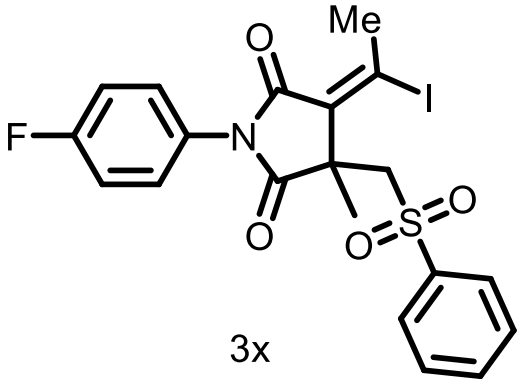
3v

***(E)*-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)-1-(p-tolyl)pyrrolidine-2,5-dione (3v):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3v** as white solid in 75% yield (168 mg), mp 195-197 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.87-7.85 (m, 2H), 7.68-7.63 (m, 1H), 7.55 (t, *J* = 7.8 Hz, 2H), 7.34-7.29 (m, 4H), 4.55 (d, *J* = 14.8 Hz, 1H), 3.74 (d, *J* = 14.8 Hz, 1H), 3.22 (s, 3H), 2.40 (s, 3H), 1.65 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.0, 165.7, 140.2, 139.0, 134.0, 132.1, 129.9, 129.4, 129.0, 128.3, 126.7, 121.5, 58.3, 48.0, 34.7, 22.4, 21.3; **MS (ESI)** *m/z* 510 $[M+H]^+$; HRMS Calculated for $C_{21}H_{21}INO_4S^+$ 510.0231; Found: 510.0254 $[M+H]^+$.



3w

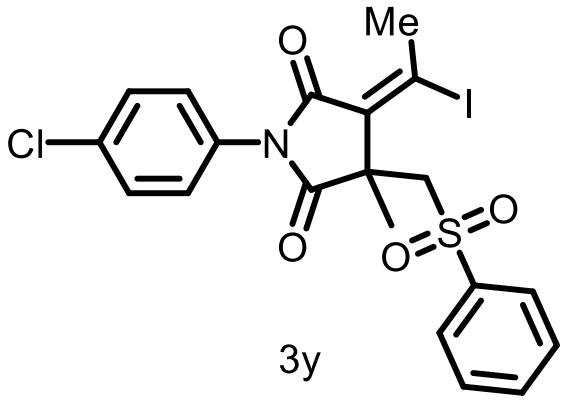
***(E)*-4-(1-iodoethylidene)-1-(4-methoxyphenyl)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3w):** Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **3w** as yellow solid in 78% yield (180 mg), mp 178-180 ^{o}C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.86-7.84 (m, 2H), 7.68-7.64 (m, 1H), 7.57-7.53 (m, 2H), 7.38-7.34 (m, 2H), 7.03-6.97 (m, 2H), 4.54 (d, *J* = 14.7 Hz, 1H), 3.83 (s, 3H), 3.73 (d, *J* = 14.7 Hz, 1H), 3.21 (s, 3H), 1.64 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.0, 165.7, 159.7, 140.1, 133.9, 132.1, 129.3, 128.8, 128.2, 128.1, 124.2, 121.3, 114.7, 114.5, 58.2, 55.5, 47.8, 34.6, 22.3; **MS (ESI)** *m/z* 526 $[M+H]^+$; HRMS Calculated for $C_{21}H_{21}INO_5S^+$ 526.0180; Found: 526.0189 $[M+H]^+$.



3x

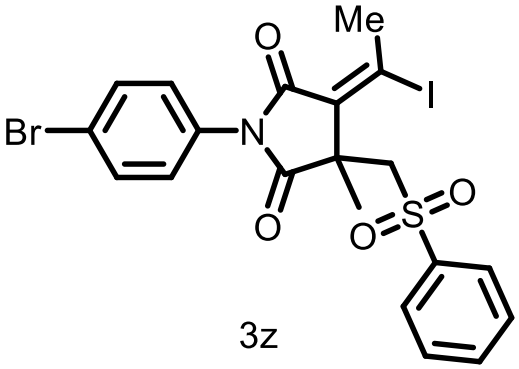
***(E)*-1-(4-fluorophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3x):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3x** as white solid in 70% yield (158 mg),

mp 192-194 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.86-7.84 (m, 2H), 7.66 (t, *J* = 6.9 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 2H), 7.47-7.42 (m, 2H), 7.22-7.17 (m, 2H), 4.55 (d, *J* = 14.8 Hz, 1H), 3.73 (d, *J* = 14.8 Hz, 1H), 3.23 (s, 3H), 1.65 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 13C-NMR (101 MHz, CHLOROFORM-D) δ 176.9, 165.4, 162.5 (d, $J_{C\text{-}F}$ = 247.0 Hz, 1C), 140.1, 134.0, 131.9, 129.4, 128.9 (d, $J_{C\text{-}F}$ = 8.7 Hz, 1C), 128.3, 127.6, 127.6, 121.9, 116.2 (d, $J_{C\text{-}F}$ = 22.4 Hz, 1C), 58.4, 48.0, 34.7, 22.3; **^{19}F NMR (376 MHz, $CDCl_3$)** δ −112.9 (s, 1F); **MS (ESI)** *m/z* 514 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}FINO_4S^+$ 513.9980; Found: 514.0008 $[M+H]^+$.



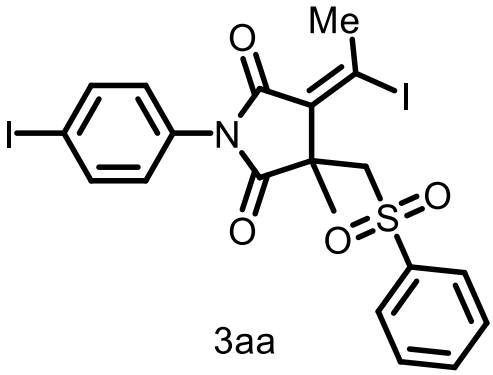
3y

***(E)*-1-(4-chlorophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3y):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3y** as white solid in 72% yield (167 mg), mp 182-184 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.90-7.81 (m, 3H), 7.68 (dd, *J* = 7.9, 5.9 Hz, 1H), 7.60 (t, *J* = 6.9 Hz, 2H), 7.49-7.42 (m, 3H), 4.08 (d, *J* = 15.0 Hz, 1H), 3.81 (d, *J* = 14.8 Hz, 1H), 2.65 (s, 3H), 1.58 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** *δ* 177.1, 165.6, 140.5, 134.5, 132.8, 132.2, 131.1, 129.8, 129.0, 128.7, 123.4, 122.6, 58.8, 48.5, 35.2, 22.7; **MS (ESI)** *m/z* 529 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}ClINO_4S^+$ 529.9684; Found: 529.9684 $[M+H]^+$.



3z

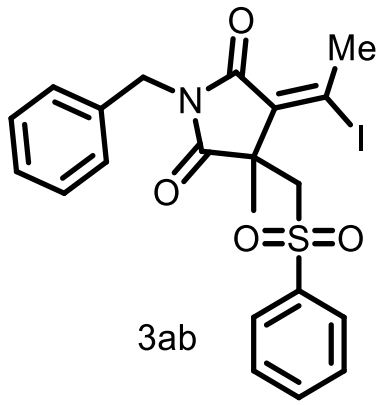
***(E)*-1-(4-bromophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3z):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3z** as white solid in 76% yield (191 mg), mp 188-190 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.86-7.84 (m, 2H), 7.69-7.62 (m, 3H), 7.57 (t, *J* = 7.6 Hz, 2H), 7.35 (dt, *J* = 9.3, 2.4 Hz, 2H), 4.55 (d, *J* = 14.8 Hz, 1H), 3.73 (d, *J* = 14.8 Hz, 1H), 3.23 (s, 3H), 1.66 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.7, 165.2, 140.0, 134.1, 132.4, 131.8, 130.7, 129.4, 128.6, 128.3, 122.9, 122.2, 58.4, 48.0, 34.8, 22.3; **MS (ESI)** *m/z* 573 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}BrINO_4S^+$ 573.9179; Found: 573.9196 $[M+H]^+$.



3aa

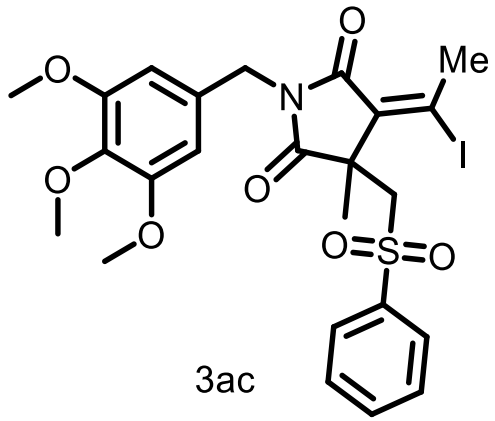
***(E)*-4-(1-iodoethylidene)-1-(4-iodophenyl)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (3aa):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3aa** as white solid in 85% yield (144 mg), mp 182-184 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.79-7.76 (m, 4H), 7.62-7.47 (m, 3H),

7.17-7.13 (m, 2H), 4.48 (d, *J* = 14.8 Hz, 1H), 3.66 (d, *J* = 14.8 Hz, 1H), 3.16 (s, 3H), 1.58 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.6, 165.1, 140.1, 138.4, 134.0, 131.9, 131.4, 129.4, 128.7, 128.3, 122.1, 121.5, 94.6, 58.4, 48.0, 34.8, 22.3; **MS (ESI)** *m/z* 621 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}I_2NO_4S^+$ 621.9040; Found: 621.9040 $[M+H]^+$.



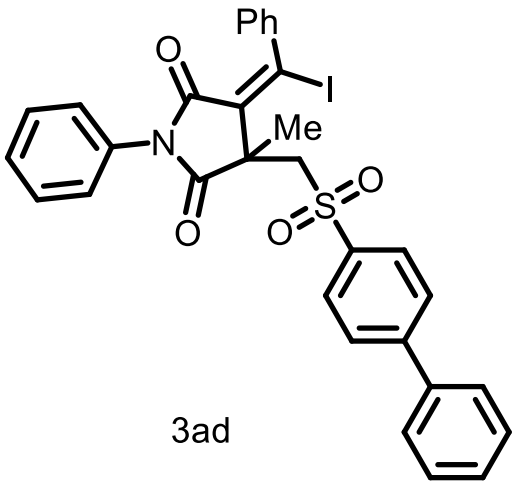
3ab

***(E)*-3-methyl-4-((methylthio)(phenyl)methylene)-1-(*p*-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione (3ab):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ab** as white solid in 70% yield (157 mg), mp 205-207 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.78-7.76 (m, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.42 (d, *J* = 7.0 Hz, 2H), 7.35-7.27 (m, 3H), 4.78 (s, 2H), 4.47 (d, *J* = 14.8 Hz, 1H), 3.67 (d, *J* = 14.8 Hz, 1H), 3.19 (s, 3H), 1.50 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 177.2, 166.0, 140.1, 135.5, 134.0, 132.2, 129.3, 128.7, 128.7, 128.3, 127.9, 120.6, 57.9, 48.0, 42.8, 34.4, 22.4. **MS (ESI)** *m/z* 510 $[M+H]^+$; HRMS Calculated for $C_{21}H_{21}INO_4S^+$ 510.0231; Found: 510.0238 $[M+H]^+$.



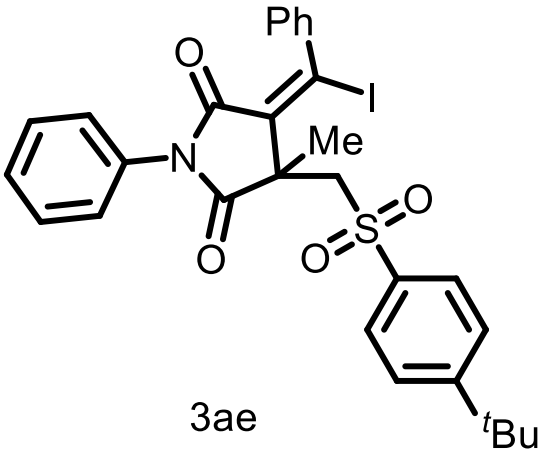
3ac

***(E)*-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)-1-(3,4,5-trimethoxybenzyl)pyrrolidine-2,5-dione (3ac):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ac** as white solid in 78% yield (205 mg), mp 208-210 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.75 (d, *J* = 7.0 Hz, 2H), 7.66-7.63 (m, 1H), 7.53 (d, *J* = 13.8 Hz, 2H), 6.68 (s, 2H), 4.77 (d, *J* = 14.3 Hz, 1H), 4.64 (d, *J* = 14.3 Hz, 1H), 4.49 (d, *J* = 15.0 Hz, 1H), 3.85 (s, 6H), 3.80 (s, 3H), 3.67 (d, *J* = 14.8 Hz, 1H), 3.19 (s, 3H), 1.51 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.3, 165.9, 153.2, 140.1, 137.5, 133.9, 132.1, 130.9, 129.3, 128.2, 120.5, 105.6, 60.7, 57.8, 56.1, 48.0, 43.0, 34.4, 22.4; **MS (ESI)** *m/z* 600 $[M+H]^+$; HRMS Calculated for $C_{24}H_{27}INO_7S^+$ 600.0547; Found: 600.0587 $[M+H]^+$.

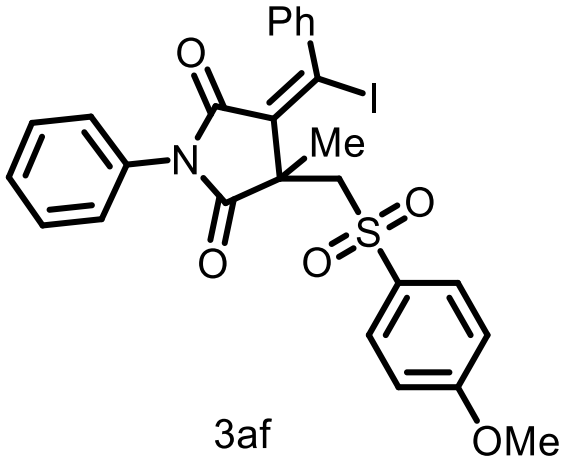


3ad

***(E)*-3-(([1,1'-biphenyl]-4-ylsulfonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenylpyrrolidine-2,5-dione (3ad):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ad** as pale yellow solid in 77% yield (170 mg), mp 212-214 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 8.02 (d, *J* = 8.5 Hz, 2H), 7.78 (d, *J* = 8.1 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.54-7.49 (m, 3H), 7.47-7.40 (m, 5H), 7.38-7.35 (m, 5H), 4.72 (d, *J* = 14.2 Hz, 1H), 3.84 (d, *J* = 14.3 Hz, 1H), 1.83 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.0, 163.6, 147.1, 144.7, 139.0, 138.7, 134.2, 131.6, 129.1, 128.9, 128.9, 128.8, 128.7, 128.5, 128.4, 128.4, 128.1, 128.1, 127.4, 126.8, 126.7, 126.7, 126.6, 119.4, 58.2, 47.9, 22.4 ; **MS (ESI)** *m/z* 634 $[M+H]^+$; HRMS Calculated for $C_{31}H_{25}INO_4S^+$ 634.0543; Found: 634.0562 $[M+H]^+$.

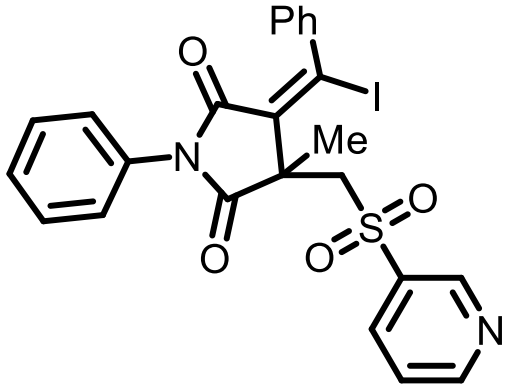


***(E)*-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenylpyrrolidine-2,5-dione (3ae):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ae** as pale yellow solid in 70% yield (148.7 mg), mp 209-211 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.81-7.79 (m, 2H), 7.71-7.69 (m, 1H), 7.51-7.49 (m, 3H), 7.45-7.44 (m, 1H), 7.34-7.31 (m, 3H), 7.29-7.27 (m, 4H), 4.57 (d, *J* = 14.2 Hz, 1H), 3.70 (d, *J* = 14.2 Hz, 1H), 1.72 (s, 3H), 1.27 (s, 9H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.1, 163.7, 158.1, 144.8, 137.3, 134.3, 131.7, 129.2, 129.1, 129.0, 128.9, 128.7, 128.2, 128.1, 127.8, 127.8, 126.9, 126.8, 126.7, 126.6, 126.5, 119.2, 58.2, 47.9, 35.3, 31.1, 22.4; **MS (ESI)** *m/z* 614 $[M+H]^+$; HRMS Calculated for $C_{29}H_{29}INO_4S^+$ 614.0857; Found: 614.0818 $[M+H]^+$.



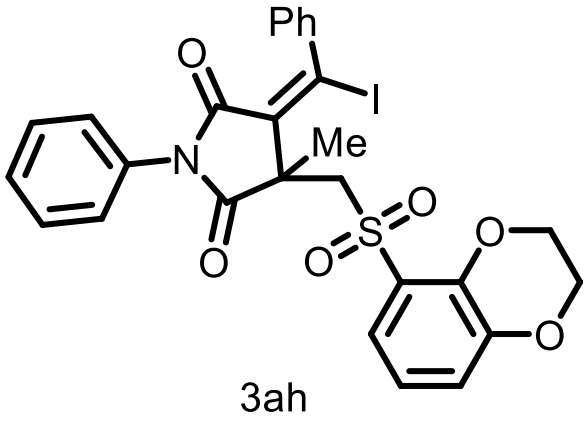
***(E)*-4-(iodo(phenyl)methylene)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-methyl-1-phenylpyrrolidine-2,5-dione (3af):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3af** as pale yellow solid in 74% yield (150 mg), mp 219-221 °C; **^{1}H-**

NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.3, 1.5 Hz, 4H), 7.67 (s, 1H), 7.51-7.49 (m, 2H), 7.39-7.28 (m, 4H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 9.0 Hz, 2H), 3.88 (s, 3H), 3.71 (d, *J* = 14.3 Hz, 1H), 3.17 (d, *J* = 14.3 Hz, 1H), 1.18 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 171.7, 164.3, 160.0, 140.3, 138.1, 132.6, 130.3, 129.9, 129.5, 129.2, 128.7, 128.6, 126.2, 124.4, 120.8, 114.9, 59.8, 55.8, 34.8, 17.5; **MS (ESI)** *m/z* 588 $[M+H]^+$; HRMS Calculated for $C_{26}H_{23}INO_5S^+$ 588.0336; Found: 588.0361. $[M+H]^+$.



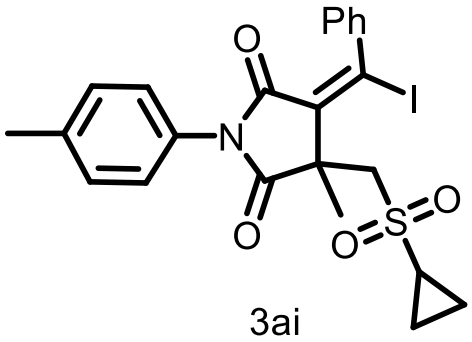
3ag

***(E)*-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-((pyridin-3-ylsulfonyl)methyl)pyrrolidine-2,5-dione (3ag):** Purification by silica gel chromatography (PE:EA=80:20) afforded the desired **3ag** as pale yellow solid in 68% yield (135 mg), mp 209-211 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 9.22 (d, *J* = 2.3 Hz, 1H), 8.94 (dd, *J* = 5.0, 1.5 Hz, 1H), 8.25 (dt, *J* = 8.2, 1.9 Hz, 1H), 7.57-7.53 (m, 1H), 7.49-7.44 (m, 2H), 7.41-7.38 (m, 7H), 7.34-7.30 (m, 1H), 4.77 (d, *J* = 14.3 Hz, 1H), 3.84 (d, *J* = 14.3 Hz, 1H), 1.84 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.9, 163.5, 154.7, 149.0, 148.8, 144.5, 136.8, 135.7, 134.0, 131.5, 129.3, 129.2, 129.1, 128.9, 128.2, 126.8, 126.7, 126.7, 124.1, 119.7, 58.5, 48.1, 22.7, 22.4; **MS (ESI)** *m/z* 559 $[M+H]^+$; HRMS Calculated for $C_{24}H_{20}IN_2O_4S^+$ 559.0183; Found: 559.0155 $[M+H]^+$.



3ah

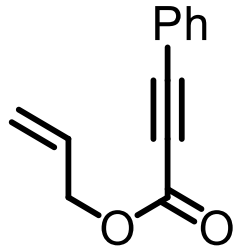
***(E)*-3-(((2,3-dihydrobenzo[b][1,4]dioxin-5-yl)sulfonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenylpyrrolidine-2,5-dione (3ah):** Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **3ah** as pale yellow solid in 72% yield (153 mg), mp 199-201 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.48 (d, *J* = 2.0 Hz, 1H), 7.46-7.40 (m, 3H), 7.38-7.33 (m, 8H), 7.01 (d, *J* = 8.5 Hz, 1H), 4.63 (d, *J* = 14.3 Hz, 1H), 4.31 (dd, *J* = 13.5, 5.3 Hz, 4H), 3.76 (d, *J* = 14.3 Hz, 1H), 1.80 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.0, 163.6, 148.6, 144.8, 143.8, 134.2, 132.7, 131.6, 129.1, 129.0, 128.7, 128.1, 126.9, 126.7, 121.6, 119.2, 118.2, 117.5, 64.6, 64.1, 58.3, 47.9, 22.4; **MS (ESI)** *m/z* 616 $[M+H]^+$; HRMS Calculated for $C_{27}H_{23}INO_6S^+$ 616.0285; Found: 616.0283 $[M+H]^+$.



3ai

***(E)*-3-((cyclopropylsulfonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenylpyrrolidine-2,5-dione (3ai):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **3ai** as white solid in 75% yield (139 mg), mp 182-184 °C; **^{1}H-NMR (400**

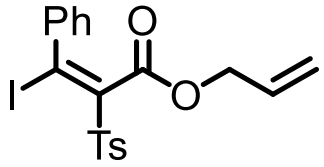
MHz, $CDCl_3$) δ 7.34-7.27 (m, 5H), 7.20-7.15 (m, 4H), 4.63 (d, J = 14.2 Hz, 1H), 3.81 (d, J = 14.2 Hz, 1H), 2.53-2.47 (m, 1H), 2.32 (s, 3H), 1.82 (s, 3H), 1.36-1.25 (m, 2H), 1.13-1.03 (m, 2H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.3, 164.6, 158.6, 145.0, 137.7, 135.8, 133.4, 131.5, 130.0, 130.0, 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* 536 $[M+H]^+$; HRMS Calculated for $C_{23}H_{23}INO_4S^+$ 536.0387; Found: 536.0399 $[M+H]^+$.



4

Compound **4** was prepared using the reported literature.[2]

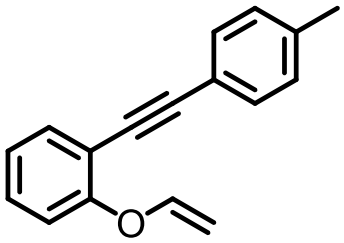
allyl 3-phenylpropiolate (4): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **4** as pale yellow solid in 80% yield (103 mg), mp 142-144 ^oC; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.48-7.46 (m, 2H), 7.36-7.33 (m, 1H), 7.27 (t, *J* = 7.4 Hz, 2H), 5.94-5.84 (m, 1H), 5.32 (dd, *J* = 17.1, 1.4 Hz, 1H), 5.22 (dd, *J* = 10.4, 1.1 Hz, 1H), 4.65-4.64 (m, 2H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 157.02, 148.78, 138.48, 133.55, 131.56, 129.46, 129.11, 123.38, 120.45, 117.34, 115.08, 94.93, 94.44, 21.54. **MS (ESI)** *m/z* 187 $[M+H]^+$; HRMS Calculated for $C_{12}H_{11}O_2^+$ 187.0754; Found: 187.0755 $[M+H]^+$.



5

allyl (Z)-3-iodo-3-phenyl-2-tosylacrylate (5): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **5** as offwhite solid in 75% yield (188 mg), mp 156-158 ^oC; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.27-7.23 (m, 2H), 7.23-7.18 (m, 2H), 7.17-7.14 (m, 1H),

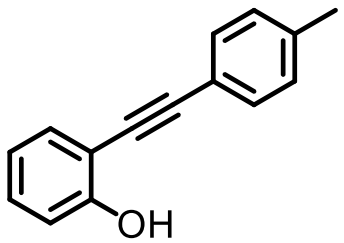
7.06-7.04 (m, 2H), 7.02-6.99 (m, 2H), 6.03-5.93 (m, 1H), 5.43 (dq, *J* = 17.2, 1.4 Hz, 1H), 5.29 (dq, *J* = 10.4, 1.1 Hz, 1H), 4.78 (dt, *J* = 6.0, 1.2 Hz, 2H), 2.31 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 163.41, 146.44, 145.00, 139.76, 137.08, 130.90, 129.68, 129.40, 128.34, 127.86, 127.36, 120.03, 114.50, 67.74, 21.71. **MS (ESI)** *m/z* 468 $[M+H]^+$; HRMS Calculated for $C_{19}H_{18}IO_4S^+$ 468.9965; Found: 468.9969 $[M+H]^+$.



6

Compound **6** was prepared using the reported literature.[3]

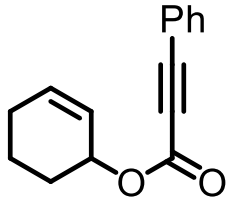
1-(p-tolylethynyl)-2-(vinyloxy)benzene (6): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **6** as colourless liquid in 70% yield (52 mg); **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.56 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.31 (td, *J* = 7.9, 1.5 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.12-7.04 (m, 2H), 6.72 (dd, *J* = 13.8, 6.3 Hz, 1H), 4.83 (dd, *J* = 13.8, 1.8 Hz, 1H), 4.50 (dd, *J* = 6.0, 1.8 Hz, 1H), 2.39 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 153.49, 132.88, 131.28, 130.70, 128.59, 119.40, 119.13, 86.39, 80.54, 66.40. **MS (ESI)** *m/z* 235 $[M+H]^+$; HRMS Calculated for $C_{17}H_{15}O^+$ 235.1117; Found: 235.1119 $[M+H]^+$.



7

2-(p-tolylethynyl)phenol (7): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **7** as white solid in 75% yield (56 mg), mp 170-172 °C; **^{1}H-NMR (400**

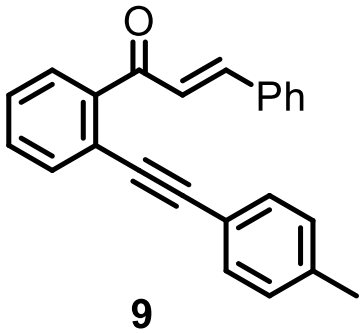
MHz, $CDCl_3$) δ 7.35 (td, *J* = 7.9, 1.6 Hz, 3H), 7.20-7.16 (m, 1H), 7.10 (d, *J* = 7.8 Hz, 2H), 6.90 (dd, *J* = 8.2, 1.0 Hz, 1H), 6.83 (td, *J* = 7.6, 1.1 Hz, 1H), 5.78 (s, 1H), 2.30 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 156.5, 139.1, 131.6, 131.5, 130.3, 129.3, 120.4, 119.3, 114.7, 109.8, 96.6, 82.4, 21.6. **MS (ESI)** *m/z* 209 $[M+H]^+$; HRMS Calculated for $C_{15}H_{13}O^+$ 209.0961; Found: 209.0963 $[M+H]^+$.



8

Compound **8** was prepared using the reported literature.[4]

Cyclohex-2-en-1-yl 3-phenylpropiolate (8): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **8** as colourless liquid in 85% yield (132 mg); **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.39-7.36 (m, 2H), 7.25 (td, *J* = 7.4, 1.3 Hz, 1H), 7.21-7.17 (m, 2H), 5.86-5.82 (m, 1H), 5.64 (dd, *J* = 10.2, 1.9 Hz, 1H), 5.24 (t, *J* = 1.6 Hz, 1H), 1.96-1.59 (m, 5H), 1.49-1.44 (m, 1H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 152.9, 132.9, 132.2, 130.0, 128.0, 124.2, 119.0, 85.0, 80.5, 69.4, 27.5, 24.2, 18.1. **MS (ESI)** *m/z* 227 $[M+H]^+$; HRMS Calculated for $C_{15}H_{15}O_2^+$ 227.1067; Found: 227.1066 $[M+H]^+$.

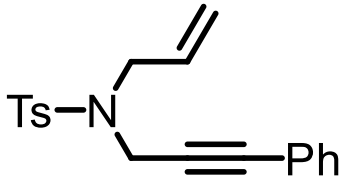


9

Compound **9** was prepared using the reported literature.[5]

(E)-3-phenyl-1-(2-(p-tolylethynyl)phenyl)prop-2-en-1-one (9): Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **9** as yellow-white solid in 72% yield

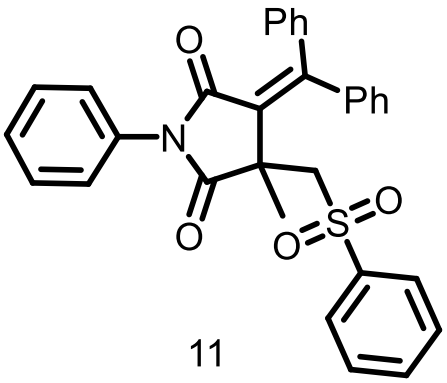
(69 mg), mp 202-204 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.76-7.72 (m, 2H), 7.67-7.59 (m, 4H), 7.54-7.36 (m, 5H), 7.28 (d, *J* = 7.8 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 2.33 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 193.8, 144.3, 141.9, 138.8, 135.0, 133.1, 131.5, 130.8, 130.5, 129.0, 128.9, 128.8, 128.6, 128.2, 125.9, 121.9, 119.6, 95.9, 87.4, 21.5. **MS (ESI)** *m/z* 323 $[M+H]^+$; HRMS Calculated for $C_{24}H_{19}O^+$ 323.1430; Found: 323.1432 $[M+H]^+$.



10

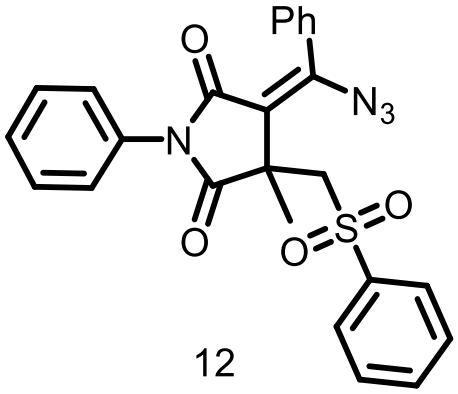
Compound **10** was prepared using the reported literature.[6]

***N*-allyl-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (10):** Purification by silica gel chromatography (PE:EA=88:12) afforded the desired **10** as white solid in 88% yield (100 mg), mp 182-184 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.24 (d, *J* = 8.3 Hz, 2H), 7.15-7.07 (m, 2H), 6.89 (d, *J* = 7.3 Hz, 2H), 5.85-5.75 (m, 1H), 5.34 (dd, *J* = 17.0, 1.3 Hz, 1H), 5.27-5.25 (m, 1H), 4.31 (s, 2H), 3.91 (d, *J* = 6.3 Hz, 2H), 2.32 (s, 3H), 2.28 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 143.6, 137.8, 132.9, 132.1, 132.0, 129.6, 129.3, 128.6, 128.1, 127.8, 122.0, 119.9, 85.9, 81.3, 49.3, 36.8, 21.4, 21.2; **MS (ESI)** *m/z* 326 $[M+H]^+$; HRMS Calculated for $C_{19}H_{20}NO_2S^+$ 326.1209; Found: 326.1210 $[M+H]^+$.



11

4-(diphenylmethylene)-3-methyl-1-phenyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (11): Purification by silica gel chromatography (PE:EA=80:20) afforded the desired **11** as white solid in 70% yield (64 mg), mp 212-214 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.89-7.82 (m, 5H), 7.54-7.47 (m, 6H), 7.46-7.34 (m, 9H), 4.11 (d, *J* = 14.8 Hz, 1H), 3.71 (d, *J* = 14.8 Hz, 1H), 1.59 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 176.4, 141.6, 140.6, 133.7, 133.1, 132.8, 132.0, 132.0, 131.4, 130.5, 129.4, 129.1, 128.8, 128.0, 127.9, 127.7, 127.2, 126.9, 62.5, 46.3, 26.7; **MS (ESI)** *m/z* 508 $[M+H]^+$; HRMS Calculated for $C_{31}H_{26}NO_4S^+$ 508.1577; Found: 508.1598 $[M+H]^+$.



12

(E)-4-(azido(phenyl)methylene)-3-methyl-1-phenyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione (12): Purification by silica gel chromatography (PE:EA=80:20) afforded the desired **12** as white solid in 60% yield (50.8 mg), mp 212-214 °C; **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 8.26-8.24 (m, 1H), 7.92-7.78 (m, 2H),

7.74-7.60 (m, 4H), 7.57-7.38 (m, 8H), 3.77 (d, *J* = 15.3 Hz, 1H), 3.15 (d, *J* = 15.0 Hz, 1H), 1.43 (s, 3H); **^{13}C-NMR (100 MHz, $CDCl_3$)** δ 177.3, 157.7, 140.9, 134.5, 134.3, 134.0, 132.1, 131.4, 130.3, 129.9, 129.6, 129.4, 129.3, 129.2, 129.1, 128.9, 128.6, 127.5, 127.3, 126.7, 126.3, 61.6, 44.8, 20.9; **MS (ESI)** *m/z* 473 $[M+H]^+$; HRMS Calculated for $C_{25}H_{21}N_4O_4S^+$ 473.1278; Found: 473.1298 $[M+H]^+$.

(9) References

1) Y Gu, L. Dai, K. Mao, J. Zhang, C. Wang, L. Zhao, L. Rong, *Org. Lett.* 2020, **22**, 2956.

2) B. Wang, J. Singh, Y. Deng, *Org. Lett.* 2023, **25**, 9219.

3) Z. Chen, W. Huang, Y. Su, H. Jiang, W. Wu, *Chem. Comm.*, 2023, **29**, 4523.

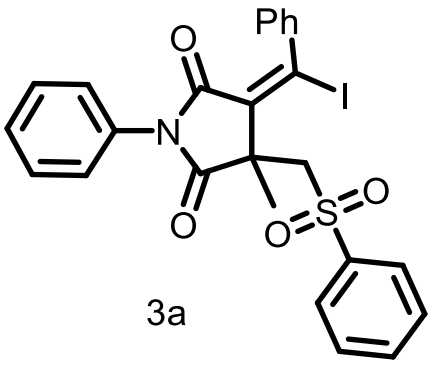
4) X. Chen, Z. Luo, Y. Chen, Y. Zhang, *Org. Lett.* 2020, **24**, 9200.

5) M. Mandal, A. K. Mahapatra, A. Kar, *Analyst*, 2021, **146**, 2998.

6) M. R. Mutra, J. Li, Y.-T. Chen, J.-J. Wang, *Chem. Eur. J.*, 2022, **28**, e202200742.

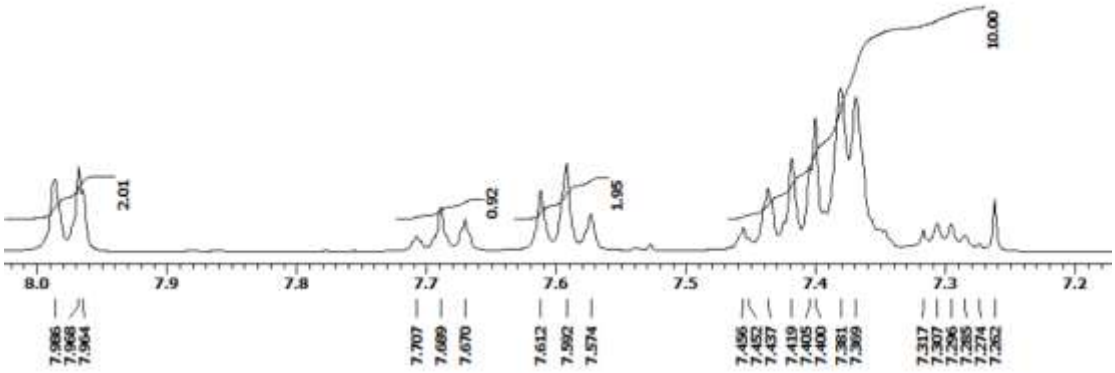
(10) Copies of ^{1}H NMR, ^{13}C NMR, ^{19}F NMR and Mass Spectra

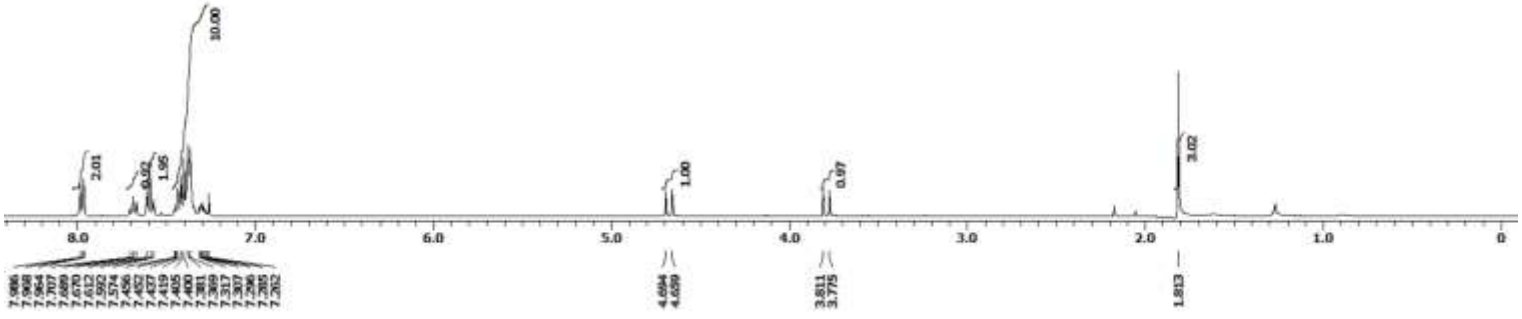
^{1}H NMR spectrum of 3a (400 MHz, $CDCl_3$)



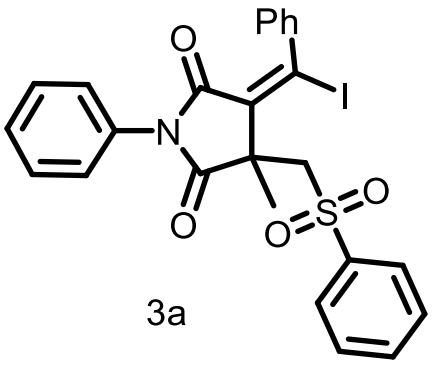
3a

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



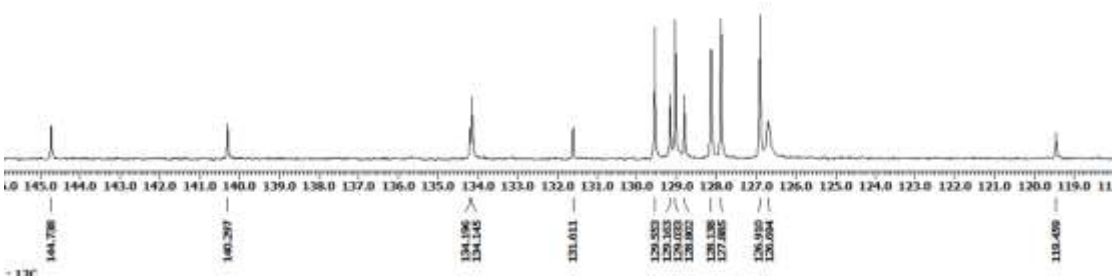


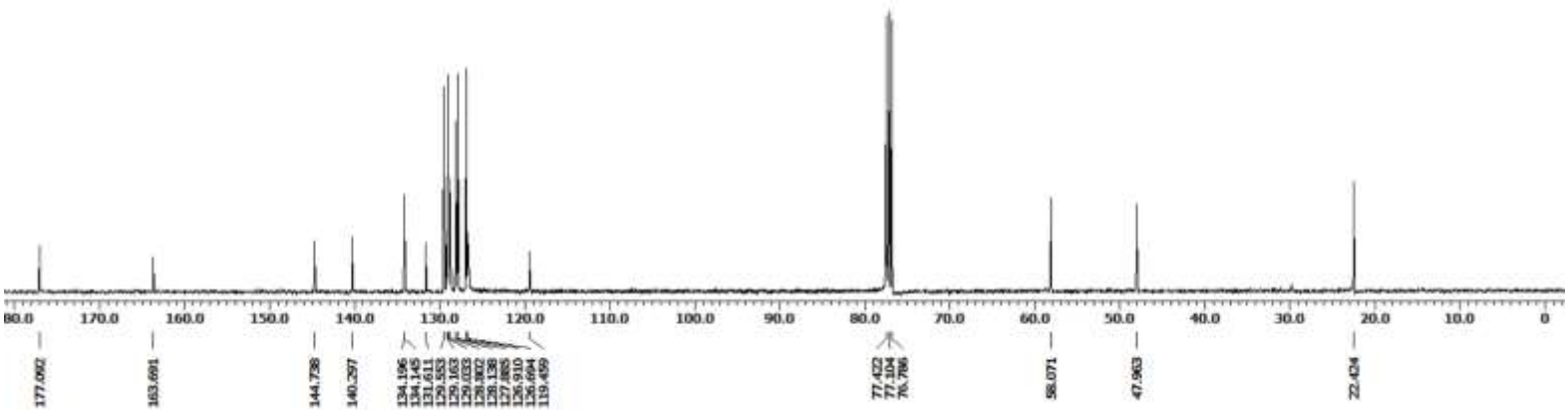
^{13}C NMR spectrum of 3a (100 MHz, $CDCl_3$)



3a

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





HRMS Spectrum of 3a

Qualitative Compound Report

Data File	SMT-160.d	**Sample Name**	SMT-160
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	06-06-2024 10:56:36
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	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C25 H20 I N O4 S	0.367	557.0126	4932	C25 H20 I N O4 S	557.0158	-5.81	C25 H20 I N O4 S	C25 H20 I N O4 S

Compound Label	m/z	RT	Algorithm	Mass
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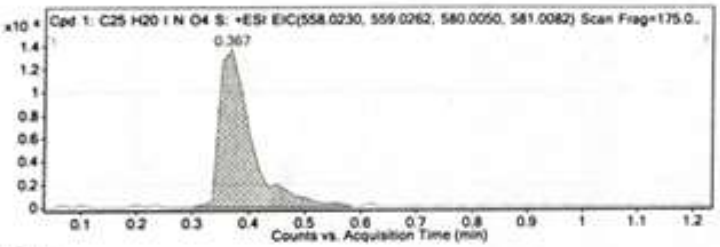
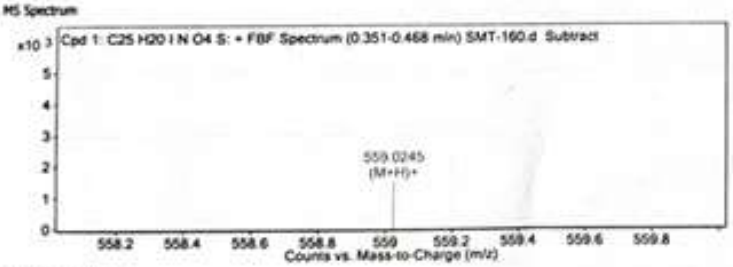
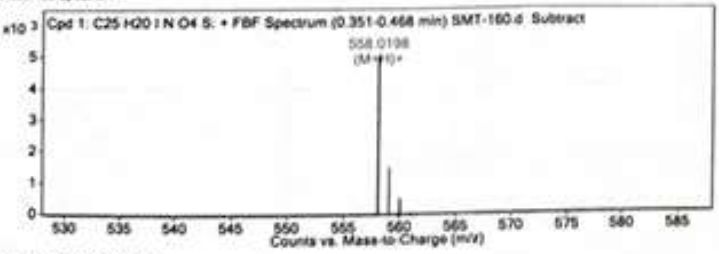


MS Spectrum



MS Zoomed Spectrum

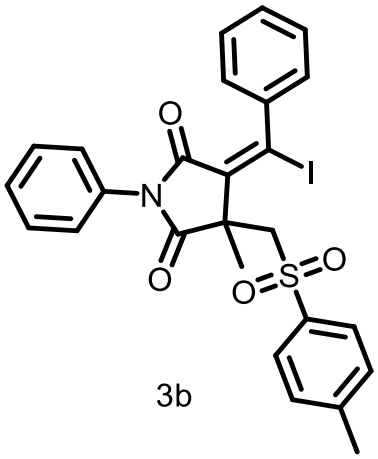


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
558.0198	1	4931.52	C25H21INO4S	(M+H)+
559.0245	1	1511.64	C25H21INO4S	(M+H)+
560.018	1	451.21	C25H21INO4S	(M+H)+

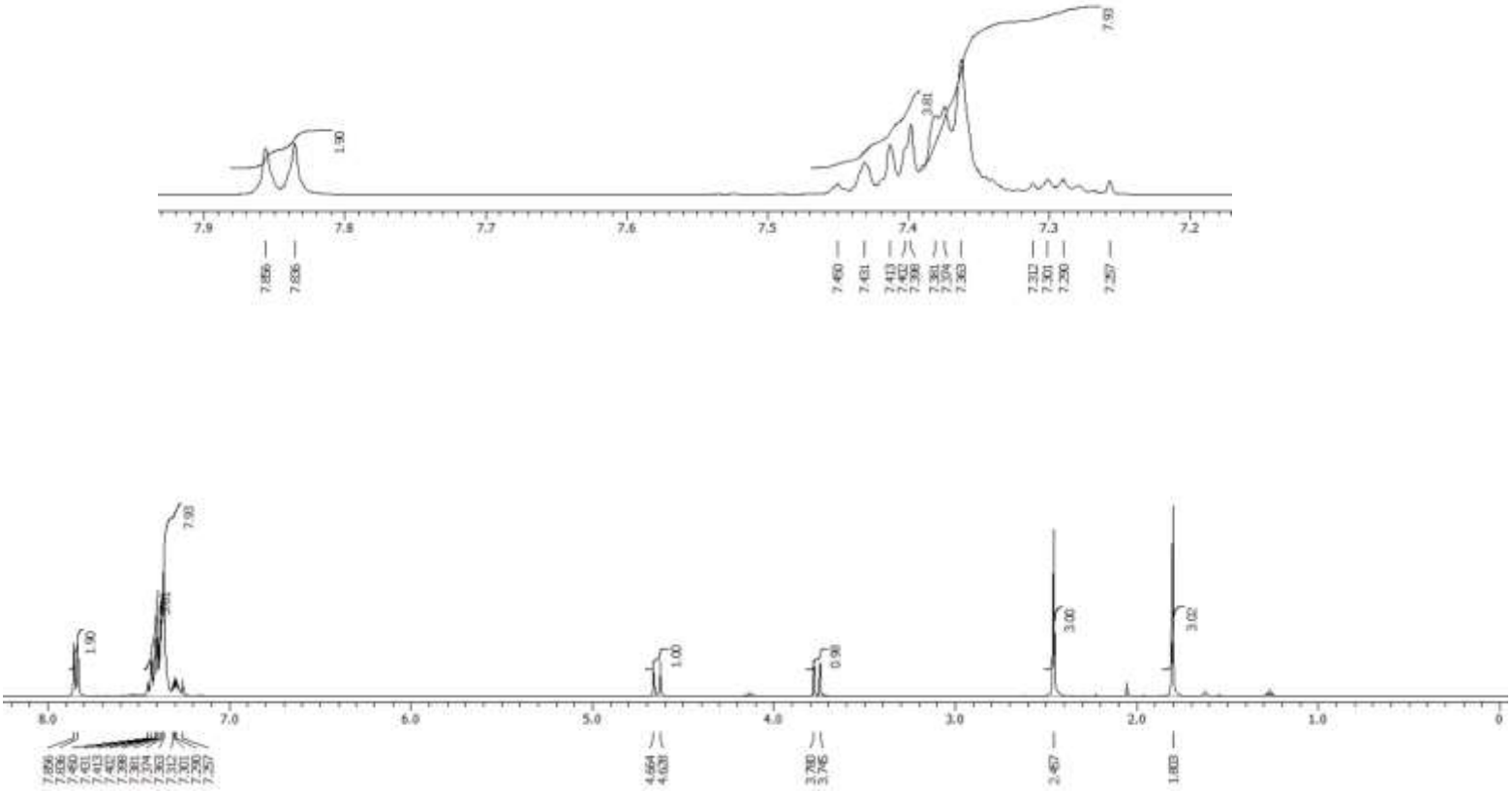
--- End Of Report ---

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

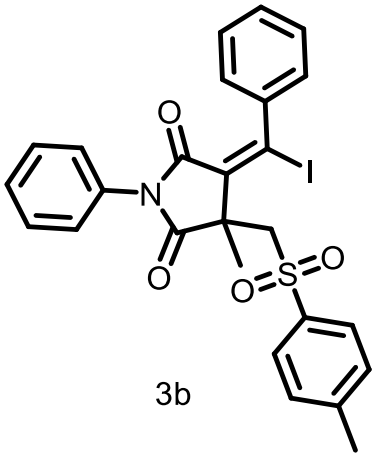


3b

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

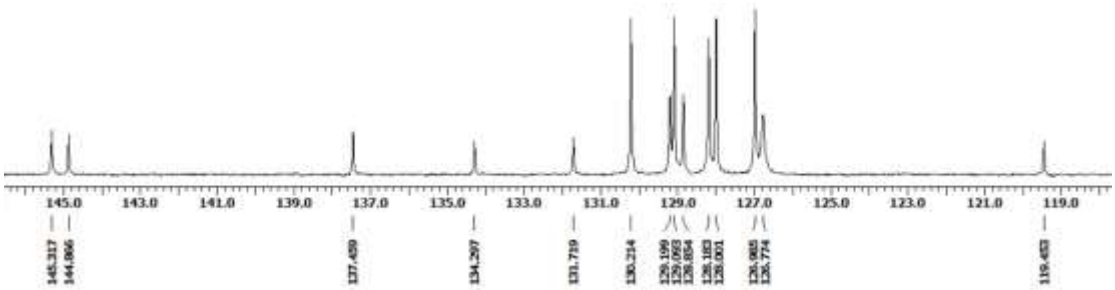


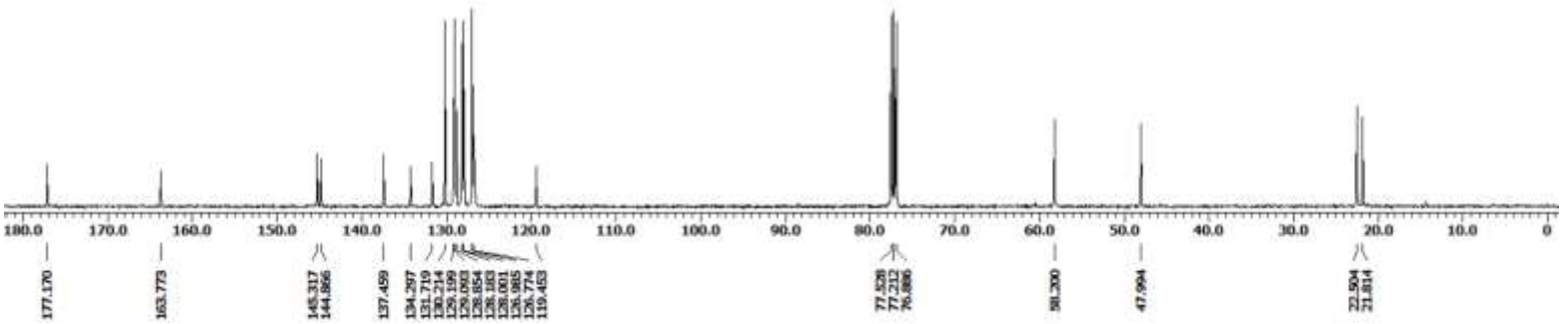
^{13}C NMR spectrum of 3b (100 MHz, $CDCl_3$)



3b

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





HRMS Spectrum of 3b

3 b

Qualitative Compound Report

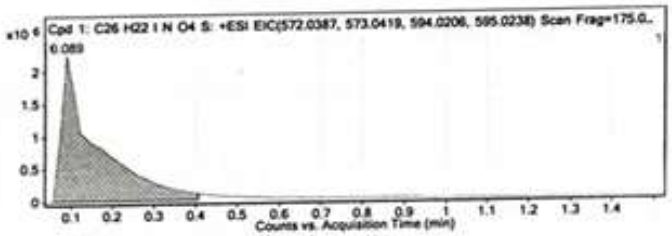
Data File	SMT-160.d	Sample Name	SMT-160
Sample Type	Sample	Position	P1-B3
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	17-10-2022 13:10:39
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

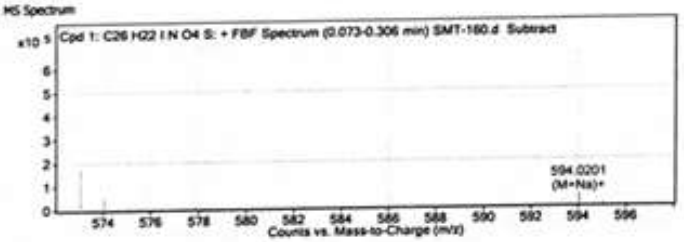
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H22 I N O4 S	0.089	571.0314	595894	C26 H22 I N O4 S	571.0314	-0.03	C26 H22 I N O4 S	C26 H22 I N O4 S

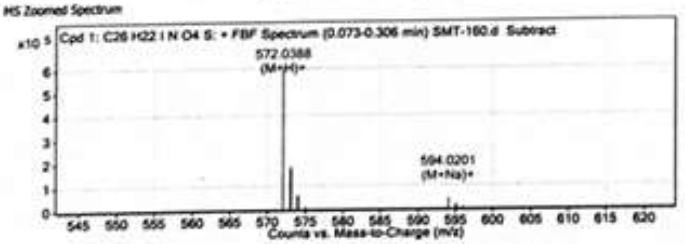
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H22 I N O4 S	572.0388	0.089	Find By Formula	571.0314



MS Spectrum



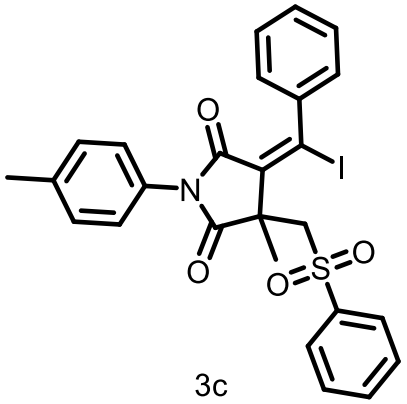
MS Zoomed Spectrum



MS Spectrum Peak List

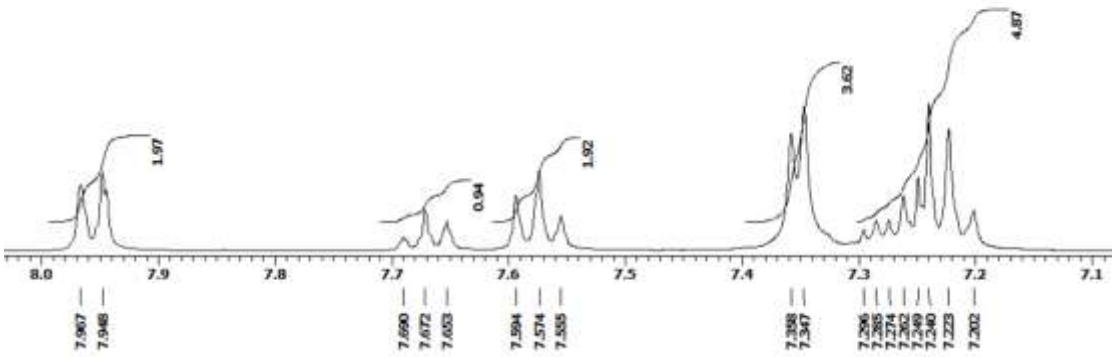
m/z	z	Abund	Formula	Ion
572.0388	1	595893.75	C26H23INO4S	(M+H)+
573.0417	1	170346.25	C26H23INO4S	(M+H)+
574.0395	1	50446.83	C26H23INO4S	(M+H)+
575.0406	1	9973.11	C26H23INO4S	(M+H)+
576.0425	1	1506.78	C26H23INO4S	(M+H)+
594.0201	1	44584.1	C26H22INNaO4S	(M+Na)+
595.0231	1	12519.06	C26H22INNaO4S	(M+Na)+
596.0219	1	3935.14	C26H22INNaO4S	(M+Na)+
597.0252	1	851.24	C26H22INNaO4S	(M+Na)+
598.0229	1	46.79	C26H22INNaO4S	(M+Na)+

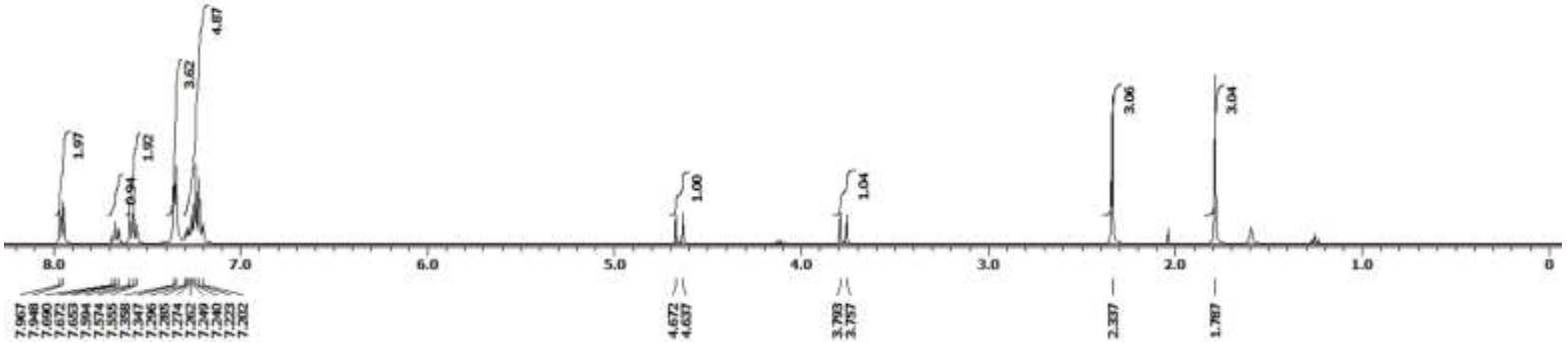
^{1}H NMR spectrum of 3c (400 MHz, $CDCl_3$)



