Supporting Information

Transition-Metal Free, Radical Oxidation of 1,6-Enyne Cyclopropanation: Synthesis of aza-bicyclo[4.1.0]heptane Derivatives

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(1) General Information.

All reagents were purchased (unless specified) at highest commercial quality and used as received. Reaction mixtures were stirred magnetically. All require temperature for reactions were achieved using a 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).

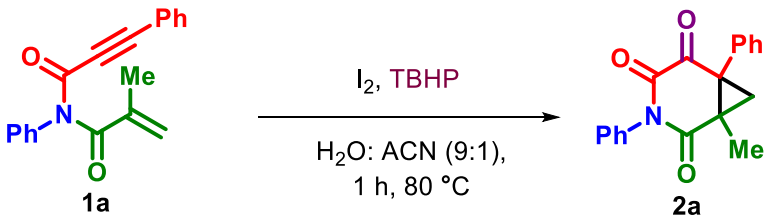
(2) Reaction Optimization

We commenced our investigation by employing *N*-(3-phenylpropioloyl)-*N*-(*p*-tolyl)methacrylamide **1a** as a model substrate. The reaction of **1a** in the presence of I_2, TBHP as an oxidant, and MeCN as a solvent gave the product **2a** in 75% yield (Table 1, entry 1). When PIDA was used product **2a** was observed in 65% yield, however, the use of *N*-iodosuccinimide (NIS) gave a 60% yield of **2a** (Table 1, entry 2-3) which shows that molecular iodine was the best iodine source for this conversion.

The use of other oxidants, DTBP and $K_2S_2O_8$ provided the desired product **2a** in 40 and 10% yields (entries 4-5). When the reaction was performed under an N_2 atmosphere (entry 6) product **2a** was obtained in 75% yield. This concluded that TBHP was the optimal oxidant for the reaction. Product **2a** was formed in 60% yield when the reaction was conducted in H_2O as solvent. The use of other solvents like dioxane, toluene, THF, and DMSO, was found inferior/unsuitable for the reaction (entries 8-11).

When the reaction was performed without iodine, we did not observe the desired product **2a** (entry 12). Also, the reaction did not proceed without the oxidant TBHP (entry 13). These observations indicate that both iodine and TBHP were necessary for the reaction. The yield of the product was further enhanced when a mixture of H_2O: MeCN (9:1) was used (entry 14). Subsequent adjustments in the reaction temperature revealed that deviations from the optimal temperature adversely affected the yield of product **2a**. Reduction to 40 °C and 60 °C resulted in the product **2a** in 50% and 60% yield, respectively. An increase in temperature to 100 °C and 120 °C proved to be unfavorable, leading to decreased yields of **2a** in 30% and 25%, respectively.

Table S1. Optimization of Reaction Conditions[a]



Entry	I_2 Source (0.5 equiv.)	Oxidant (3.0 equiv.)	Solvent	Yield[b] 2a (%)
1	I_2	TBHP	ACN	75
2	PIDA	TBHP	ACN	65
3	NIS	TBHP	ACN	60
4	I_2	DTBP	ACN	40
5	I_2	$K_2S_2O_8$	ACN	10
6	I_2	TBHP	ACN	75[c]
7	I_2	TBHP	H_2O	60
8	I_2	TBHP	Dioxane	0
9	I_2	TBHP	Toluene	20

10	I_2	TBHP	THF	40
11	I_2	TBHP	DMSO	0
12		TBHP	ACN	0
13	I_2		ACN	0
14	I_2	TBHP	H_2O:ACN (9:1)	85[d]
15	I_2	TBHP	H_2O:ACN (1:1)	80
16	I_2	TBHP	H_2O:ACN (9:1)	50[e], 60[f], 30[g], 25[h]

[a]Reaction Conditions: **1a** (0.346 mmol, 1.0 equiv.), Iodine (0.173 mmol, 0.5 equiv.), Oxidant (1.038 mmol, 3.0 equiv.) in a solvent at 80 °C for 1 h under an air atmosphere. [b]Isolated yield, [c]N_2 atmosphere, [d]ACN was added to increase the solubility of the substrates, [e]40 °C, [f]60 °C, [g]100 °C, [h]120 °C.

(3) Real time mass monitoring studies:

(3.1) Experimental Section

All chemicals were obtained from commercial sources. LC-MS grade solvents were obtained from Thermo Fisher Scientific for online ESI–MS Study. The online ESI-MS study for real-time detection of reactive intermediates was performed using a custom-built pressurized sample infusion method, originally described by McIndoe and coworkers.[1] The experimental setup diagram is presented in the upper panel of Figure 2. Briefly, the reaction in a Schlenk flask was performed at a 0.346 mmol scale (containing **1a**) in 2 mL (9: 1) of solvent (H2O: ACN) at 80 °C. The reaction flask was pressurized by nitrogen gas with a backpressure of 4 psi for transferring the reaction mixture through a borosilicate capillary to a T-junction, where it was mixed with acetonitrile delivered by a Hamilton syringe (30 µL/min flow) connected to a high voltage (+5 kV) DC power source. The diluted reaction mixture from the T-junction was transferred to a custom-made electrospray source for spraying it to a high-resolution mass spectrometer (Orbitrap Exploris 120, Thermo Fisher Scientific). An inner fused silica capillary (100 µm i.d. and 360 µm o.d.) was utilized for solvent delivery, and an outer (coaxial) stainless steel capillary (0.5 mm i.d. and 1.6 mm o.d.) was employed for the nitrogen sheath gas supply (at 110 psi back pressure) in the customized spray source. To improve nebulization through the spray nozzle, the inner silica capillary tip was placed 1 mm outside the coaxial stainless steel capillary orifice. The stream of charged microdroplets from the spray nozzle was directed to the MS inlet capillary (300 oC), which caused the desolvation of the analyte ions for mass spectrometric detection. The maximum ion injection period with a single microscan was set to 500 ms, and the distance between the spray tip and the MS inlet was maintained at 15 mm. The mass resolution was set to 120,000. In order to obtain the highest ion current, other ion optics were further tuned. Thermo Fisher Scientific's XCalibur software was used for data acquisition.

The dead time (time taken by the reaction mixture to travel from the reaction vial to the electrospray nozzle) is approximately 45 seconds and does not account for the onset of the reaction seen in Figure 2. The extracted ion chronogram of all the detected species (Figures 2a-h) is normalized to 1 as there is no cross-correlation between species for comparing their concentrations with ion signal intensities because of their differences in ionization efficiencies in the gas phase.

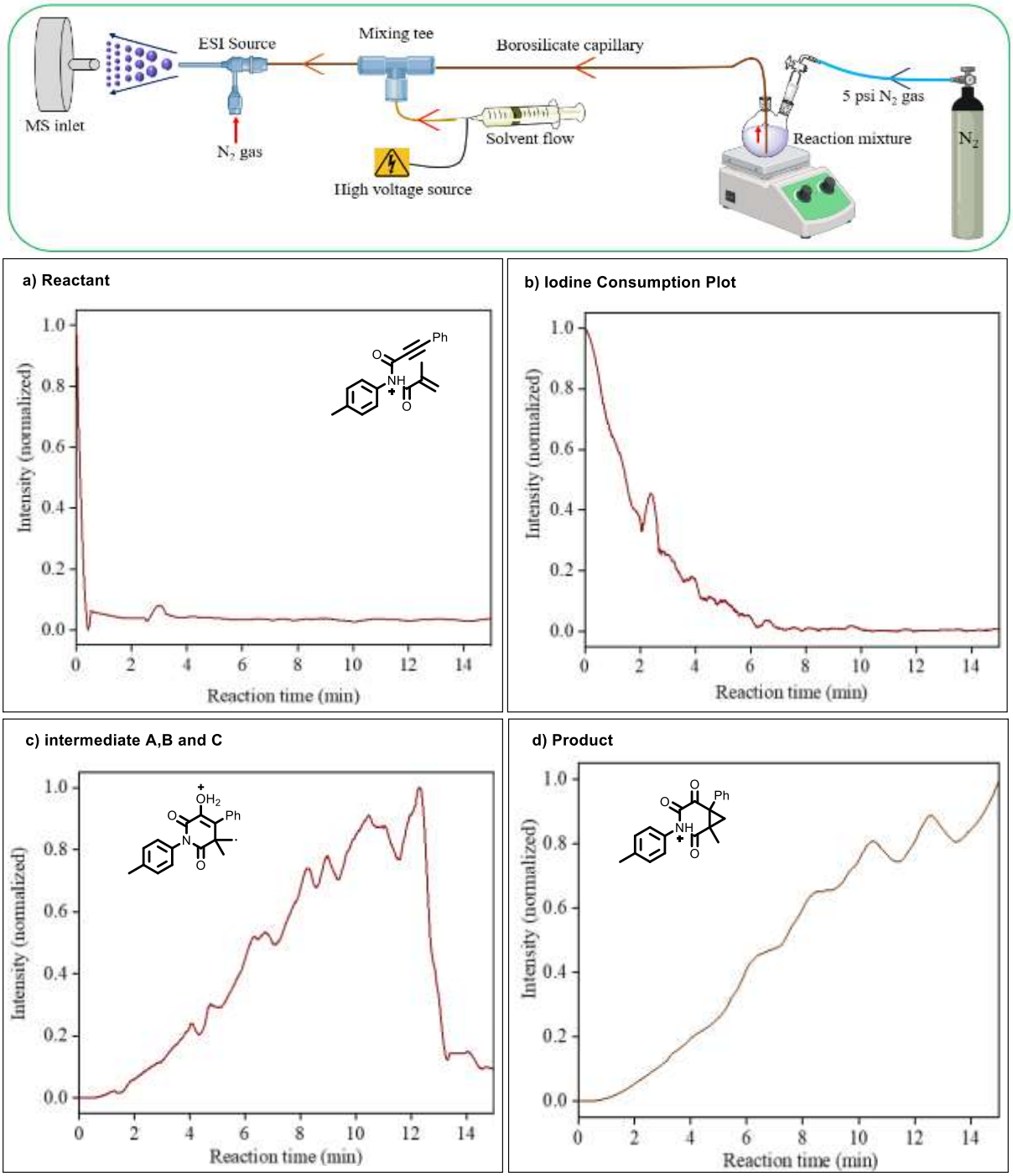


Figure S1. Custom-built online ESI-MS setup (upper panel) for real-time monitoring of the abundance of reactants, intermediates, and products in the positive ion mode during the progress of the reaction. All species are characterized by high mass accuracy, resolution, and isotopic distribution pattern (Figure S1).

(3.2) Reaction Setup

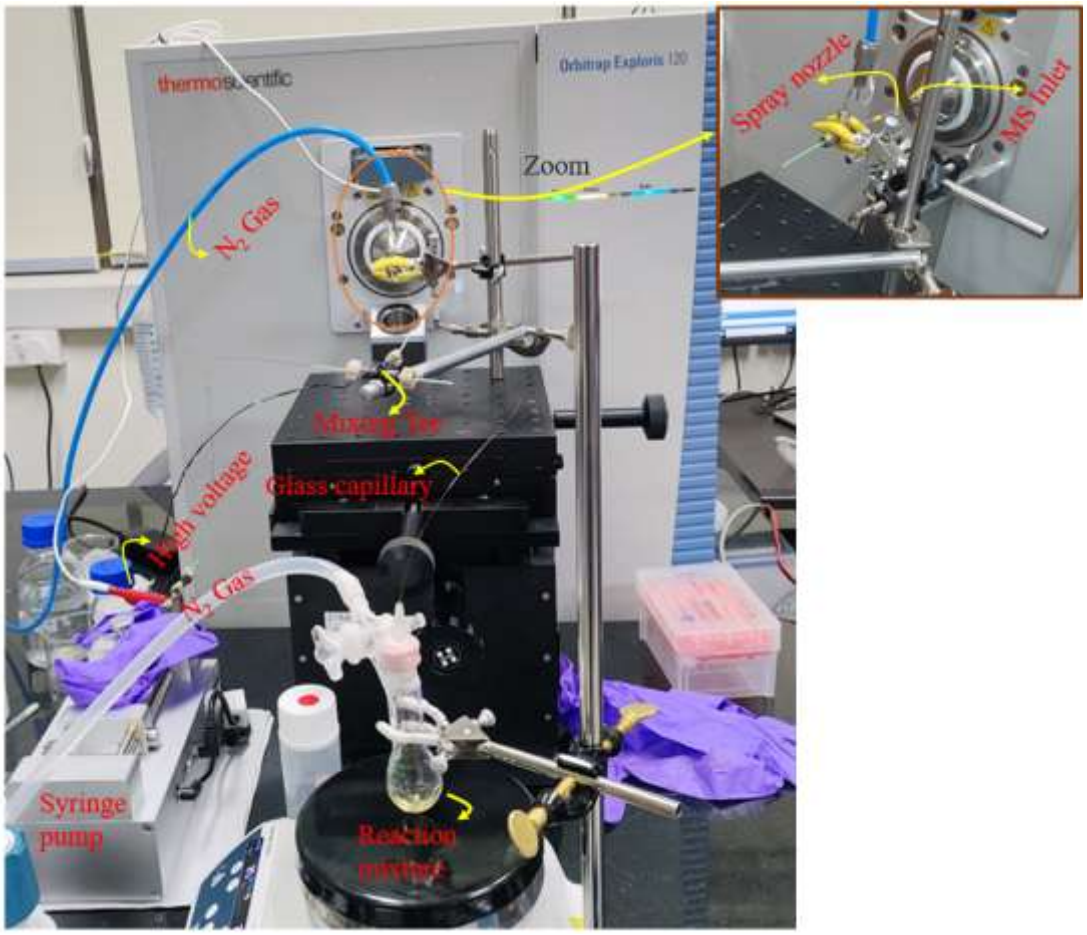
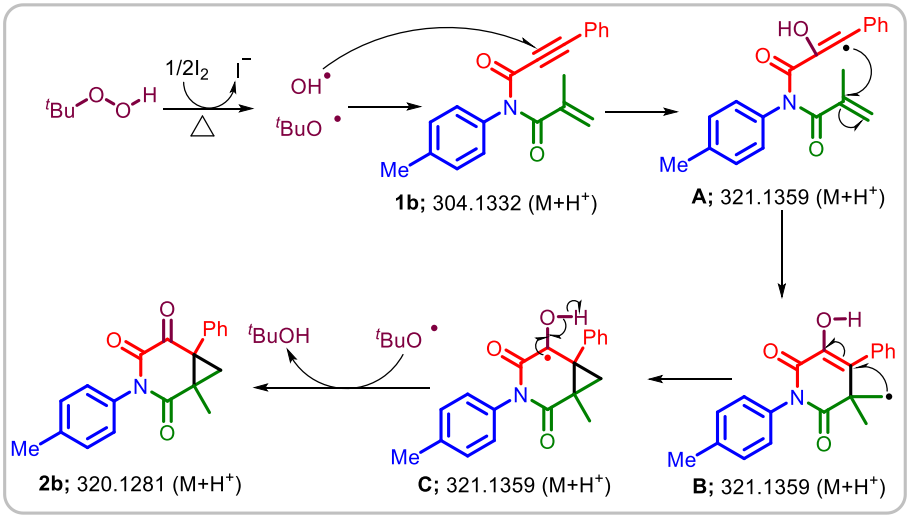
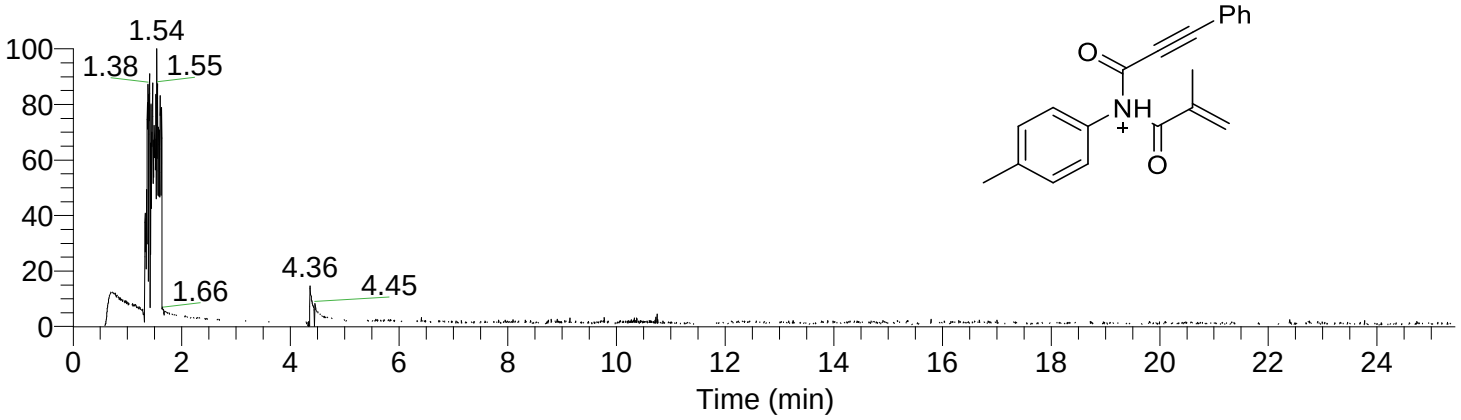


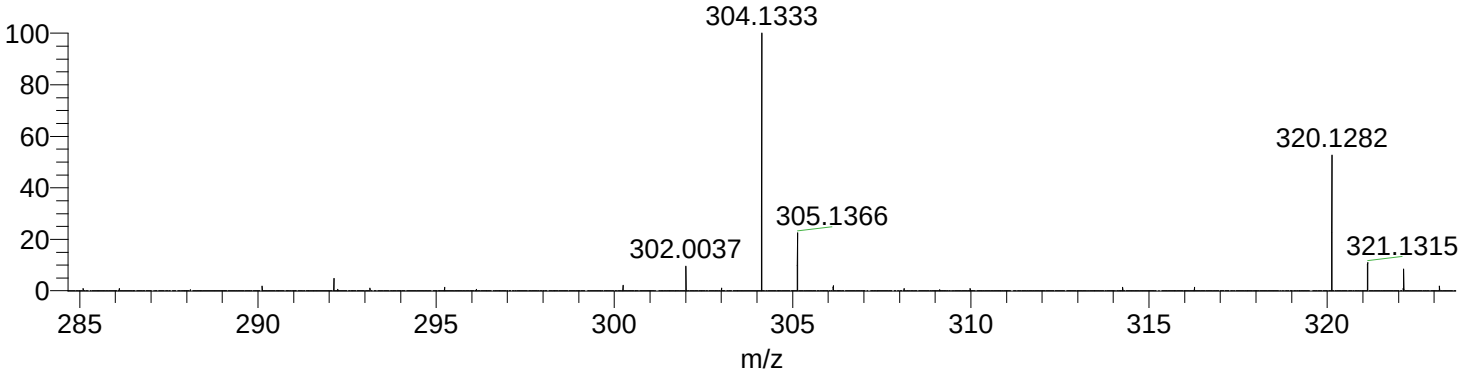
Figure S2: Online ESI-MS with pressurized sample infusion setup used monitoring to track different species S4 MS with pressurized sample infusion setup used for realmonitoring to track different species formed during the progress of the reaction.



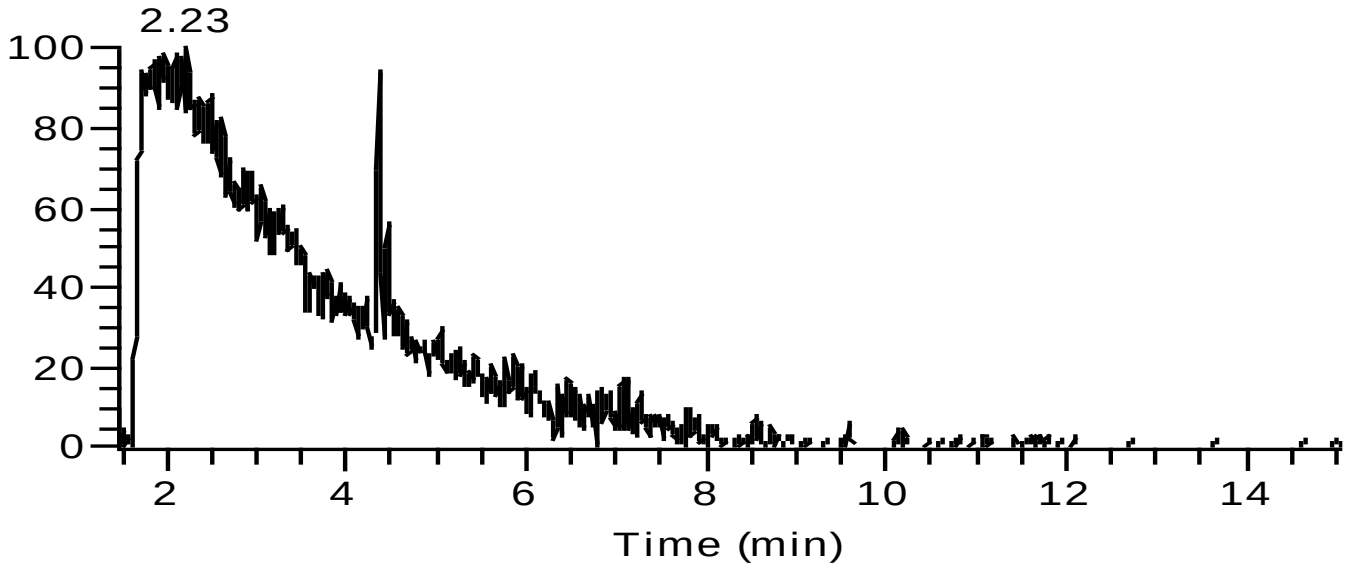
(a) Chronogram showing the consumption of 1



MS Data



(b) Chronogram showing the consumption of Iodine



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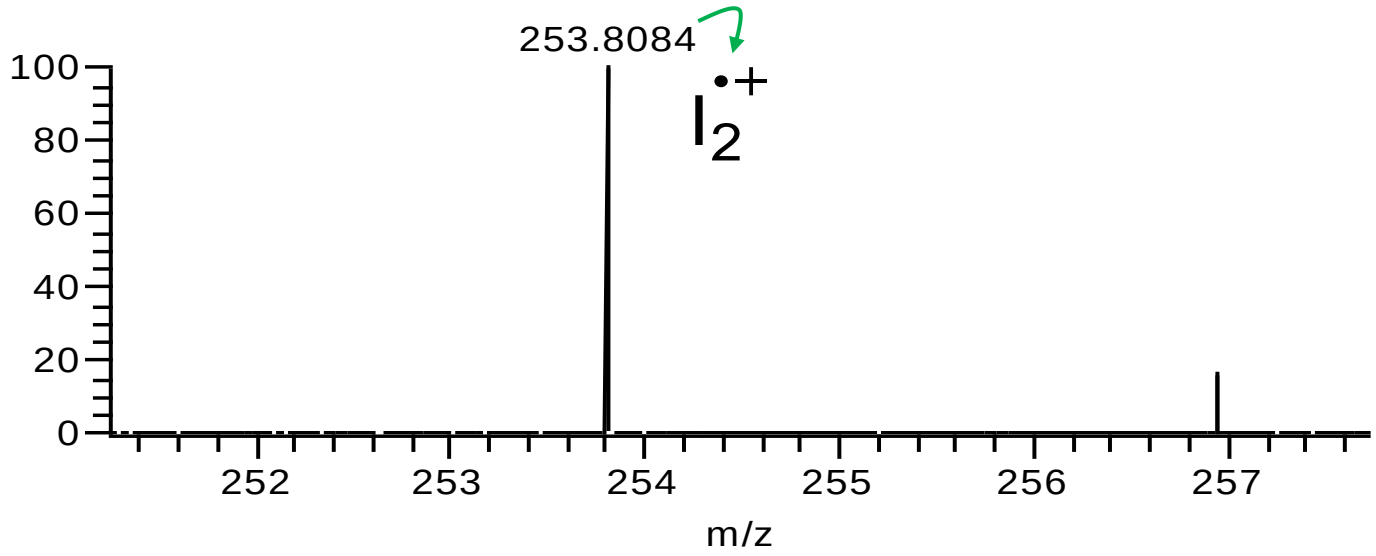
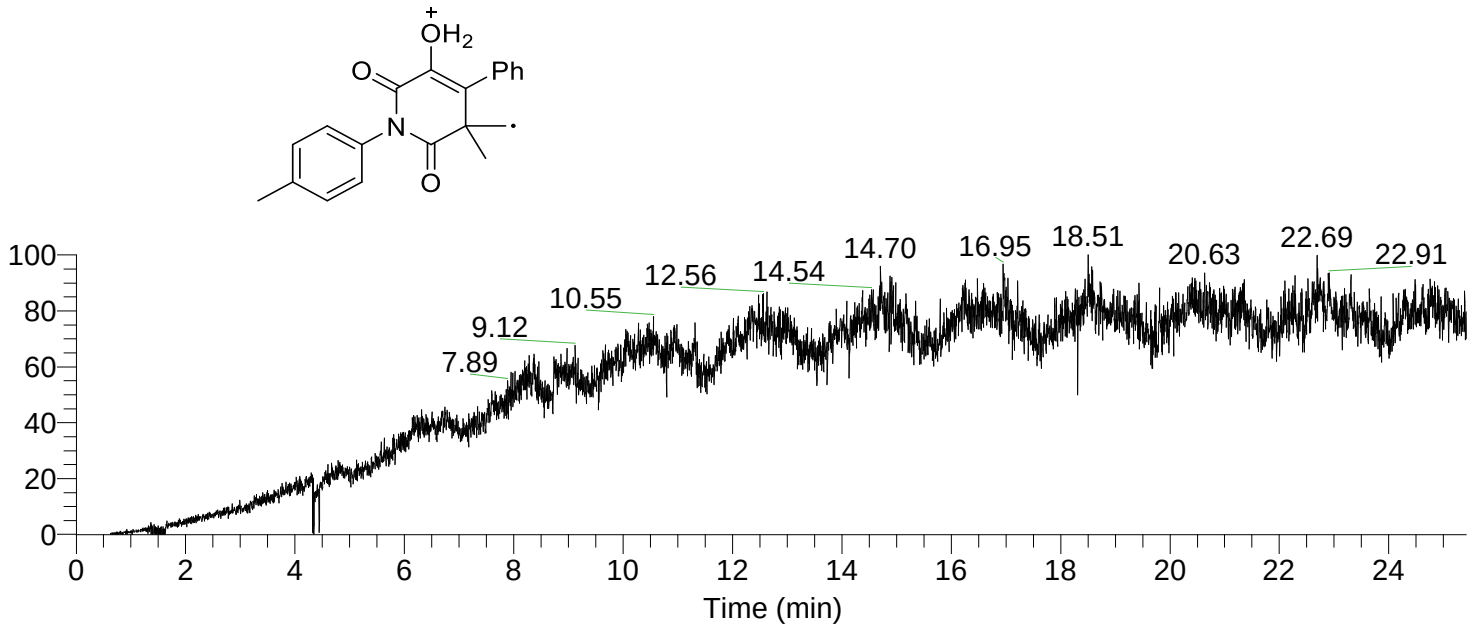
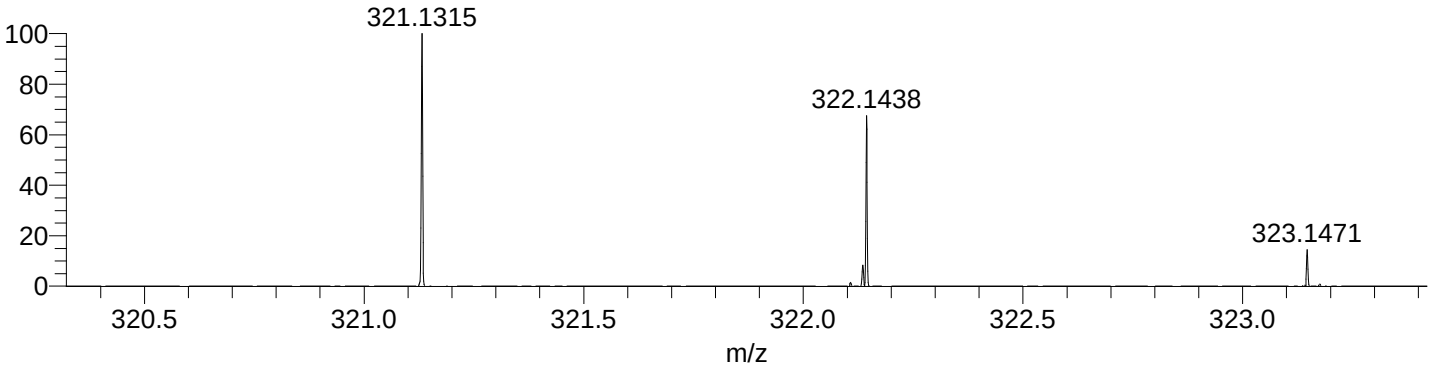


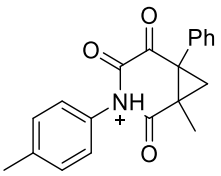
(c) Chronogram showing the formation of intermediates A, B and C

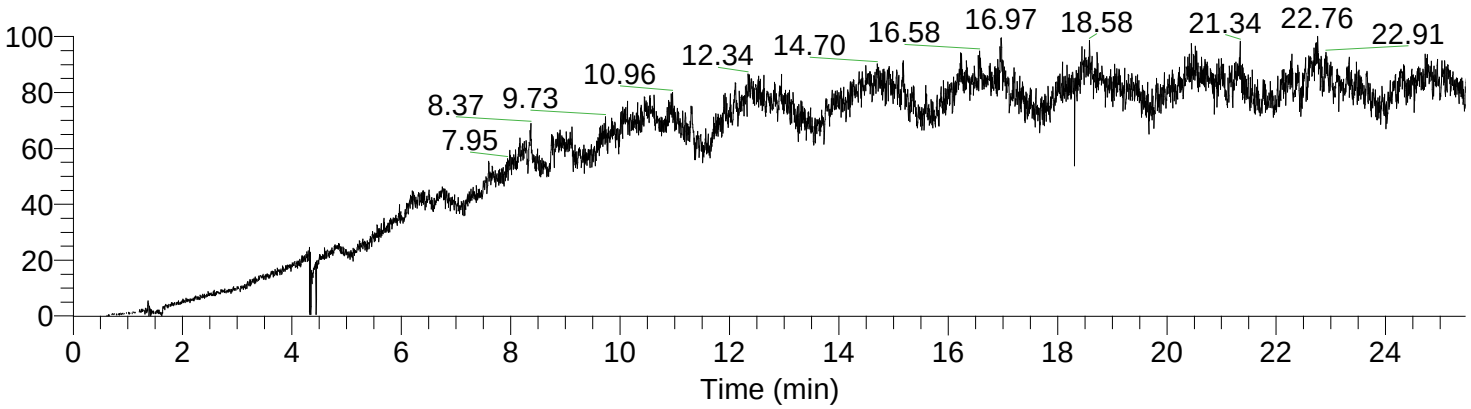


MS Data

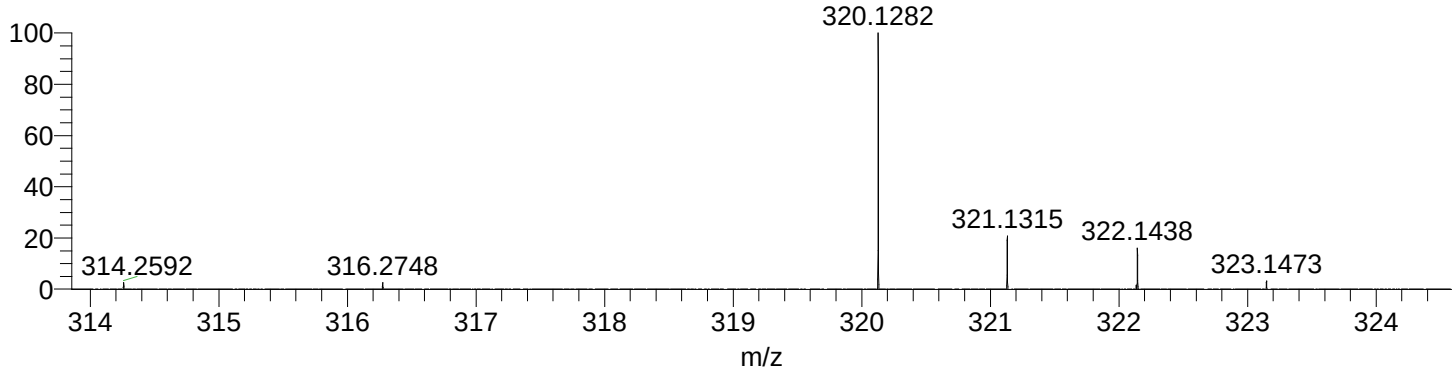


(d) Chronogram showing the formation of 2





MS Data



(4) X-Ray Crystallographic Data of 2a, 2j and 4j:

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.[12] Non-hydrogen atoms were refined anisotropicallyusing the WinGX (version 1.80.05) program package.[13] All non-hydrogen atoms were refined anisotropically and hydrogen atoms were treated as riding atoms using SHELX default parameters. Molecular structures have drawn using ORTEP software shown in figure S2, S3 and S4. Further information on the crystal structure determination (excluding structure factors) has been given as table S1, S2 and S3 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.

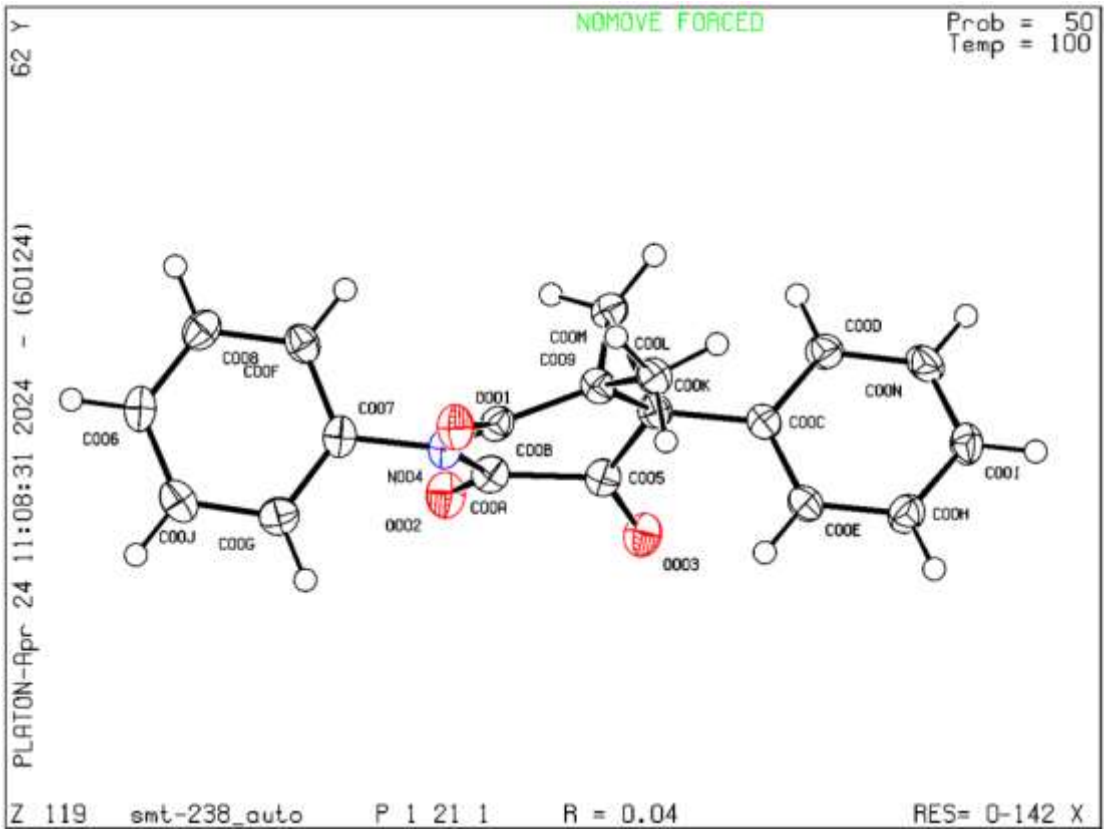


Figure S2: Ellipsoid plot

Table S2: Crystallographic description of 1-methyl-3,6-diphenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2a):

Identification code	SMT-238_auto	
Empirical formula	C_{19} H_{15} NO_3	
Formula weight	305.32	
Temperature	100 K	
Wavelength	0.71073	
Crystal system	monoclinic	
Space group	P21	
Unit cell dimensions	a = 10.2750(5) Å	a= 90°.
	b = 6.3644(3)Å	b= 112.449(6)°.
	c = 12.1715(6) Å	g = 90°.
Volume	735.63(7) $Å^3$	
Z	2	
Density (calculated)	1.378 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	320.0	
Crystal size	0.20 x 0.24 x 0.18 mm^3	
Theta range for data collection	6.588 to 52.712°.	
Index ranges	$-12 \leq h \leq 12$, $-7 \leq k \leq 7$, $-15 \leq l \leq 13$	
Reflections collected	7187	
Independent reflections	2879 [Rint = 0.0310, Rsigma = 0.0364]	
Completeness to theta = 27.71°	100 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2879/1/210	
Goodness-of-fit on F^2	1.069	
Final R indices [I>2sigma(I)]	R_1 = 0.0355, wR_2 = 0.0813	
R indices (all data)	R_1 = 0.0390, wR_2 = 0.0832	
Largest diff. peak and hole	0.19 and -0.16 $e.Å^{-3}$	
CCDC	2350836	

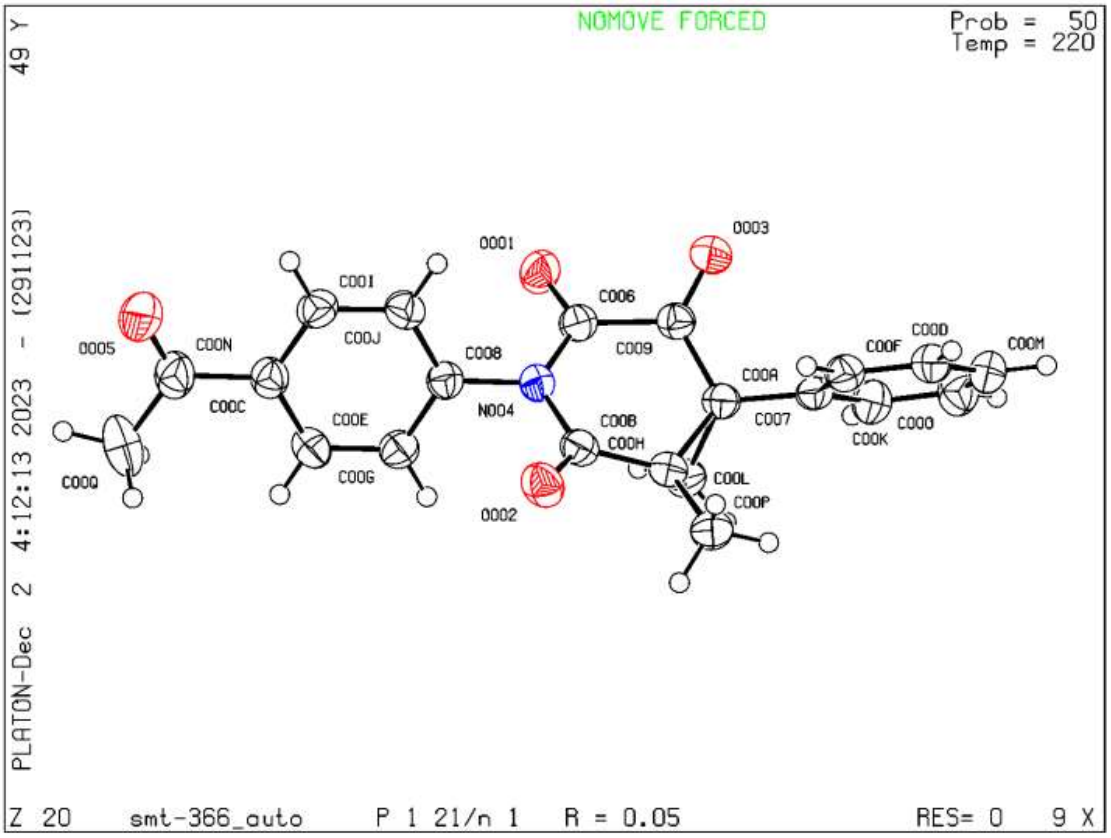


Figure S3: Ellipsoid plot

Table S3: Crystallographic description of 3-(4-acetylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2j):

Identification code	SMT-366_auto	
Empirical formula	$C_{21}H_{17}NO_4$	
Formula weight	347.36	
Temperature/K	224(40)	
Wavelength	0.71073	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 14.2969(17) Å	α= 90°.
	b = 6.8015(6) Å	β= 112.036(14)°.
	c = 18.834(2) Å	γ = 90°.
Volume	1697.6(4)$Å^3$	
Z	4	
Density (calculated)	1.359 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	728.0	

Crystal size	0.20 x 0.18 x 0.16 mm^3
Theta range for data collection	6.428 to 61.838°.
Index ranges	-17<=h<=18, -7<=k<=9,-26<=l<=22
Reflections collected	10835
Independent reflections	3870 [R(int) = 0.0569, R(sigma) = 0.0714]
Completeness to theta = 25.242°	100 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3870 / 0 / 237
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R_1 = 0.0543, wR_2 = 0.1310
R indices (all data)	R_1 = 0.0865, wR_2 = 0.1469
Largest diff. peak and hole	0.20 and -0.19 e.$Å^{-3}$
CCDC	2311799

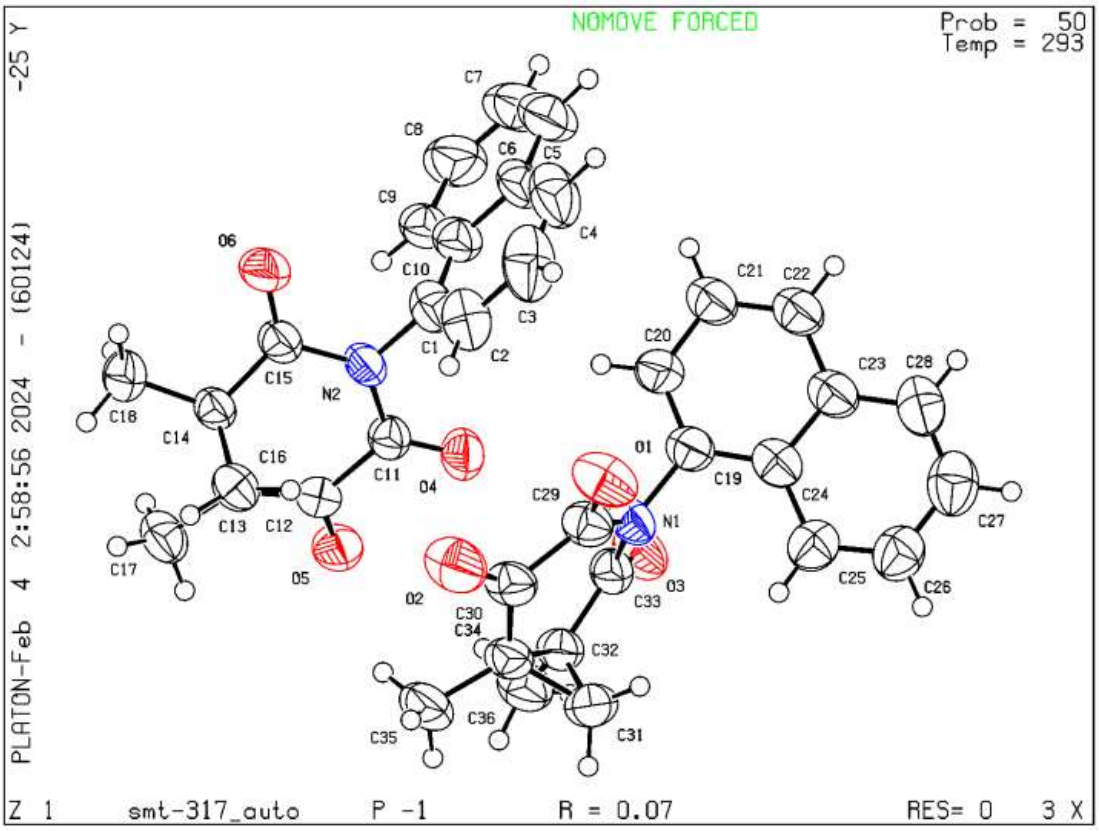


Figure S4: Ellipsoid plot

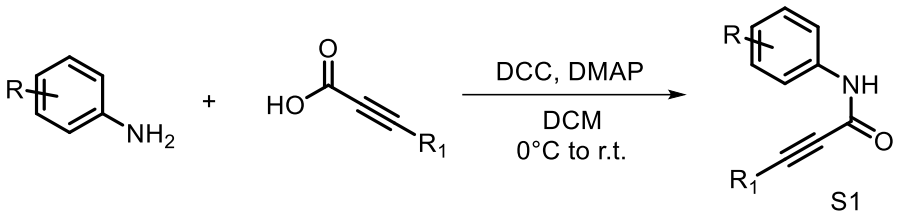
Table S4: Crystallographic description of 1,6-dimethyl-3-(naphthalen-1-yl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4i):

Identification code	SMT-317_auto	
Empirical formula	C_{18} H_{15} NO_3	
Formula weight	293.31	
Temperature	293 K	
Wavelength	0.71073	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.6199(4) Å	a= 103.773° (4)°.
	b = 10.8504(5)Å	b= 97.032(3) °.
	c = 15.1555(6) Å	g = 114.529(4).
Volume	1493.92(12) $Å^3$	
Z	4	
Density (calculated)	1.304 g/cm^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	616.0	
Crystal size	0.24 x 0.19 x 0.18 mm^3	
Theta range for data collection	6.26 to 52.742°.	
Index ranges	$-13 \leq h \leq 13$, $-13 \leq k \leq 12$, $-18 \leq l \leq 18$	
Reflections collected	21311	
Independent reflections	6120 [Rint = 0.0447, Rsigma = 0.0486]	
Completeness to theta = 27.71°	100 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6120/28/383	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R_1 = 0.0652, wR_2 = 0.1858	
R indices (all data)	R_1 = 0.1049, wR_2 = 0.2094	
Largest diff. peak and hole	0.57 and -0.28 $e.Å^{-3}$	
CCDC	2330995	

(5) Synthesis of Substrates 1:

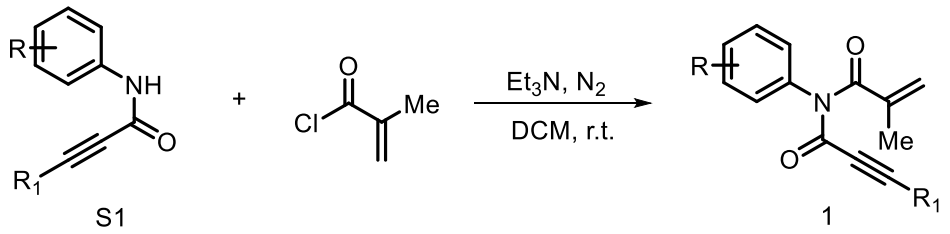
Substrates **1** were prepared following the reported procedure.[2]

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



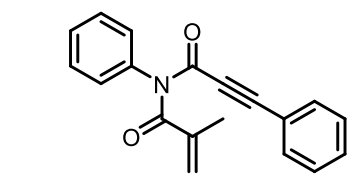
Phenylpropiolic acid (1 equiv) and DMAP (10 mol%) were charged into an oven-dried round-bottom flask, which was then purged with nitrogen gas for 10 minutes. After dissolving the mixture in DCM, amine (1.1 equiv) was added. The mixture was cooled to 0°C and a saturated solution of DCC (1.0 equiv) in 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**.

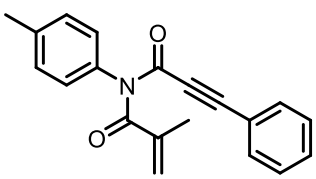
(ii) Methallylation of S1

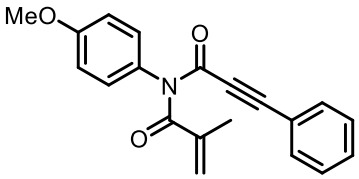


An oven-dried round-bottom flask equipped with a magnetic stir bar was charged with S1 (1.0 equiv) then sealed with septum and purged with nitrogen gas for 10 minutes. Afterwards DCM were added. Then, Methacryloyl chloride (1.5 equiv) and Et_3N (2.0 equiv) were added successively in dropwise manner while 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 to afford pure product **1**. The prepared substrates are as follows:


1a


1b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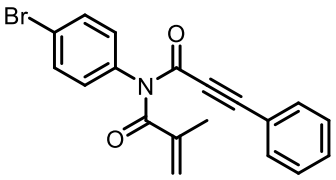
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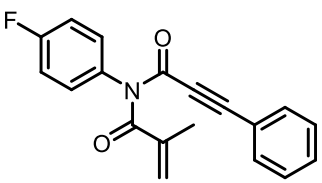
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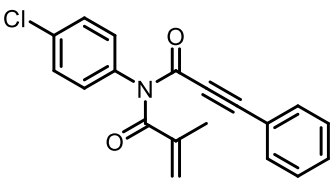
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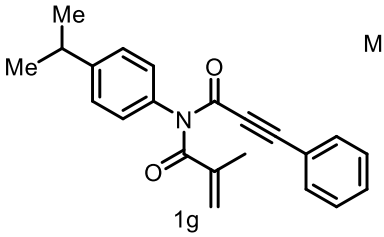
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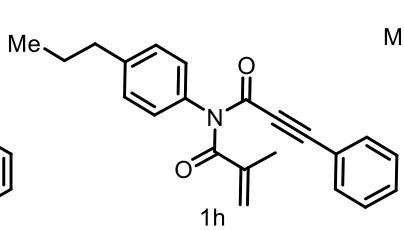
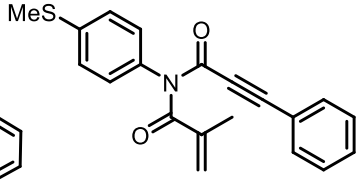

1h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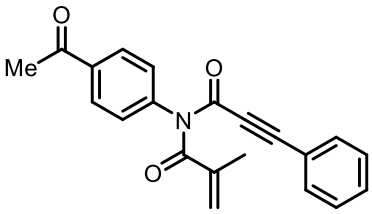
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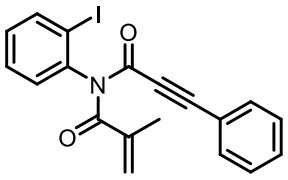
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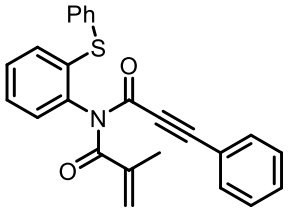
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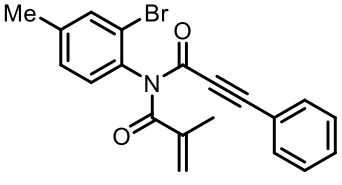
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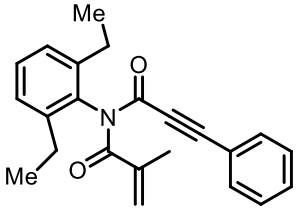
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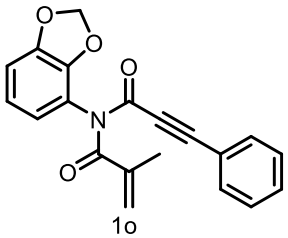
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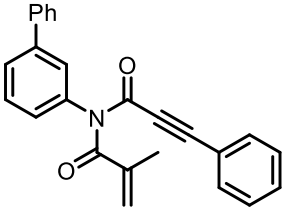
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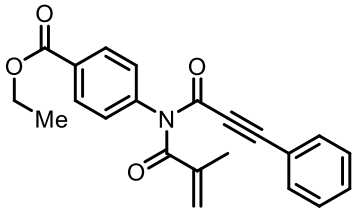
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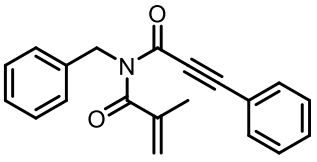
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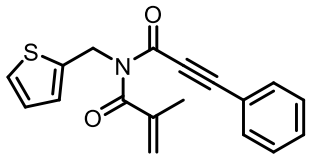
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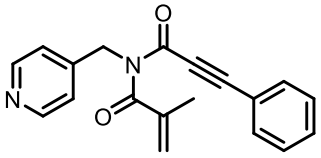
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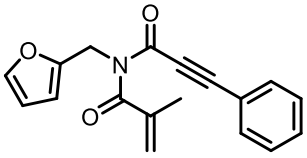
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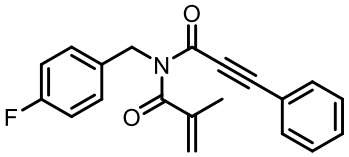
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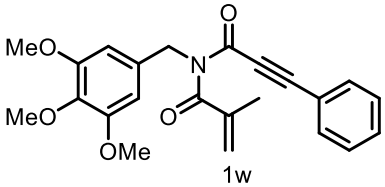
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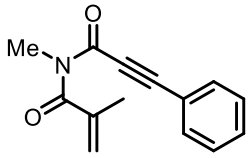
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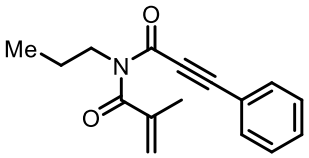
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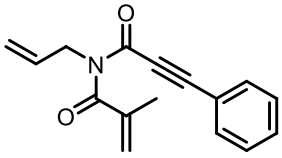
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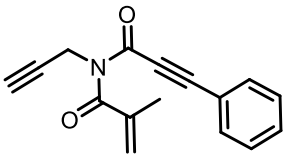
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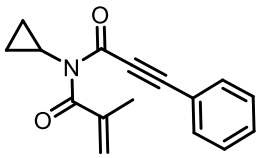
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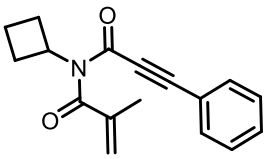
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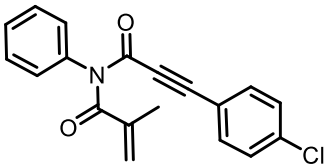
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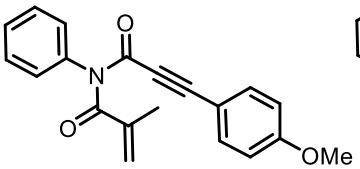
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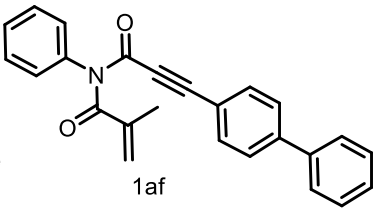
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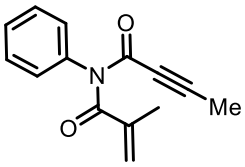
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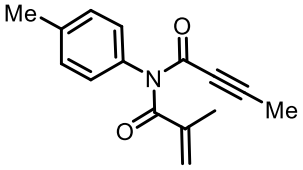
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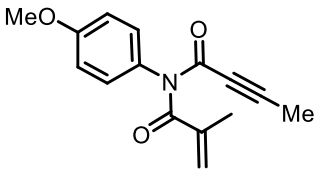
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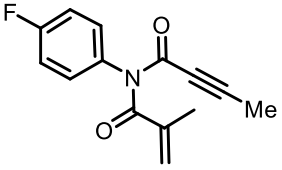
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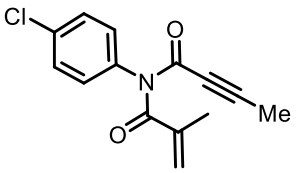
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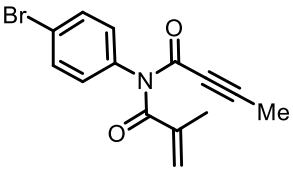
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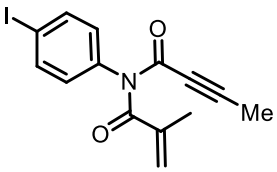
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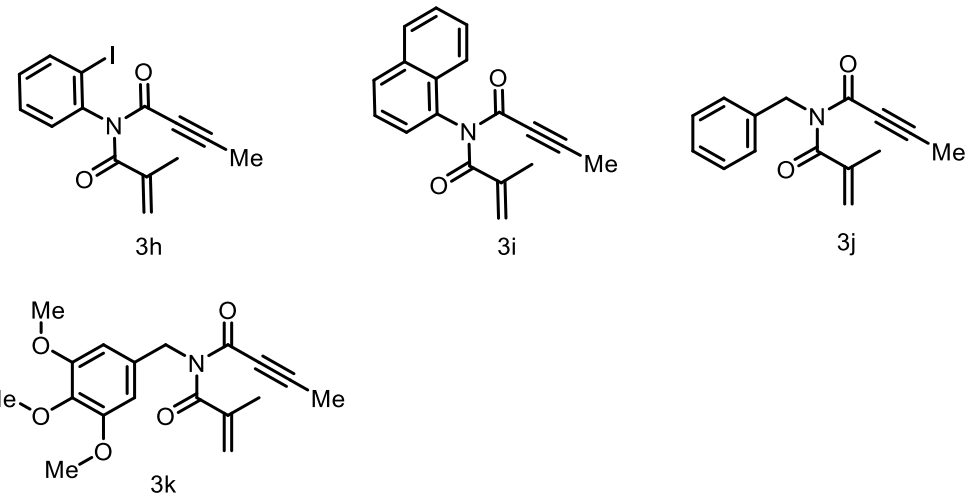
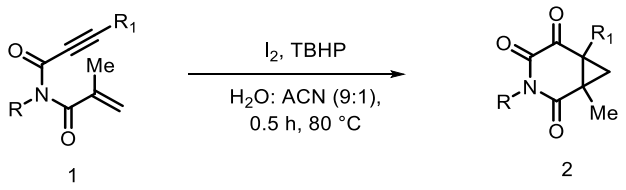


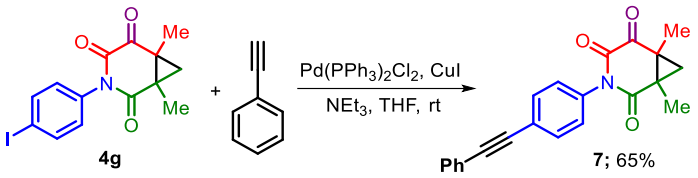
(6) General procedure for the Synthesis of bicyclo[4.1.0]heptane



An oven-dried round bottom flask equipped with a magnetic stir bar was charged with **1** (100 mg, 0.346 mmol) then I_2, TBHP, H_2O: ACN solution was added. The reaction mixture was then stirred at 80 °C oil bath for 0.5hrs (monitored reactions by TLC). Afterwards the solvent was removed under reduced pressure and the resulting residue was purified by silica gel column chromatography to afford pure product **2**.

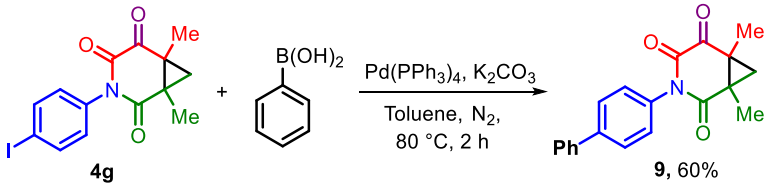
(7) General procedure for post functionalization of products

(7.1) Sonogashira Coupling



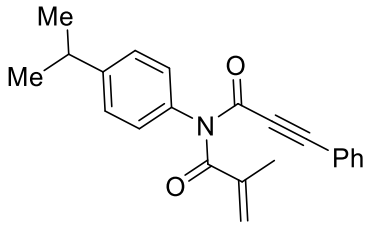
To a solution of the compound **4g** (0.2 mmol) and phenylacetylene (0.3 mmol) in NEt_3 (1.5 mL) and THF (1.5 mL) was added $PdCl_2(PPh_3)_2$ (7.02 mg, 0.01 mmol) and CuI (2.85 mg, 0.015 mmol) under an argon atmosphere. The reaction mixture was stirred at room temperature. The reaction progress was monitored by TLC. After completion of the reaction, the residue was extracted with EtOAc (10 mL x 3). The combined organic phases were dried over anhydrous Na_2SO_4 and evaporated under reduced pressure to remove the solvent. The given residue was purified by flash chromatography using a mixture of EtOAc and P.E. as eluent to provide the substrates **7**.

(7.2) Suzuki- Miyaura Coupling



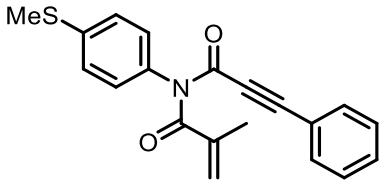
To a solution of compound **4g** (0.2 mmol,0.274 mmol), $Pd(OAc)_2$ (0.1 equiv, 0.02 mmol) in DMF (4 mL)and water (1 mL) was added phenylboronic acid (2 equiv, 0.4 mmol) and K_2CO_3 (2equiv, 0.4 mmol) and the mixture was stirred under reflux at 85°C. The reaction progress was monitored by TLC. After 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 (EtOAc/PE) to afford the desired product **9**.

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



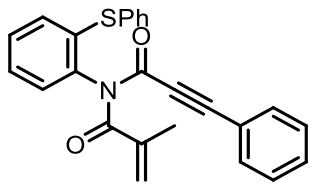
1g

***N*-(4-isopropylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide (1g):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1g** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.27 (t, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.18-7.15 (m, 1H), 7.13 (dd, *J* = 4.6, 2.1 Hz, 2H), 7.11-7.08 (m, 3H), 5.61 (s, 1H), 5.41 (s, 1H), 2.90-2.83 (m, 1H), 1.96 (s, 3H), 1.18 (d, J = 7.0 Hz, 6H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.2, 154.4, 149.5, 141.3, 135.4, 132.7, 132.4, 130.7, 128.4, 128.3, 127.3, 127.2, 126.6, 122.0, 119.9, 119.3, 94.3, 82.6, 33.7, 23.7, 18.6, 17.7; **MS** (ESI) *m/z* 332 $[M+H]^+$; HRMS Calculated for $C_{22}H_{22}NO_2^+$ 332.1645; Found: 332.1652. $[M+H]^+$.



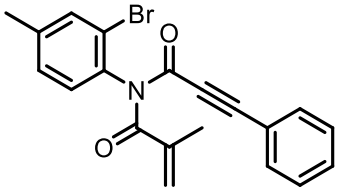
1i

***N*-(2,6-diethylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide (1i):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1i** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.44-7.38 (m, 1H), 7.33-7.28 (m, 6H), 7.22-7.19 (m, 2H), 5.71 (s, 1H), 5.54 (s, 1H), 2.49 (s, 3H), 2.05 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.1, 154.3, 141.3, 139.9, 134.4, 132.7, 132.4, 130.8, 129.7, 128.8, 128.5, 128.1, 127.5, 126.7, 122.5, 119.3, 94.5, 82.6, 18.7, 15.5; **MS** (ESI) *m/z* 336 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}NO_2S^+$ 336.1083; Found: 336.1115. $[M+H]^+$.



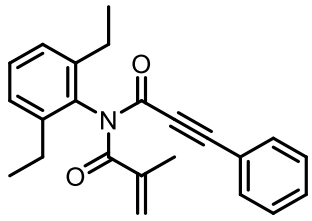
1l

***N*-(3-phenylpropioloyl)-*N*-(2-(phenylthio)phenyl)methacrylamide (1l):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1l** as brown solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.42-7.33 (m, 6H), 7.32-7.26 (m, 3H), 7.25-7.22 (m, 5H), 5.78 (s, 1H), 5.47 (d, *J* = 1.5 Hz, 1H), 2.12 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 172.5, 154.2, 141.3, 137.4, 137.3, 133.7, 132.9, 132.3, 132.1, 130.8, 130.6, 129.8, 129.3, 128.5, 127.8, 127.7, 121.2, 119.4, 94.0, 82.8, 19.0; **MS** (ESI) *m/z* 398 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}NO_2S^+$ 398.1209; Found: 398.1239. $[M+H]^+$.



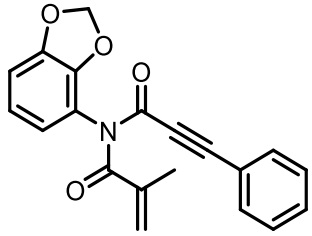
1m

***N*-(2-bromo-4-methylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide (1m):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1m** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.56 (s, 1H), 7.44-7.40 (m, 1H), 7.35-7.23 (m, 6H), 5.78 (s, 1H), 5.50 (s, 1H), 2.41 (s, 3H), 2.14 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 172.1, 154.0, 141.2, 141.1, 134.3, 133.9, 132.8, 130.9, 130.8, 129.1, 128.5, 123.5, 121.2, 119.4, 94.1, 82.5, 20.9, 19.0; **MS** (ESI) *m/z* 382 $[M+H]^+$; HRMS Calculated for $C_{20}H_{17}BrNO_2^+$ 382.0437; Found: 382.0440. $[M+H]^+$.



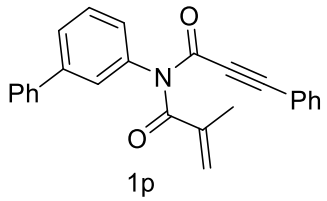
1n

***N*-(2,6-diethylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide (1n):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1n** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.45-7.39 (m, 2H), 7.32-7.26 (m, 4H), 7.16 (d, *J* = 8.0 Hz, 2H), 5.60 (s, 1H), 5.47 (s, 1H), 2.63 (q, *J* = 7.5 Hz, 4H), 2.18 (s, 3H), 1.26 (t, *J* = 7.6 Hz, 6H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 172.6, 155.3, 142.5, 142.1, 134.9, 133.1, 130.9, 129.7, 128.5, 126.6, 119.4, 119.2, 93.9, 82.6, 29.7, 24.4, 19.4, 14.3; **MS** (ESI) *m/z* 346 $[M+H]^+$; HRMS Calculated for $C_{23}H_{24}NO_2^+$ 346.1842; Found: 386.1869. $[M+H]^+$.



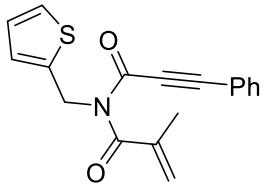
1o

***N*-(2,6-diethylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide (1o):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1o** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.41-7.30 (m, 5H), 6.91-6.86 (m, 2H), 6.78-6.76 (m, 1H), 5.98 (s, 2H), 5.74 (s, 1H), 5.52 (d, *J* = 1.0 Hz, 1H), 2.06 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 172.7, 153.8, 148.9, 143.9, 141.0, 132.9, 132.7, 131.0, 128.7, 122.7, 122.1, 121.9, 120.2, 119.5, 109.1, 101.9, 93.7, 82.5, 18.8; **MS** (ESI) *m/z* 334 $[M+H]^+$; HRMS Calculated for $C_{20}H_{16}NO_4^+$ 334.1074; Found: 334.1082. $[M+H]^+$.



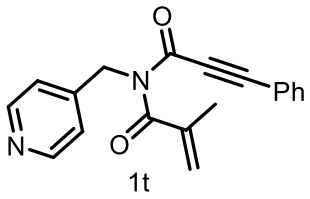
1p

***N*-([1,1'-biphenyl]-3-yl)-*N*-(3-phenylpropioloyl)methacrylamide (1p):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1p** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.3 Hz, 1H), 7.63-7.55 (m, 4H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.41-7.37 (m, 2H), 7.34-7.29 (m, 5H), 5.81 (s, 1H), 5.60 (s, 1H), 2.13 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.2, 154.3, 142.6, 141.3, 139.7, 138.2, 132.7, 130.8, 129.6, 128.8, 128.4, 127.7, 127.4, 127.3, 127.2, 127.1, 122.5, 119.3, 94.5, 82.6, 18.7; **MS** (ESI) *m/z* 366 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}NO_2^+$ 366.1489; Found: 366.1497. $[M+H]^+$.



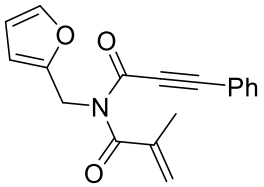
1s

***N*-(3-phenylpropioloyl)-*N*-(thiophen-2-ylmethyl)methacrylamide (1s):** Purification by silica gel chromatography (PE:EA=90:10) afforded the desired **1s** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 2H), 7.20 (t, *J* = 4.0 Hz, 1H), 7.09 (d, *J* = 2.3 Hz, 1H), 6.92 (t, *J* = 4.1 Hz, 1H), 5.44 (s, 1H), 5.38 (s, 1H), 5.21 (s, 2H), 2.06 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.6, 154.2, 142.0, 138.2, 132.6, 132.3, 130.7, 129.4, 128.8, 128.6, 128.2, 127.8, 127.5, 126.8, 126.6, 126.5, 125.8, 122.3, 119.3, 94.5, 82.6, 42.4, 18.7; **MS** (ESI) *m/z* 310 $[M+H]^+$; HRMS Calculated for $C_{18}H_{16}NO_2S^+$ 310.0896; Found: 310.0899. $[M+H]^+$.



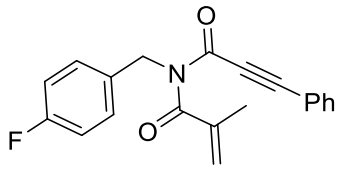
1t

***N*-(3-phenylpropioloyl)-*N*-(pyridin-4-ylmethyl)methacrylamide (1t):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1t** as purple solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, DMSO-*d6*) δ 8.51 (d, *J* = 1.2 Hz, 2H), 7.75 (d, *J* = 3.4 Hz, 2H), 7.51 (s, 2H), 7.39 (d, *J* = 4.7 Hz, 3H), 6.91 (s, 1H), 6.65 (s, 1H), 5.36 (s, 1H), 5.29 (s, 1H), 1.89 (s, 3H); **^{13}C-NMR** (100 MHz, DMSO-*d6*) δ 168.6, 168.6, 161.4, 150.0, 145.9, 140.4, 131.1, 130.0, 128.9, 128.7, 127.9, 122.8, 119.9, 119.5, 62.4, 18.5; **MS** (ESI) *m/z* 305 $[M+H]^+$; HRMS Calculated for $C_{19}H_{17}N_2O_2^+$ 305.1285; Found: 305.1522. $[M+H]^+$.



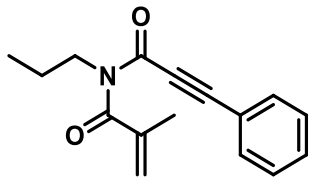
1u

***N*-(furan-2-ylmethyl)-*N*-(3-phenylpropioloyl)methacrylamide (1u):** Purification by silica gel chromatography (PE:EA=90:10) afforded the desired **1u** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.3 Hz, 2H), 7.44-7.41 (m, 1H), 7.37 (q, *J* = 3.7 Hz, 2H), 7.22-7.20 (m, 1H), 7.09 (s, 1H), 6.91 (t, *J* = 3.5 Hz, 1H), 5.44 (s, 1H), 5.38 (s, 1H), 5.21 (s, 2H), 2.06 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.7, 154.4, 142.1, 138.3, 132.4, 130.8, 128.7, 127.9, 126.6, 125.9, 122.4, 119.5, 94.6, 82.7, 42.6, 18.7; **MS** (ESI) *m/z* 294 $[M+H]^+$; HRMS Calculated for $C_{18}H_{16}NO_3^+$ 294.1125; Found: 294.1138. $[M+H]^+$.



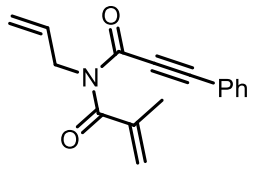
1v

***N*-(4-fluorobenzyl)-*N*-(3-phenylpropioloyl)methacrylamide (1v):** Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **1v** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.50-7.45 (m, 2H), 7.44-7.36 (m, 5H), 7.01 (t, *J* = 8.8 Hz, 2H), 5.47 (s, 1H), 5.37 (s, 1H), 5.02 (s, 2H), 2.09 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 174.1, 163.5, 161.0, 154.8, 142.3, 132.4, 130.8, 130.5, 130.4, 128.7, 128.0, 122.6, 119.5, 115.7, 115.5, 115.3, 94.6, 82.9, 47.2, 18.8; **^{19}F NMR** (376 MHz, $CDCl_3$) δ −112.9 (s, 1F); **MS** (ESI) *m/z* 322 $[M+H]^+$; HRMS Calculated for $C_{20}H_{17}FNO_2^+$ 322.1238; Found: 322.1242. $[M+H]^+$.



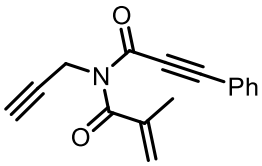
1y

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



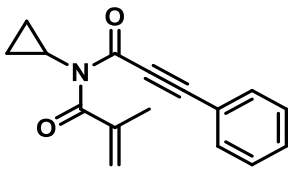
1z

***N*-allyl-*N*-(3-phenylpropioloyl)methacrylamide (1z):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1z** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.38-7.36 (m, 2H), 7.34-7.28 (m, 1H), 7.26-7.21 (m, 2H), 5.83-5.72 (m, 1H), 5.37-5.36 (m, 2H), 5.15 (dq, *J* = 17.1, 1.3 Hz, 1H), 5.07 (dq, *J* = 10.3, 1.2 Hz, 1H), 4.35-4.33 (m, 2H), 1.95 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.3, 171.7, 158.4, 130.9, 130.7, 130.6, 128.9, 119.6, 45.5, 43.7, 34.8, 29.1, 16.1; **MS** (ESI) *m/z* 254 $[M+H]^+$; HRMS Calculated for $C_{16}H_{16}NO_2^+$ 254.1176; Found: 254.1168. $[M+H]^+$.



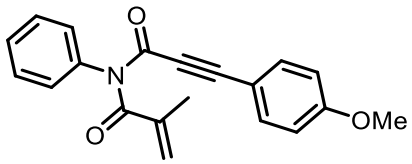
1aa

***N*-(3-phenylpropioloyl)-*N*-(prop-2-yn-1-yl)methacrylamide (1aa):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1aa** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.48-7.39 (m, 3H), 7.35-7.31 (m, 2H), 5.55-5.51 (m, 2H), 4.56 (d, *J* = 2.5 Hz, 2H), 2.25 (t, *J* = 2.5 Hz, 1H), 2.04 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.6, 154.4, 142.2, 132.4, 132.2, 130.8, 128.7, 121.7, 119.5, 93.7, 82.8, 47.0, 18.9; **MS** (ESI) *m/z* 252 $[M+H]^+$; HRMS Calculated for $C_{16}H_{14}NO_2^+$ 252.1019; Found: 252.1012. $[M+H]^+$.



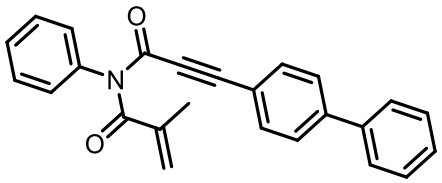
1ab

***N*-cyclopropyl-*N*-(3-phenylpropioloyl)methacrylamide (1ab):** Purification by silica gel chromatography (PE:EA=98:2) afforded the desired **1ab** as yellow semisolid in 80% yield (1.52 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.53-7.51 (m, 2H), 7.45-7.41 (m, 1H), 7.38-7.34 (m, 2H), 5.54-5.52 (m, 2H), 2.91-2.86 (m, 1H), 2.01 (s, 3H), 1.07 (q, *J* = 6.8 Hz, 2H), 0.75-0.71 (m, 2H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 175.3, 155.7, 142.4, 132.7, 130.8, 128.7, 123.2, 120.0, 93.3, 82.8, 28.1, 18.3, 9.2; **MS** (ESI) *m/z* 254 $[M+H]^+$; HRMS Calculated for $C_{16}H_{16}NO_2^+$ 254.1176; Found: 254.1197. $[M+H]^+$.



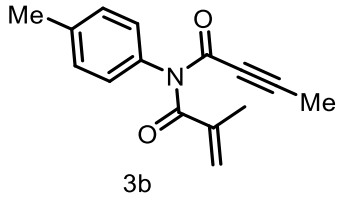
1ae

***N*-(3-(4-methoxyphenyl)propioloyl)-*N*-phenylmethacrylamide (1ae):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1ae** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.3 Hz, 1H), 7.51-7.43 (m, 3H), 7.34-7.29 (m, 3H), 7.17 (dd, *J* = 6.9, 1.9 Hz, 1H), 6.80 (dd, *J* = 7.0, 2.0 Hz, 1H), 5.69 (s, 1H), 5.51 (d, *J* = 1.3 Hz, 1H), 3.79 (s, 3H), 2.07 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.4, 161.7, 154.7, 141.6, 138.1, 134.9, 134.4, 131.4, 129.3, 129.0, 128.8, 128.8, 122.0, 120.4, 114.3, 111.3, 95.7, 82.5, 55.4, 18.8; **MS** (ESI) *m/z* 320 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}NO_3^+$ 320.1281; Found: 320.1287. $[M+H]^+$.



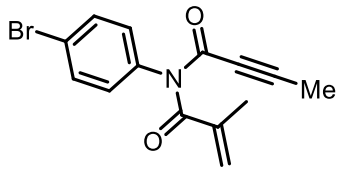
1af

***N*-(3-([1,1'-biphenyl]-4-yl)propioloyl)-*N*-phenylmethacrylamide (1af):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **1af** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.57-7.52 (m, 4H), 7.51-7.44 (m, 5H), 7.41-7.33 (m, 5H), 5.75 (s, 1H), 5.57 (d, *J* = 1.3 Hz, 1H), 2.10 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.4, 154.5, 143.7, 141.5, 139.7, 138.0, 133.4, 133.1, 129.4, 129.0, 128.9, 128.8, 128.3, 127.2, 127.1, 122.4, 120.0, 118.3, 94.7, 83.4, 30.3, 29.8, 25.3, 18.9, 18.8; **MS** (ESI) *m/z* 366 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}NO_2^+$ 366.1489; Found: 366.1498. $[M+H]^+$.



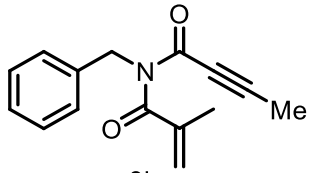
3b

***N*-methacryloyl-*N*-(p-tolyl)but-2-ynamide (3b):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **3b** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.15 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.2 Hz, 2H), 5.60 (s, 1H), 5.43 (s, 1H), 2.29 (s, 3H), 1.94 (s, 3H), 1.78 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.5, 154.4, 141.4, 138.5, 135.1, 129.9, 128.0, 122.5, 93.7, 74.6, 21.1, 18.6, 4.0; **MS** (ESI) *m/z* 242 $[M+H]^+$; HRMS Calculated for $C_{15}H_{16}NO_2^+$ 242.1176; Found: 242.1181. $[M+H]^+$.



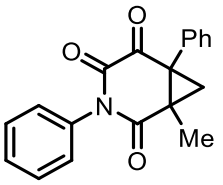
3f

***N*-(4-bromophenyl)-*N*-methacryloylbut-2-ynamide (3f):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **3f** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.4 Hz, 1H), 7.07(d, *J* = 8.8 Hz, 1H), 5.65 (s, 1H), 5.35 (s, 2H), 2.00 (s, 3H), 1.90 (s, 3H)); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 173.2, 153.9, 141.3, 136.7, 132.6, 132.0, 131.9, 129.9, 123.1, 122.6, 121.7, 121.4, 94.4, 74.5, 18.7, 4.3; **MS** (ESI) *m/z* 306 $[M+H]^+$; HRMS Calculated for $C_{14}H_{13}BrNO_2^+$ 306.0124; Found: 306.0140. $[M+H]^+$.



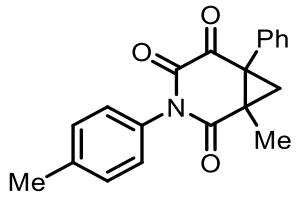
3j

***N*-benzyl-*N*-methacryloylbut-2-ynamide (3j):** Purification by silica gel chromatography (PE:EA=75:25) afforded the desired **3j** as white solid in 85% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.37-7.28 (m, 4H), 5.38 (s, 1H), 5.29 (s, 1H), 5.00 (s, 2H), 2.02 (s, 3H), 1.99 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 170.3, 150.7, 149.0, 138.5, 133.2, 128.4, 117.6, 101.4, 90.0, 70.9, 56.6, 51.9, 44.0, 14.5; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{15}H_{16}NO_2^+$ 242.1176; Found: 242.1179. $[M+H]^+$.



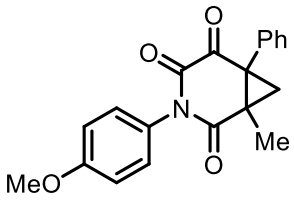
2a

1-methyl-3,6-diphenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2a): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2a** as white solid in 85% yield (89.70 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.54-7.45 (m, 6H), 7.29-7.27 (m, 2H), 7.21-7.18 (m, 2H), 2.58 (d, *J* = 6.0 Hz, 1H), 2.24 (d, *J* = 6.0 Hz, 1H), 1.30 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.7, 172.2, 158.8, 134.0, 130.8, 130.7, 129.5, 129.3, 129.0, 129.0, 128.5, 127.9, 45.8, 35.3, 29.1, 16.2; **MS** (ESI) *m/z* 306 $[M+H]^+$; HRMS Calculated for $C_{19}H_{16}NO_3^+$ 306.1125; Found: 306.1136 $[M+H]^+$.



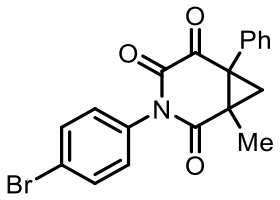
2b

1-methyl-6-phenyl-3-(*p*-tolyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2b): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2b** as white solid in 82% yield (90.60 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.41-7.34 (m, 3H), 7.25-7.20 (m, 2H), 7.18-7.15 (m, 2H), 6.92-7.03 (2H), 2.46 (d, J = 6.0 Hz, 1H), 2.33 (s, 3H), 2.12 (s, 1H), 1.19 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.7, 172.3, 158.9, 139.3, 131.3, 130.8, 130.6, 130.2, 128.9, 127.4, 45.7, 35.2, 29.0, 21.2, 16.2; **MS** (ESI) *m/z* 320 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}NO_3^+$ 320.1281; Found: 320.1266. $[M+H]^+$.



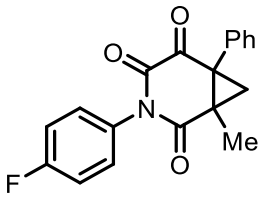
2c

3-(4-methoxyphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2c): Purification by silica gel chromatography (PE:EA=80:20) afforded the desired **2c** as white solid in 80% yield (92.74 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.46-7.42 (m, 3H), 7.25-7.23 (m, 2H), 7.09-7.06 (m, 2H), 7.01-6.98 (m, 2H), 3.84 (s, 3H), 2.52 (d, *J* = 6.0 Hz, 1H), 2.20 (d, *J* = 5.9 Hz, 1H), 1.27 (s, 3H**)**; **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.7, 172.3, 159.9, 159.0, 130.8, 130.7, 129.0, 128.8, 126.4, 114.8, 55.5, 45.8, 35.2, 29.0, 16.2; **MS** (ESI) *m/z* 336 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}NO_4^+$ 336.1230; Found: 336.1209. $[M+H]^+$.



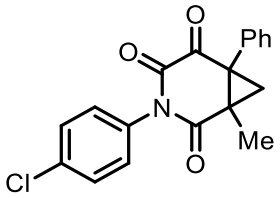
2d

3-(4-bromophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2d): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2d** as brown solid in 75% yield (99.69 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.64-7.60 (m, 2H), 7.47-7.43 (m, 3H), 7.25-7.22 (m, 2H), 7.07-7.03 (m, 2H), 2.54 (d, *J* = 6.0 Hz, 1H), 2.22 (d, *J* = 6.0 Hz, 1H), 1.27 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.3, 171.9, 158.5, 132.8, 132.7, 130.6, 129.6, 129.1, 129.0, 123.3, 45.8, 35.2, 29.1, 16.2; **MS** (ESI) *m/z* 384 $[M+H]^+$; HRMS Calculated for $C_{19}H_{15}BrNO_3^+$ 384.0230; Found: 384.0208. $[M+H]^+$.



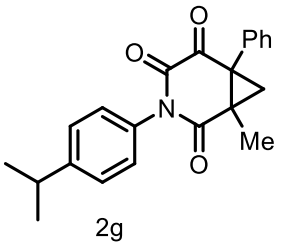
2e

3-(4-fluorophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2e): Purification by silica gel chromatography (PE:EA=80:20) afforded the desired **2e** as white solid in 70% yield (78.3 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.46-7.43 (m, 3H), 7.25-7.23 (m, 2H), 7.20-7.14 (m, 4H), 2.53 (d, J = 6.2 Hz, 1H), 2.22 (d, J = 6.2 Hz, 1H), 1.24-1.28 (s, 3H**)**; **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.4, 172.1, 160.1 (d, $J_{C\text{-}F}$ = 266.4 Hz, 1C), 130.6, 130.1, 129.7 (d, $J_{C\text{-}F}$ = 8.7 Hz, 1C), 129.1, 129.0, 128.5, 116.6 (d, $J_{C\text{-}F}$ = 23 Hz, 1C), 45.8, 35.2, 29.1, 16.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ −111.5 (s, 1F) **MS** (ESI) *m/z* 324 $[M+H]^+$; HRMS Calculated for $C_{19}H_{15}FNO_3^+$ 324.1030; Found: 324.1009. $[M+H]^+$.



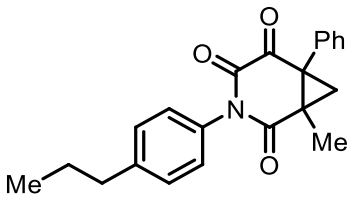
2f

3-(4-chlorophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2f): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2f** as white solid in 82% yield (96.39 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.45-7.42 (m, 5H), 7.23-7.21 (m, 2H), 7.10 (d, J = 8.7 Hz, 2H), 2.55 (d, J = 6.0 Hz, 1H), 2.19 (d, J = 6.0 Hz, 1H), 1.25 (s, 3H**)**; **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.4, 172.0, 158.5, 135.2, 132.3, 130.6, 129.7, 129.3, 129.0, 129.0, 45.8, 35.2, 29.7, 29.1, 16.2; **MS** (ESI) *m/z* 340 $[M+H]^+$; HRMS Calculated for $C_{19}H_{15}ClNO_3^+$ 340.0735; Found: 340.0748. $[M+H]^+$.



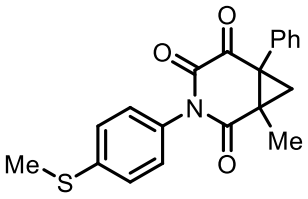
2g

3-(4-*iso*propylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2g): Purification by silica gel chromatography (PE:EA=83:17) afforded the desired **2g** as white solid in 73% yield (87.73 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.49-7.45 (m, 3H), 7.37 (d, *J* = 8.3 Hz, 2H), 7.29-7.26 (m, 2H), 7.10 (d, *J* = 8.3 Hz, 2H), 3.02-2.95 (m, 1H), 2.57 (d, *J* = 6.0 Hz, 1H), 2.24 (d, *J* = 6.0 Hz, 1H), 1.30 (d, *J* = 7.0 Hz, 6H), 0.91 (t, *J* = 7.0 Hz, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 207.1, 186.8, 172.4, 158.9, 149.9, 131.5, 130.9, 130.7, 129.0, 127.6, 127.5, 45.8, 33.9, 31.0, 29.1, 23.9, 16.3, 14.2; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{22}H_{22}NO_3^+$ 348.1594; Found: 348.1589. $[M+H]^+$.



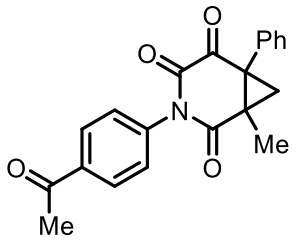
2h

1-methyl-6-phenyl-3-(4-propylphenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2h): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2h** as white solid in 81% yield (97.66 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.37-7.33 (m, 3H), 7.21 (s, 1H), 7.19 (s, 1H), 7.17-7.14 (m, 2H), 6.99-6.96 (m, 2H), 2.57-2.53 (m, 2H), 2.46 (d, *J* = 6.0 Hz, 1H), 2.11 (d, *J* = 6.2 Hz, 1H), 1.62-1.55 (m, 2H), 1.17 (s, 3H), 0.89 (t, *J* = 7.4 Hz, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.7, 172.2, 158.8, 143.8, 131.4, 130.8, 130.6, 129.4, 128.9, 127.4, 45.7, 37.6, 35.1, 29.0, 24.2, 16.1, 13.8; **MS** (ESI) *m/z* 348 $[M+H]^+$; HRMS Calculated for $C_{22}H_{22}NO_3^+$ 348.1594; Found: 348.1578. $[M+H]^+$.



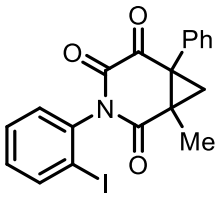
2i

1-methyl-3-(4-(methylthio)phenyl)-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2i): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2i** as brown solid in 78% yield (94.83 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.47-7.43 (m, 3H), 7.35-7.32 (m, 2H), 7.26-7.23 (m, 2H), 7.10-7.06 (m, 2H), 2.54 (d, *J* = 6.0 Hz, 1H), 2.51 (s, 3H), 2.22 (d, *J* = 6.0 Hz, 1H), 1.27 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.6, 172.2, 158.8, 140.5, 130.7, 130.6, 130.6, 129.0, 128.1, 126.9, 45.8, 35.2, 29.1, 16.2, 15.5; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}NO_3S^+$ 352.1002; Found: 352.0992. $[M+H]^+$.



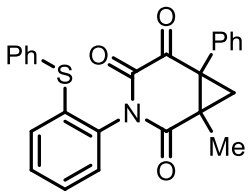
2j

3-(4-acetylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2j): Purification by silica gel chromatography (PE:EA=80:20) afforded the desired **2j** as colourless oil in 69% yield (82.92 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 8.02-7.99 (m, 2H), 7.40-7.36 (m, 3H), 7.23-7.20 (m, 2H), 7.19-7.17 (m, 2H), 2.57 (s, 3H), 2.49 (d, *J* = 6.2 Hz, 1H), 2.18 (d, *J* = 6.0 Hz, 1H), 1.21 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 196.9, 186.2, 171.9, 158.4, 138.0, 137.5, 130.6, 130.6, 129.5, 129.1, 129.0, 128.3, 45.9, 35.3, 29.1, 26.7, 16.2; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{21}H_{18}NO_4^+$ 348.1230; Found: 348.1223. $[M+H]^+$.



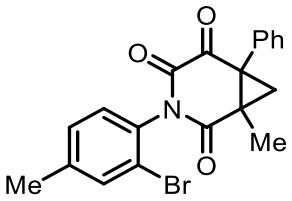
2k

3-(2-iodophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2k): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2k** as white solid in 80% yield (119.35 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.44-7.36 (m, 4H), 7.21-7.18 (m, 2H), 7.14-7.10 (m, 2H), 3.06 (d, *J* = 6.2 Hz, 1H), 2.19 (d, *J* = 6.0 Hz, 1H), 1.24 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.2, 171.0, 157.8, 139.9, 137.2, 131.0, 131.0, 130.6, 129.9, 129.6, 129.0, 97.3, 46.2, 35.7, 29.3, 16.3; **MS** (ESI) *m/z* 432 $[M+H]^+$; HRMS Calculated for $C_{19}H_{15}INO_3^+$ 432.0091; Found: 432.0083. $[M+H]^+$.



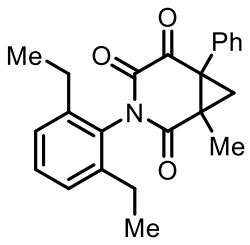
2l

1-methyl-6-phenyl-3-(2-(phenylthio)phenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2l): Purification by silica gel chromatography (PE:EA=80:20) afforded the desired **2l** as white solid in 67% yield (95.85 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.47-7.42 (m, 4H), 7.40 (d, *J* = 3.8 Hz, 2H), 7.35-7.34 (m, 4H), 7.32-7.25 (m, 4H), 2.95 (d, *J* = 5.9 Hz, 1H), 2.20 (d, *J* = 6.0 Hz, 1H), 1.28 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.8, 171.8, 158.4, 134.8, 134.4, 134.3, 133.8, 131.2, 131.1, 130.7, 130.4, 129.7, 129.5, 129.0, 128.8, 127.6, 46.2, 35.6, 29.3, 16.2; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}NO_3S^+$ 414.1158; Found: 414.1159. $[M+H]^+$.



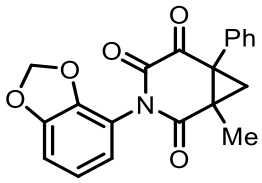
2m

3-(2-bromo-4-methylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2m): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2m** as white solid in 74% yield (106.22 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ7.56 (d, *J* = 6.8 Hz, 1H), 7.50-7.45 (m, 3H), 7.29-7.26 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 1H), 2.95 (d, *J* = 6.0 Hz, 1H), 2.42 (s, 3H), 2.26 (d, *J* = 6.0 Hz, 1H), 1.30 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.5, 171.3, 158.0, 141.7, 133.9, 131.0, 130.7, 130.0, 129.5, 129.0, 121.6, 46.1, 35.5, 29.2, 21.0, 16.2; **MS** (ESI) *m/z* 398 $[M+H]^+$; HRMS Calculated for $C_{20}H_{17}BrNO_3^+$ 398.0386; Found: 398.0400. $[M+H]^+$.



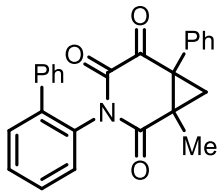
2n

3-(2-bromo-4-methylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2n): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2n** as white solid in 76% yield (97.78 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.51-7.46 (m, 3H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.30-7.23 (m, 4H), 2.60 (d, *J* = 6.0 Hz, 1H), 2.56-2.46 (m, 2H), 2.44-2.32 (m, 2H), 2.29 (d, *J* = 6.0 Hz, 1H), 1.32 (s, 3H), 1.24 (t, *J* = 7.6 Hz, 3H), 1.20 (t, *J* = 7.6 Hz, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.5, 171.3, 158.0, 141.7, 133.9, 131.0, 130.7, 130.0, 129.5, 129.0, 121.6, 46.1, 35.5, 29.2, 21.0, 16.2; **MS** (ESI) *m/z* 362 $[M+H]^+$; HRMS Calculated for $C_{23}H_{24}NO_3^+$ 362.1751; Found: 362.1768. $[M+H]^+$.



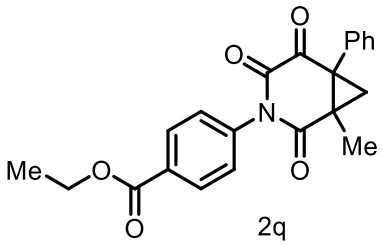
2o

3-(benzo[*d*][1,3]dioxol-4-yl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2o): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2o** as white solid in 80% yield (96.6 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.0 Hz, 3H), 7.29-7.26 (m, 3H), 6.94 (q, *J* = 7.9 Hz, 2H), 6.04 (d, *J* = 6.0 Hz, 2H), 2.60 (d, *J* = 6.0 Hz, 1H), 2.24 (d, *J* = 5.8 Hz, 1H), 1.30 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.6, 171.4, 148.9, 130.8, 130.7, 129.1, 129.0, 122.1, 121.5, 109.5, 102.0, 45.9, 35.3, 29.3, 16.2; **MS** (ESI) *m/z* 350 $[M+H]^+$; HRMS Calculated for $C_{20}H_{16}NO_5^+$ 350.1023; Found: 350.1020. $[M+H]^+$.



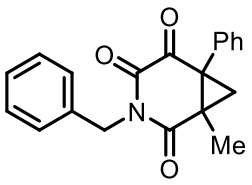
2p

3-([1,1'-biphenyl]-2-yl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2p): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2p** as white solid in 60% yield (79.18 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 1H), 7.58-7.52 (m, 3H), 7.45-7.41 (m, 5H), 7.37-7.34 (m, 2H), 7.26-7.23 (m, 2H), 7.13 (s, 1H), 2.58 (d, *J* = 6.0 Hz, 1H), 2.23 (d, *J* = 6.0 Hz, 1H), 1.27 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.7, 172.3, 158.8, 142.9, 139.9, 134.4, 130.8, 130.7, 129.9, 129.1, 129.0, 128.9, 128.0, 127.8, 127.3, 126.7, 126.5, 45.9, 35.3, 29.2, 16.3; **MS** (ESI) *m/z* 382 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}NO_3^+$ 382.1438; Found: 382.1440. $[M+H]^+$.



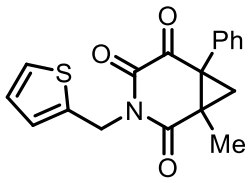
2q

ethyl 4-(1-methyl-2,4,5-trioxo-6-phenyl-3-azabicyclo[4.1.0]heptan-3-yl)benzoate (2q): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2q** as white solid in 65% yield (84.87 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.8 Hz, 2H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.66 (d, *J* = 7.0 Hz, 1H), 7.52-7.44 (m, 3H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.24 (s, 1H), 4.43-4.35 (m, 2H), 2.56 (d, *J* = 6.3 Hz, 1H), 2.25 (d, *J* = 6.3 Hz, 1H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.28 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 207.2, 186.3, 171.8, 165.5, 137.7, 130.8, 130.7, 129.1, 129.0, 128.2, 128.1, 128.0, 122.8, 61.3, 35.3, 30.1, 29.0, 16.3, 14.1; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{22}H_{20}NO_5^+$ 378.1336; Found: 378.1327. $[M+H]^+$.



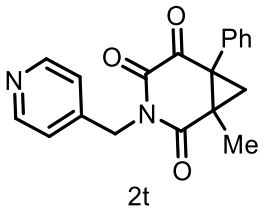
2r

3-benzyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2r): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2r** as white solid in 78% yield (90.73 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.44-7.41 (m, 2H), 7.40-7.37 (m, 3H), 7.36-7.29 (m, 3H), 7.17-7.14 (m, 2H), 5.05 (d, *J* = 13.7 Hz, 1H), 4.94 (d, *J* = 13.6 Hz, 1H), 2.17 (d, *J* = 6.2 Hz, 1H), 2.02 (d, *J* = 5.9 Hz, 1H), 1.21 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.3, 171.9, 158.7, 135.8, 133.1, 131.0, 130.9, 130.5, 129.2, 128.9, 128.6, 128.5, 128.0, 127.7, 127.6, 45.5, 44.8, 34.8, 28.9, 16.1; **MS** (ESI) *m/z* 320 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}NO_3^+$ 320.1281 ; Found: 320.1281. $[M+H]^+$.



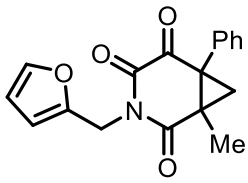
2s

1-methyl-6-phenyl-3-(thiophen-3-ylmethyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2s): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2s** as yellow solid in 70% yield (78.80 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.42-7.39 (m, 4H), 7.17-7.14 (m, 3H), 6.96 (dd, *J* = 5.1, 3.6 Hz, 1H), 5.27 (d, *J* = 14.3 Hz, 1H), 5.09 (d, *J* = 14.3 Hz, 1H), 2.17 (d, *J* = 5.9 Hz, 1H), 2.04 (d, *J* = 5.9 Hz, 1H), 1.24 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.2, 171.7, 158.2, 148.7, 142.5, 131.0, 130.6, 128.9, 110.5, 109.7, 45.6, 37.5, 34.8, 29.0, 16.0; **MS** (ESI) *m/z* 326 $[M+H]^+$; HRMS Calculated for $C_{18}H_{16}NO_3S^+$ 326.0845; Found: 326.0851. $[M+H]^+$.