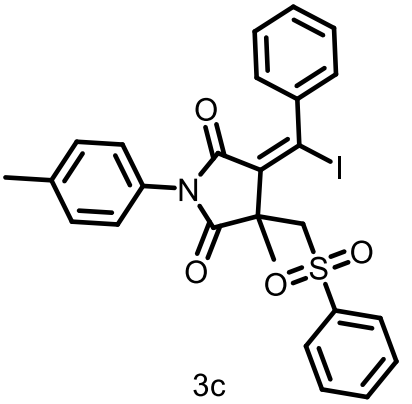
3c

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



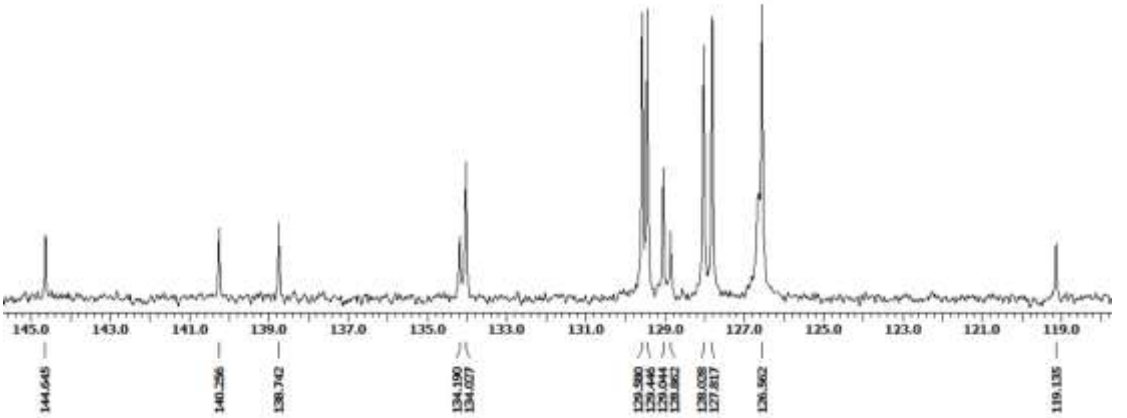


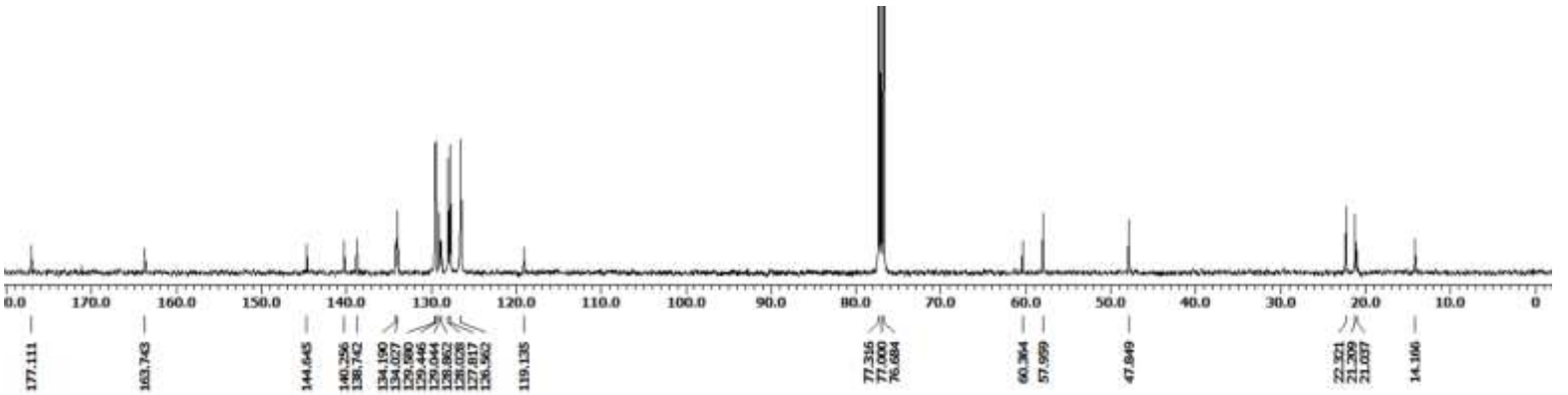
^{13}C NMR spectrum of 3c (100 MHz, $CDCl_3$)



3c

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





HRMS Spectrum of 3c

3c

Qualitative Compound Report

Data File	SMT-194.d	Sample Name	SMT-194
Sample Type	Sample	Position	P1-A7
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IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

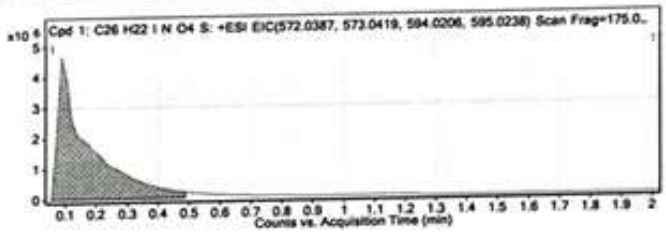
Sample Group — Info. 3

Acquisition SW Version: 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

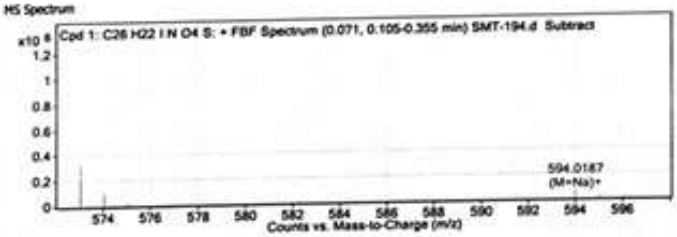
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H22 I N O4 S	0.088	571.0302	1085465	C26 H22 I N O4 S	571.0314	-2.09	C26 H22 I N O4 S	C26 H22 I N O4 S

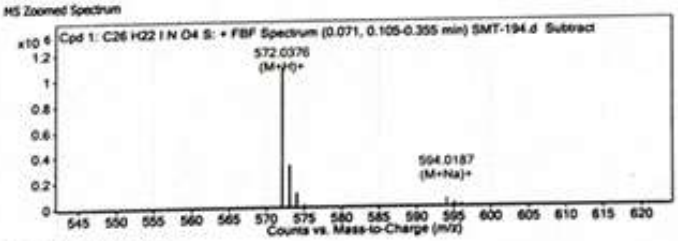
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H22 I N O4 S	572.0376	0.088	Find By Formula	571.0302



MS Spectrum



MS Zoomed Spectrum

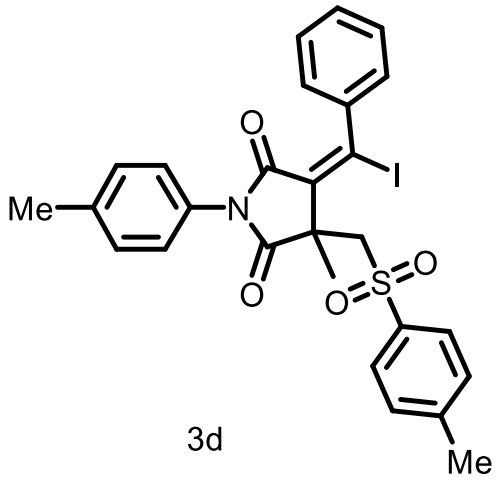


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
572.0376	1	1085465.13	C26H23INO4S	(M+H)+
573.0406	1	322910.97	C26H23INO4S	(M+H)+
574.0386	1	96945.81	C26H23INO4S	(M+H)+
575.039	1	19122.98	C26H23INO4S	(M+H)+
576.0407	1	2822.33	C26H23INO4S	(M+H)+
594.0187	1	58851.18	C26H22INaO4S	(M+Na)+
595.0217	1	17132.49	C26H22INaO4S	(M+Na)+
596.0198	1	5150.85	C26H22INaO4S	(M+Na)+
597.0218	1	1036.77	C26H22INaO4S	(M+Na)+
598.0262	1	134.78	C26H22INaO4S	(M+Na)+

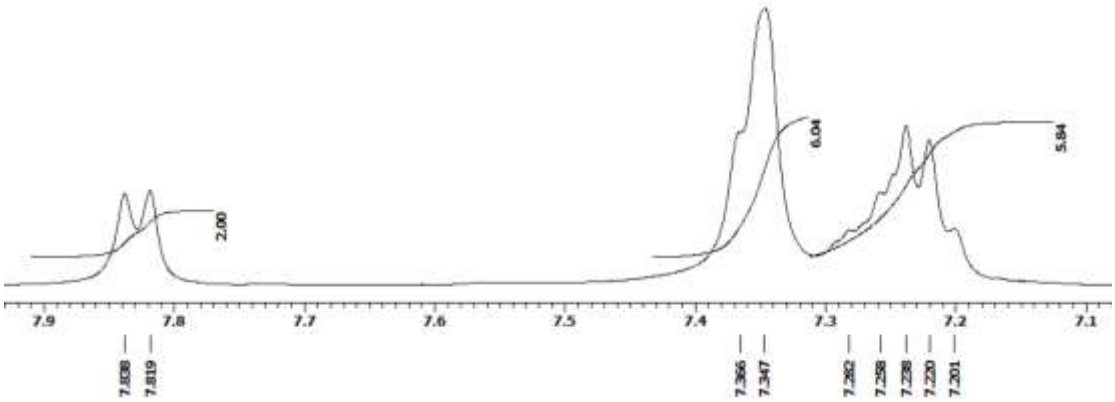
Agilent Technologies — Page 1 of 2 — Printed at: 14:21 on:13-10-2022

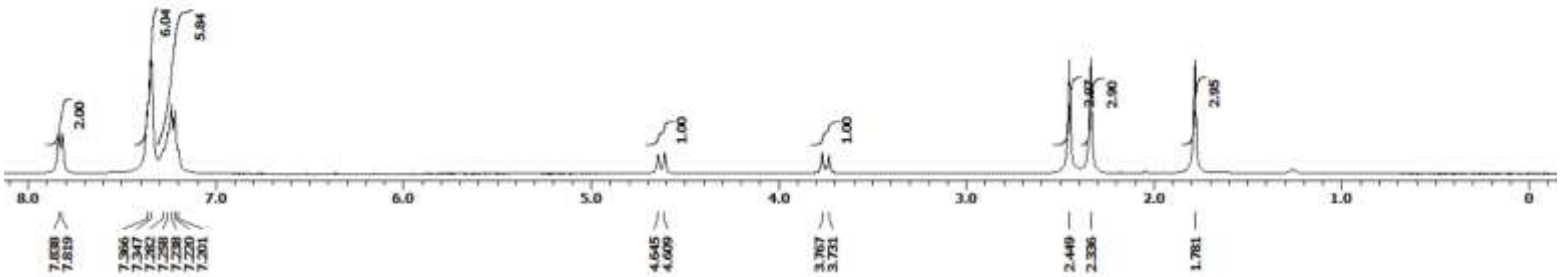
^{1}H NMR spectrum of 3d (400 MHz, $CDCl_3$)



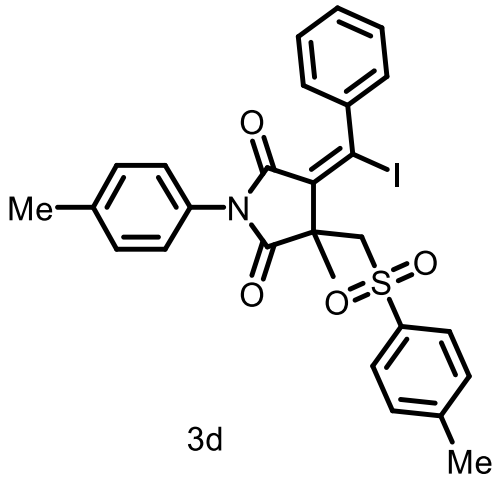
3d

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



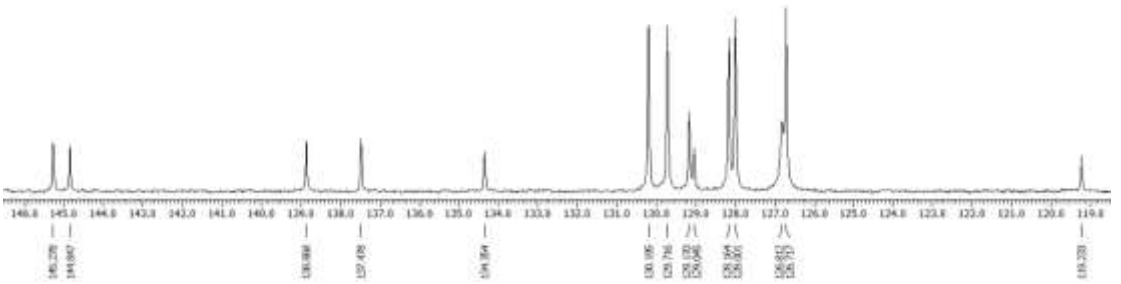


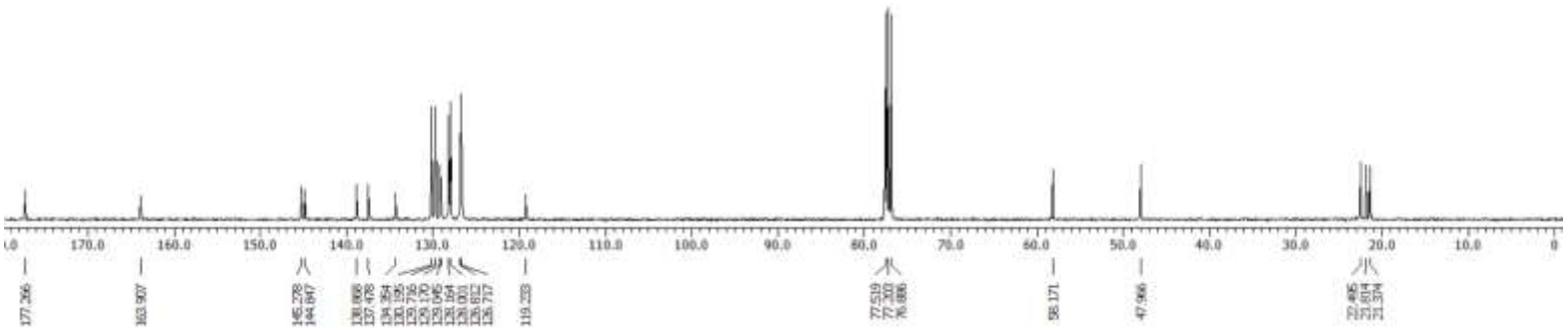
^{13}C NMR spectrum of 3d (100 MHz, $CDCl_3$)



3d

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





HRMS Spectrum of 3d

3d

Qualitative Compound Report

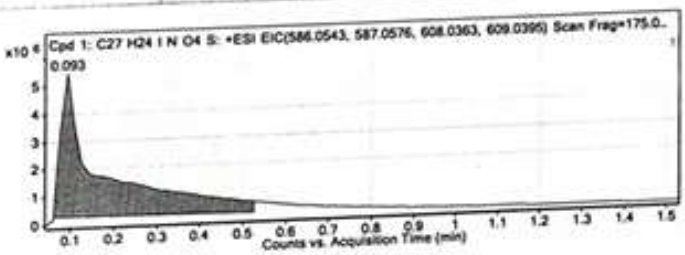
Data File	SMT-161.d	Sample Name	SMT-161
Sample Type	Sample	Position	P1-B6
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	19-10-2022 13:23:38
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

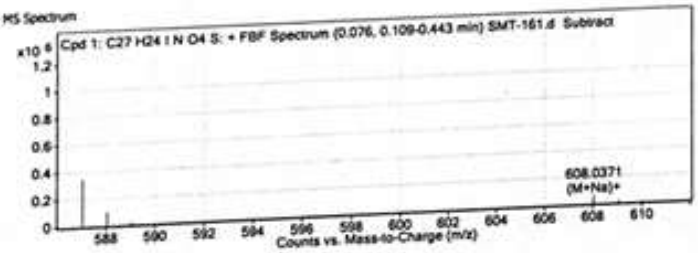
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C27 H24 I N O4 S	0.093	585.0491	55032	C27 H24 I N O4 S	585.0471	3.47	C27 H24 I N O4 S	C27 H24 I N O4 S

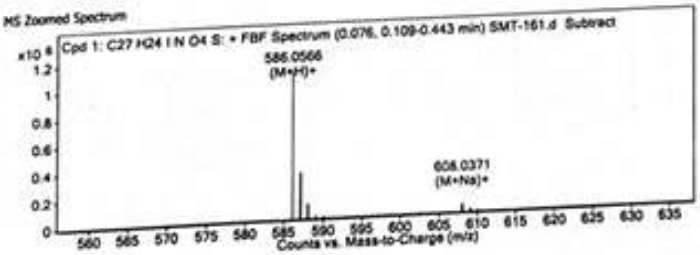
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C27 H24 I N O4 S	608.0371	0.093	Find By Formula	585.0491



MS Spectrum



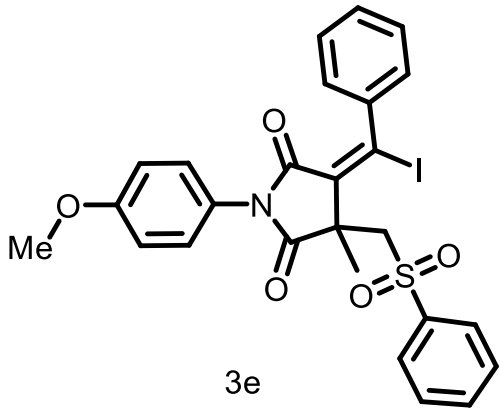
MS Zoomed Spectrum



MS Spectrum Peak List

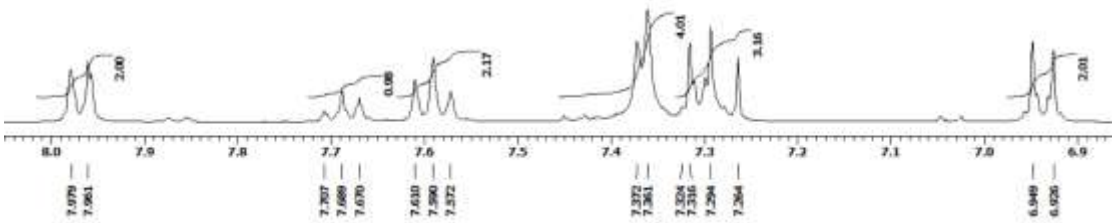
m/z	z	Abund	Formula	Ion
586.0566	1	1081560.13	C27H25INO4S	(M+H)+
587.0594	1	341044.53	C27H25INO4S	(M+H)+
588.0575	1	99728.45	C27H25INO4S	(M+H)+
589.0581	1	19938.63	C27H25INO4S	(M+H)+
590.0591	1	2990.24	C27H25INO4S	(M+H)+
608.0371	1	55031.58	C27H24INNaO4S	(M+Na)+
609.04	1	16748.64	C27H24INNaO4S	(M+Na)+
610.0385	1	5023.69	C27H24INNaO4S	(M+Na)+
611.04	1	1121.47	C27H24INNaO4S	(M+Na)+
612.0448	1	147.35	C27H24INNaO4S	(M+Na)+

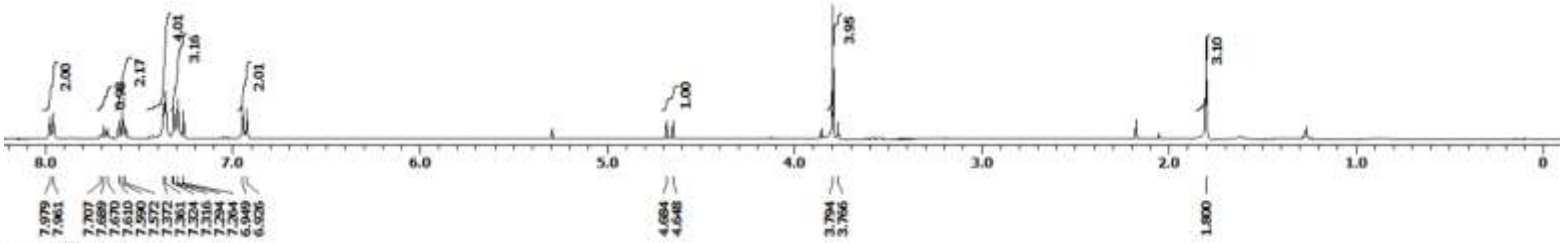
^{1}H NMR spectrum of 3e (400 MHz, $CDCl_3$)



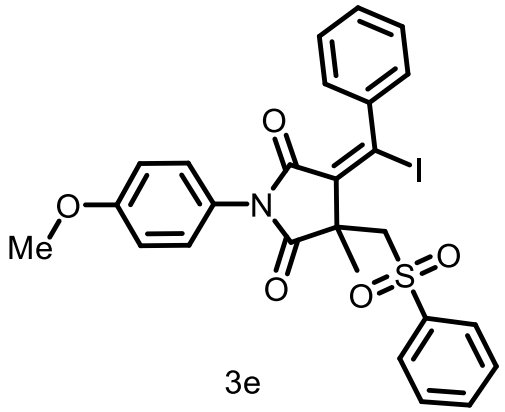
3e

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



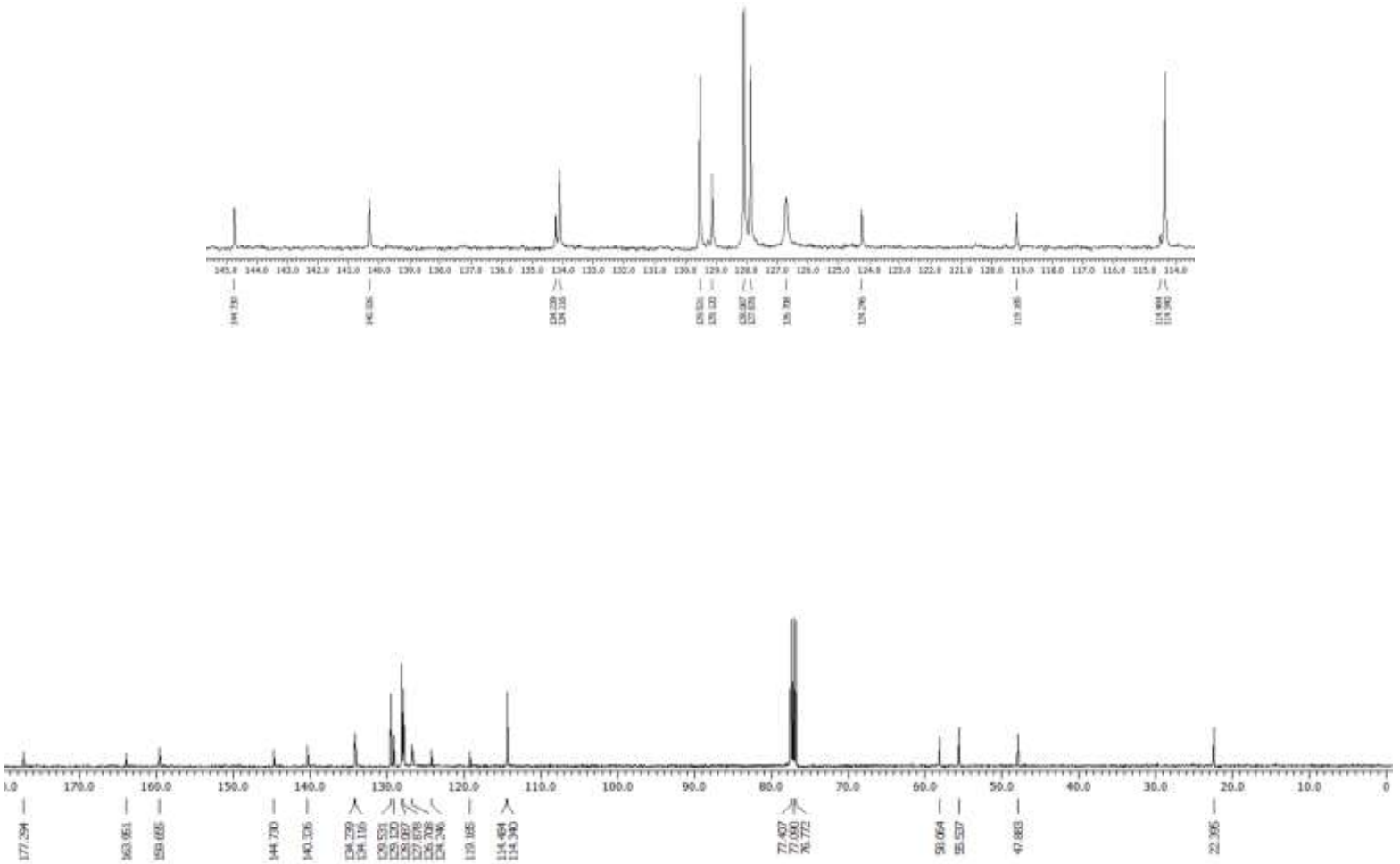


^{13}C NMR spectrum of 3e (100 MHz, $CDCl_3$)



3e

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



HRMS Spectrum of 3e

3a

Qualitative Compound Report

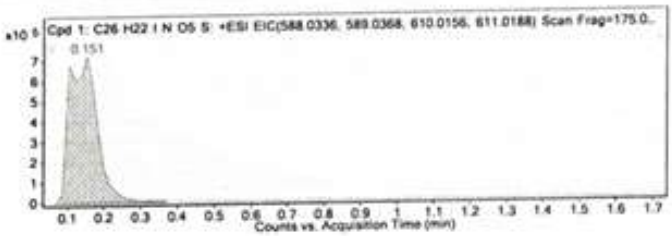
Data File	SMT-422.d	**Sample Name**	SMT-422
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	10-02-2024 12:17:33
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

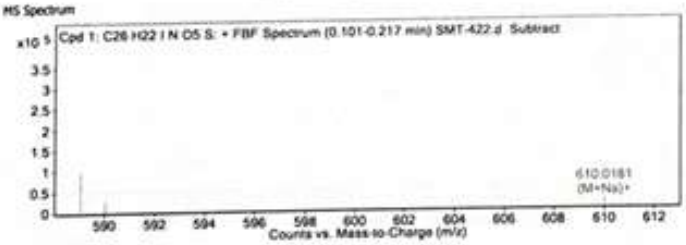
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H22 I N O5 S	0.151	587.0286	343979	C26 H22 I N O5 S	587.0263	3.78	C26 H22 I N O5 S	C26 H22 I N O5 S

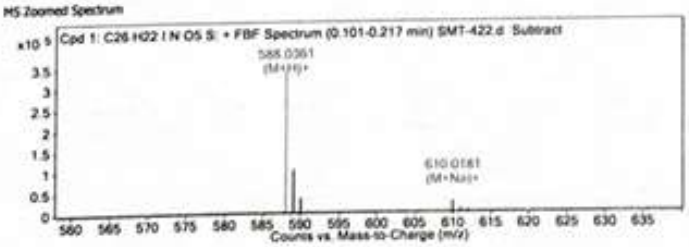
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H22 I N O5 S	588.0361	0.151	Find By Formula	587.0286



MS Spectrum



MS Zoomed Spectrum

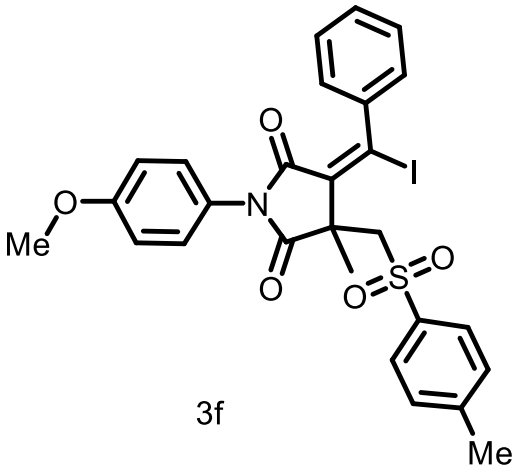


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
588.0361	1	343978.75	C26H23INO5S	(M+H)+
589.0389	1	98272.41	C26H23INO5S	(M+H)+
590.0367	1	30175.5	C26H23INO5S	(M+H)+
610.0181	1	20568.38	C26H22INNaO5S	(M+Na)+
611.0215	1	6647.8	C26H22INNaO5S	(M+Na)+
611.9994	1	3214.13	C26H22INNaO5S	(M+Na)+
613.0008	1	1014.48	C26H22INNaO5S	(M+Na)+

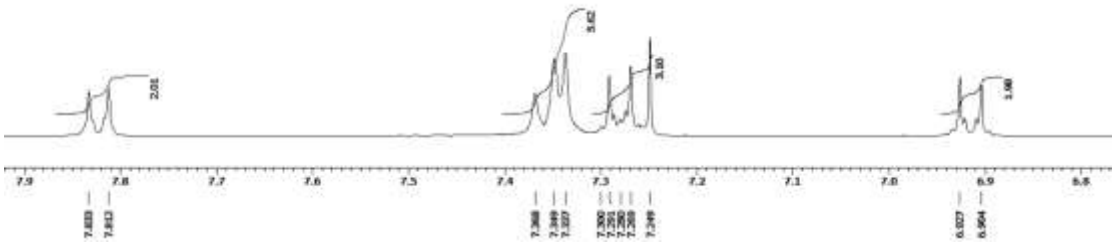
--- End Of Report ---

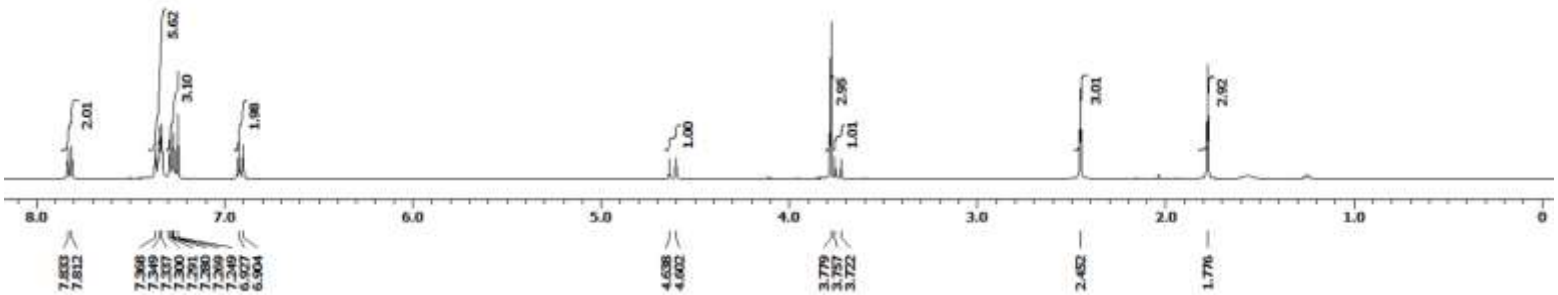
^{1}H NMR spectrum of 3f (400 MHz, $CDCl_3$)



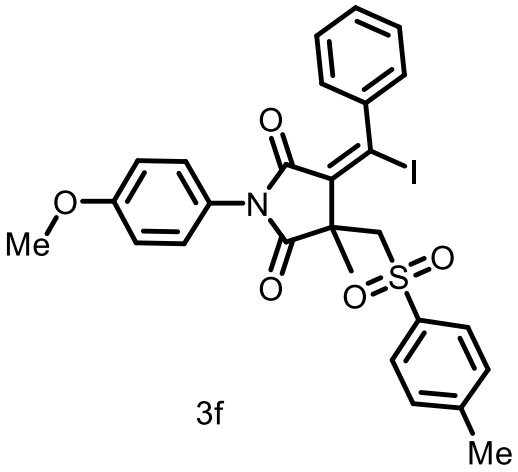
3f

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



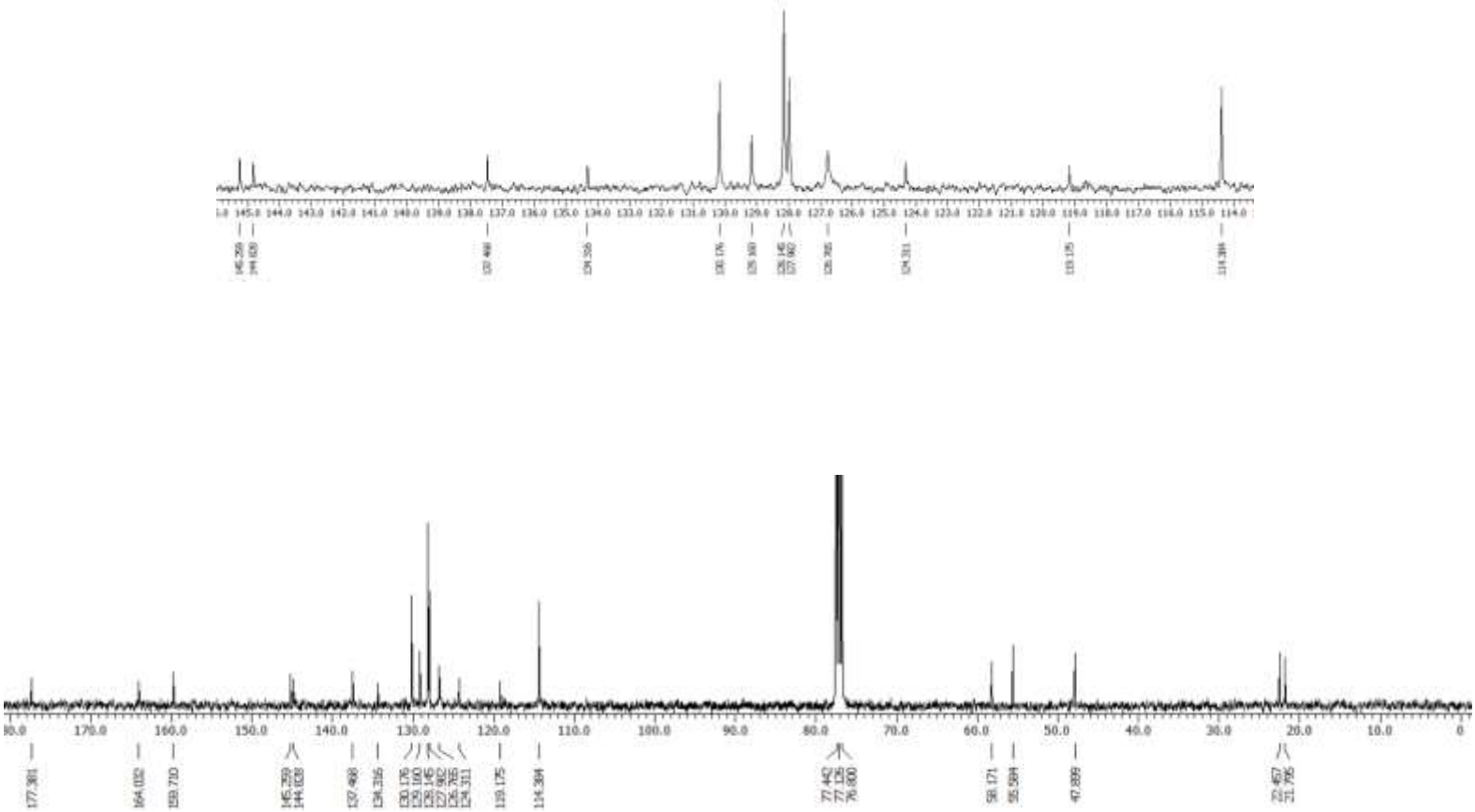


^{13}C NMR spectrum of 3f (100 MHz, $CDCl_3$)



3f

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



HRMS Spectrum of 3f

3f

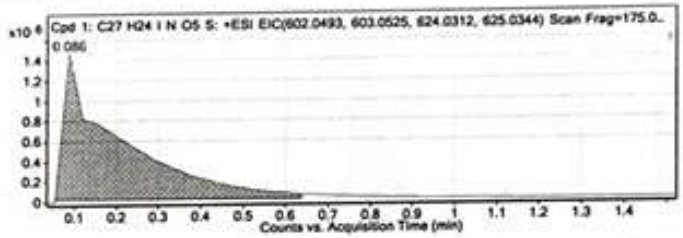
Qualitative Compound Report

Data File	SMT-162.d	Sample Name	SMT-162
Sample Type	Sample	Position	P1-C8
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-10-2022 14:24:05
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

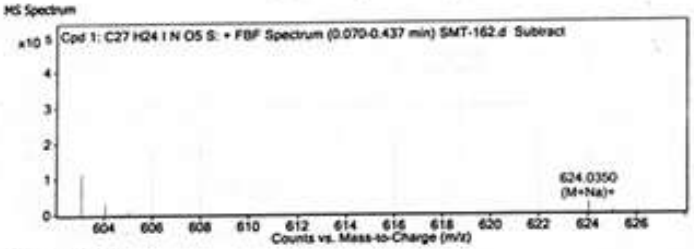
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C27 H24 I N O5 S	0.086	601.0463	28466	C27 H24 I N O5 S	601.042	7.23	C27 H24 I N O5 S	C27 H24 I N O5 S

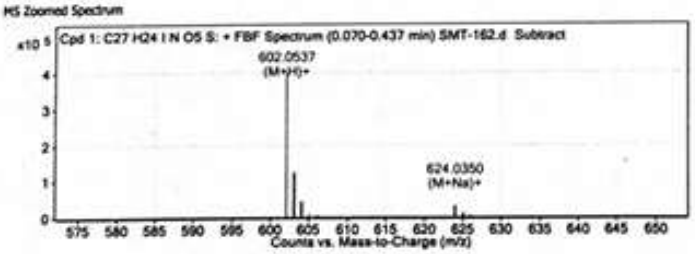
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C27 H24 I N O5 S	624.035	0.086	Find By Formula	601.0463



MS Spectrum



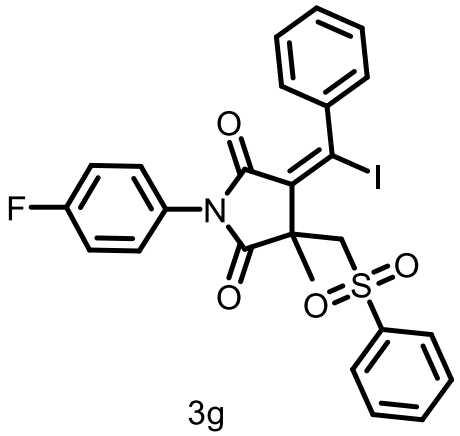
MS Zoomed Spectrum



MS Spectrum Peak List

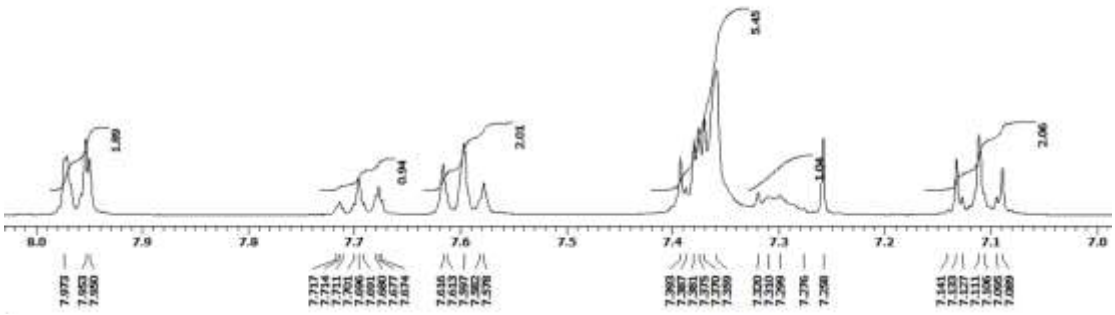
m/z	z	Abund	Formula	Ion
602.0537	1	400548.34	C27H25INO5S	(M+H)+
603.0566	1	117963.08	C27H25INO5S	(M+H)+
604.0548	1	35486.55	C27H25INO5S	(M+H)+
605.0567	1	8408.53	C27H25INO5S	(M+H)+
606.0593	1	1569.39	C27H25INO5S	(M+H)+
607.0647	1	235.7	C27H25INO5S	(M+H)+
624.035	1	28465.54	C27H24INNaO5S	(M+Na)+
625.038	1	8310.5	C27H24INNaO5S	(M+Na)+
626.0366	1	2773.52	C27H24INNaO5S	(M+Na)+
627.0378	1	596.74	C27H24INNaO5S	(M+Na)+
628.0375	1	75.31	C27H24INNaO5S	(M+Na)+

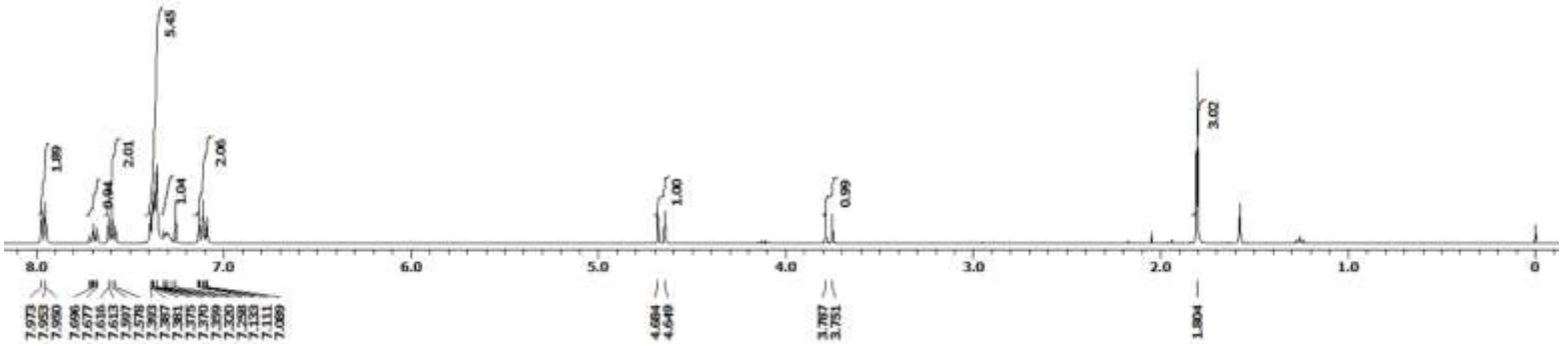
^{1}H NMR spectrum of 3g (400 MHz, $CDCl_3$)



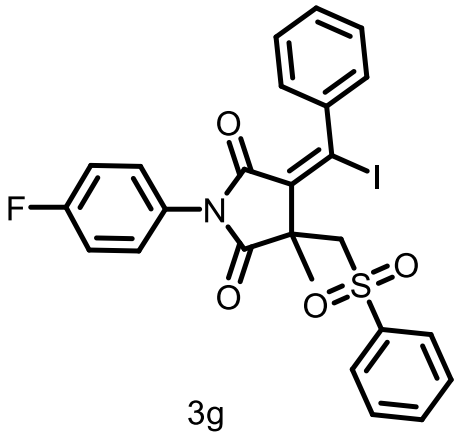
3g

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



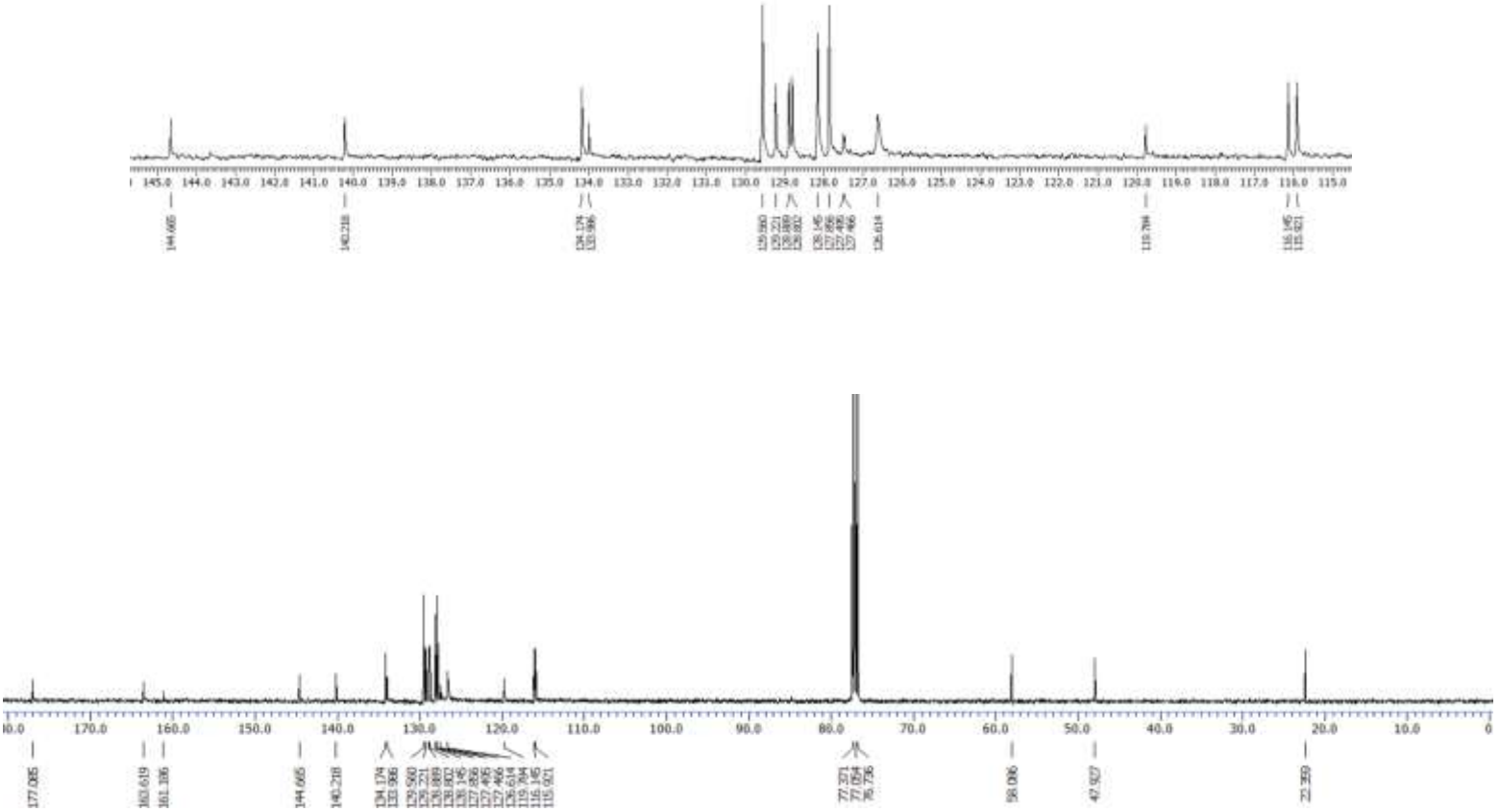


^{13}C NMR spectrum of 3g (100 MHz, $CDCl_3$)

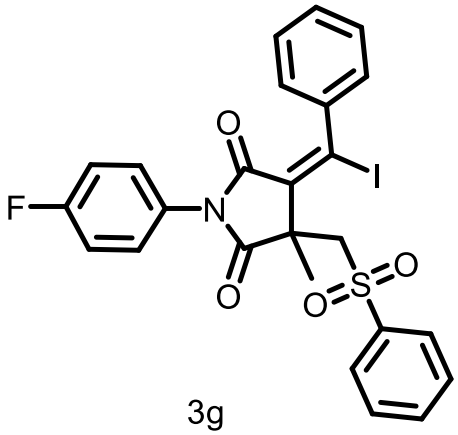


3g

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

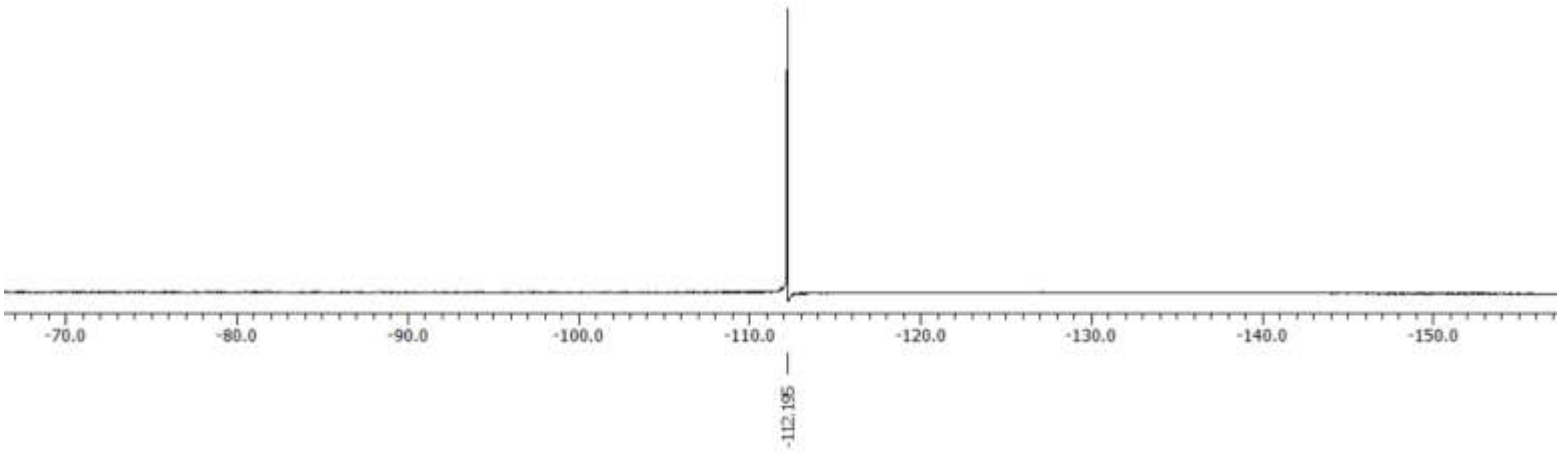


^{19}F NMR spectrum of 3g (376 MHz, $CDCl_3$)



3g

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



HRMS Spectrum of 3g

Qualitative Compound Report

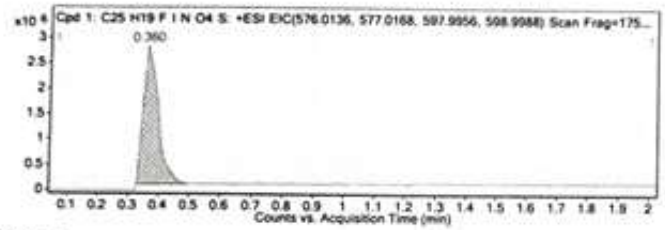
Data File	SMT-169.d	Sample Name	SMT-169
Sample Type	Sample	Position	P1-A2
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	30-05-2024 13:01:47
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

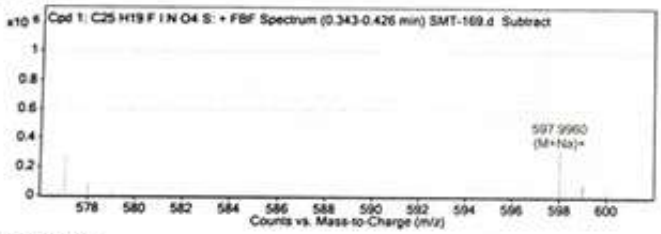
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C25 H19 F I N O4 S	0.36	575.0069	322445	C25 H19 F I N O4 S	575.0064	1.03	C25 H19 F I N O4 S	C25 H19 F I N O4 S

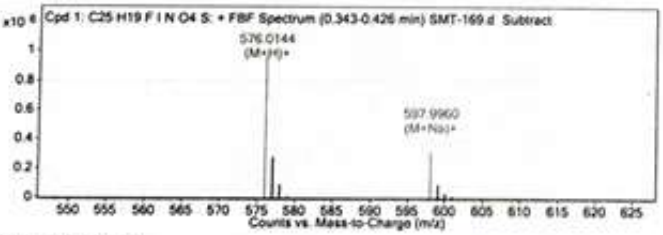
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C25 H19 F I N O4 S	597.996	0.36	Find By Formula	575.0069



MS Spectrum



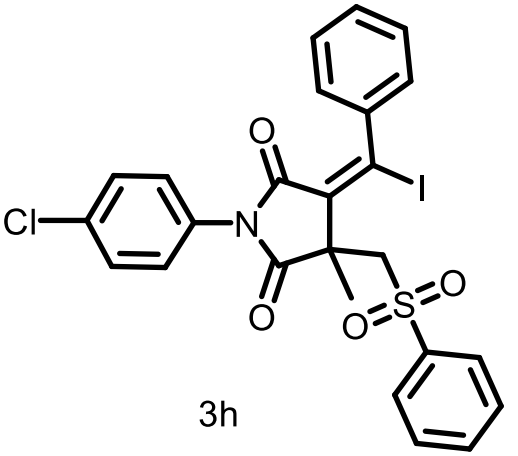
MS Zoomed Spectrum



MS Spectrum Peak List

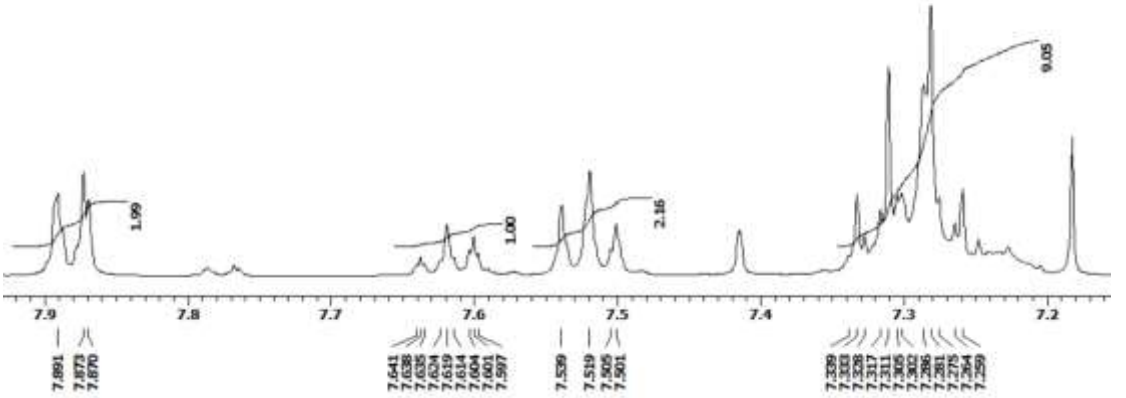
m/z	z	Abund	Formula	Ion
576.0144	1	980541.44	C25H20FINO4S	(M+H)+
577.0172	1	273318.53	C25H20FINO4S	(M+H)+
578.0151	1	79775.9	C25H20FINO4S	(M+H)+
579.0154	1	15727.16	C25H20FINO4S	(M+H)+
580.0163	1	2690.31	C25H20FINO4S	(M+H)+
597.996	1	322444.91	C25H19FINNaO4S	(M+Na)+
598.9988	1	86133.88	C25H19FINNaO4S	(M+Na)+
599.9974	1	25399.93	C25H19FINNaO4S	(M+Na)+
600.998	1	5171.04	C25H19FINNaO4S	(M+Na)+
601.9982	1	731.2	C25H19FINNaO4S	(M+Na)+

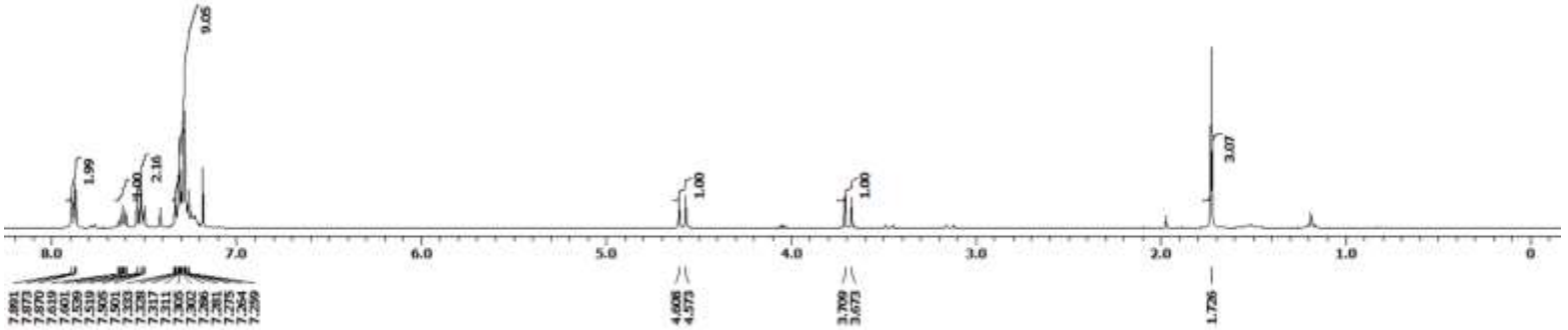
^{1}H NMR spectrum of 3h (400 MHz, $CDCl_3$)



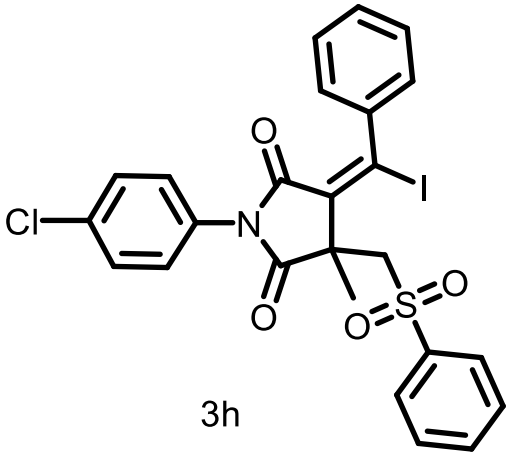
3h

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



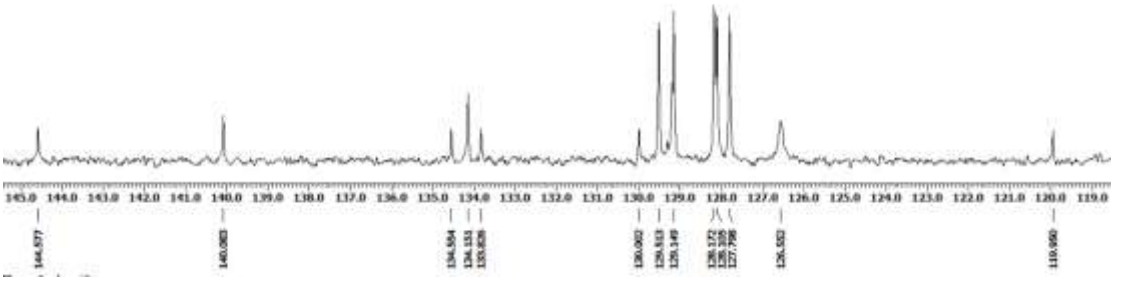


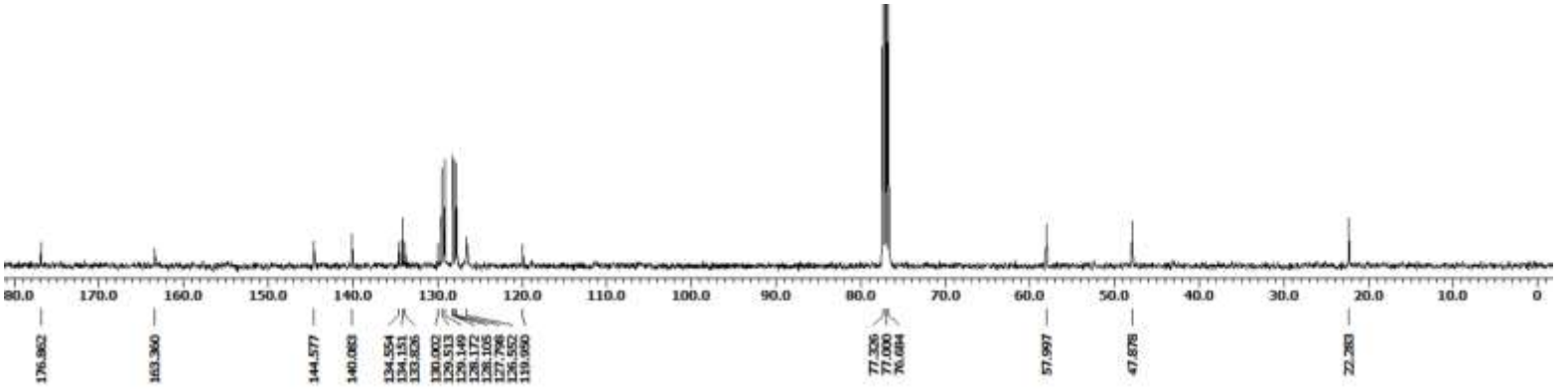
^{13}C NMR spectrum of 3h (100 MHz, $CDCl_3$)



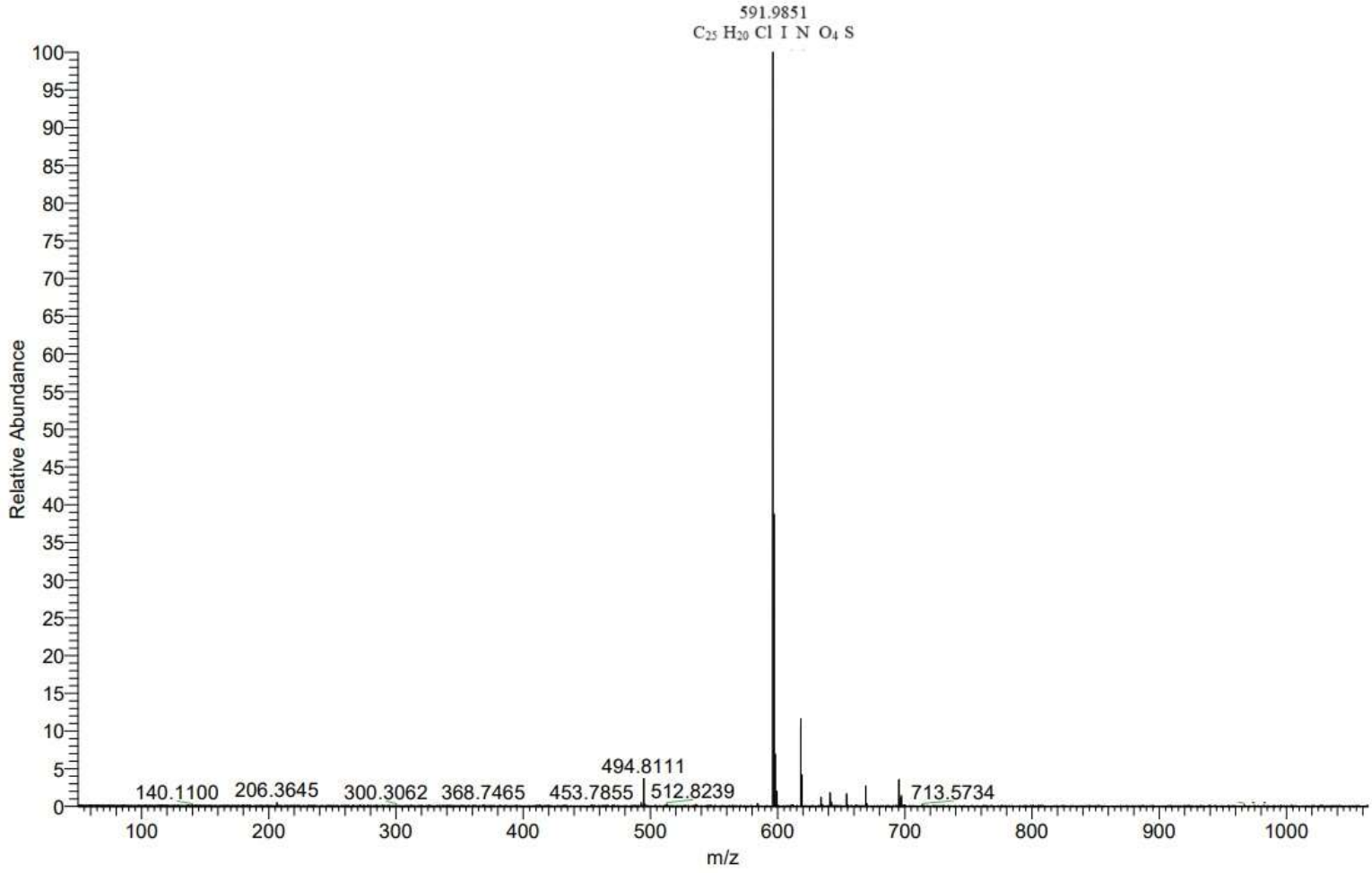
3h

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

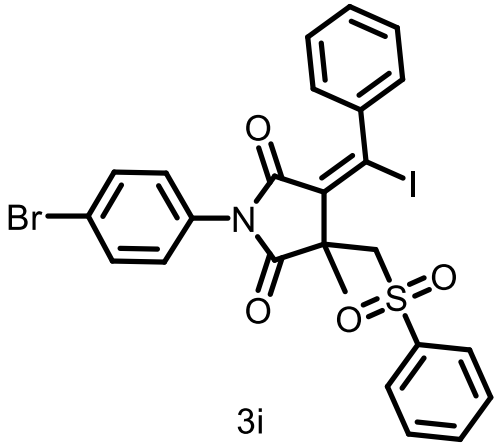




HRMS Spectrum of 3h

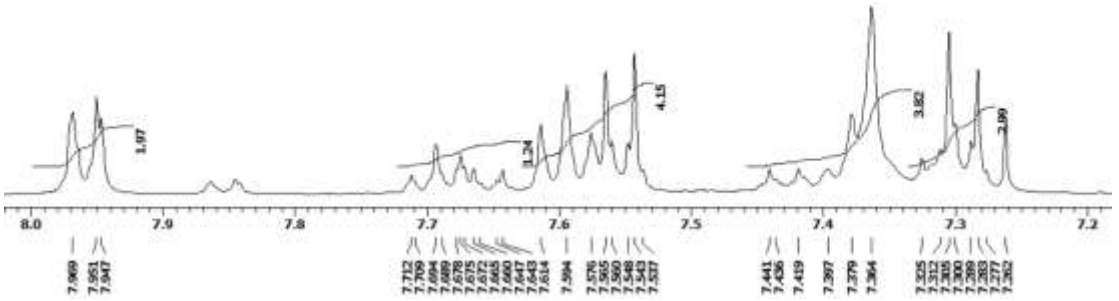


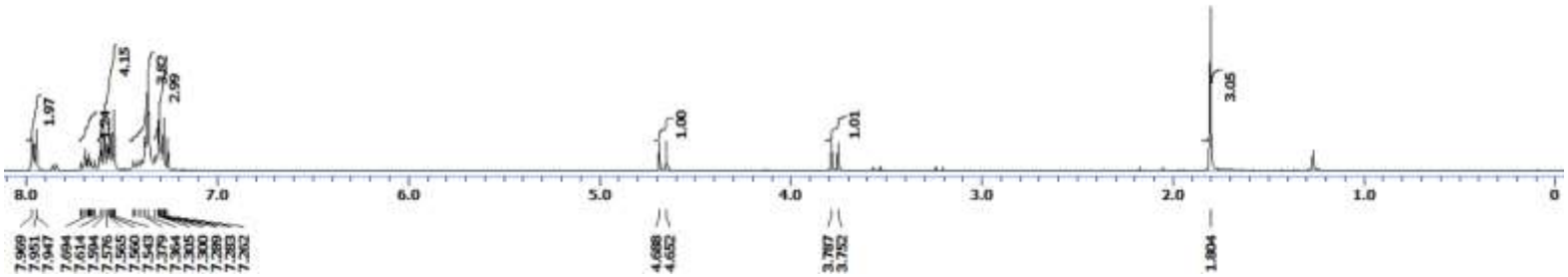
^{1}H NMR spectrum of 3i (400 MHz, $CDCl_3$)



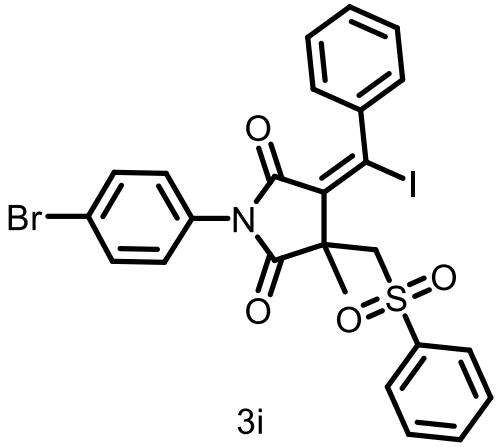
3i

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



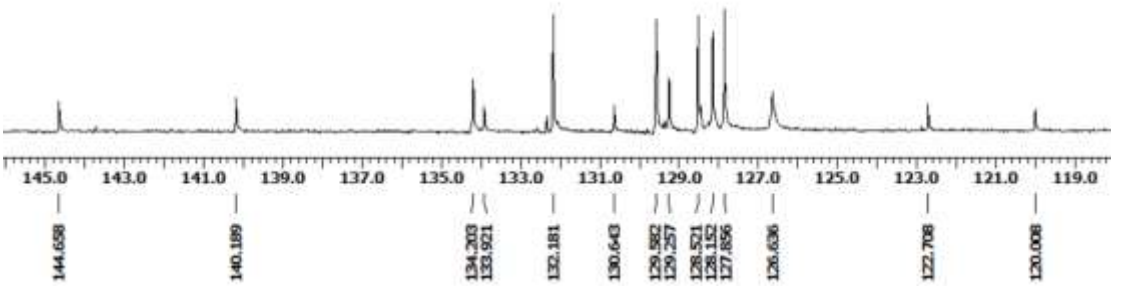


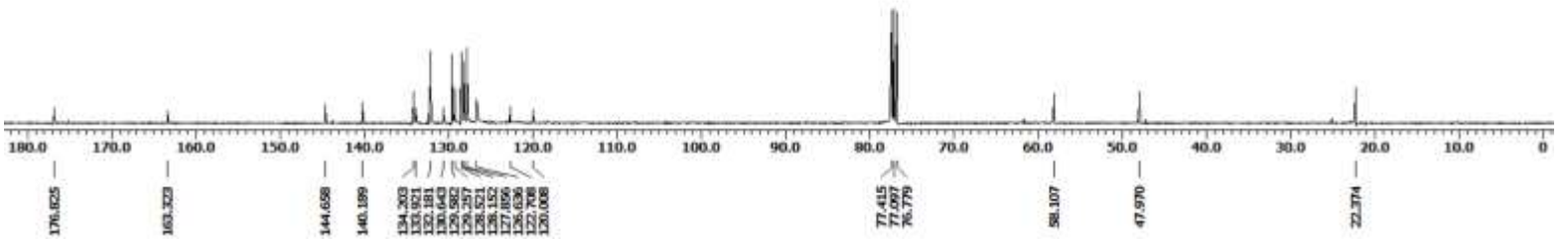
^{13}C NMR spectrum of 3i (100 MHz, $CDCl_3$)



3i

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





HRMS Spectrum of 3i

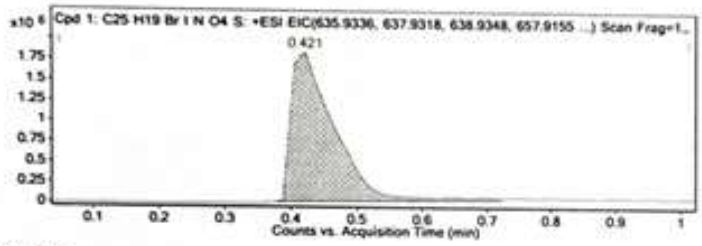
Qualitative Compound Report

Data File	ANU-2.d	Sample Name	ANU-2
Sample Type	Sample	Position	P1-D9
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	29-05-2024 15:44:49
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)		

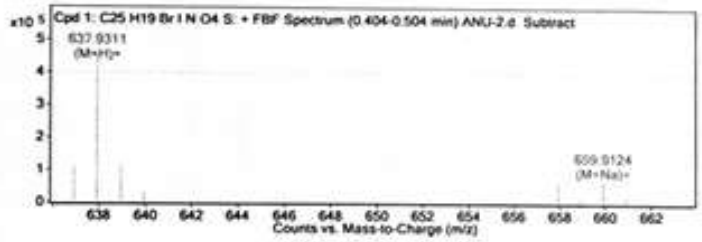
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C25 H19 Br I N O4 S	0.421	634.9255	452296	C25 H19 Br I N O4 S	634.9263	-1.27	C25 H19 Br I N O4 S	C25 H19 Br I N O4 S

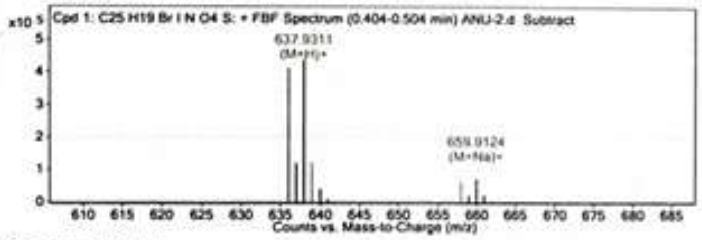
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C25 H19 Br I N O4 S	637.9311	0.421	Find By Formula	634.9255



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
635.9329	1	417279.41	C25H20BrINO4S	(M+H)+
636.9358	1	111180.09	C25H20BrINO4S	(M+H)+
637.9311	1	452295.84	C25H20BrINO4S	(M+H)+
638.9338	1	116863.17	C25H20BrINO4S	(M+H)+
639.9317	1	32584.09	C25H20BrINO4S	(M+H)+
640.9318	1	6078.62	C25H20BrINO4S	(M+H)+
641.9338	1	1087.86	C25H20BrINO4S	(M+H)+
657.9148	1	66018.15	C25H19BrINNaO4S	(M+Na)+
658.9179	1	18269.51	C25H19BrINNaO4S	(M+Na)+
659.9124	1	69347.98	C25H19BrINNaO4S	(M+Na)+
660.9155	1	18418.81	C25H19BrINNaO4S	(M+Na)+

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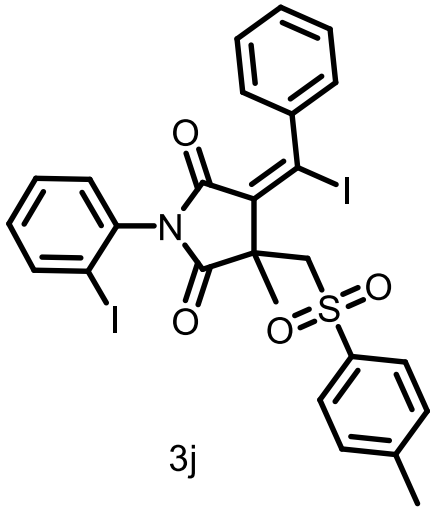
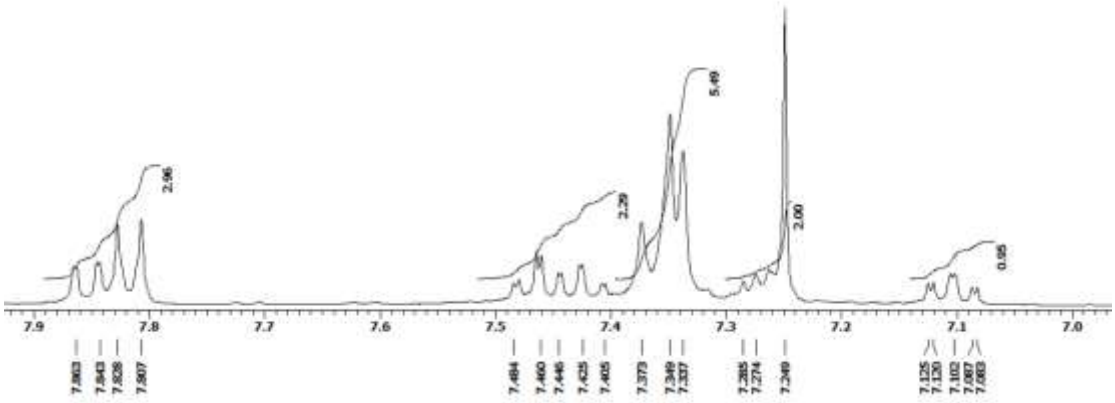
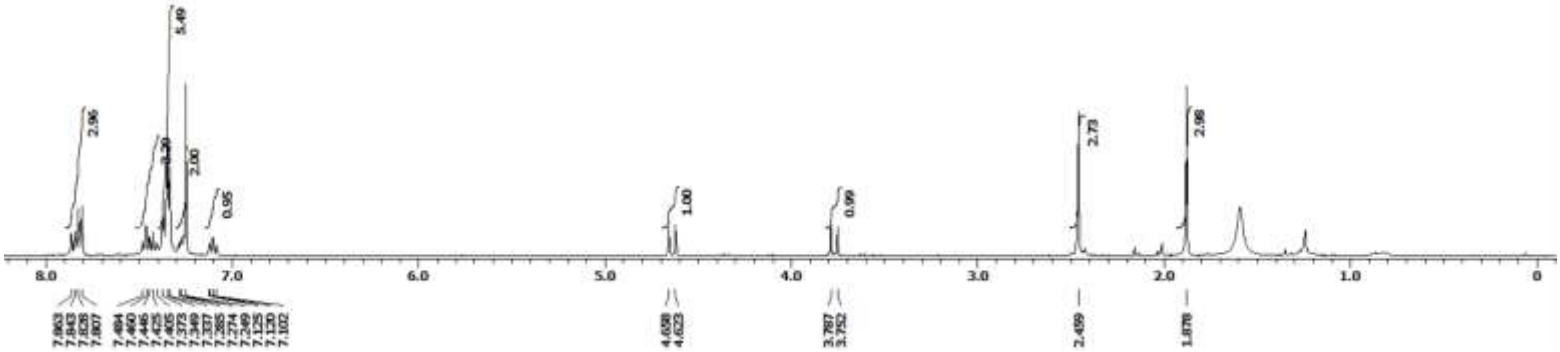
^{1}H NMR spectrum of 3j (400 MHz, $CDCl_3$)



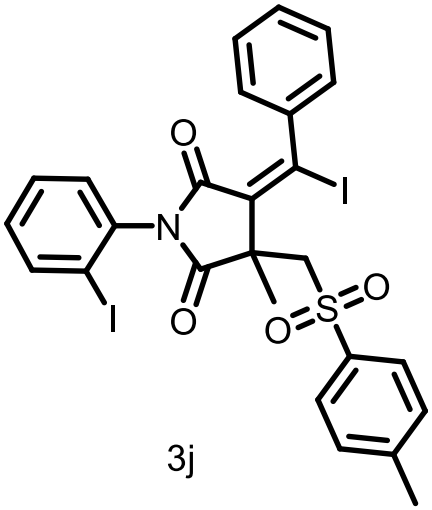
3j

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



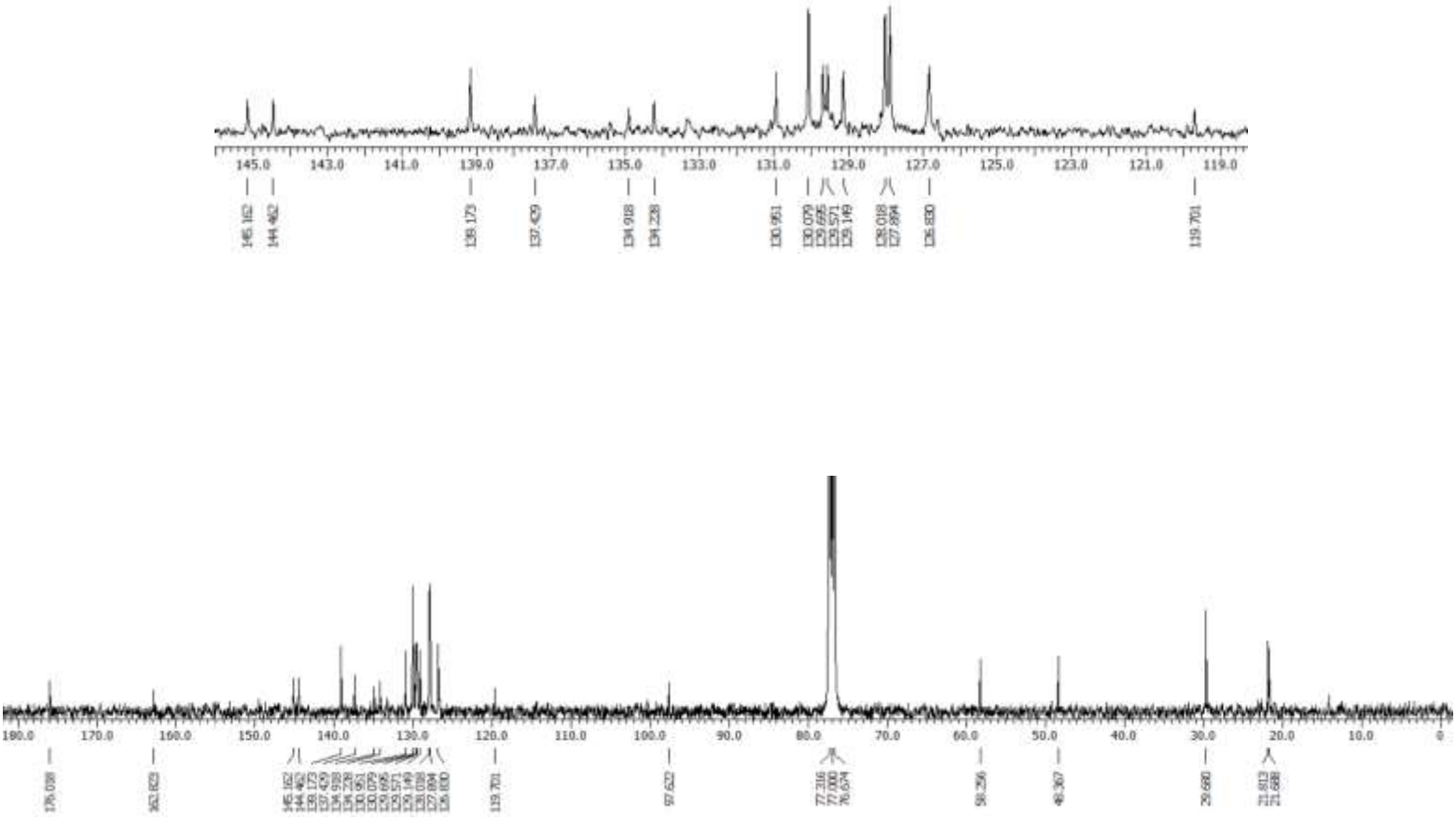


^{13}C NMR spectrum of 3j (100 MHz, $CDCl_3$)



3j

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



HRMS spectrum of 3j

3k

Qualitative Compound Report

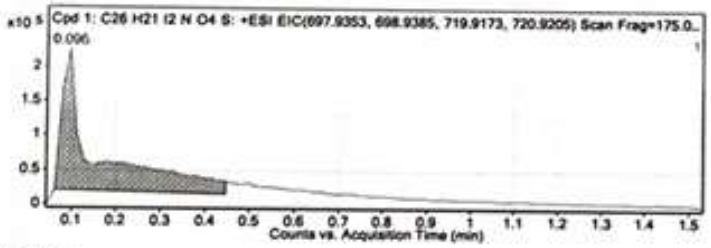
Data File	SMT-163.d	Sample Name	SMT-163
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	17-10-2022 13:06:54
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

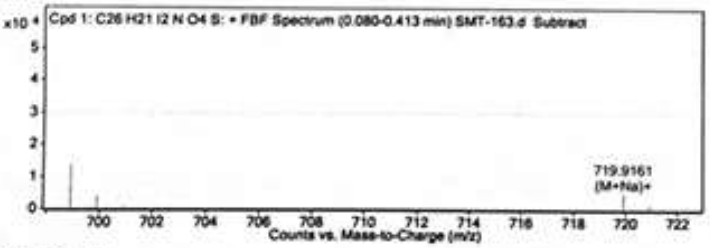
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H21 I2 N O4 S	0.096	696.927	47162	C26 H21 I2 N O4 S	696.9281	-1.6	C26 H21 I2 N O4 S	C26 H21 I2 N O4 S

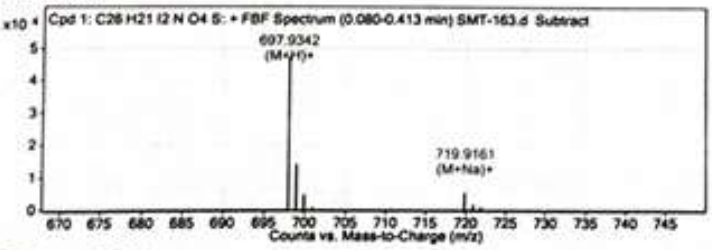
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H21 I2 N O4 S	697.9342	0.096	Find By Formula	696.927



MS Spectrum



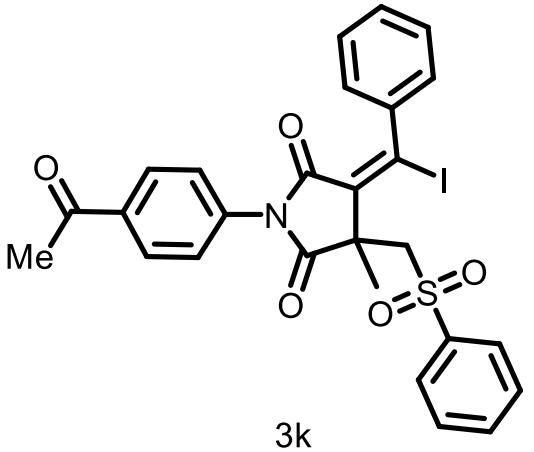
MS Zoomed Spectrum



MS Spectrum Peak List

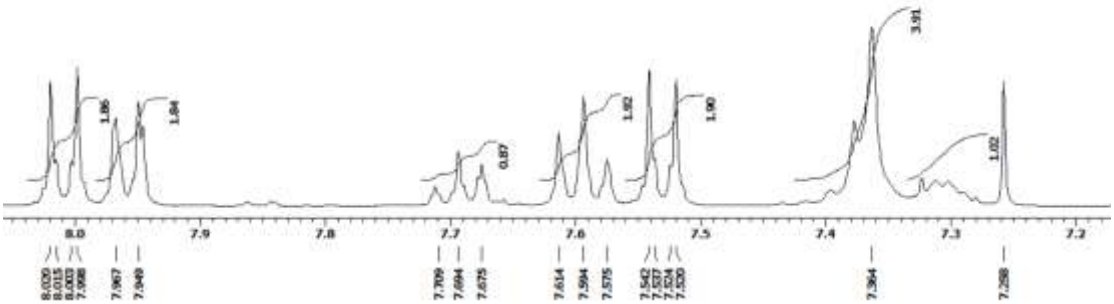
m/z	z	Abund	Formula	Ion
697.9342	1	47162.39	C26H22I2NO4S	(M+H)+
698.9374	1	13697.79	C26H22I2NO4S	(M+H)+
699.9354	1	4334.56	C26H22I2NO4S	(M+H)+
700.9363	1	906.64	C26H22I2NO4S	(M+H)+
719.9161	1	5021.69	C26H21I2NNaO4S	(M+Na)+
720.9197	1	1511.36	C26H21I2NNaO4S	(M+Na)+
721.9173	1	530.21	C26H21I2NNaO4S	(M+Na)+
722.9173	1	66.88	C26H21I2NNaO4S	(M+Na)+

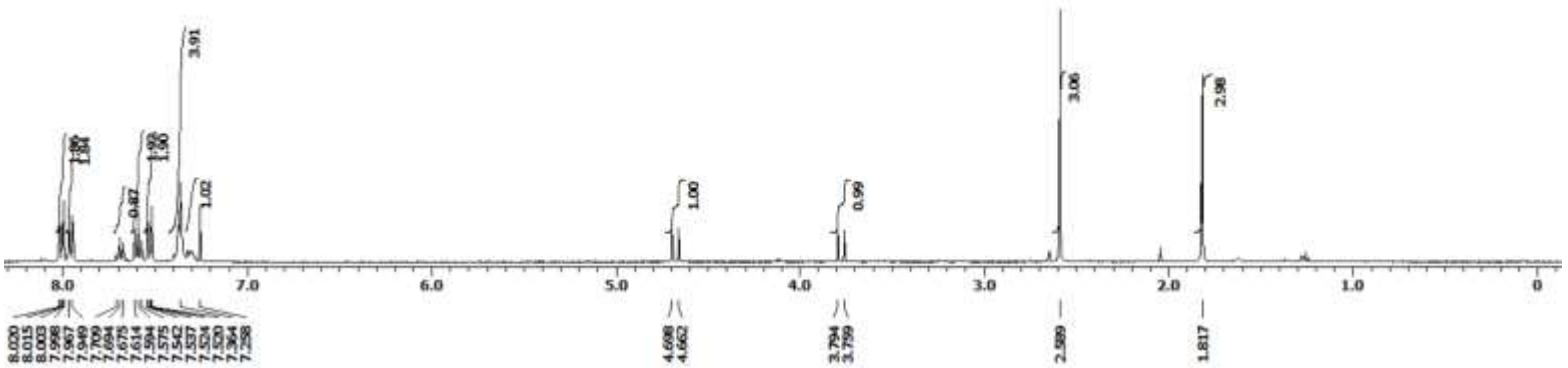
^{1}H NMR spectrum of 3k (400 MHz, $CDCl_3$)



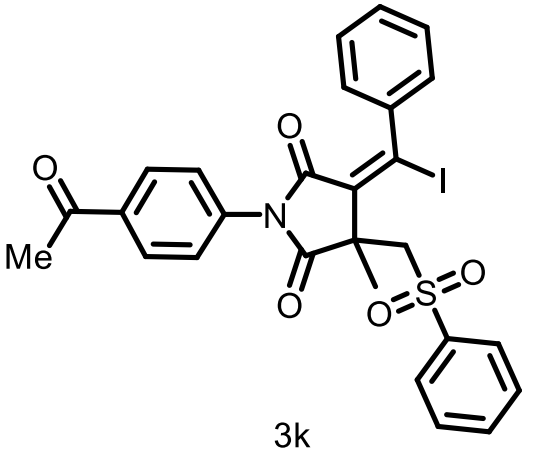
3k

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



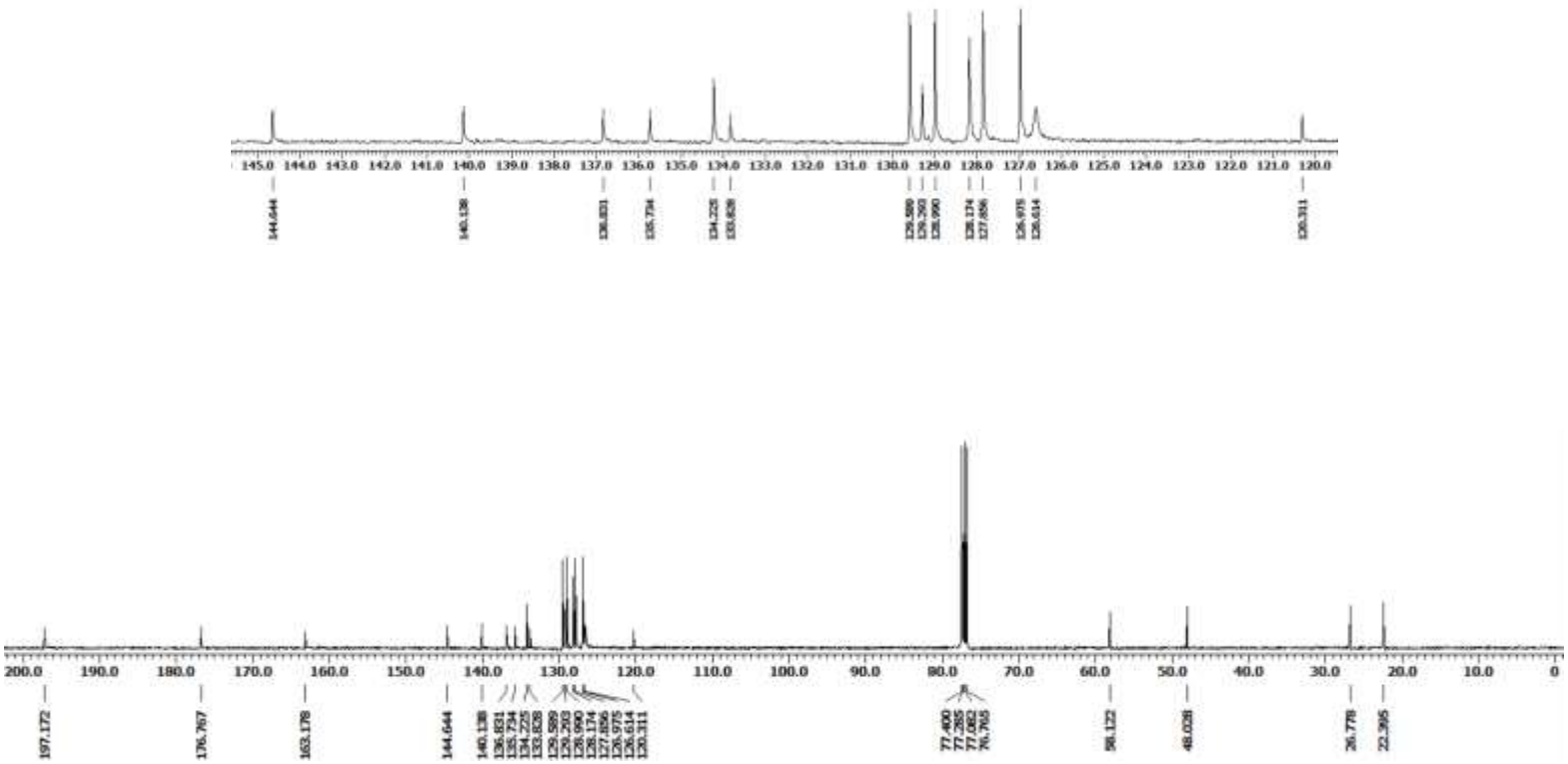


^{13}CNMR spectrum of 3k (100 MHz, $CDCl_3$)



3k

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



HRMS spectrum of 3k

Qualitative Compound Report

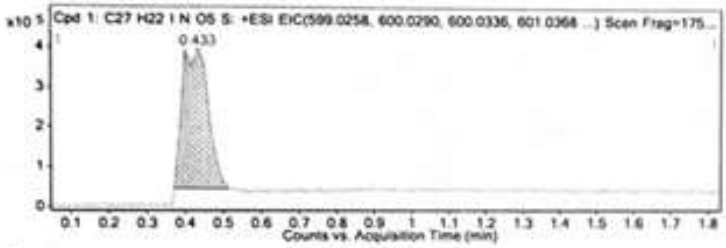
Data File	SMT-398.d	**Sample Name**	SMT-398
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-06-2024 13:47:03
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

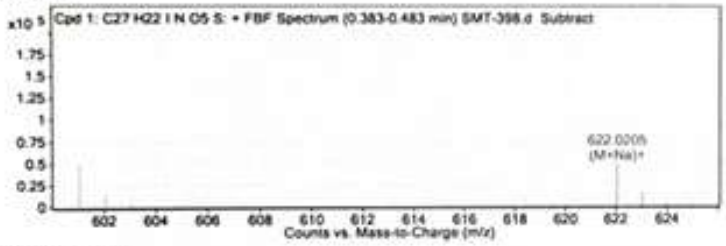
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	DIF (ppm)	MFG Formula	DB Formula
Cpd 1: C27 H22 I N O5 S	0.433	599.0312	173003	C27 H22 I N O5 S	599.0263	8.18	C27 H22 I N O5 S	C27 H22 I N O5 S

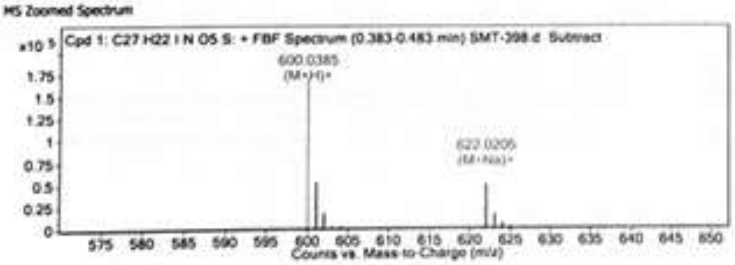
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C27 H22 I N O5 S	600.0385	0.433	Find By Formula	599.0312



MS Spectrum



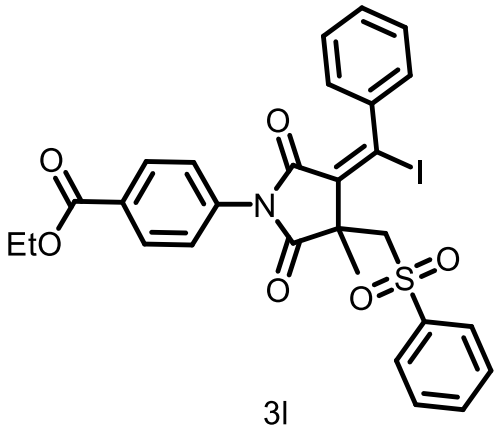
MS Zoomed Spectrum



MS Spectrum Peak List

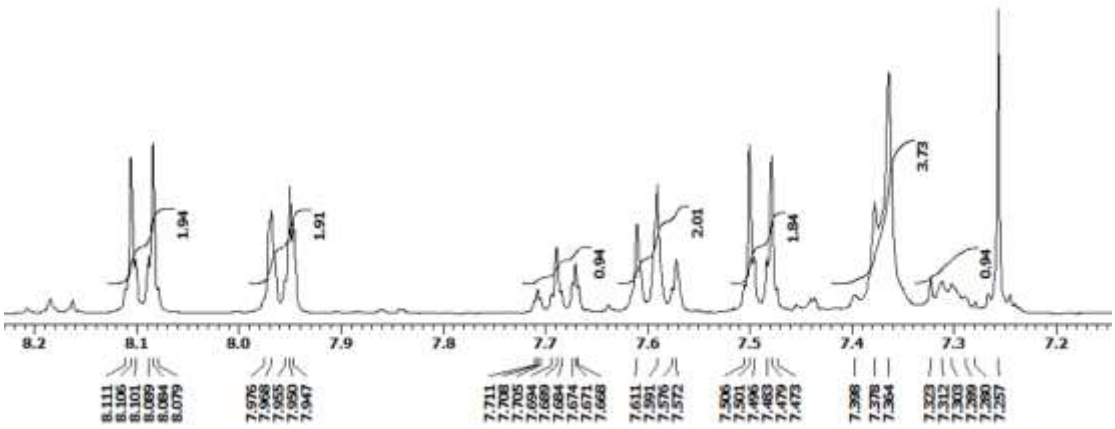
m/z	z	Abund	Formula	Ion
600.0385	1	173003.16	C27H23INO5S	(M+H)+
601.0415	1	50152.28	C27H23INO5S	(M+H)+
602.0403	1	15406.43	C27H23INO5S	(M+H)+
603.0411	1	3250.88	C27H23INO5S	(M+H)+
604.0438	1	623.77	C27H23INO5S	(M+H)+
622.0205	1	48435.31	C27H22INNaO5S	(M+Na)+
623.0237	1	15799.64	C27H22INNaO5S	(M+Na)+
624.0216	1	4634.73	C27H22INNaO5S	(M+Na)+
625.0333	1	1044.74	C27H22INNaO5S	(M+Na)+
626.0475	1	30.11	C27H22INNaO5S	(M+Na)+

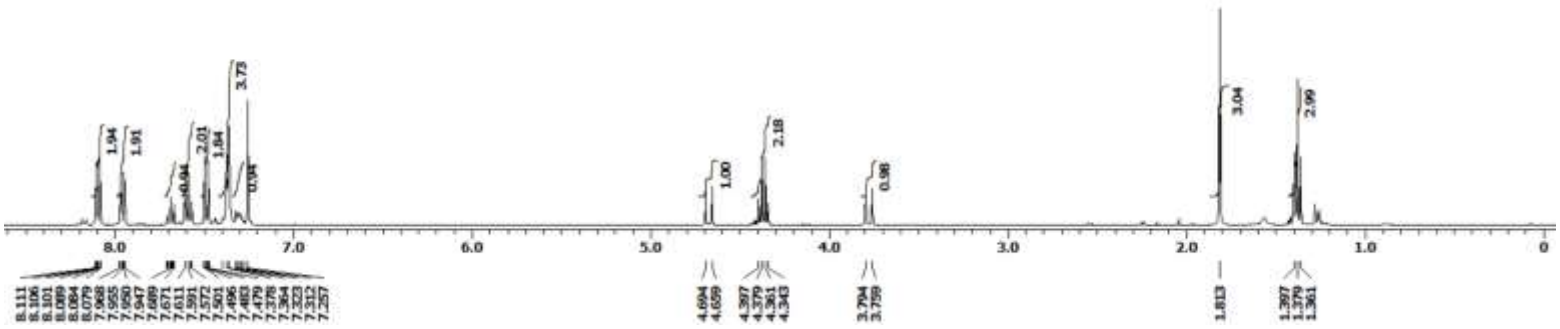
^{1}H NMR spectrum of 3l (400 MHz, $CDCl_3$)



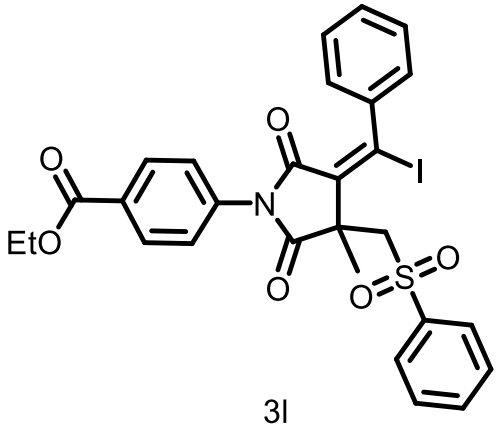
3l

ethyl (*E*)-4-(4-(iodo(phenyl)methylene)-3-methyl-2,5-dioxo-3-((phenylsulfonyl)methyl)pyrrolidin-1-yl)benzoate



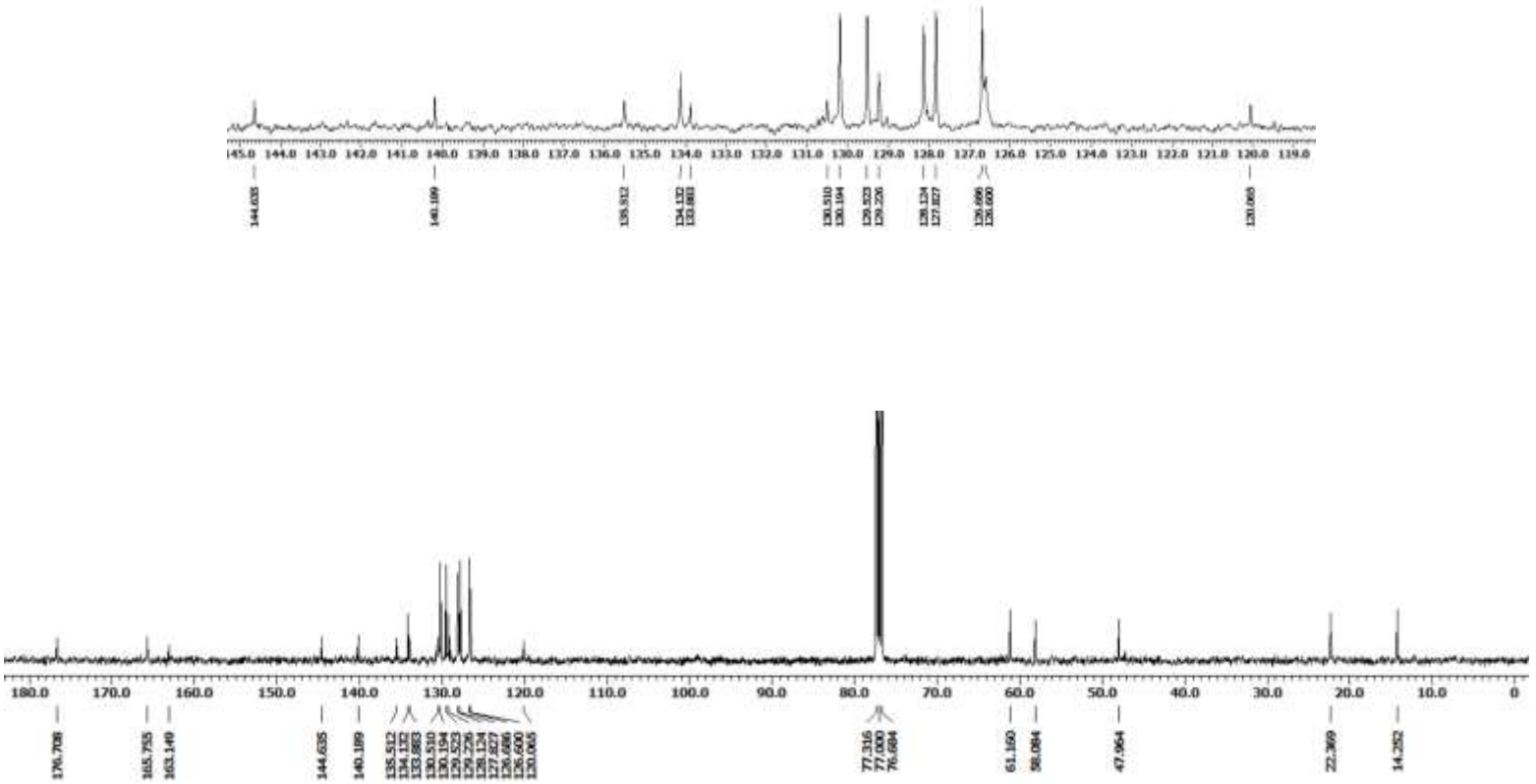


^{13}C NMR spectrum of 3l (100 MHz, $CDCl_3$)



3l

ethyl (*E*)-4-(4-(iodo(phenyl)methylene)-3-methyl-2,5-dioxo-3-((phenylsulfonyl)methyl)pyrrolidin-1-yl)benzoate



HRMS spectrum of 3l

Qualitative Compound Report

Data File	SMT-456.d	**Sample Name**	SMT-456
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	06-06-2024 10:58:44
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

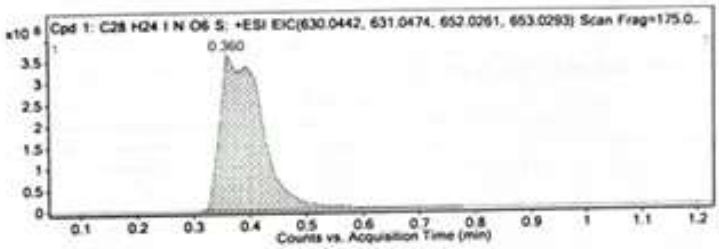
Sample Group **Info.** 3

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

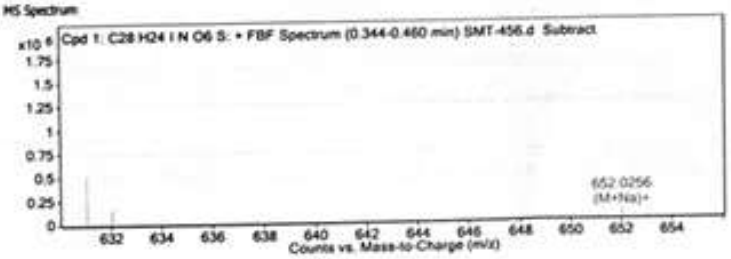
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C28 H24 I N O6 S	0.36	629.0368	1586942	C28 H24 I N O6 S	629.0369	-0.09	C28 H24 I N O6 S	C28 H24 I N O6 S

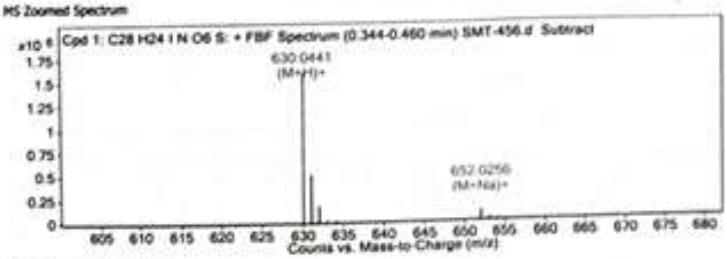
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C28 H24 I N O6 S	630.0441	0.36	Find By Formula	629.0368



MS Spectrum



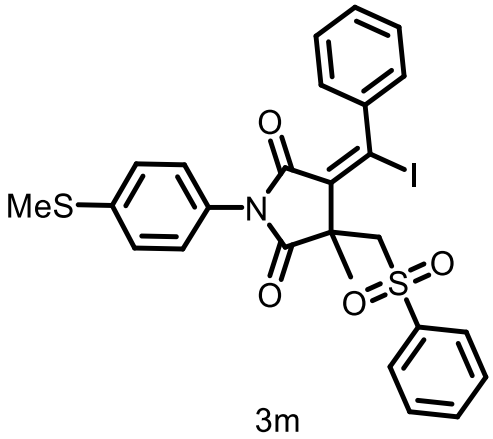
MS Zoomed Spectrum



MS Spectrum Peak List

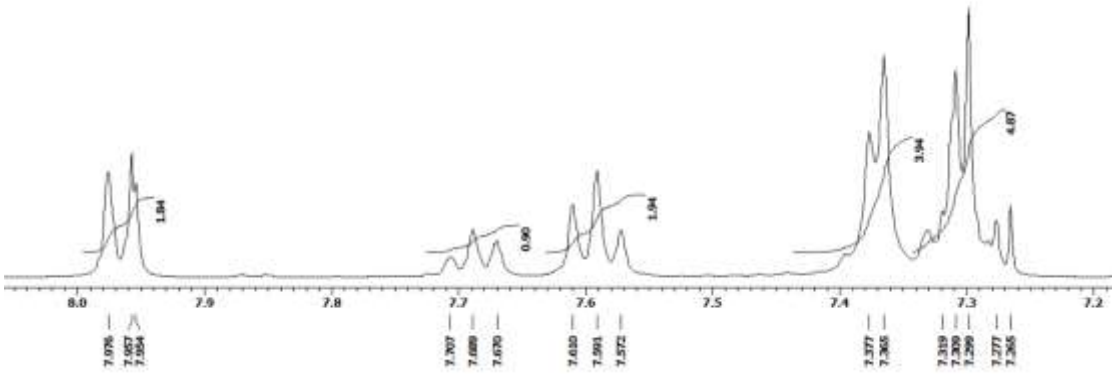
m/z	z	Abund	Formula	Ion
630.0441	1	1586942.38	C28H25INO6S	(M+H)+
631.0476	1	515417.91	C28H25INO6S	(M+H)+
632.0459	1	159115.91	C28H25INO6S	(M+H)+
633.0463	1	33015.09	C28H25INO6S	(M+H)+
634.0466	1	4995.1	C28H25INO6S	(M+H)+
652.0256	1	95254.29	C28H24INNaO6S	(M+Na)+
653.0288	1	29406.32	C28H24INNaO6S	(M+Na)+
654.027	1	9136.26	C28H24INNaO6S	(M+Na)+
655.0288	1	1956.07	C28H24INNaO6S	(M+Na)+
656.0236	1	276.82	C28H24INNaO6S	(M+Na)+

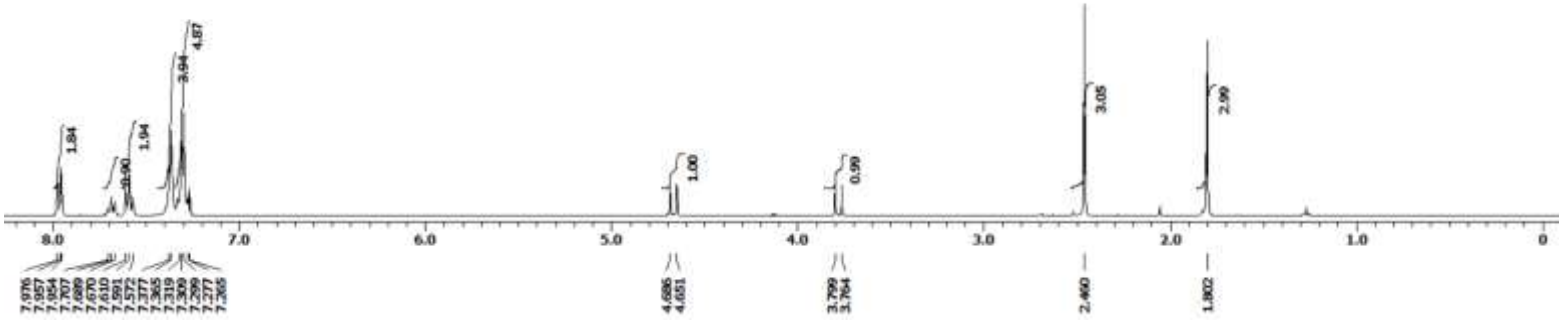
^{1}H NMR spectrum of 3m (400 MHz, $CDCl_3$)



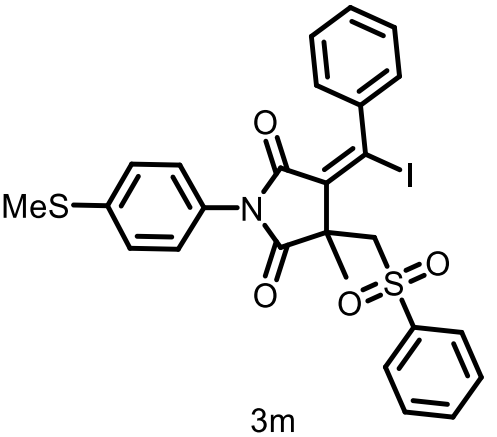
3m

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



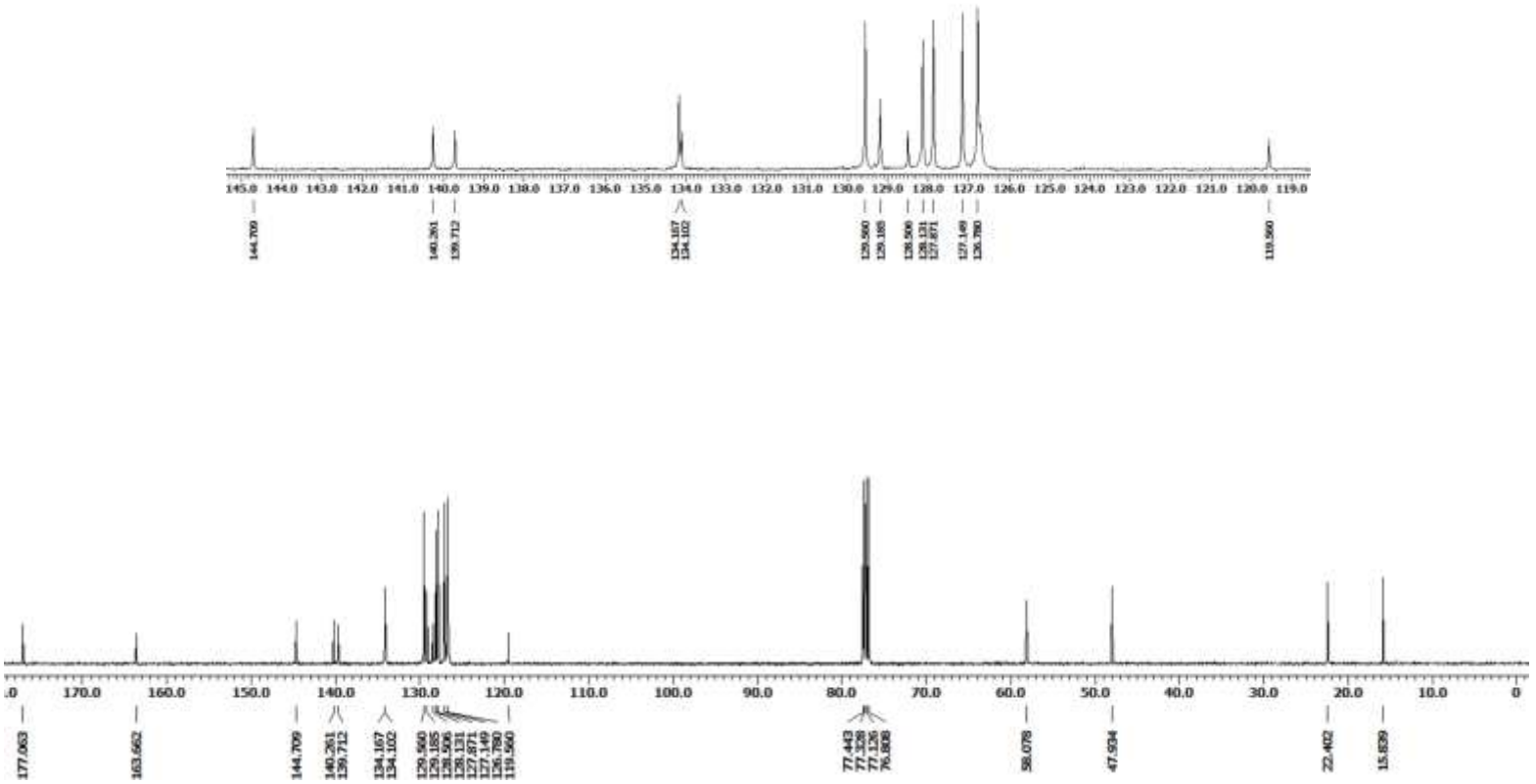


^{13}C NMR spectrum of 3m (100 MHz, $CDCl_3$)



3m

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



HRMS spectrum of 3m

3n

Qualitative Compound Report

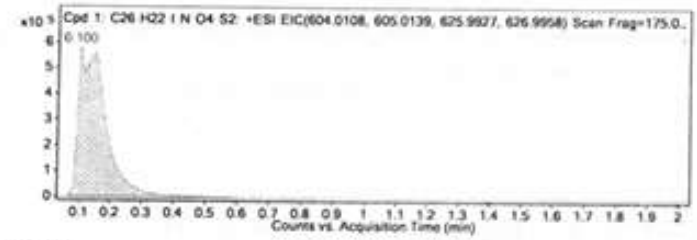
Data File	SMT-409.d	**Sample Name**	SMT-409
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	07-02-2024 12:18:15
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

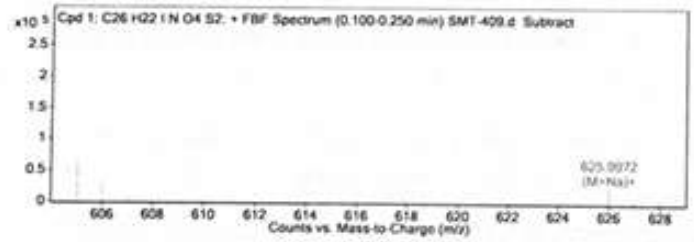
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H22 I N O4 S2	0.1	603.0082	24458	C26 H22 I N O4 S2	603.0035	7.84	C26 H22 I N O4 S2	C26 H22 I N O4 S2