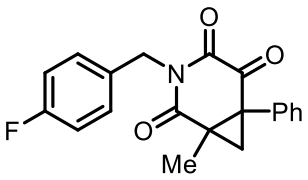
2t

3-(2-bromo-4-methylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2t): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2t** as white solid in 71% yield (3.56 g); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 8.53-8.44 (m, 2H), 7.55-7.52 (m, 1H), 7.36 (dd, *J* = 4.5, 1.6 Hz, 1H), 7.32-7.21 (m, 4H), 7.06 (dd, *J* = 4.5, 1.6 Hz, 1H), 5.38-5.31 (m, 2H), 1.97 (d, *J* = 5.9 Hz, 1H), 1.23 (m, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$) *δ* 186.8, 171.6, 158.4, 140.5, 137.8, 131.7, 131.6, 131.3, 130.6, 130.2, 129.6, 47.1, 46.9, 36.3, 29.9, 16.9; **MS** (ESI) *m/z* 321 $[M+H]^+$; HRMS Calculated for $C_{19}H_{17}N_2O_3^+$ 321.1234; Found: 321.1227. $[M+H]^+$.



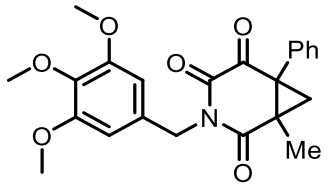
2u

3-(furan-3-ylmethyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2u): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2u** as white solid in 73% yield (78.07 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.42-7.39 (m, 3H), 7.26-7.25 (m, 3H), 7.17-7.15 (m, 2H), 6.96 (dd, *J* = 5.2, 3.5 Hz, 1H), 5.27 (d, *J* = 14.3 Hz, 1H), 5.09 (d, *J* = 14.3 Hz, 1H), 2.18 (d, *J* = 5.9 Hz, 1H), 2.04 (d, *J* = 5.9 Hz, 1H), 1.24 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.1, 171.7, 158.2, 148.7, 142.5, 130.9, 130.6, 129.0, 110.6, 109.7, 45.6, 37.5, 34.8, 29.1, 16.1; **MS** (ESI) *m/z* 310 $[M+H]^+$; HRMS Calculated for $C_{18}H_{16}NO_4^+$ 310.1074; Found: 310.1080. $[M+H]^+$.



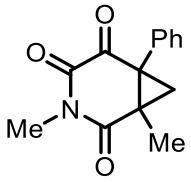
2v

3-(4-fluorobenzyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2v): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2v** as white solid in 74% yield (86.36 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.46-7.39 (m, 5H), 7.17-7.15 (m, 2H), 7.05-6.99 (m, 2H), 5.02 (d, *J* = 13.7 Hz, 1H), 4.91 (d, *J* = 13.7 Hz, 1H), 2.15 (d, *J* = 5.9 Hz, 1H), 2.04 (d, *J* = 5.9 Hz, 1H), 1.22 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.2, 171.9, 162.5 (d, J_{C-F} = 245.3 Hz, 1C), 158.7, 131.6, 131.4 (d, J_{C-F} = 8.6 Hz, 1C), 130.8, 130.5, 129.0, 115.6 (d, J_{C-F} = 22 Hz, 1C), 45.5, 44.1, 34.8, 29.7, 29.0, 16.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ −111.5 (s, 1F); **MS** (ESI) *m/z* 338 $[M+H]^+$; HRMS Calculated for $C_{20}H_{17}FNO_3^+$ 338.1187; Found: 338.1179. $[M+H]^+$.



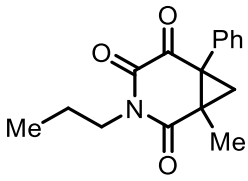
2w

3-(4-fluorobenzyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2w): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2w** as white solid in 68% yield (96.32 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.43-7.38 (m, 3H), 7.16 (dd, *J* = 4.3, 3.2 Hz, 2H), 6.70 (s, 2H), 4.96 (d, *J* = 13.5 Hz, 1H), 4.87 (d, *J* = 13.5 Hz, 1H), 3.85 (d, *J* = 3.7 Hz, 6H), 3.83 (d, J = 2.7 Hz, 3H), 2.17 (d, *J* = 5.8 Hz, 1H), 2.05 (d, *J* = 5.9 Hz, 1H), 1.22 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.3, 171.9, 158.7, 153.4, 153.1, 137.7, 131.3, 130.8, 130.5, 128.9, 128.5, 128.5, 106.7, 104.5, 60.8, 56.1, 45.5, 45.0, 43.9, 34.8, 29.0, 16.1; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{23}H_{24}NO_6^+$ 410.1598; Found: 410.1594 $[M+H]^+$.



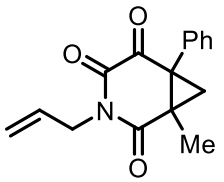
2x

1,3-dimethyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2x): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2x** as white solid in 78% yield (65.65 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.44-7.40 (m, 3H), 7.19-7.16 (m, 2H), 3.27 (s, 3H), 2.28 (d, *J* = 5.9 Hz, 1H), 2.09 (d, *J* = 5.9 Hz, 1H), 1.23 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.1, 172.3, 158.9, 130.9, 130.5, 128.9, 45.4, 34.7, 29.2, 28.1, 16.2; **MS** (ESI) *m/z* 244 $[M+H]^+$; HRMS Calculated for $C_{14}H_{14}NO_3^+$ 244.0968; Found: 244.0978. $[M+H]^+$.



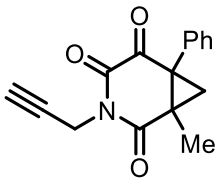
2y

1-methyl-6-phenyl-3-propyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2y): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2y** as white solid in 78% yield (73.21 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.64-7.62 (m, 1H), 7.43-7.39 (m, 3H), 7.19-7.17 (m, 1H), 2.24 (d, J = 5.8 Hz, 1H), 2.08 (d, J = 5.9 Hz, 1H), 1.70-1.59 (m, 4H), 1.23 (s, 3H), 1.00-0.93 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.5, 172.1, 158.8, 133.1, 131.1, 130.9, 130.6, 128.9, 128.7, 43.2, 34.7, 29.2, 22.2, 21.0, 16.2, 11.3; **MS** (ESI) *m/z* 272 $[M+H]^+$; HRMS Calculated for $C_{16}H_{18}NO_3^+$ 272.1281; Found: 272.1296. $[M+H]^+$.



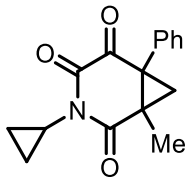
2z

1,3-dimethyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2z): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2z** as white solid in 73% yield (68.01 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.43-7.40 (m, 3H), 7.19-7.16 (m, 2H), 5.89-5.79 (m, 1H), 5.33-5.23 (m, 2H), 4.51 (dd, *J* = 14.2, 6.5 Hz, 1H), 4.36 (dd, *J* = 15.4, 5.8 Hz, 1H), 2.27 (d, *J* = 5.9 Hz, 1H), 2.09 (d, *J* = 5.9 Hz, 1H), 1.23 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.3, 171.7, 158.4, 130.9, 130.7, 130.6, 128.9, 119.6, 45.5, 43.7, 34.8, 29.1, 16.1; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{16}H_{16}NO_3^+$ 270.1125; Found: 270.1117. $[M+H]^+$.



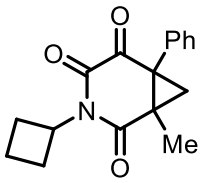
2aa

1-methyl-6-phenyl-3-(prop-2-yn-1-yl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2aa): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2aa** as brown solid in 72% yield (66.57 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.42-7.39 (m, 3H), 7.18-7.16 (m, 2H), 4.64 (dd, *J* = 16.6, 2.5 Hz, 1H), 4.53 (dd, *J* = 16.5, 2.5 Hz, 1H), 2.31 (d, *J* = 6.0 Hz, 1H), 2.23 (t, *J* = 2.5 Hz, 1H), 2.11 (d, *J* = 6.0 Hz, 1H), 1.24 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 185.7, 171.1, 157.5, 130.7, 130.5, 128.9, 76.9, 71.7, 45.6, 34.8, 30.6, 29.0, 16.0; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{16}H_{14}NO_3^+$ 268.0968; Found: 268.0971. $[M+H]^+$.



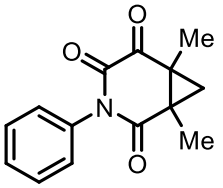
2ab

3-cyclopropyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2ab): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2ab** as white solid in 68% yield (63.35 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.44-7.39 (m, 3H), 7.18-7.15 (m, 2H), 2.74-2.68 (m, 1H), 2.18 (d, *J* = 5.9 Hz, 1H), 2.07 (d, *J* = 5.9 Hz, 1H), 1.25-1.15 (m, 4H), 1.12-1.05 (m, 1H), 0.91-0.83 (m, 1H), 0.66-0.59 (m, 1H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.3, 173.0, 159.4, 131.0, 130.5, 128.9, 45.8, 35.0, 29.1, 25.3, 16.0, 9.0, 7.1; **MS** (ESI) *m/z* 270 $[M+H]^+$; HRMS Calculated for $C_{16}H_{16}NO_3^+$ 270.1125; Found: 270.1133. $[M+H]^+$.



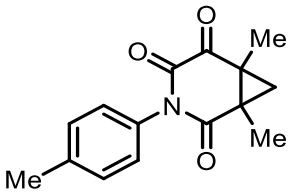
2ac

3-cyclobutyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (2ac): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **2ac** as white solid in 65% yield (63.71 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.42-7.38 (m, 3H), 7.18-7.15 (m, 2H), 4.92-4.83 (m, 1H), 2.70-2.59 (m, 2H), 2.35-2.29 (m, 3H), 2.08 (d, *J* = 5.9 Hz, 1H), 1.92-1.85 (m, 1H), 1.82-1.74 (m, 1H), 1.20 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.7, 172.6, 159.0, 132.0, 130.6, 130.1, 128.9, 128.8, 49.2, 45.6, 35.1, 29.2, 28.7, 27.7, 16.1, 15.4; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{17}H_{18}NO_3^+$ 284.1281; Found: 284.1287. $[M+H]^+$.



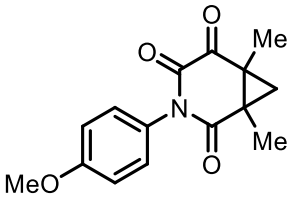
4a

1,6-dimethyl-3-(*p*-tolyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4a): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4a** as white solid in 80% yield (67.33 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.47-7.39 (m, 3H), 7.08-7.05 (m, 2H), 2.23 (d, *J* = 5.8 Hz, 1H), 1.57 (s, 3H), 1.55-1.53 (m, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.3, 172.5, 158.3, 133.9, 129.3, 129.0, 127.7, 36.0, 34.0, 31.2, 14.1, 12.2; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{14}H_{14}NO_3^+$ 244.0968; Found: 244.0962. $[M+H]^+$.



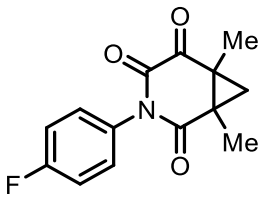
4b

1,6-dimethyl-3-(*p*-tolyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4b): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4b** as white solid in 83% yield (73.88 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.18 (d, *J* = 7.6 Hz, 2H), 6.88 (d, *J* = 10.6 Hz, 2H), 2.31 (s, 3H), 2.15 (d, *J* = 5.8 Hz, 1H), 1.51 (s, 3H), 1.48 (d, *J* = 6.2 Hz, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.4, 172.5, 158.5, 139.1, 131.2, 130.0, 127.4, 36.0, 34.0, 31.2, 21.2, 14.2, 12.3; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{15}H_{16}NO_3^+$ 258.1125; Found: 258.1120. $[M+H]^+$.



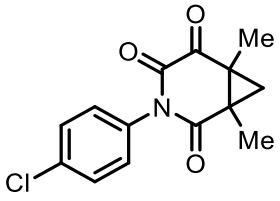
4c

3-(4-methoxyphenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4c): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4c** as white solid in 78% yield (73.75 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.01-6.94 (m, 4H), 3.81 (s, 3H), 2.21 (d, *J* = 5.8 Hz, 1H), 1.59 (s, 3H), 1.55 (d, *J* = 5.8 Hz, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.5, 172.7, 159.8, 158.8, 128.8, 126.5, 121.7, 114.7, 114.2, 55.5, 36.1, 34.0, 31.3, 14.3, 12.4; **MS** (ESI) *m/z* 274 $[M+H]^+$; HRMS Calculated for $C_{15}H_{16}NO_4^+$ 274.1074; Found: 274.1076. $[M+H]^+$.



4d

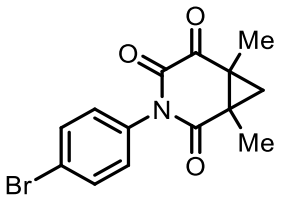
3-(4-methoxyphenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4d): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4d** as white solid in 80% yield (72.31 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.17-7.11 (m, 2H), 7.08-7.04 (m, 2H), 2.22 (d, *J* = 5.8 Hz, 1H), 1.60 (s, 3H), 1.57 (d, *J* = 5.8 Hz, 1H), 1.55 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.1, 172.5, 162.6 (d, J_{C-F} = 247.0 Hz, 1C), 158.4, 129.7 (d, J_{C-F} = 8.7 Hz, 1C) , 129.6, 116.5 (d, J_{C-F} = 22.4 Hz, 1C), 77.4, 36.2, 34.1, 31.3, 14.3, 12.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ −111.5 (s, 1F);s **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{14}H_{13}FNO_3^+$ 262.0874; Found: 262.0867. $[M+H]^+$.



4e

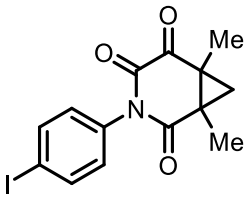
3-(4-chlorophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4e): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4e** as white solid in 81% yield (77.82 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.45-7.42 (m, 2H), 7.05-7.01 (m, 2H), 2.22 (d, *J* = 5.8 Hz, 1H), 1.61 (s, 3H), 1.58 (d, *J* = 5.8 Hz, 1H), 1.57 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.0, 172.3, 158.2, 135.2, 132.3, 129.7, 129.2, 129.1, 36.2, 34.1,

31.3, 14.3, 12.4; **MS** (ESI) *m/z* 278 $[M+H]^+$; HRMS Calculated for $C_{14}H_{13}ClNO_3^+$ 278.0578; Found: 278.0587. $[M+H]^+$.



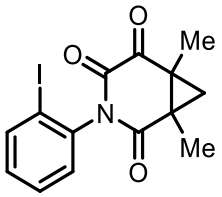
4f

3-(4-chlorophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4f): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4f** as brown solid in 78% yield (86.93 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.90-7.60 (m, 2H), 7.01-6.97 (m, 2H), 2.24 (d, *J* = 5.8 Hz, 1H), 1.62 (s, 3H), 1.60 (d, *J* = 5.8 Hz, 1H), 1.58 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.0, 172.3, 158.2, 132.9, 132.7, 132.1, 129.6, 123.3, 36.2, 34.1, 31.3, 14.3, 12.4; **MS** (ESI) *m/z* 322 $[M+H]^+$; HRMS Calculated for $C_{14}H_{13}BrNO_3^+$ 322.0073; Found: 322.0072. $[M+H]^+$.



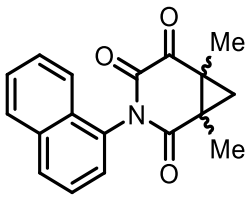
4g

3-(4-iodophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4g): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4g** as white solid in 78% yield (102.17 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 2.23 (d, *J* = 5.8 Hz, 1H), 1.60 (s, 3H), 1.60 (d, *J* = 5.8 Hz, 1H), 1.59 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.0, 172.3, 158.2, 138.7, 138.0, 133.6, 129.7, 121.6, 95.0, 36.2, 34.1, 31.3, 14.3, 12.4; **MS** (ESI) *m/z* 370 $[M+H]^+$; HRMS Calculated for $C_{14}H_{13}INO_3^+$ 369.9935; Found: 369.9934. $[M+H]^+$.



4h

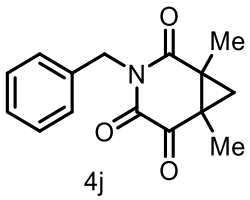
3-(4-iodophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4h): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4h** as white solid in 70% yield (99.6 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.47-7.43 (m, 1H), 7.18-7.09 (m, 2H), 2.84 (d, *J* = 5.8 Hz, 1H), 1.64 (s, 3H), 1.60 (d, *J* = 5.8 Hz, 1H), 1.59 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 187.9, 171.3, 157.6, 139.9, 130.9, 129.9, 129.6, 121.6, 97.3, 36.5, 34.5, 31.5, 14.5, 12.7; **MS** (ESI) *m/z* 370 $[M+H]^+$; HRMS Calculated for $C_{14}H_{13}INO_3^+$ 369.9935; Found: 369.9946. $[M+H]^+$.



4i

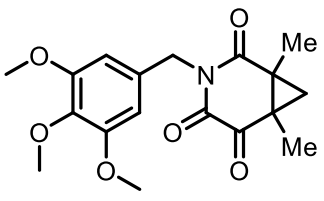
1,6-dimethyl-3-(naphthalen-1-yl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (*dr*: 1:1) (4i): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4i** as white solid in 75% yield (76.11 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.89-7.83 (m, 4H), 7.49-7.41 (m, 5H), 7.40-7.32 (m, 2H), 7.19-7.16 (m, 3H), 2.45 (d, J = 5.8 Hz, 1H), 2.31 (d, J = 5.8 Hz, 1H), 1.67 (d, J = 5.8 Hz, 1H), 1.59-1.58 (m, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.6, 188.3, 172.7, 172.2, 159.0, 158.6, 134.5, 134.4, 131.2, 130.5, 130.1, 129.9, 129.5, 129.3, 129.0, 128.6, 127.5, 127.4, 126.9, 126.6, 126.4, 125.6, 125.5, 125.3, 121.7, 120.8, 36.3, 36.1, 34.4, 34.1, 31.6, 31.5,

14.5, 14.3, 12.5, 12.4; **MS** (ESI) *m/z* 294 $[M+H]^+$; HRMS Calculated for $C_{18}H_{16}NO_3^+$ 294.1125; Found: 294.1129. $[M+H]^+$.



4j

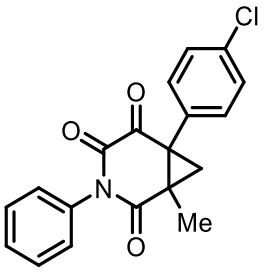
3-benzyl-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4j): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4j** as white solid in 71% yield (63.19 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 7.0 Hz, 2H), 7.24-7.19 (m, 3H), 4.91 (d, *J* = 13.7 Hz, 1H), 4.81 (d, *J* = 13.7 Hz, 1H), 1.80 (d, *J* = 5.6 Hz, 1H), 1.48 (s, 3H), 1.41 (s, 3H), 1.31 (d, J = 5.6 Hz, 1H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.0, 172.3, 158.5, 135.9, 129.1, 128.6, 128.0, 44.6, 35.7, 33.7, 31.2, 14.3, 12.3; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{15}H_{15}NNaO_3^+$ 280.0944; Found: 280.0937. $[M+Na]^+$.



4k

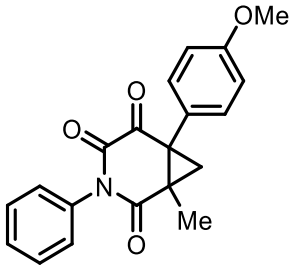
3-benzyl-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (4k): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **4k** as white solid in 82% yield (98.55 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 6.64 (s, 2H), 4.88 (d, *J* = 13.6 Hz, 1H), 4.81 (d, *J* = 13.6 Hz, 1H), 3.82 (s, 6H), 3.80 (s, 3H), 1.86 (d, *J* = 5.5 Hz, 1H), 1.56 (s, 3H), 1.48 (s, 3H), 1.40 (d, J = 5.8 Hz, 1H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 187.9, 172.3, 158.5, 153.1, 137.7, 131.3,

106.6, 60.7, 56.1, 44.8, 35.7, 33.7, 31.2, 14.2, 12.3; **MS** (ESI) *m/z* 348 $[M+H]^+$; HRMS Calculated for $C_{18}H_{22}NO_6^+$ 348.1442; Found: 348.1445. $[M+H]^+$.



5a

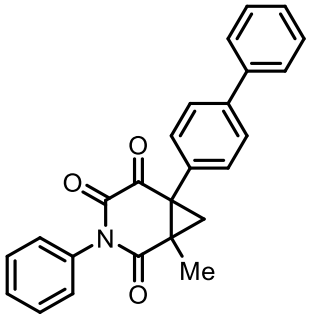
6-(4-chlorophenyl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (5a): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **5a** as white solid in 72% yield (84.64 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.38-7.35 (m, 5H), 7.13-7.07 (m, 4H), 2.48 (d, *J* = 6.0 Hz, 1H), 2.11 (d, *J* = 7.8 Hz, 1H), 1.21 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.4, 171.8, 158.5, 135.2, 133.8, 132.0, 129.5, 129.3, 129.2, 127.8, 45.1, 35.2, 29.0, 16.2; **MS** (ESI) *m/z* 340 $[M+H]^+$; HRMS Calculated for $C_{19}H_{15}ClNO_3^+$ 340.0735; Found: 340.0758. $[M+H]^+$.



5b

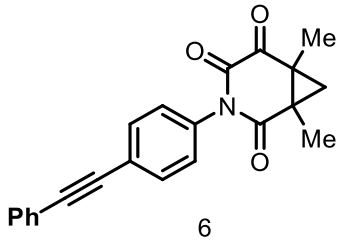
6-(4-methoxyphenyl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (5b): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **5b** as white solid in 75% yield (87.01 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.52-7.45 (m, 3H), 7.18-7.17 (m, 2H), 7.16-7.12 (m, 2H), 6.99-6.96 (m, 2H), 3.85 (s, 3H), 2.52 (d, *J* = 5.9 Hz, 1H), 2.19 (d, *J* = 6.0 Hz, 1H), 1.28 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 187.1, 172.3, 160.0, 158., 134.0,

131.8, 129.5, 129.3, 127.8, 122.5, 114.5, 55.4, 45.3, 35.6, 29.4, 16.2; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}NO_4^+$ 336.1230; Found: 336.1223. $[M+H]^+$.



5c

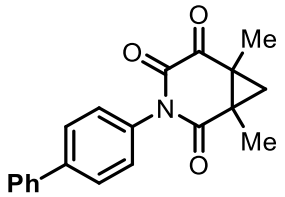
6-([1,1'-biphenyl]-4-yl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (5c): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **5c** as white solid in 71% yield (93.69 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.5 Hz, 2H), 7.64-7.61 (m, 2H), 7.53-7.45 (m, 5H), 7.41-7.37 (m, 1H), 7.33 (d, *J* = 8.3 Hz, 2H), 7.20-7.17 (m, 2H), 2.59 (d, *J* = 6.3 Hz, 1H), 2.27 (d, *J* = 6.3 Hz, 1H), 1.33 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 186.8, 172.2, 158.8, 142.0, 140.2, 134.0, 131.1, 129.7, 129.5, 129.3, 128.9, 127.9, 127.7, 127.2, 45.6, 35.4, 29.2, 16.3; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{25}H_{20}NO_3^+$ 382.1438; Found: 382.1430. $[M+H]^+$.



6

1,6-dimethyl-3-(4-(phenylethynyl)phenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (6): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **6** as dark brown solid in 65% yield (71.75 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.61-7.58 (m, 2H), 7.54-7.51

(m, 2H), 7.36-7.33 (m, 3H), 7.08-7.05 (m, 2H), 2.23 (d, J = 5.8 Hz, 1H), 1.60 (s, 3H), 1.56 (d, J = 4.8 Hz, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 188.1, 172.3, 158.2, 133.5, 132.5, 131.7, 128.5, 128.4, 127.9, 124.4, 122.8, 90.7, 88.3, , 36.1, 34.1, 31.2, 14.3, 12.4; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{22}H_{18}NO_3^+$ 344.1281; Found: 344.1274. $[M+H]^+$.

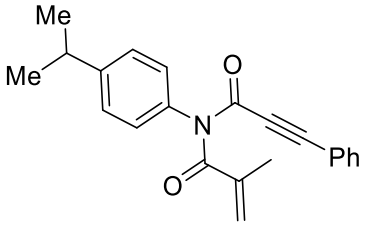


7

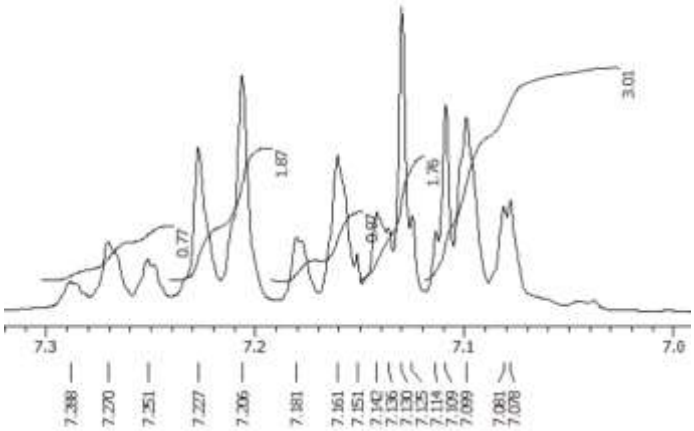
3-([1,1'-biphenyl]-4-yl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione (7): Purification by silica gel chromatography (PE:EA=85:15) afforded the desired **7** as white solid in 60% yield (114.26 mg); **^{1}H-NMR** (400 MHz, $CDCl_3$) δ 7.67-7.64 (m, 2H), 7.59-7.57 (m, 2H), 7.46-7.42 (m, 2H), 7.39-7.35 (m, 1H), 7.18-7.15 (m, 2H), 2.26 (d, *J* = 5.8 Hz, 1H), 1.63 (s, 3H), 1.59 (d, *J* = 7.4 Hz, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$) δ 13C-NMR (101 MHz, CHLOROFORM-D) δ 188.6, 172.8, 158.7, 134.0, 133.0, 132.2, 129.0, 128.8, 128.4, 124.9, 123.3, 36.6, 34.6, 31.7, 14.8, 12.9; **MS** (ESI) *m/z* 255 $[M+H]^+$; HRMS Calculated for $C_{20}H_{18}NO_3^+$ 320.1281; Found: 320.1270. $[M+H]^+$.

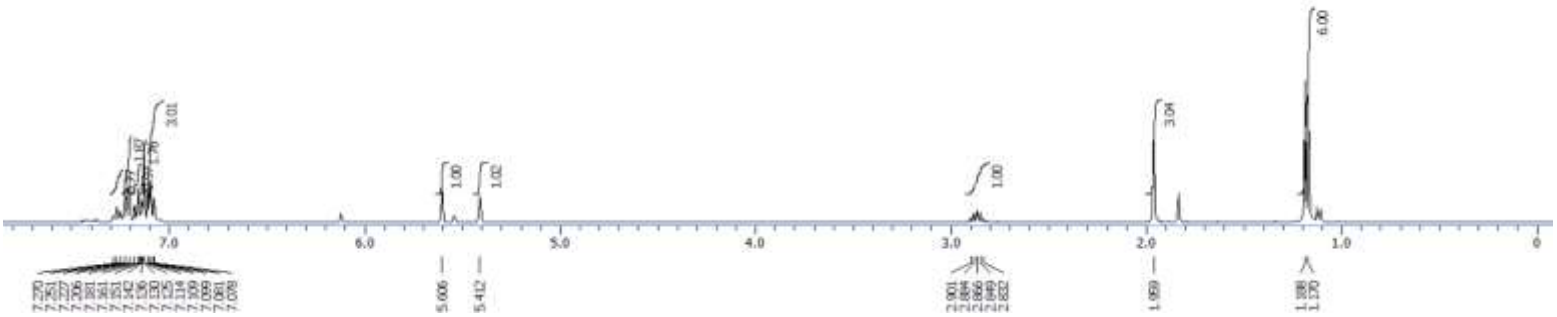
(9) Copies of ^{1}H NMR, ^{13}C NMR, ^{19}F NMR and Mass Spectra

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

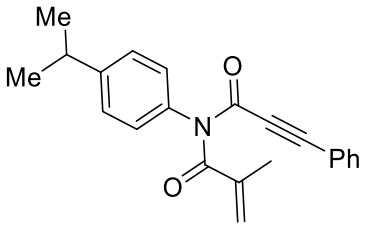


N-(4-isopropylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide

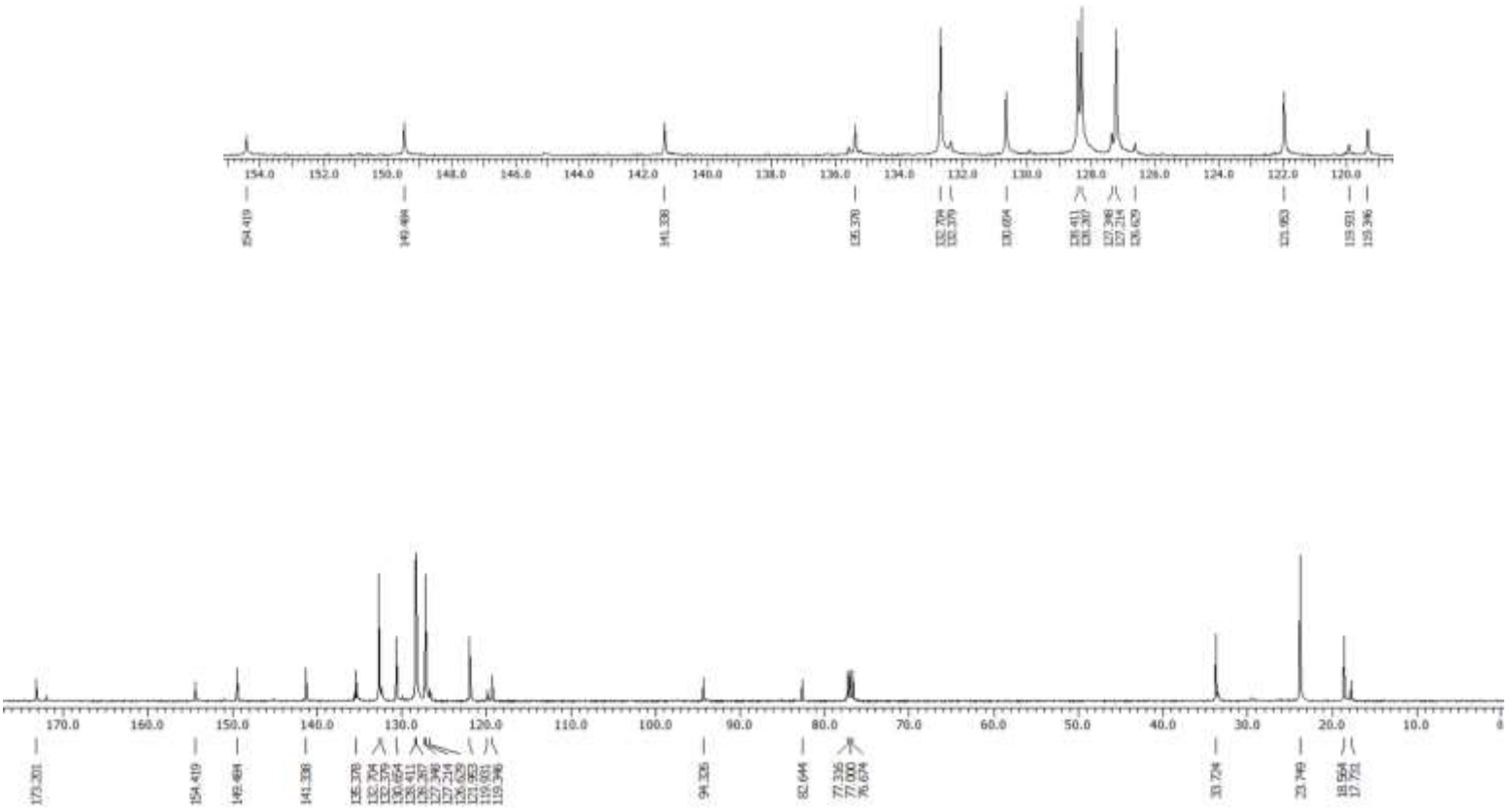




^{13}C NMR spectrum of 1g (100 MHz, $CDCl_3$)



N-(4-isopropylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide



HRMS spectrum of 1g

Qualitative Compound Report

Data File	348-A.d	**Sample Name**	348-A
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 13:28:32
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: C22 H21 N O2	0.353	331.1579	1180221	C22 H21 N O2	331.1572	1.9	C22 H21 N O2	C22 H21 N O2

Compound Label	m/z	RT	Algorithm	Mass
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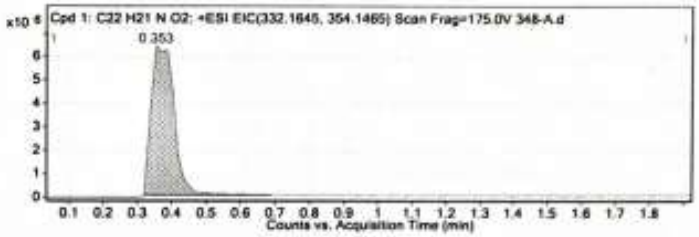
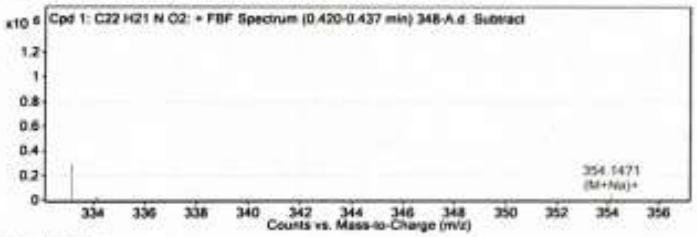
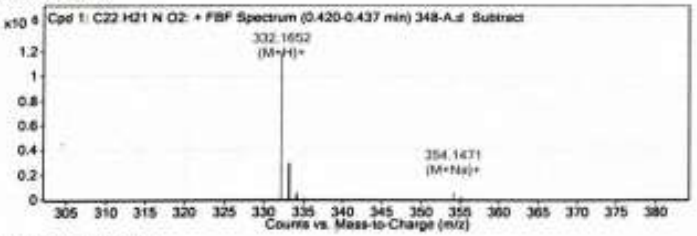


MS Spectrum



MS Zoomed Spectrum

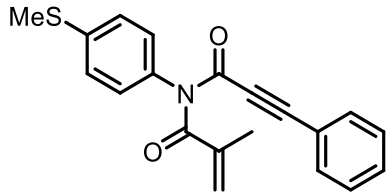


MS Spectrum Peak List

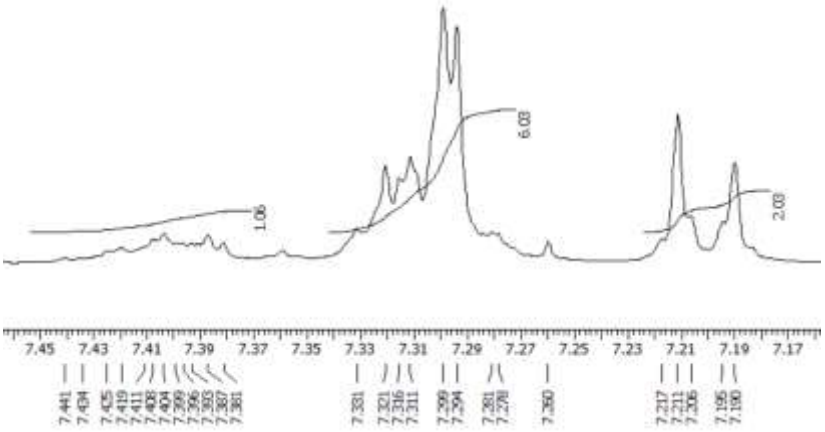
m/z	z	Abund	Formula	Ion
332.1652	1	1180221.13	C22H22NO2	(M+H)+
333.1684	1	297861.06	C22H22NO2	(M+H)+
334.1707	1	38231.71	C22H22NO2	(M+H)+
335.1737	1	4033.71	C22H22NO2	(M+H)+
336.174	1	726.23	C22H22NO2	(M+H)+
354.1471	1	51403.02	C22H21NNaO2	(M+Na)+
355.1512	1	13572.05	C22H21NNaO2	(M+Na)+
356.1531	1	3627.28	C22H21NNaO2	(M+Na)+
357.1675	1	768.45	C22H21NNaO2	(M+Na)+

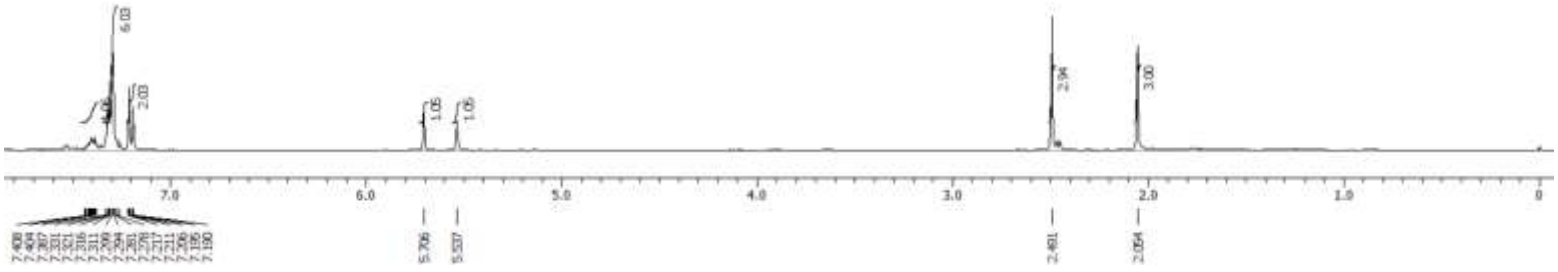
--- End Of Report ---

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

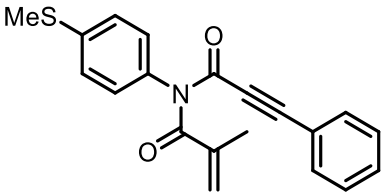


N-(4-(methylthio)phenyl)-*N*-(3-phenylpropioloyl)methacrylamide

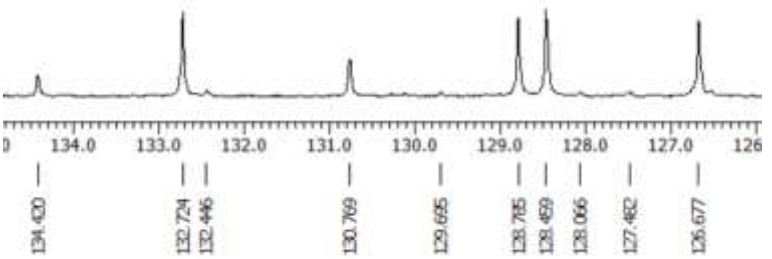


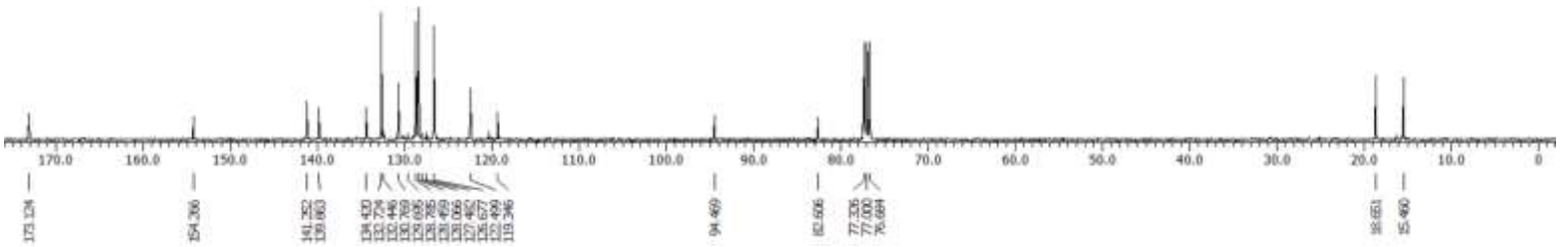


^{13}C NMR spectrum of 1i (100 MHz, $CDCl_3$)



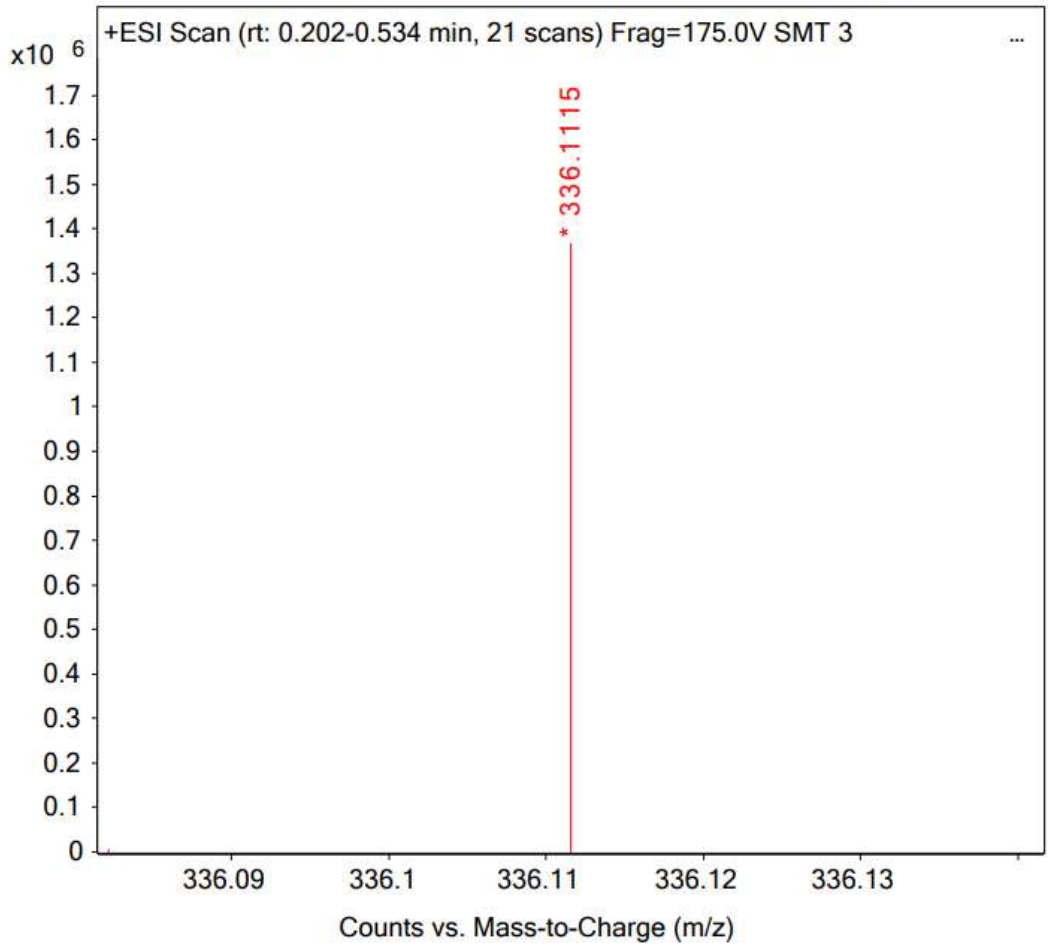
N-(4-(methylthio)phenyl)-*N*-(3-phenylpropioloyl)methacrylamide



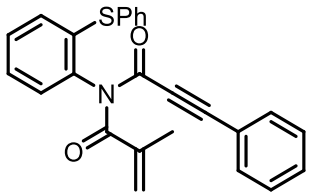


HRMS spectrum of 1i

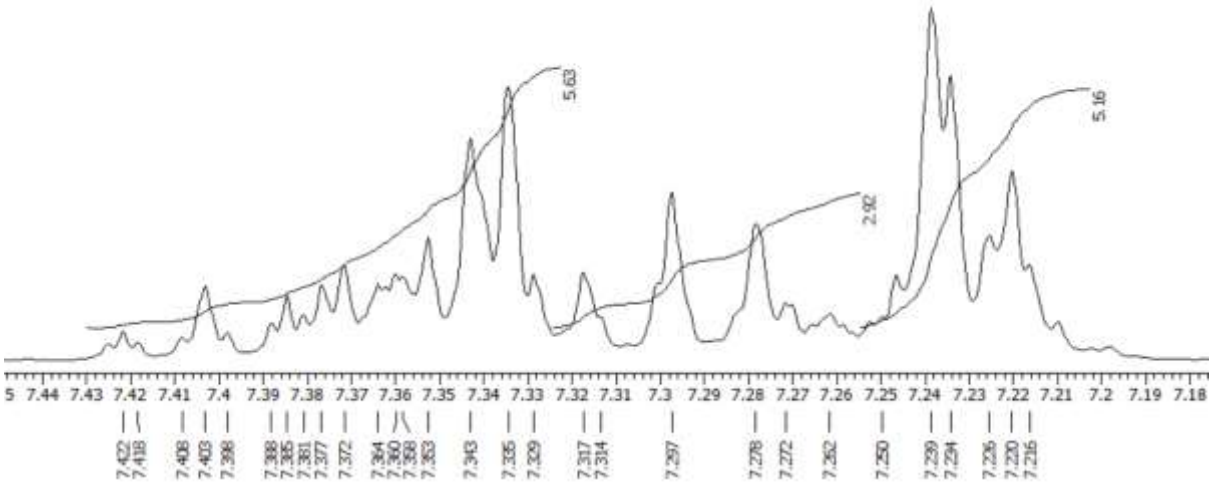
Sample Name	SMT 346(A)	**Position**	P1-B5	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 346(A).d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:38:47 (UTC+05:30)

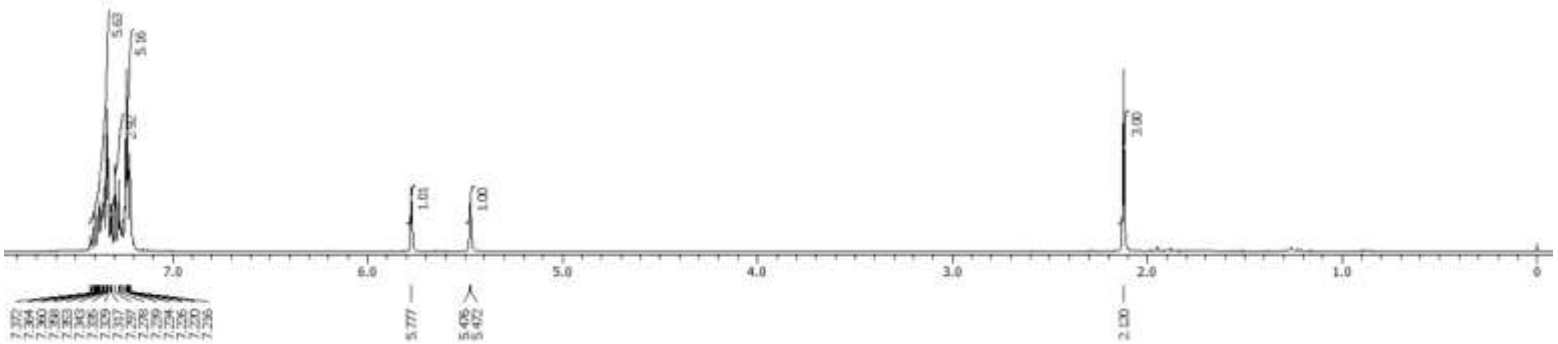


^{1}H NMR spectrum of 1l (400 MHz, $CDCl_3$)

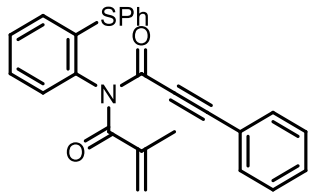


N-(3-phenylpropioloyl)-*N*-(2-(phenylthio)phenyl)methacrylamide

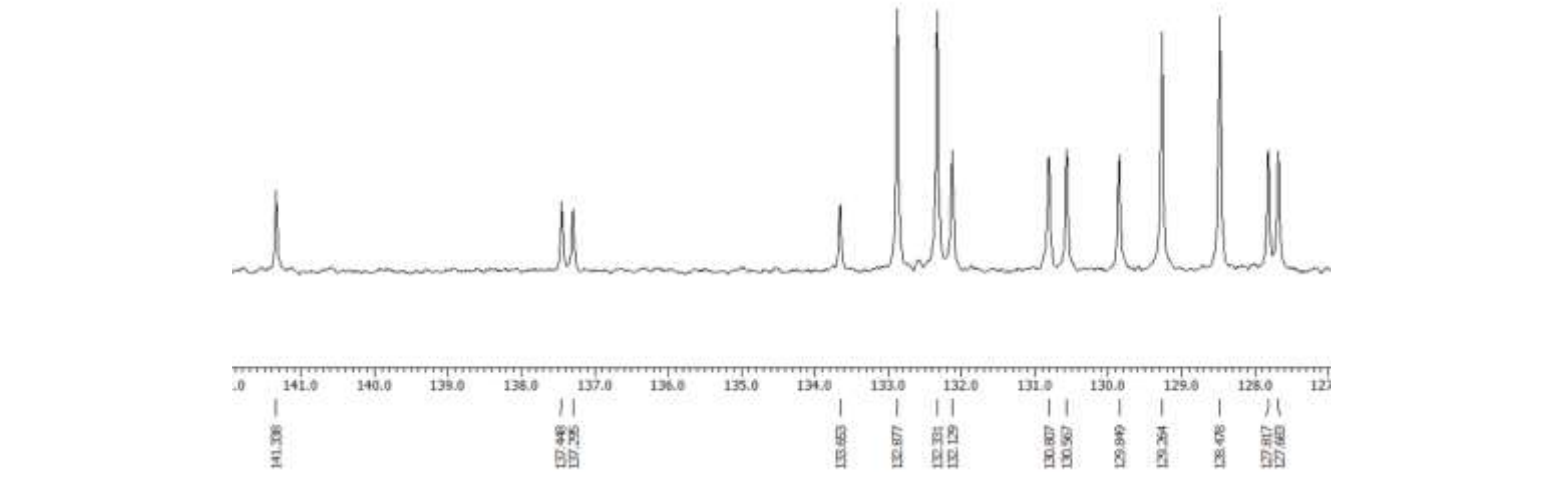


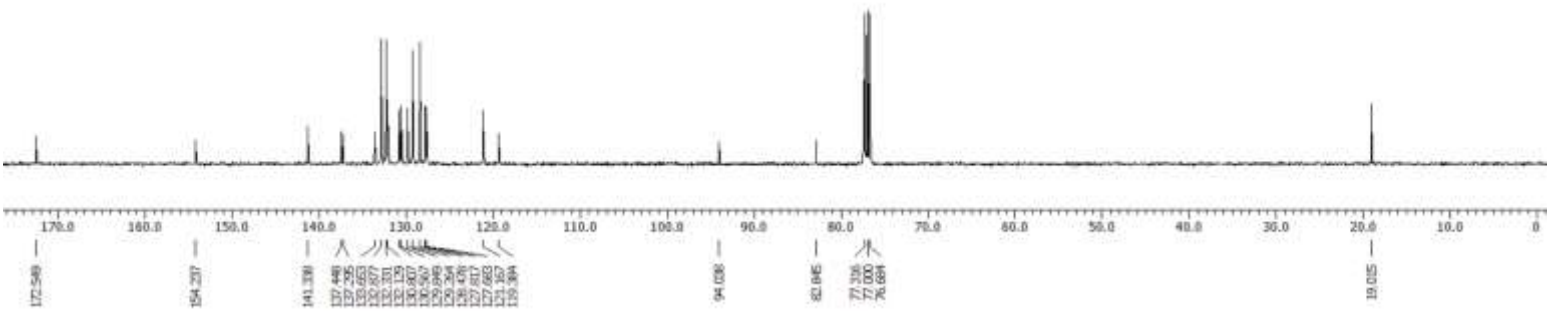


^{13}C NMR spectrum of 1l (100 MHz, $CDCl_3$)



N-(3-phenylpropioloyl)-*N*-(2-(phenylthio)phenyl)methacrylamide





HRMS spectrum of 1l

Qualitative Compound Report

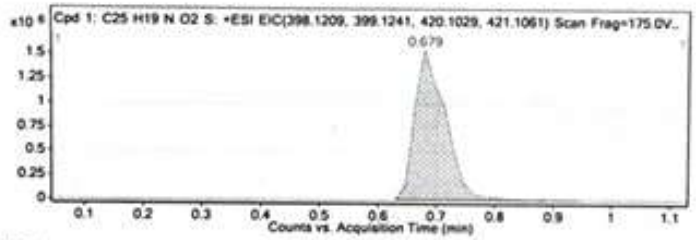
Data File	ST-349-A.d	**Sample Name**	ST-349-A
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	11-05-2024 12:26:28
ERM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

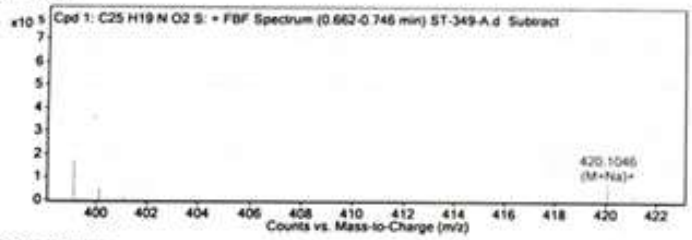
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C25 H19 N O2 S	0.679	397.1164	80023	C25 H19 N O2 S	397.1136	6.98	C25 H19 N O2 S	C25 H19 N O2 S

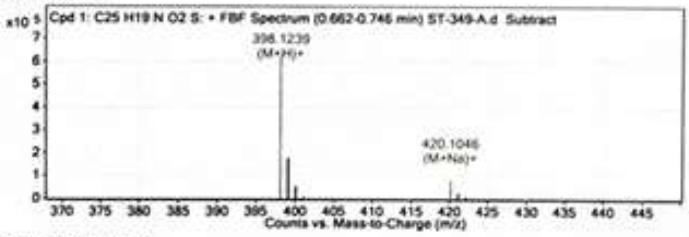
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C25 H19 N O2 S	420.1046	0.679	Find By Formula	397.1164



MS Spectrum



MS Zoomed Spectrum

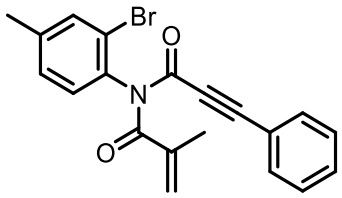


MS Spectrum Peak List

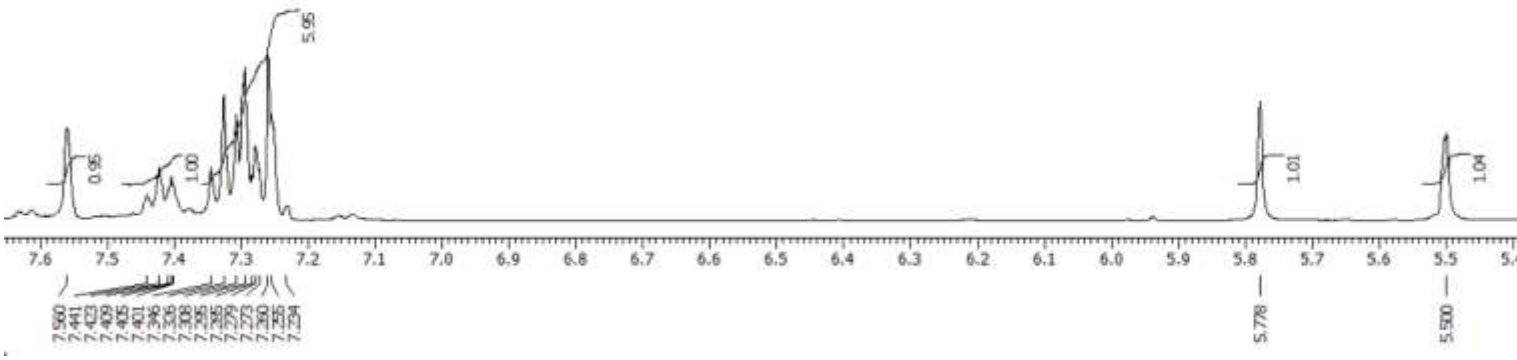
m/z	z	Abund	Formula	Ion
398.1239	1	630825.88	C25H20NO2S	(M+H)+
399.1266	1	172347.55	C25H20NO2S	(M+H)+
400.1244	1	49340.97	C25H20NO2S	(M+H)+
401.1253	1	10554.12	C25H20NO2S	(M+H)+
402.1353	1	1845.54	C25H20NO2S	(M+H)+
420.1046	1	80023.44	C25H19NNaO2S	(M+Na)+
421.1081	1	22635.56	C25H19NNaO2S	(M+Na)+
422.1065	1	6917.5	C25H19NNaO2S	(M+Na)+
423.1108	1	1321.02	C25H19NNaO2S	(M+Na)+

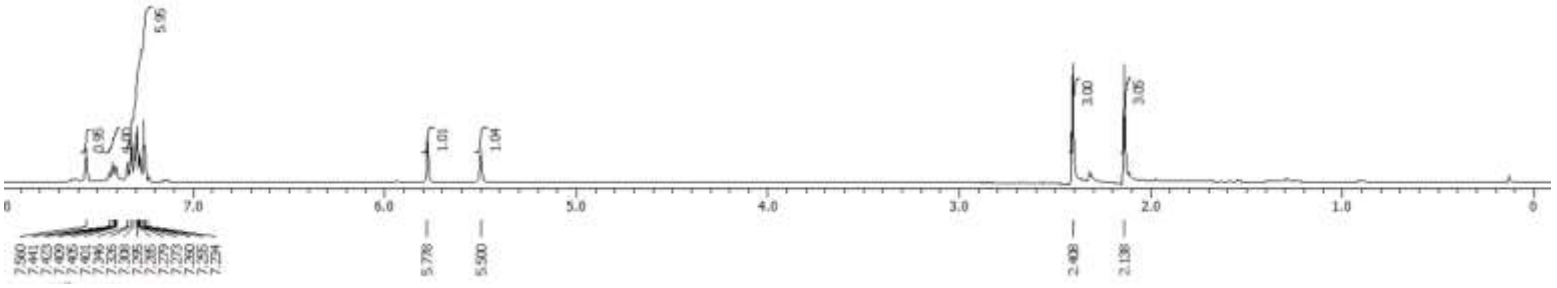
— End Of Report —

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

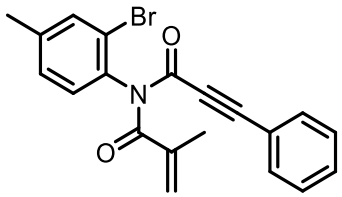


N-(2-bromo-4-methylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide

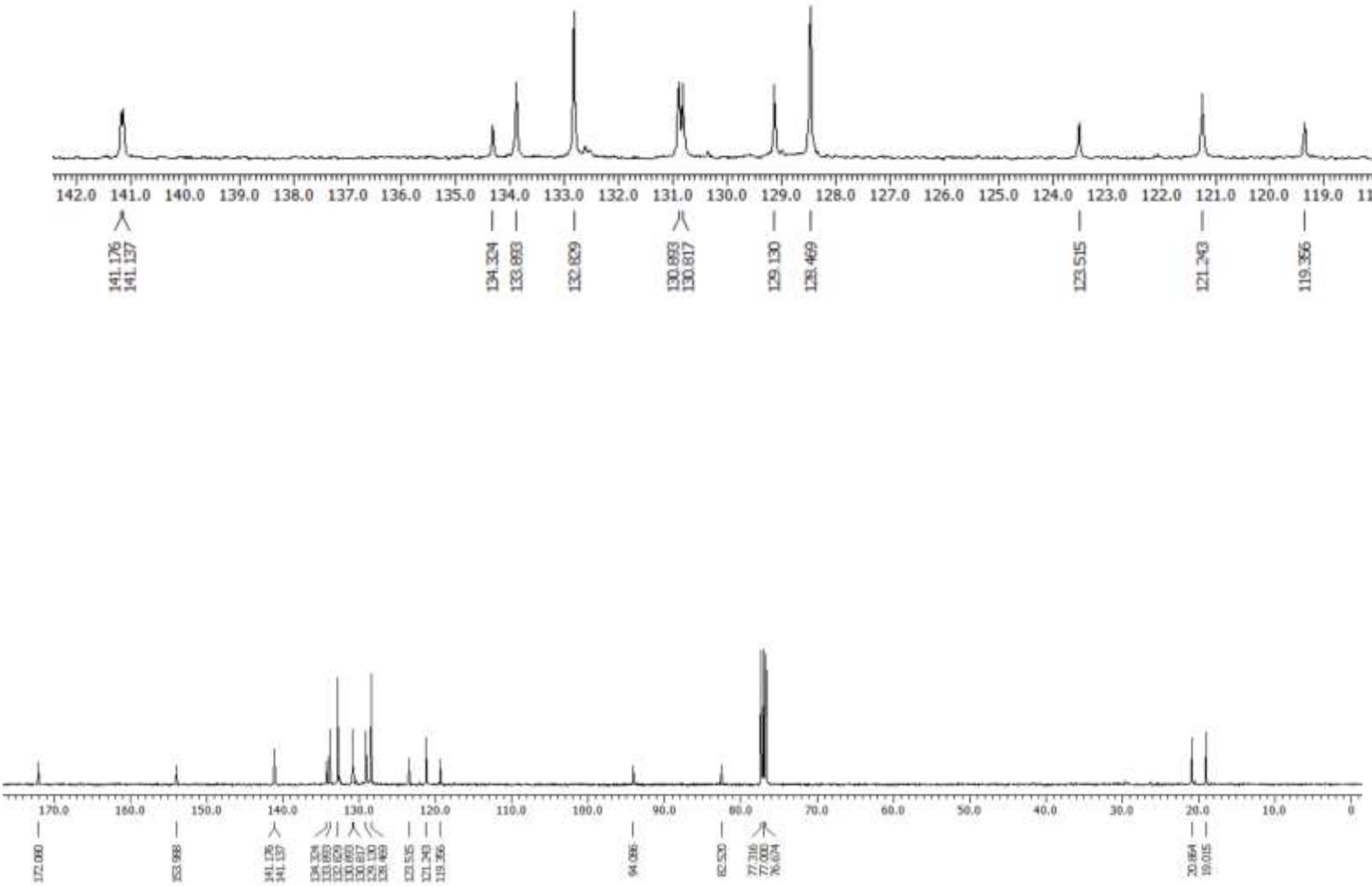




^{13}C NMR spectrum of 1m (100 MHz, $CDCl_3$)



N-(2-bromo-4-methylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide



HRMS spectrum of 1m

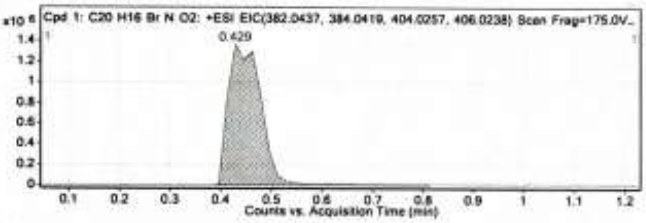
Qualitative Compound Report

Data File	281-A.d	**Sample Name**	281-A
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 16:16:10
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)		

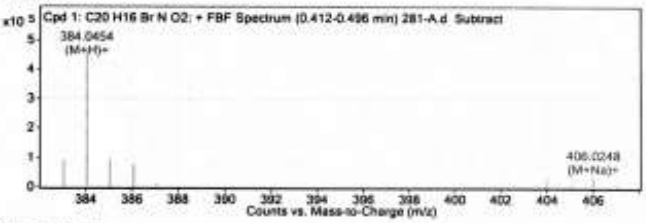
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	DiM (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H16 Br N O2	0.429	381.0388	37453	C20 H16 Br N O2	381.0364	6.33	C20 H16 Br N O2	C20 H16 Br N O2

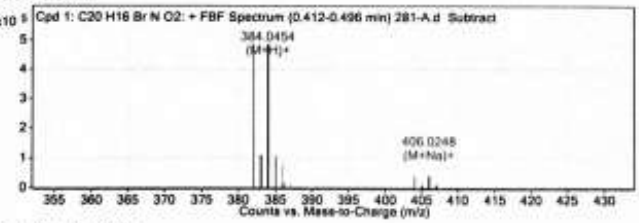
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H16 Br N O2	406.0248	0.429	Find By Formula	381.0388



MS Spectrum



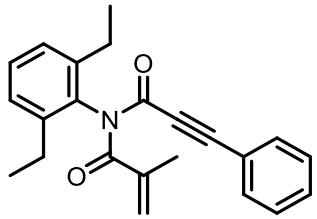
MS Zoomed Spectrum



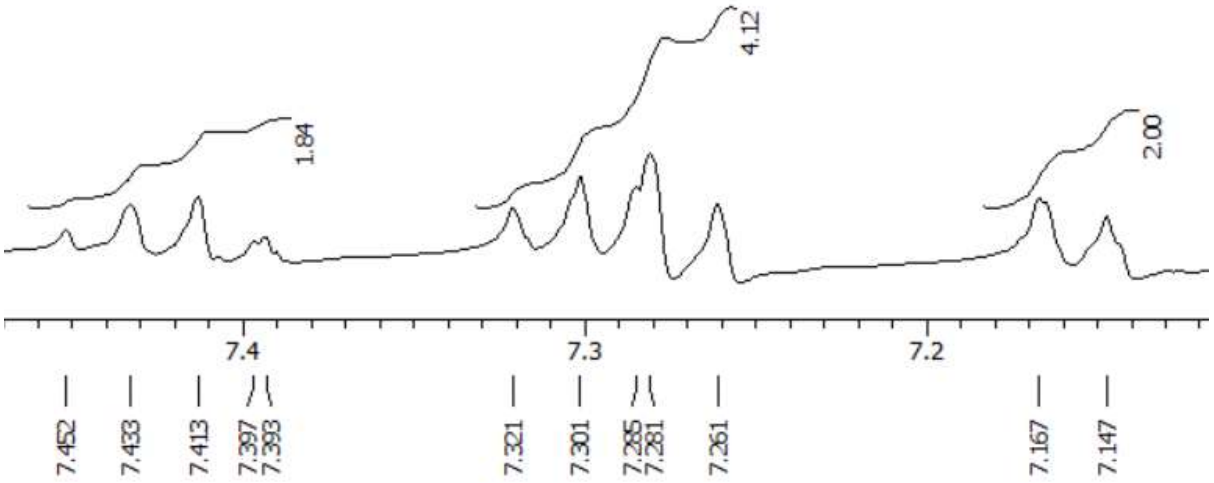
MS Spectrum Peak List

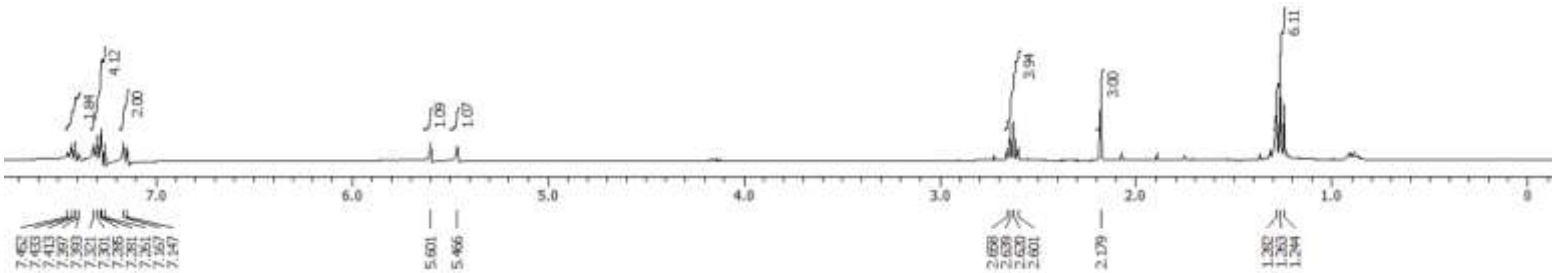
m/z	z	Abund	Formula	Ion
382.044	1	451917.72	C20H17BrNO2	(M+H)+
383.0472	1	93936.3	C20H17BrNO2	(M+H)+
384.0454	1	461409.97	C20H17BrNO2	(M+H)+
385.0482	1	96072.84	C20H17BrNO2	(M+H)+
386.0571	1	77821.27	C20H17BrNO2	(M+H)+
387.061	1	15068.45	C20H17BrNO2	(M+H)+
388.0597	1	3513.4	C20H17BrNO2	(M+H)+
404.0268	1	37138.53	C20H16BrNNaO2	(M+Na)+
405.0303	1	8518.6	C20H16BrNNaO2	(M+Na)+
406.0248	1	37453.49	C20H16BrNNaO2	(M+Na)+
407.0289	1	8358.58	C20H16BrNNaO2	(M+Na)+

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

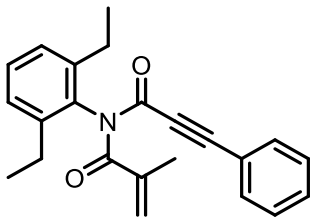


N-(2,6-diethylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide

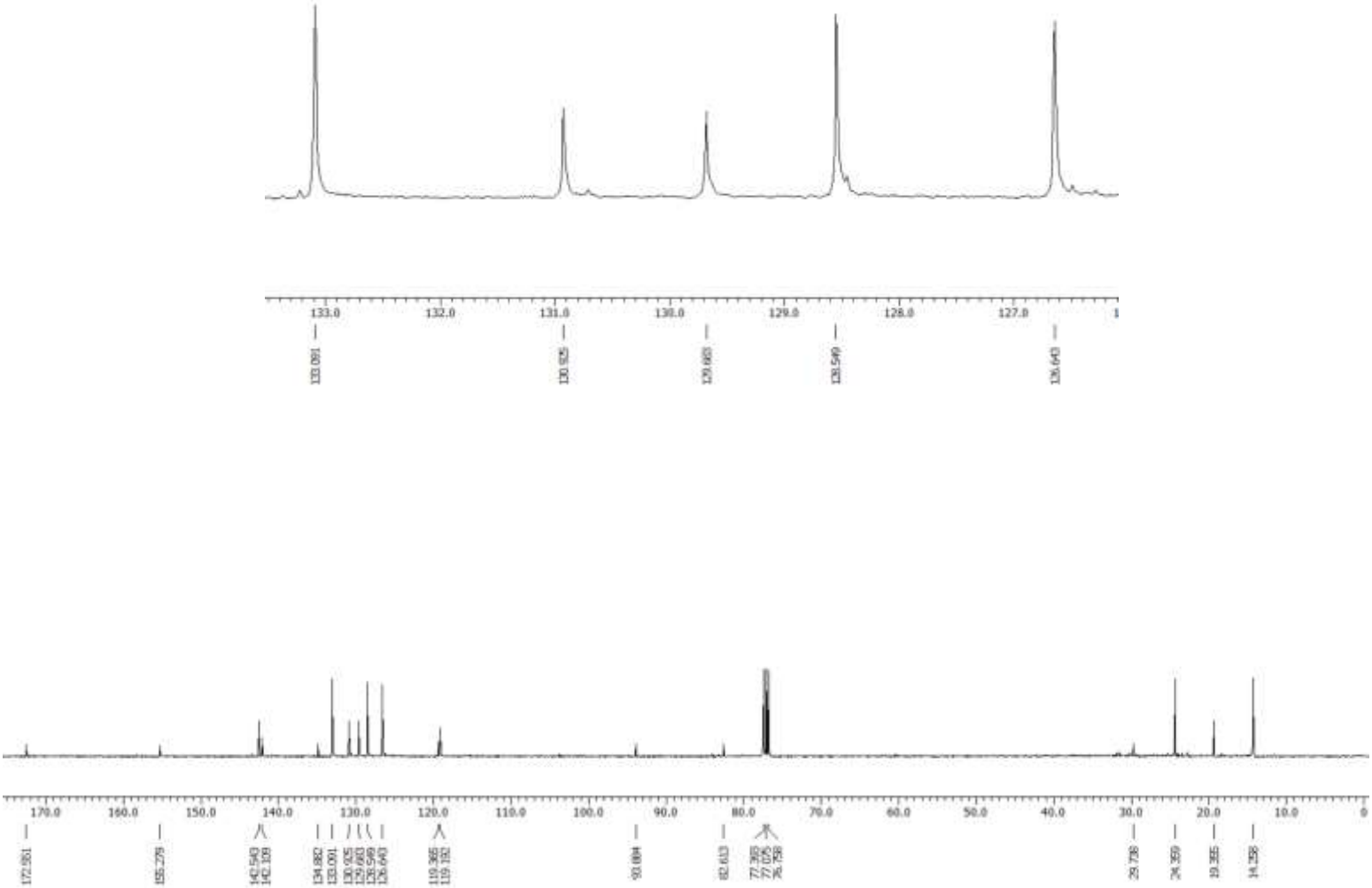




^{13}C NMR spectrum of 1n (100 MHz, $CDCl_3$)

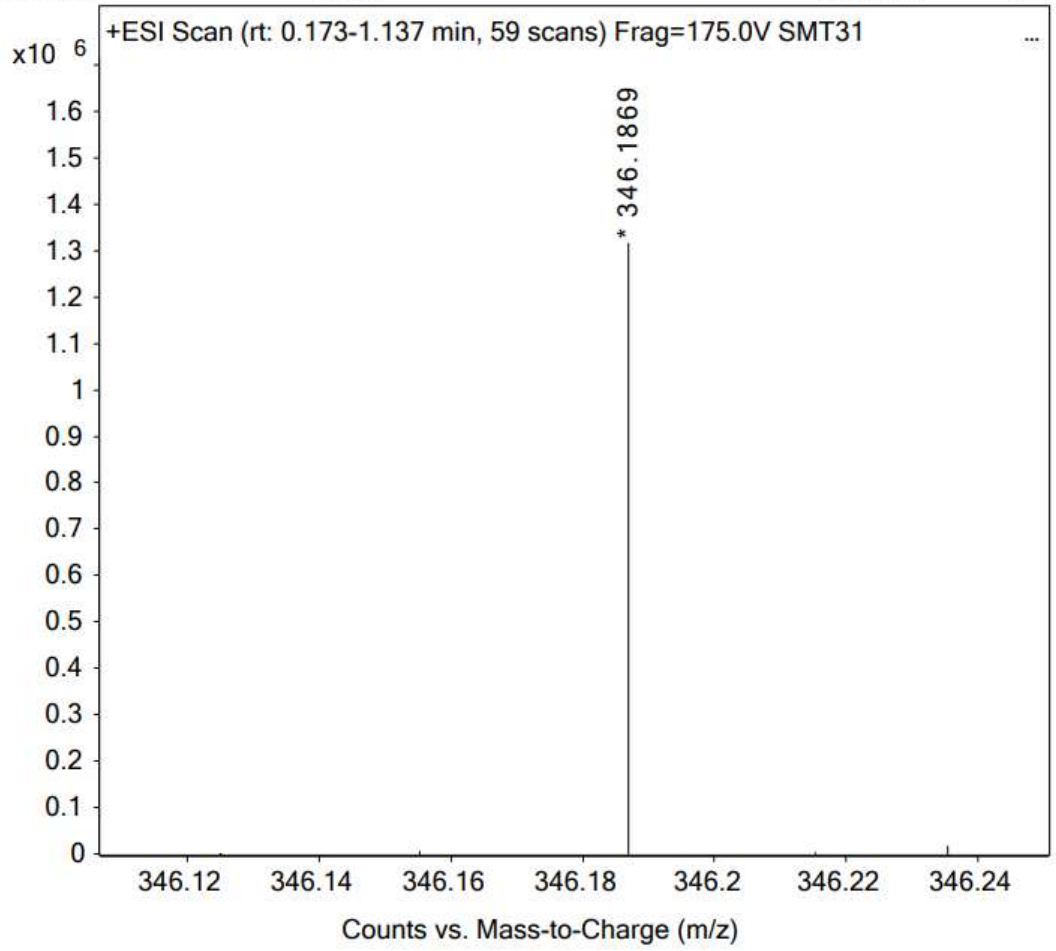


N-(2,6-diethylphenyl)-*N*-(3-phenylpropioloyl)methacrylamide

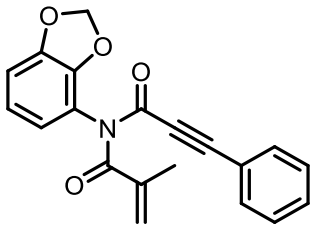


HRMS spectrum of 1n

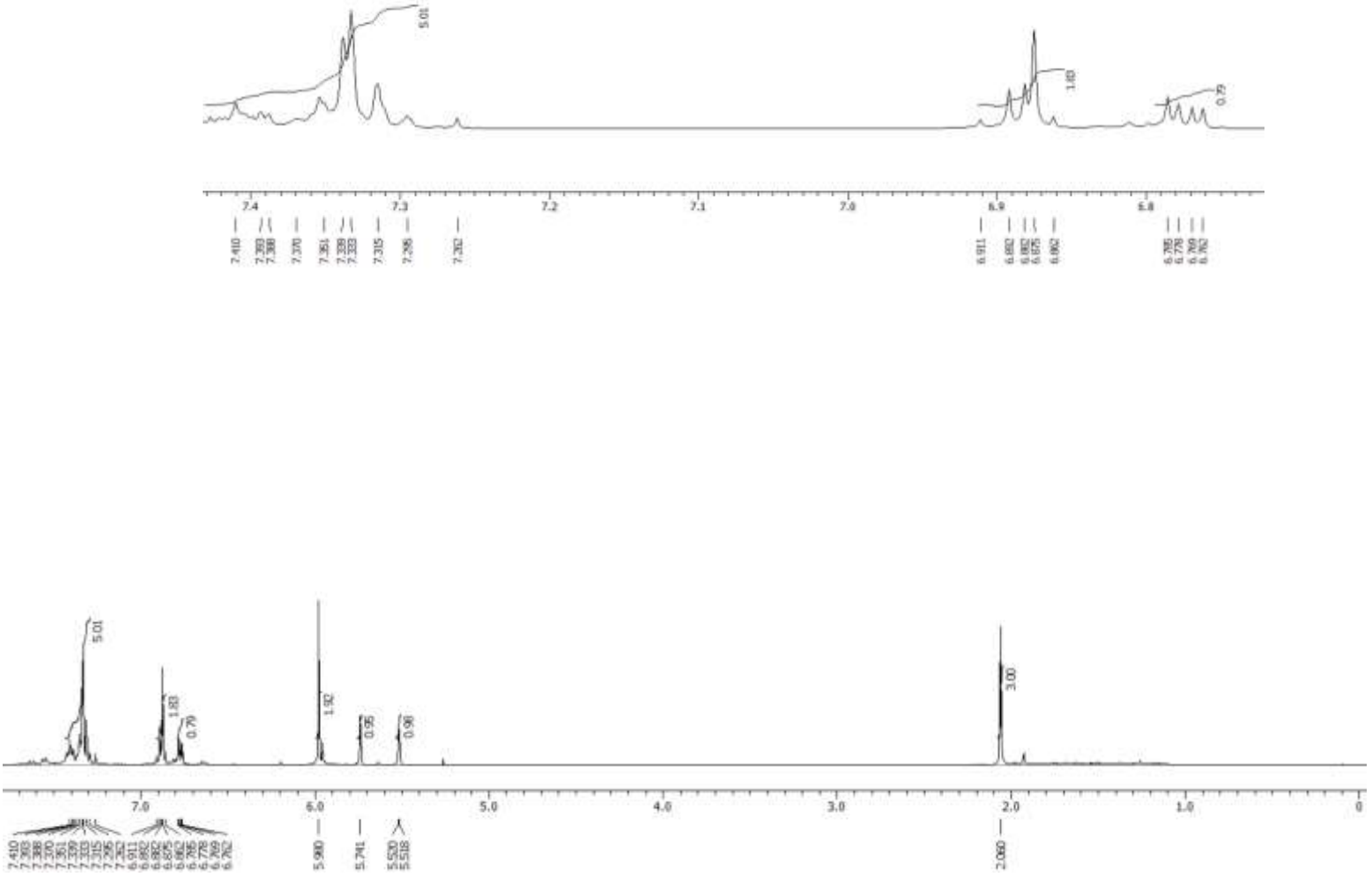
Sample Name	SMT 316(A)	**Position**	P1-C9	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT316(A).d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 13:36:51 (UTC+05:30)



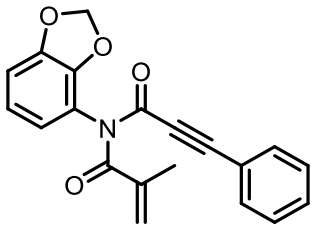
^{1}H NMR spectrum of 1o (400 MHz, $CDCl_3$)



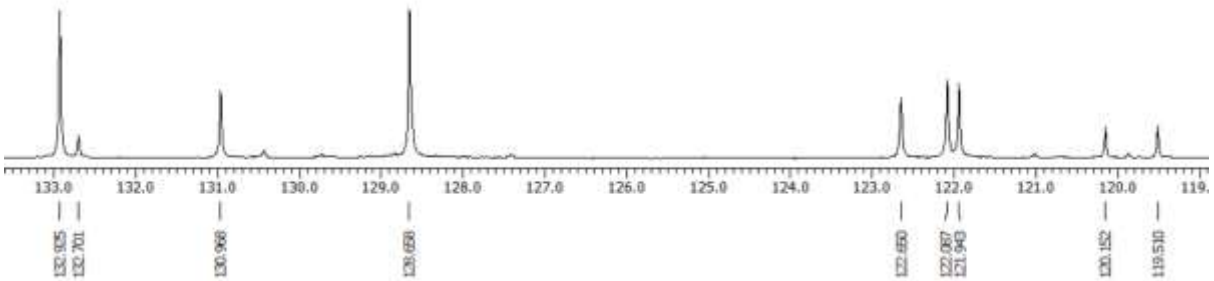
N-(benzo[*d*][1,3]dioxol-4-yl)-*N*-(3-phenylpropioloyl)methacrylamide

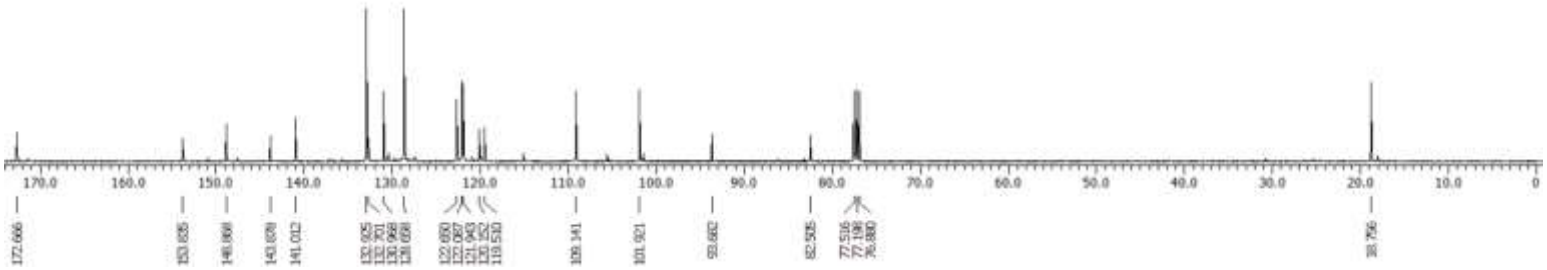


^{13}C NMR spectrum of 1o (100 MHz, $CDCl_3$)



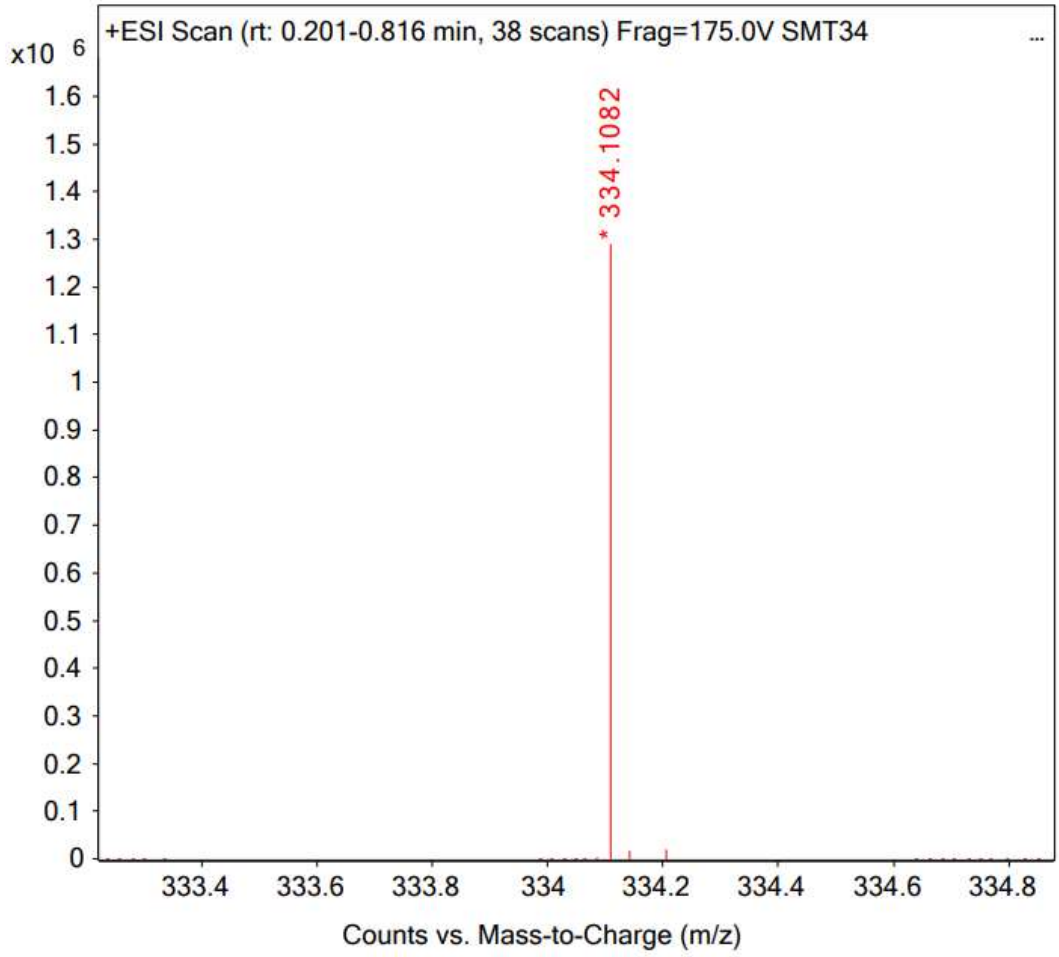
N-(benzo[*d*][1,3]dioxol-4-yl)-*N*-(3-phenylpropioloyl)methacrylamide



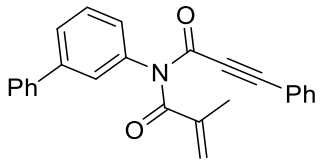


HRMS spectrum of 1o

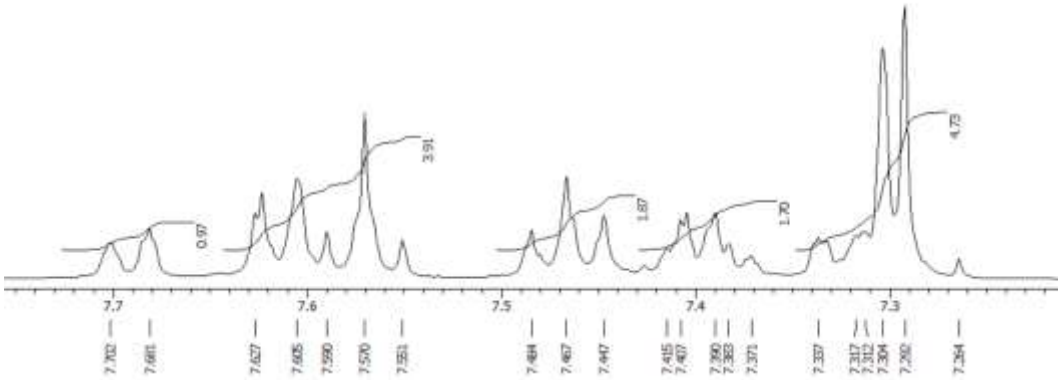
Sample Name	SMT 345(A)	**Position**	P1-C8	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT345(A).d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 13:32:58 (UTC+05:30)

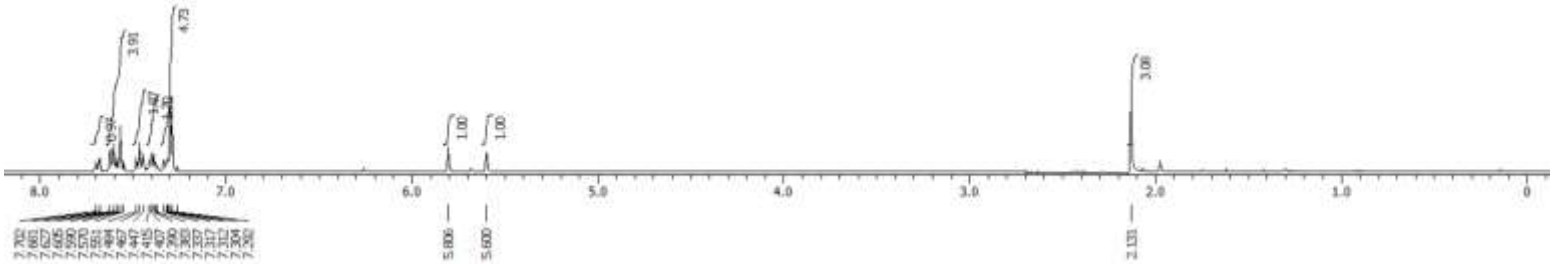


^{1}H NMR spectrum of 1p (400 MHz, $CDCl_3$)

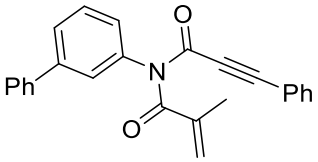


N-([1,1'-biphenyl]-3-yl)-*N*-(3-phenylpropioloyl)methacrylamide

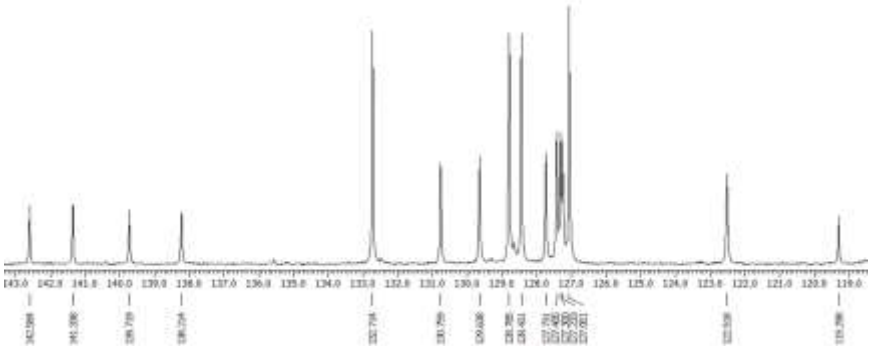


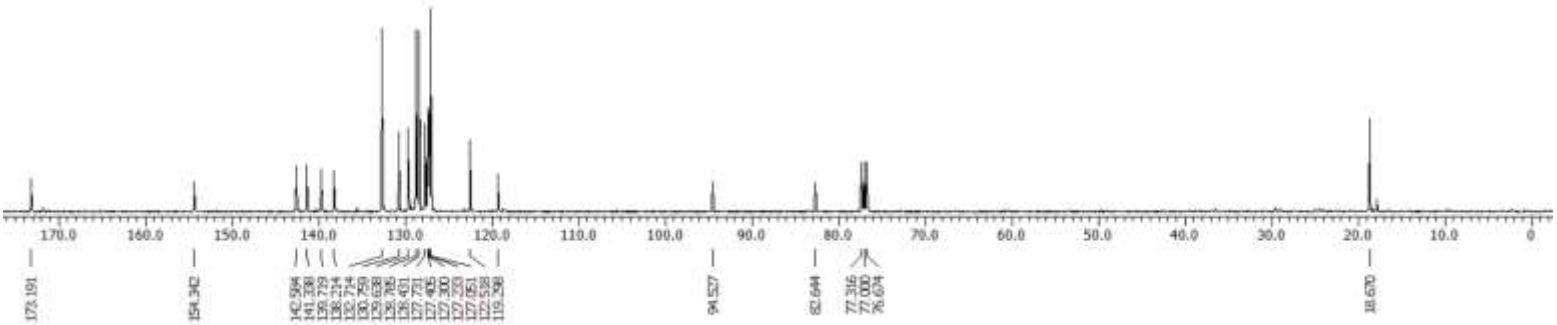


^{13}C NMR spectrum of 1p (100 MHz, $CDCl_3$)



N-([1,1'-biphenyl]-3-yl)-*N*-(3-phenylpropioloyl)methacrylamide





Mass spectrum of 1p

Qualitative Compound Report

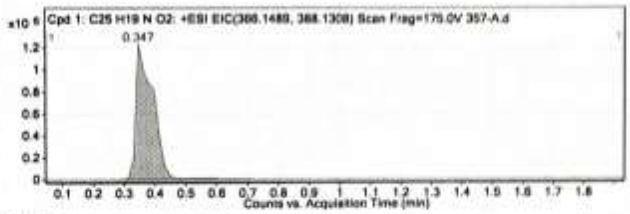
Data File	357-A.d	**Sample Name**	357-A
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 13:48:10
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

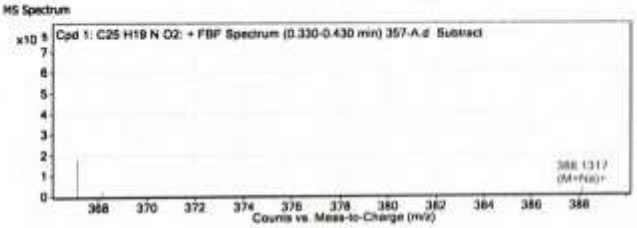
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C25 H19 N O2	0.347	365.1423	628825	C25 H19 N O2	365.1416	2.11	C25 H19 N O2	C25 H19 N O2

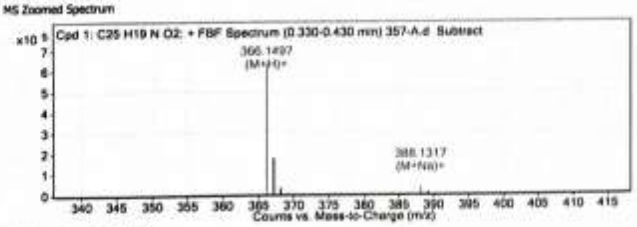
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C25 H19 N O2	366.1497	0.347	Find By Formula	365.1423



MS Spectrum



MS Zoomed Spectrum

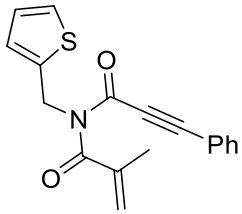


MS Spectrum Peak List

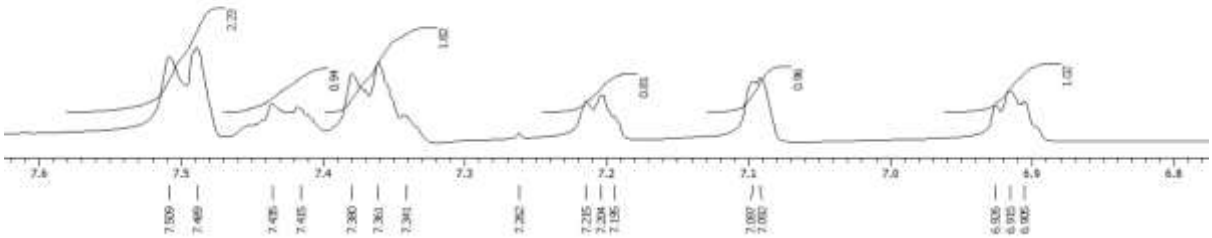
m/z	z	Abund	Formula	Ion
366.1497	1	628824.94	C25H20NO2	(M+H)+
367.1528	1	176375.03	C25H20NO2	(M+H)+
368.1558	1	25977.41	C25H20NO2	(M+H)+
369.159	1	2902.28	C25H20NO2	(M+H)+
388.1317	1	33282.09	C25H19NNaO2	(M+Na)+
389.1355	1	9540.02	C25H19NNaO2	(M+Na)+
390.1376	1	1454.76	C25H19NNaO2	(M+Na)+

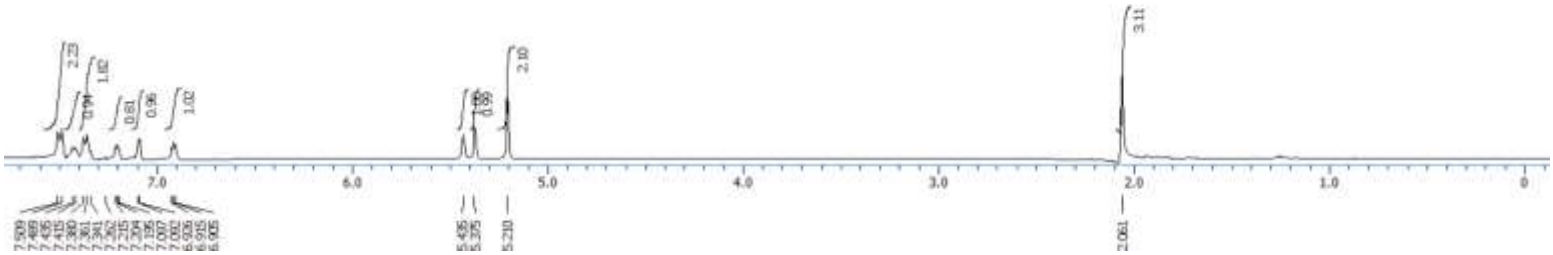
--- End Of Report ---

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

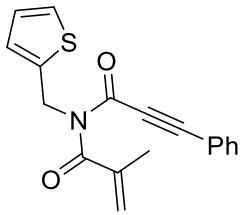


N-(3-phenylpropioloyl)-*N*-(thiophen-2-ylmethyl)methacrylamide

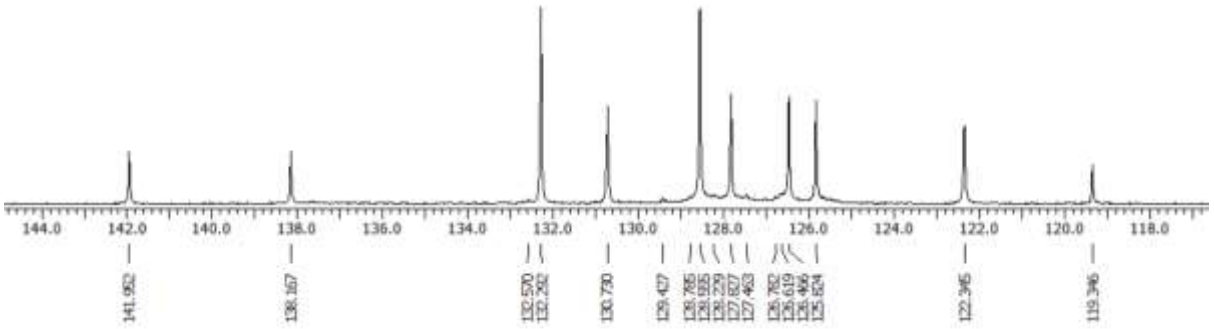


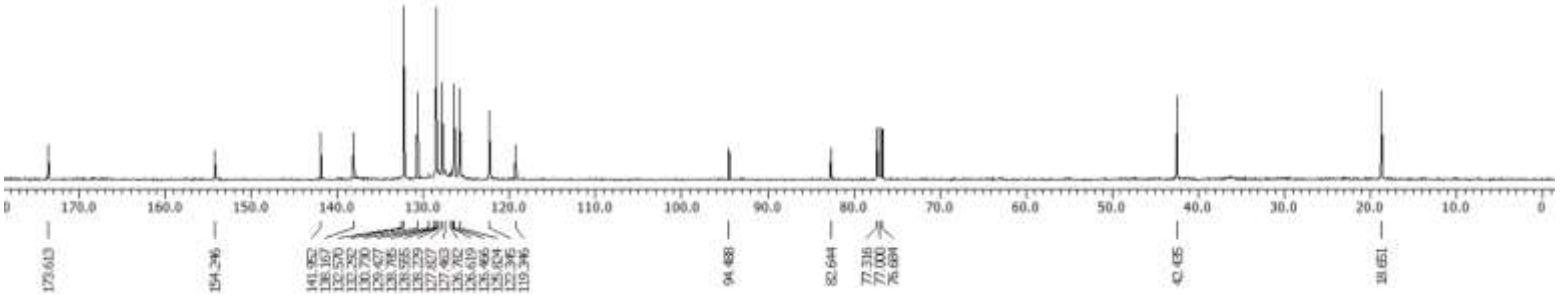


^{13}C NMR spectrum of 1s (100 MHz, $CDCl_3$)