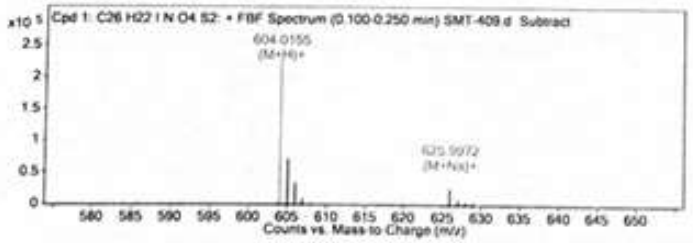
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H22 I N O4 S2	625.9972	0.1	Find By Formula	603.0082



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
604.0155	1	233508.53	C26H23INO4S2	(M+H)+
605.0185	1	66941.74	C26H23INO4S2	(M+H)+
606.0152	1	29634.96	C26H23INO4S2	(M+H)+
607.0182	1	10024.48	C26H23INO4S2	(M+H)+
625.9972	1	24458.18	C26H22INNaO4S2	(M+Na)+
627.0006	1	7666.93	C26H22INNaO4S2	(M+Na)+
627.9955	1	3544.85	C26H22INNaO4S2	(M+Na)+
629.0042	1	391.77	C26H22INNaO4S2	(M+Na)+

--- End Of Report ---

Agilent Technologies

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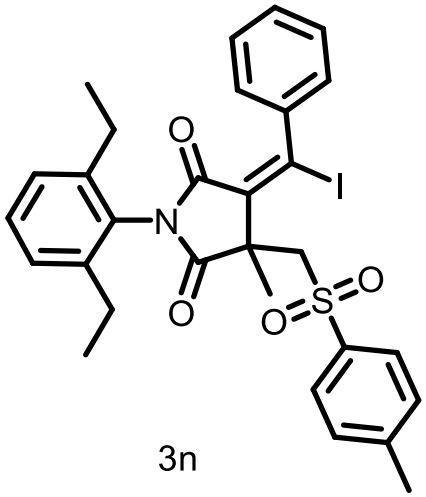
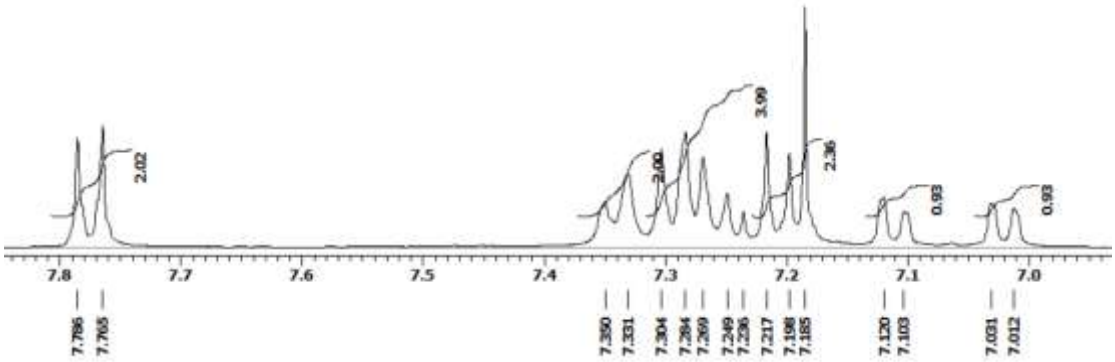
Printed at: 15:34 on:07-02-2024

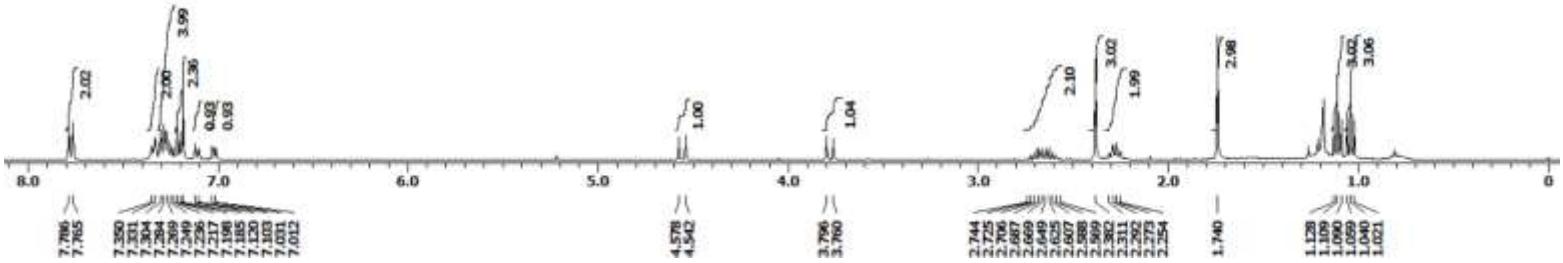
^{1}H NMR spectrum of 3n (400 MHz, $CDCl_3$)



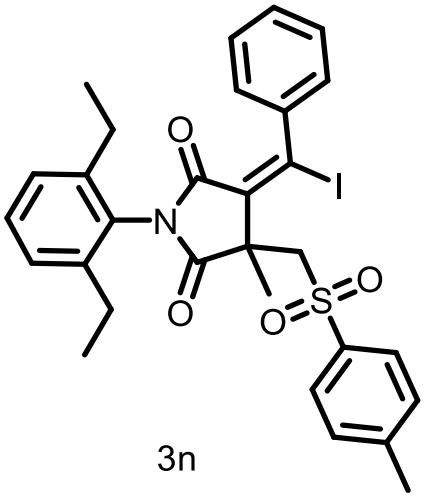
3n

(*E*)-1-(2,6-diethylphenyl)-4-(iodo(phenyl)methylene)-
3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione



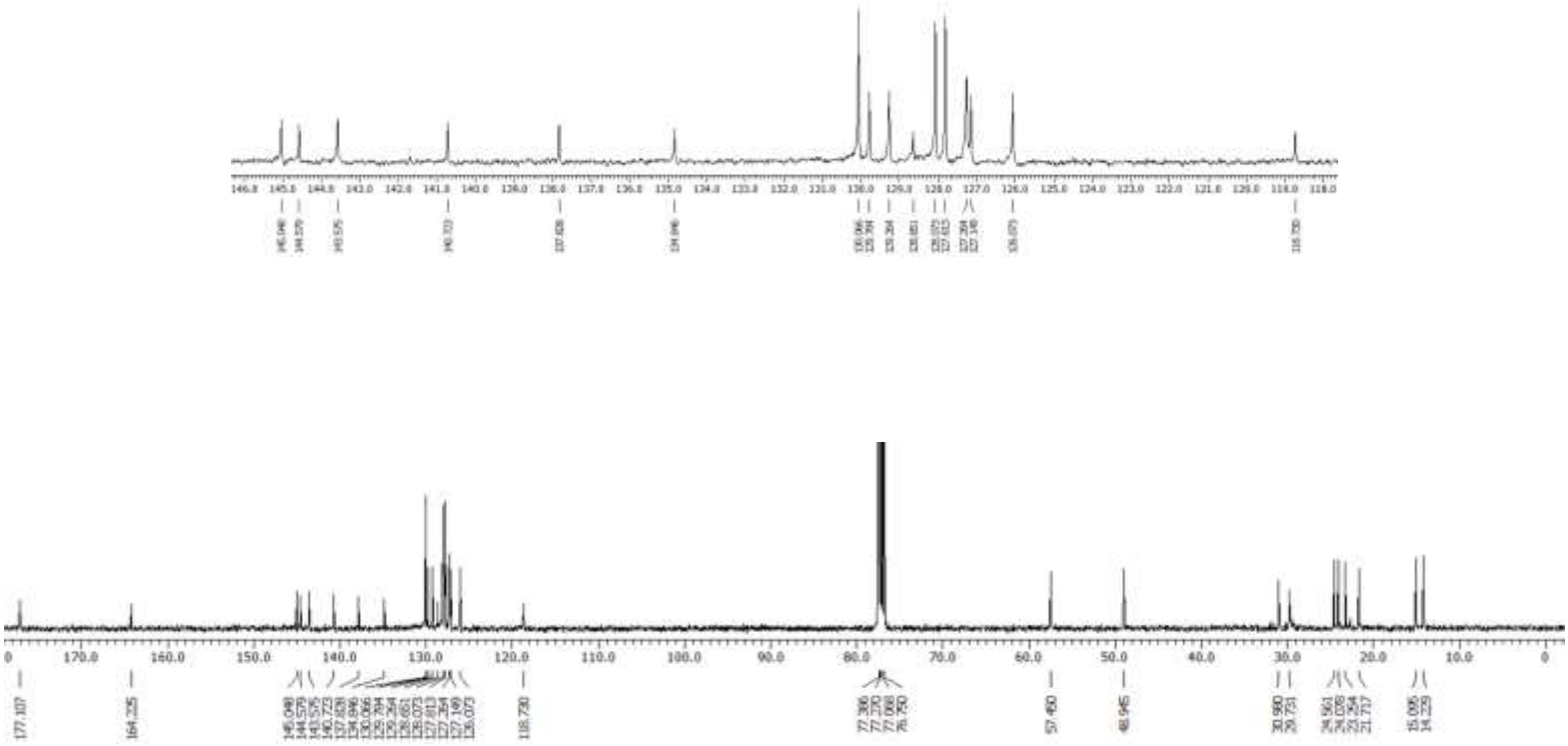


^{13}C NMR spectrum of 3n (100 MHz, $CDCl_3$)



3n

(*E*)-1-(2,6-diethylphenyl)-4-(iodo(phenyl)methylene)-
3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione



HRMS spectrum of 3n

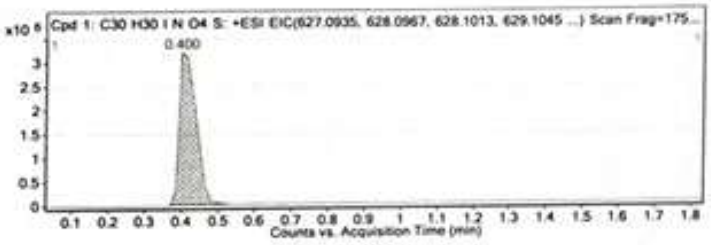
Qualitative Compound Report

Data File	SMT-370.d	**Sample Name**	SMT-370
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-06-2024 13:46:09
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 (B5125)		

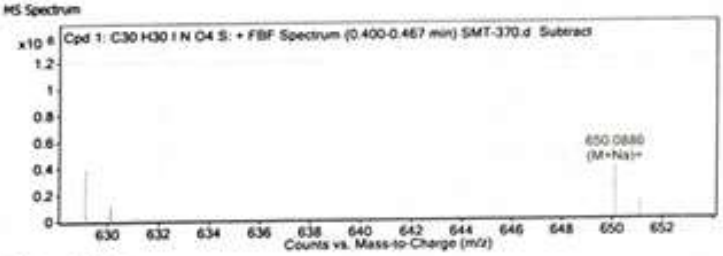
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C30 H30 I N O4 S	0.4	627.0994	390354	C30 H30 I N O4 S	627.094	8.55	C30 H30 I N O4 S	C30 H30 I N O4 S

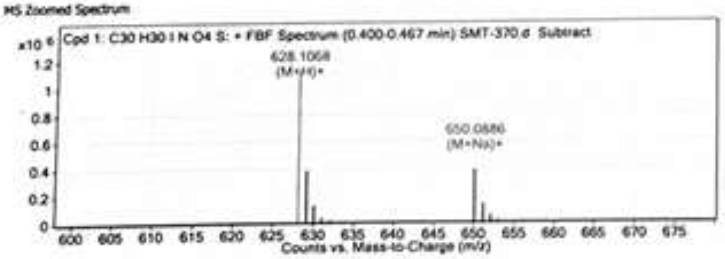
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C30 H30 I N O4 S	650.0886	0.4	Find By Formula	627.0994



MS Spectrum



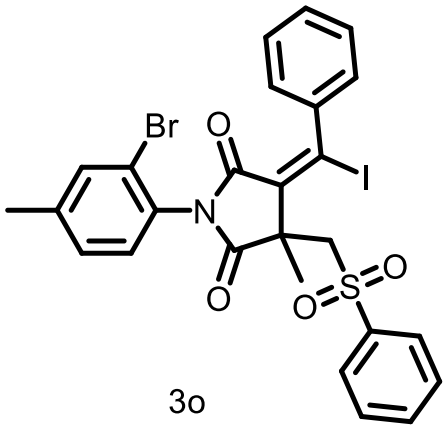
MS Zoomed Spectrum



MS Spectrum Peak List

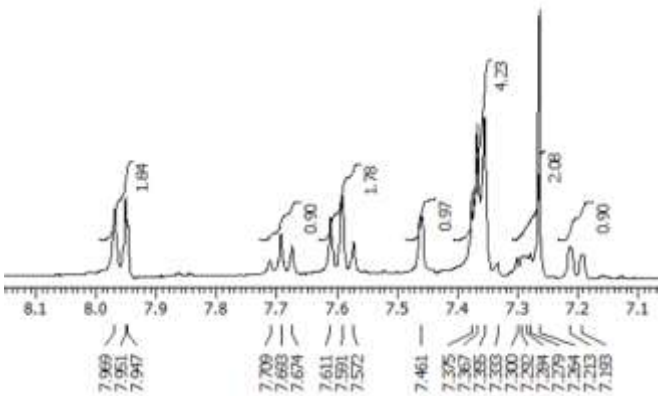
m/z	z	Abund	Formula	Ion
628.1068	1	1117485	C30H31INO4S	(M+H)+
629.1099	1	384884.88	C30H31INO4S	(M+H)+
630.1084	1	112972.77	C30H31INO4S	(M+H)+
631.1088	1	24229.33	C30H31INO4S	(M+H)+
632.1096	1	3934.13	C30H31INO4S	(M+H)+
650.0886	1	390354.22	C30H30INNaO4S	(M+Na)+
651.0916	1	124983.08	C30H30INNaO4S	(M+Na)+
652.0902	1	36693.48	C30H30INNaO4S	(M+Na)+
653.0911	1	7913.26	C30H30INNaO4S	(M+Na)+
654.0888	1	1251.99	C30H30INNaO4S	(M+Na)+

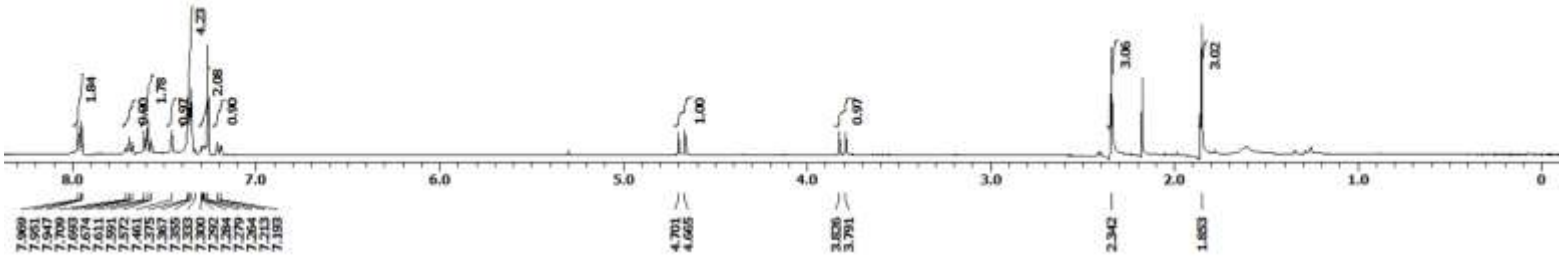
^{1}H NMR spectrum of 3o (400 MHz, $CDCl_3$)



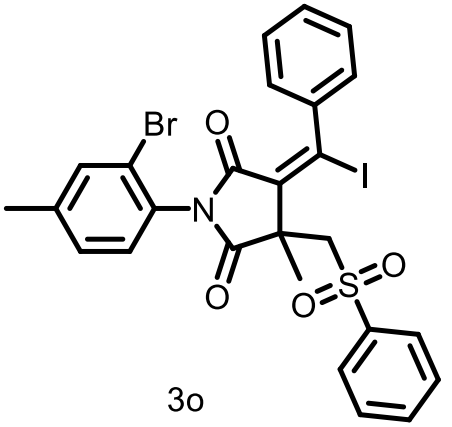
3o

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



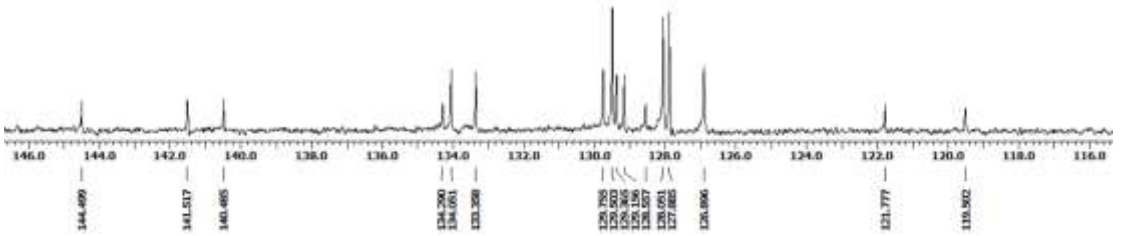


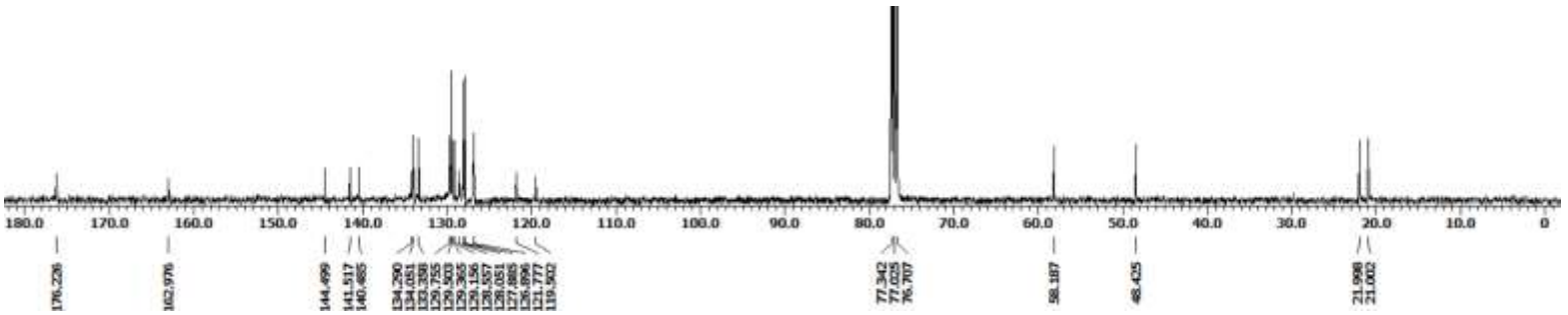
^{13}C NMR spectrum of 3o (100 MHz, $CDCl_3$)



3o

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





HRMS spectrum of 3o

Qualitative Compound Report

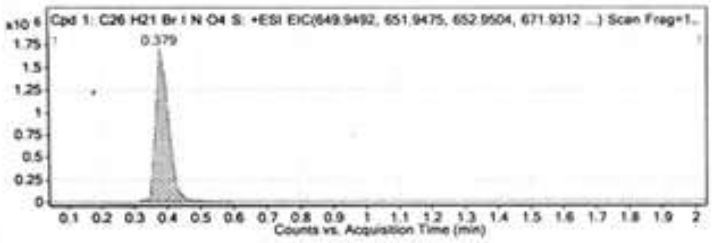
Data File	SMT-416.d	**Sample Name**	SMT-416
Sample Type	Sample	**Position**	P1-D5
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	07-06-2024 13:50:16
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

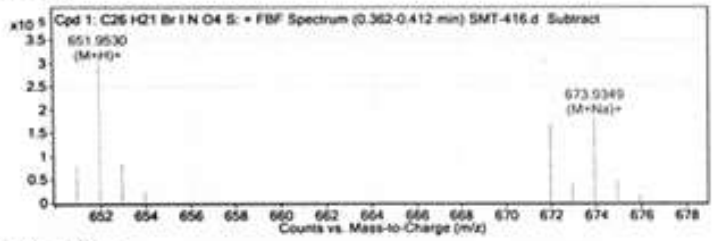
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H21 Br I N O4 S	0.379	648.9474	181724	C26 H21 Br I N O4 S	648.9419	8.37	C26 H21 Br I N O4 S	C26 H21 Br I N O4 S

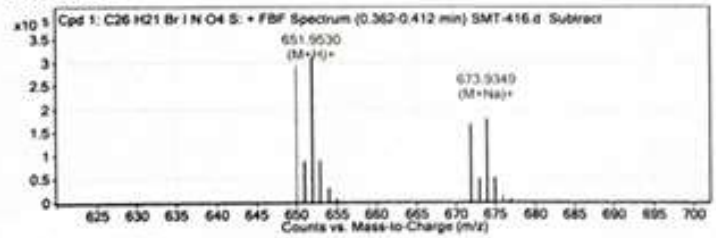
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H21 Br I N O4 S	673.9349	0.379	Find By Formula	648.9474



MS Spectrum



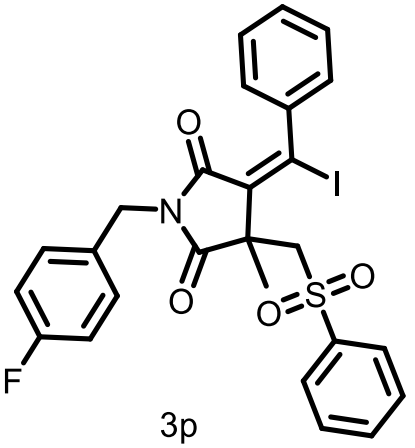
MS Zoomed Spectrum



MS Spectrum Peak List

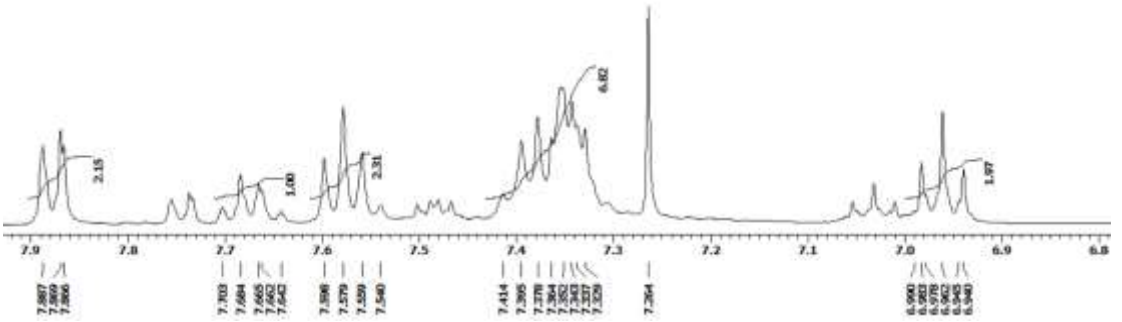
m/z	z	Abund	Formula	Ion
649.9547	1	294064.91	C26H22BrINO4S	(M+H)+
650.9577	1	81060.84	C26H22BrINO4S	(M+H)+
651.953	1	334669.13	C26H22BrINO4S	(M+H)+
652.9556	1	85430.91	C26H22BrINO4S	(M+H)+
653.954	1	25274.59	C26H22BrINO4S	(M+H)+
654.955	1	4506.78	C26H22BrINO4S	(M+H)+
655.9553	1	756.83	C26H22BrINO4S	(M+H)+
671.9366	1	169363.41	C26H21BrINNaO4S	(M+Na)+
672.9396	1	46507.19	C26H21BrINNaO4S	(M+Na)+
673.9349	1	181724.03	C26H21BrINNaO4S	(M+Na)+
674.9378	1	47758.2	C26H21BrINNaO4S	(M+Na)+

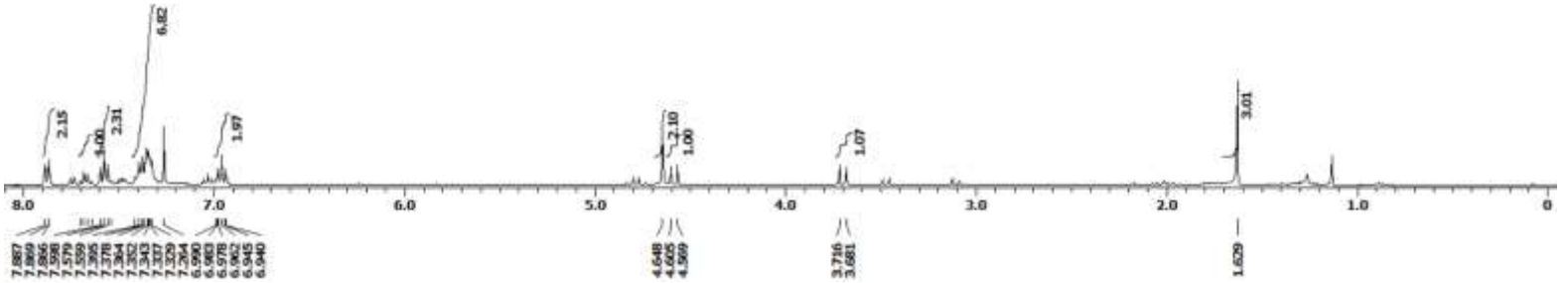
^{1}H NMR spectrum of 3p (400 MHz, $CDCl_3$)



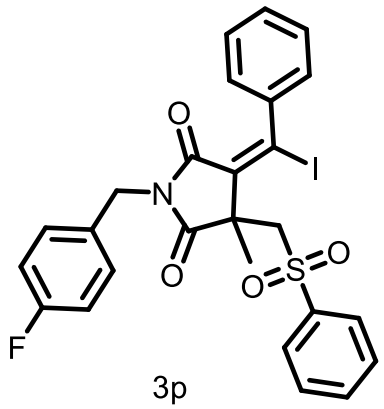
3p

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



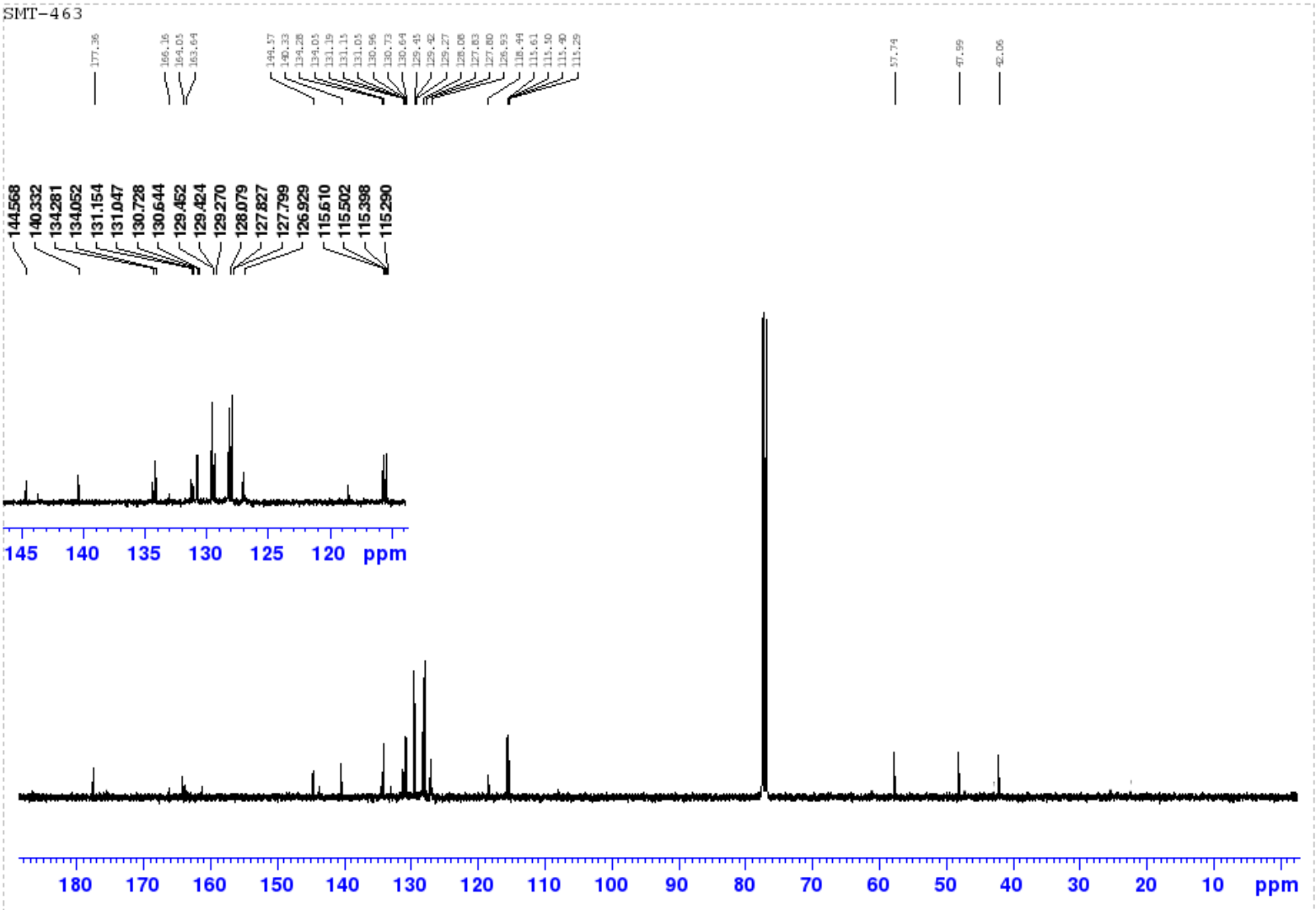


^{13}C NMR spectrum of 3p (100 MHz, $CDCl_3$)

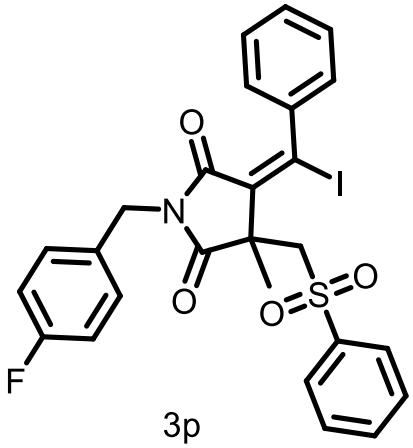


3p

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

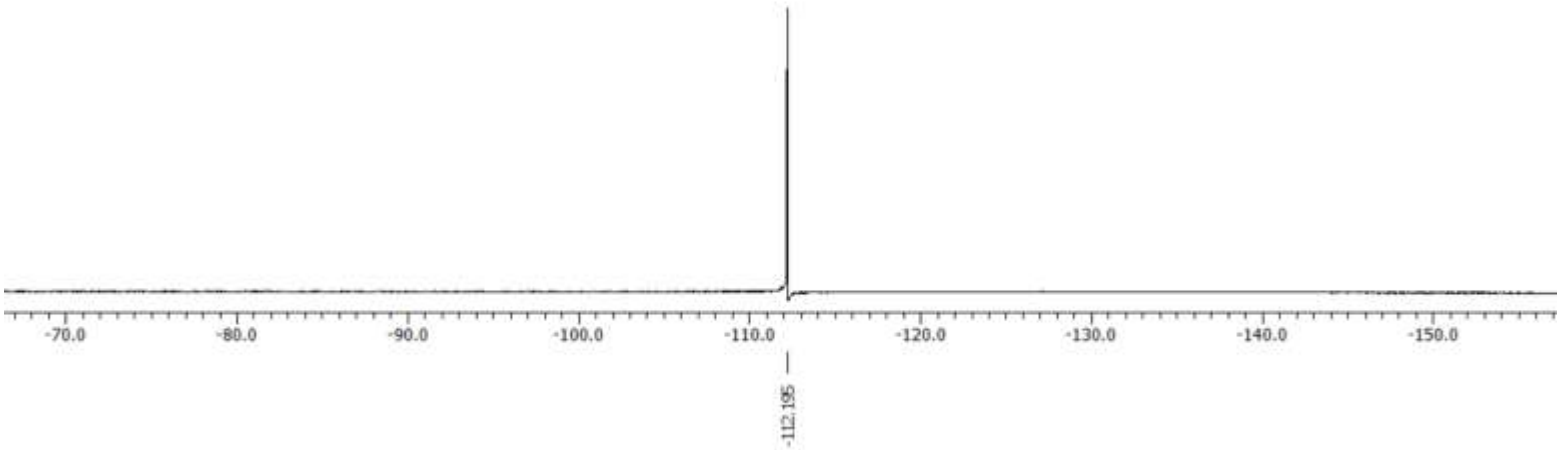


^{19}F NMR spectrum of 3p (376 MHz, $CDCl_3$)



3p

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



HRMS spectrum of 3p

Qualitative Compound Report

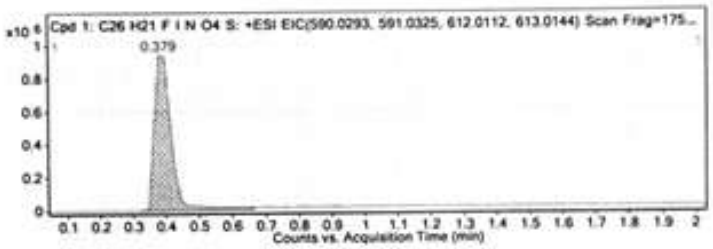
Data File	SMT-463.d	**Sample Name**	SMT-463
Sample Type	Sample	**Position**	P1-D6
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	07-06-2024 13:55:08
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

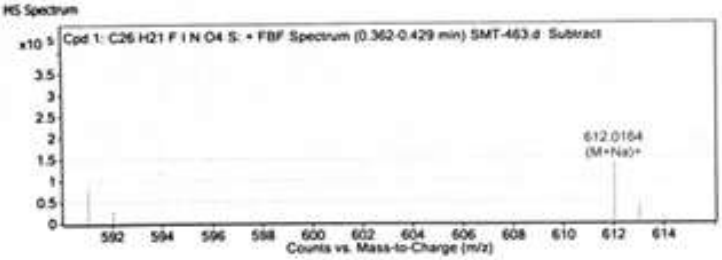
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H21 F I N O4 S	0.379	589.0271	139996	C26 H21 F I N O4 S	589.022	8.65	C26 H21 F I N O4 S	C26 H21 F I N O4 S

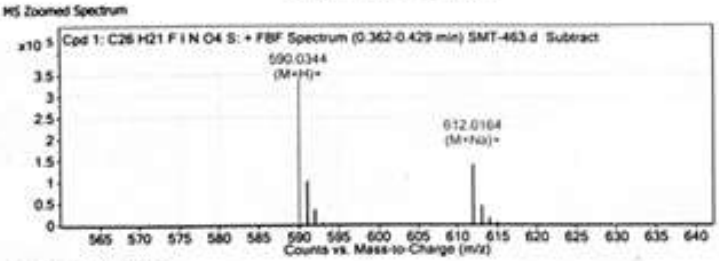
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H21 F I N O4 S	612.0164	0.379	Find By Formula	589.0271



MS Spectrum



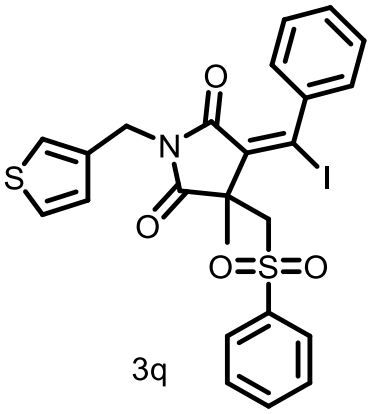
MS Zoomed Spectrum



MS Spectrum Peak List

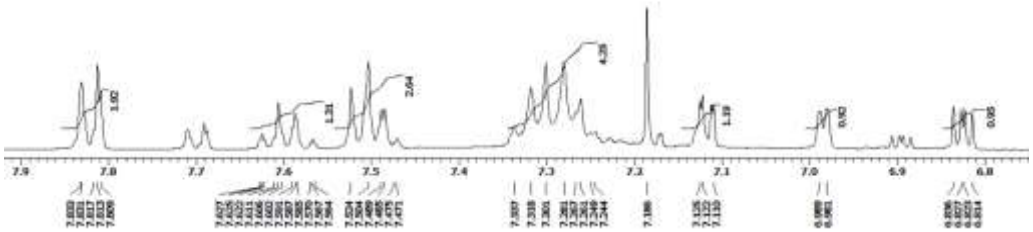
m/z	z	Abund	Formula	Ion
590.0344	1	348442.84	C26H22FINO4S	(M+H)+
591.0373	1	95485.11	C26H22FINO4S	(M+H)+
592.0356	1	28674.05	C26H22FINO4S	(M+H)+
593.0374	1	5975.65	C26H22FINO4S	(M+H)+
594.0387	1	1158.83	C26H22FINO4S	(M+H)+
612.0164	1	139995.73	C26H21FINNaO4S	(M+Na)+
613.0193	1	40175.28	C26H21FINNaO4S	(M+Na)+
614.0178	1	12554.09	C26H21FINNaO4S	(M+Na)+
615.0205	1	2531.56	C26H21FINNaO4S	(M+Na)+
616.0174	1	508	C26H21FINNaO4S	(M+Na)+

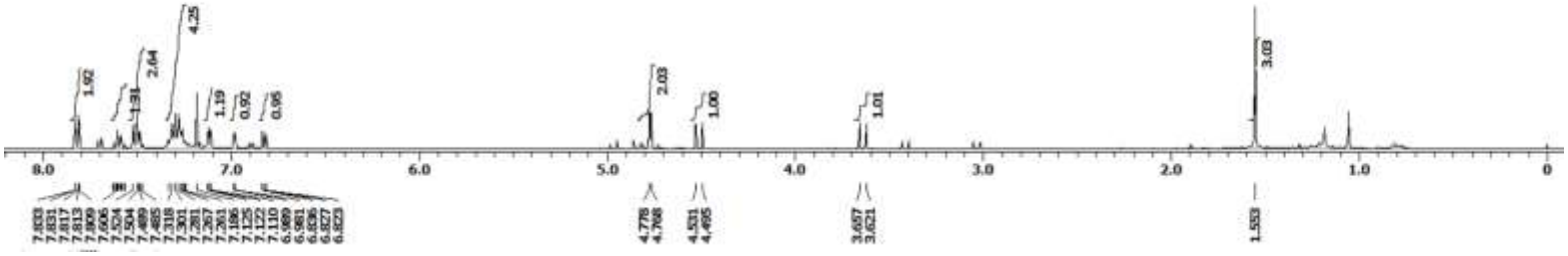
^{1}H NMR spectrum of 3q (400 MHz, $CDCl_3$)



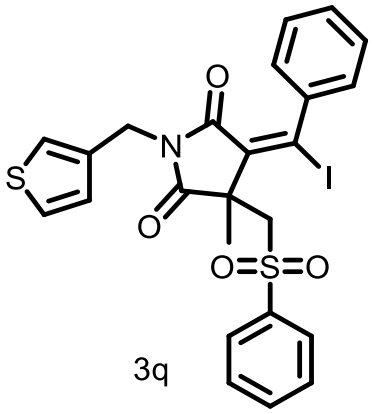
3q

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



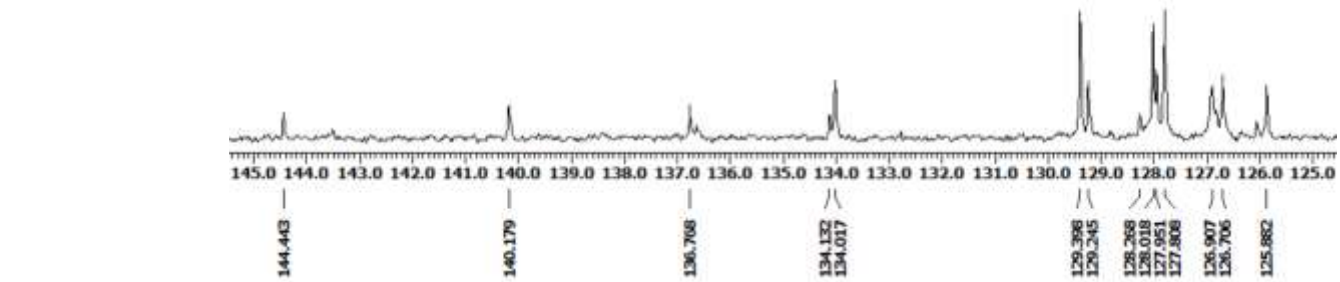


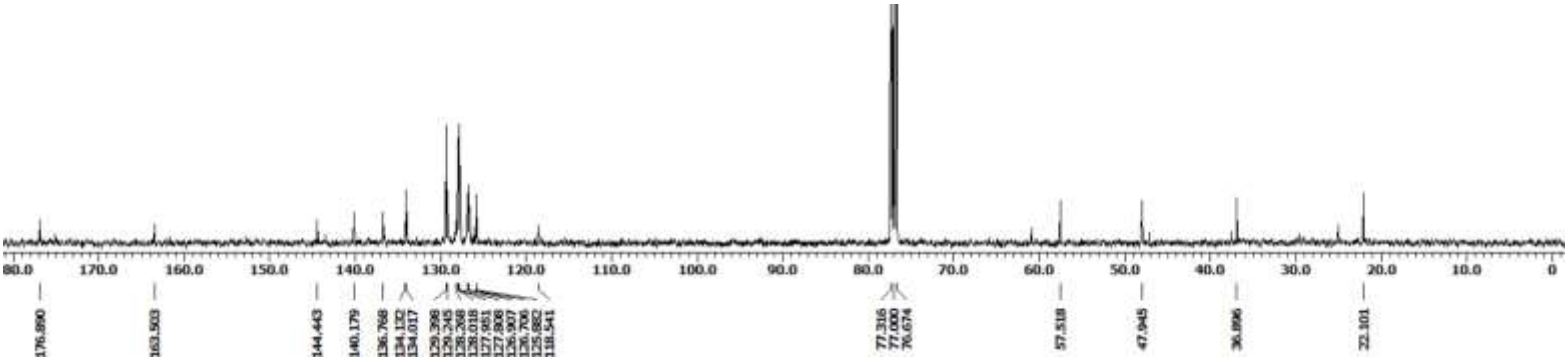
^{13}C NMR spectrum of 3q (100 MHz, $CDCl_3$)



3q

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





HRMS spectrum of 3q

Qualitative Compound Report

Data File	SMT-476.d	**Sample Name**	SMT-476
Sample Type	Sample	**Position**	P1-D7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	07-06-2024 13:58:00
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

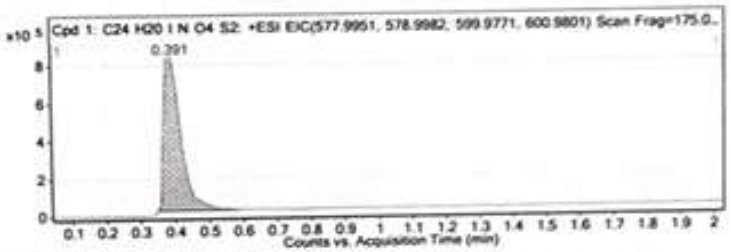
Sample Group **Info.** 3

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

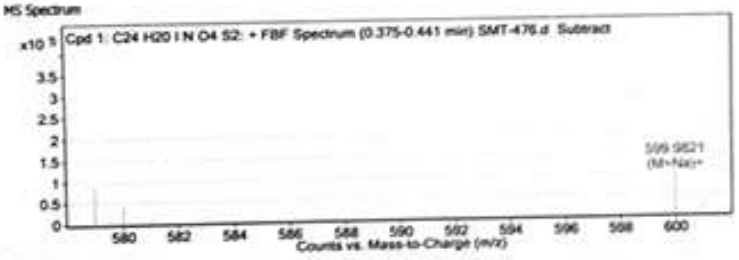
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C24 H20 I N O4 S2	0.391	576.9929	352136	C24 H20 I N O4 S2	576.9878	8.69	C24 H20 I N O4 S2	C24 H20 I N O4 S2

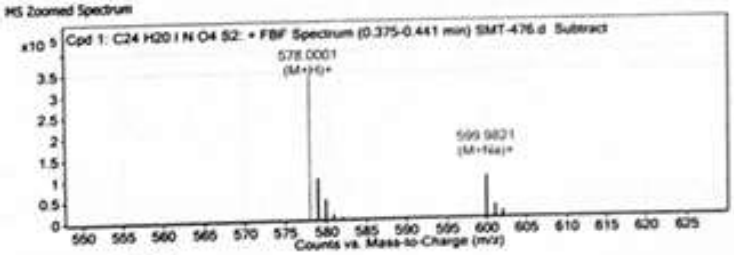
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C24 H20 I N O4 S2	578.0001	0.391	Find By Formula	576.9929



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
578.0001	1	352135.69	C24H21INO4S2	(M+H)+
579.003	1	93392.46	C24H21INO4S2	(M+H)+
579.9993	1	41578	C24H21INO4S2	(M+H)+
581.0011	1	9043.03	C24H21INO4S2	(M+H)+
581.9999	1	2014.35	C24H21INO4S2	(M+H)+
582.9989	1	352.81	C24H21INO4S2	(M+H)+
599.9821	1	98377.14	C24H20INaO4S2	(M+Na)+
600.9856	1	26857.03	C24H20INaO4S2	(M+Na)+
601.9818	1	12190.38	C24H20INaO4S2	(M+Na)+

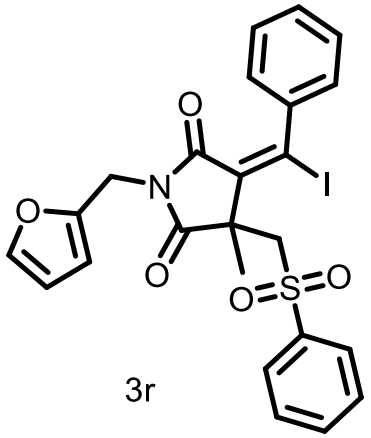
— End Of Report —

Agilent Technologies

Page 1 of 1

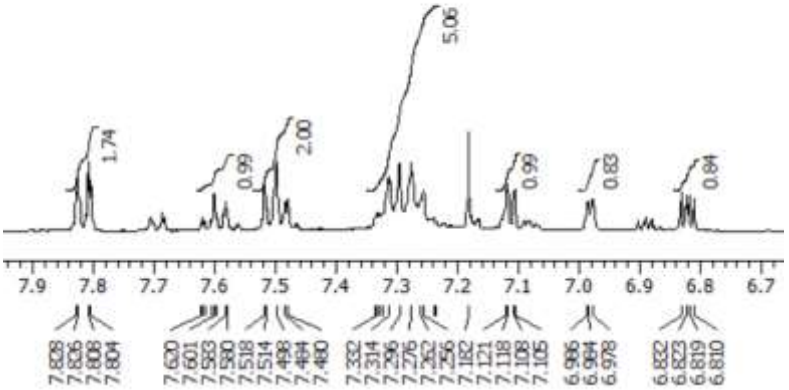
Printed at: 14:39 on:07-06-2024

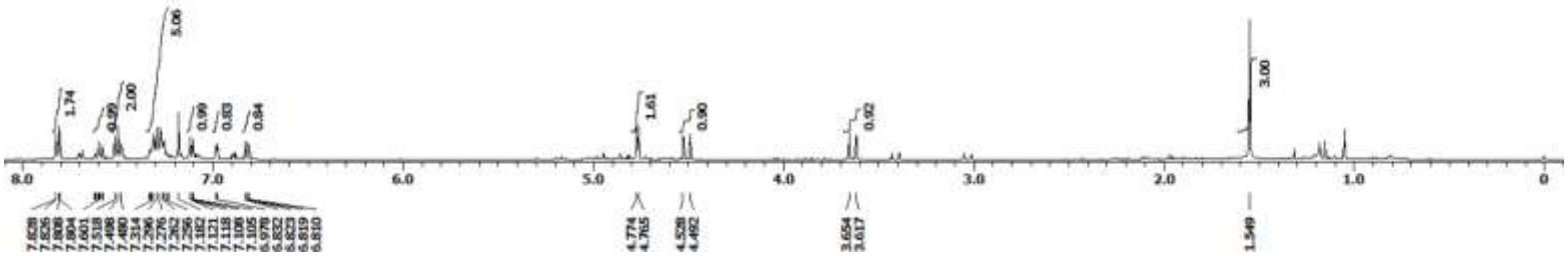
^{1}H NMR spectrum of 3r (400 MHz, $CDCl_3$)



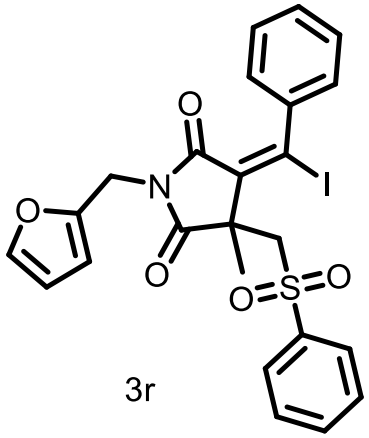
3r

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



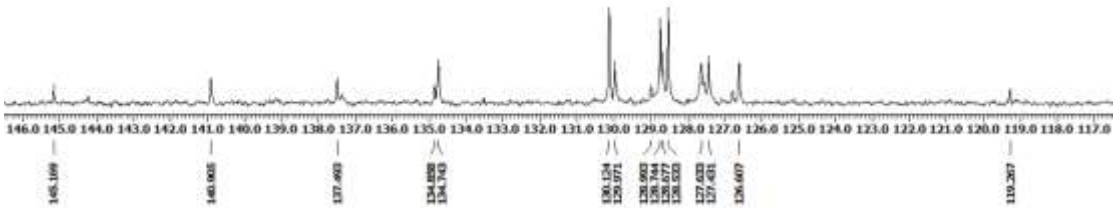


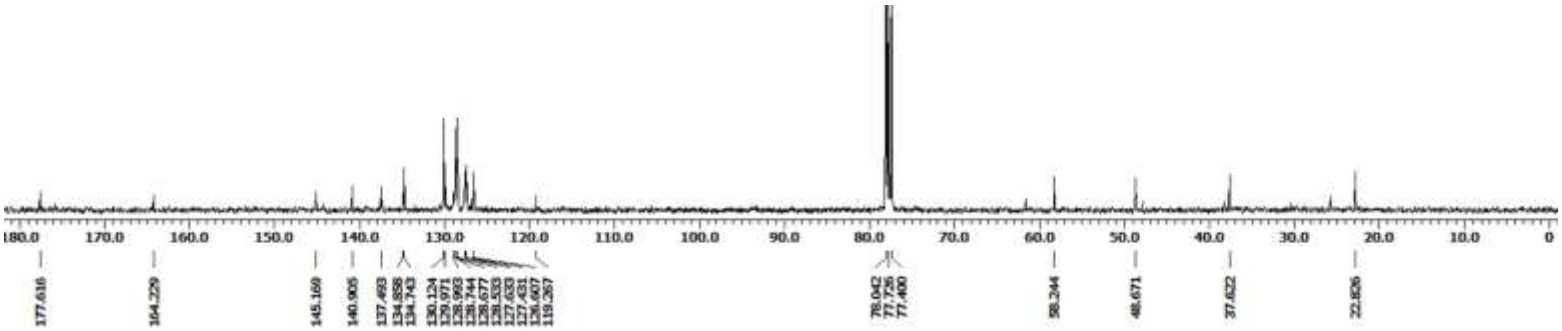
^{13}C NMR spectrum of 3r (100 MHz, $CDCl_3$)



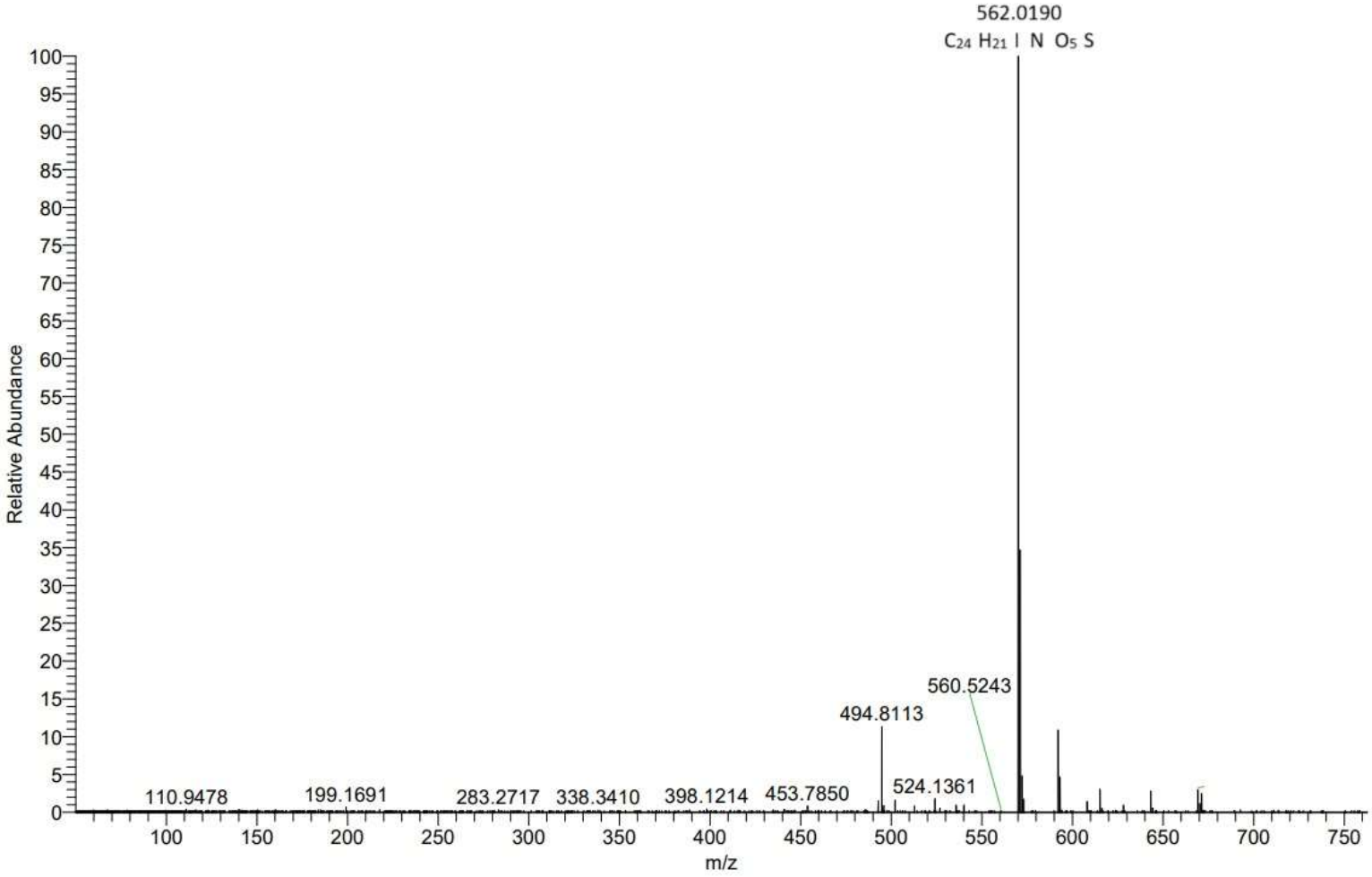
3r

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

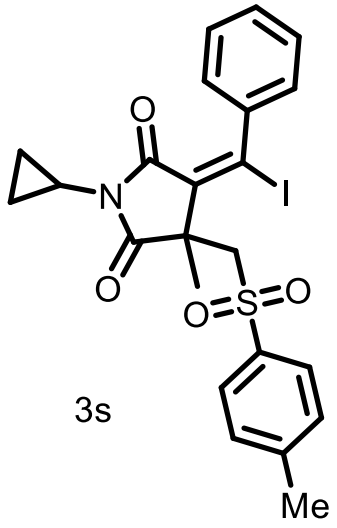




HRMS spectrum of 3r

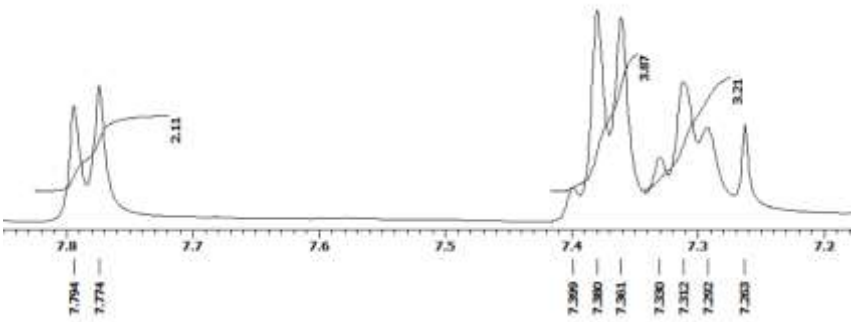


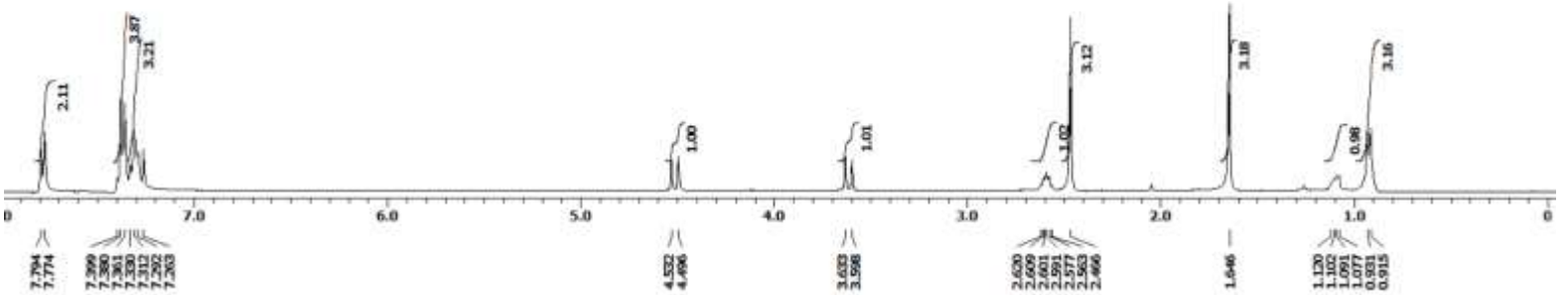
^{1}H NMR spectrum of 3s (400 MHz, $CDCl_3$)