N-(3-phenylpropioloyl)-*N*-(thiophen-2-ylmethyl)methacrylamide





HRMS spectrum of 1s

Qualitative Compound Report

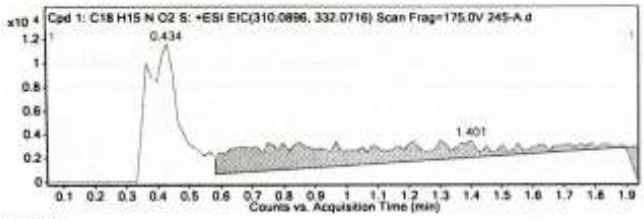
Data File	245-A.d	**Sample Name**	245-A
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 13:35:07
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

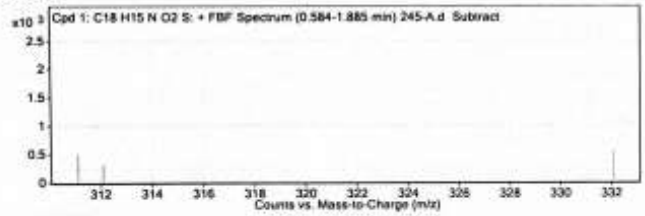
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C18 H15 N O2 S	1.401	309.0834	2346	C18 H15 N O2 S	309.0823	3.47	C18 H15 N O2 S	C18 H15 N O2 S

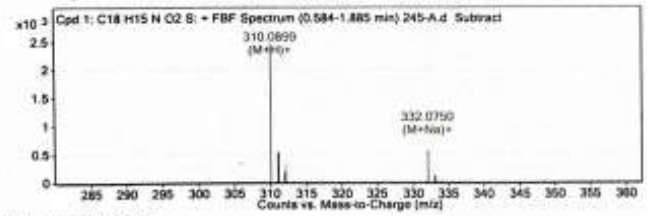
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H15 N O2 S	310.0899	1.401	Find By Formula	309.0834



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
310.0899	1	2346.48	C18H16NO2S	(M+H)+
311.0936	1	498.29	C18H16NO2S	(M+H)+
312.0912	1	316.06	C18H16NO2S	(M+H)+
332.075	1	556.16	C18H15NNaO2S	(M+Na)+
333.0779	1	122.65	C18H15NNaO2S	(M+Na)+

--- End Of Report ---

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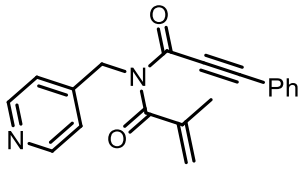
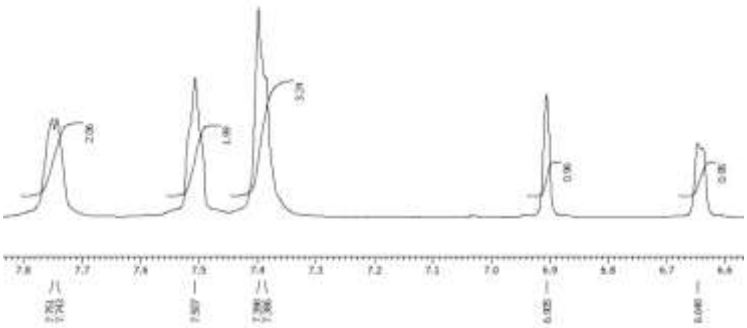
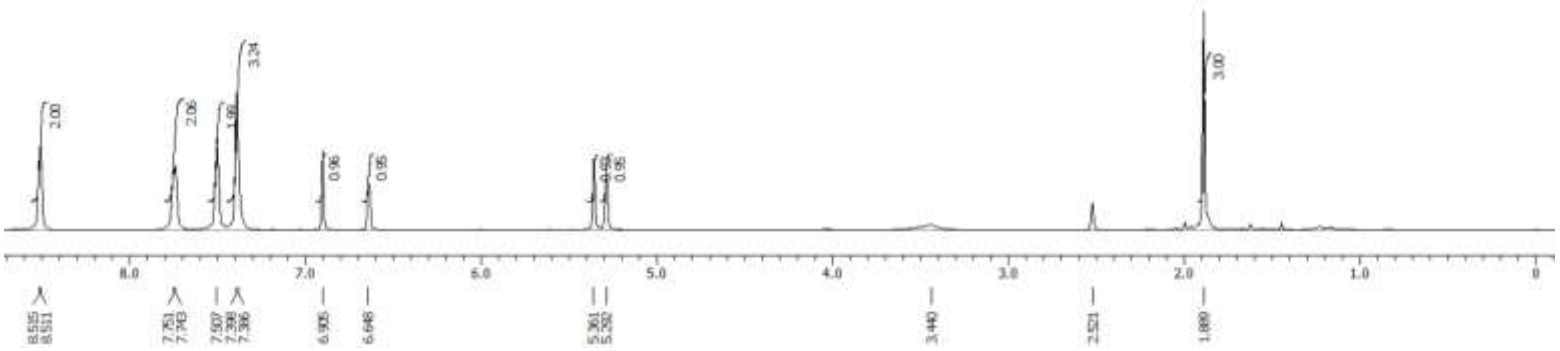
^{1}H NMR spectrum of 1t (400 MHz, DMSO-*d6*)

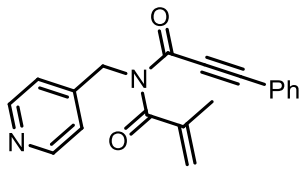


N-(3-phenylpropioloyl)-*N*-(pyridin-4-ylmethyl)methacrylamide

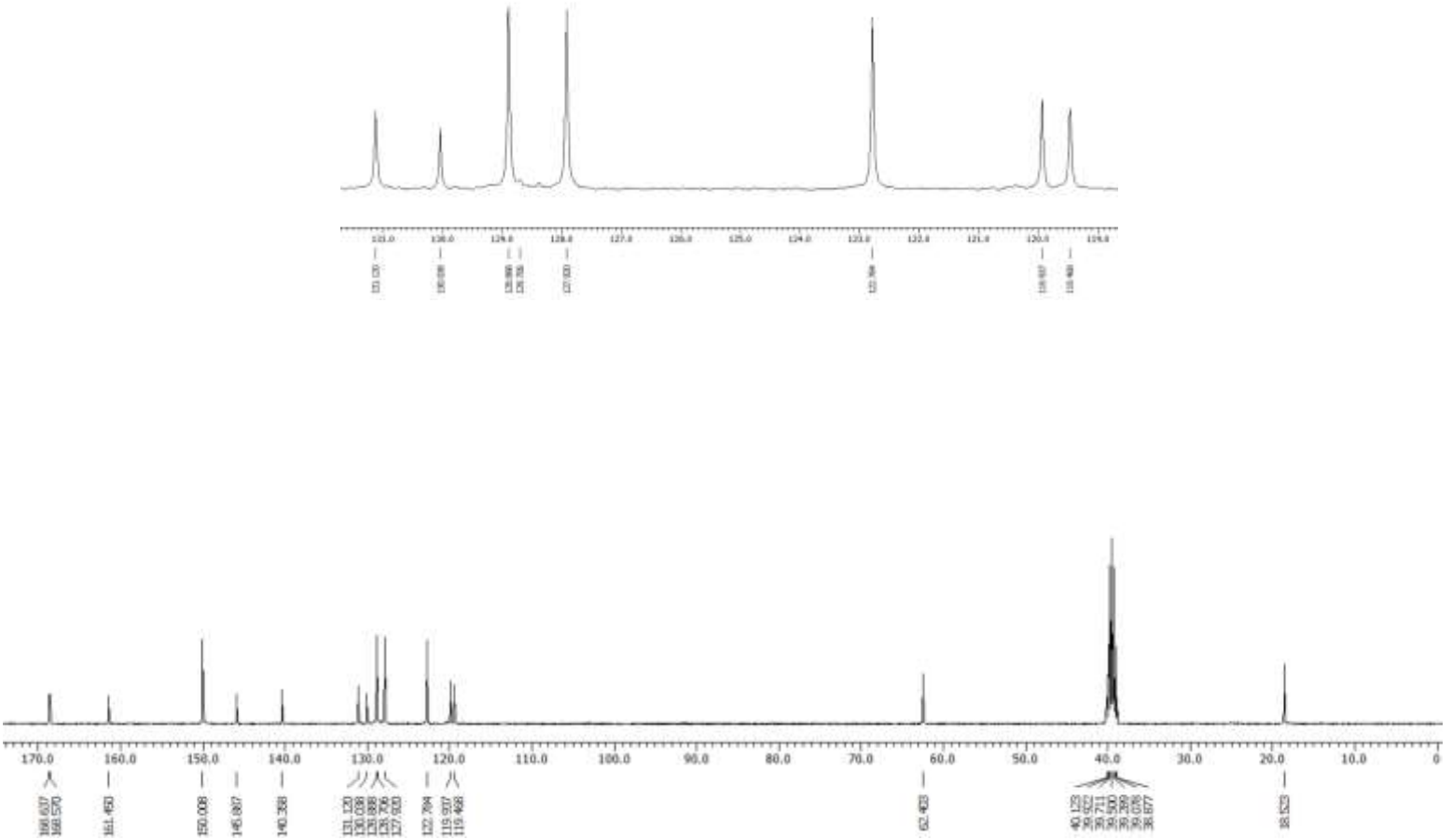




^{13}C NMR spectrum of 1t (100 MHz, DMSO-*d6*)

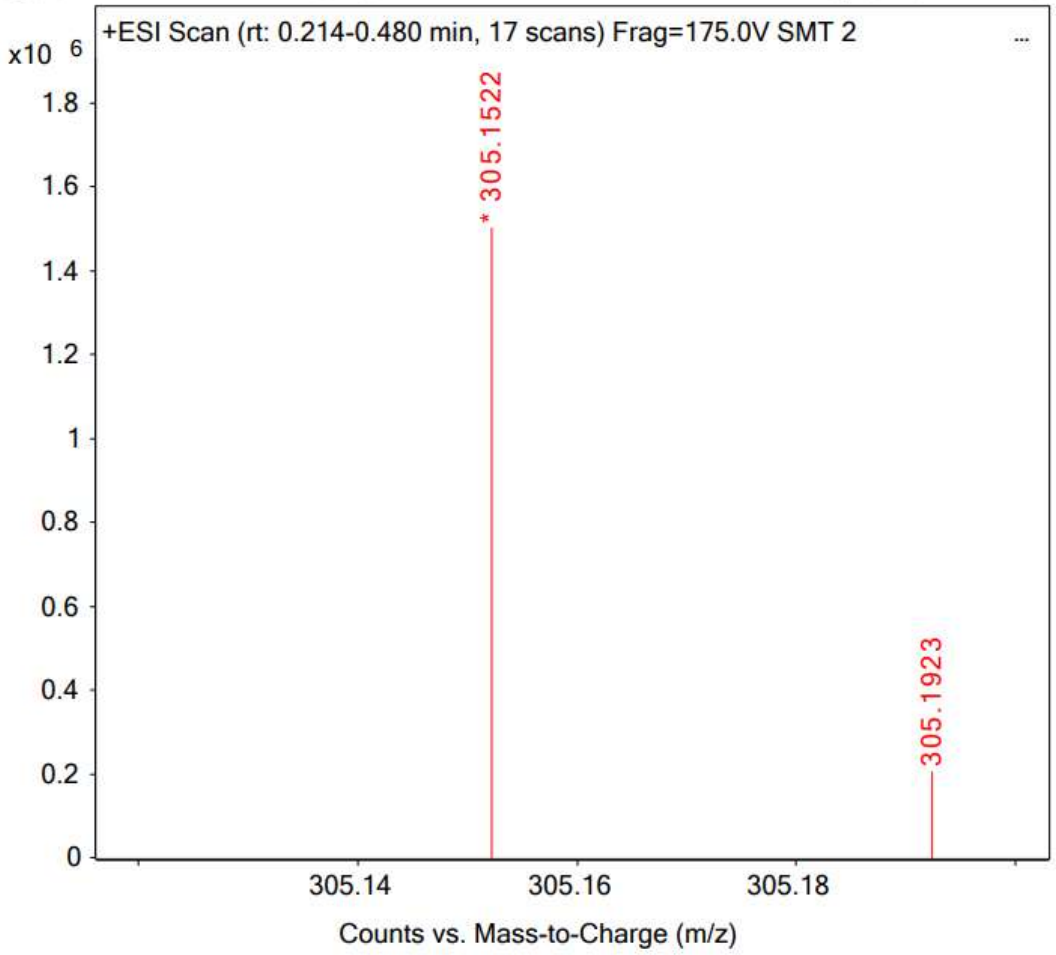


N-(3-phenylpropioloyl)-*N*-(pyridin-4-ylmethyl)methacrylamide

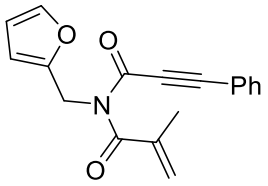


HRMS spectrum of 1t

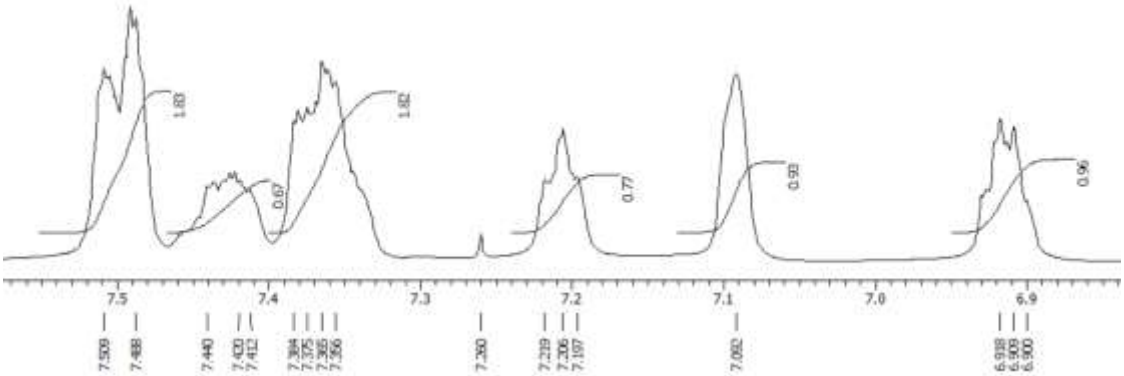
Sample Name	SMT 259(A)	**Position**	P1-A7	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 259(A).d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:03:59 (UTC+05:30)

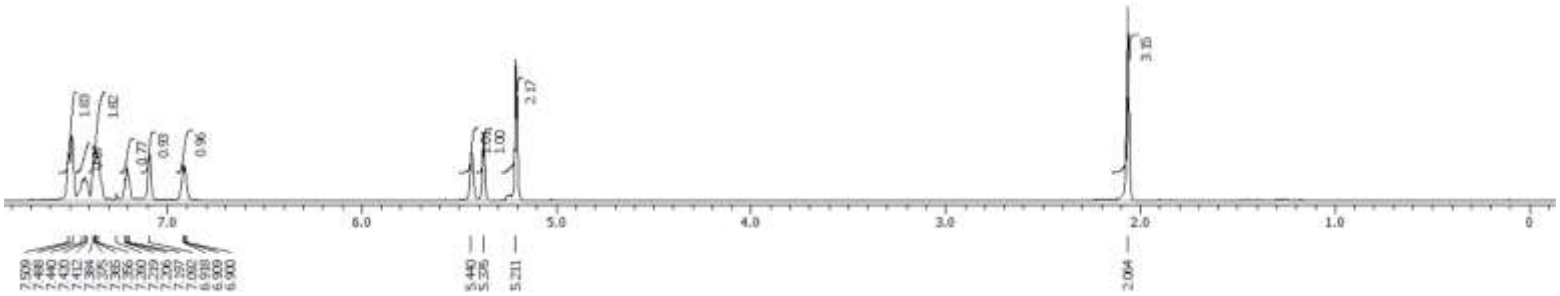


^{1}H NMR spectrum of 1u (400 MHz, $CDCl_3$)

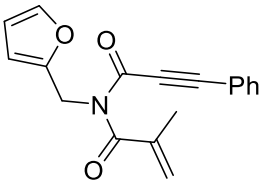


N-(furan-2-ylmethyl)-*N*-(3-phenylpropioloyl)methacrylamide

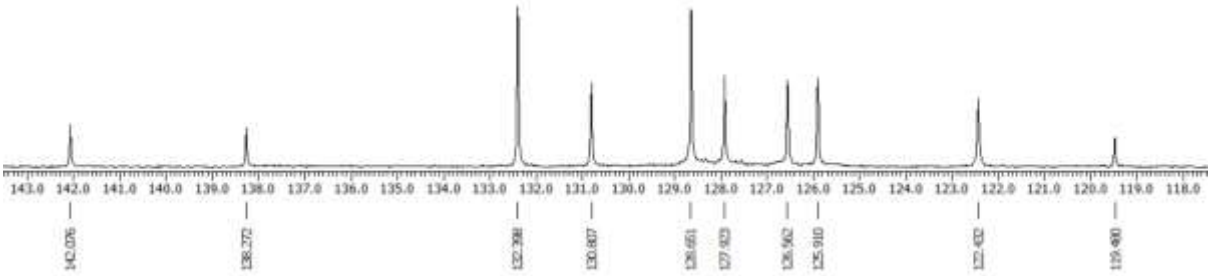


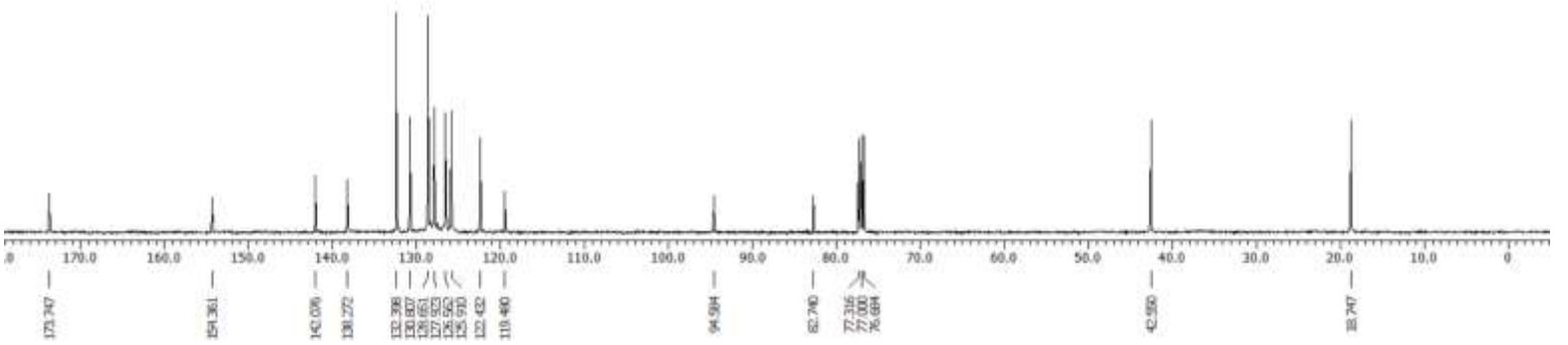


^{13}C NMR spectrum of 1u (100 MHz, $CDCl_3$)



N-(furan-2-ylmethyl)-*N*-(3-phenylpropioloyl)methacrylamide





HRMS spectrum of 1u

Qualitative Compound Report

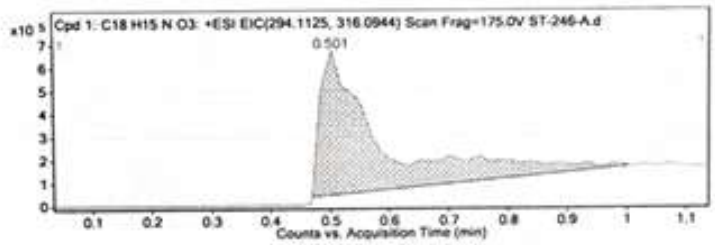
Data File	ST-246-A.d	**Sample Name**	ST-246-A
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	11-05-2024 12:23:38
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

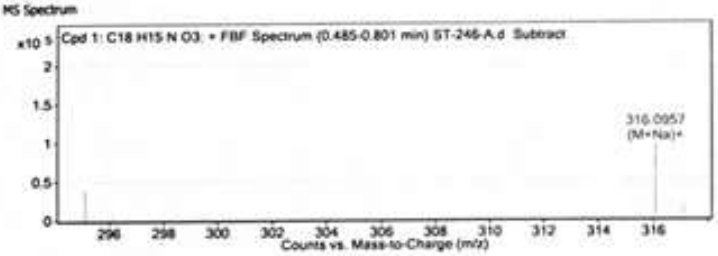
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C18 H15 N O3	0.501	293.1066	95314	C18 H15 N O3	293.1052	4.89	C18 H15 N O3	C18 H15 N O3

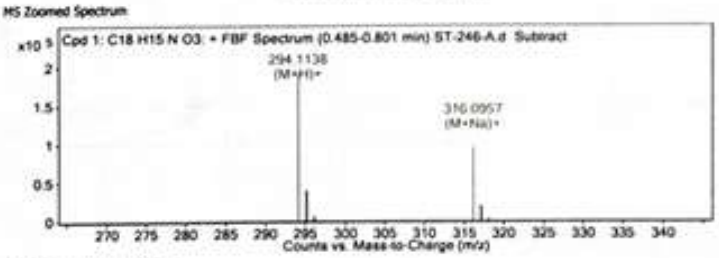
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H15 N O3	316.0957	0.501	Find By Formula	293.1066



MS Spectrum



MS Zoomed Spectrum

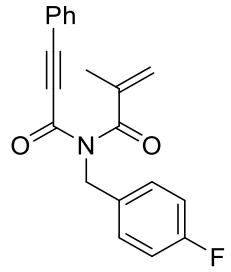


MS Spectrum Peak List

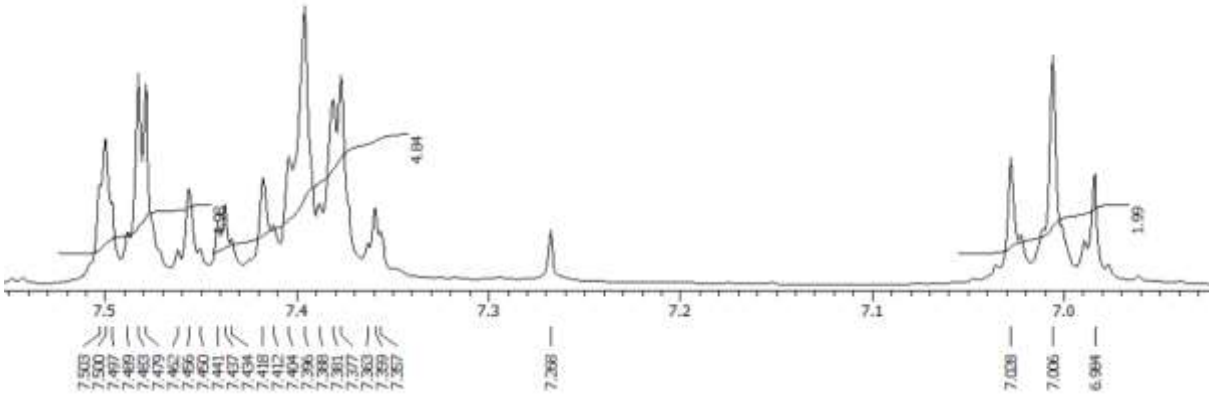
m/z	z	Abund	Formula	Ion
294.1138	1	189636.41	C18H16NO3	(M+H)+
295.1176	1	40339.96	C18H16NO3	(M+H)+
296.1213	1	5406.94	C18H16NO3	(M+H)+
297.1275	1	633.02	C18H16NO3	(M+H)+
316.0957	1	95314.3	C18H15NNaO3	(M+Na)+
317.0993	1	18664.03	C18H15NNaO3	(M+Na)+
318.1036	1	2517.46	C18H15NNaO3	(M+Na)+

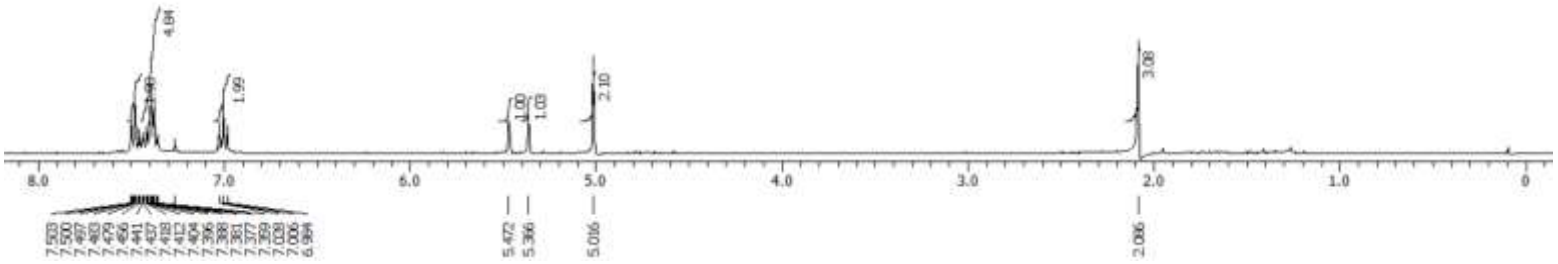
--- End Of Report ---

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

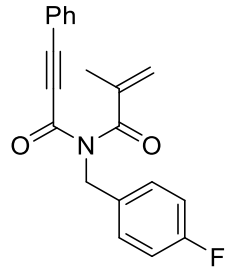


N-(4-fluorobenzyl)-*N*-(3-phenylpropioloyl)methacrylamide

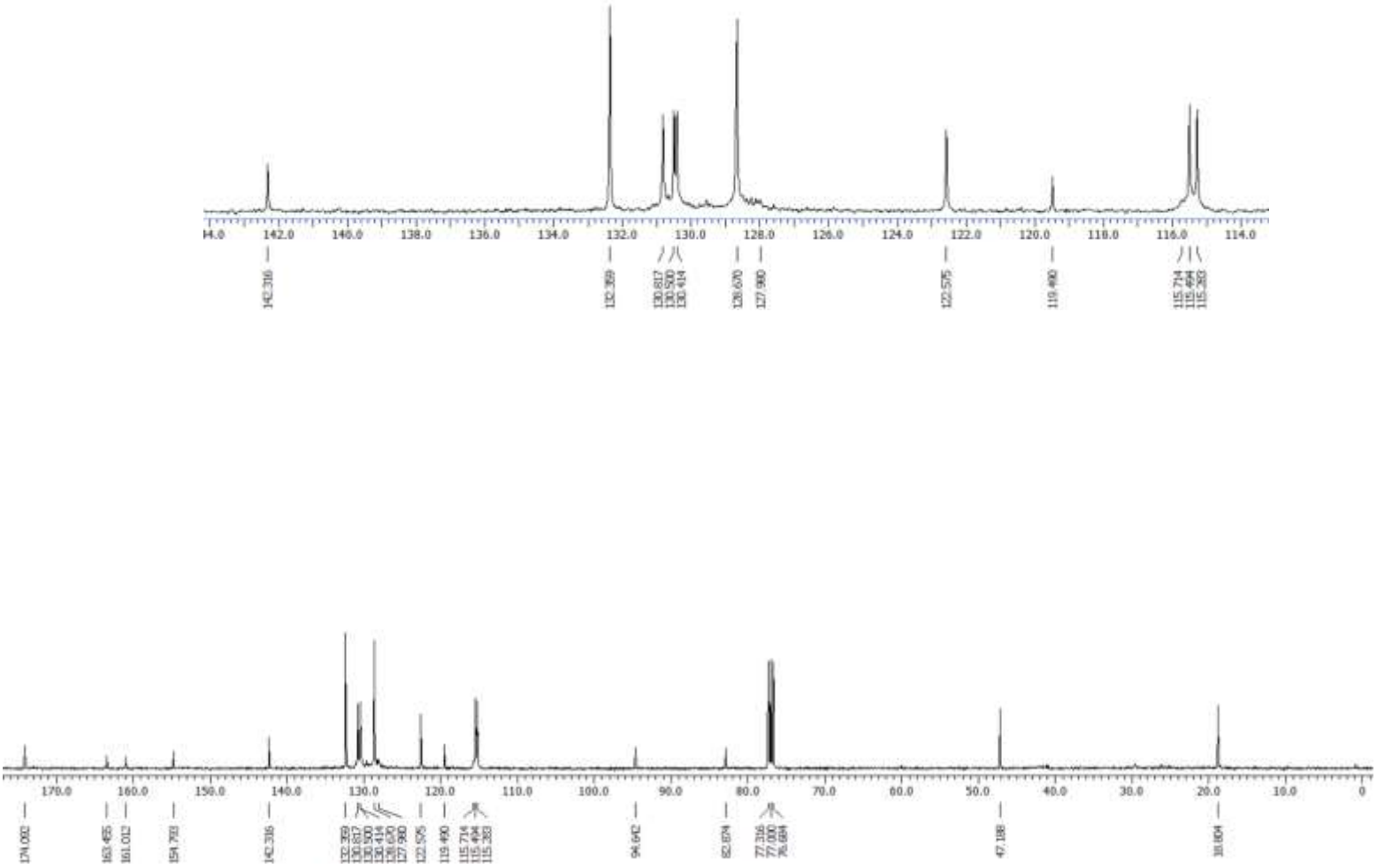




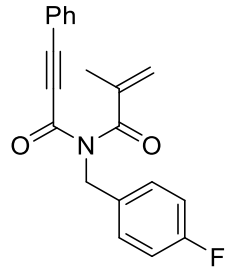
^{13}C NMR spectrum of 1v (100 MHz, $CDCl_3$)



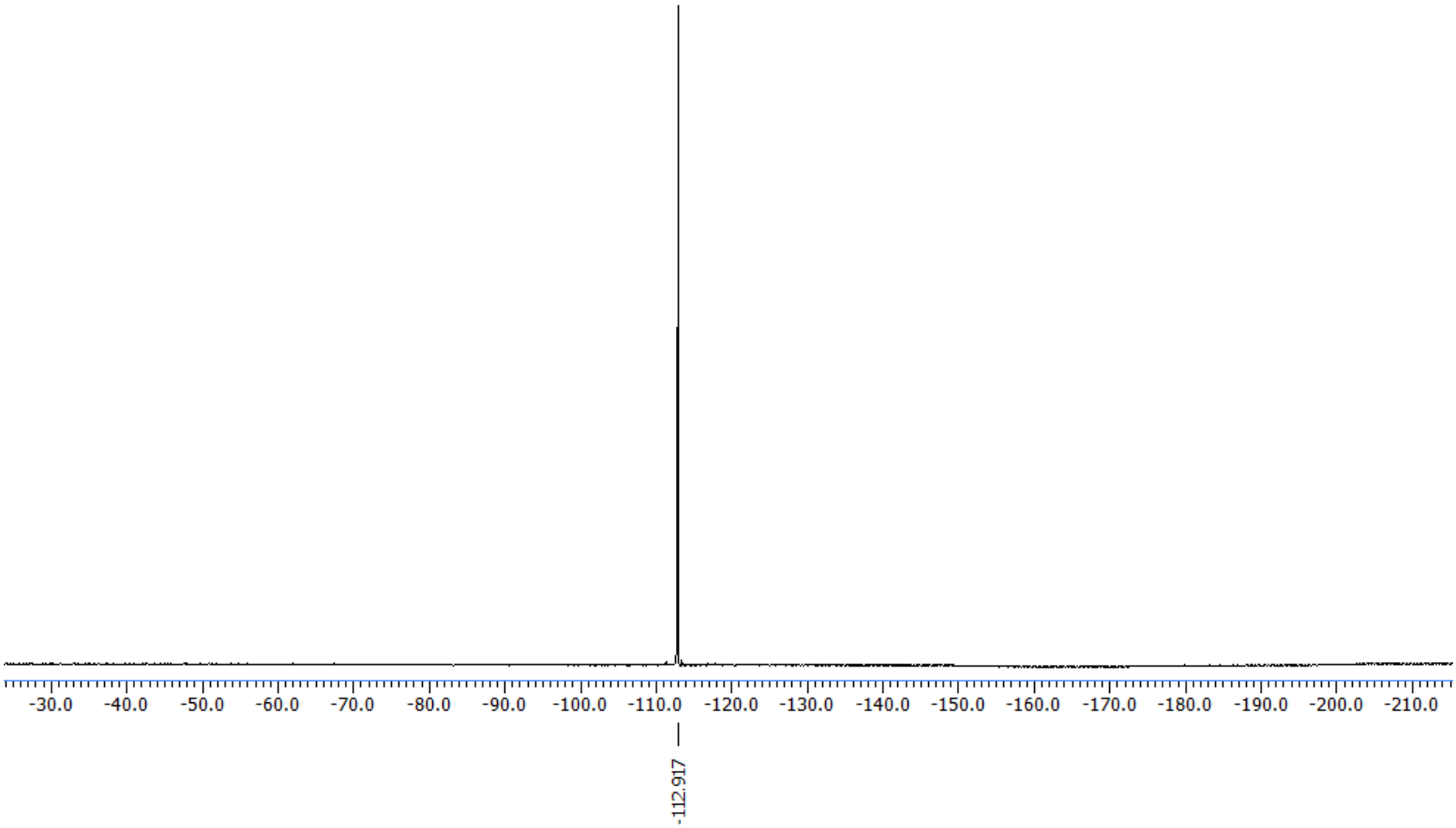
N-(4-fluorobenzyl)-*N*-(3-phenylpropioloyl)methacrylamide



^{19}F NMR spectrum of 1v (100 MHz, $CDCl_3$)



N-(4-fluorobenzyl)-*N*-(3-phenylpropioloyl)methacrylamide



Mass spectrum of 1v

Qualitative Compound Report

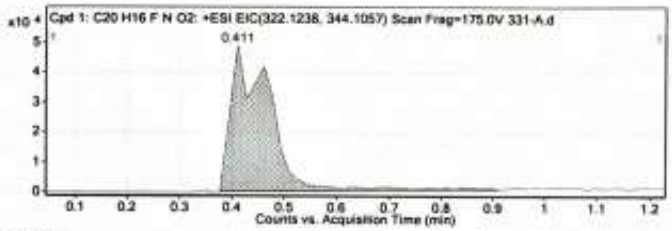
Data File	331-A.d	**Sample Name**	331-A
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 16:18:17
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

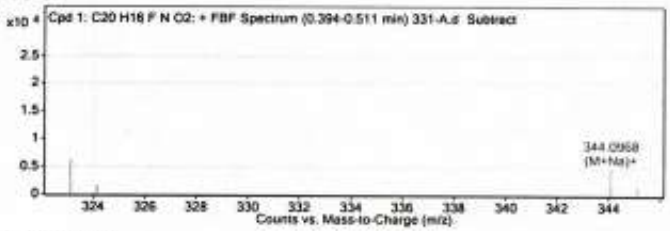
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H16 F N O2	0.411	321.1152	25446	C20 H16 F N O2	321.1165	-4	C20 H16 F N O2	C20 H16 F N O2

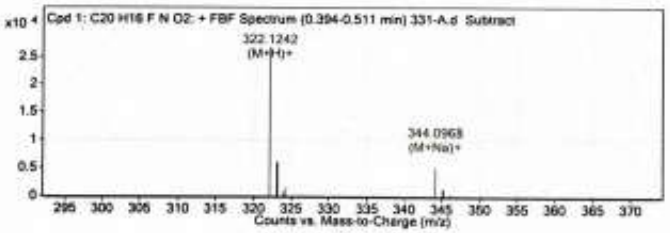
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H16 F N O2	322.1242	0.411	Find By Formula	321.1152



MS Spectrum



MS Zoomed Spectrum

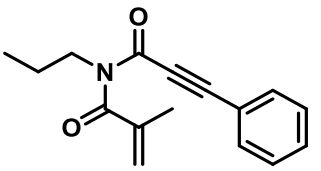


MS Spectrum Peak List

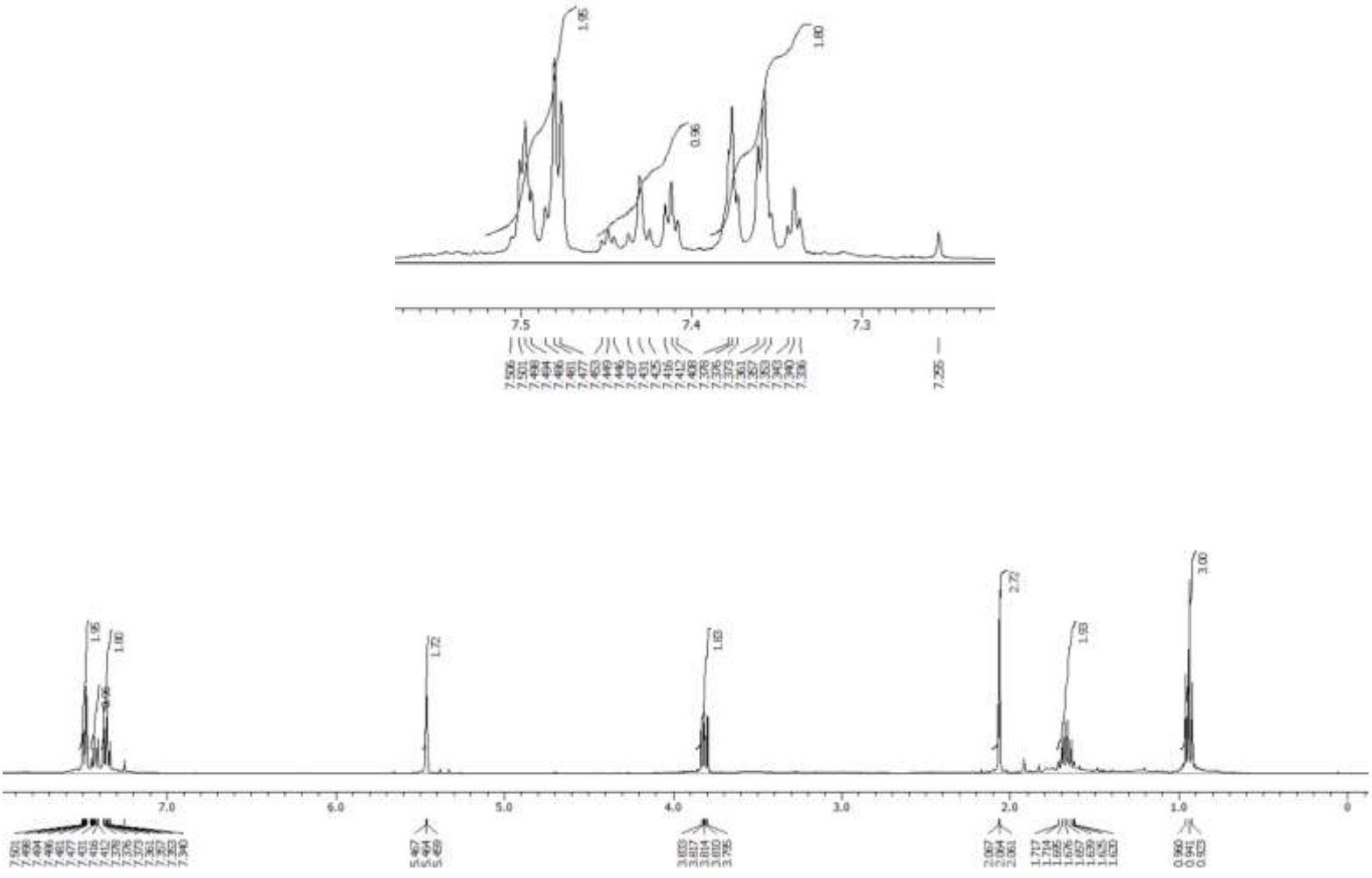
m/z	z	Abund	Formula	Ion
322.1242	1	25445.97	C20H17FNO2	(M+H)+
323.1285	1	6285.22	C20H17FNO2	(M+H)+
324.1229	1	1729.27	C20H17FNO2	(M+H)+
344.0968	1	4901.5	C20H16FNNaO2	(M+Na)+
345.1004	1	1368.83	C20H16FNNaO2	(M+Na)+
346.0998	1	160.6	C20H16FNNaO2	(M+Na)+

--- End Of Report ---

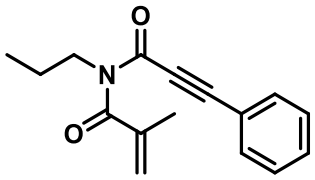
^{1}H NMR spectrum of 1y (400 MHz, $CDCl_3$)



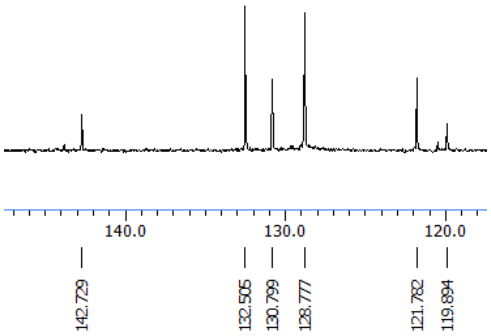
N-(3-phenylpropioloyl)-*N*-propylmethacrylamide

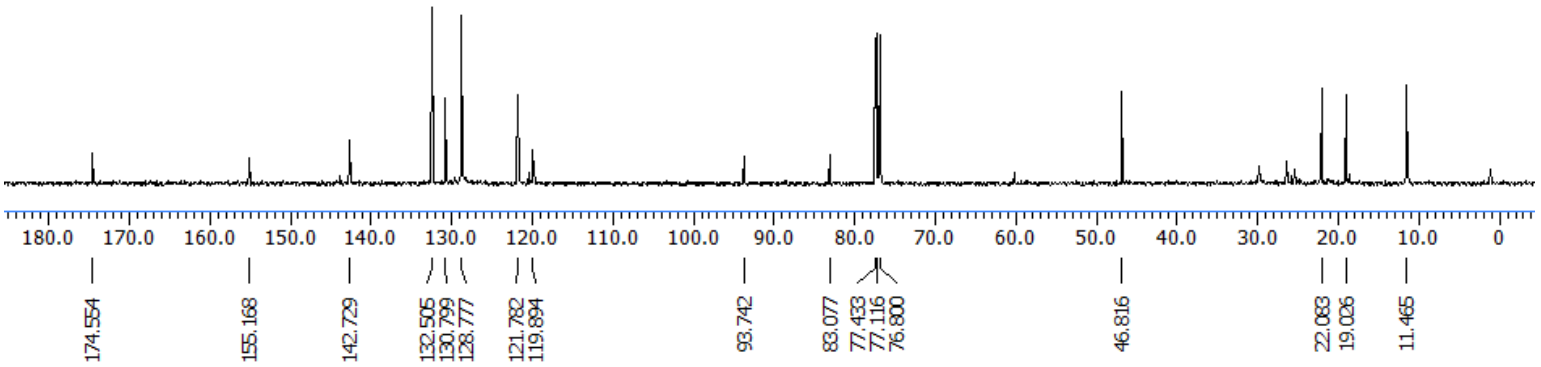


^{13}C NMR spectrum of 1y (100 MHz, $CDCl_3$)

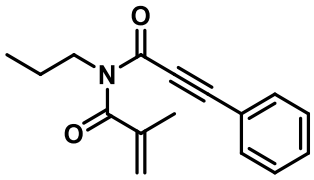


N-(3-phenylpropioloyl)-*N*-propylmethacrylamide

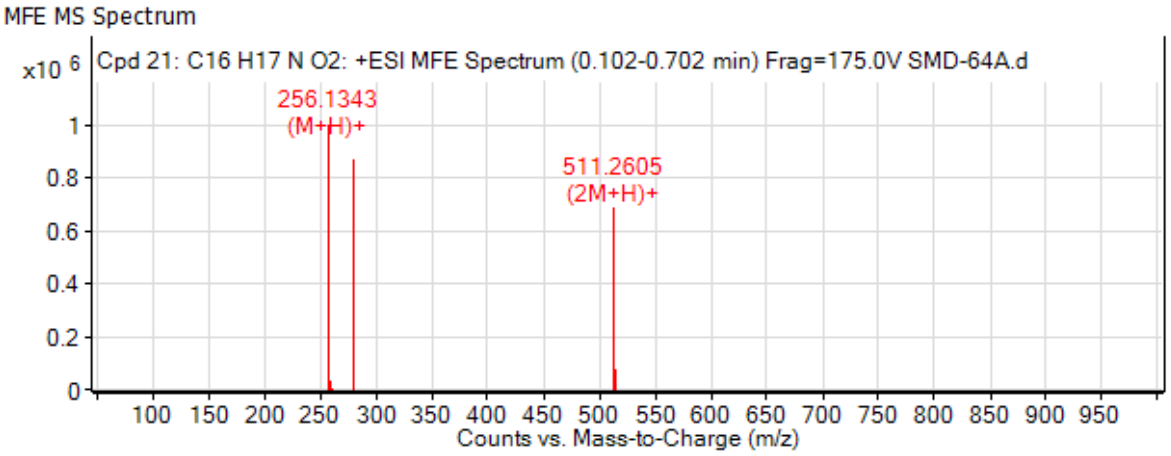


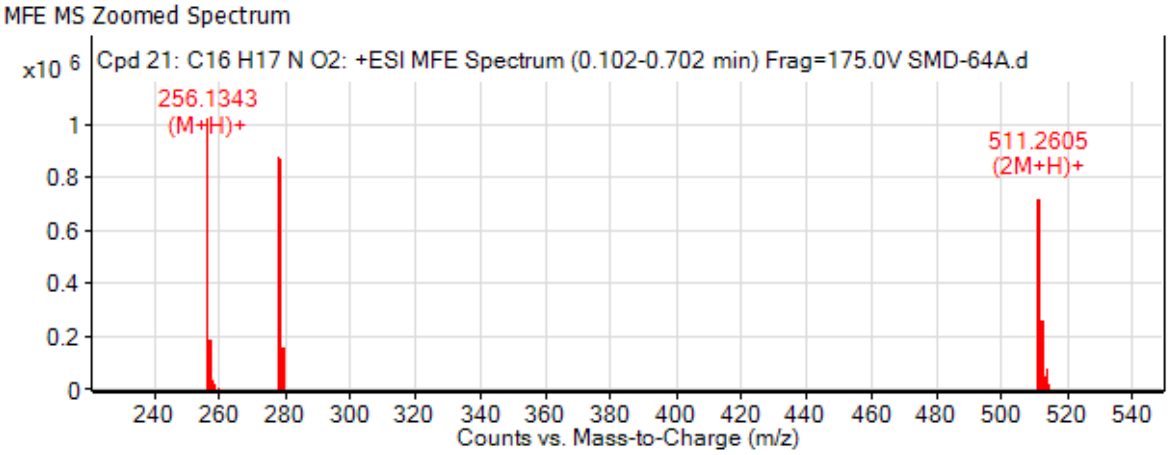


Mass spectrum of 1y

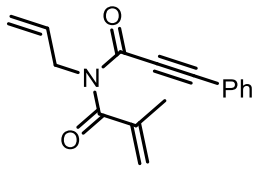


N-(3-phenylpropioloyl)-*N*-propylmethacrylamide

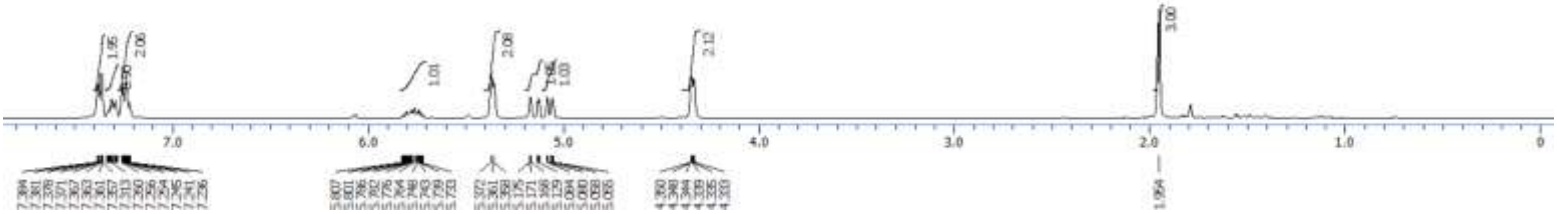




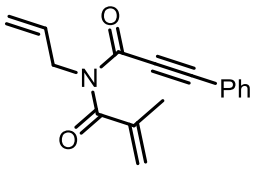
^{1}H NMR spectrum of 1z (400 MHz, $CDCl_3$)



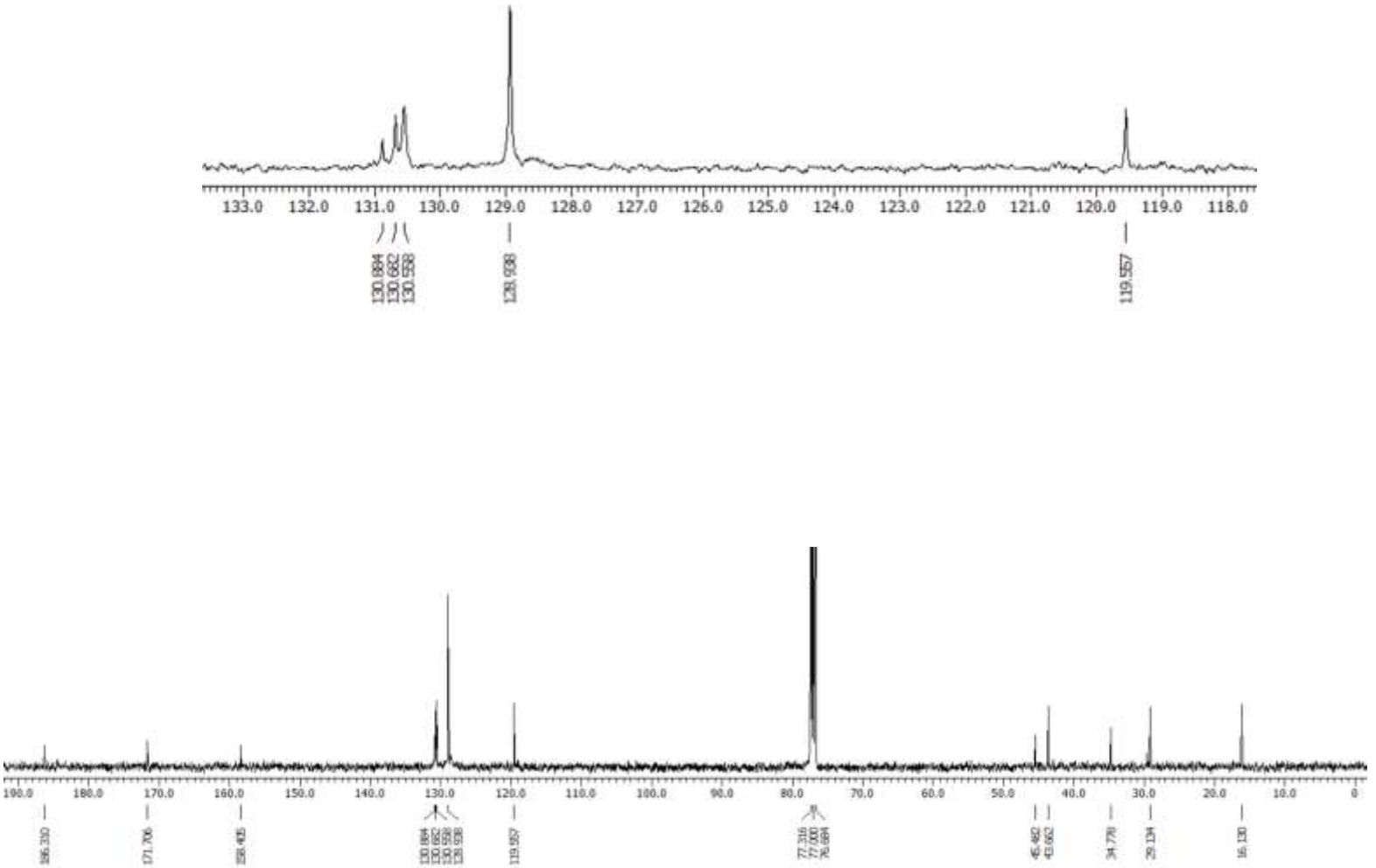
N-allyl-*N*-(3-phenylpropioloyl)methacrylamide



^{13}C NMR spectrum of 1z (100 MHz, $CDCl_3$)

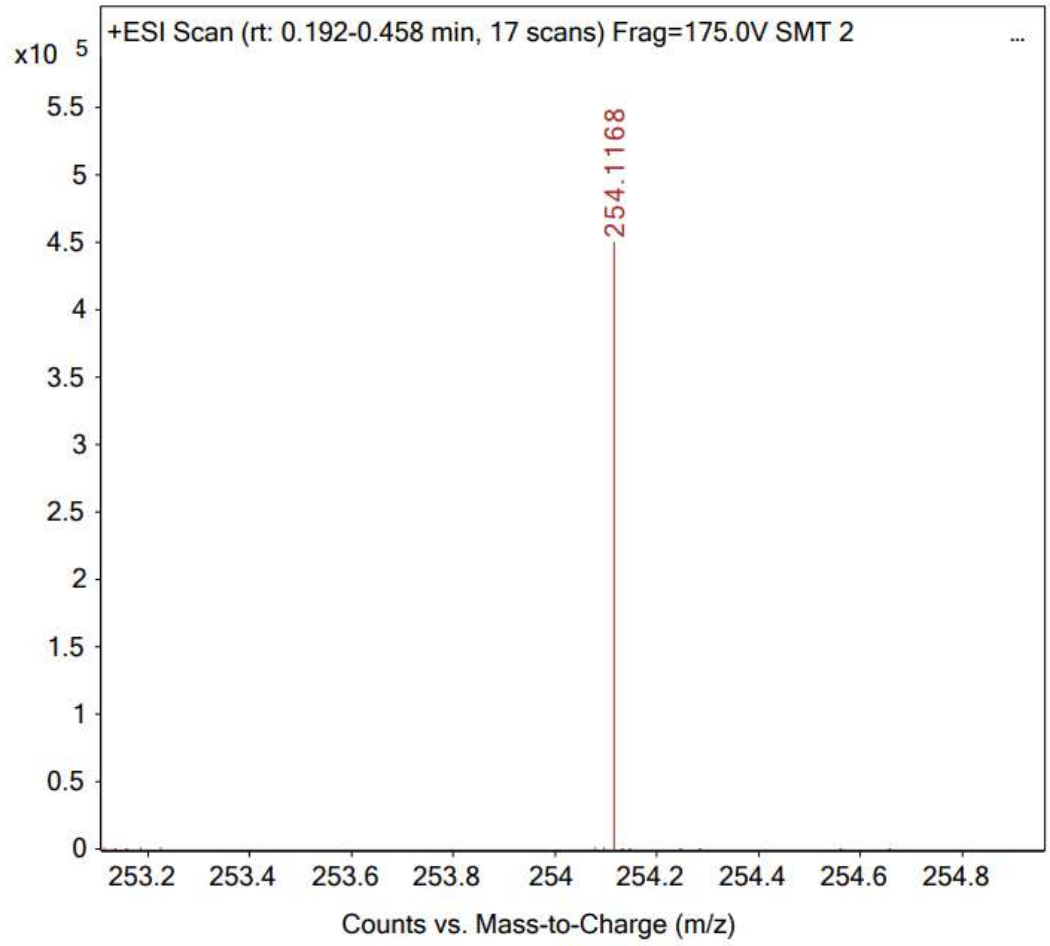


N-allyl-*N*-(3-phenylpropioloyl)methacrylamide

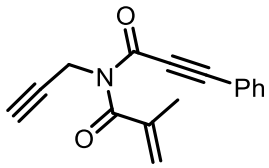


HRMS spectrum of 1z

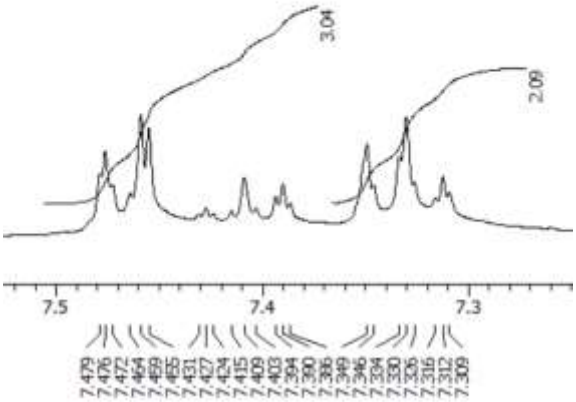
Sample Name	SMT 288(A)	**Position**	P1-A6	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 288(A).d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:00:09 (UTC+05:30)

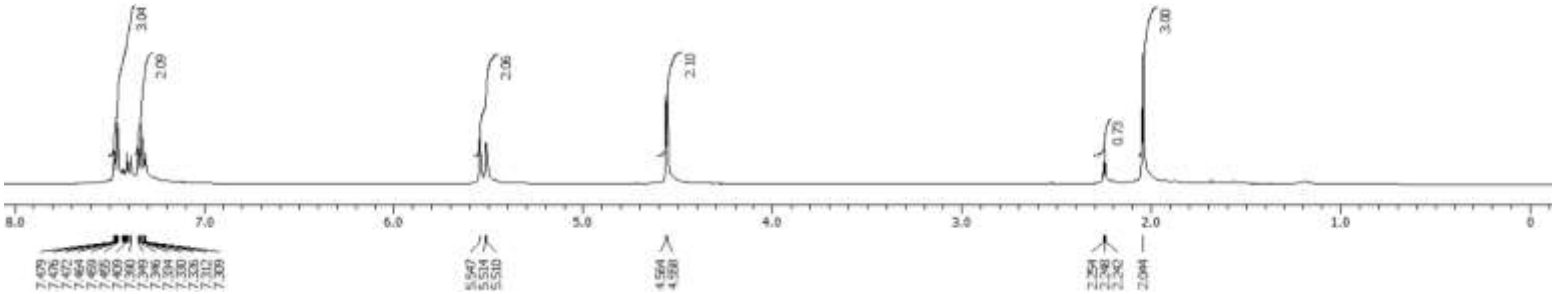


^{1}H NMR spectrum of 1aa (400 MHz, $CDCl_3$)

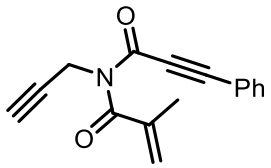


N-(3-phenylpropioloyl)-*N*-(prop-2-yn-1-yl)methacrylamide

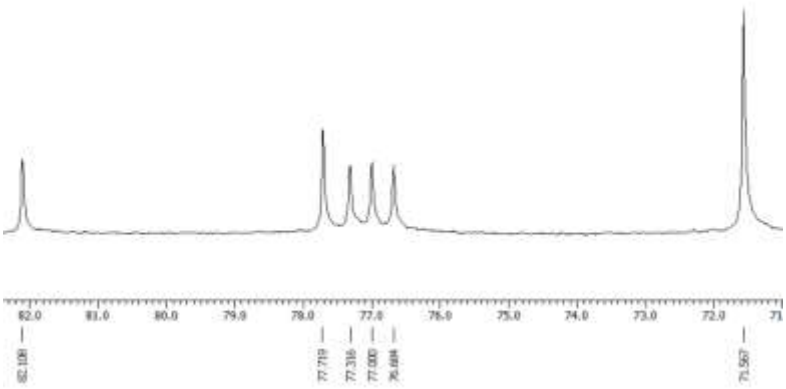


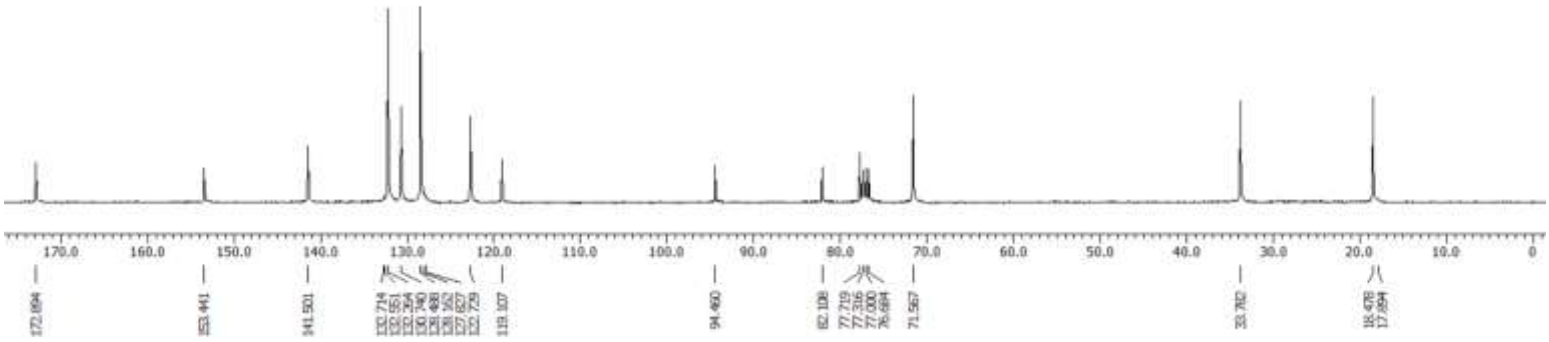


^{13}C NMR spectrum of 1aa (100 MHz, $CDCl_3$)



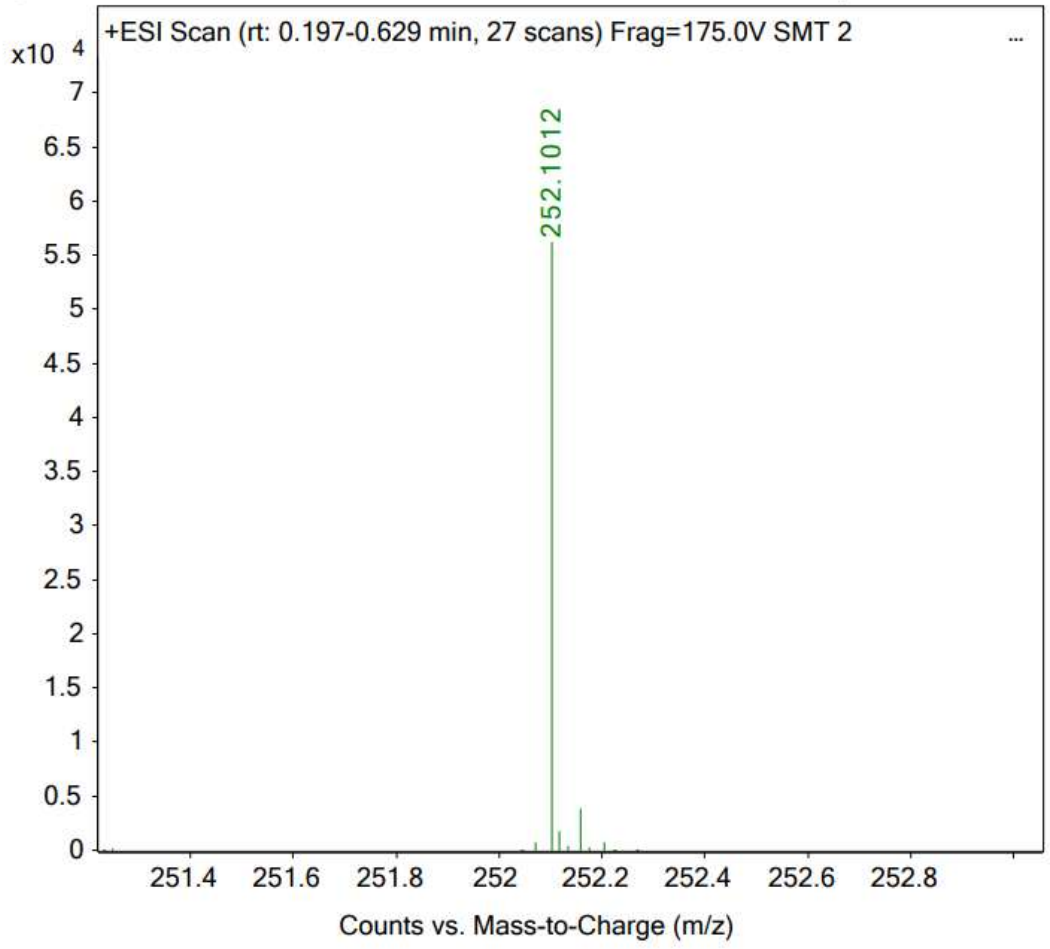
N-(3-phenylpropioloyl)-*N*-(prop-2-yn-1-yl)methacrylamide



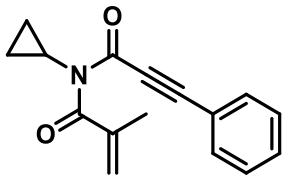


HRMS spectrum of 1aa

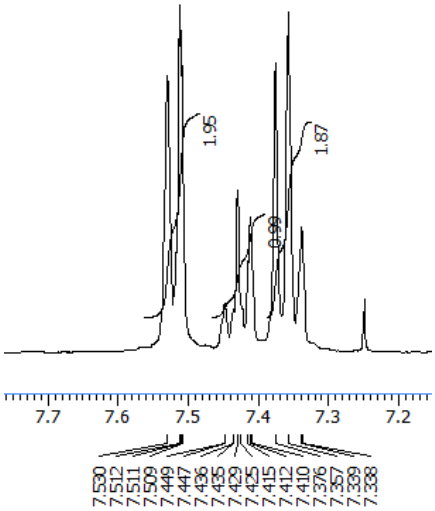
Sample Name	SMT 268(A)	**Position**	P1-C7	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 268(A).d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 13:29:05 (UTC+05:30)

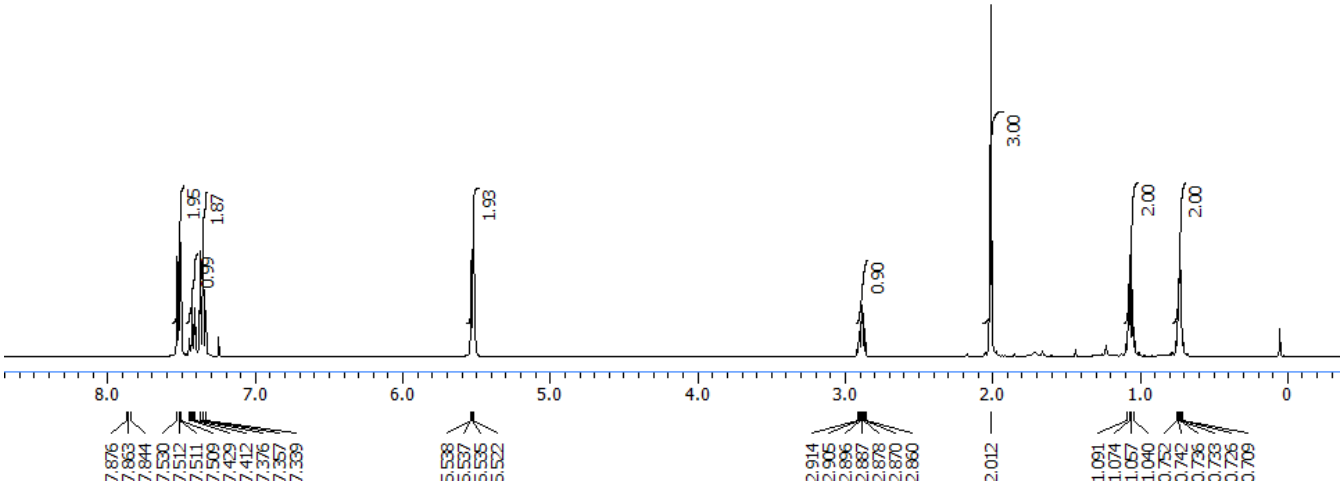


^{1}H NMR spectrum of 1ab (400 MHz, $CDCl_3$)

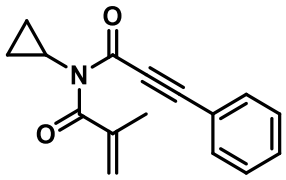


N-cyclopropyl-N-(3-phenylpropioloyl)methacrylamide

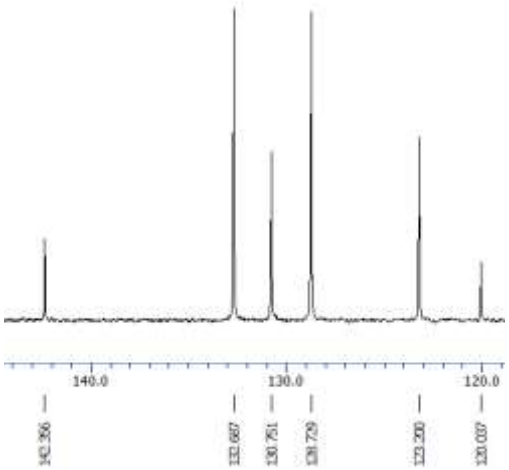


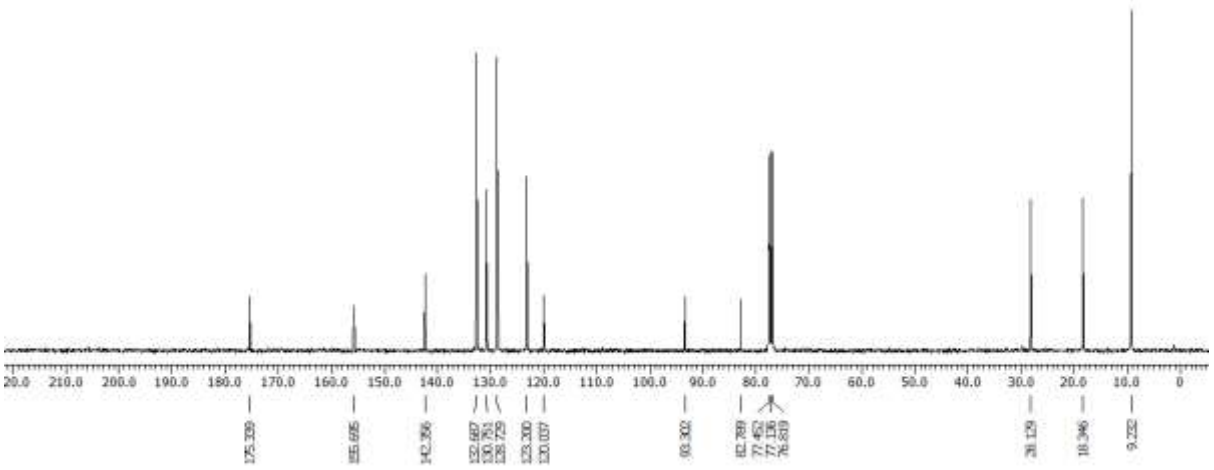


^{13}C NMR spectrum of 1ab (100 MHz, $CDCl_3$)

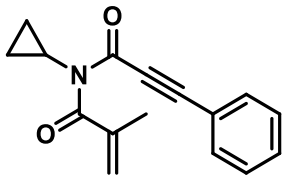


N-cyclopropyl-N-(3-phenylpropioloyl)methacrylamide

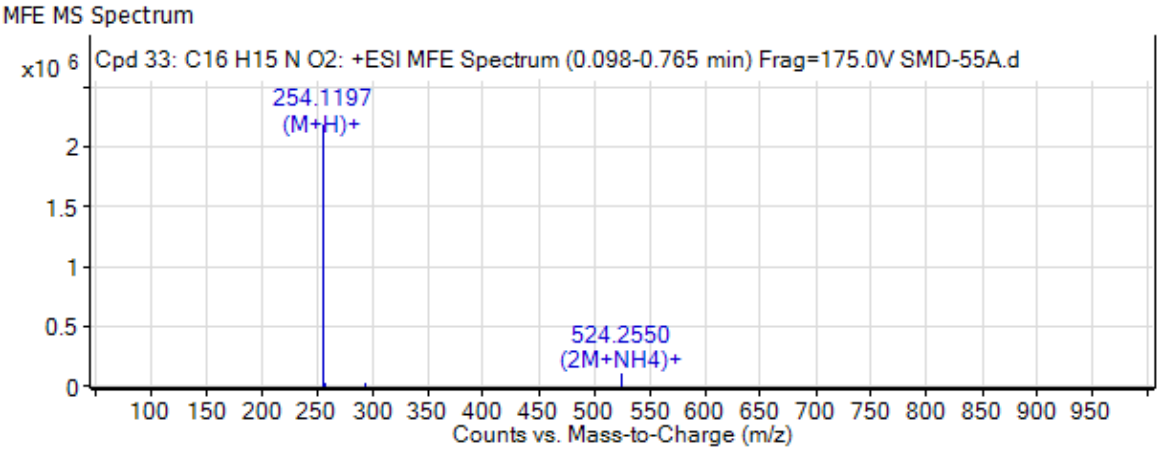


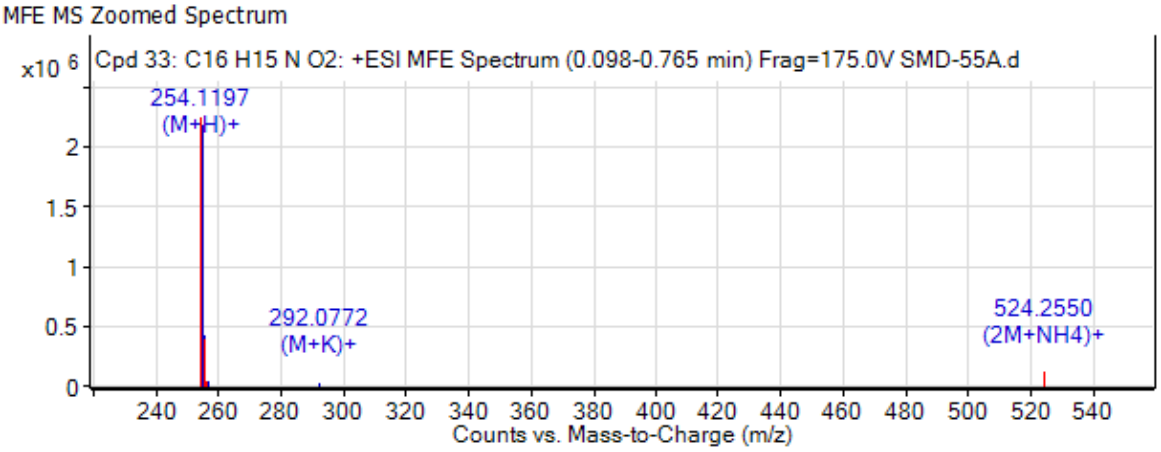


Mass Spectrum of 1ab

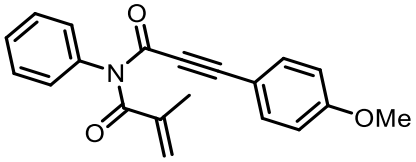


N-cyclopropyl-N-(3-phenylpropioloyl)methacrylamide

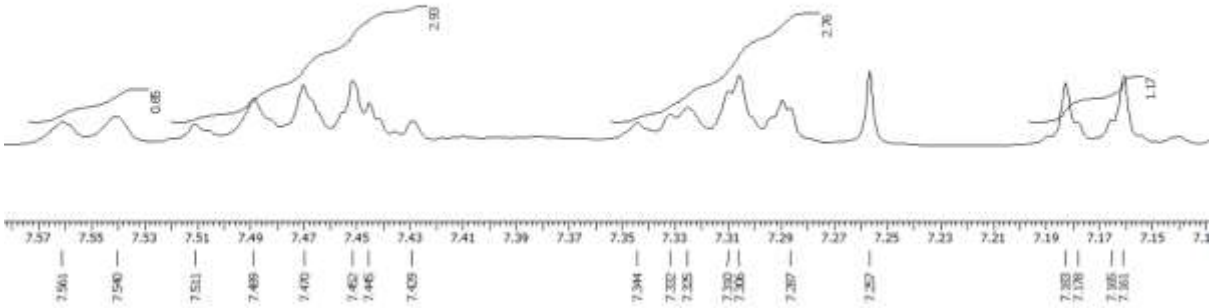


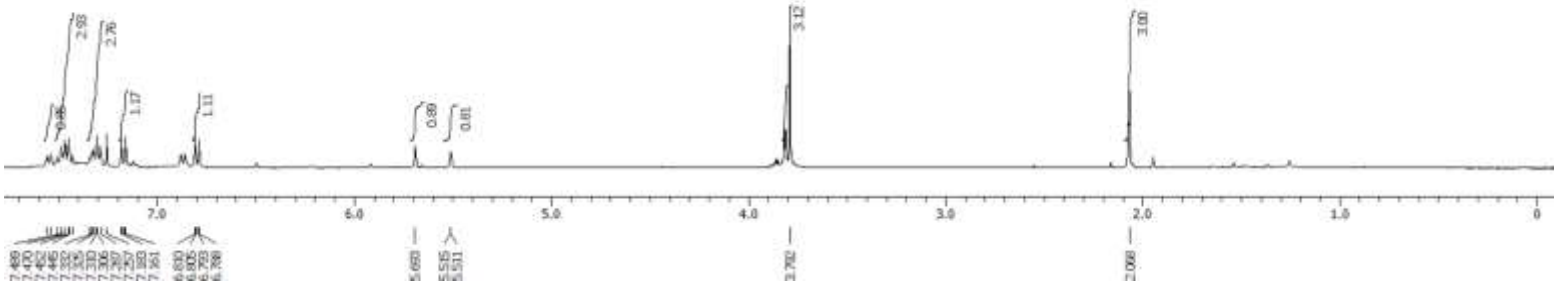


^{1}H NMR spectrum of 1ae (400 MHz, $CDCl_3$)

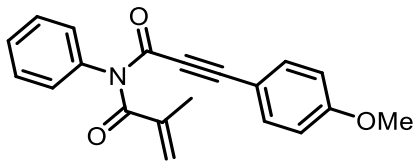


N-(3-(4-methoxyphenyl)propioloyl)-*N*-phenylmethacrylamide

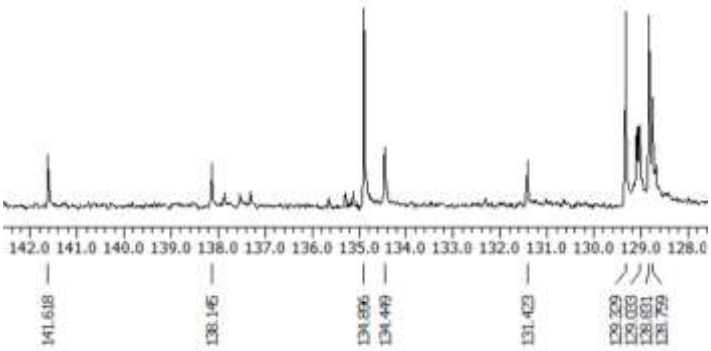


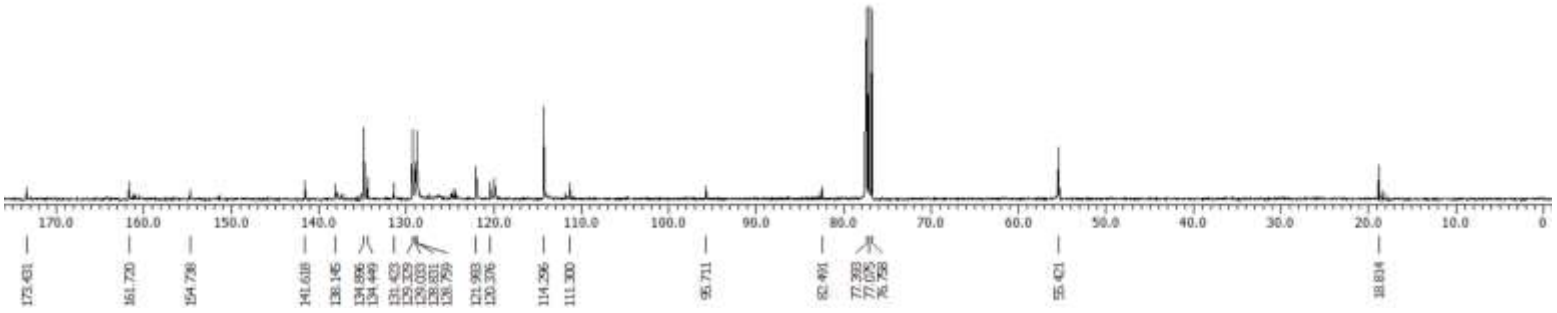


^{13}C NMR spectrum of 1ae (100 MHz, $CDCl_3$)



N-(3-(4-methoxyphenyl)propioloyl)-*N*-phenylmethacrylamide





HRMS spectrum of 1ae

Qualitative Compound Report

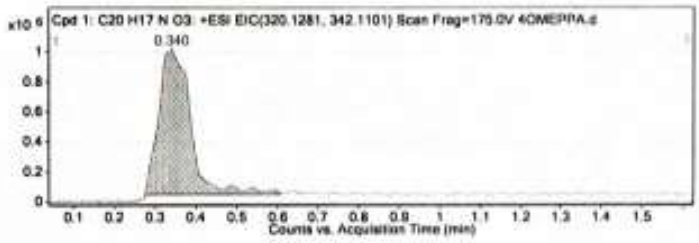
Data File	4OMEPPA.d	**Sample Name**	4OMEPPA
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	01-05-2024 13:35:23
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

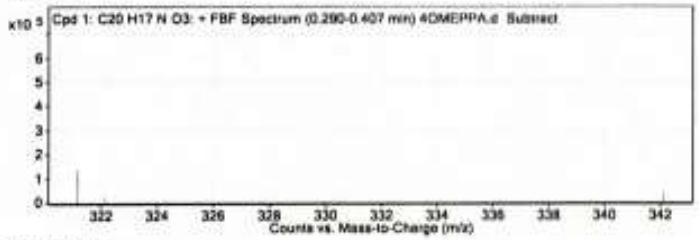
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H17 N O3	0.34	319.1215	610515	C20 H17 N O3	319.1208	2.1	C20 H17 N O3	C20 H17 N O3

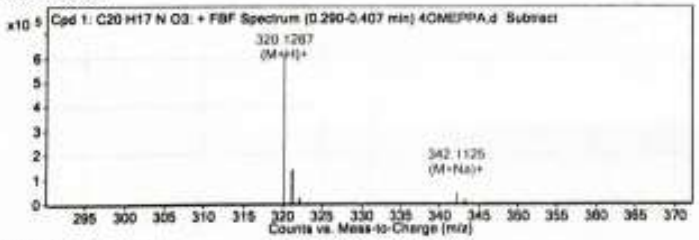
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H17 N O3	320.1287	0.34	Find By Formula	319.1215



MS Spectrum



MS Zoomed Spectrum

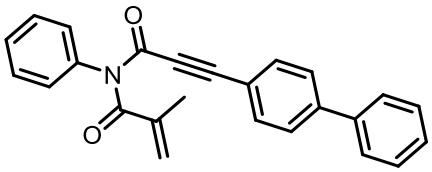


MS Spectrum Peak List

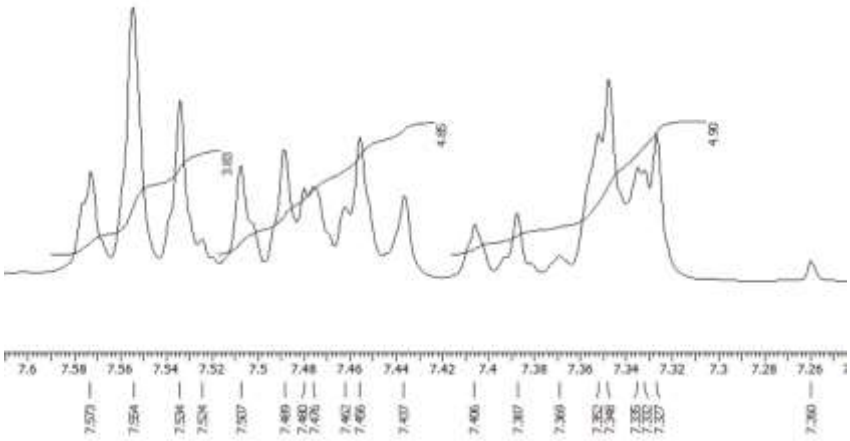
m/z	z	Abund	Formula	Ion
320.1287	1	610515.13	C20H18NO3	(M+H)+
321.1319	1	133285.97	C20H18NO3	(M+H)+
322.1337	1	21906.9	C20H18NO3	(M+H)+
323.1375	1	3654.61	C20H18NO3	(M+H)+
342.1125	1	41305.99	C20H17NNaO3	(M+Na)+
343.119	1	10981.56	C20H17NNaO3	(M+Na)+

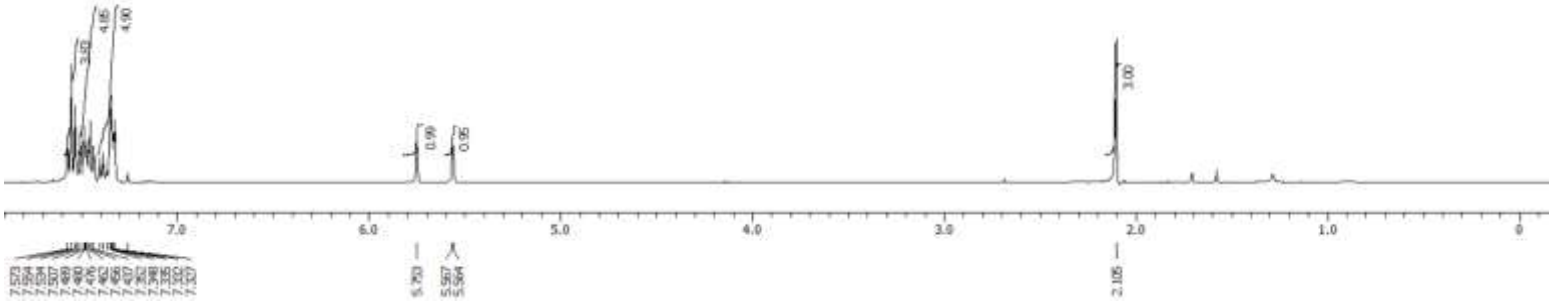
--- End Of Report ---

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

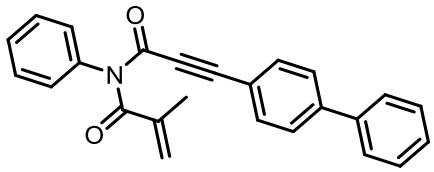


N-(3-([1,1'-biphenyl]-4-yl)propioloyl)-*N*-phenylmethacrylamide

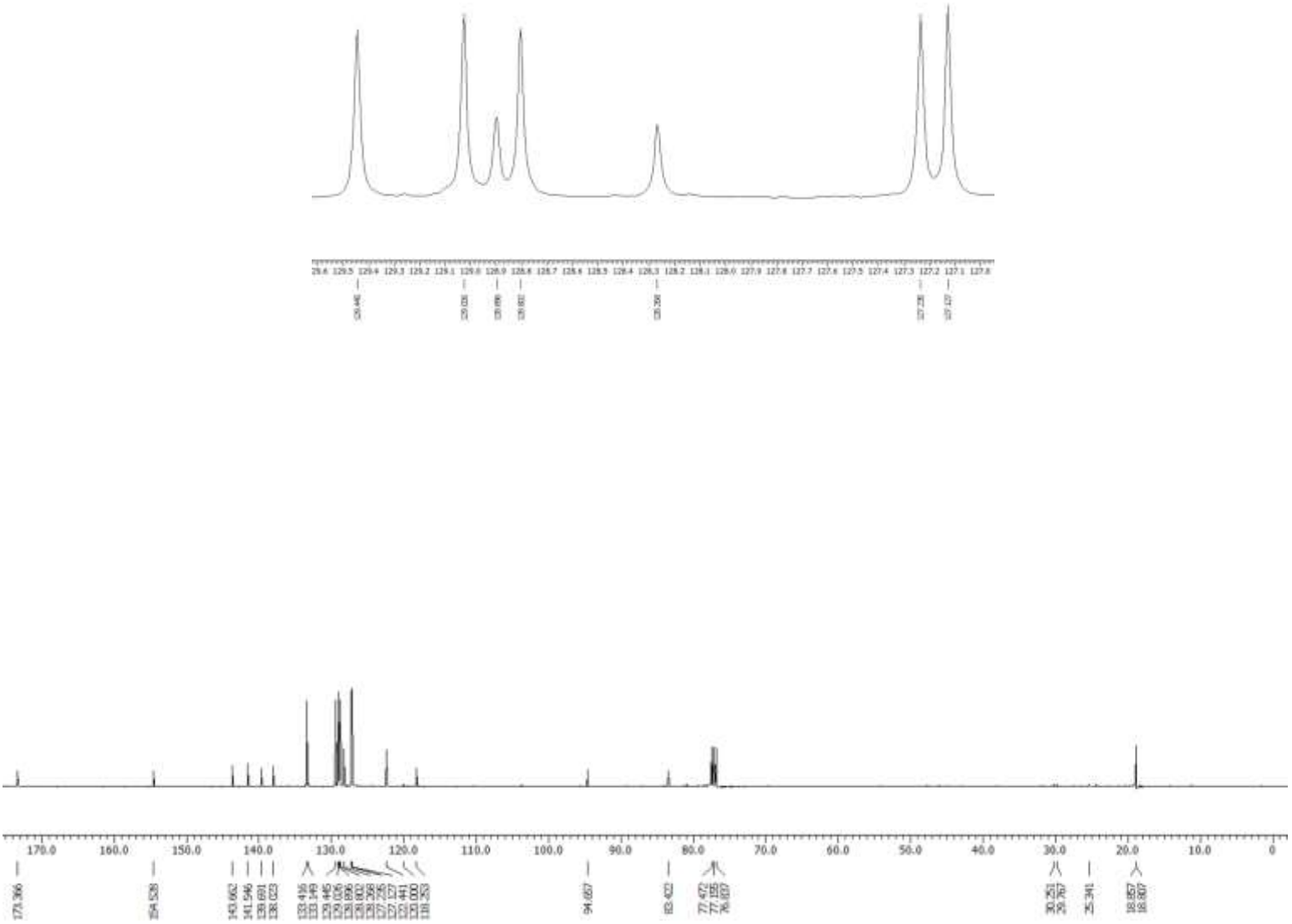




^{13}C NMR spectrum of 1af (100 MHz, $CDCl_3$)



N-(3-([1,1'-biphenyl]-4-yl)propioloyl)-*N*-phenylmethacrylamide



HRMS spectrum of 1af

Qualitative Compound Report

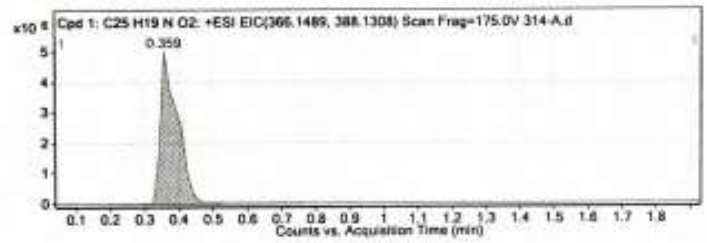
Data File	314-A.d	**Sample Name**	314-A
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 13:50:56
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

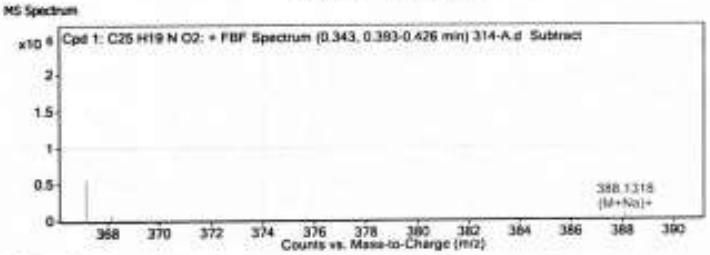
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C25 H19 N O2	0.359	365.1426	2003384	C25 H19 N O2	365.1416	2.7	C25 H19 N O2	C25 H19 N O2

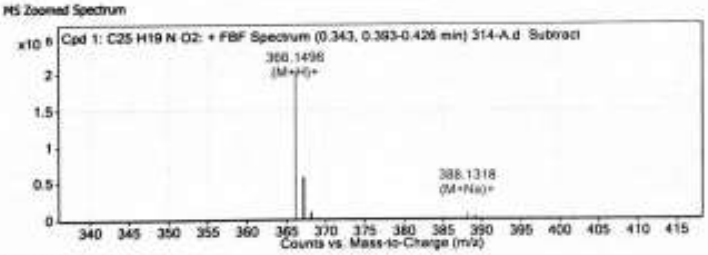
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C25 H19 N O2	366.1498	0.359	Find By Formula	365.1426



MS Spectrum



MS Zoomed Spectrum

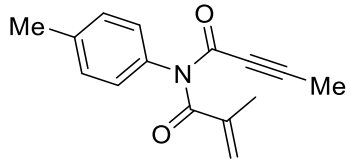


MS Spectrum Peak List

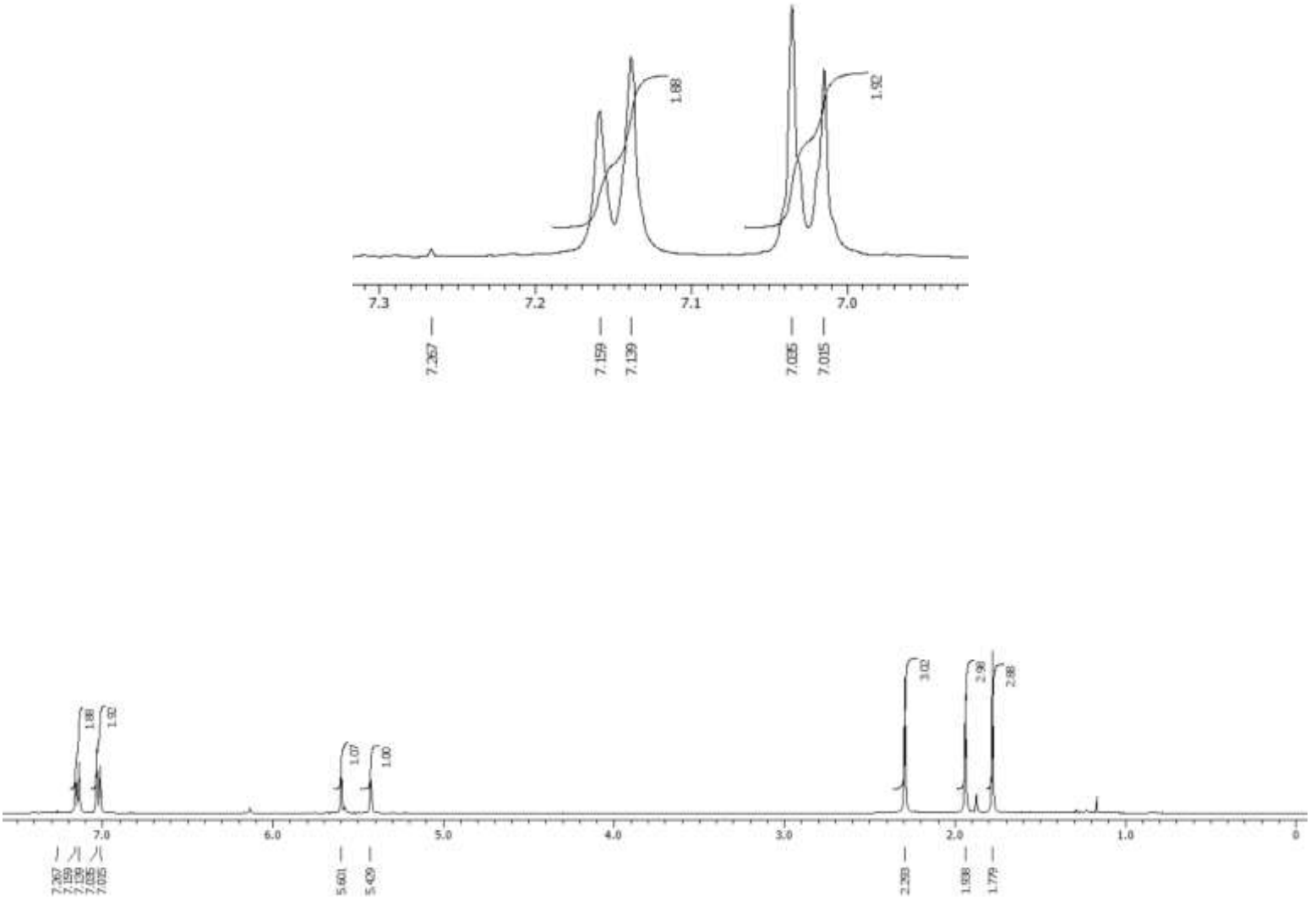
m/z	z	Abund	Formula	Ion
366.1498	1	2003383.75	C25H20NO2	(M+H)+
367.1532	1	564809.31	C25H20NO2	(M+H)+
368.1557	1	82827.2	C25H20NO2	(M+H)+
369.158	1	8330.13	C25H20NO2	(M+H)+
388.1318	1	69122.83	C25H19NNaO2	(M+Na)+
389.1395	1	20041.17	C25H19NNaO2	(M+Na)+
390.1474	1	3543.41	C25H19NNaO2	(M+Na)+
391.1477	1	909.3	C25H19NNaO2	(M+Na)+

--- End Of Report ---

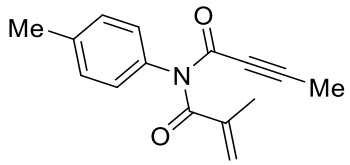
^{1}H NMR spectrum of 3b (400 MHz, $CDCl_3$)