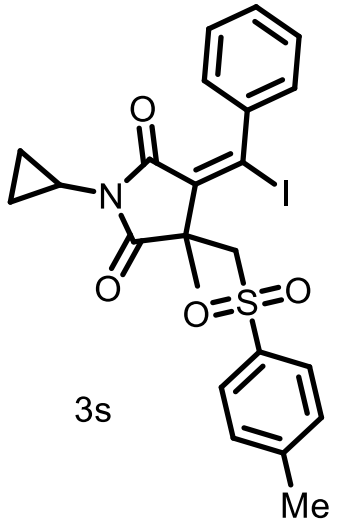
3s

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



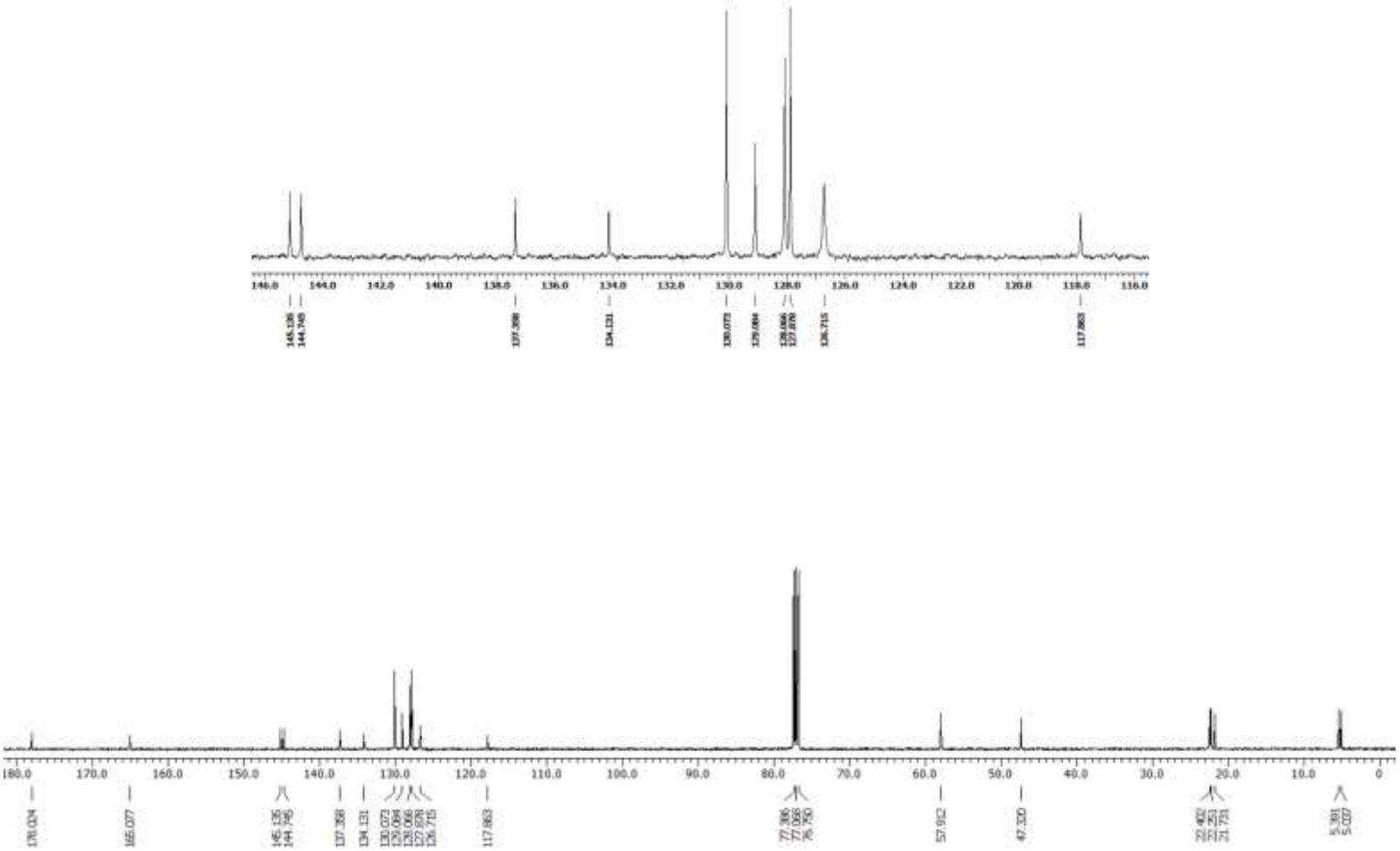


^{13}C NMR spectrum of 3s (100 MHz, $CDCl_3$)



3s

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



HRMS spectrum of 3s

at

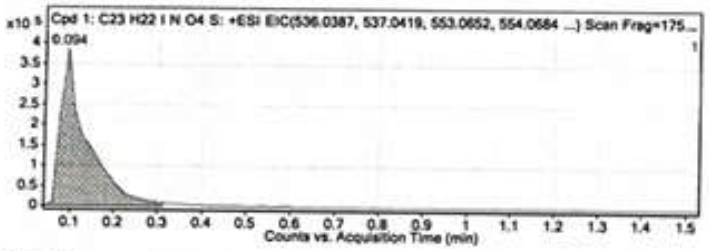
Qualitative Compound Report

Data File	SAM-1.d	Sample Name	SAM-1
Sample Type	Sample	Position	P1-B7
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	02-11-2022 13:12:42
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			
Sample Group		Info.	}
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

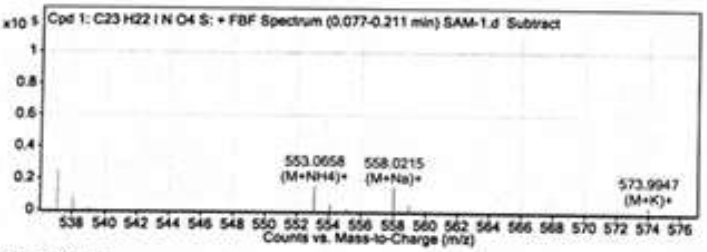
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C23 H22 I N O4 S	0.094	535.032	95894	C23 H22 I N O4 S	535.0314	1.04	C23 H22 I N O4 S	C23 H22 I N O4 S

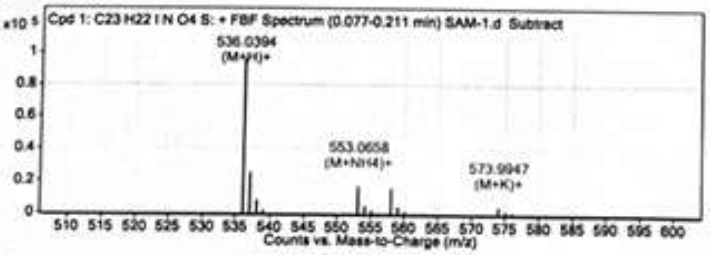
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C23 H22 I N O4 S	536.0394	0.094	Find By Formula	535.032



MS Spectrum



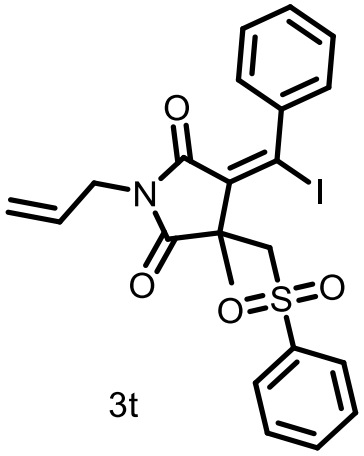
MS Zoomed Spectrum



MS Spectrum Peak List

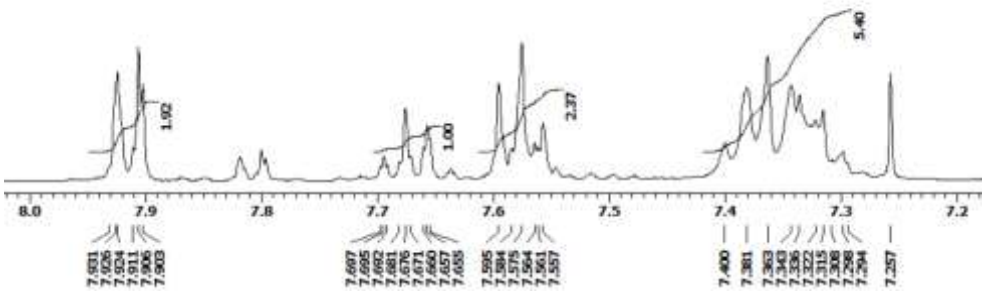
m/z	z	Abund	Formula	Ion
536.0394	1	95894.24	C23H23INO4S	(M+H)+
537.0422	1	24570.77	C23H23INO4S	(M+H)+
538.0403	1	7752.1	C23H23INO4S	(M+H)+
539.0401	1	1630.37	C23H23INO4S	(M+H)+
553.0658	1	16315.02	C23H26IN2O4S	(M+NH4)+
554.0677	1	4756.58	C23H26IN2O4S	(M+NH4)+
555.0669	1	1571.81	C23H26IN2O4S	(M+NH4)+
558.0215	1	15498.62	C23H22INNaO4S	(M+Na)+
559.0238	1	4252.36	C23H22INNaO4S	(M+Na)+

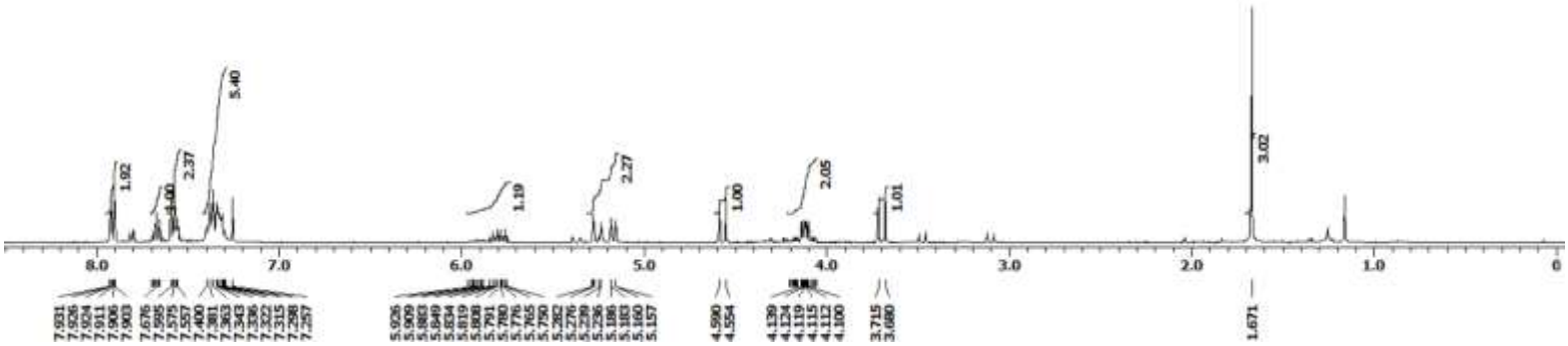
^{1}H NMR spectrum of 3t (400 MHz, $CDCl_3$)



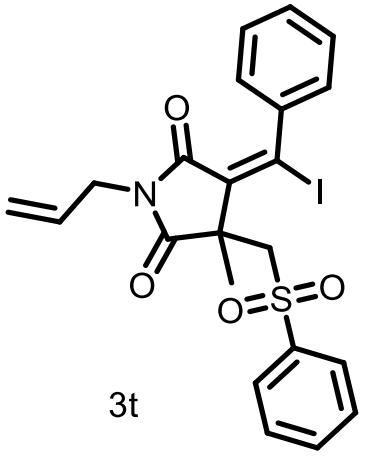
3t

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



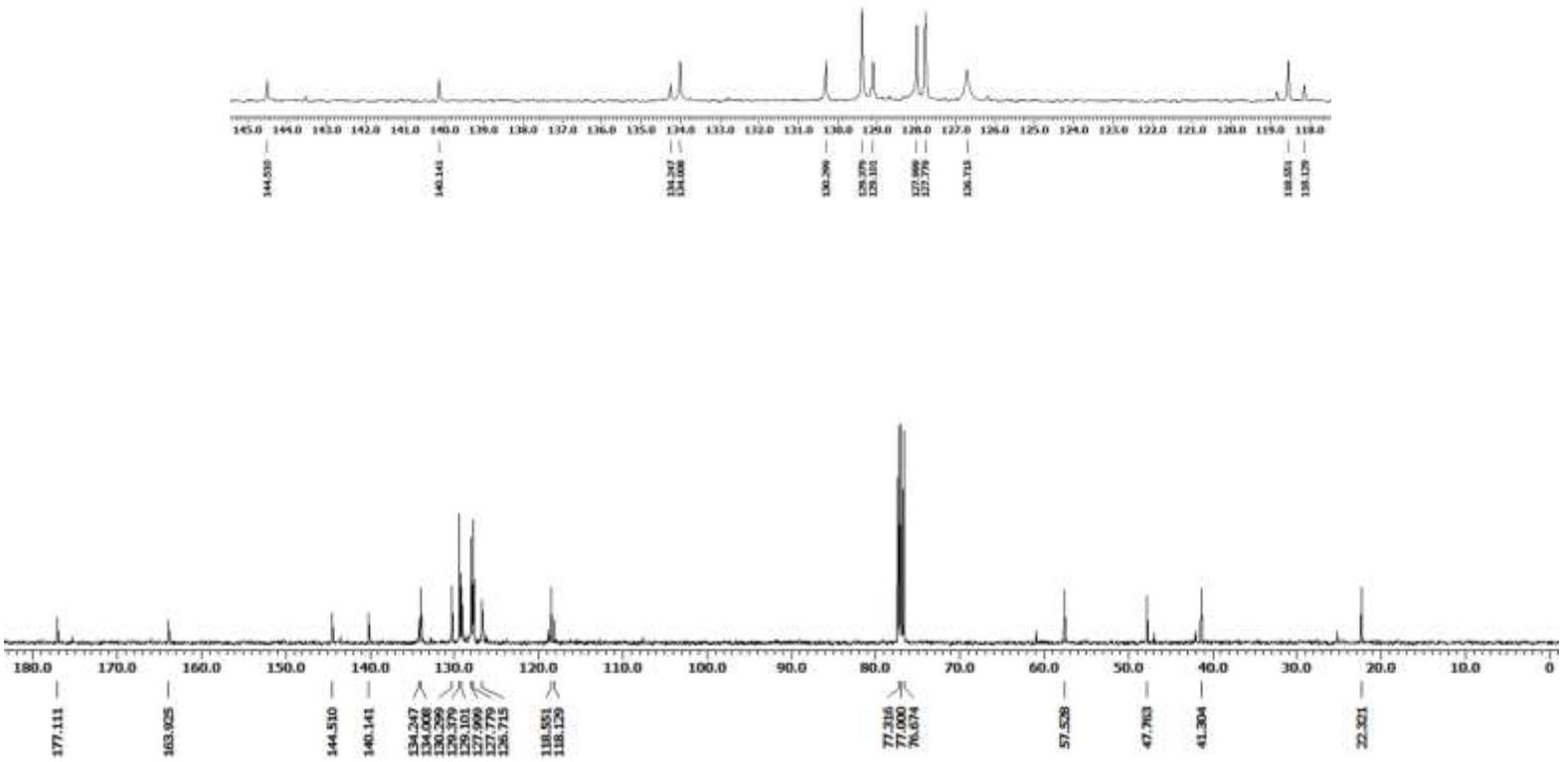


^{13}C NMR spectrum of 3t (100 MHz, $CDCl_3$)



3t

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



HRMS spectrum of 3t

3u

Qualitative Compound Report

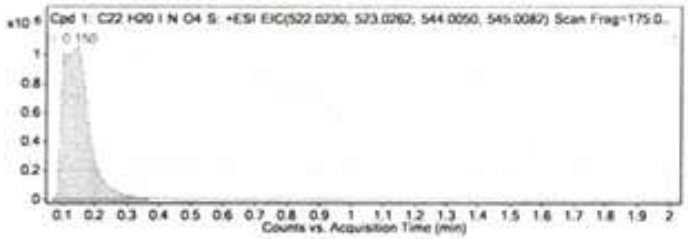
Data File	SMT-408.d	**Sample Name**	SMT-408
Sample Type	Sample	**Position**	P1-C9
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	07-02-2024 12:16:24
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

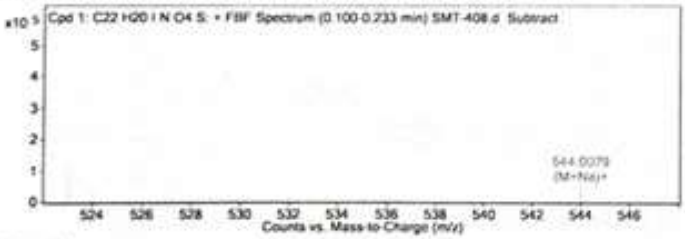
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C22 H20 I N O4 S	0.15	521.0189	54650	C22 H20 I N O4 S	521.0158	6.01	C22 H20 I N O4 S	C22 H20 I N O4 S

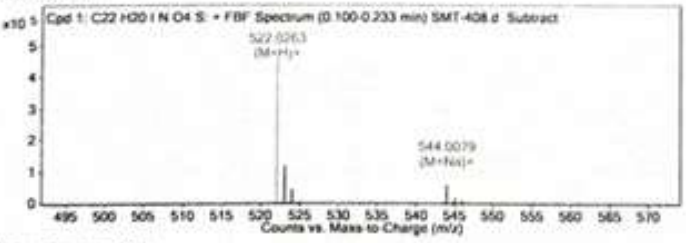
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C22 H20 I N O4 S	544.0079	0.15	Find By Formula	521.0189



MS Spectrum



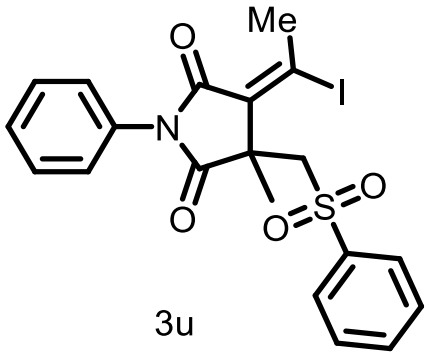
MS Zoomed Spectrum



MS Spectrum Peak List

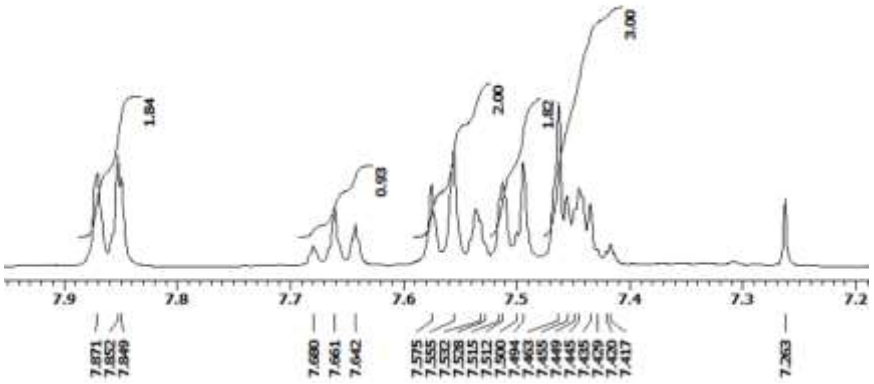
m/z	z	Abund	Formula	Ion
522.0263	1	471853.84	C22H21INO4S	(M+H)+
523.0291	1	111611.79	C22H21INO4S	(M+H)+
524.0265	1	34076.64	C22H21INO4S	(M+H)+
525.0275	1	6357.69	C22H21INO4S	(M+H)+
526.0302	1	1074.38	C22H21INO4S	(M+H)+
544.0079	1	54649.52	C22H20INNaO4S	(M+Na)+
545.0111	1	13091.87	C22H20INNaO4S	(M+Na)+
546.0089	1	4255.01	C22H20INNaO4S	(M+Na)+
547.011	1	842.83	C22H20INNaO4S	(M+Na)+
548.0172	1	112.45	C22H20INNaO4S	(M+Na)+

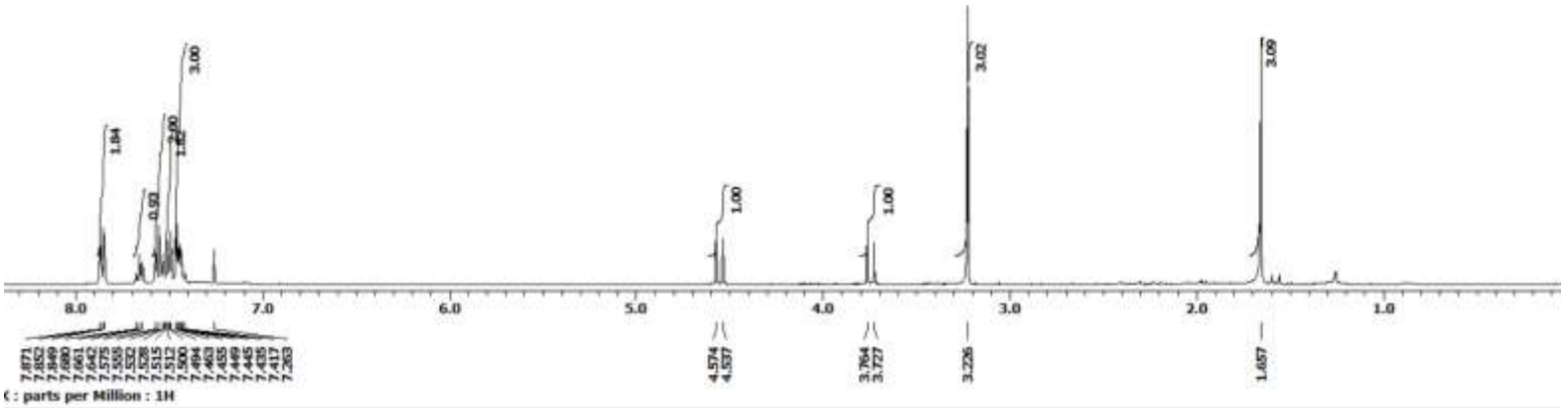
^{1}H NMR spectrum of 3u (400 MHz, $CDCl_3$)



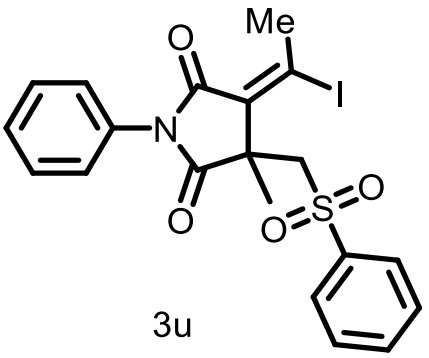
3u

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



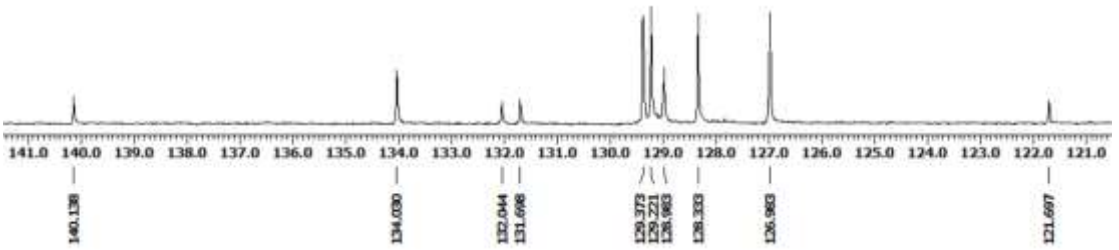


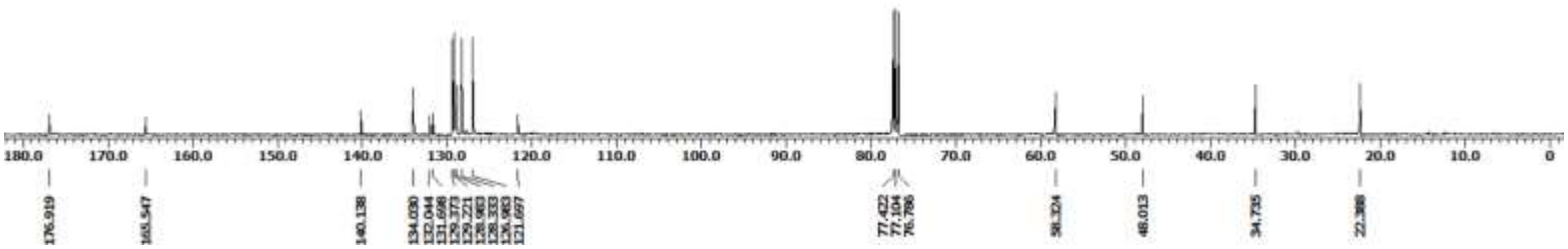
^{13}C NMR spectrum of 3u (100 MHz, $CDCl_3$)



3u

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





HRMS Spectrum of 3u

Qualitative Compound Report

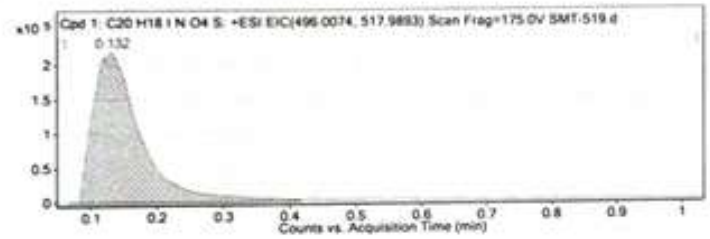
Data File	SMT-519.d	**Sample Name**	SMT-519
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	08.06.2024 13:17:30
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

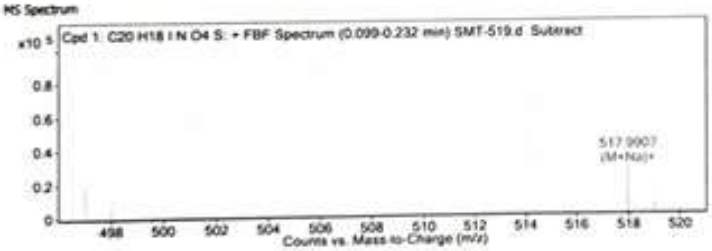
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H18 I N O4 S	0.132	495.0016	2704.7	C20 H18 I N O4 S	495.0001	2.89	C20 H18 I N O4 S	C20 H18 I N O4 S

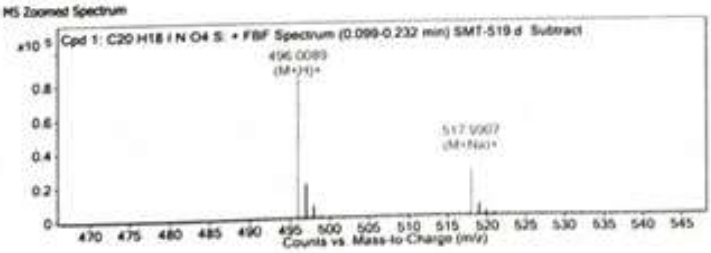
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H18 I N O4 S	517.9907	0.132	Find By Formula	495.0016



MS Spectrum



MS Zoomed Spectrum



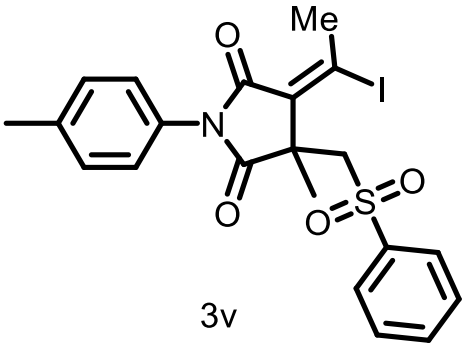
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
496.0089	1	86910.7	C20H19INO4S	(M+H)+
497.0118	1	18830.14	C20H19INO4S	(M+H)+
498.0092	1	6228.16	C20H19INO4S	(M+H)+
499.0125	1	1066.46	C20H19INO4S	(M+H)+
500.0116	1	96.79	C20H19INO4S	(M+H)+
517.9907	1	27046.57	C20H18INNaO4S	(M+Na)+
518.9939	1	6005.16	C20H18INNaO4S	(M+Na)+
519.9904	1	1961.41	C20H18INNaO4S	(M+Na)+
520.9957	1	288.74	C20H18INNaO4S	(M+Na)+

--- End Of Report ---

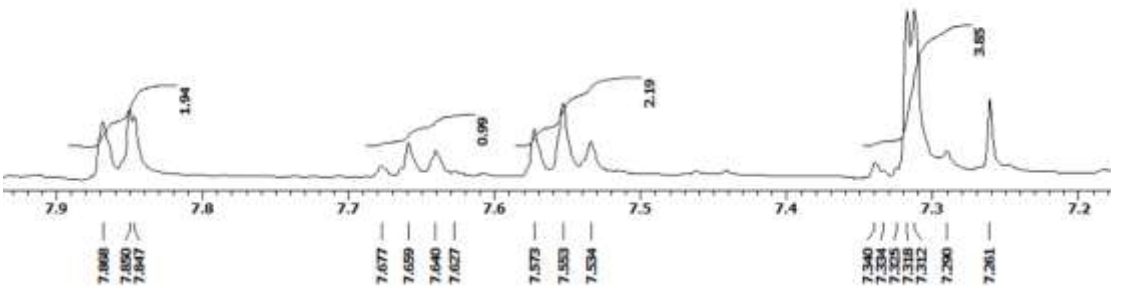
Printed at: 13:28 on:08-06-2024

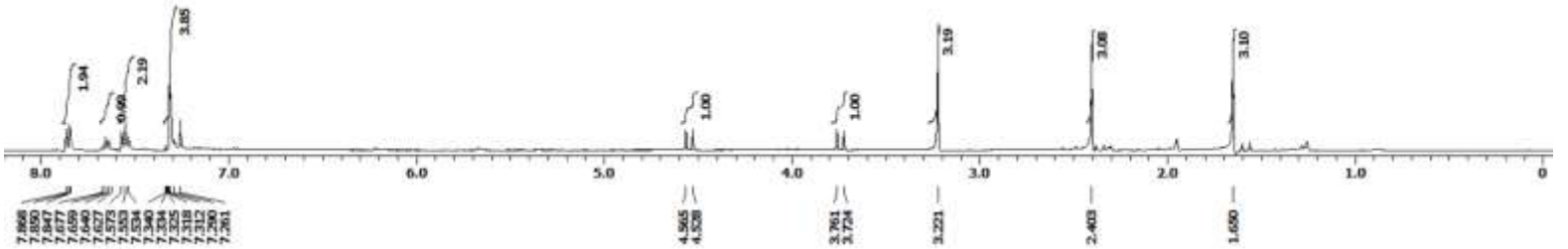
^{1}H NMR spectrum of 3v (400 MHz, $CDCl_3$)



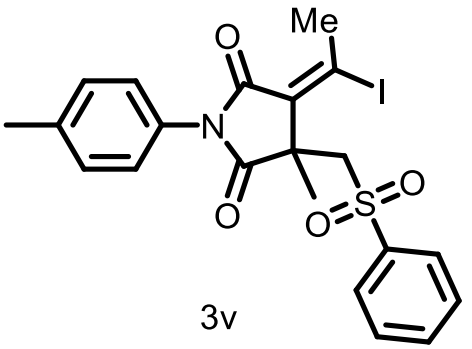
3v

(*E*)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)-1-(*p*-tolyl)pyrrolidine-2,5-dione



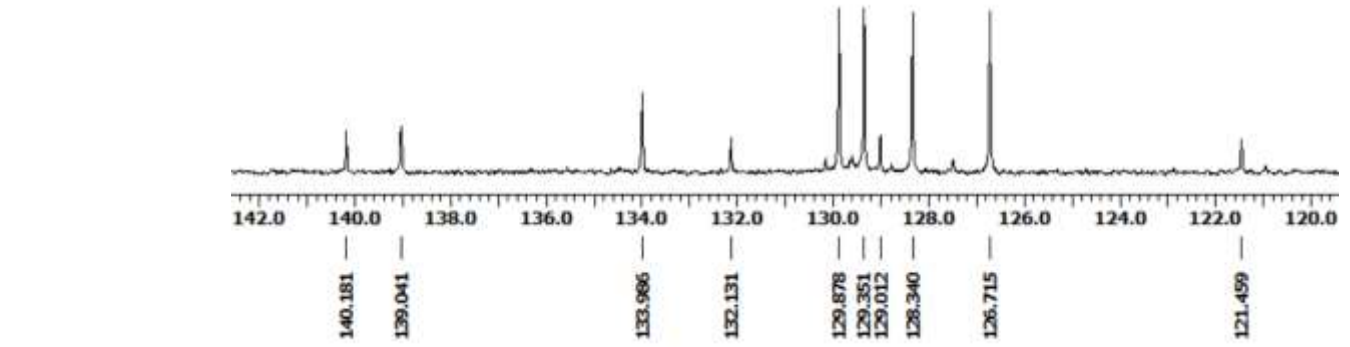


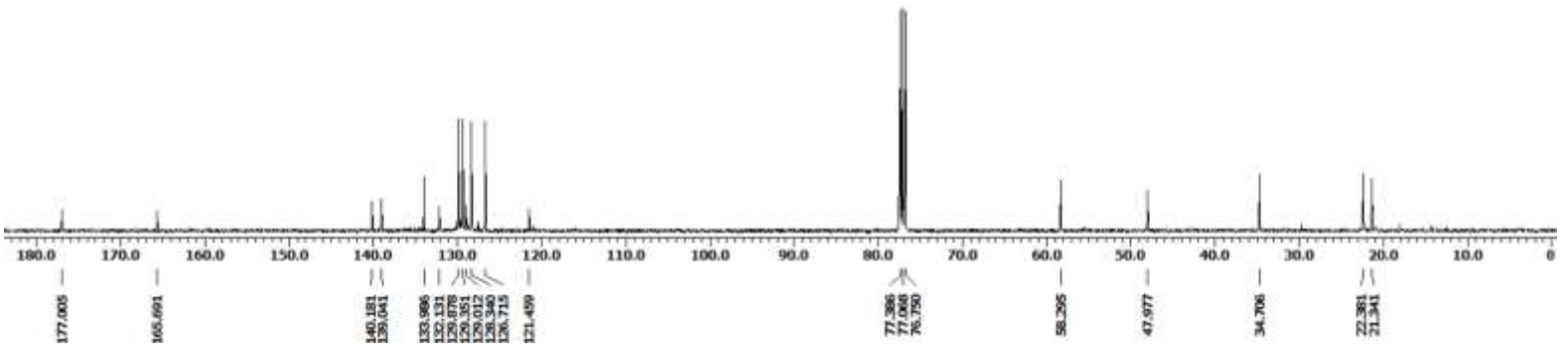
^{13}C NMR spectrum of 3v (100 MHz, $CDCl_3$)



3v

(*E*)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)-1-(*p*-tolyl)pyrrolidine-2,5-dione





HRMS Spectrum of 3v

Qualitative Compound Report

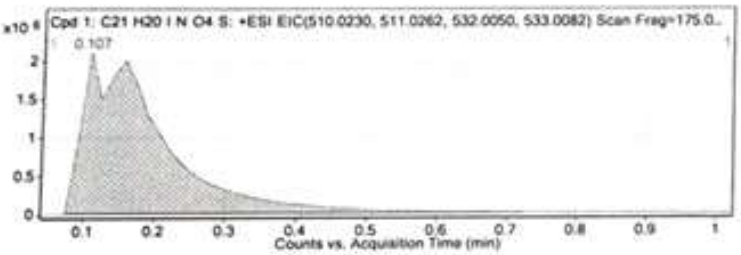
Data File	SMT-521.d	**Sample Name**	SMT-521
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	08-06-2024 13:21:15
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

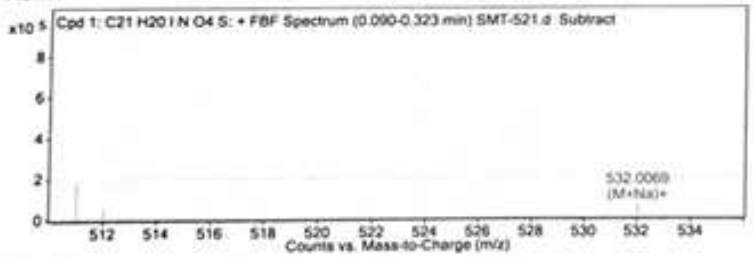
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C21 H20 I N O4 S	0.107	509.018	64273	C21 H20 I N O4 S	509.0158	4.44	C21 H20 I N O4 S	C21 H20 I N O4 S

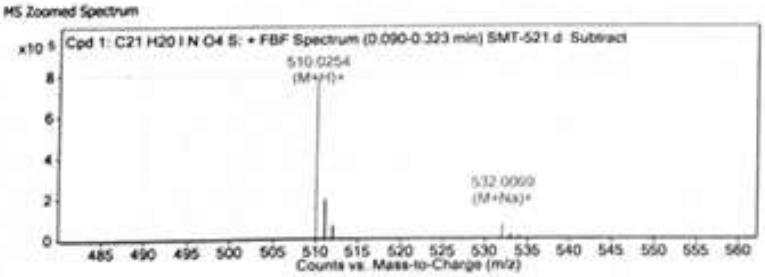
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C21 H20 I N O4 S	532.0069	0.107	Find By Formula	509.018



MS Spectrum



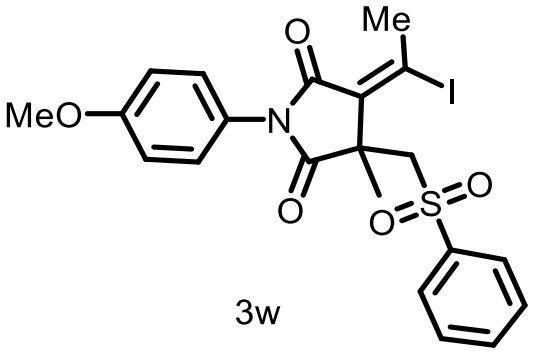
MS Zoomed Spectrum



MS Spectrum Peak List

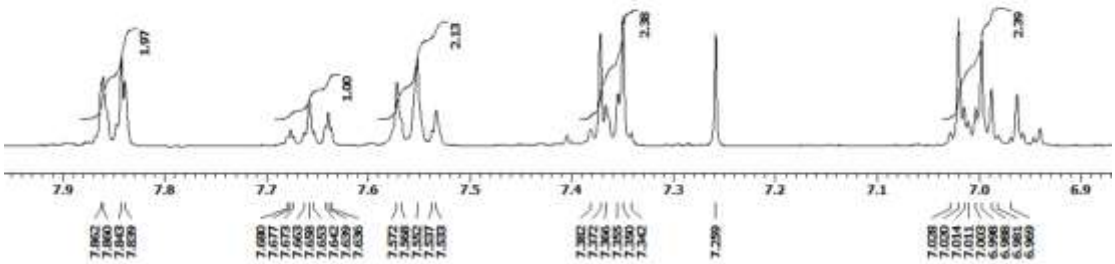
m/z	z	Abund	Formula	Ion
510.0254	1	775834.38	C21H21INO4S	(M+H)+
511.0282	1	185887.33	C21H21INO4S	(M+H)+
512.0255	1	55056.55	C21H21INO4S	(M+H)+
513.0294	1	13812.57	C21H21INO4S	(M+H)+
514.0316	1	2452.78	C21H21INO4S	(M+H)+
515.0338	1	613.48	C21H21INO4S	(M+H)+
532.0069	1	64273.11	C21H20INNaO4S	(M+Na)+
533.0101	1	14685.36	C21H20INNaO4S	(M+Na)+
534.0069	1	4809.74	C21H20INNaO4S	(M+Na)+

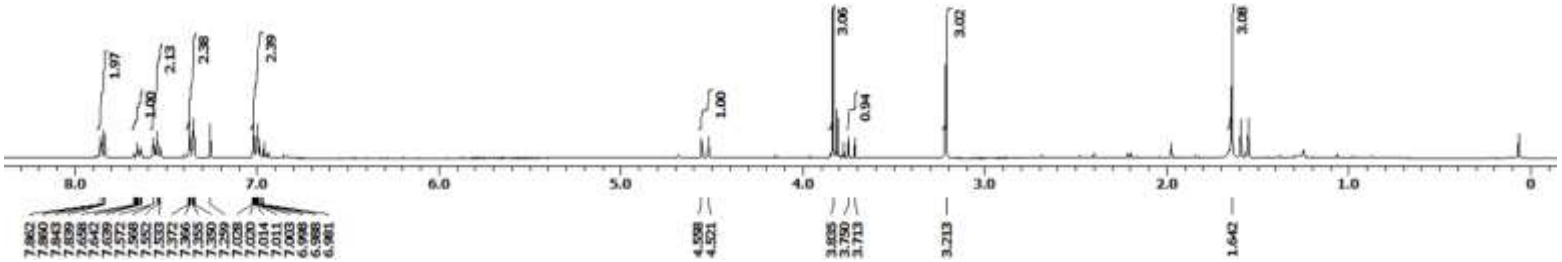
^{1}H NMR spectrum of 3w (400 MHz, $CDCl_3$)



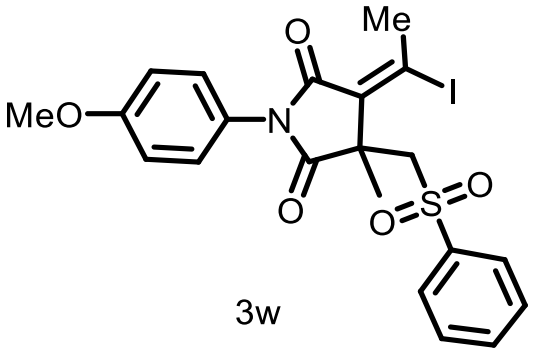
3w

(*E*)-4-(1-iodoethylidene)-1-(4-methoxyphenyl)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



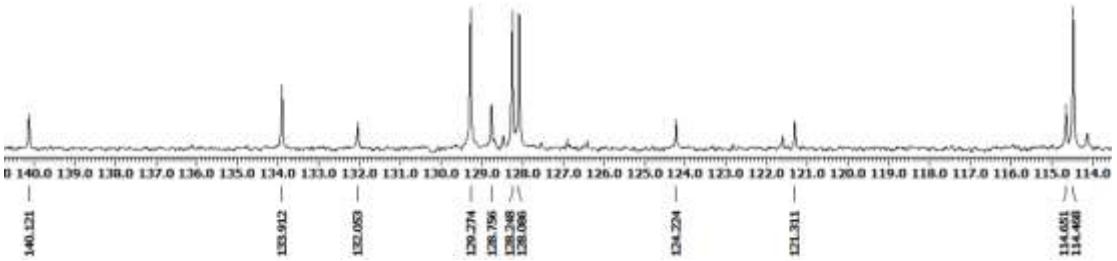


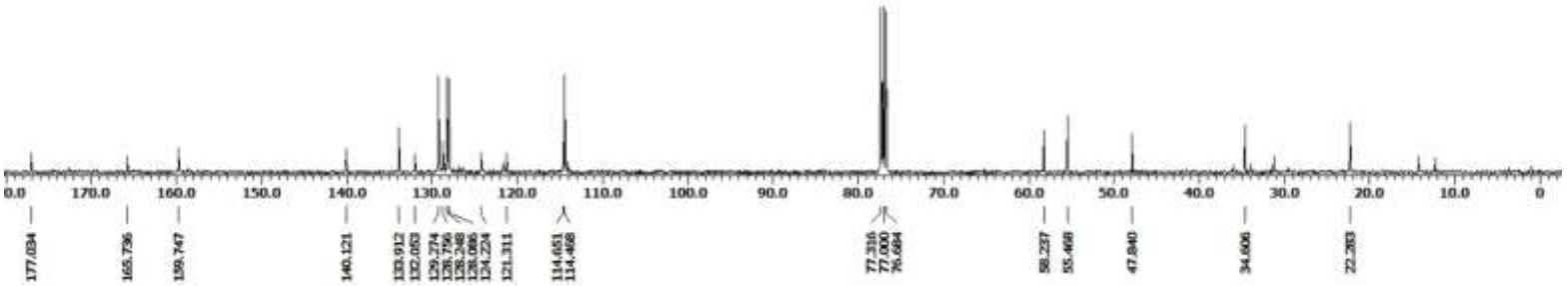
^{13}C NMR spectrum of 3w (100 MHz, $CDCl_3$)



3w

(*E*)-4-(1-iodoethylidene)-1-(4-methoxyphenyl)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione





HRMS Spectrum of 3w

Qualitative Compound Report

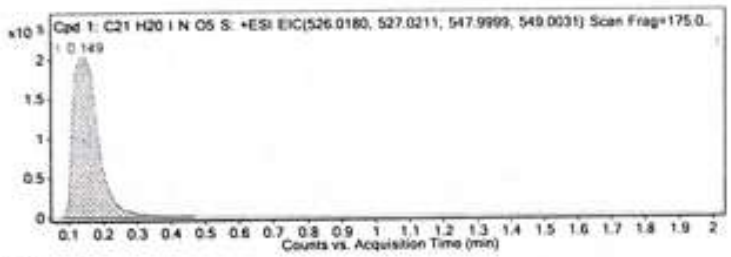
Data File	SMT-466.d	**Sample Name**	SMT-466
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	13-06-2024 13:49:29
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

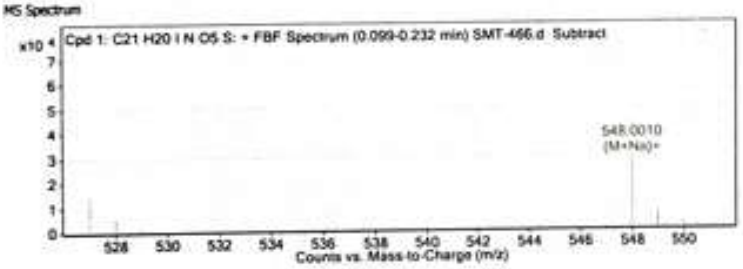
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C21 H20 I N O5 S	0.149	525.0116	63190	C21 H20 I N O5 S	525.0107	1.81	C21 H20 I N O5 S	C21 H20 I N O5 S

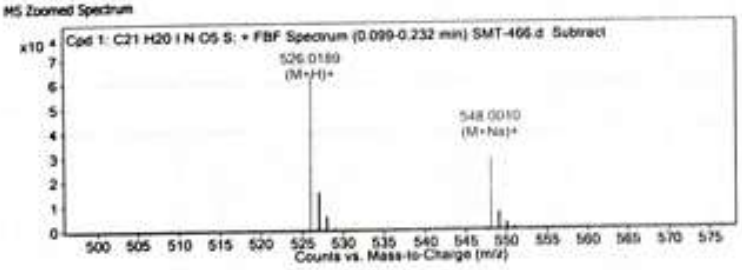
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C21 H20 I N O5 S	526.0189	0.149	Find By Formula	525.0116



MS Spectrum



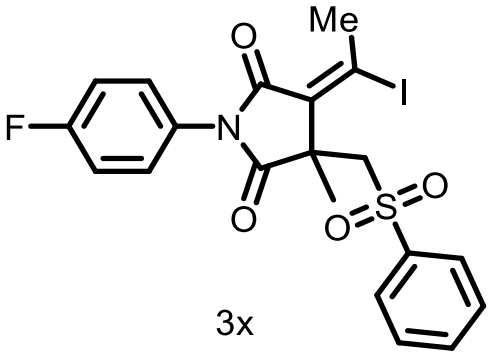
MS Zoomed Spectrum



MS Spectrum Peak List

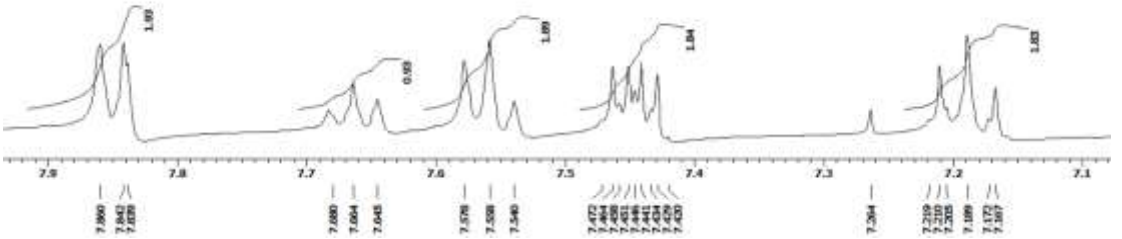
m/z	z	Abund	Formula	Ion
526.0189	1	63189.96	C21H21INO5S	(M+H)+
527.0219	1	14929.21	C21H21INO5S	(M+H)+
528.0187	1	5165.72	C21H21INO5S	(M+H)+
529.0218	1	994.35	C21H21INO5S	(M+H)+
530.0141	1	50.17	C21H21INO5S	(M+H)+
548.001	1	28979.22	C21H20INNaO5S	(M+Na)+
549.0038	1	6577.33	C21H20INNaO5S	(M+Na)+
550.0014	1	2306.74	C21H20INNaO5S	(M+Na)+
551.0051	1	440.48	C21H20INNaO5S	(M+Na)+
551.9996	1	65.41	C21H20INNaO5S	(M+Na)+

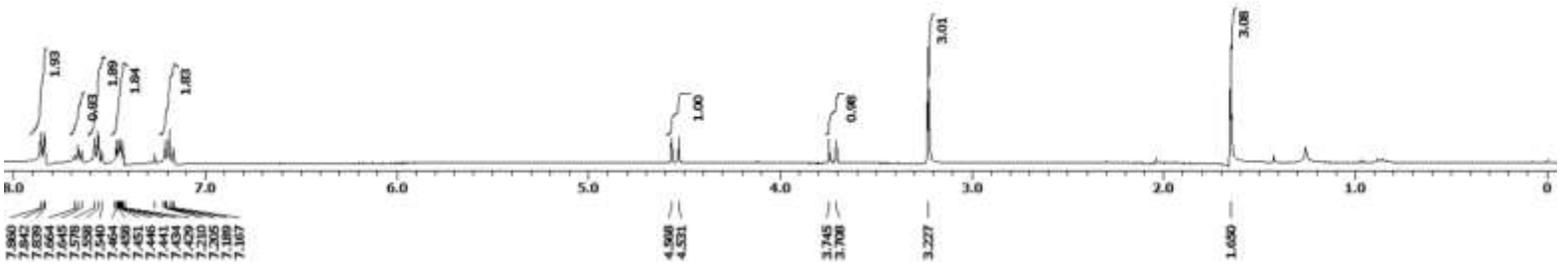
^{1}H NMR spectrum of 3x (400 MHz, $CDCl_3$)



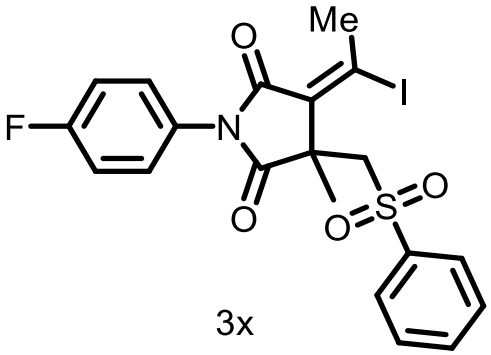
3x

(*E*)-1-(4-fluorophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



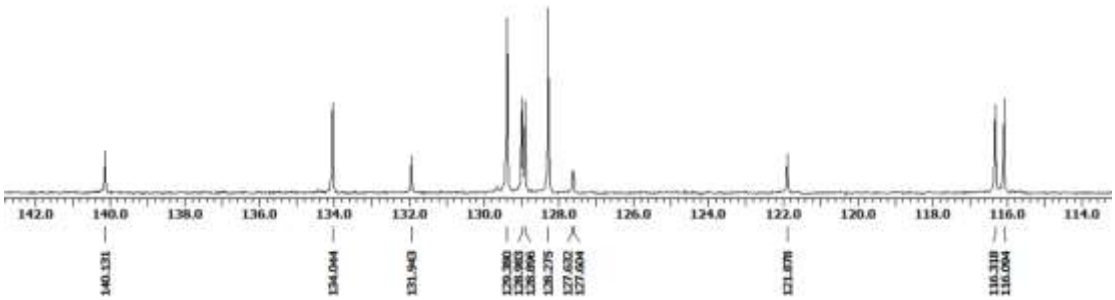


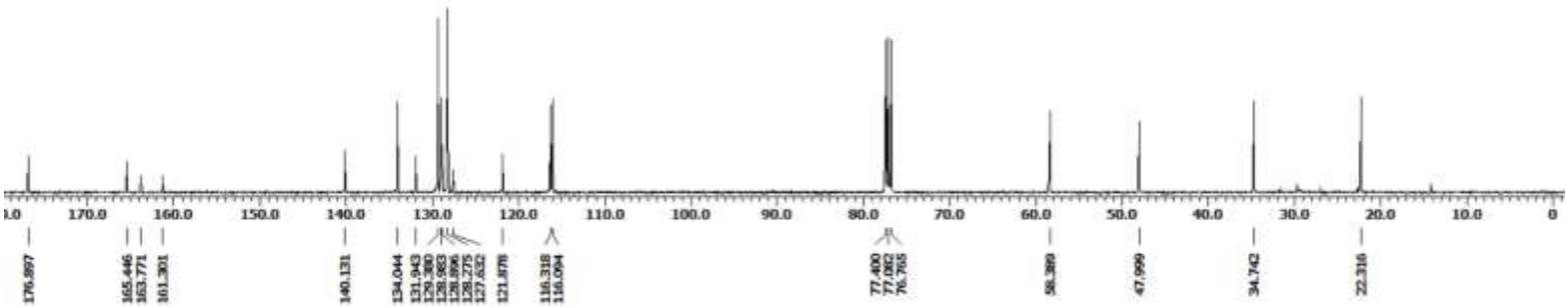
^{13}C NMR spectrum of 3x (100 MHz, $CDCl_3$)



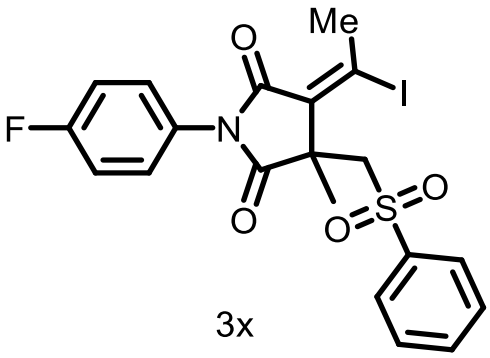
3x

(*E*)-1-(4-fluorophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



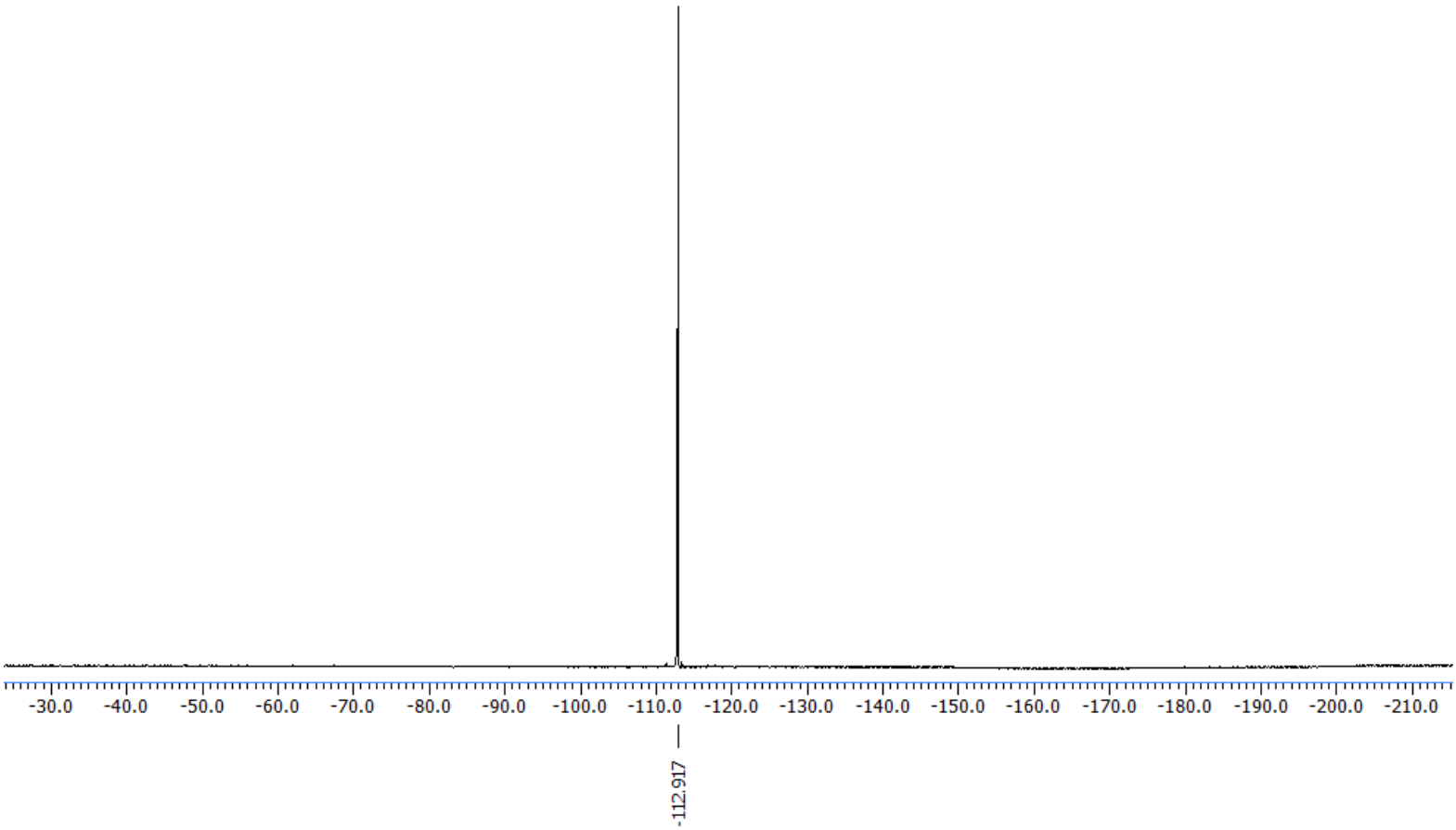


^{19}F NMR spectrum of 3x (376 MHz, $CDCl_3$)



3x

(*E*)-1-(4-fluorophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3x

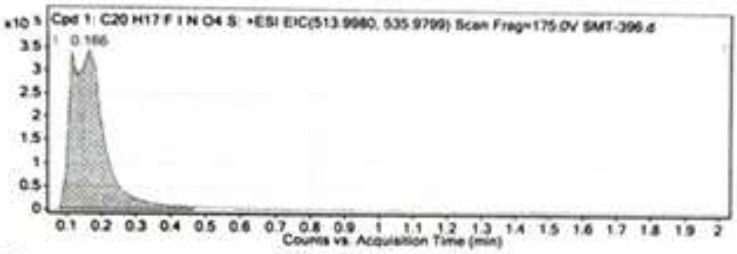
Qualitative Compound Report

Data File	SMT-396.d	**Sample Name**	SMT-396
Sample Type	Sample	**Position**	P1-C8
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	13-06-2024 14:21:27
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

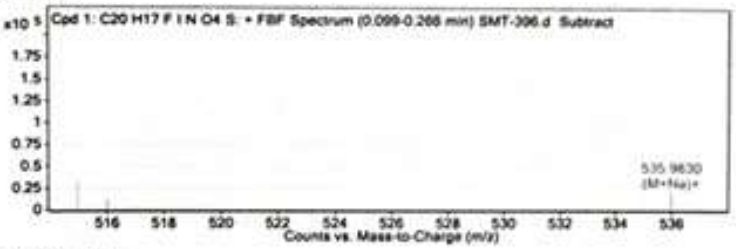
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H17 F I N O4 S	0.166	512.9937	174821	C20 H17 F I N O4 S	512.9907	5.88	C20 H17 F I N O4 S	C20 H17 F I N O4 S

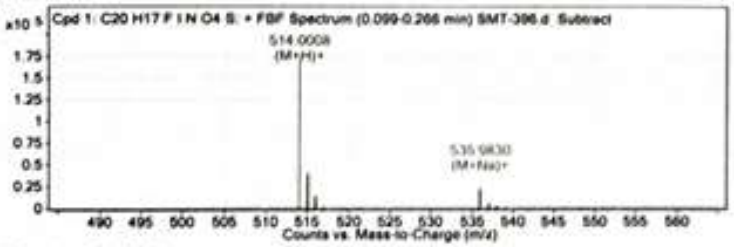
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H17 F I N O4 S	514.0008	0.166	Find By Formula	512.9937