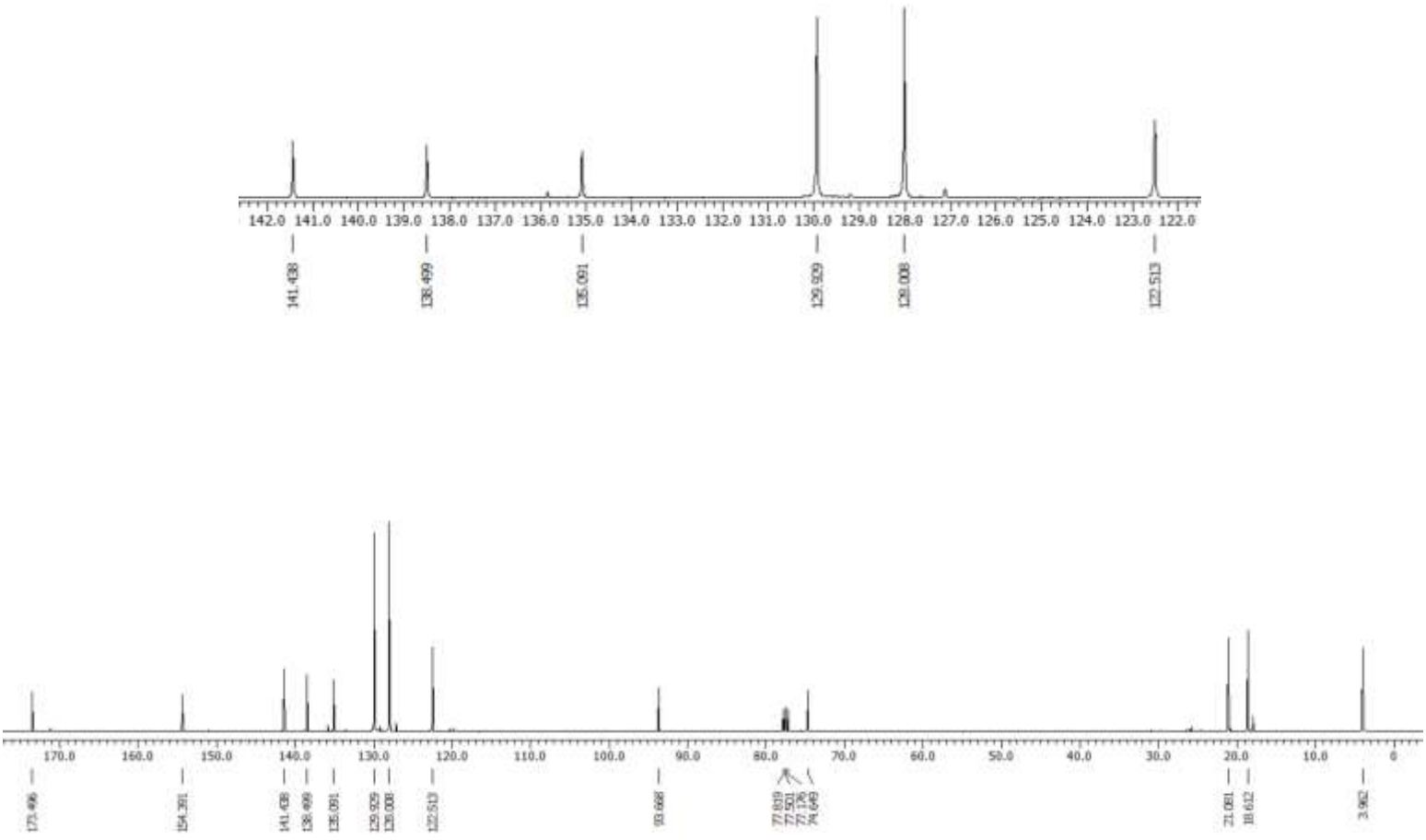
N-methacryloyl-*N*-(*p*-tolyl)but-2-ynamide



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



N-methacryloyl-*N*-(*p*-tolyl)but-2-ynamide



HRMS spectrum of 3b

Qualitative Compound Report

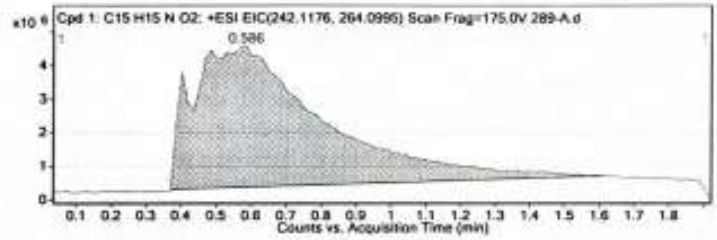
Data File	289-A.d	**Sample Name**	289-A
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 13:34:10
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

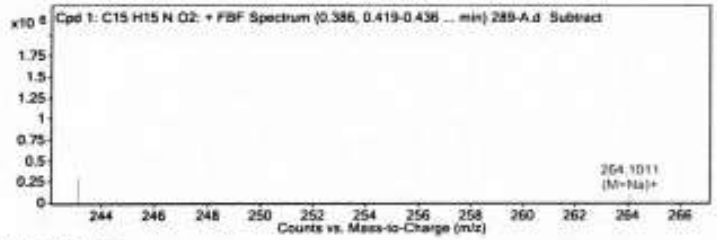
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C15 H15 N O2	0.586	241.1108	103810	C15 H15 N O2	241.1103	2.34	C15 H15 N O2	C15 H15 N O2

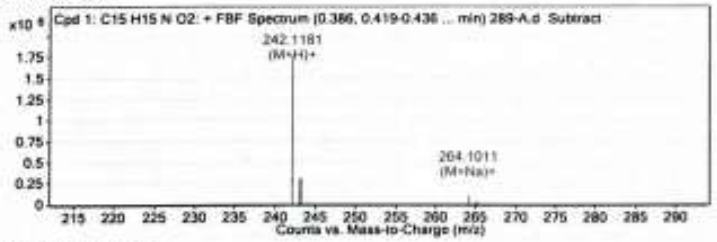
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C15 H15 N O2	264.1011	0.586	Find By Formula	241.1108



MS Spectrum



MS Zoomed Spectrum

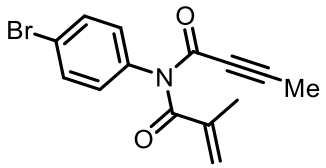


MS Spectrum Peak List

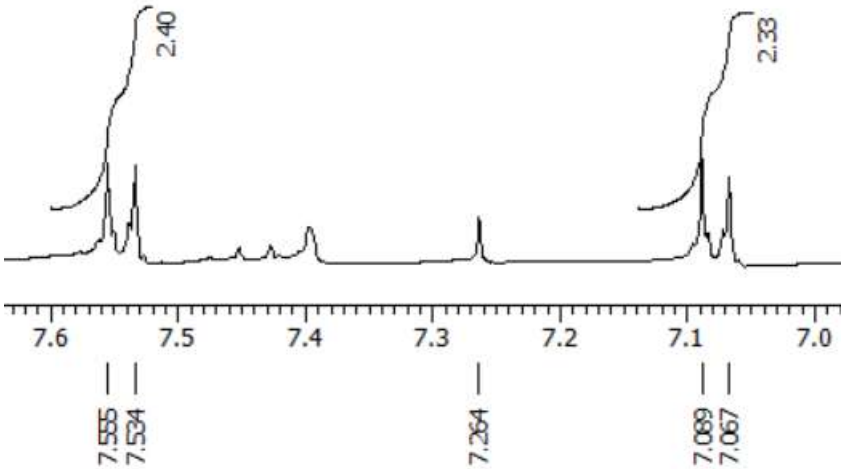
m/z	z	Abund	Formula	Ion
242.1181	1	1764747.75	C15H16NO2	(M+H)+
243.1212	1	300927.28	C15H16NO2	(M+H)+
264.1011	1	103809.88	C15H15NNaO2	(M+Na)+
265.1046	1	17338.39	C15H15NNaO2	(M+Na)+
266.1088	1	1806.65	C15H15NNaO2	(M+Na)+
267.112	1	102.84	C15H15NNaO2	(M+Na)+

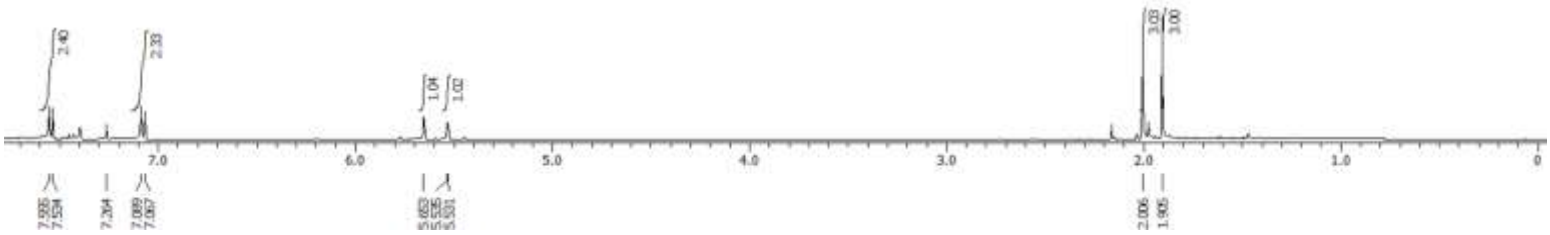
--- End Of Report ---

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

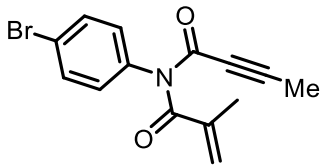


N-(4-bromophenyl)-*N*-methacryloylbut-2-ynamide

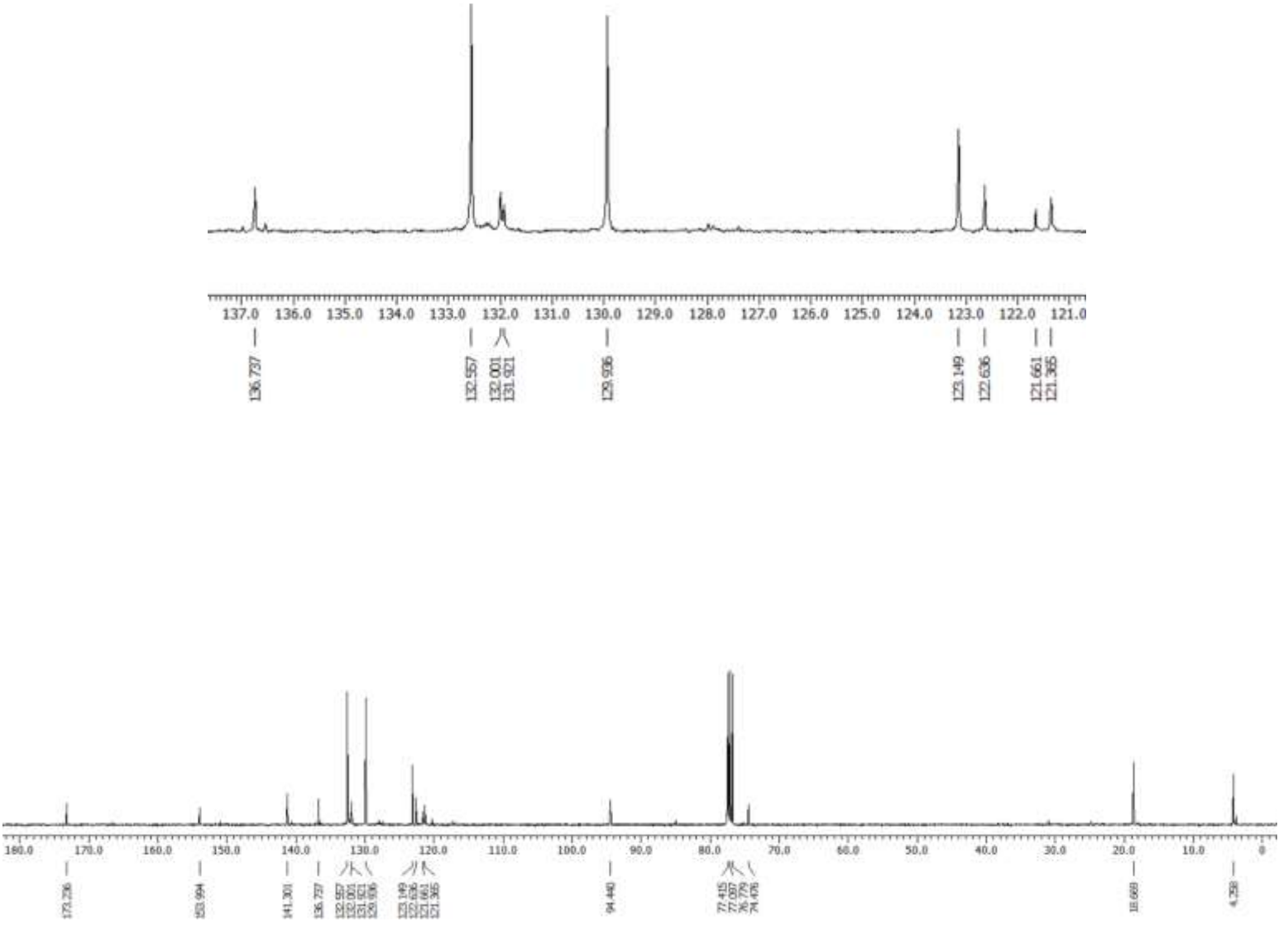




^{13}C NMR spectrum of 3f (100 MHz, $CDCl_3$)



N-(4-bromophenyl)-*N*-methacryloylbut-2-ynamide



HRMS spectrum of 3f

Qualitative Compound Report

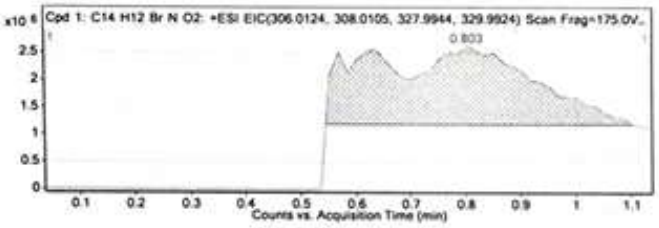
Data File	ST-296-A.d	**Sample Name**	ST-296-A
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	11-05-2024 12:25:37
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

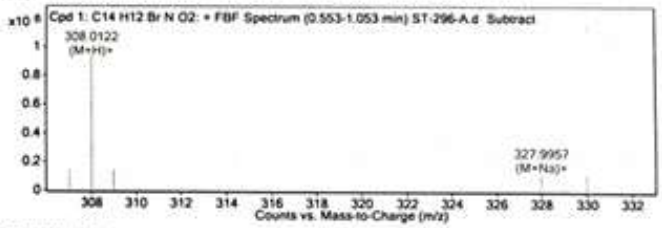
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H12 Br N O2	0.803	305.0067	115520	C14 H12 Br N O2	305.0051	5.16	C14 H12 Br N O2	C14 H12 Br N O2

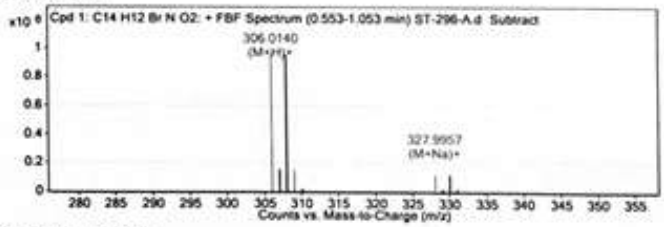
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C14 H12 Br N O2	327.9957	0.803	Find By Formula	305.0067



MS Spectrum



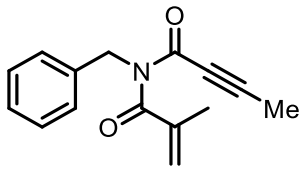
MS Zoomed Spectrum



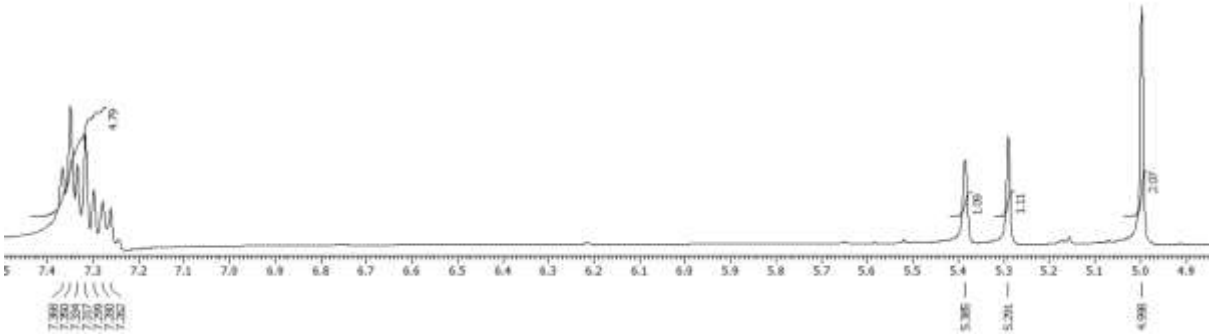
MS Spectrum Peak List

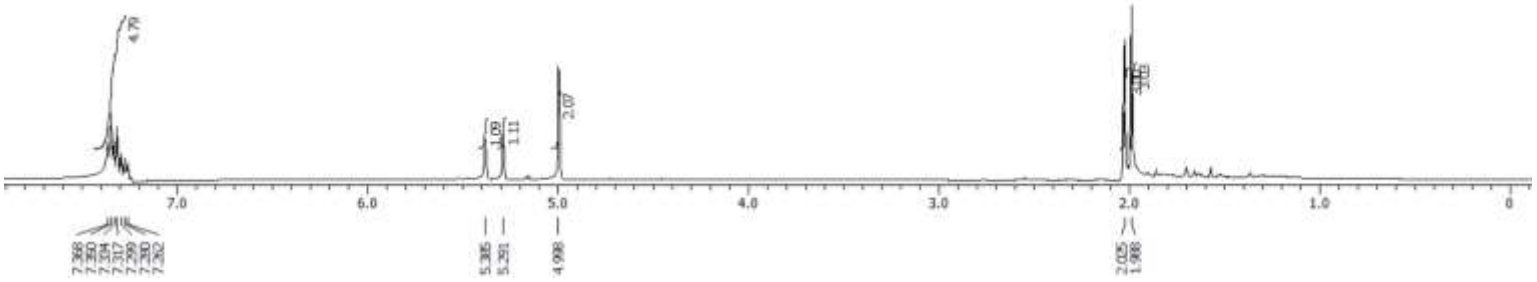
m/z	z	Abund	Formula	Ion
306.014	1	964470.94	C14H13BrNO2	(M+H)+
307.0169	1	143638.41	C14H13BrNO2	(M+H)+
308.0122	1	957175.19	C14H13BrNO2	(M+H)+
309.0151	1	145578.98	C14H13BrNO2	(M+H)+
310.0197	1	16641.71	C14H13BrNO2	(M+H)+
327.9957	1	115520.27	C14H12BrNNaO2	(M+Na)+
328.9989	1	17230.08	C14H12BrNNaO2	(M+Na)+
329.9939	1	113081.05	C14H12BrNNaO2	(M+Na)+
330.997	1	16866.98	C14H12BrNNaO2	(M+Na)+
332.0003	1	2003.74	C14H12BrNNaO2	(M+Na)+

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

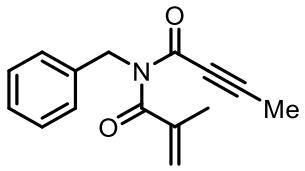


N-benzyl-*N*-methacryloylbut-2-ynamide

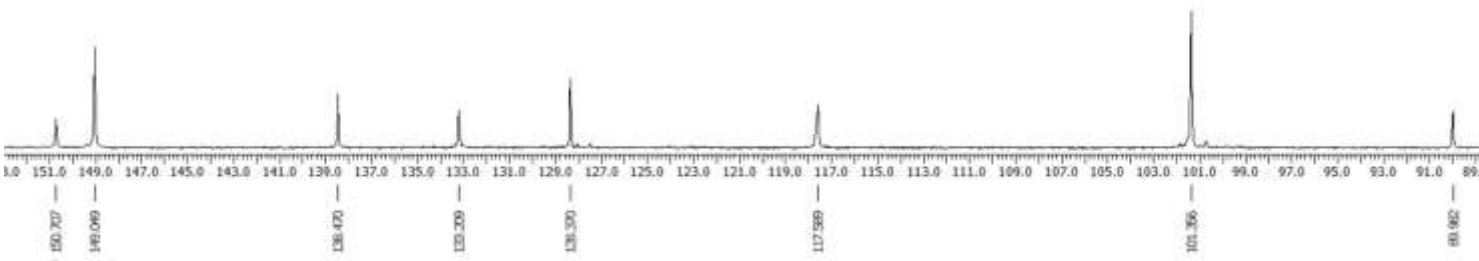


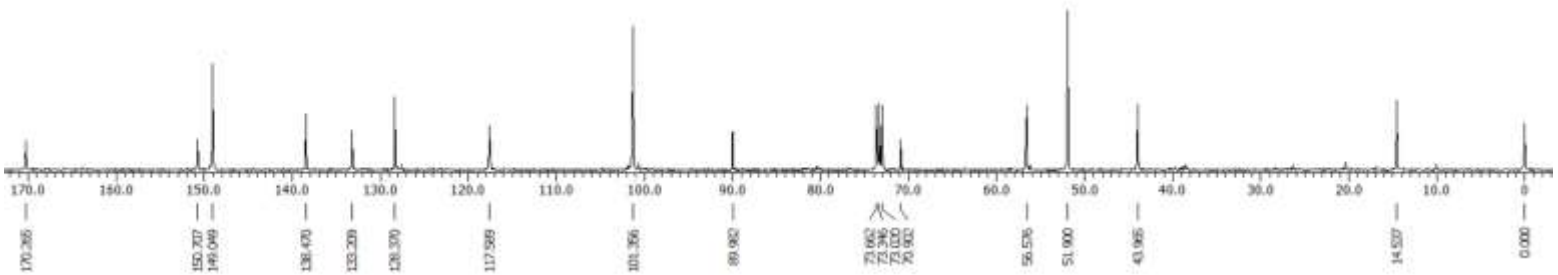


^{13}C NMR spectrum of 3j (100 MHz, $CDCl_3$)



N-benzyl-*N*-methacryloylbut-2-ynamide





HRMS spectrum of 3j

Qualitative Compound Report

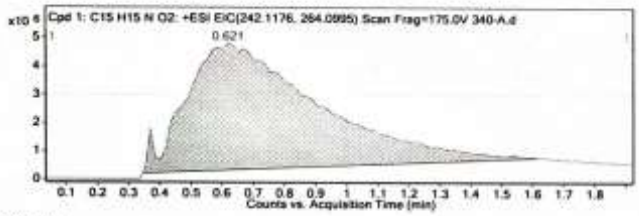
Data File	340-A.d	**Sample Name**	340-A
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 13:29:28
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

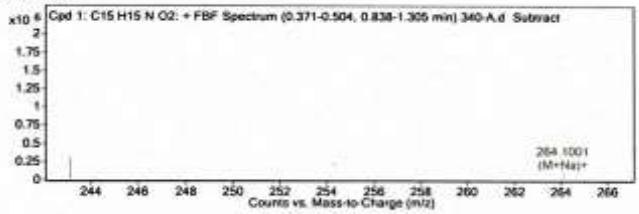
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C15 H15 N O2	0.621	241.1106	1800411	C15 H15 N O2	241.1103	1.4	C15 H15 N O2	C15 H15 N O2

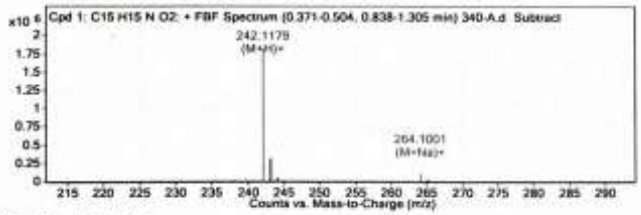
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C15 H15 N O2	242.1179	0.621	Find By Formula	241.1106



MS Spectrum



MS Zoomed Spectrum

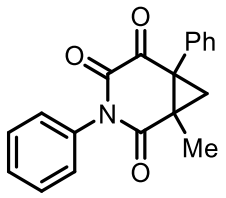


MS Spectrum Peak List

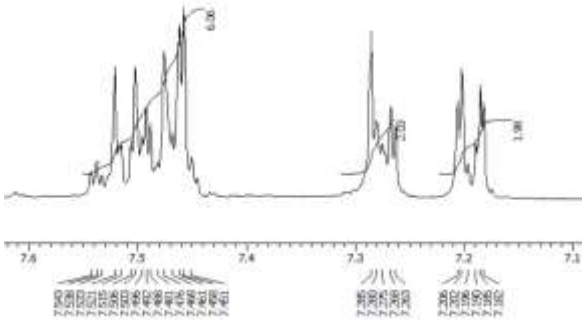
m/z	z	Abund	Formula	Ion
242.1179	1	1800411	C15H16NO2	(M+H)+
243.121	1	307773.16	C15H16NO2	(M+H)+
244.1252	1	31442.27	C15H16NO2	(M+H)+
245.1288	1	3096.14	C15H16NO2	(M+H)+
264.1001	1	110312.05	C15H15NNaO2	(M+Na)+
265.1033	1	18253.43	C15H15NNaO2	(M+Na)+
266.1055	1	2119.56	C15H15NNaO2	(M+Na)+
267.1028	1	123.23	C15H15NNaO2	(M+Na)+

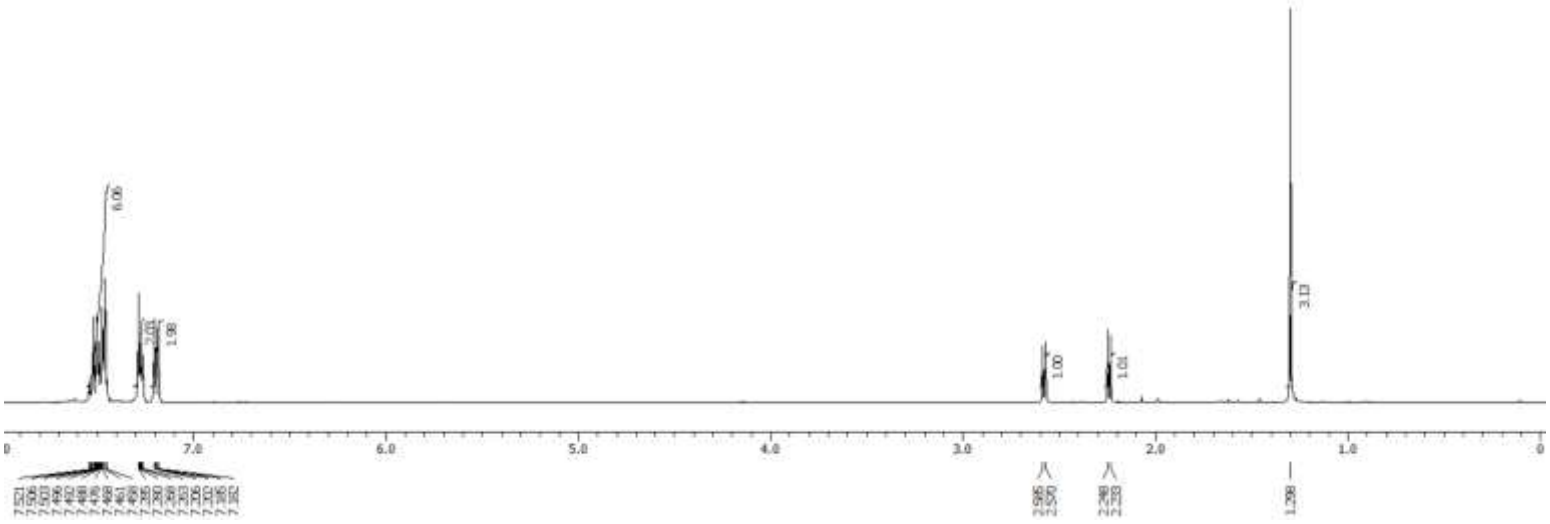
--- End Of Report ---

^{1}H NMR spectrum of 2a (400 MHz, $CDCl_3$)

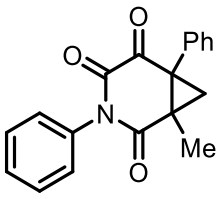


1-methyl-3,6-diphenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

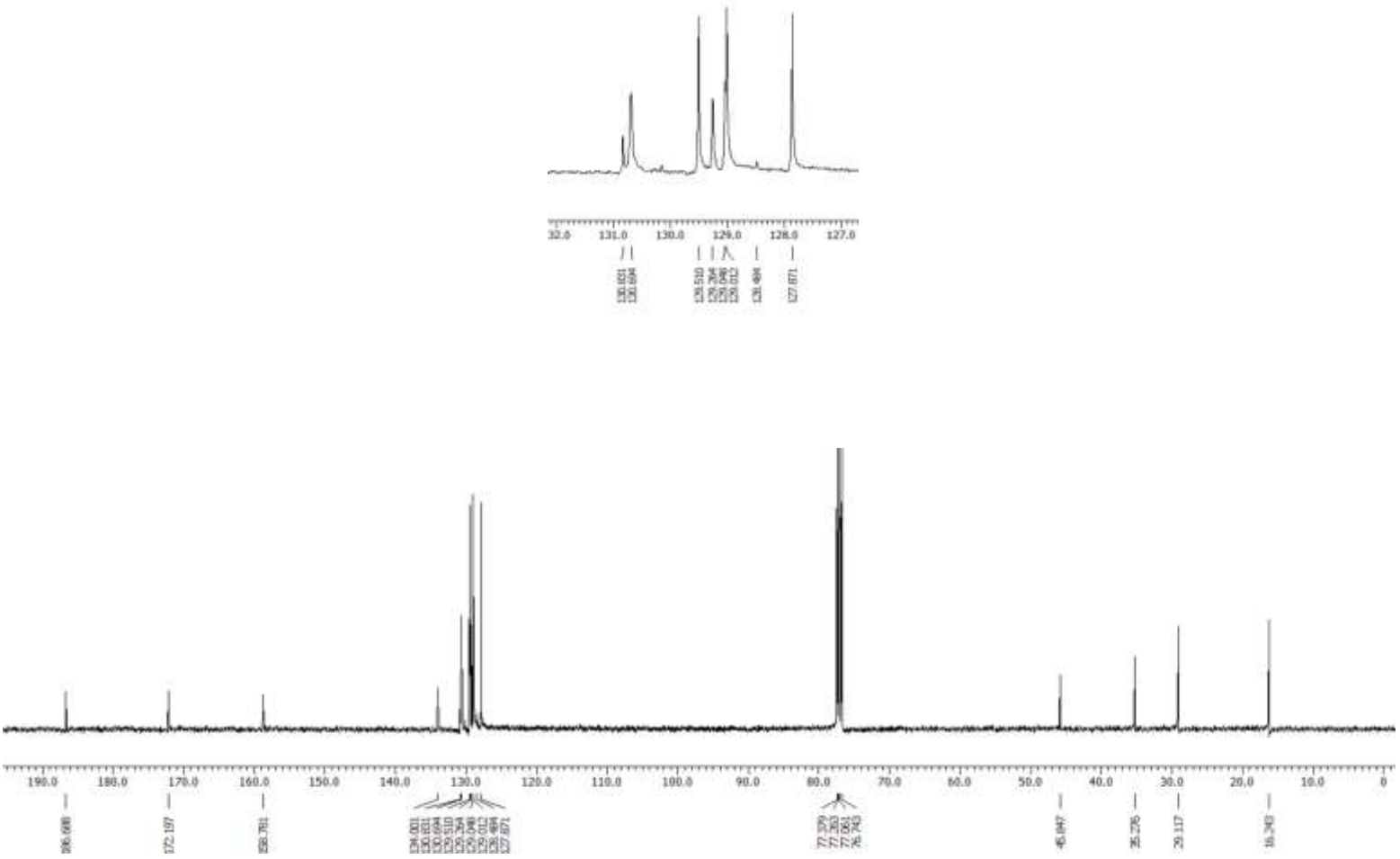




^{13}C NMR spectrum of 2a (100 MHz, $CDCl_3$)



1-methyl-3,6-diphenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2a

Qualitative Compound Report

Data File	SMT-238.d	Sample Name	SMT-238
Sample Type	Sample	Position	P1-A6
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	03-04-2023 13:13:49
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

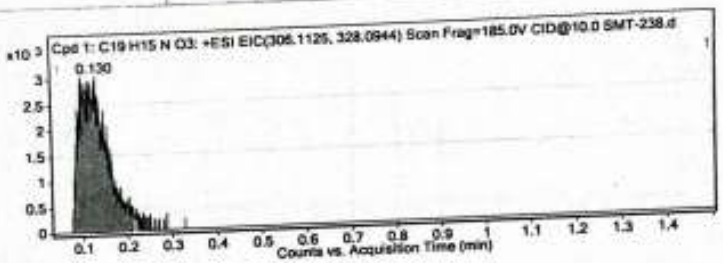
Sample Group — Info. 3

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

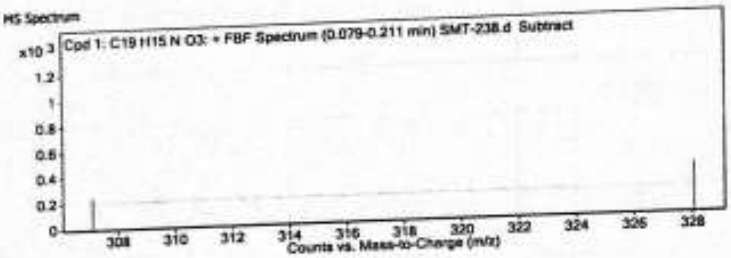
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C19 H15 N O3	0.13	305.106	1167	C19 H15 N O3	305.1052	2.58	C19 H15 N O3	C19 H15 N O3

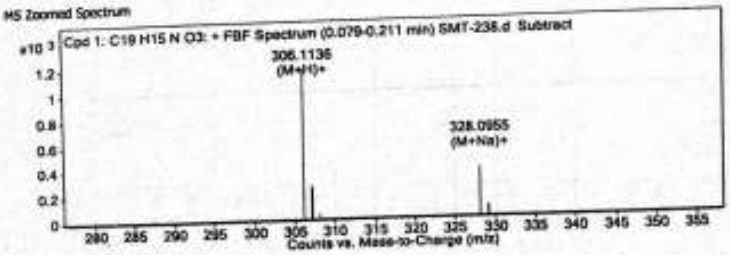
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H15 N O3	306.1136	0.13	Find By Formula	305.106



MS Spectrum



MS Zoomed Spectrum

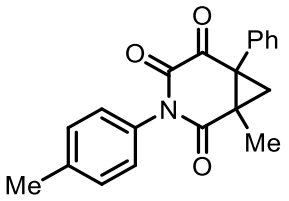


MS Spectrum Peak List

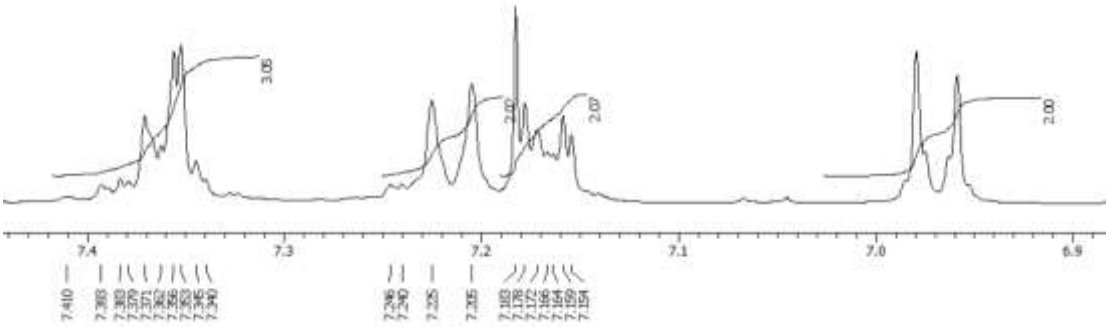
m/z	z	Abund	Formula	Ion
306.1136	1	1166.51	C19H16NO3	(M+H)+
307.1142	1	242.76	C19H16NO3	(M+H)+
328.0955	1	383.11	C19H15NNaO3	(M+Na)+
329.0993	1	44.9	C19H15NNaO3	(M+Na)+

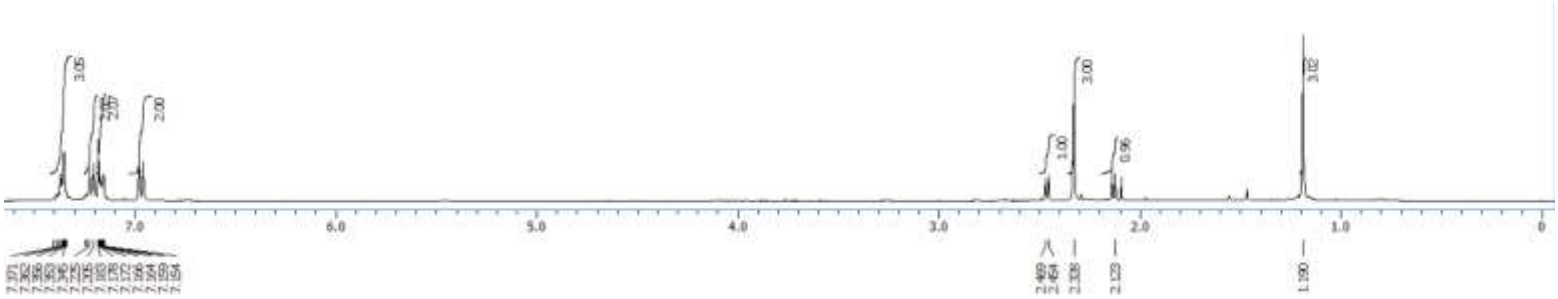
--- End Of Report ---

^{1}H NMR spectrum of 2b (400 MHz, $CDCl_3$)

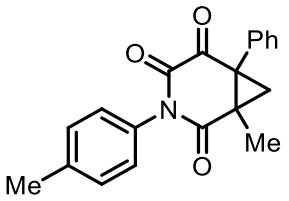


1-methyl-6-phenyl-3-(*p*-tolyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

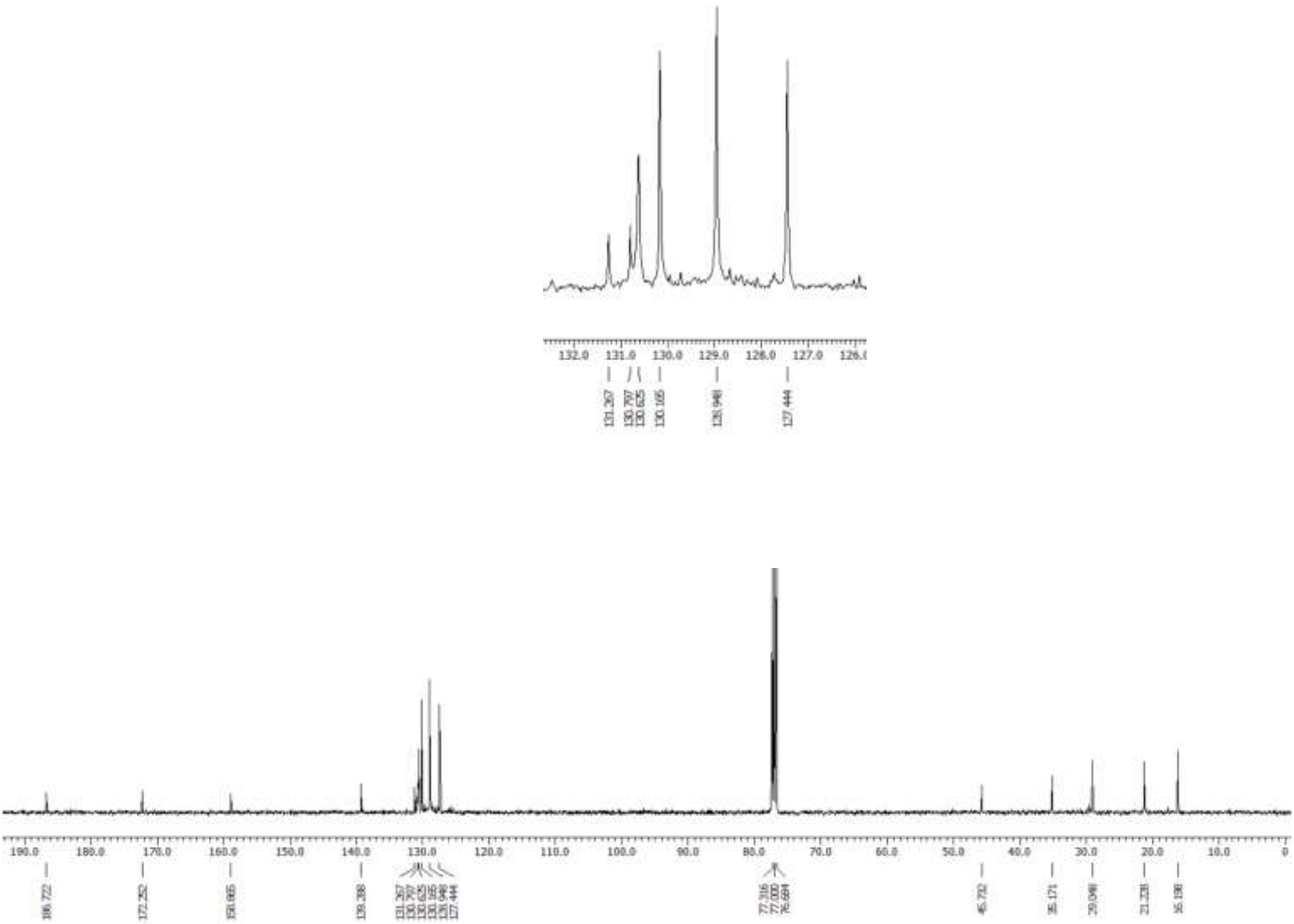




^{13}C NMR spectrum of 2b (100 MHz, $CDCl_3$)



1-methyl-6-phenyl-3-(*p*-tolyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2b (400 MHz, $CDCl_3$)

Qualitative Compound Report

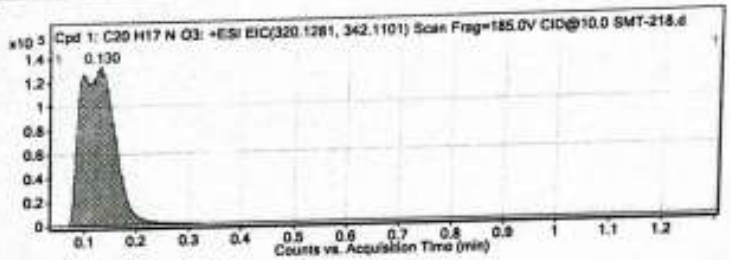
Data File	SMT-218.d	Sample Name	SMT-218
Sample Type	Sample	Position	P1-A6
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-05-2023 12:13:24
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

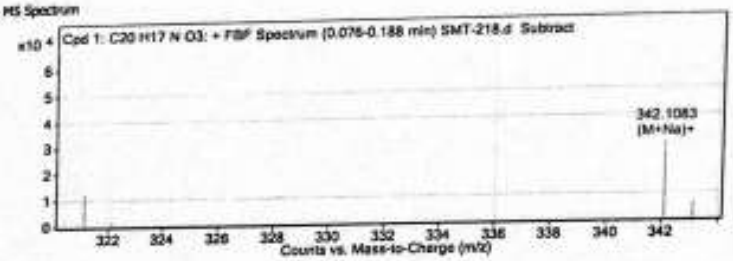
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H17 N O3	0.13	319.1192	57949	C20 H17 N O3	319.1208	-5.07	C20 H17 N O3	C20 H17 N O3

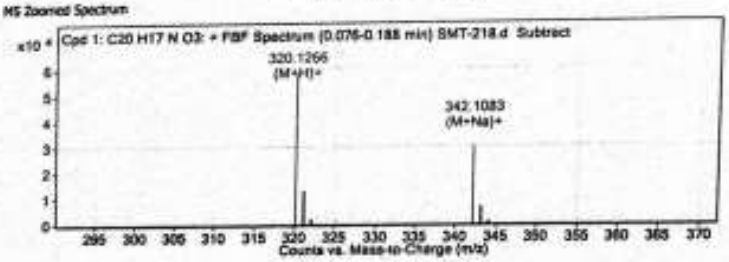
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H17 N O3	320.1266	0.13	Find By Formula	319.1192



MS Spectrum



MS Zoomed Spectrum

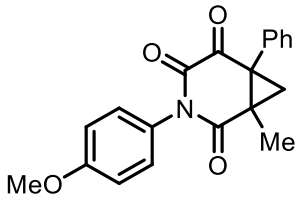


MS Spectrum Peak List

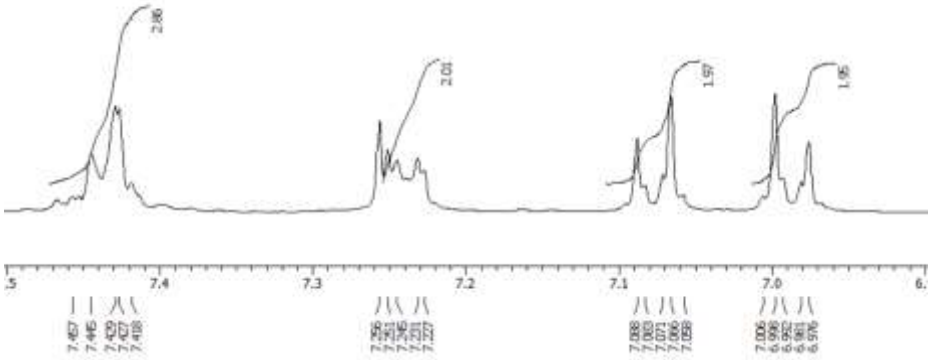
m/z	z	Abund	Formula	Ion
320.1266	1	57949	C20H18NO3	(M+H)+
321.1296	1	13630.01	C20H18NO3	(M+H)+
322.1326	1	1609.46	C20H18NO3	(M+H)+
323.1378	1	142.22	C20H18NO3	(M+H)+
342.1083	1	29859.86	C20H17NNaO3	(M+Na)+
343.1114	1	6115.92	C20H17NNaO3	(M+Na)+
344.1143	1	779.86	C20H17NNaO3	(M+Na)+

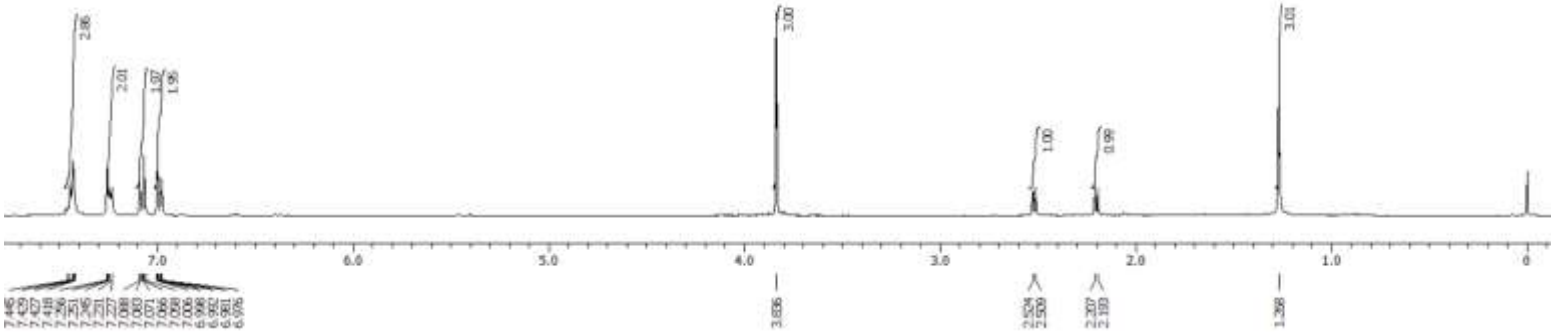
--- End Of Report ---

^{1}H NMR spectrum of 2c (400 MHz, $CDCl_3$)