MS Spectrum



MS Zoomed Spectrum

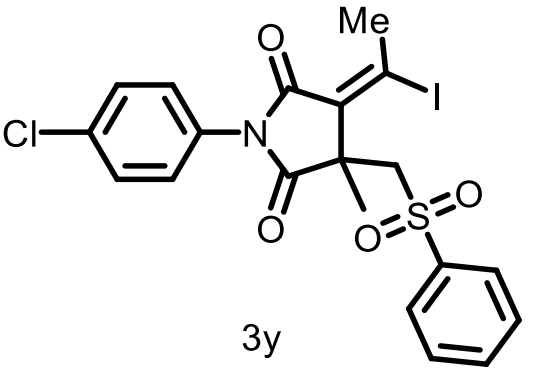


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
514.0008	1	174821.06	C20H18FINO4S	(M+H)+
515.0037	1	37705.01	C20H18FINO4S	(M+H)+
516.0014	1	12285.31	C20H18FINO4S	(M+H)+
517.0041	1	2314.37	C20H18FINO4S	(M+H)+
535.983	1	21476.02	C20H17FINaO4S	(M+Na)+
536.9898	1	5715.56	C20H17FINaO4S	(M+Na)+
537.9889	1	1991.22	C20H17FINaO4S	(M+Na)+

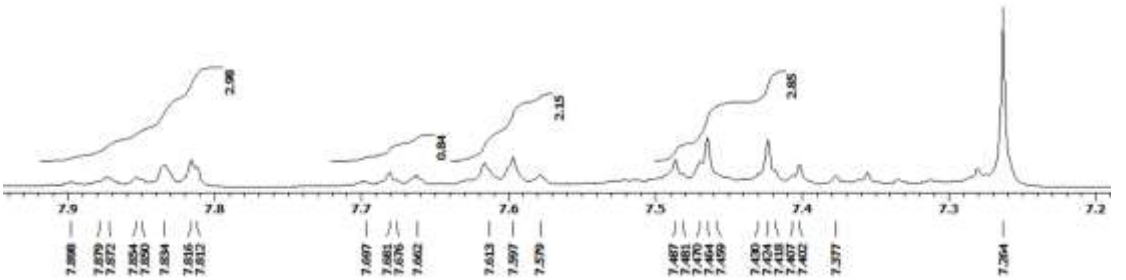
--- End Of Report ---

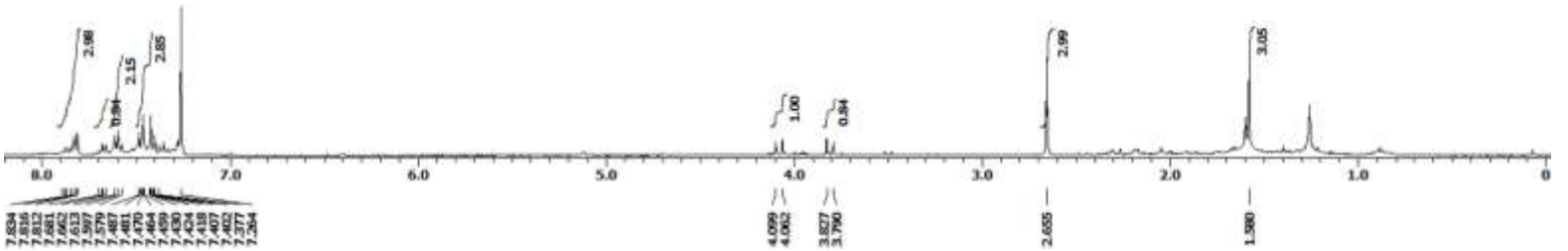
^{1}H NMR spectrum of 3y (400 MZHz, $CDCl_3$)



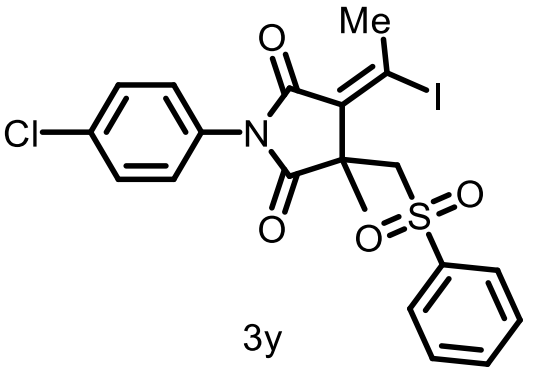
3y

(*E*)-1-(4-chlorophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



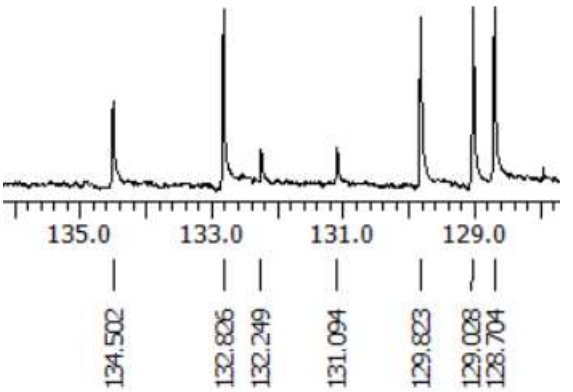


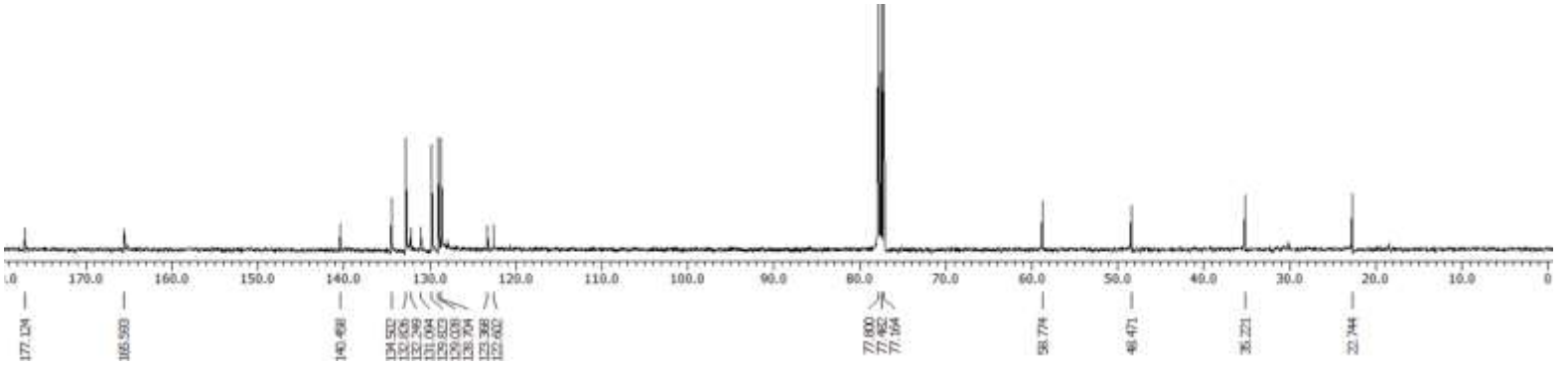
^{13}C NMR spectrum of 3y (100 MHz, $CDCl_3$)



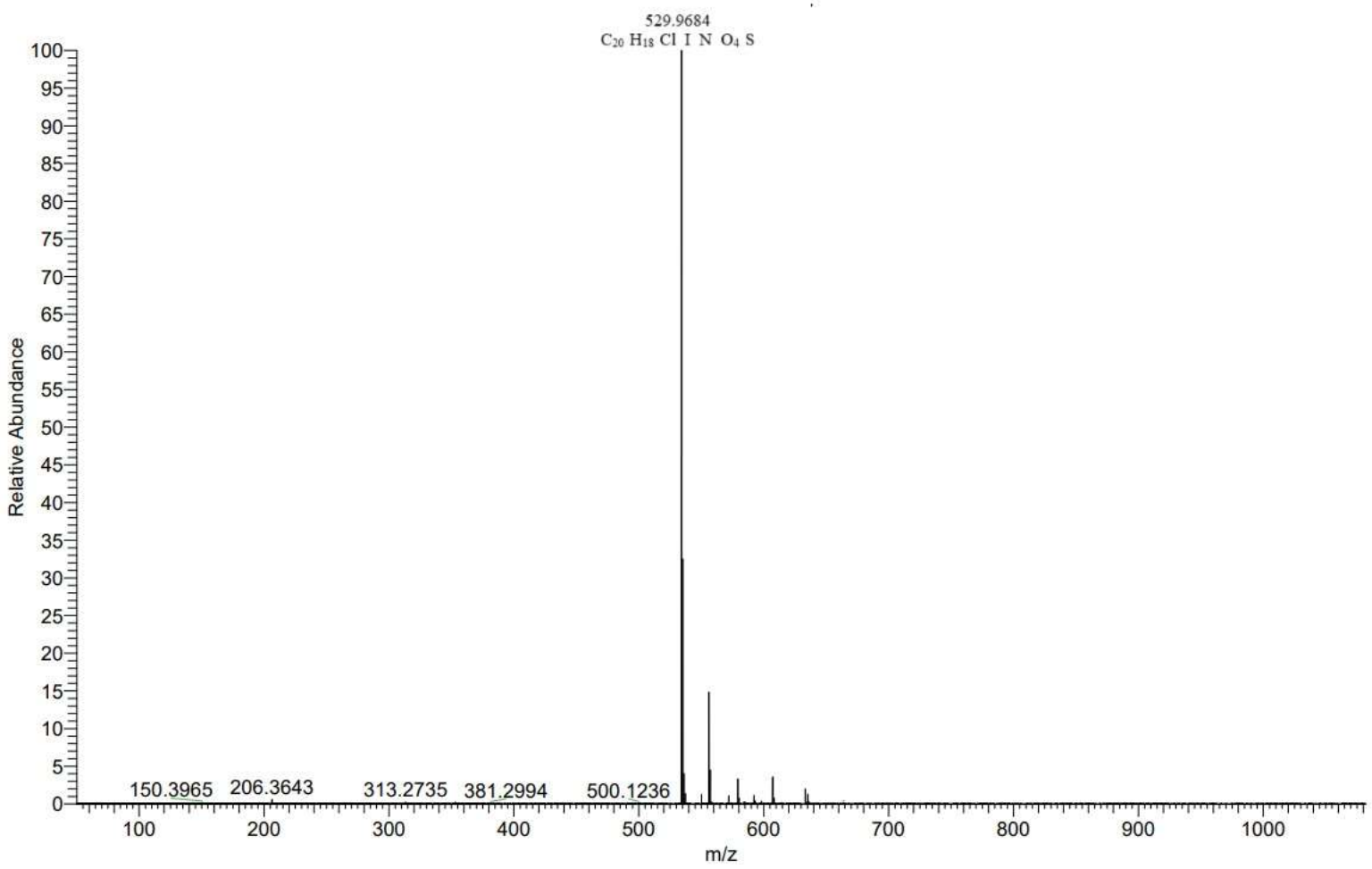
3y

(*E*)-1-(4-chlorophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione

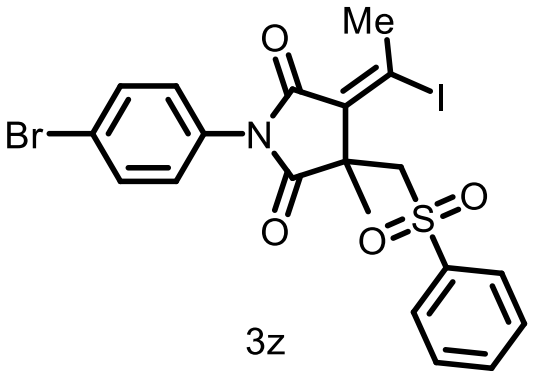




HRMS Spectrum of 3y

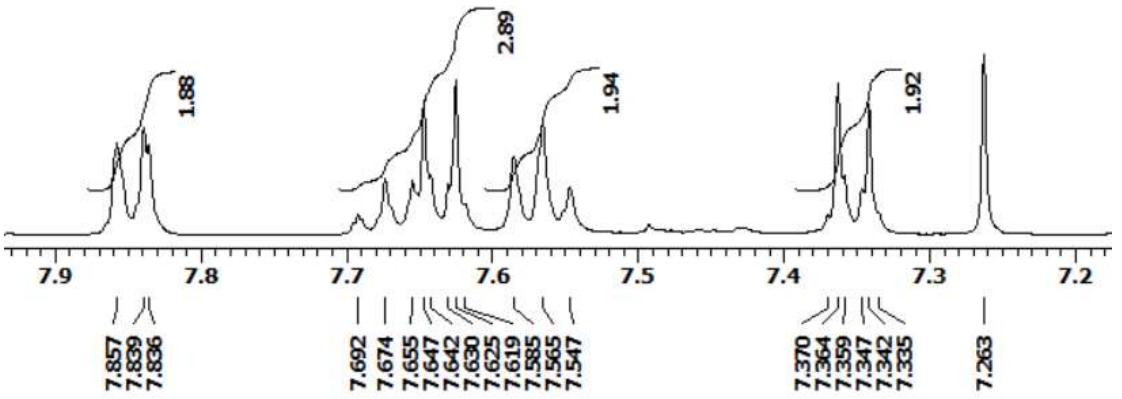


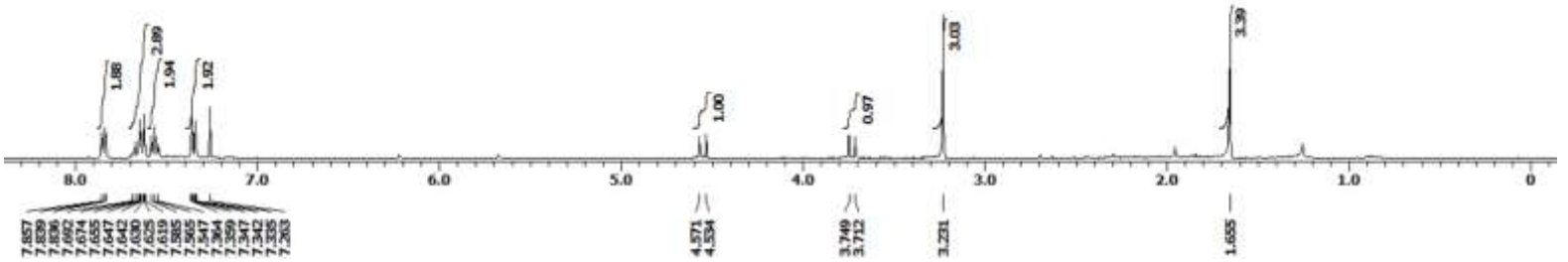
^{1}H NMR spectrum of 3z (400 MHz, $CDCl_3$)



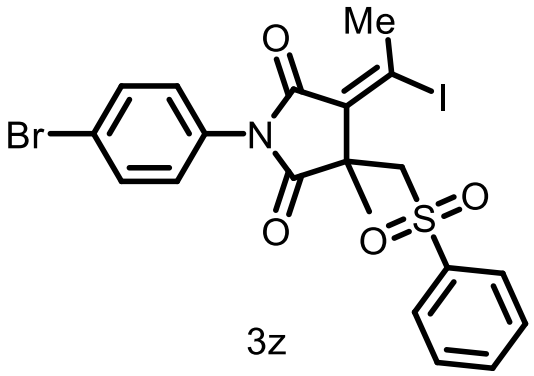
3z

(*E*)-1-(4-bromophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



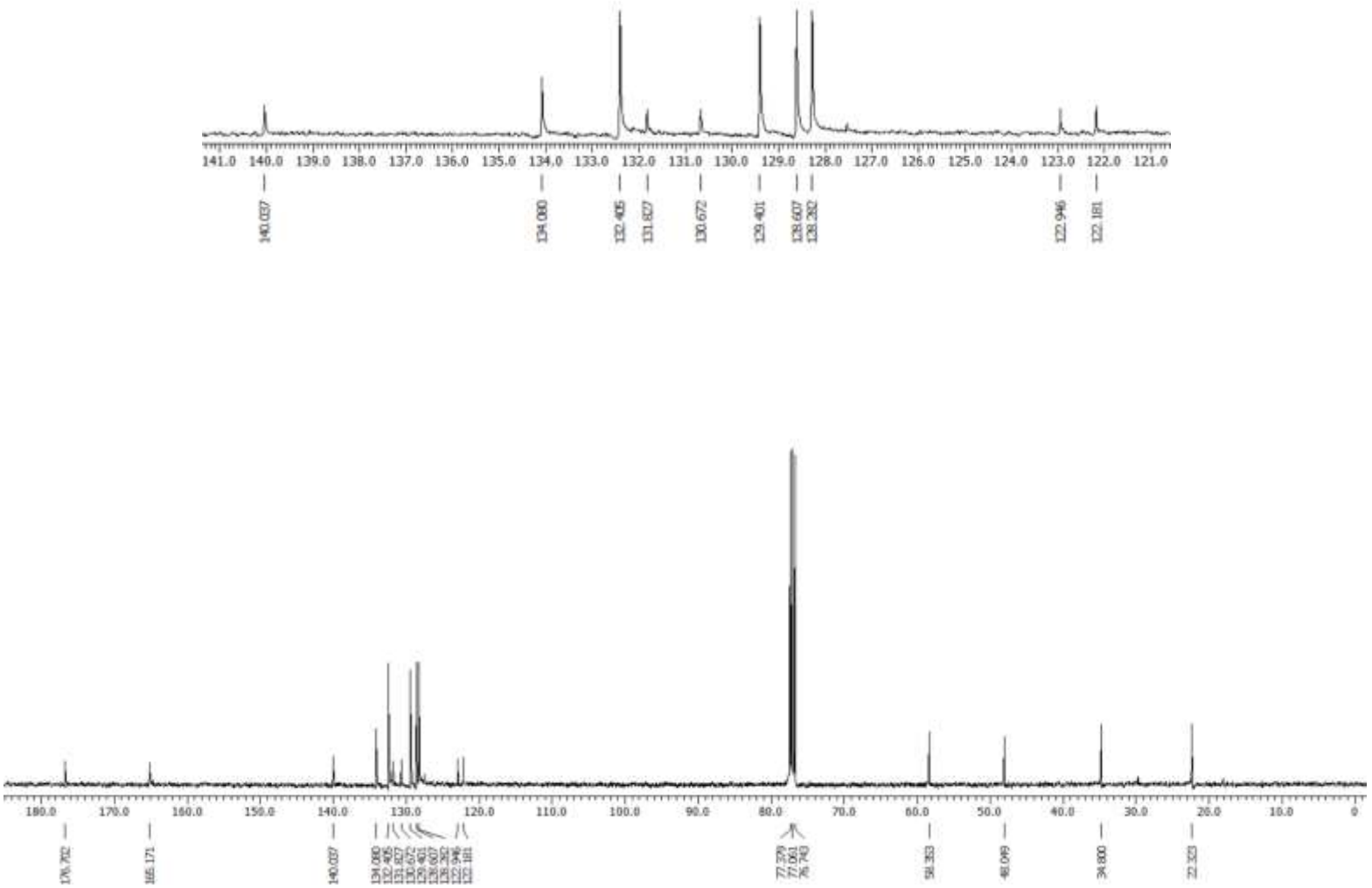


^{13}C NMR spectrum of 3z (100 MHz, $CDCl_3$)



3z

(*E*)-1-(4-bromophenyl)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



HRMS Spectrum of 3z

Qualitative Compound Report

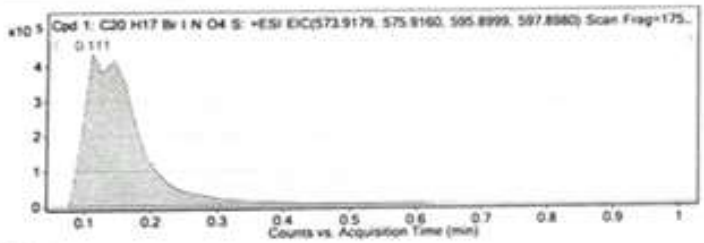
Data File	SMT-520.d	**Sample Name**	SMT-520
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	08-06-2024 13:19:23
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

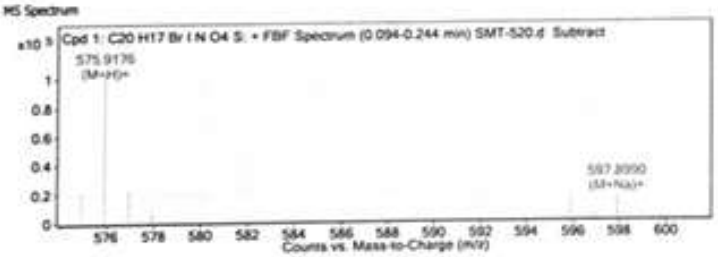
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H17 Br I N O4 S	0.111	572.9123	103388	C20 H17 Br I N O4 S	572.9106	2.89	C20 H17 Br I N O4 S	C20 H17 Br I N O4 S

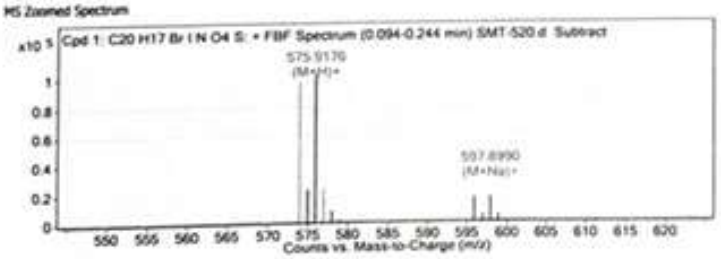
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H17 Br I N O4 S	575.9176	0.111	Find By Formula	572.9123



MS Spectrum



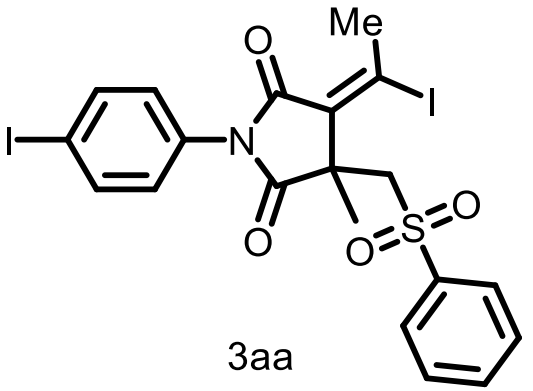
MS Zoomed Spectrum



MS Spectrum Peak List

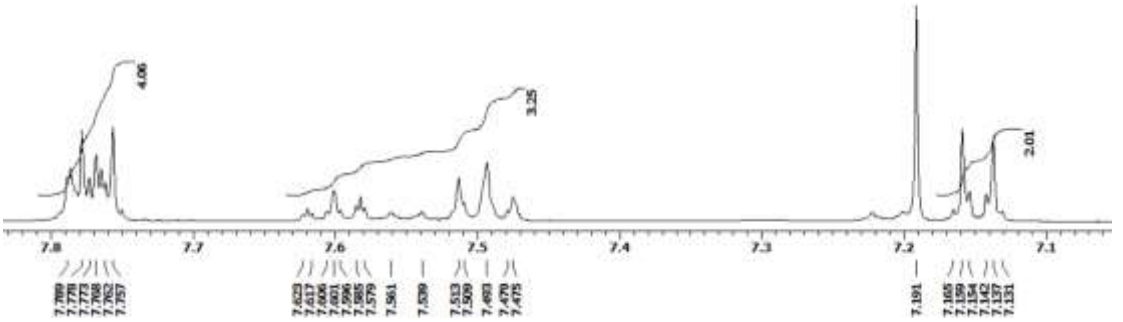
m/z	z	Abund	Formula	Ion
573.9196	1	97584.27	C20H18BrINO4S	(M+H)+
574.9221	1	21320.15	C20H18BrINO4S	(M+H)+
575.9176	1	103387.89	C20H18BrINO4S	(M+H)+
576.9207	1	22516.46	C20H18BrINO4S	(M+H)+
577.9175	1	7189.44	C20H18BrINO4S	(M+H)+
578.9189	1	1314.41	C20H18BrINO4S	(M+H)+
579.924	1	231.77	C20H18BrINO4S	(M+H)+
595.9032	1	16261.45	C20H17BrINNaO4S	(M+Na)+
596.9053	1	3901.06	C20H17BrINNaO4S	(M+Na)+
597.899	1	16488.83	C20H17BrINNaO4S	(M+Na)+
598.9023	1	3738.54	C20H17BrINNaO4S	(M+Na)+

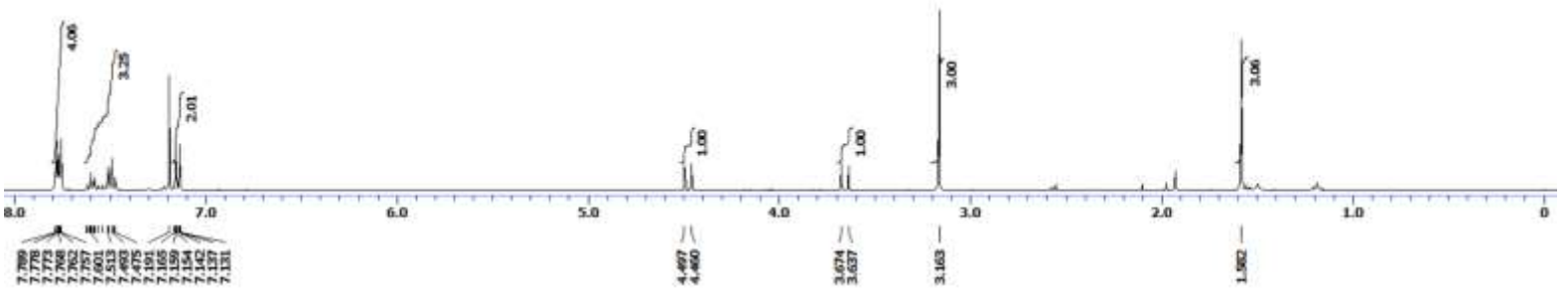
^{1}H NMR spectrum of 3aa (400 MHz, $CDCl_3$)



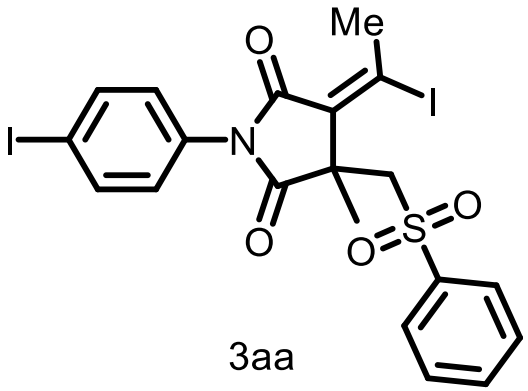
3aa

(*E*)-4-(1-iodoethylidene)-1-(4-iodophenyl)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



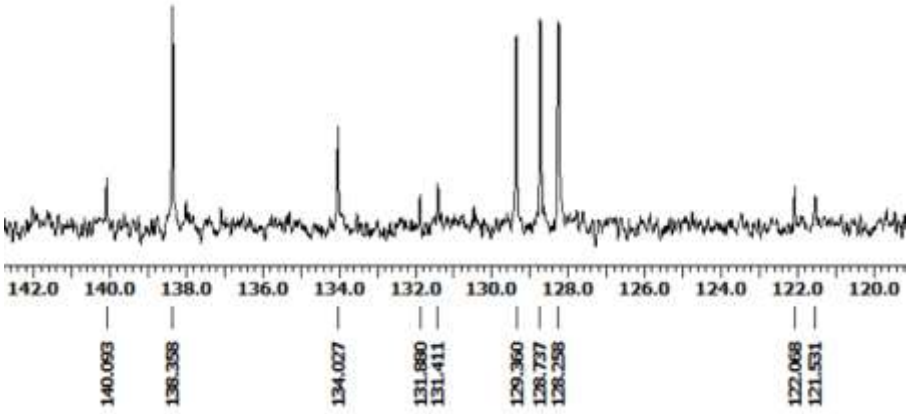


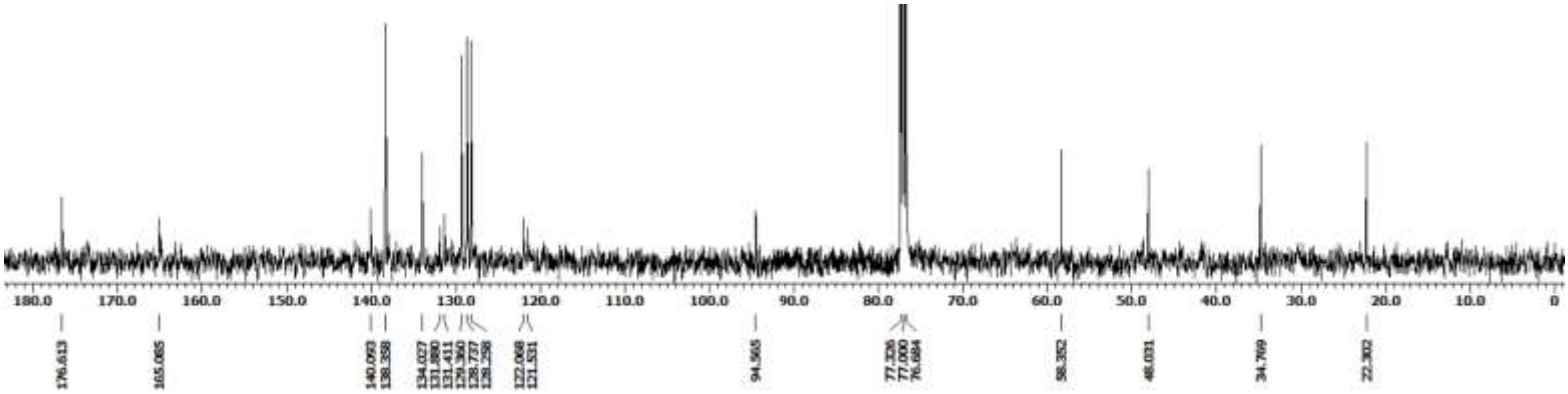
^{13}C NMR spectrum of 3aa (100 MHz, $CDCl_3$)



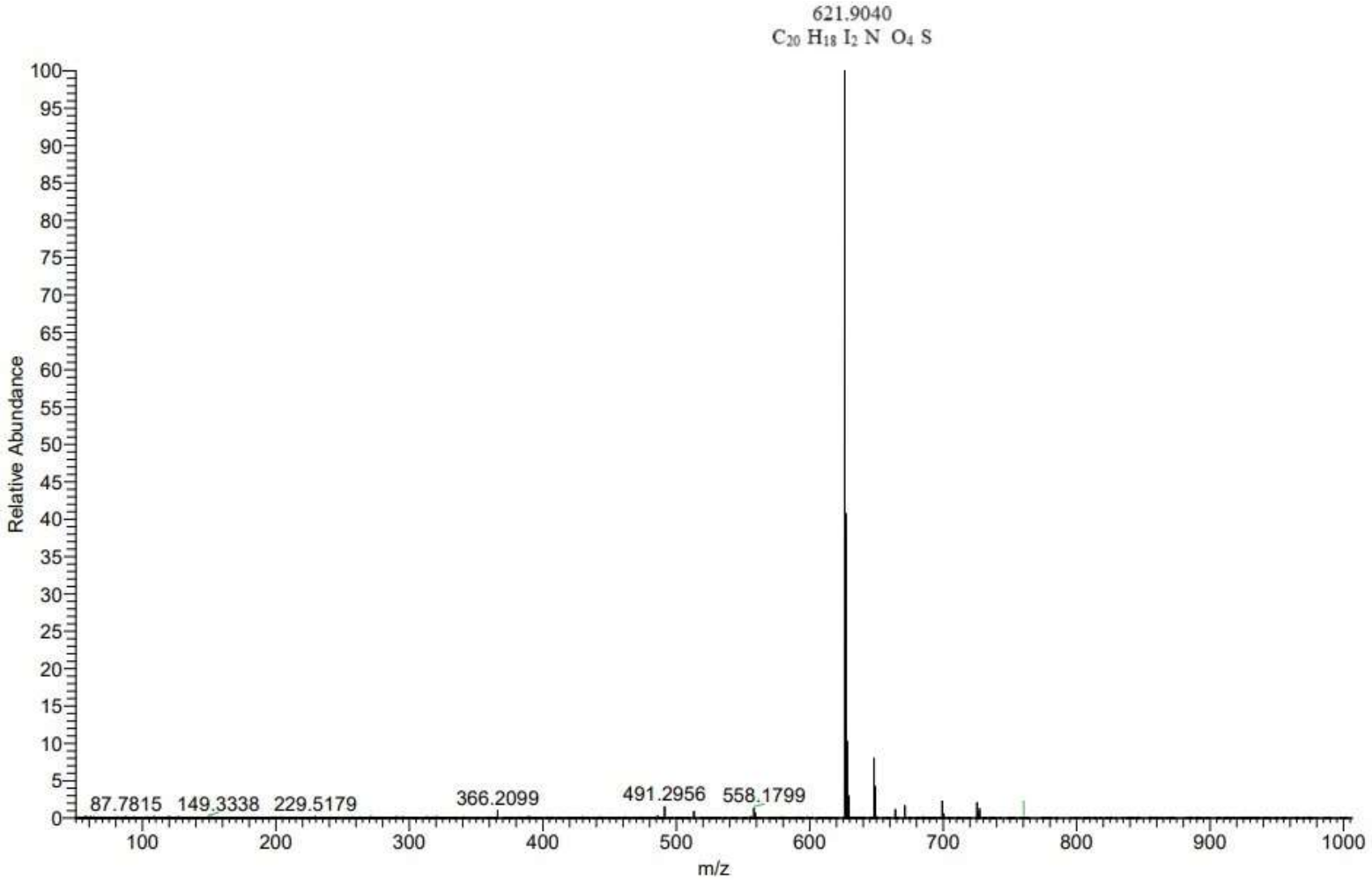
3aa

(*E*)-4-(1-iodoethylidene)-1-(4-iodophenyl)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione

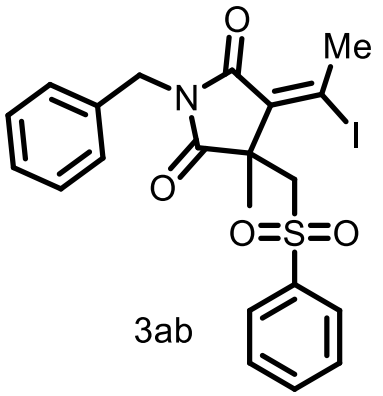




HRMS Spectrum of 3aa

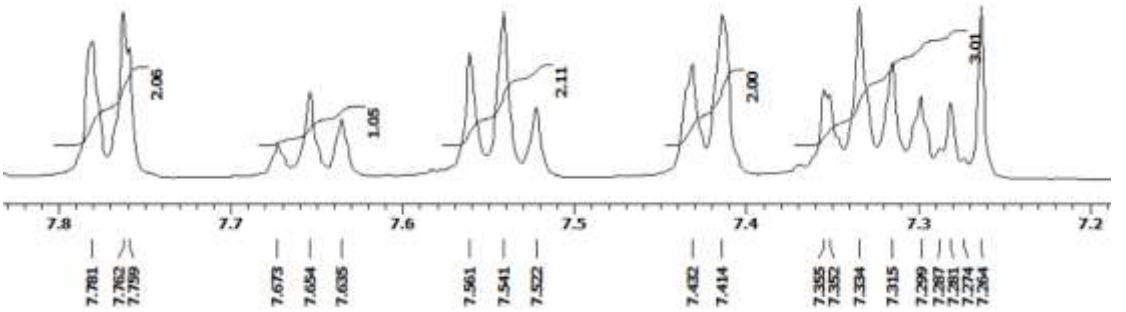


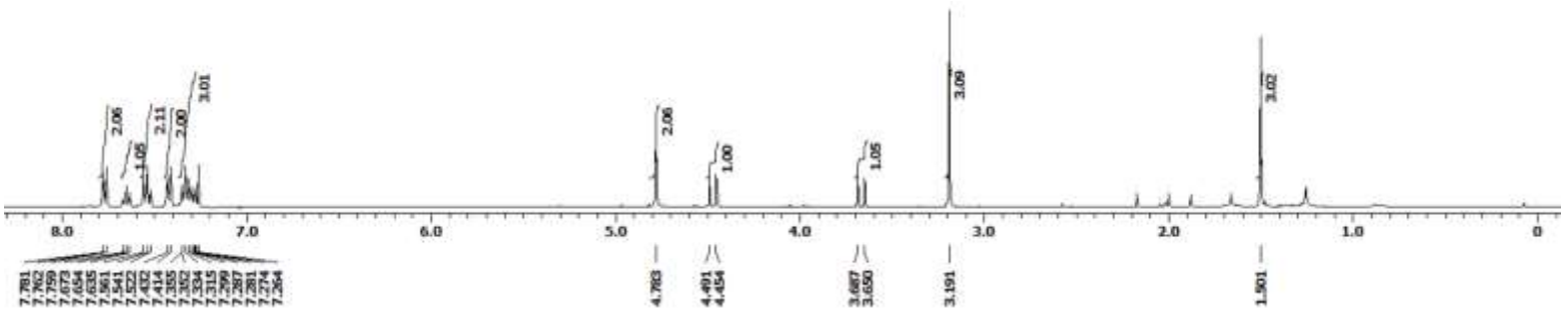
^{1}H NMR spectrum of 3ab (400 MHz, $CDCl_3$)



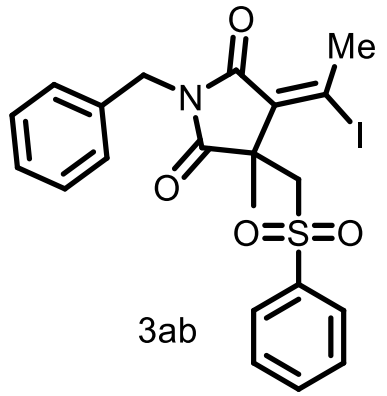
3ab

(*E*)-1-benzyl-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



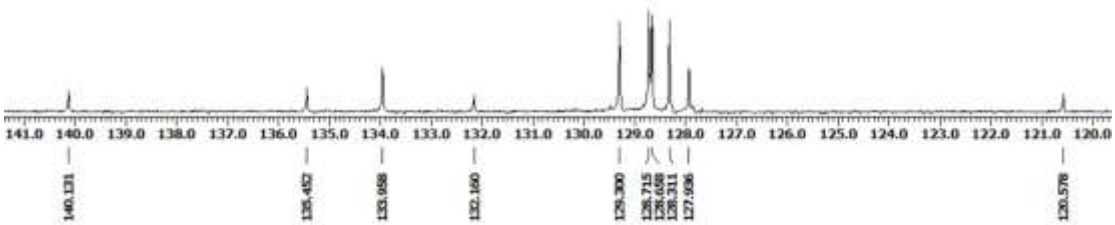


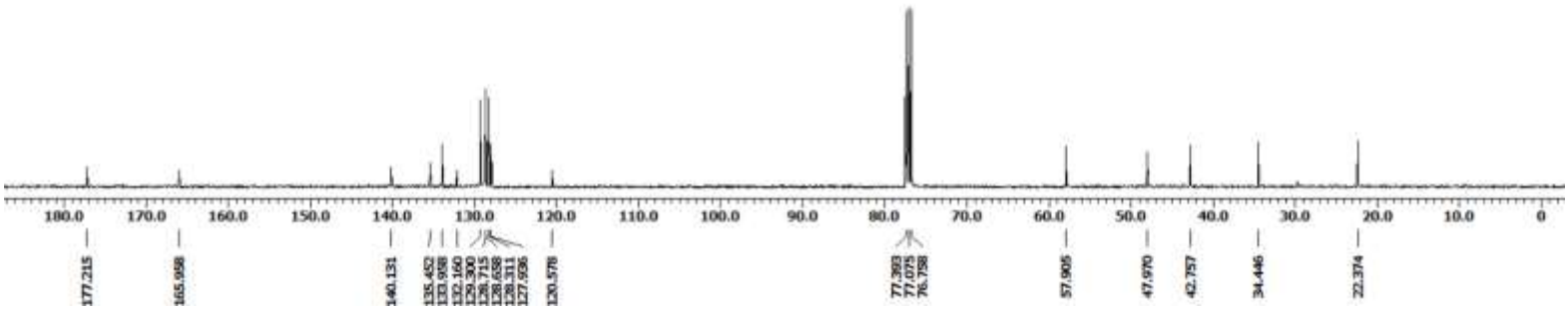
^{13}C NMR spectrum of 3ab (100 MHz, $CDCl_3$)



3ab

(*E*)-1-benzyl-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione





HRMS Spectrum of 3ab

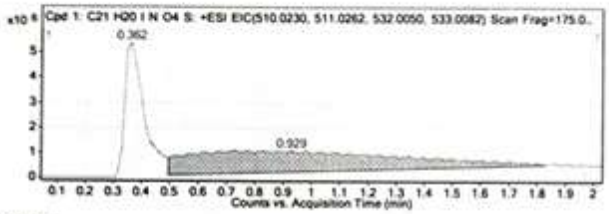
Qualitative Compound Report

Data File	SMT-393.d	**Sample Name**	SMT-393
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	30-05-2024 13:07:31
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)		

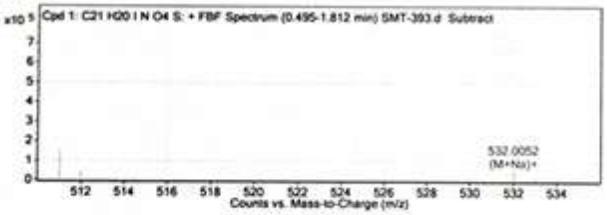
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C21 H20 I N O4 S	0.929	509.0164	52393	C21 H20 I N O4 S	509.0158	1.25	C21 H20 I N O4 S	C21 H20 I N O4 S

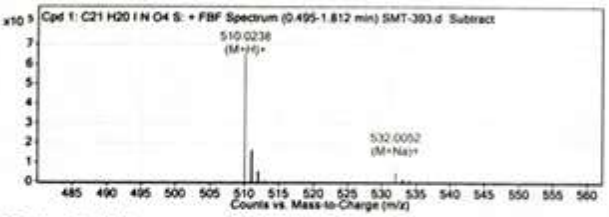
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C21 H20 I N O4 S	532.0052	0.929	Find By Formula	509.0164



MS Spectrum



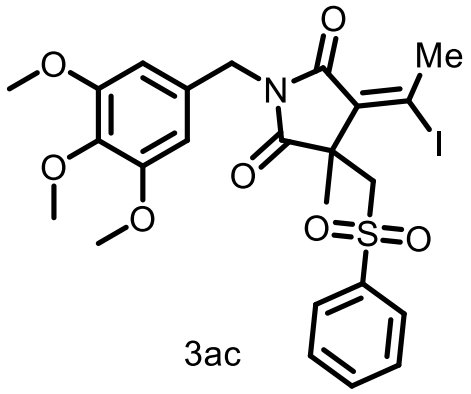
MS Zoomed Spectrum



MS Spectrum Peak List

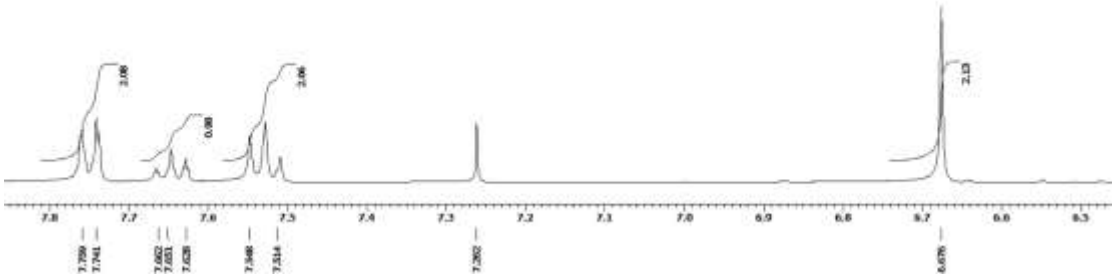
m/z	z	Abund	Formula	Ion
510.0238	1	667216.38	C21H21INO4S	(M+H)+
511.0266	1	150783.73	C21H21INO4S	(M+H)+
512.0238	1	45317.18	C21H21INO4S	(M+H)+
513.0249	1	8134.01	C21H21INO4S	(M+H)+
514.0269	1	1132.38	C21H21INO4S	(M+H)+
532.0052	1	52393.05	C21H20INNaO4S	(M+Na)+
533.0082	1	12149.68	C21H20INNaO4S	(M+Na)+
534.0056	1	4028.39	C21H20INNaO4S	(M+Na)+
535.0074	1	744.85	C21H20INNaO4S	(M+Na)+
535.9953	1	60.75	C21H20INNaO4S	(M+Na)+

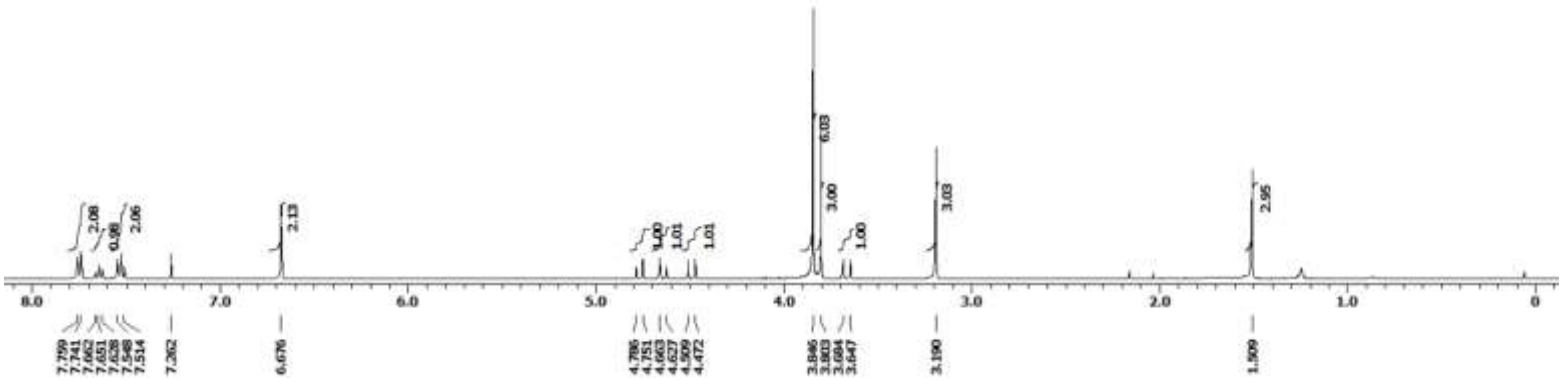
^{1}H NMR spectrum of 3ac (400 MHz, $CDCl_3$)



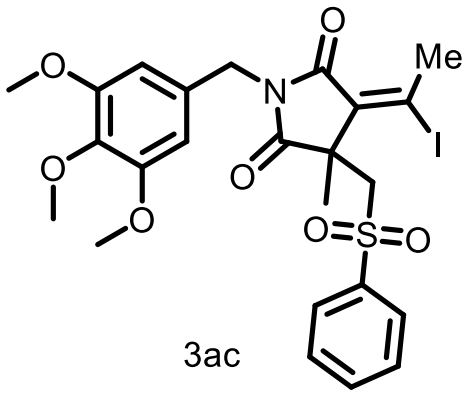
3ac

(*E*)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)-1-(3,4,5-trimethoxybenzyl)pyrrolidine-2,5-dione



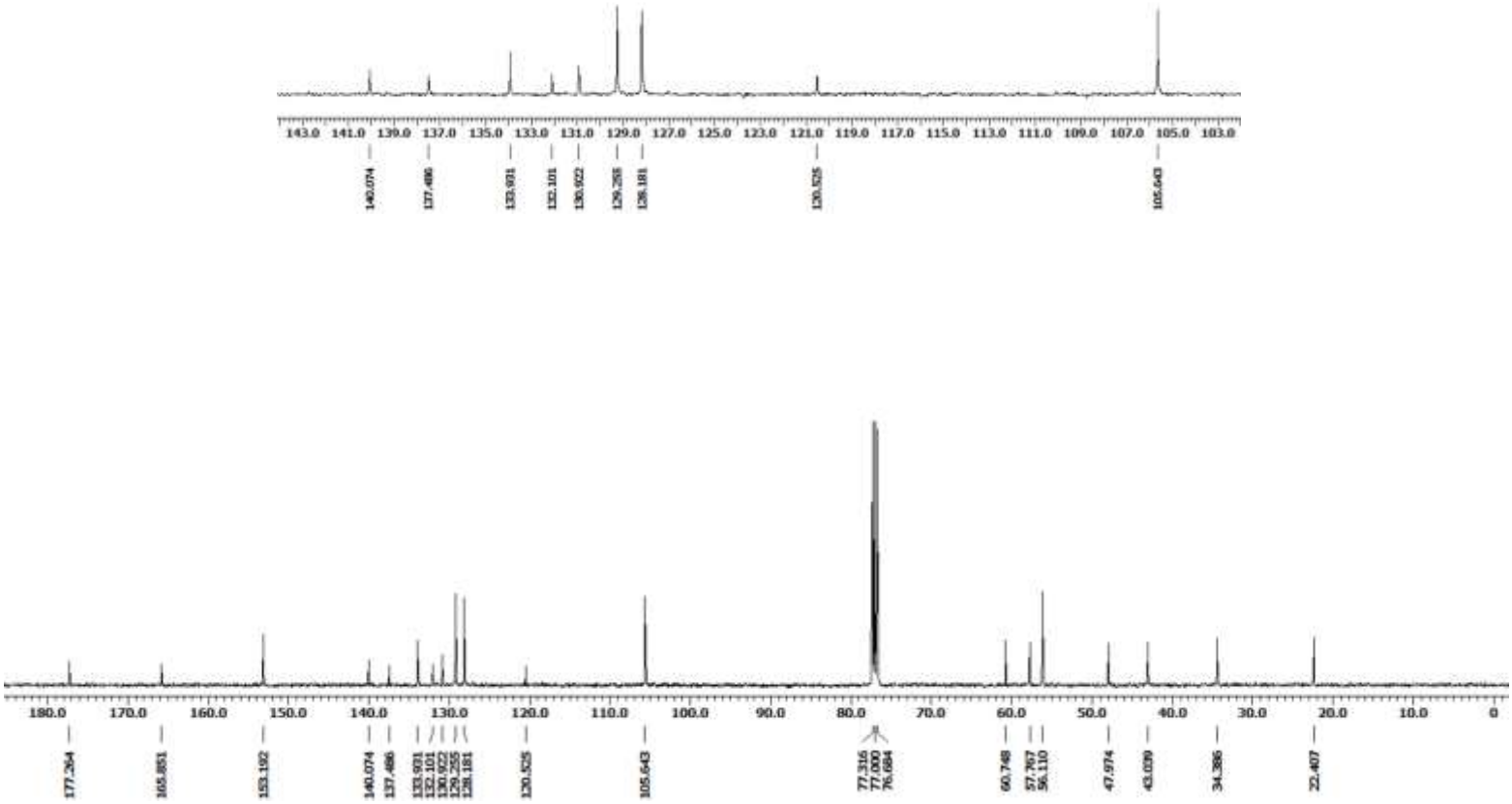


^{13}C NMR spectrum of 3ac (100 MHz, $CDCl_3$)



3ac

(*E*)-4-(1-iodoethylidene)-3-methyl-3-((phenylsulfonyl)methyl)-1-(3,4,5-trimethoxybenzyl)pyrrolidine-2,5-dione



HRMS spectrum of 3ac

Qualitative Compound Report

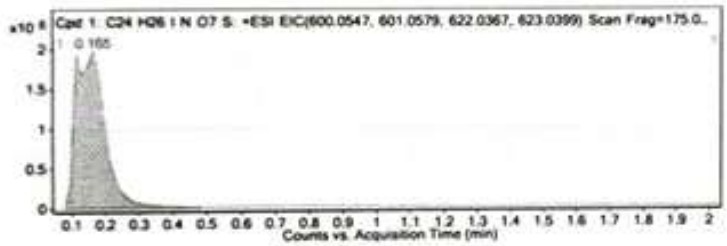
Data File	SMT-397.d	**Sample Name**	SMT-397
Sample Type	Sample	**Position**	P1-C9
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	13-06-2024 14:22:23
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

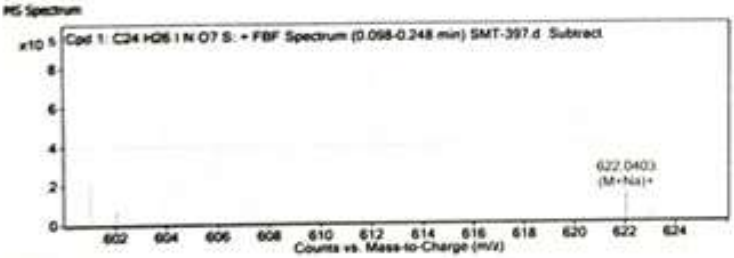
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C24 H26 I N O7 S	0.165	599.0513	148118	C24 H26 I N O7 S	599.0475	6.41	C24 H26 I N O7 S	C24 H26 I N O7 S

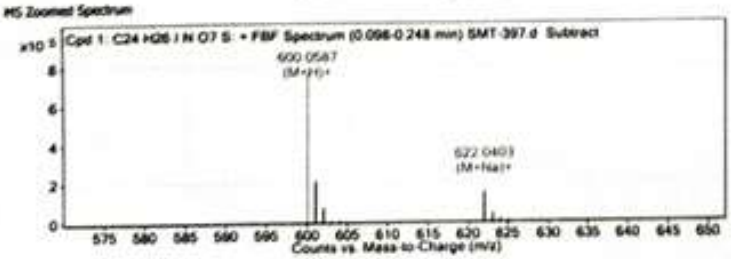
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C24 H26 I N O7 S	622.0403	0.165	Find By Formula	599.0513



MS Spectrum



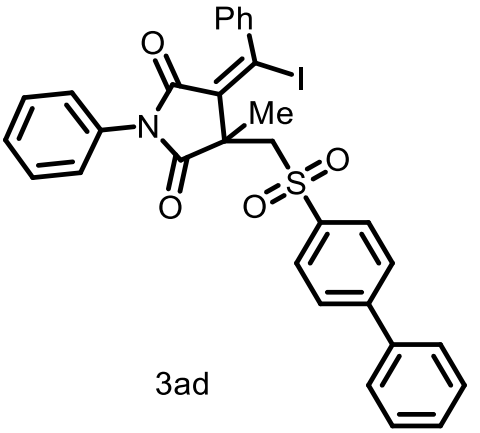
MS Zoomed Spectrum



MS Spectrum Peak List

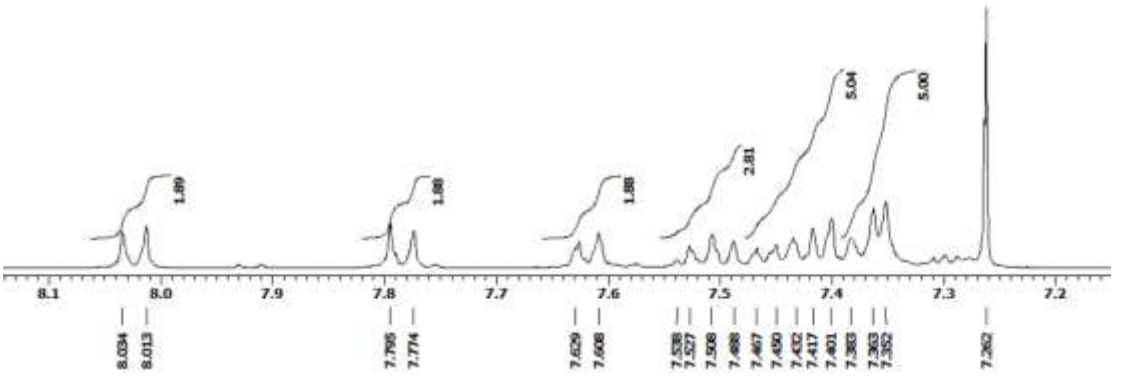
m/z	z	Abund	Formula	Ion
600.0587	1	765736.31	C24H27INO7S	(M+H)+
601.0614	1	212600.8	C24H27INO7S	(M+H)+
602.0595	1	66876.09	C24H27INO7S	(M+H)+
603.0614	1	13566.77	C24H27INO7S	(M+H)+
604.0637	1	2386.59	C24H27INO7S	(M+H)+
622.0403	1	148117.79	C24H26INNaO7S	(M+Na)+
623.0434	1	38829.15	C24H26INNaO7S	(M+Na)+
624.0418	1	12592.51	C24H26INNaO7S	(M+Na)+
625.0473	1	2454.41	C24H26INNaO7S	(M+Na)+
626.0543	1	402.81	C24H26INNaO7S	(M+Na)+

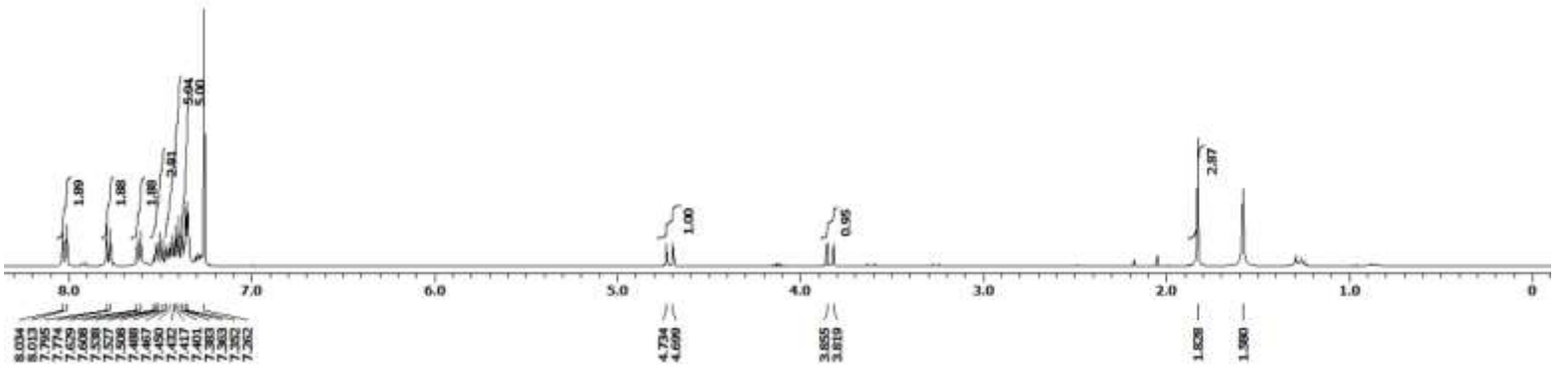
^{1}H NMR spectrum of 3ad (400 MHz, $CDCl_3$)



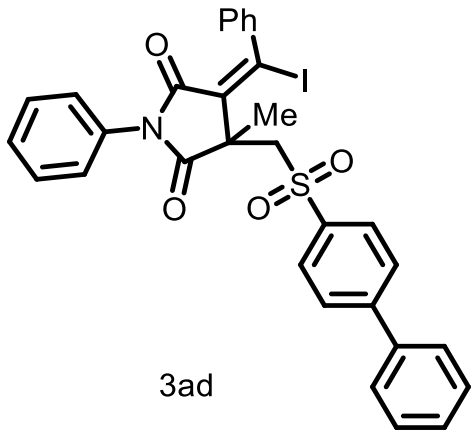
3ad

(*E*)-3-(([1,1'-biphenyl]-4-ylsulfonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenylpyrrolidine-2,5-dione



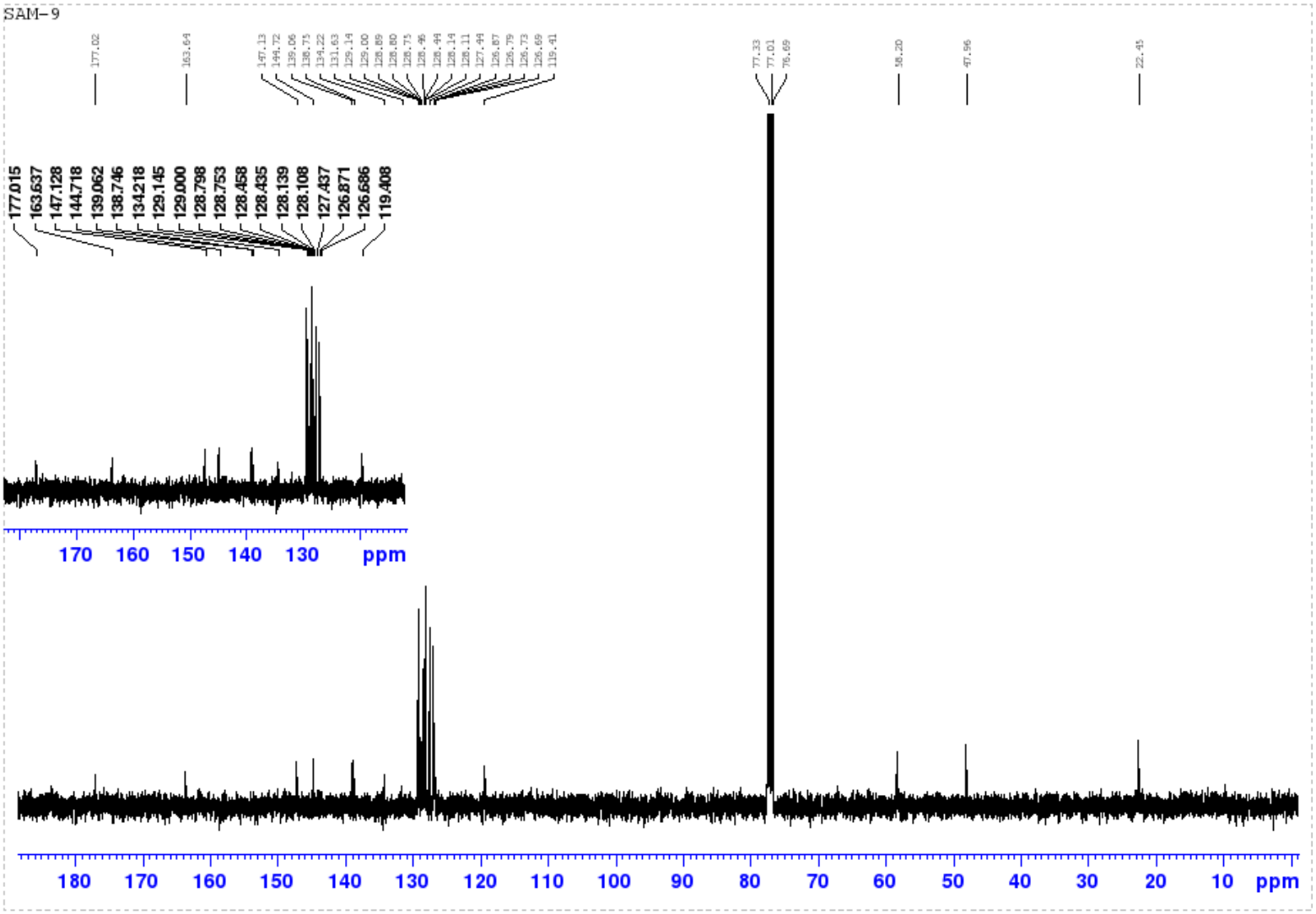


^{13}C NMR spectrum of 3ad (100 MHz, $CDCl_3$)



3ad

(*E*)-3-(([1,1'-biphenyl]-4-ylsulfonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenylpyrrolidine-2,5-dione



HRMS Spectrum of 3ad

3a & 6

Qualitative Compound Report

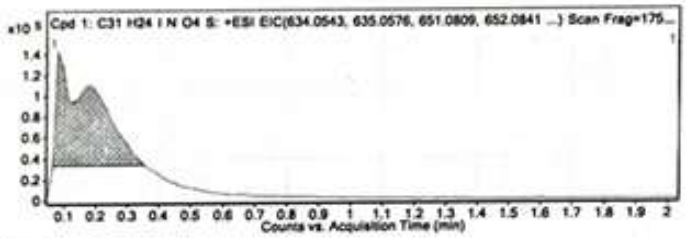
Data File	SAM-9.d	Sample Name	SAM-9
Sample Type	Sample	Position	P1-D1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	05-12-2022 16:02:28
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

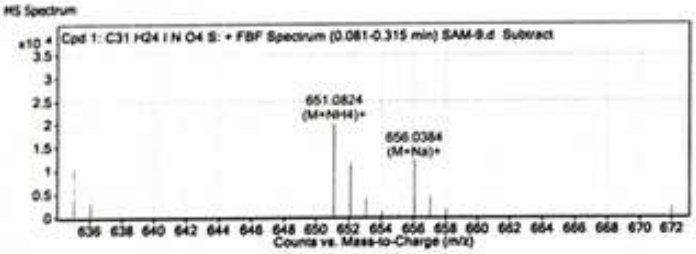
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C31 H24 I N O4 S	0.081	633.0477	12028	C31 H24 I N O4 S	633.0471	1.06	C31 H24 I N O4 S	C31 H24 I N O4 S

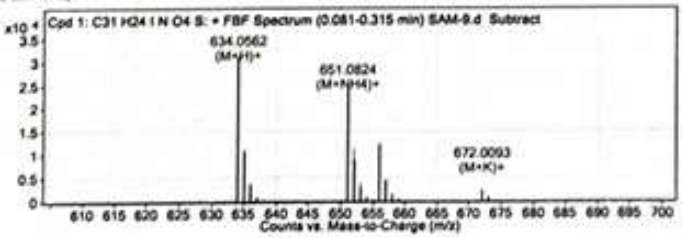
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C31 H24 I N O4 S	656.0384	0.081	Find By Formula	633.0477



MS Spectrum



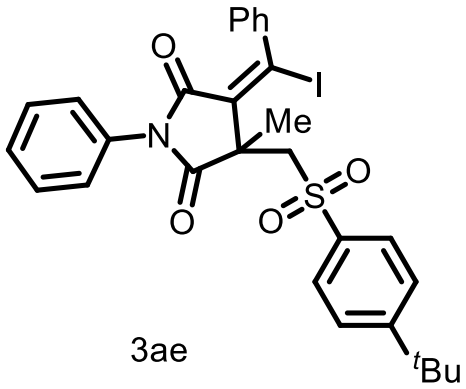
MS Zoomed Spectrum



MS Spectrum Peak List

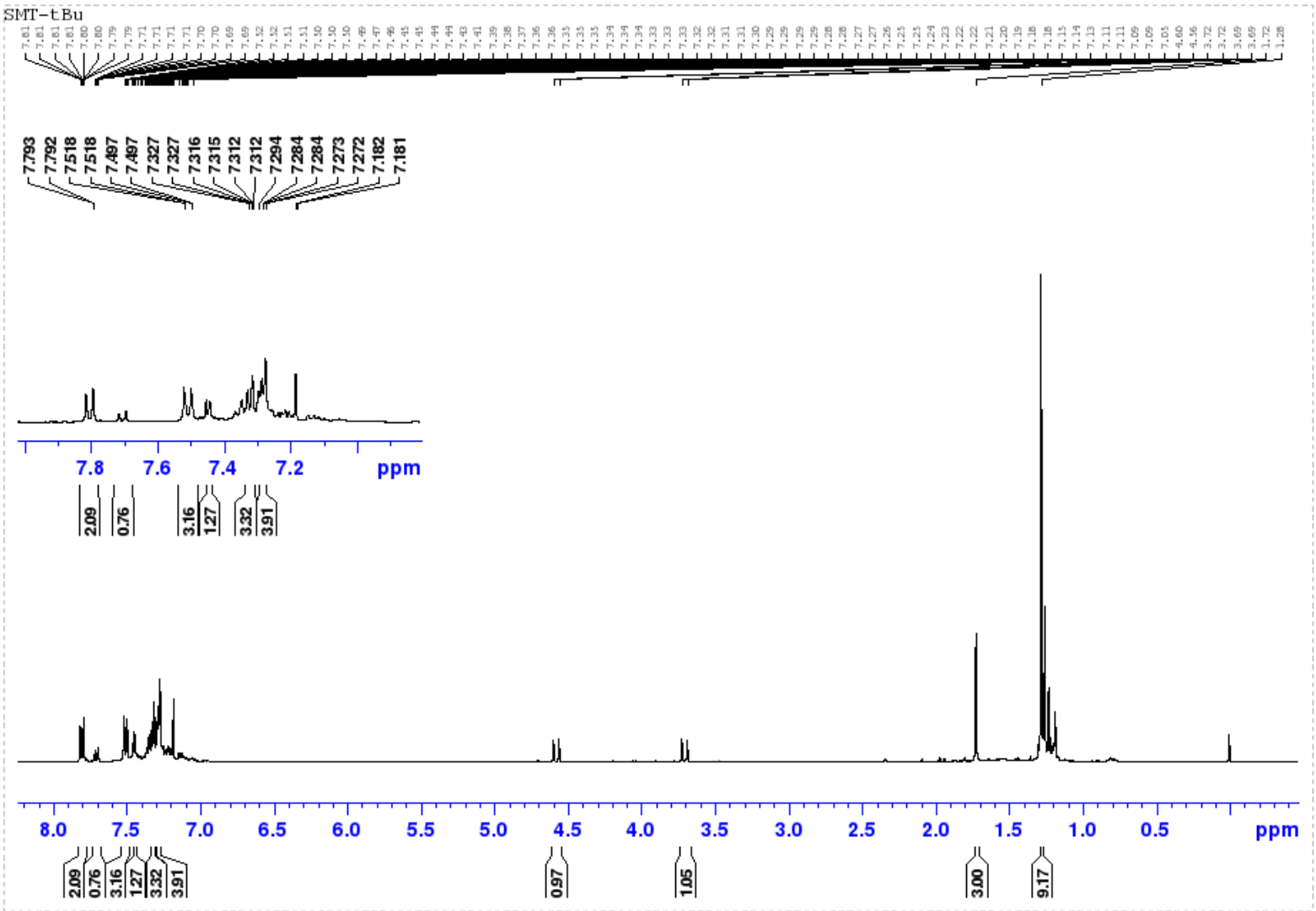
m/z	z	Abund	Formula	Ion
634.0562	1	31087.96	C31H25INO4S	(M+H)+
635.0598	1	10551.18	C31H25INO4S	(M+H)+
636.0589	1	3517.41	C31H25INO4S	(M+H)+
637.0591	1	792.26	C31H25INO4S	(M+H)+
638.0479	1	136.55	C31H25INO4S	(M+H)+
651.0824	1	20122.37	C31H28IN2O4S	(M+NH4)+
652.0788	1	11422.01	C31H28IN2O4S	(M+NH4)+
653.0786	1	4031.44	C31H28IN2O4S	(M+NH4)+
654.0782	1	1049.23	C31H28IN2O4S	(M+NH4)+
655.086	1	328.57	C31H28IN2O4S	(M+NH4)+
656.0384	1	12028.08	C31H24INNaO4S	(M+Na)+

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

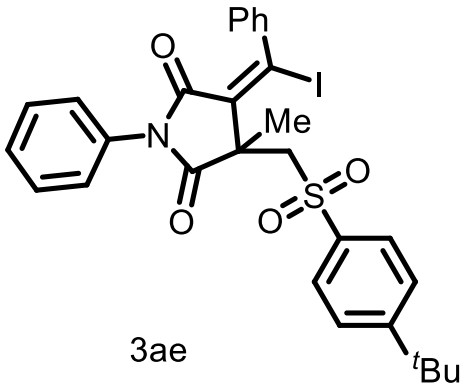


3ae

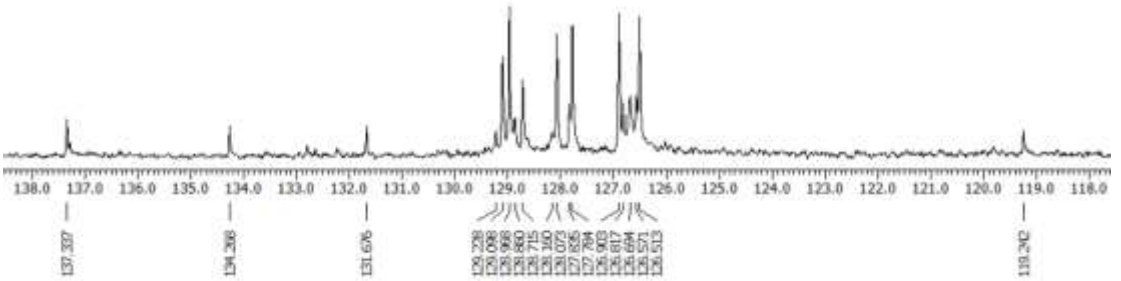
(*E*)-3-(((4-(*tert*-butyl)phenyl)sulfonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenylpyrrolidine-2,5-dione

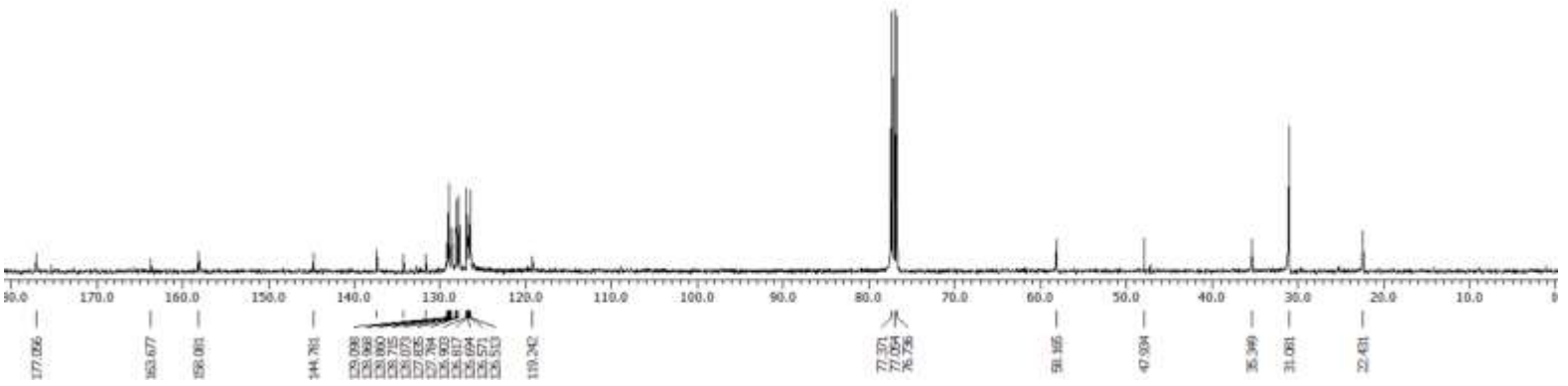


^{13}C NMR spectrum of 3ae (100 MHz, $CDCl_3$)



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





HRMS spectrum of 3ae

Qualitative Compound Report

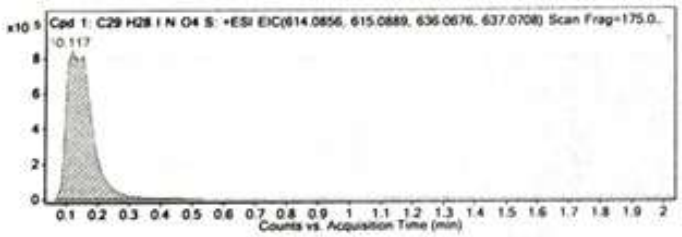
Data File	SMT-tBu.d	**Sample Name**	SMT-tBu
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	16-05-2024 13:27:40
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

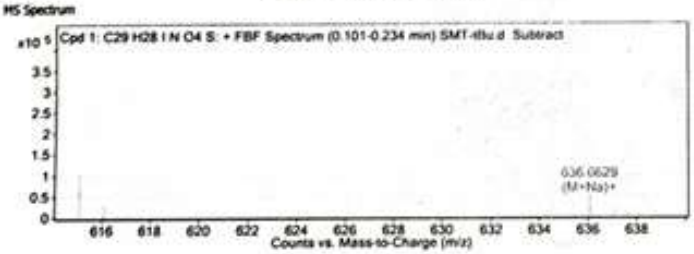
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C29 H28 I N O4 S	0.117	613.0744	345479	C29 H28 I N O4 S	613.0784	-6.54	C29 H28 I N O4 S	C29 H28 I N O4 S

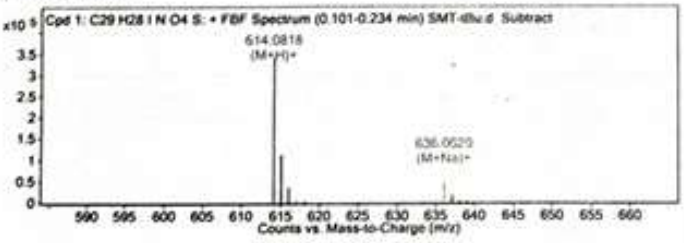
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C29 H28 I N O4 S	614.0818	0.117	Find By Formula	613.0744



MS Spectrum



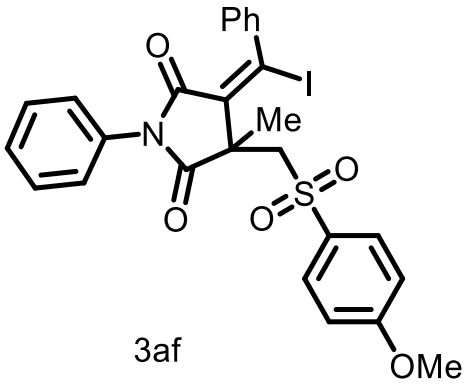
MS Zoomed Spectrum



MS Spectrum Peak List

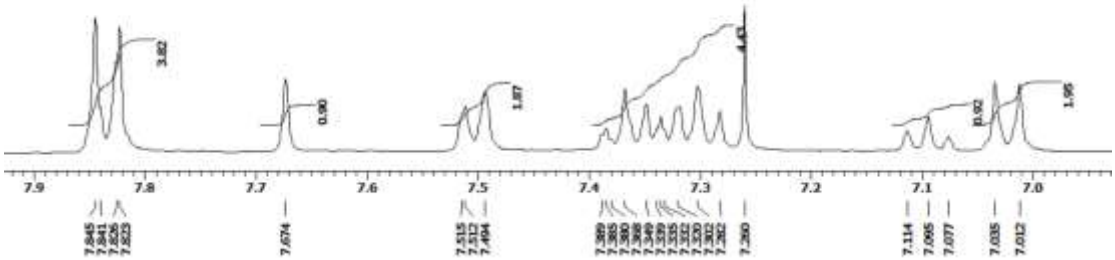
m/z	z	Abund	Formula	Ion
614.0818	1	345478.69	C29H29INO4S	(M+H)+
615.0848	1	109681.84	C29H29INO4S	(M+H)+
616.0836	1	31862.58	C29H29INO4S	(M+H)+
617.0843	1	6771.87	C29H29INO4S	(M+H)+
618.0843	1	1134.9	C29H29INO4S	(M+H)+
636.0629	1	49039.56	C29H28INNaO4S	(M+Na)+
637.0664	1	15692.91	C29H28INNaO4S	(M+Na)+
638.0647	1	5144.1	C29H28INNaO4S	(M+Na)+
639.0636	1	1104.15	C29H28INNaO4S	(M+Na)+
640.0656	1	212.47	C29H28INNaO4S	(M+Na)+

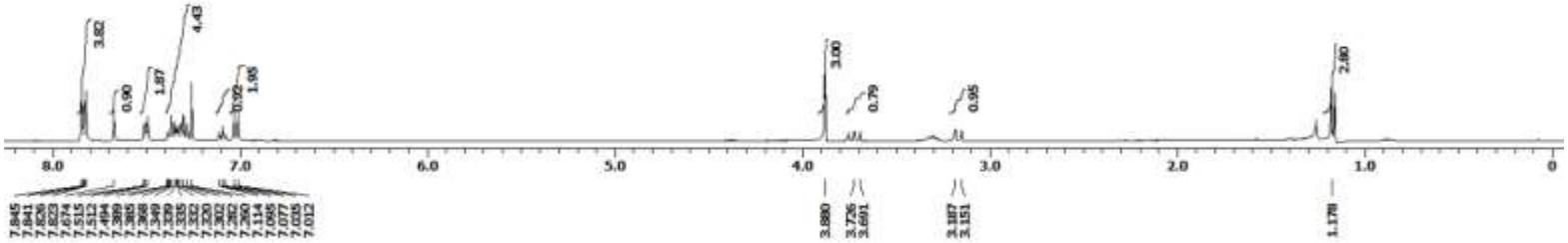
^{1}H NMR spectrum of 3af (400 MHz, $CDCl_3$)



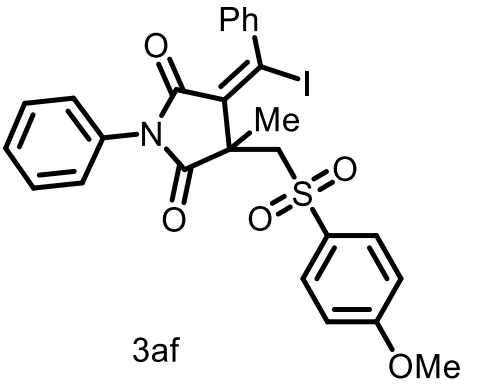
3af

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



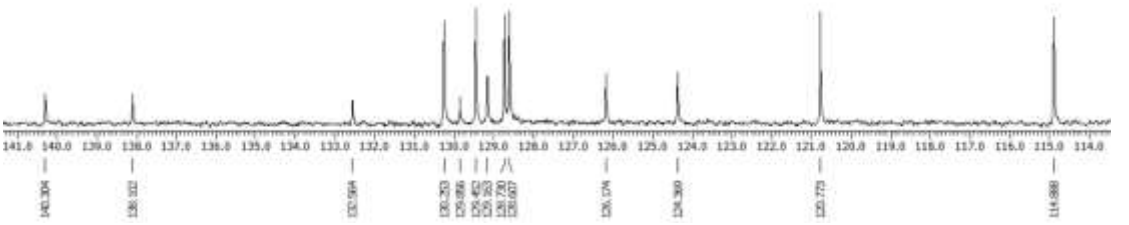


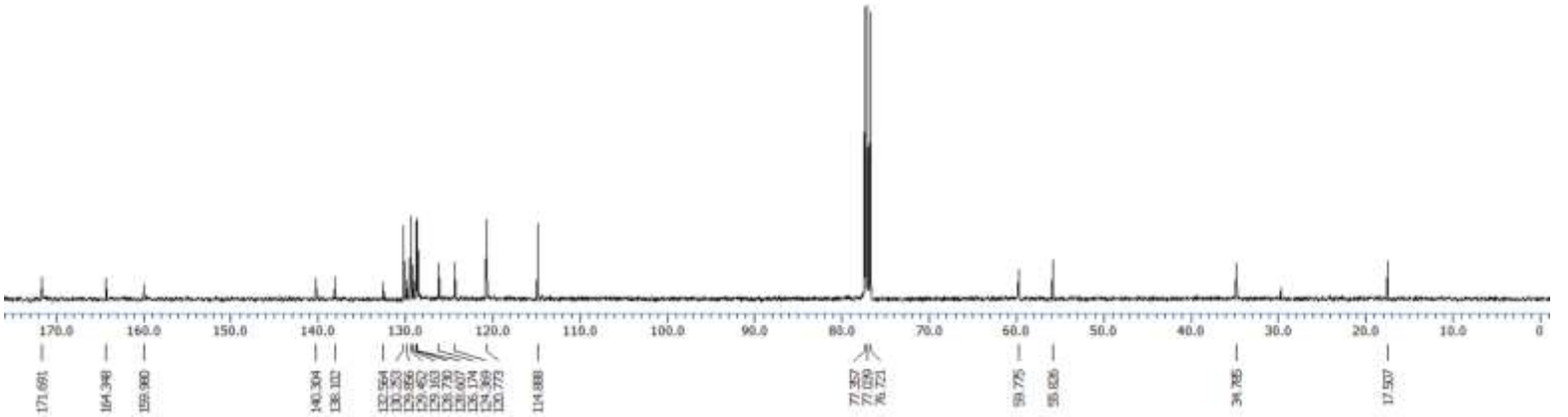
^{13}C NMR spectrum of 3af (100 MHz, $CDCl_3$)



3af

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





HRMS spectrum of 3af

3a

Qualitative Compound Report

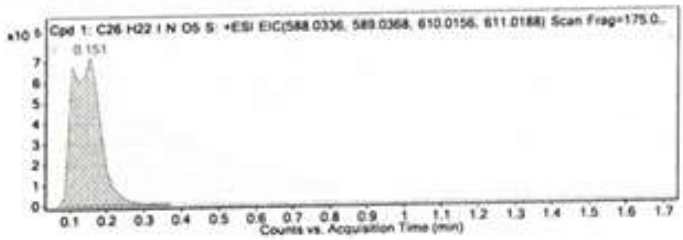
Data File	SMT-422.d	**Sample Name**	SMT-422
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	10-02-2024 12:17:33
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (05125)

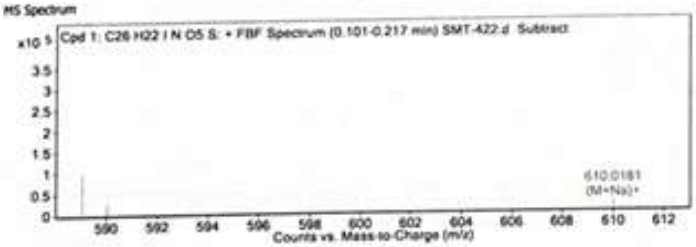
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H22 I N O5 S	0.151	587.0286	343979	C26 H22 I N O5 S	587.0263	3.78	C26 H22 I N O5 S	C26 H22 I N O5 S

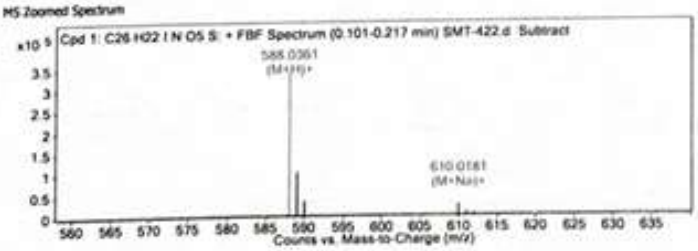
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H22 I N O5 S	588.0361	0.151	Find By Formula	587.0286



MS Spectrum



MS Zoomed Spectrum

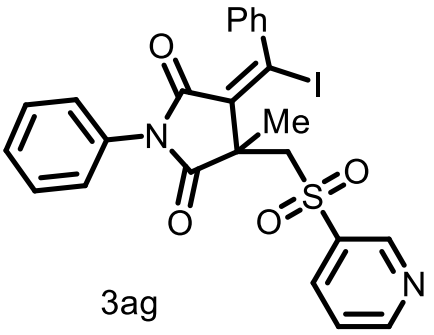


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
588.0361	1	343978.75	C26H23INO5S	(M+H)+
589.0389	1	98272.41	C26H23INO5S	(M+H)+
590.0367	1	30175.5	C26H23INO5S	(M+H)+
610.0181	1	20568.38	C26H22INNaO5S	(M+Na)+
611.0215	1	6647.8	C26H22INNaO5S	(M+Na)+
611.9994	1	3214.13	C26H22INNaO5S	(M+Na)+
613.0008	1	1014.48	C26H22INNaO5S	(M+Na)+

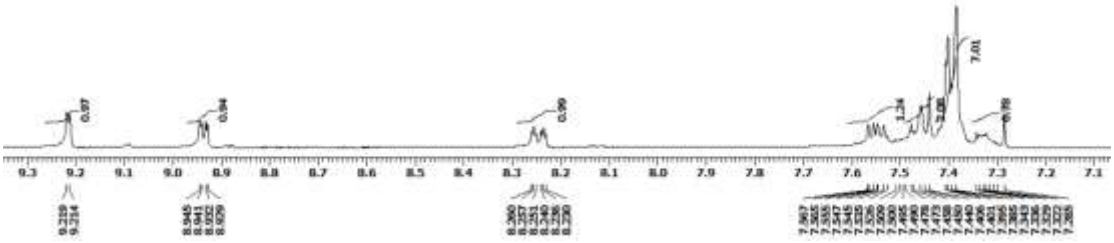
--- End Of Report ---

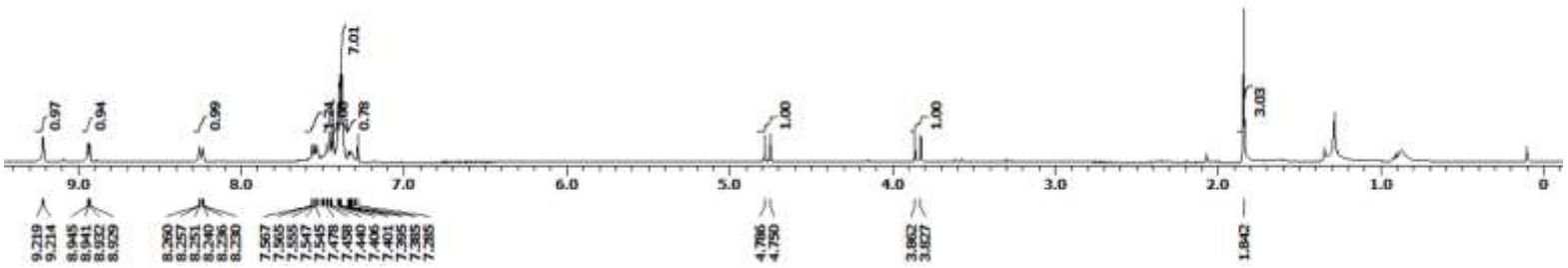
^{1}H NMR spectrum of 3ag (400 MHz, $CDCl_3$)



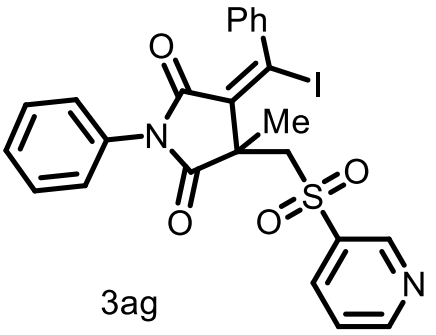
3ag

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



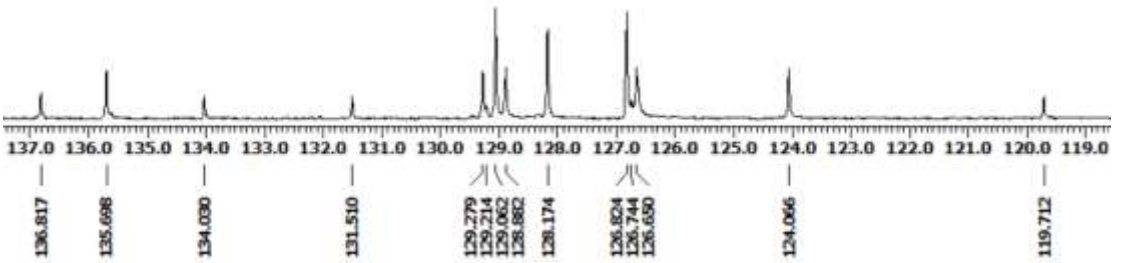


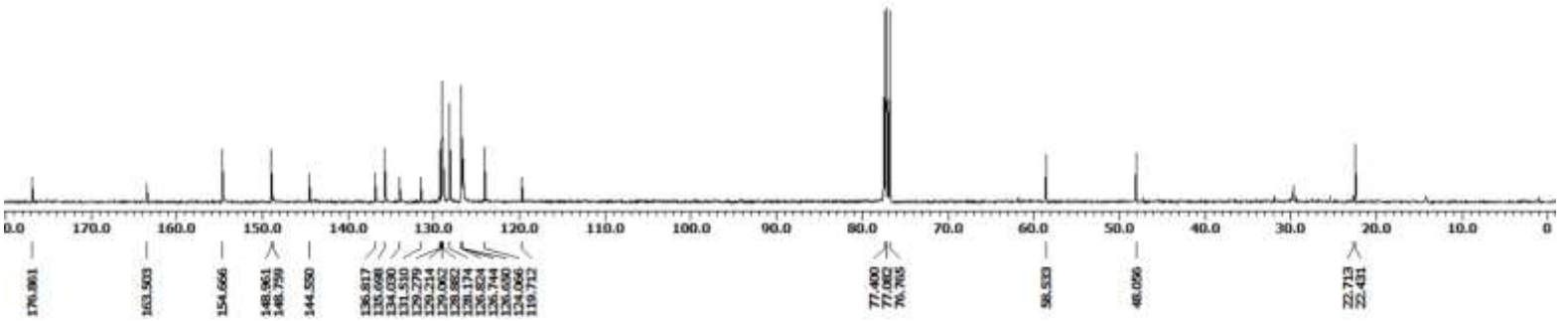
^{13}C NMR spectrum of 3ag (100 MHz, $CDCl_3$)



3ag

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





HRMS spectrum of 3ag

Qualitative Compound Report

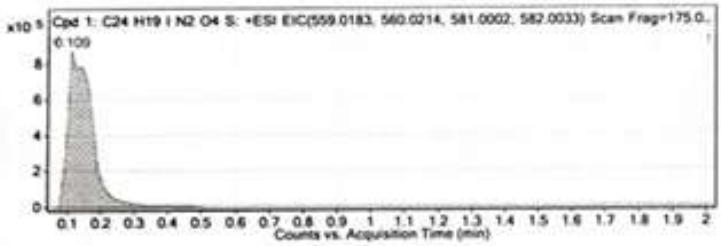
Data File	SMT-493S.d	**Sample Name**	SMT-493S
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	16-05-2024 13:33:29
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

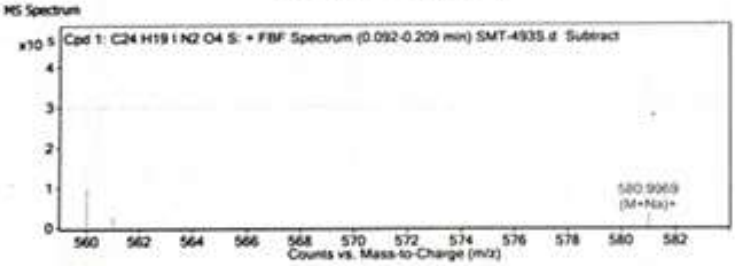
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C24 H19 I N2 O4 S	0.109	558.0081	378041	C24 H19 I N2 O4 S	558.011	-5.16	C24 H19 I N2 O4 S	C24 H19 I N2 O4 S

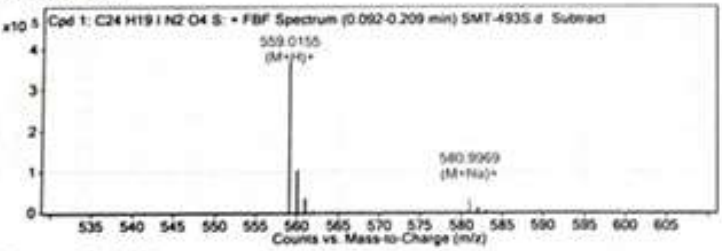
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C24 H19 I N2 O4 S	559.0155	0.109	Find By Formula	558.0081



MS Spectrum



MS Zoomed Spectrum

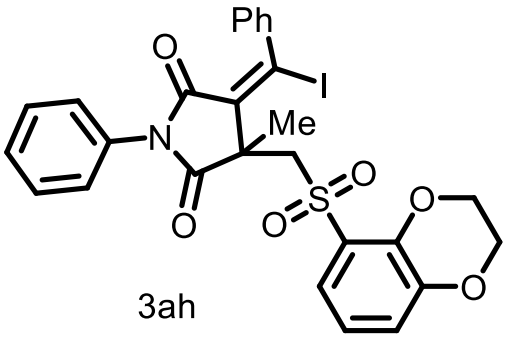


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
559.0155	1	378041.13	C24H20IN2O4S	(M+H)+
560.0184	1	97689.76	C24H20IN2O4S	(M+H)+
561.0161	1	29551.07	C24H20IN2O4S	(M+H)+
562.0174	1	6024.49	C24H20IN2O4S	(M+H)+
563.0189	1	868.04	C24H20IN2O4S	(M+H)+
580.9969	1	32633.9	C24H19IN2NaO4S	(M+Na)+
581.9997	1	8958.83	C24H19IN2NaO4S	(M+Na)+
582.9981	1	2882.22	C24H19IN2NaO4S	(M+Na)+
584.0001	1	580.07	C24H19IN2NaO4S	(M+Na)+

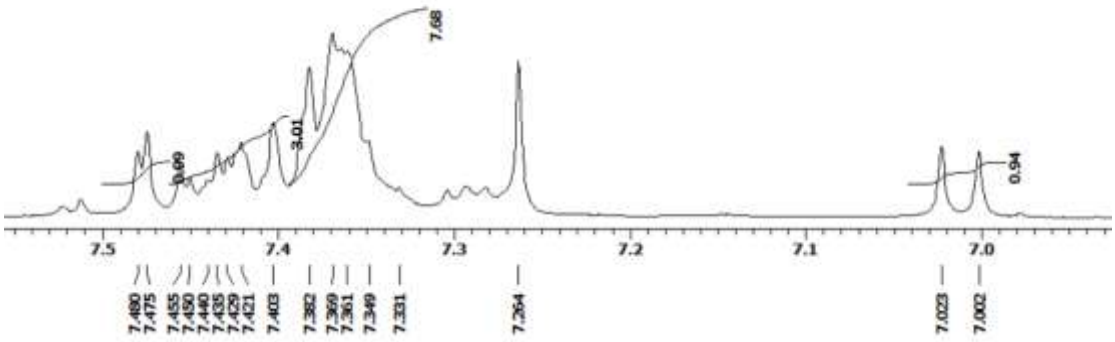
— End Of Report —

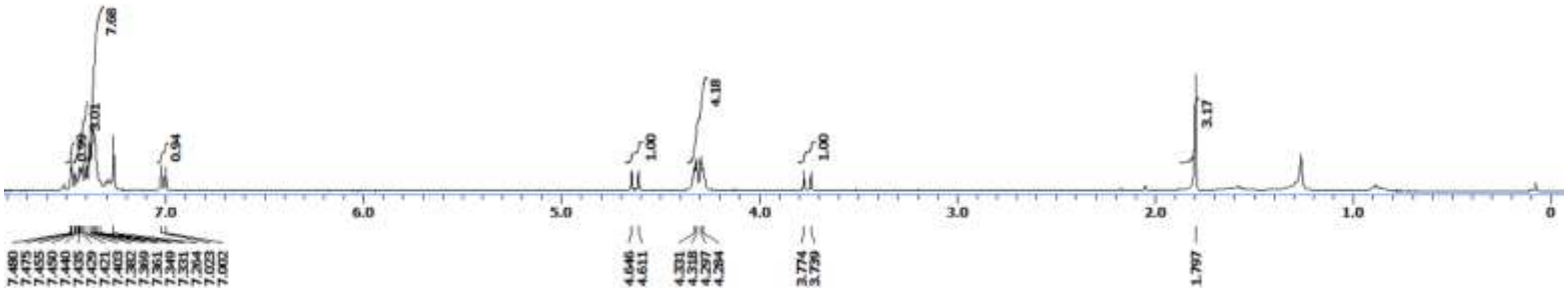
^{1}H NMR spectrum of 3ah (400 MHz, $CDCl_3$)



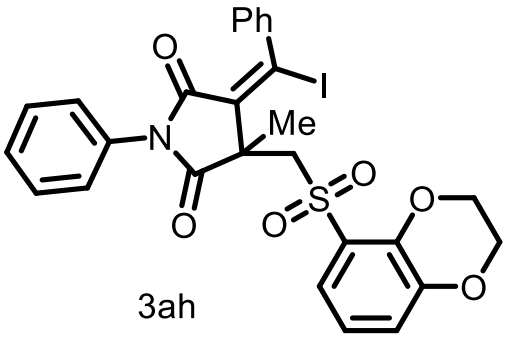
3ah

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



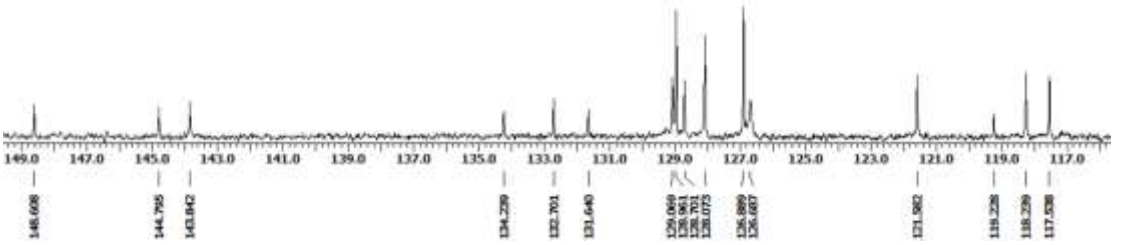


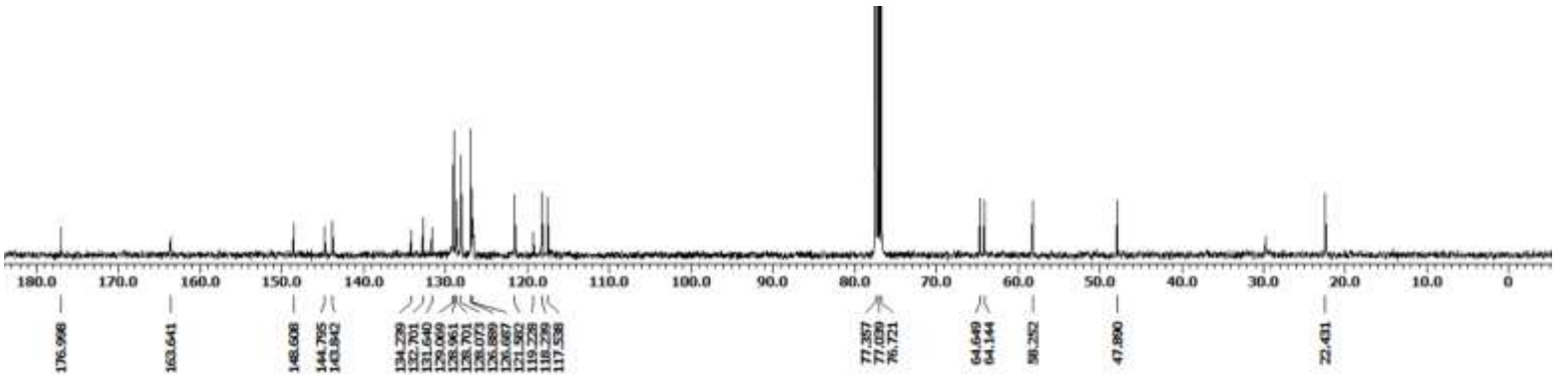
^{13}C NMR spectrum of 3ah (100 MHz, $CDCl_3$)



3ah

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





HRMS spectrum of 3ah

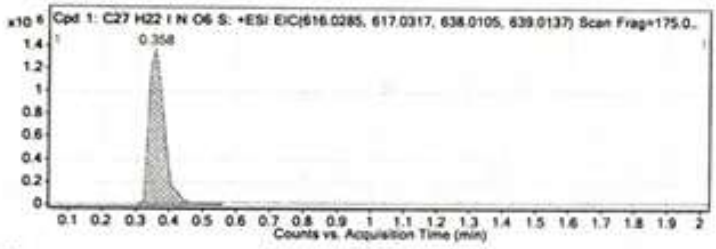
Qualitative Compound Report

Data File	SMT-492.d	**Sample Name**	SMT-492
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	30-05-2024 12:58:54
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)		

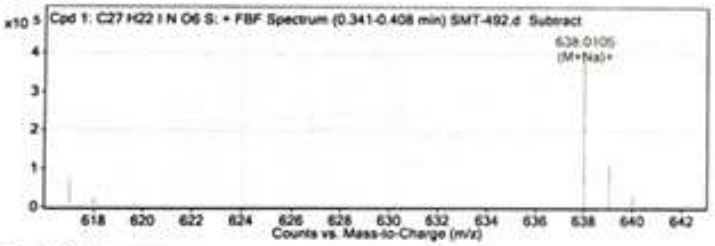
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C27 H22 I N O6 S	0.358	615.0211	390377	C27 H22 I N O6 S	615.0213	-0.3	C27 H22 I N O6 S	C27 H22 I N O6 S

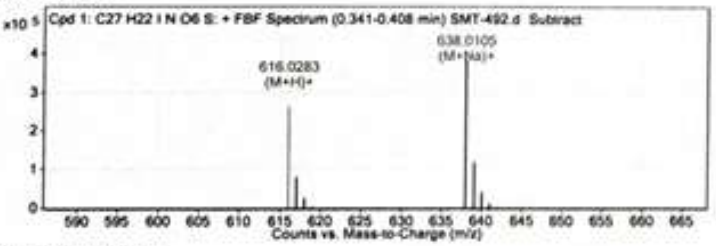
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C27 H22 I N O6 S	638.0105	0.358	Find By Formula	615.0211



MS Spectrum



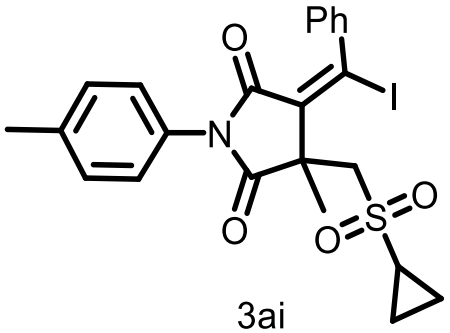
MS Zoomed Spectrum



MS Spectrum Peak List

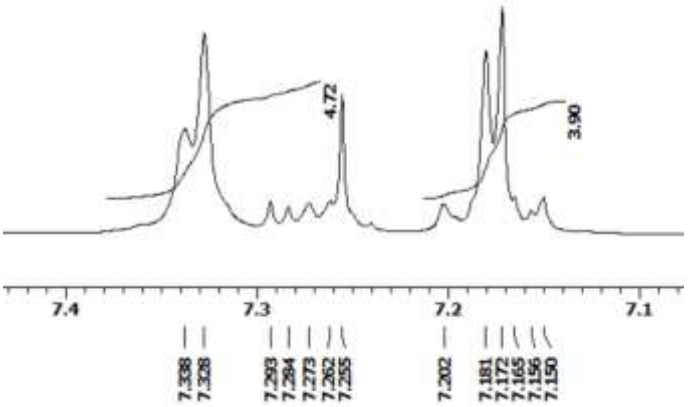
m/z	z	Abund	Formula	Ion
616.0283	1	263146.19	C27H23INO6S	(M+H)+
617.0313	1	75583.73	C27H23INO6S	(M+H)+
618.0299	1	22958.39	C27H23INO6S	(M+H)+
619.0302	1	5017.49	C27H23INO6S	(M+H)+
620.0322	1	836.01	C27H23INO6S	(M+H)+
638.0105	1	390376.69	C27H22INNaO6S	(M+Na)+
639.0133	1	112895.52	C27H22INNaO6S	(M+Na)+
640.0115	1	34480.4	C27H22INNaO6S	(M+Na)+
641.0121	1	7346	C27H22INNaO6S	(M+Na)+
642.012	1	1242.66	C27H22INNaO6S	(M+Na)+

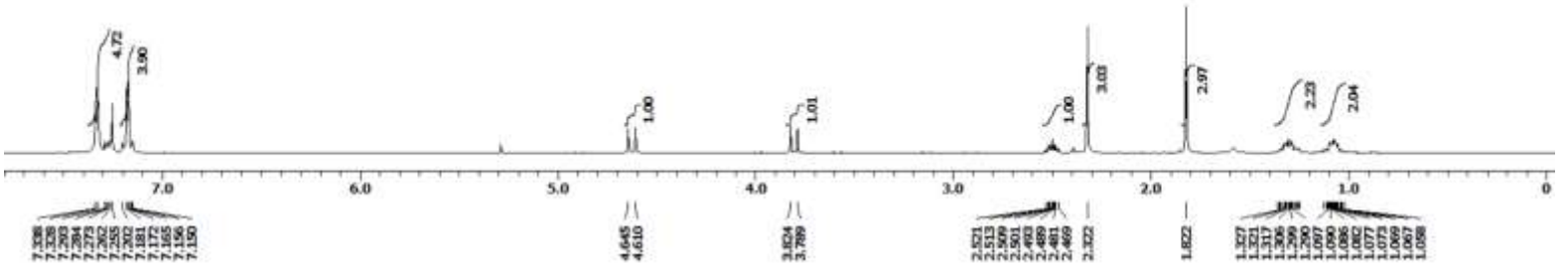
^{1}H NMR spectrum of 3ai (400 MHz, $CDCl_3$)



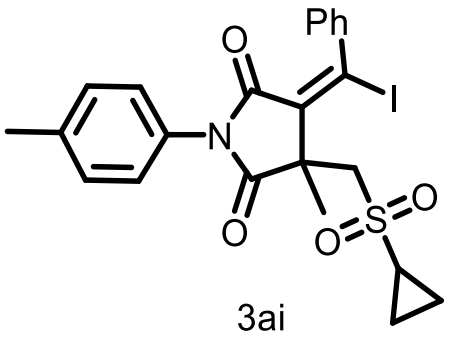
3ai

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



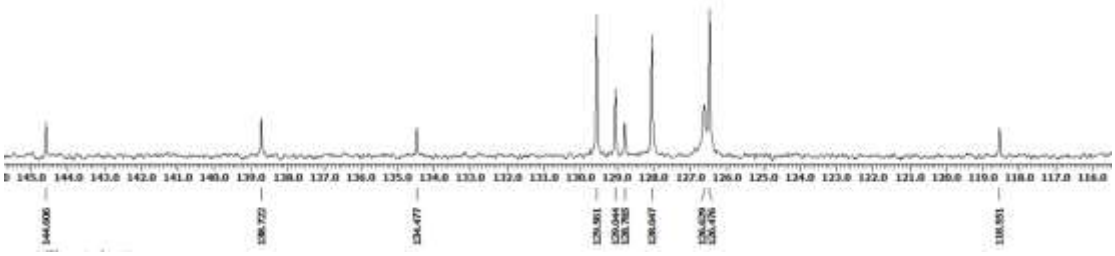


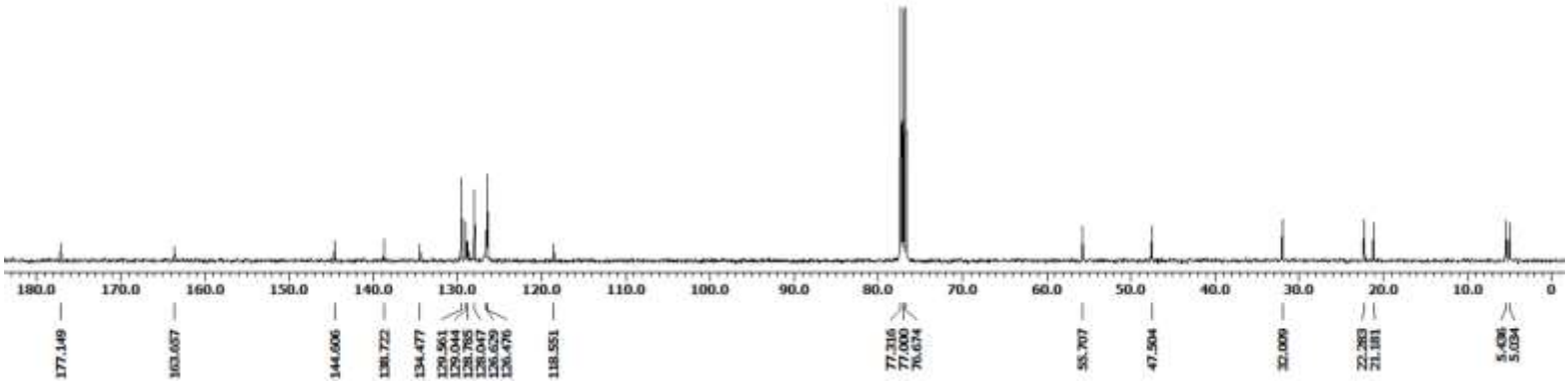
^{13}C NMR spectrum of 3ai (100 MHz, $CDCl_3$)



3ai

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





HRMS Spectrum of 3ai

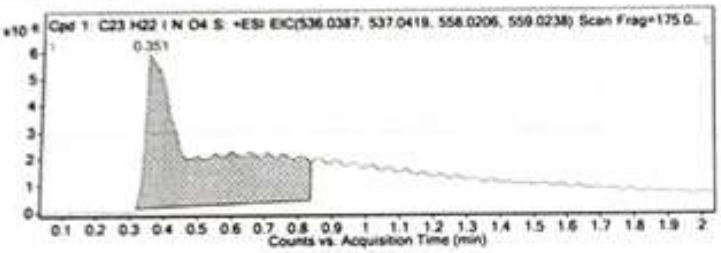
Qualitative Compound Report

Data File	SAM-13.d	**Sample Name**	SAM-13
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	30-05-2024 13:10:25
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)		

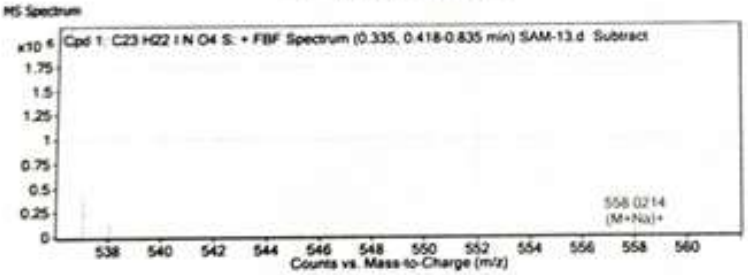
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C23 H22 I N O4 S	0.351	535.0326	54352	C23 H22 I N O4 S	535.0314	2.19	C23 H22 I N O4 S	C23 H22 I N O4 S

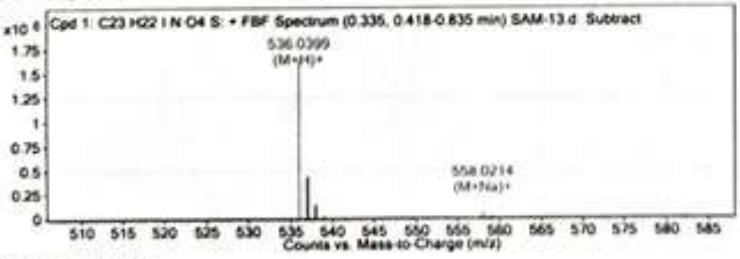
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C23 H22 I N O4 S	558.0214	0.351	Find By Formula	535.0326



MS Spectrum



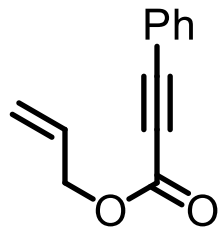
MS Zoomed Spectrum



MS Spectrum Peak List

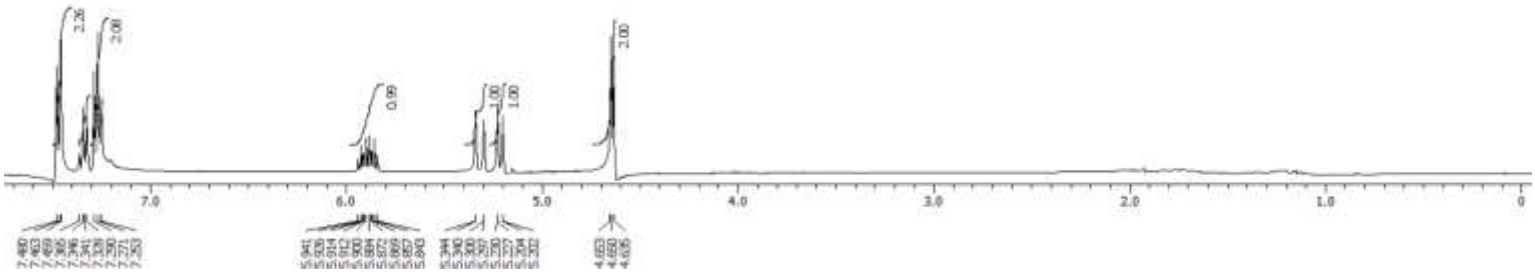
m/z	z	Abund	Formula	Ion
536.0399	1	1625752.88	C23H23INO4S	(M+H)+
537.043	1	440142.38	C23H23INO4S	(M+H)+
538.0405	1	128580.23	C23H23INO4S	(M+H)+
539.0413	1	23402.91	C23H23INO4S	(M+H)+
540.0426	1	3240.24	C23H23INO4S	(M+H)+
541.0561	1	831.71	C23H23INO4S	(M+H)+
558.0214	1	54352.11	C23H22INNaO4S	(M+Na)+
559.0241	1	14193.42	C23H22INNaO4S	(M+Na)+
560.022	1	4332.25	C23H22INNaO4S	(M+Na)+
561.0234	1	901.94	C23H22INNaO4S	(M+Na)+
562.0167	1	121.57	C23H22INNaO4S	(M+Na)+

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

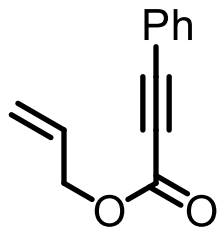


4

allyl 3-phenylpropiolate

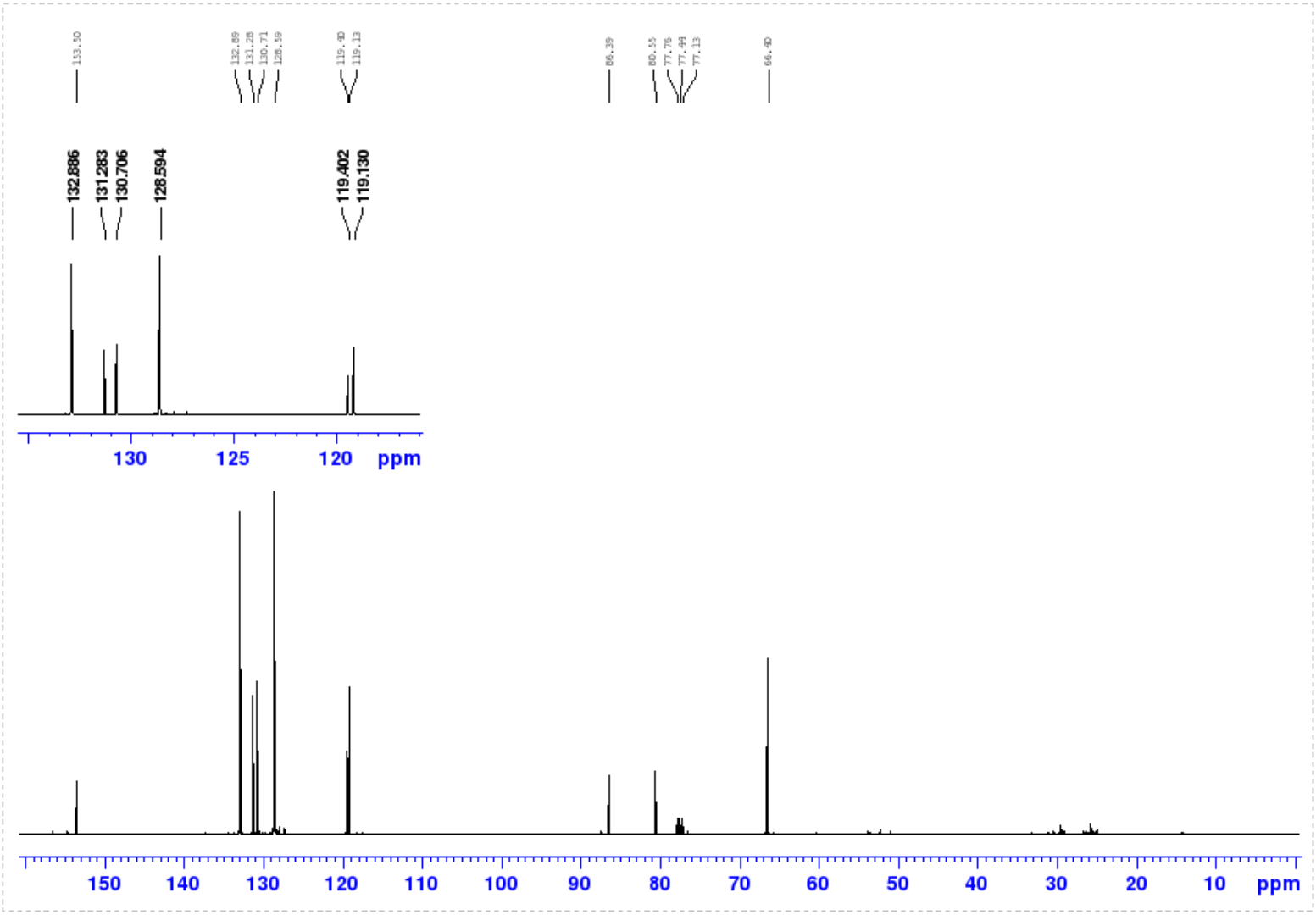


^{13}C NMR spectrum of 4 (100 MHz, $CDCl_3$)

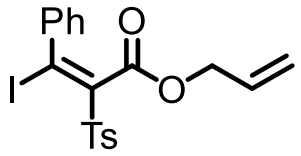


4

allyl 3-phenylpropiolate

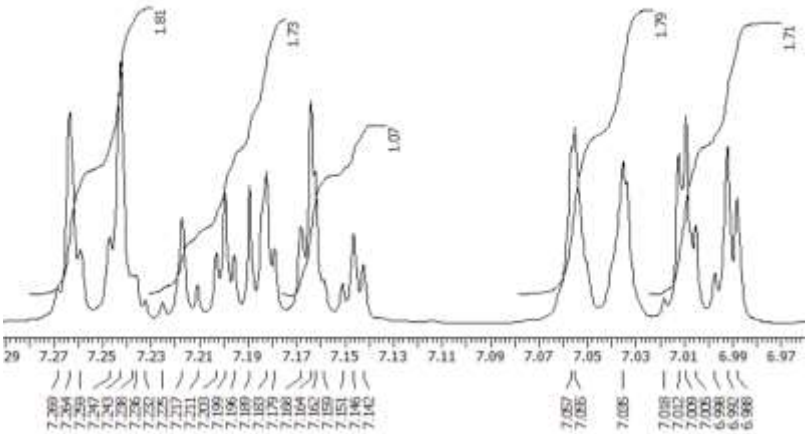


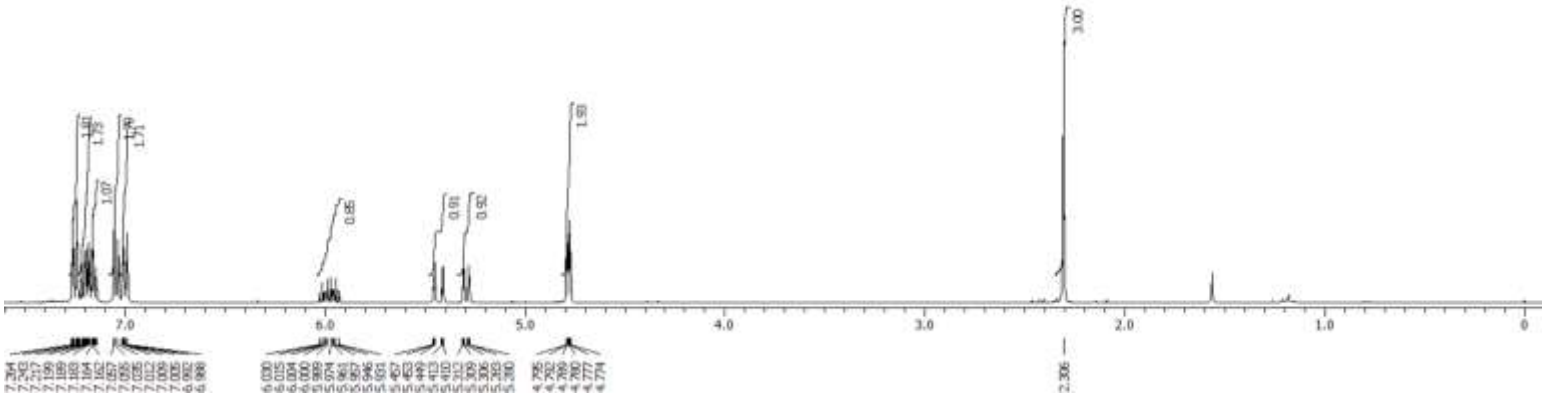
^{1}H NMR spectrum of 5 (400 MHz, $CDCl_3$)



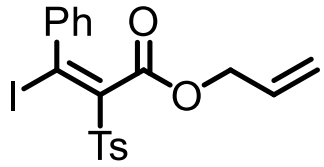
5

allyl (*Z*)-3-iodo-3-phenyl-2-tosylacrylate



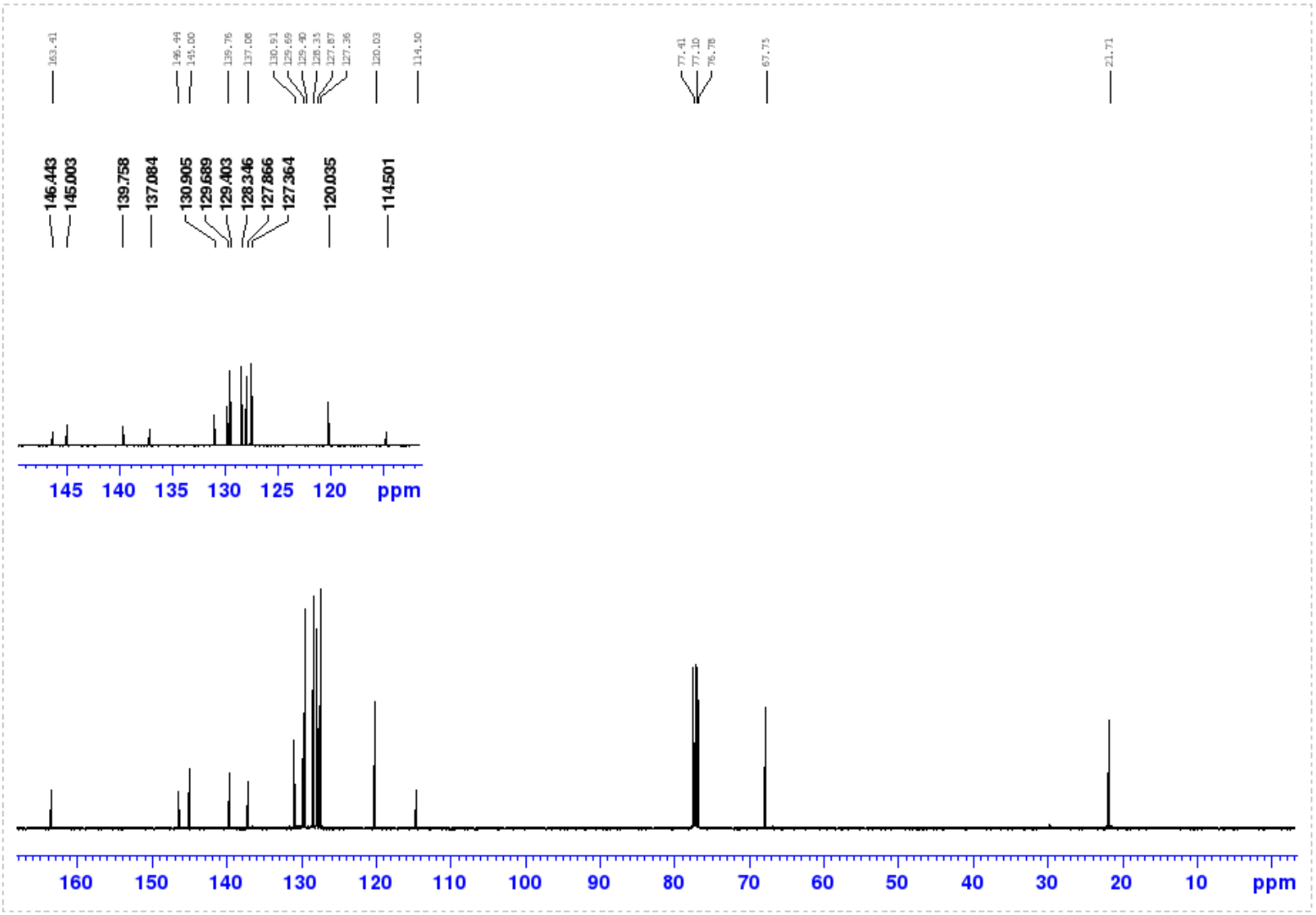


^{13}C NMR spectrum of 5 (100 MHz, $CDCl_3$)

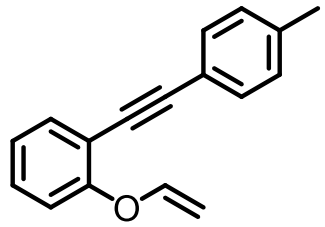


5

allyl (*Z*)-3-iodo-3-phenyl-2-tosylacrylate

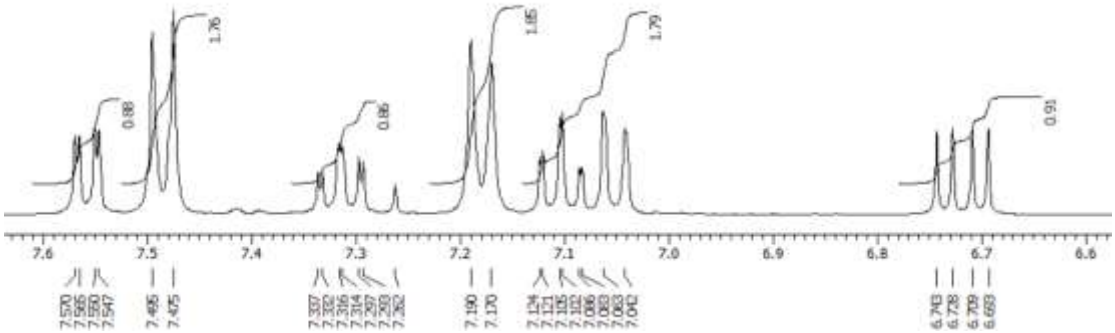


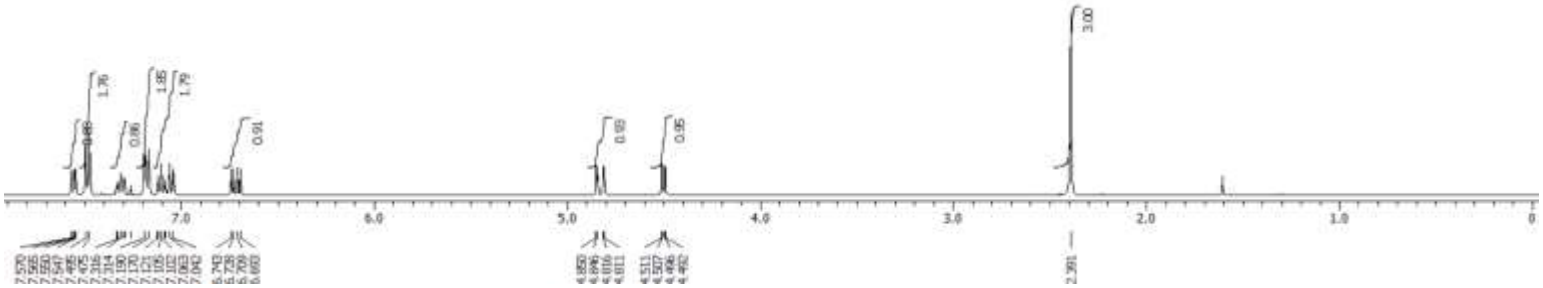
^{1}H NMR spectrum of 6 (400 MHz, $CDCl_3$)



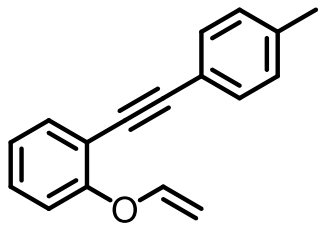
6

1-(*p*-tolylethynyl)-2-(vinyloxy)benzene



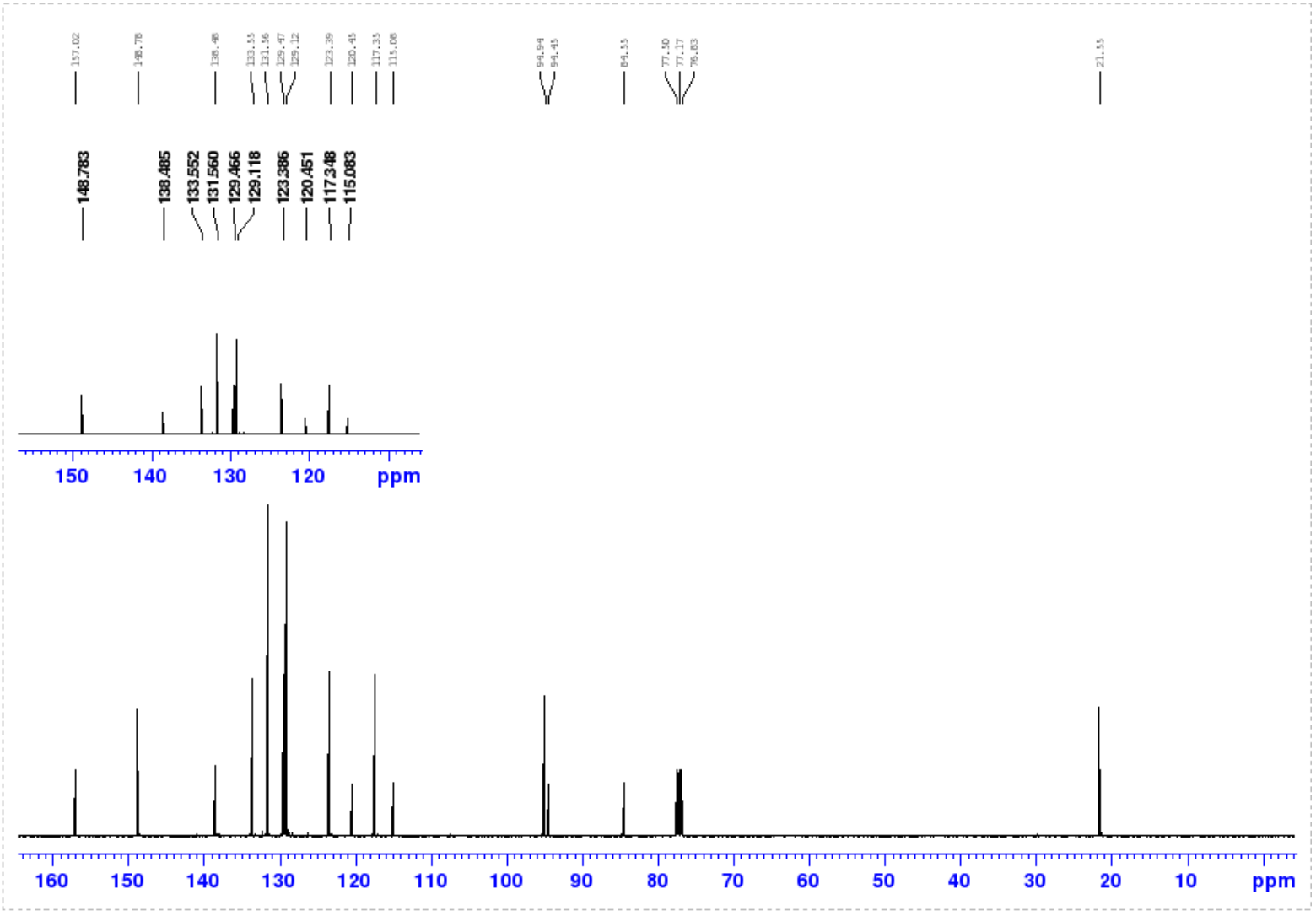


^{13}C NMR spectrum of 6 (100 MHz, $CDCl_3$)

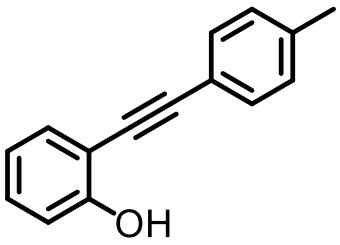


6

1-(*p*-tolylethynyl)-2-(vinyloxy)benzene

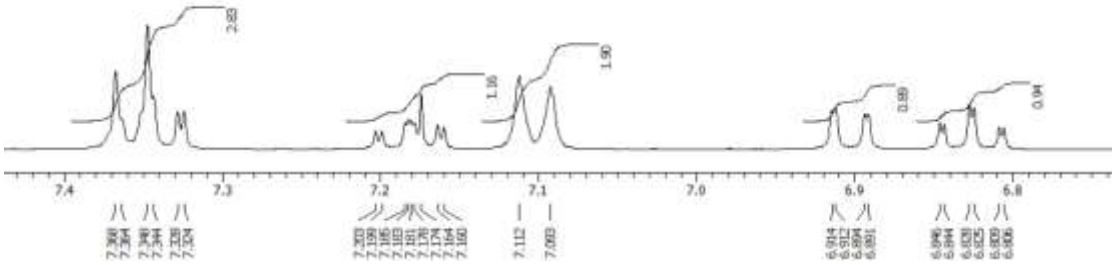


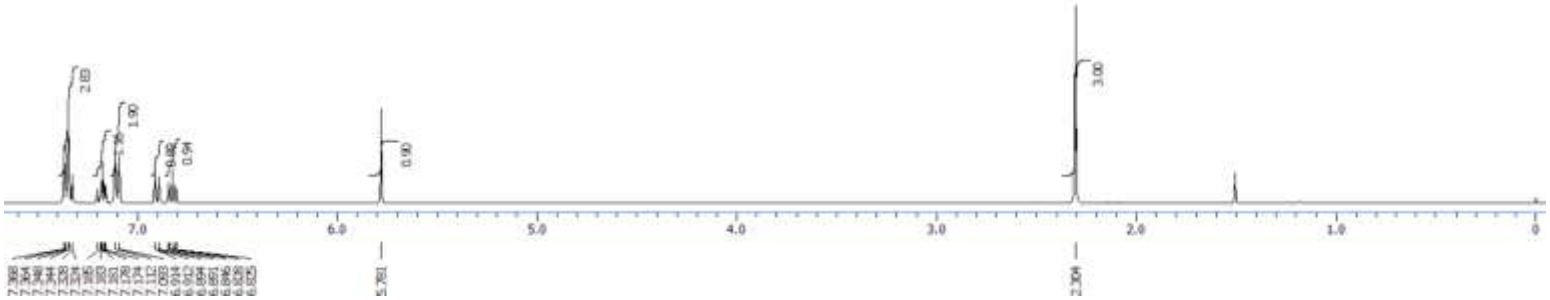
^{1}H NMR spectrum of 7 (400 MHz, $CDCl_3$)



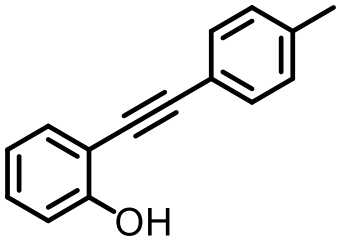
7

2-(*p*-tolylethynyl)phenol



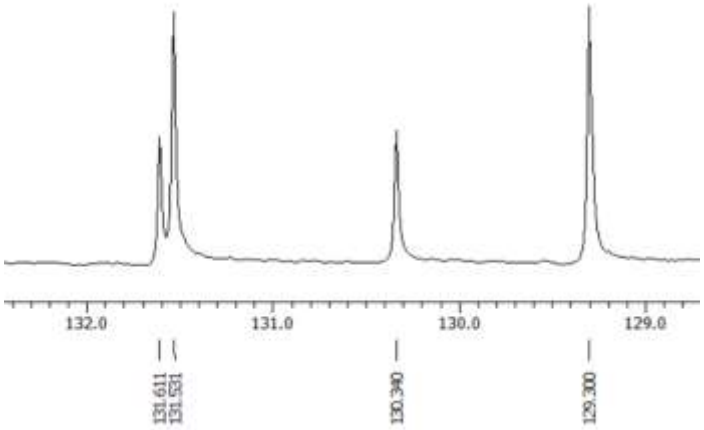


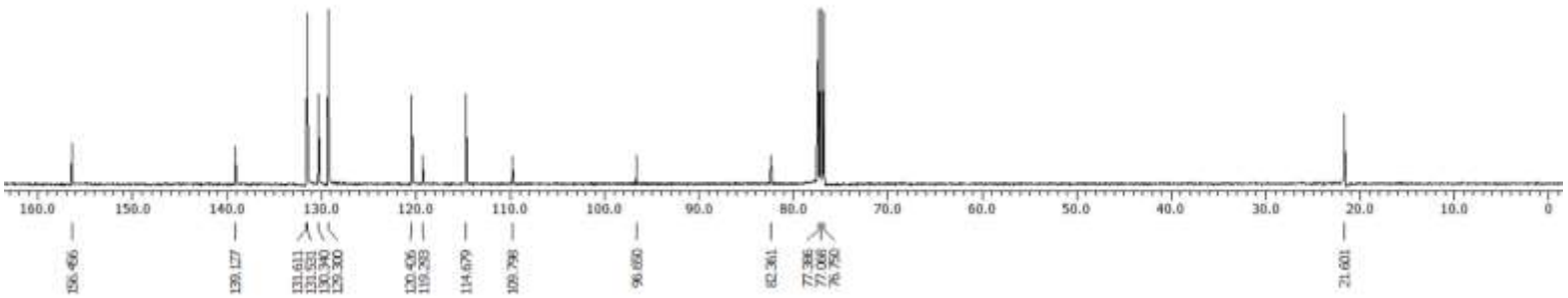
^{13}C NMR spectrum of 7 (100 MHz, $CDCl_3$)



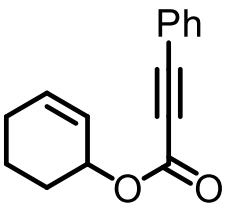
7

2-(*p*-tolylethynyl)phenol



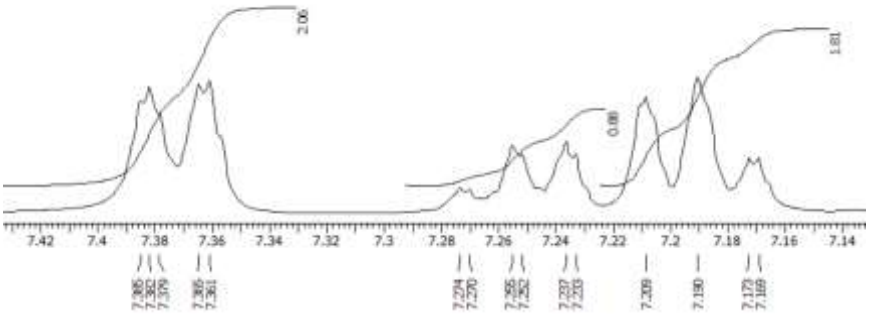


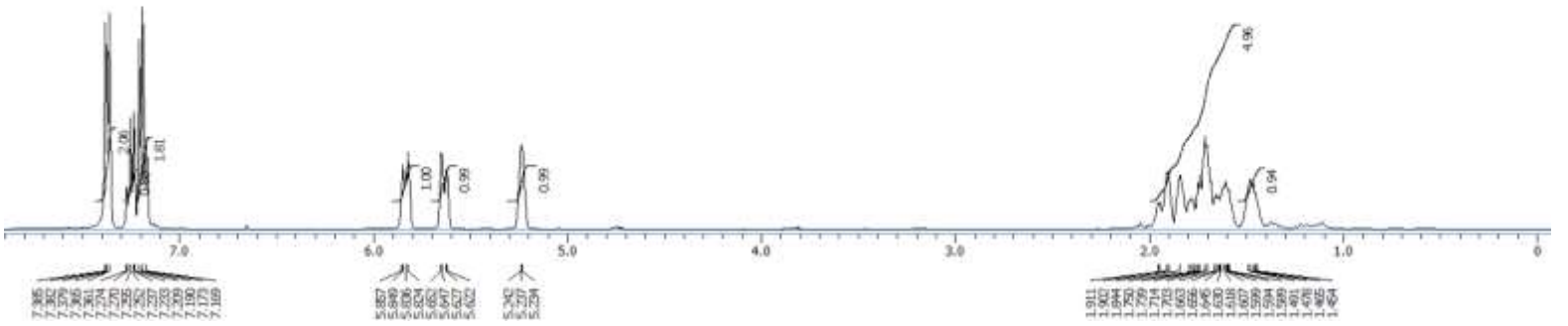
^{1}H NMR spectrum of 8 (400 MHz, $CDCl_3$)



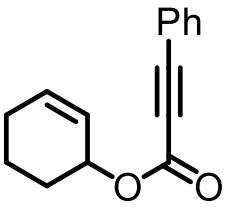
8

cyclohex-2-en-1-yl 3-phenylpropiolate



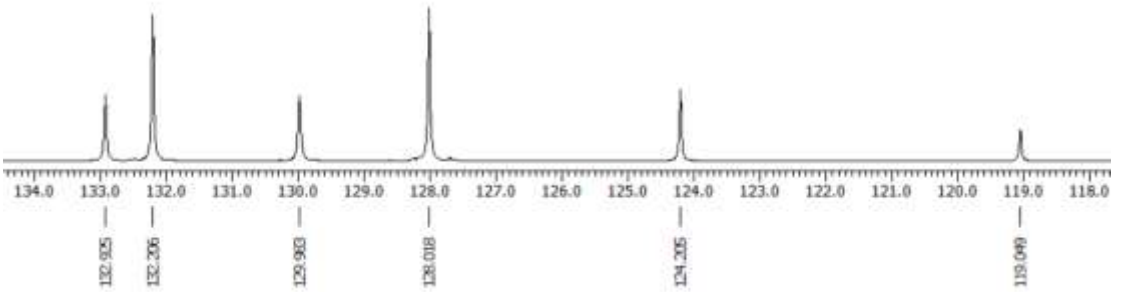


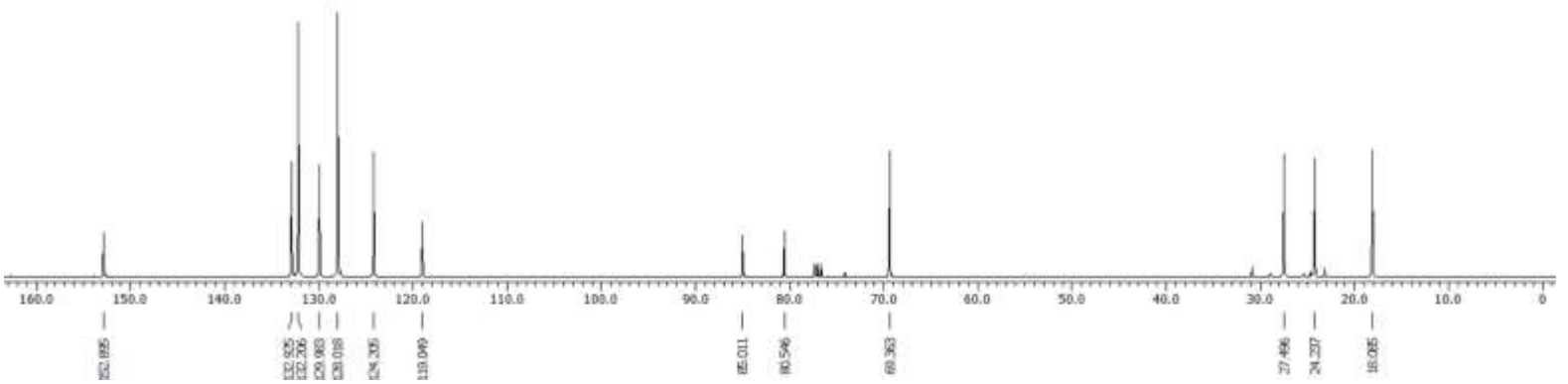
^{13}C NMR spectrum of 8 (100 MHz, $CDCl_3$)



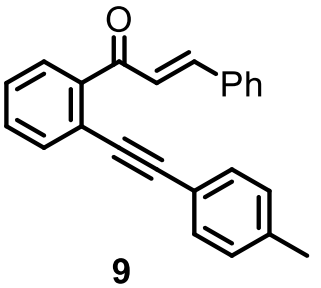
8

cyclohex-2-en-1-yl 3-phenylpropiolate



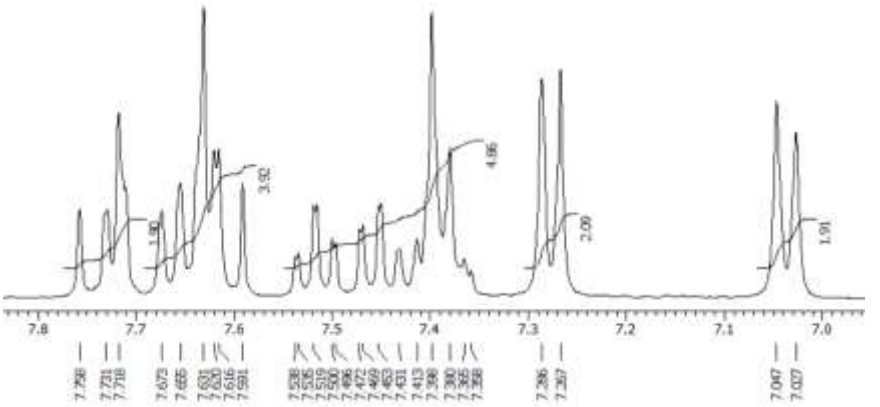


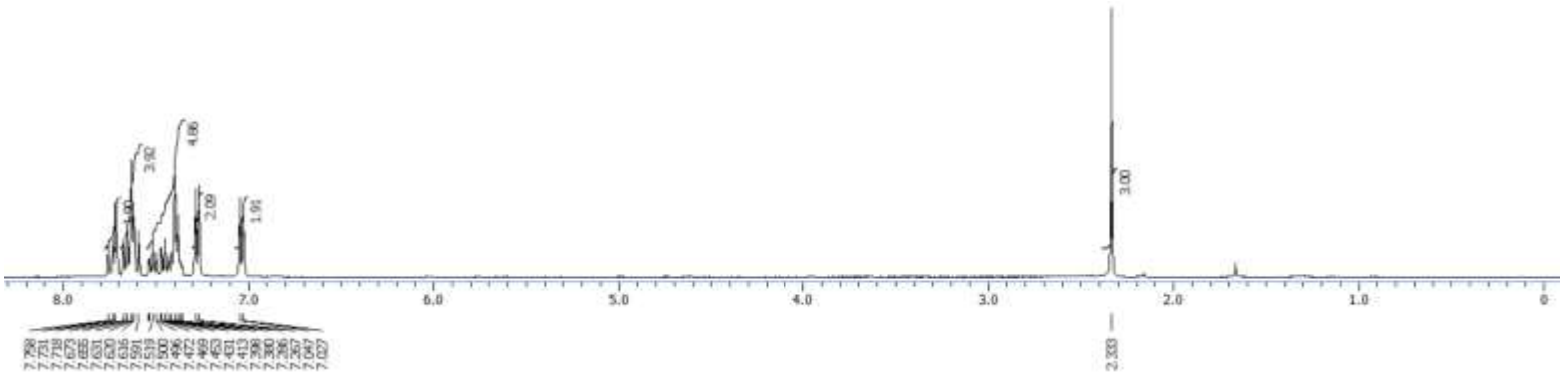
^{1}H NMR spectrum of 9 (400 MHz, $CDCl_3$)



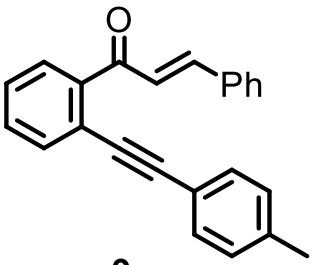
9

(*E*)-3-phenyl-1-(2-(*p*-tolylethynyl)phenyl)prop-2-en-1-one



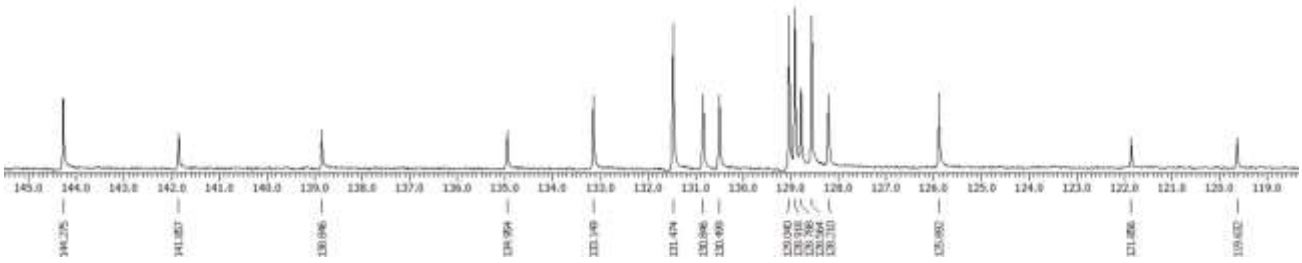


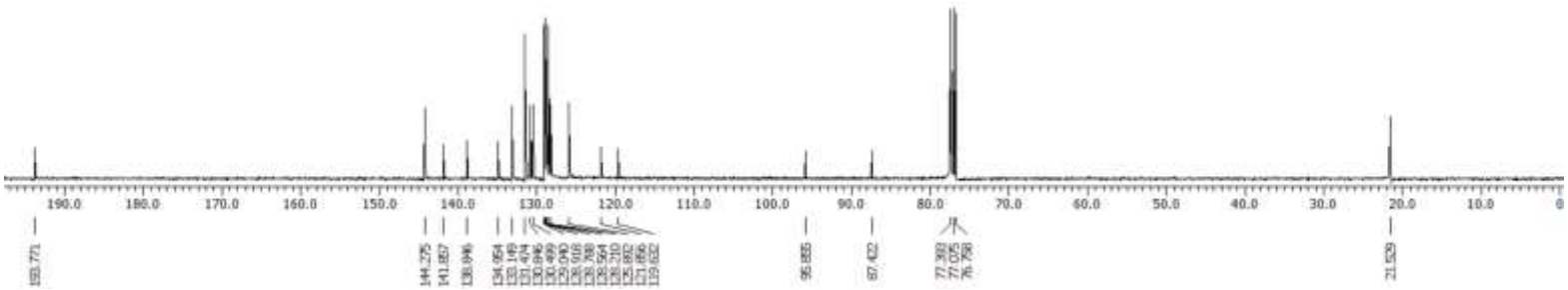
^{13}C NMR spectrum of 9 (100 MHz, $CDCl_3$)



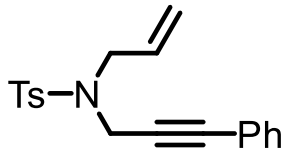
9

(*E*)-3-phenyl-1-(2-(*p*-tolylethynyl)phenyl)prop-2-en-1-one



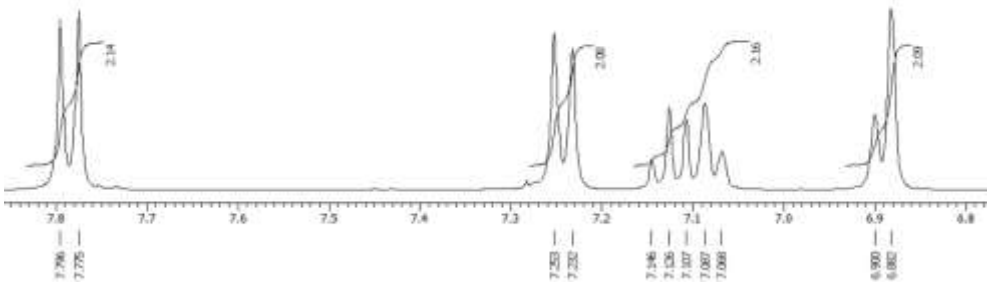


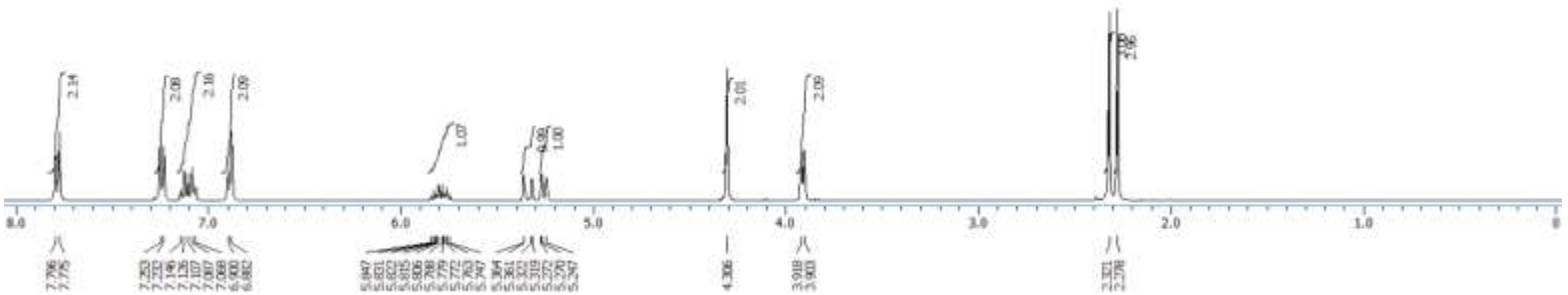
^{1}H NMR spectrum of 10 (400 MHz, $CDCl_3$)



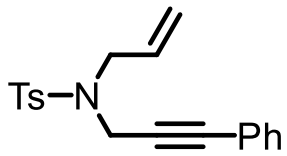
10

N-allyl-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide



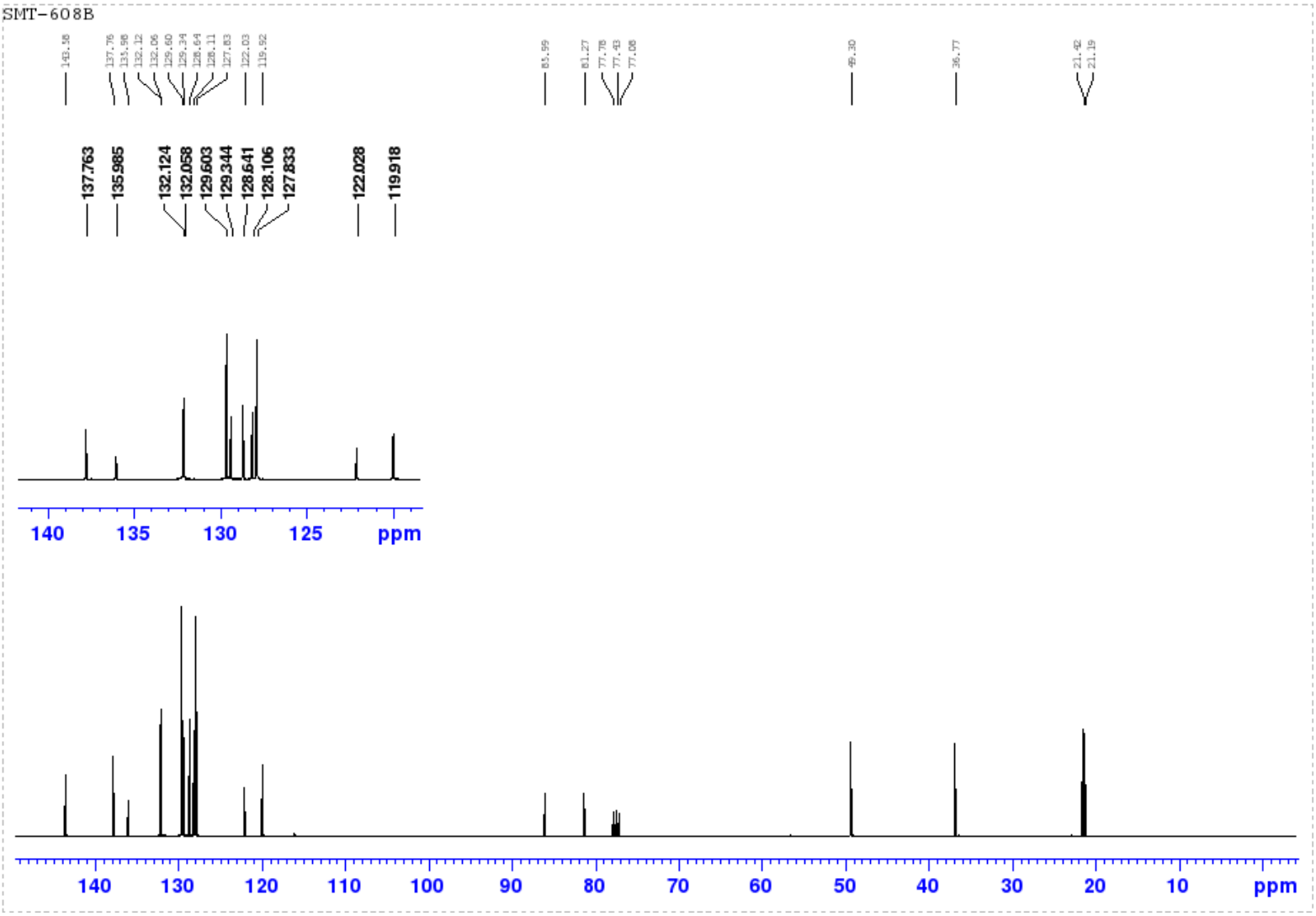


^{13}C NMR spectrum of 10 (100 MHz, $CDCl_3$)

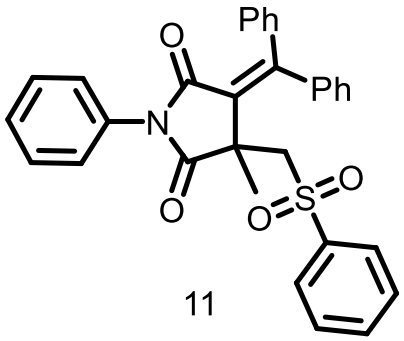


10

N-allyl-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide

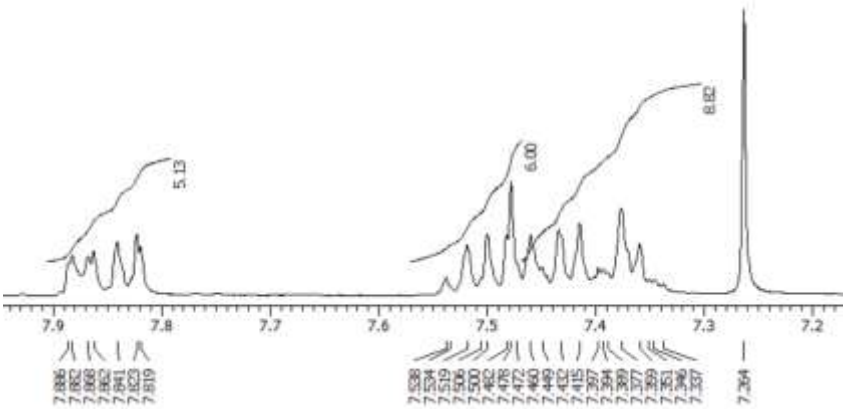


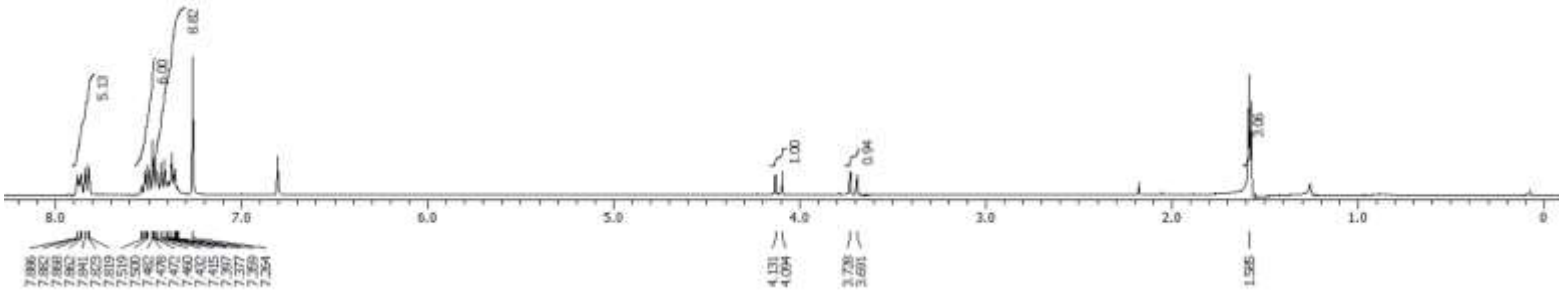
^{1}H NMR spectrum of 11 (400 MHz, $CDCl_3$)



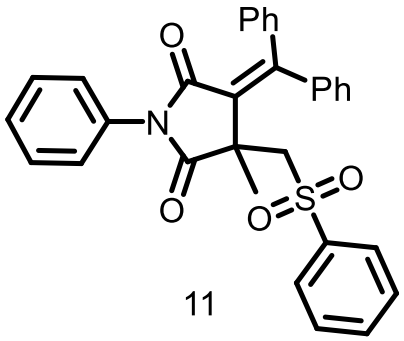
11

4-(diphenylmethylene)-3-methyl-1-phenyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



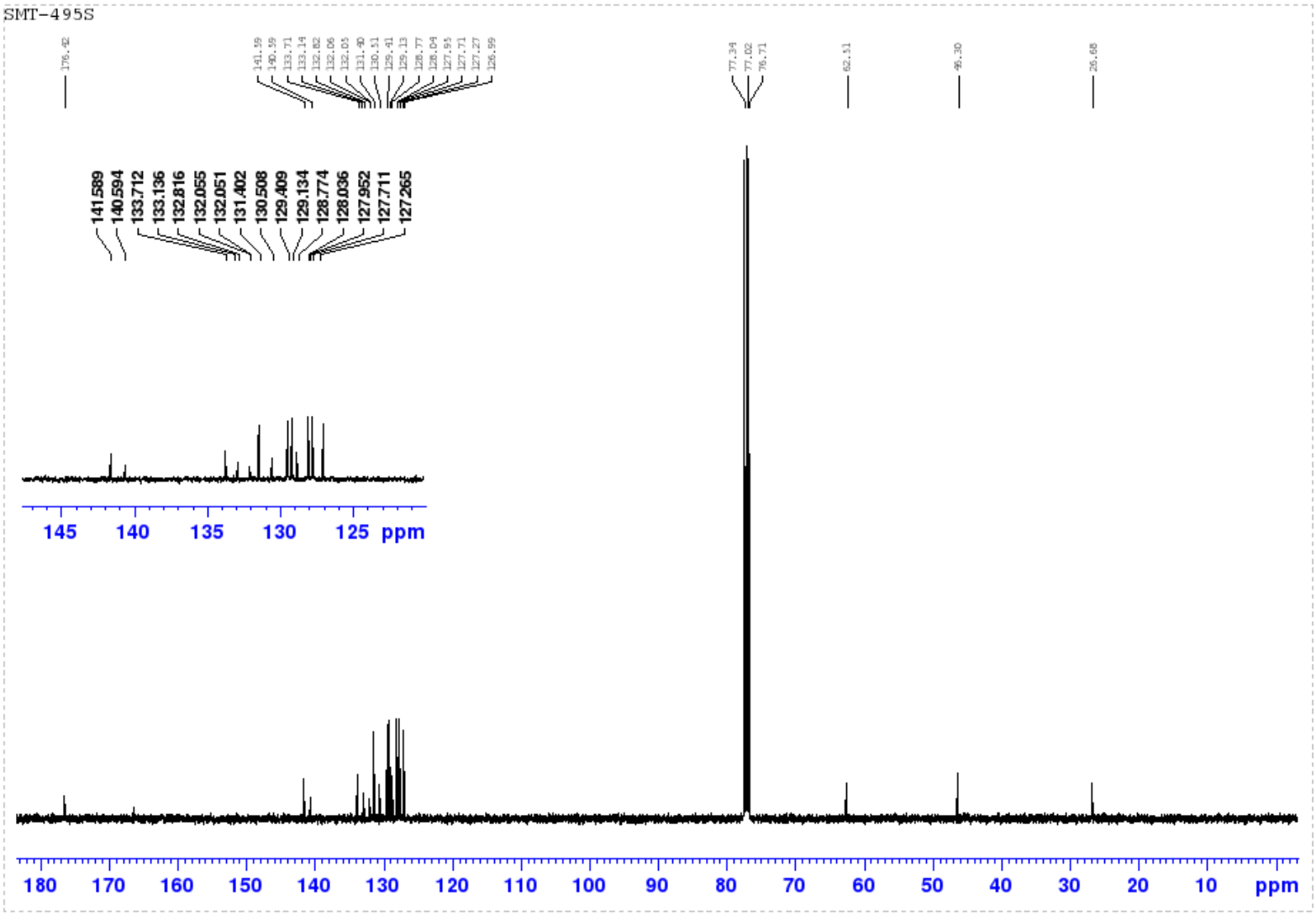


^{13}C NMR spectrum of 11 (100 MHz, $CDCl_3$)



11

4-(diphenylmethylene)-3-methyl-1-phenyl-3-((phenylsulfonyl)methyl)pyrrolidine-2,5-dione



HRMS Spectrum of 11

Qualitative Compound Report

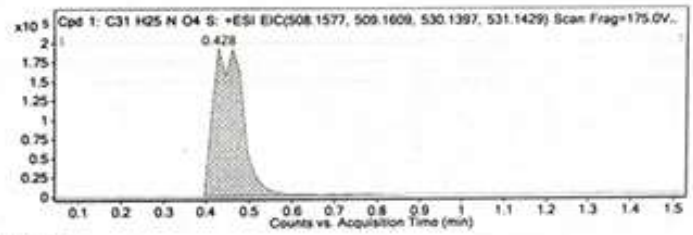
Data File	SMT-495.d	**Sample Name**	SMT-495
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	06-05-2024 13:23:51
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

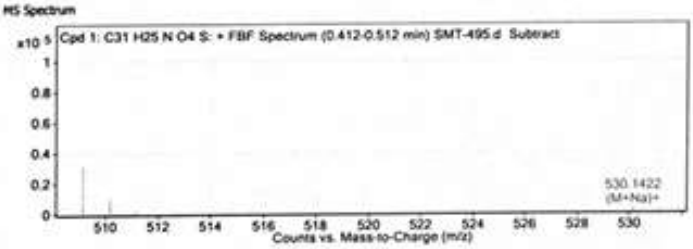
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	HFG Formula	DB Formula
Cpd 1: C31 H25 N O4 S	0.428	507.1527	92858	C31 H25 N O4 S	507.1504	4.51	C31 H25 N O4 S	C31 H25 N O4 S

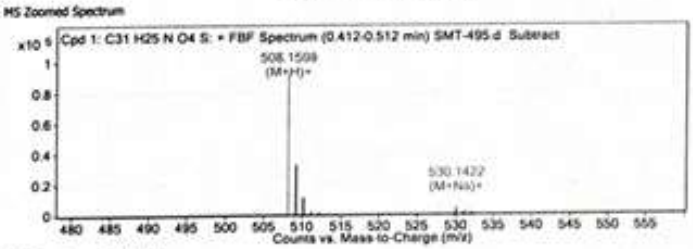
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C31 H25 N O4 S	508.1598	0.428	Find By Formula	507.1527



MS Spectrum



MS Zoomed Spectrum

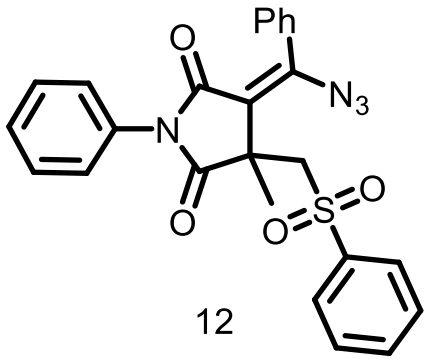


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
508.1598	1	92857.55	C31H26NO4S	(M+H)+
509.1631	1	31457.58	C31H26NO4S	(M+H)+
510.1625	1	10044.1	C31H26NO4S	(M+H)+
511.1671	1	2204.22	C31H26NO4S	(M+H)+
512.1734	1	207.11	C31H26NO4S	(M+H)+
530.1422	1	2809.28	C31H25NNaO4S	(M+Na)+
531.1446	1	1336.5	C31H25NNaO4S	(M+Na)+
532.1516	1	618.31	C31H25NNaO4S	(M+Na)+

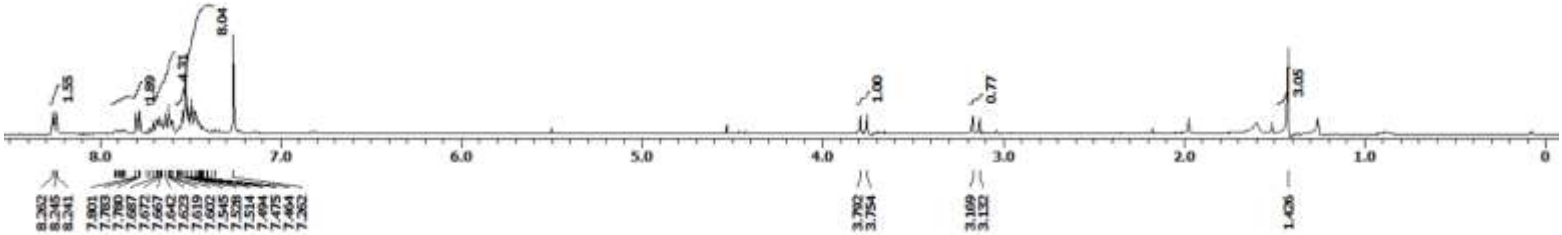
--- End Of Report ---

^{1}H NMR spectrum of 12 (400 MHz, $CDCl_3$)

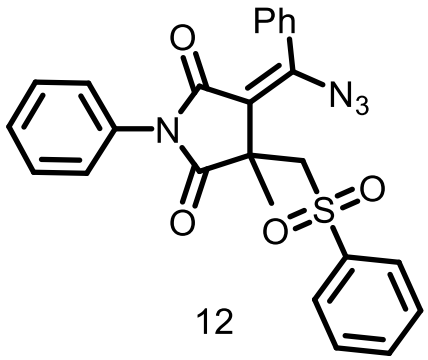


12

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

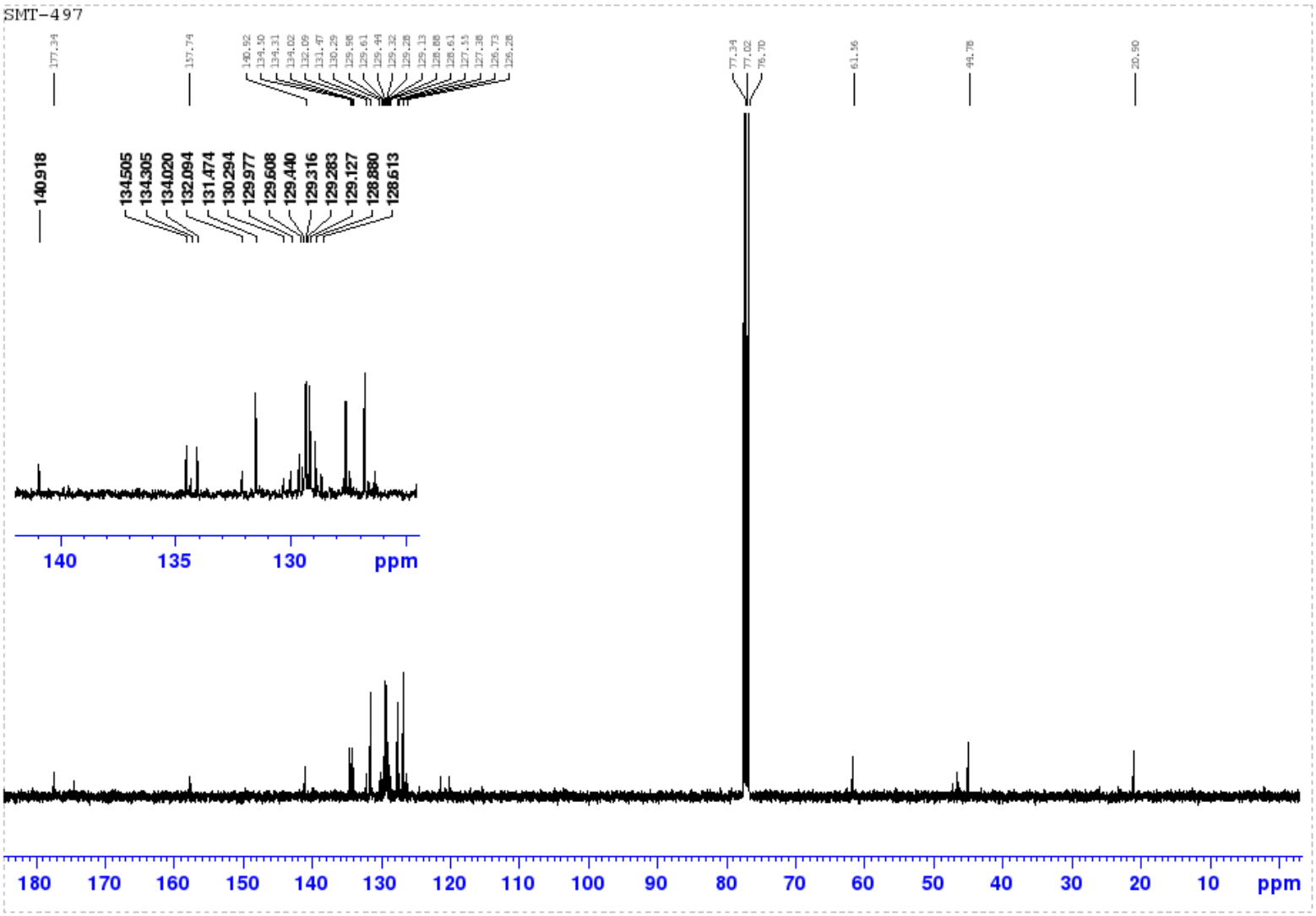


^{13}C NMR spectrum of 12 (100 MHz, $CDCl_3$)



12

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



HRMS Spectrum of 12