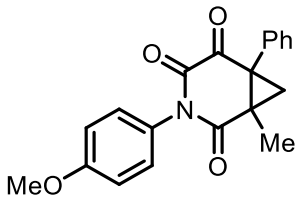


3-(4-methoxyphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

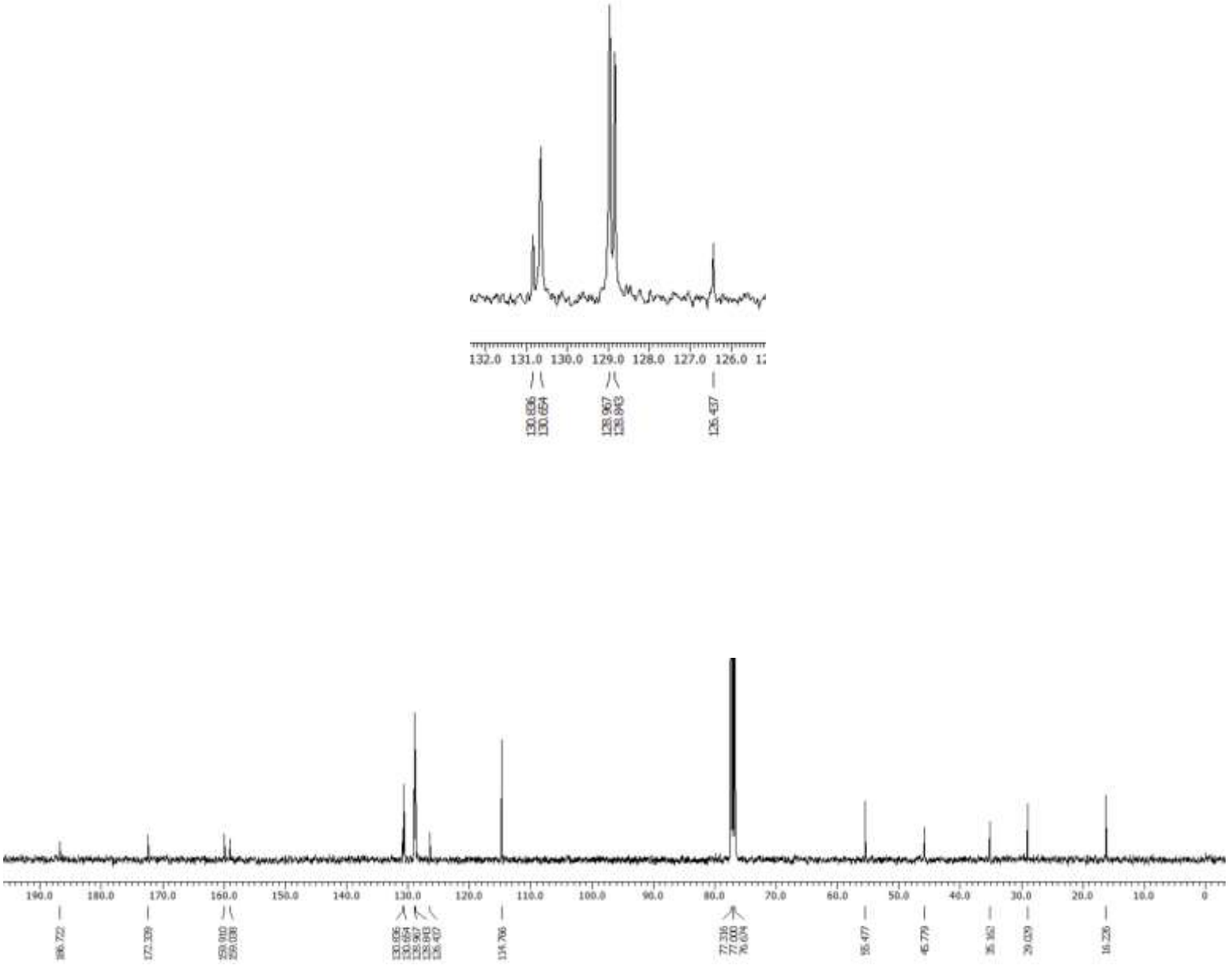




^{13}C NMR spectrum of 2c (100 MHz, $CDCl_3$)



3-(4-methoxyphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2c

Qualitative Compound Report

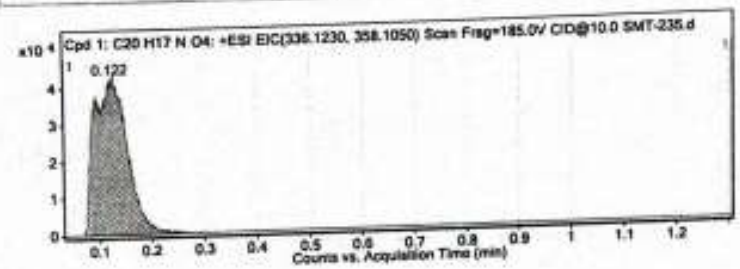
Data File	SMT-235.d	Sample Name	SMT-235
Sample Type	Sample	Position	P1-A5
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-05-2023 12:11:06
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

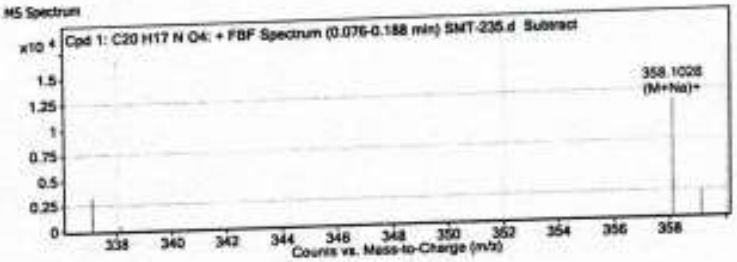
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H17 N O4	0.122	335.1137	11476	C20 H17 N O4	335.1158	-6.05	C20 H17 N O4	C20 H17 N O4

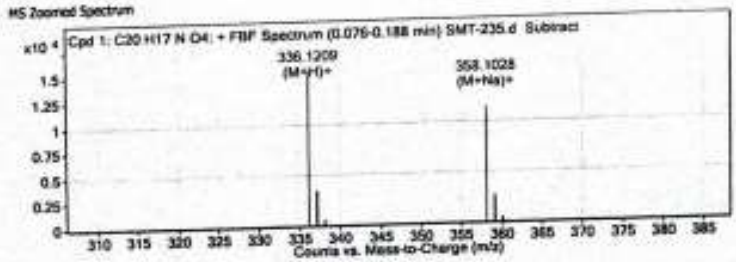
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H17 N O4	358.1028	0.122	Find By Formula	335.1137



MS Spectrum



MS Zoomed Spectrum

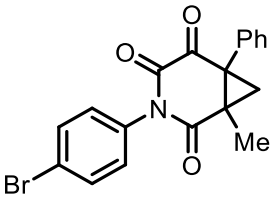


MS Spectrum Peak List

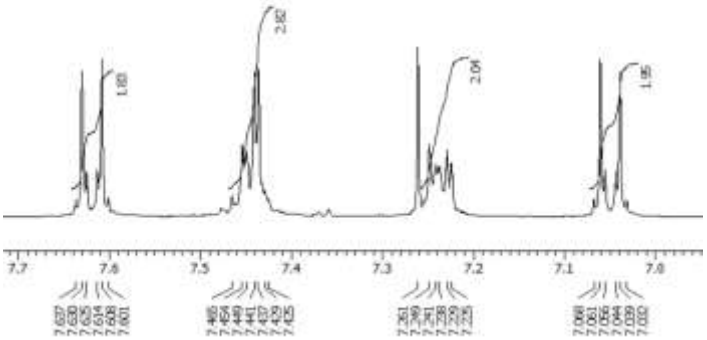
m/z	z	Abund	Formula	Ion
336.1209	1	15186.41	C20H18NO4	(M+H)+
337.124	1	3262.97	C20H18NO4	(M+H)+
338.1303	1	481.44	C20H18NO4	(M+H)+
358.1028	1	11476.42	C20H17NNaO4	(M+Na)+
359.1068	1	2435.72	C20H17NNaO4	(M+Na)+
360.1133	1	324.46	C20H17NNaO4	(M+Na)+

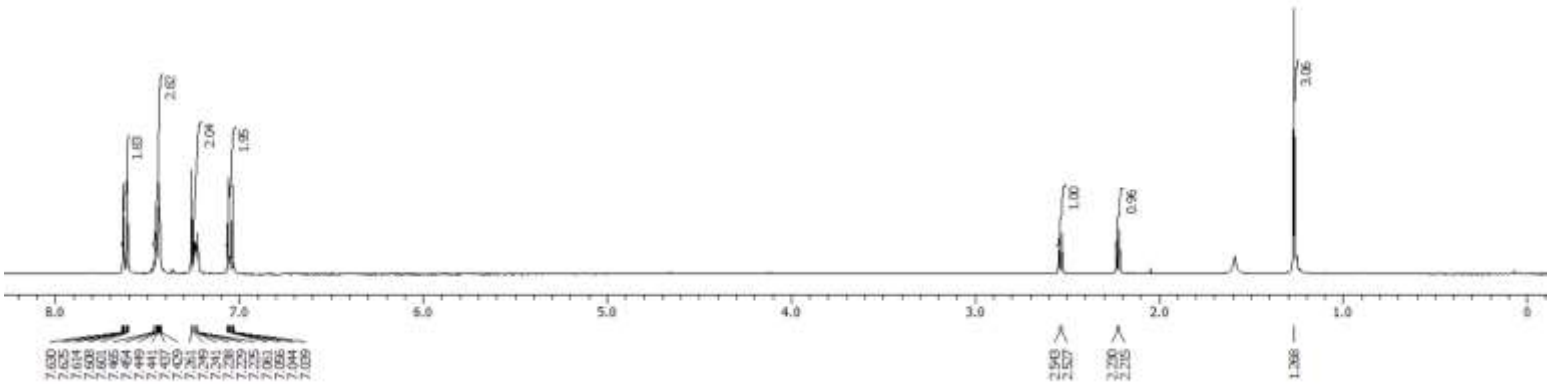
— End Of Report —

^{1}H NMR spectrum of 2d (400 MHz, $CDCl_3$)

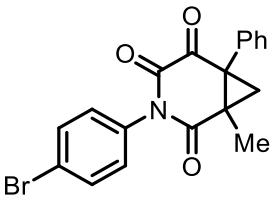


3-(4-bromophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

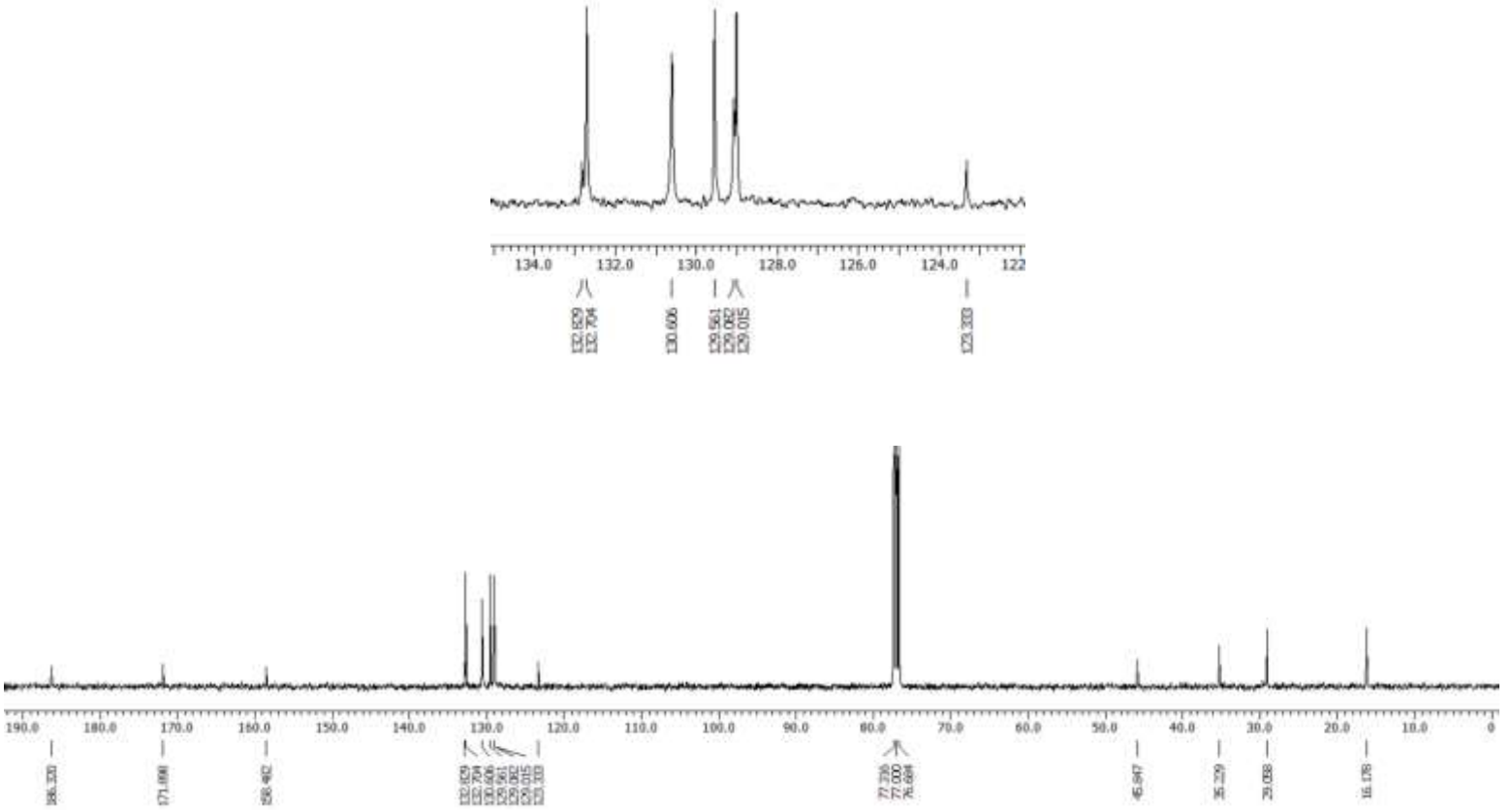




^{13}C NMR spectrum of 2d (100 MHz, $CDCl_3$)



3-(4-bromophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2d

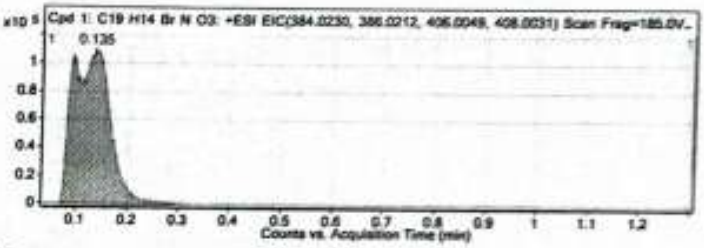
Qualitative Compound Report

Data File	SMT-234.d	Sample Name	SMT-234
Sample Type	Sample	Position	P1-A4
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-05-2023 12:08:46
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)		

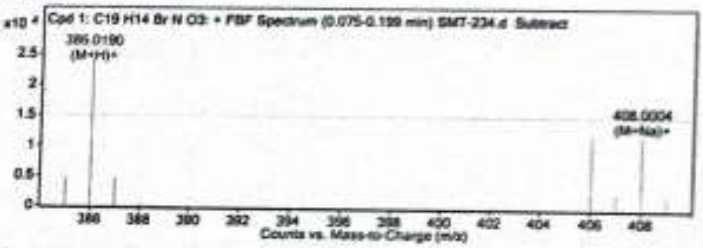
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	HiFG Formula	DB Formula
Cpd 1: C19 H14 Br N O3	0.135	383.0134	24527	C19 H14 Br N O3	383.0157	-6.14	C19 H14 Br N O3	C19 H14 Br N O3

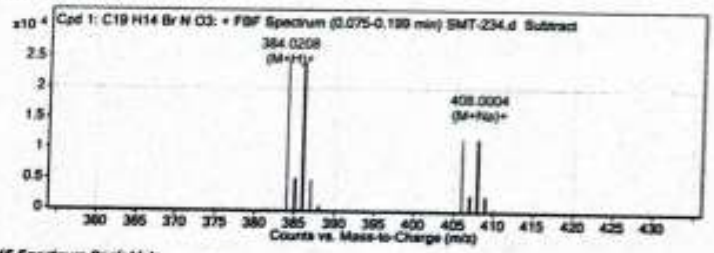
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H14 Br N O3	384.0208	0.135	Find By Formula	383.0134



MS Spectrum



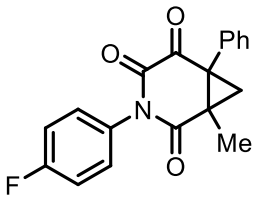
MS Zoomed Spectrum



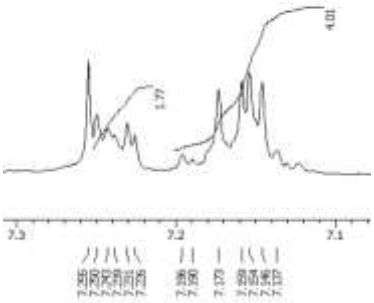
MS Spectrum Peak List

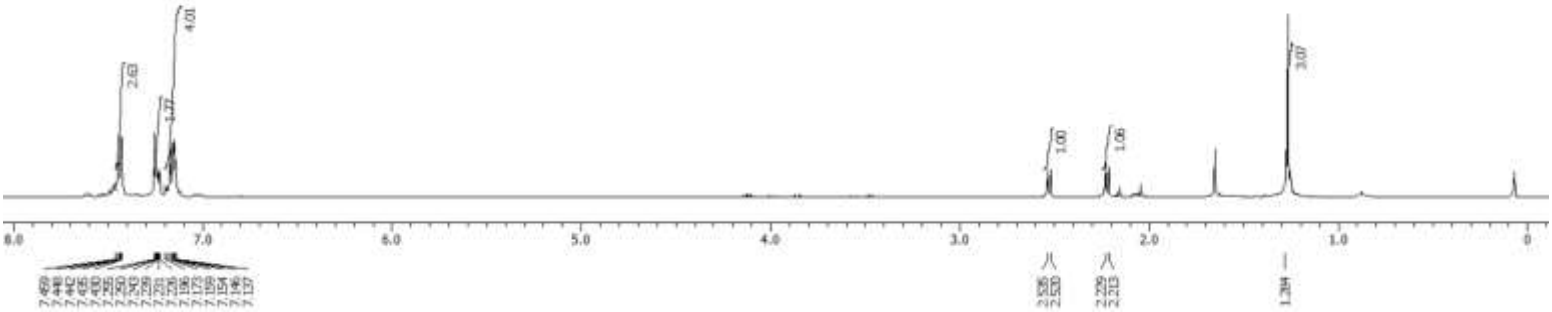
m/z	z	Abund	Formula	Ion
384.0208	1	24526.63	C19H15BrNO3	(M+H)+
385.0239	1	4718.87	C19H15BrNO3	(M+H)+
386.019	1	24330.16	C19H15BrNO3	(M+H)+
387.0217	1	4718.17	C19H15BrNO3	(M+H)+
388.027	1	635.54	C19H15BrNO3	(M+H)+
389.0322	1	48.78	C19H15BrNO3	(M+H)+
406.0023	1	11851.84	C19H14BrNNaO3	(M+Na)+
407.0053	1	2286.9	C19H14BrNNaO3	(M+Na)+
408.0004	1	11880.57	C19H14BrNNaO3	(M+Na)+
409.0032	1	2295.95	C19H14BrNNaO3	(M+Na)+

^{1}H NMR spectrum of 2e (400 MHz, $CDCl_3$)

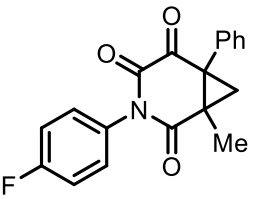


3-(4-fluorophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

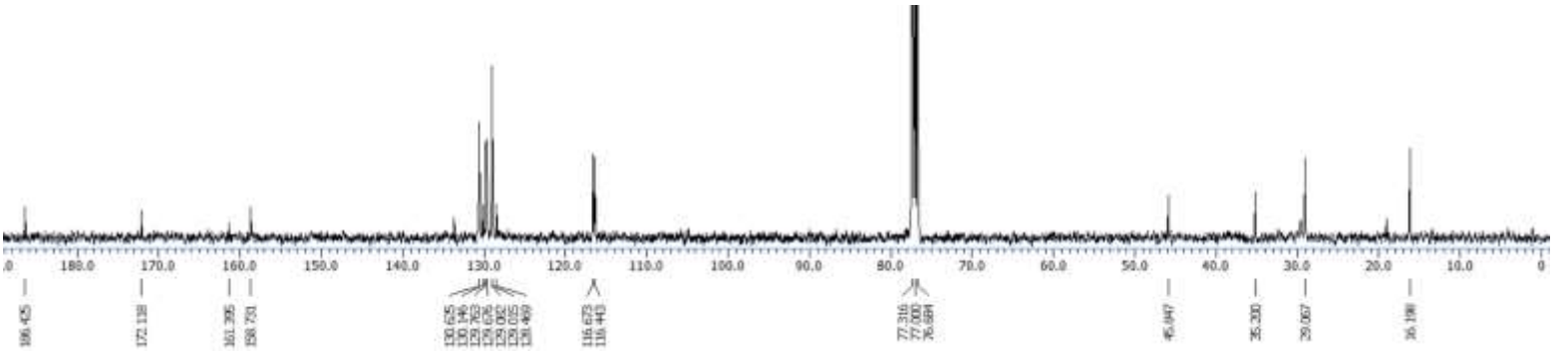




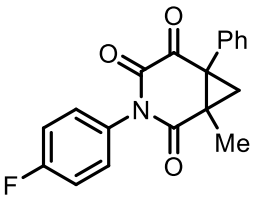
^{13}C NMR spectrum of 2e (100 MHz, $CDCl_3$)



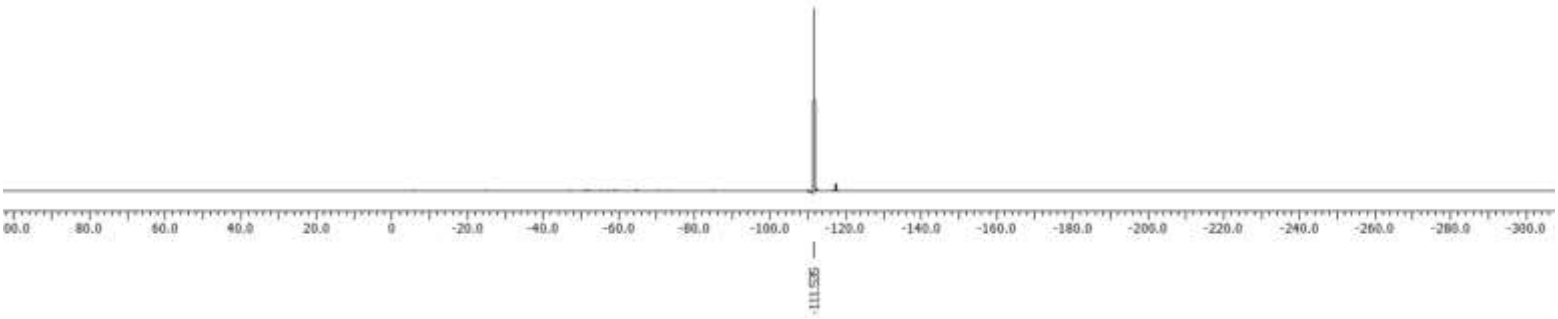
3-(4-fluorophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



^{19}F NMR spectrum of 2e (376 MHz, $CDCl_3$)



3-(4-fluorophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2e

Qualitative Compound Report

Data File	SMT-240.d	Sample Name	SMT-240
Sample Type	Sample	Position	P1-A4
Instrument Name	Instrument 1	User Name	
Acq Method	HS Scan.m	Acquired Time	24-05-2023 13:13:47
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

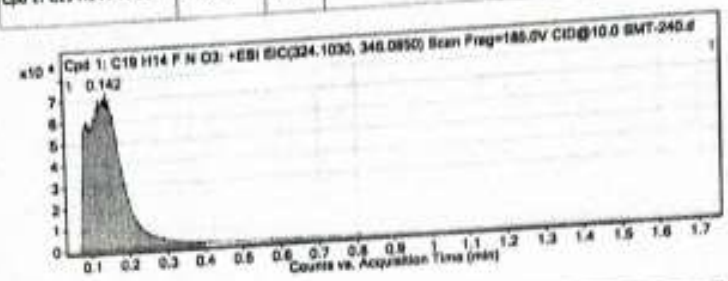
Info. 1

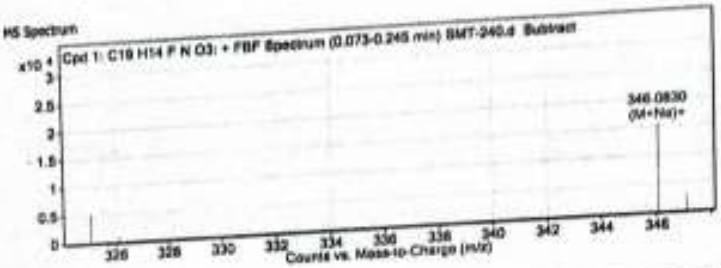
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.06.01 (B9125)

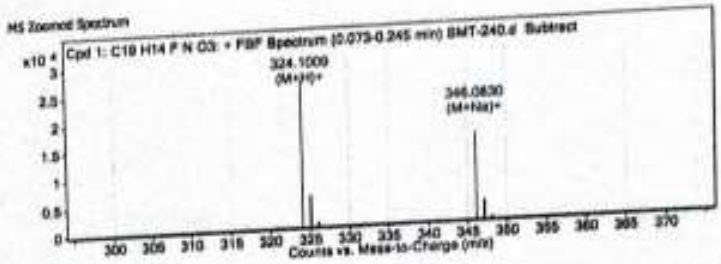
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C19 H14 F N O3	0.142	323.0937	15758	C19 H14 F N O3	323.0958	-6.42	C19 H14 F N O3	C19 H14 F N O3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H14 F N O3	346.083	0.142	Find By Formula	323.0937





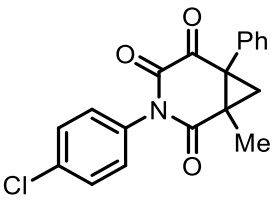


MS Spectrum Peak List

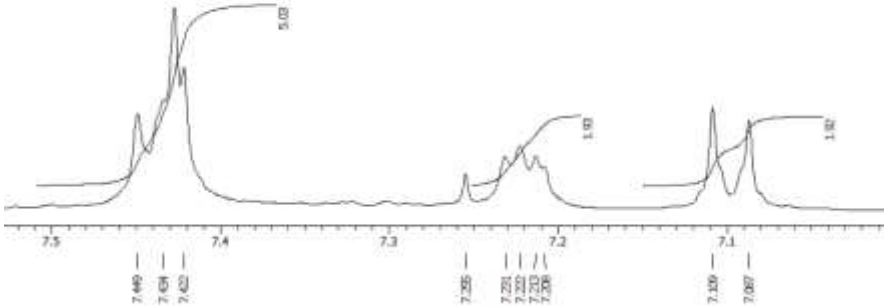
m/z	z	Abund	Formula	Ion
324.1009	1	35715.78	C19H15FNO3	(M+H)+
325.1041	1	3325.34	C19H15FNO3	(M+H)+
326.1081	1	733.99	C19H15FNO3	(M+H)+
327.1049	1	38.03	C19H15FNO3	(M+H)+
346.082	1	15757.8	C19H14FNNaO3	(M+Na)+
347.0852	1	3232.8	C19H14FNNaO3	(M+Na)+
348.0915	1	374.67	C19H14FNNaO3	(M+Na)+

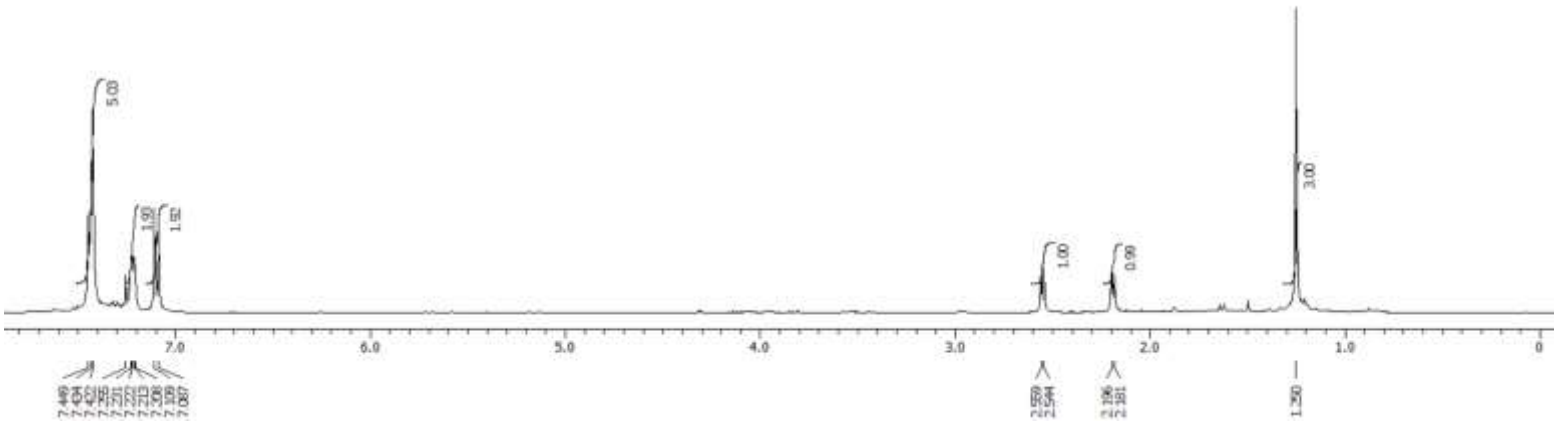
--- End Of Report ---

^{1}H NMR spectrum of 2f (400 MHz, $CDCl_3$)

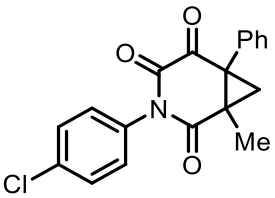


3-(4-chlorophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

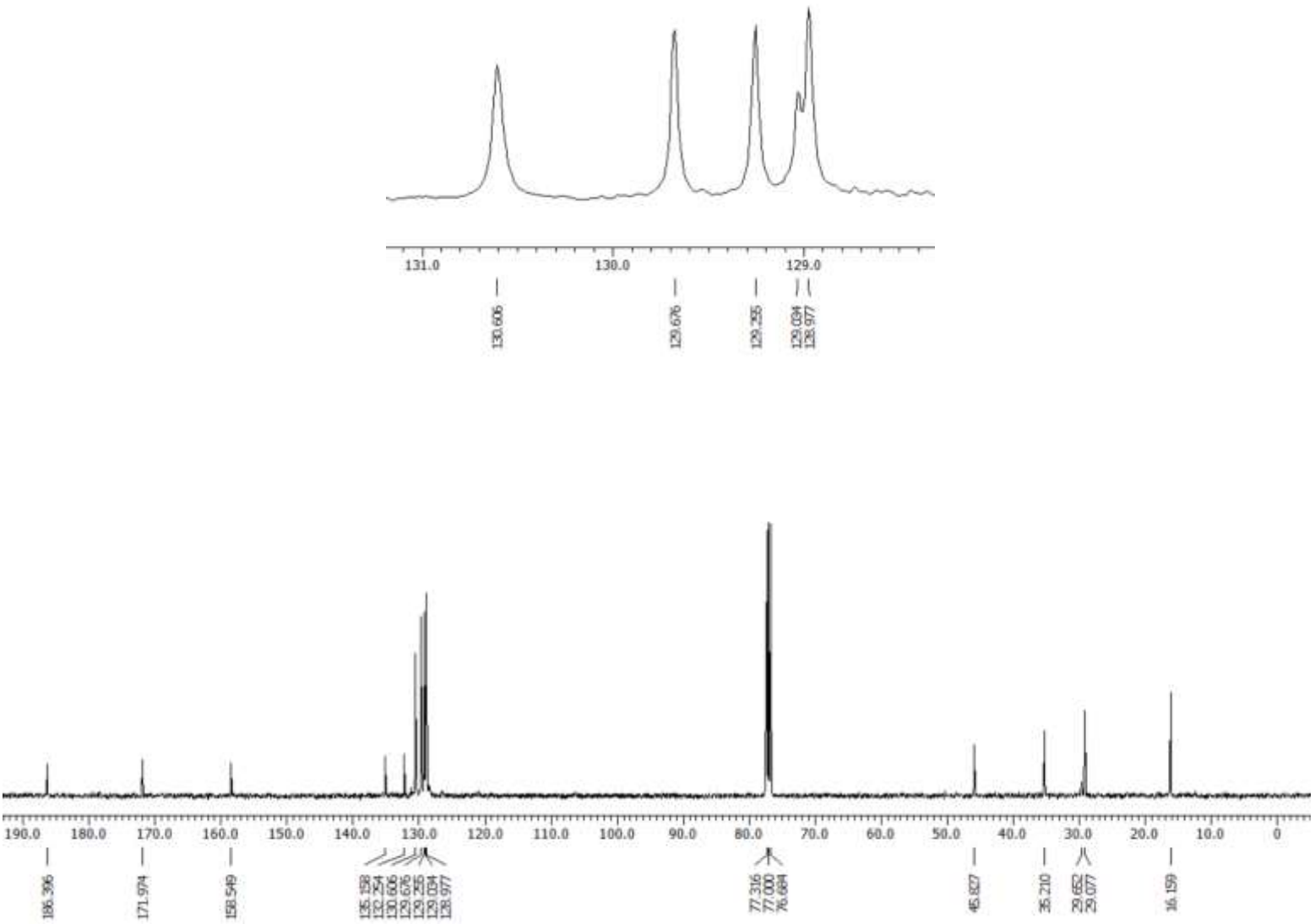




^{13}C NMR spectrum of 2f (100 MHz, $CDCl_3$)



3-(4-chlorophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2f

Qualitative Compound Report

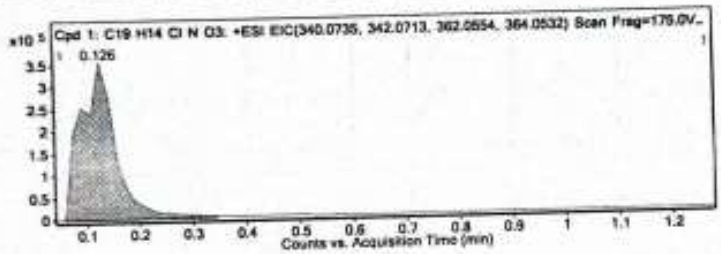
Data File	SMT-242.d	Sample Name	SMT-242
Sample Type	Sample	Position	P1-B5
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	22-07-2023 13:05:19
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

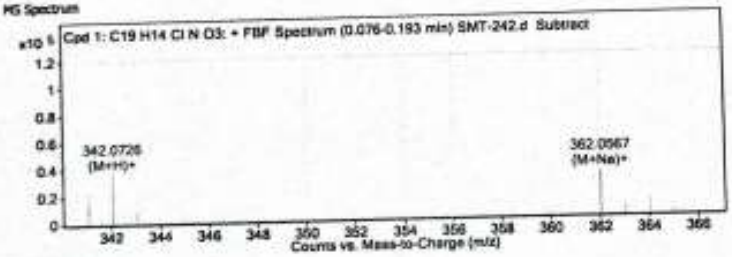
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	HFG Formula	DB Formula
Cpd 1: C19 H14 Cl N O3	0.126	339.0675	32827	C19 H14 Cl N O3	339.0662	3.84	C19 H14 Cl N O3	C19 H14 Cl N O3

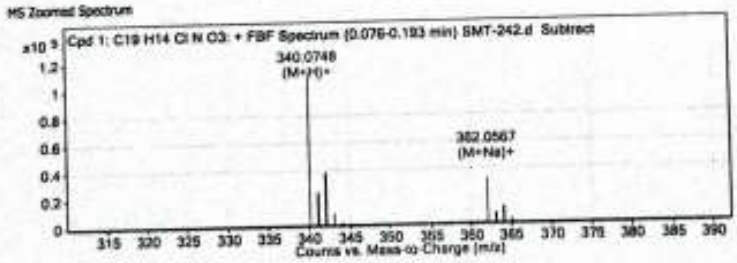
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H14 Cl N O3	362.0567	0.126	Find By Formula	339.0675



MS Spectrum



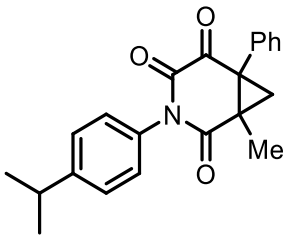
MS Zoomed Spectrum



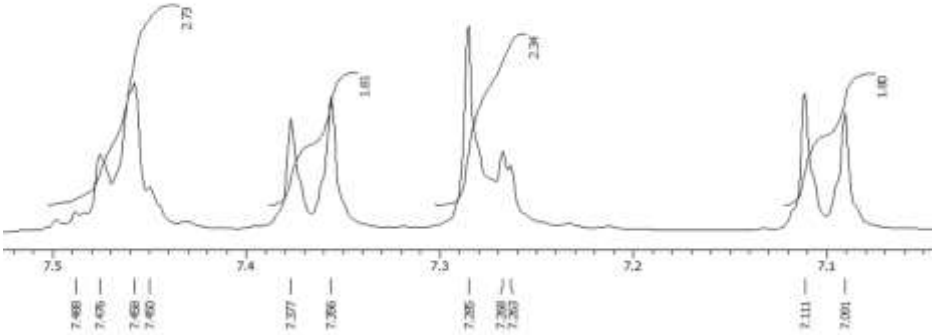
MS Spectrum Peak List

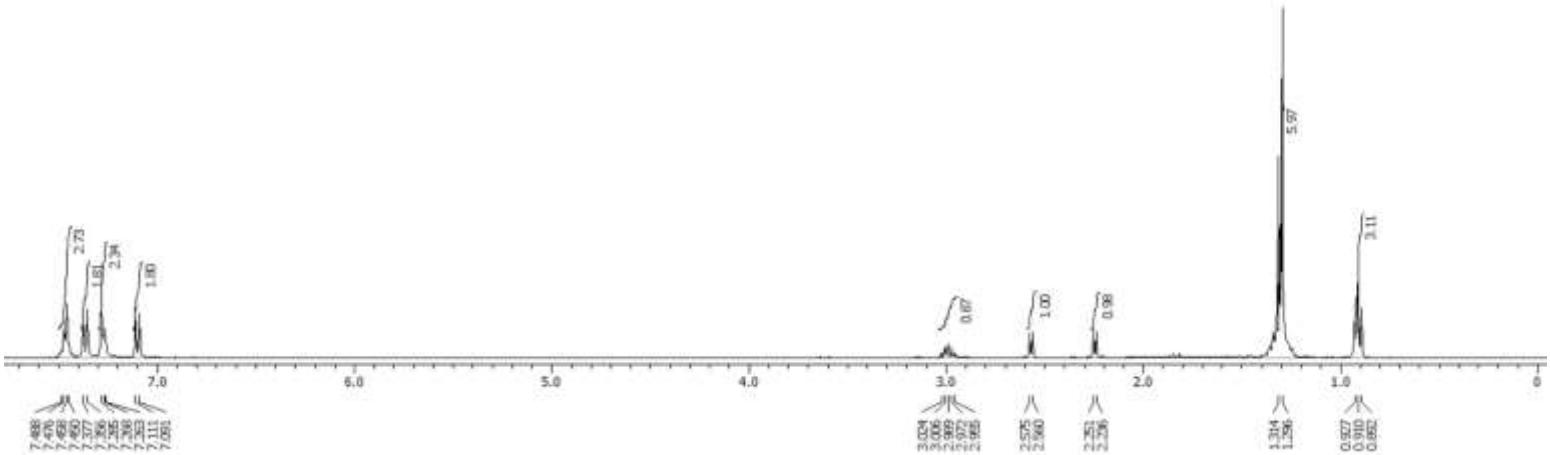
m/z	z	Abund	Formula	Ion
340.0748	1	111349.74	C19H15ClNO3	(M+H)+
341.0781	1	22860.93	C19H15ClNO3	(M+H)+
342.0726	1	37245.43	C19H15ClNO3	(M+H)+
343.0756	1	7693.04	C19H15ClNO3	(M+H)+
344.0807	1	1307.77	C19H15ClNO3	(M+H)+
345.0846	1	184.16	C19H15ClNO3	(M+H)+
362.0567	1	32827.05	C19H14ClNNaO3	(M+Na)+
363.0598	1	6730.05	C19H14ClNNaO3	(M+Na)+
364.0545	1	11288.64	C19H14ClNNaO3	(M+Na)+
365.057	1	2384.03	C19H14ClNNaO3	(M+Na)+
366.0624	1	388.24	C19H14ClNNaO3	(M+Na)+

^{1}H NMR spectrum of 2g (400 MHz, $CDCl_3$)

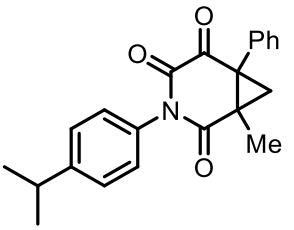


3-(4-isopropylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

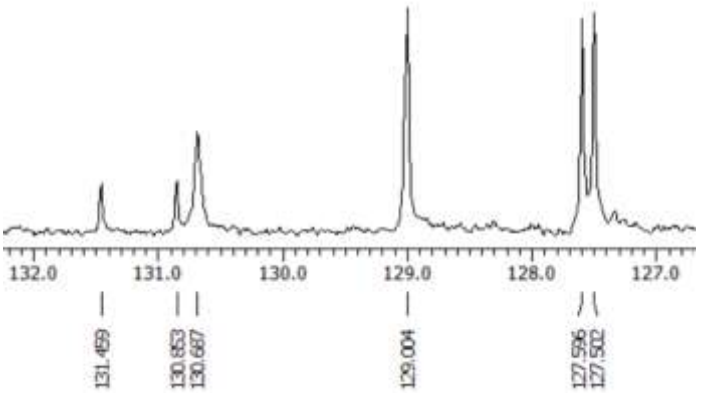


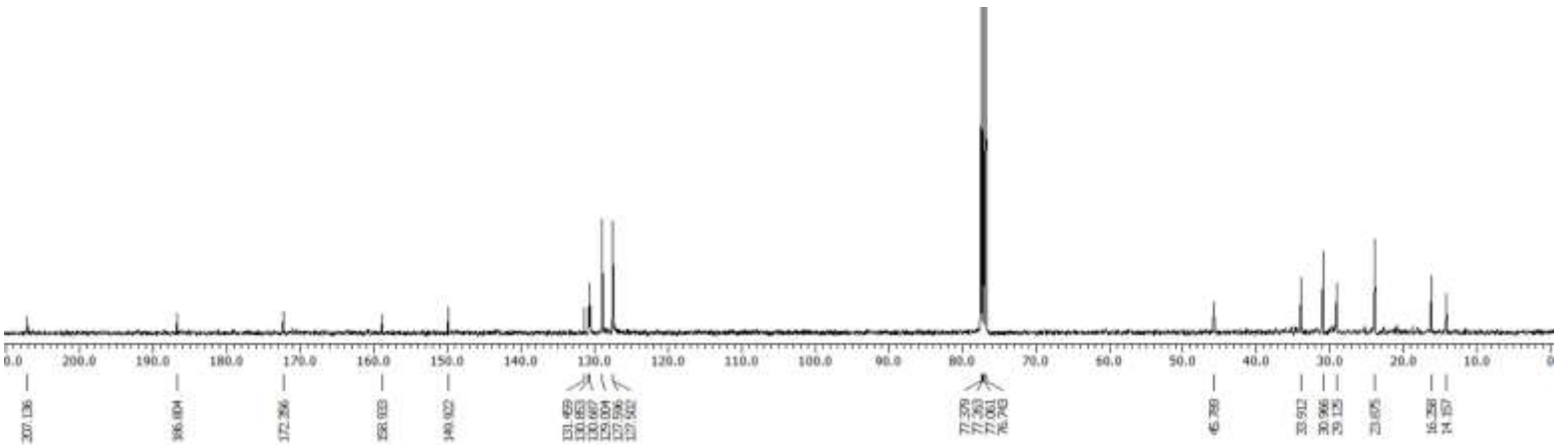


^{13}C NMR spectrum of 2g (100 MHz, $CDCl_3$)



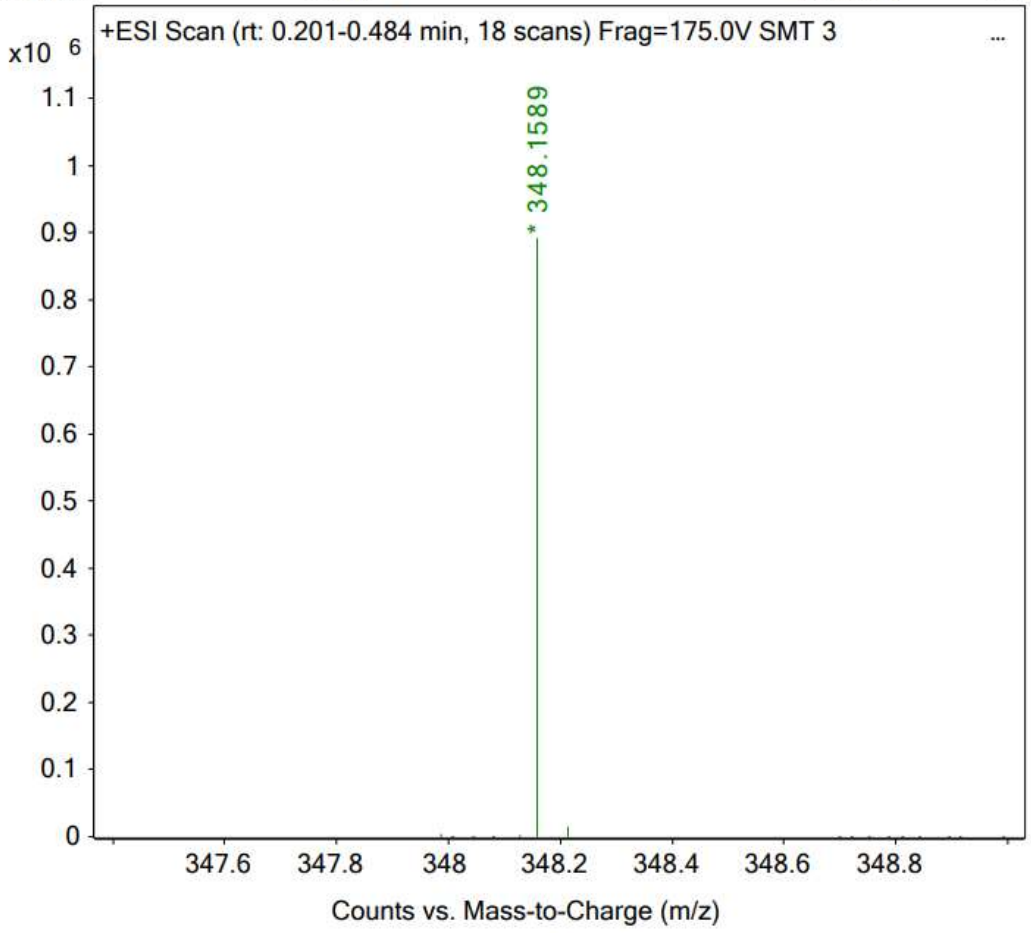
3-(4-isopropylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



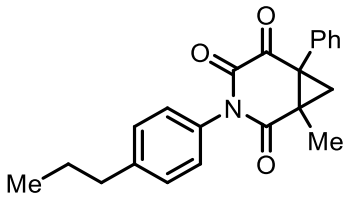


HRMS spectrum of 2g

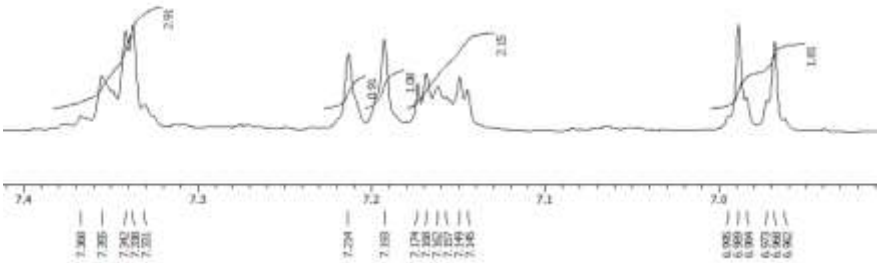
Sample Name	SMT 359	**Position**	P1-B7	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 359.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:46:32 (UTC+05:30)

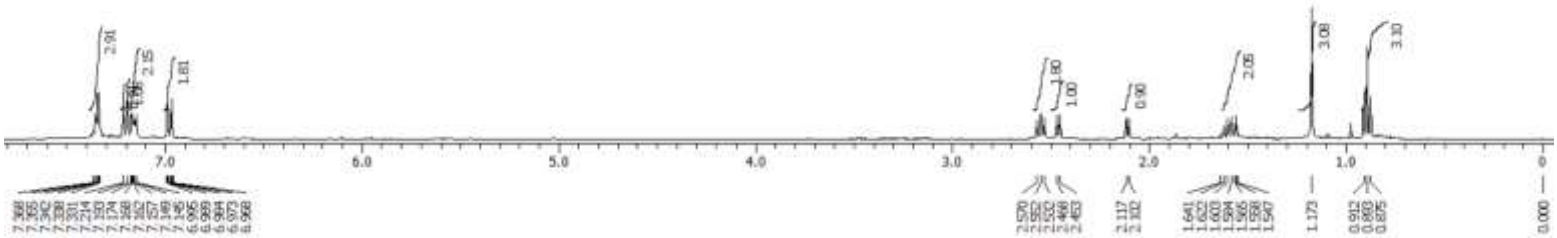


^{1}H NMR spectrum of 2h (400 MHz, $CDCl_3$)

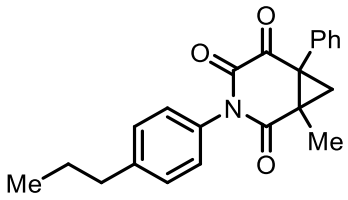


1-methyl-6-phenyl-3-(4-propylphenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

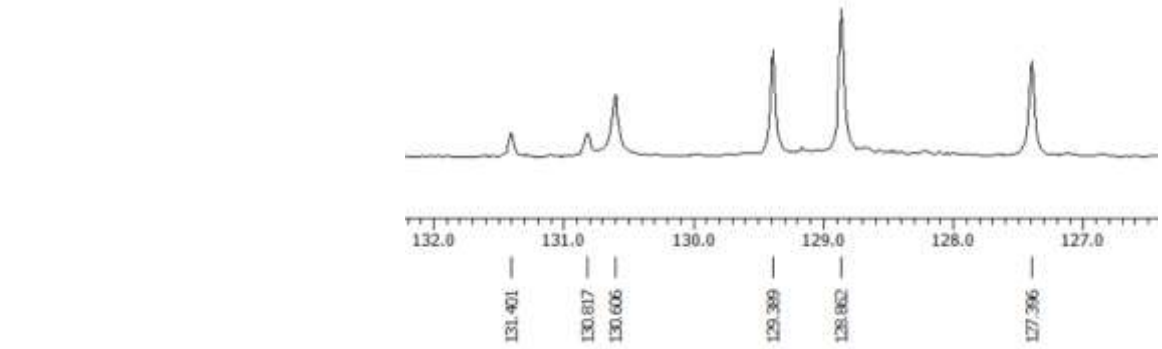


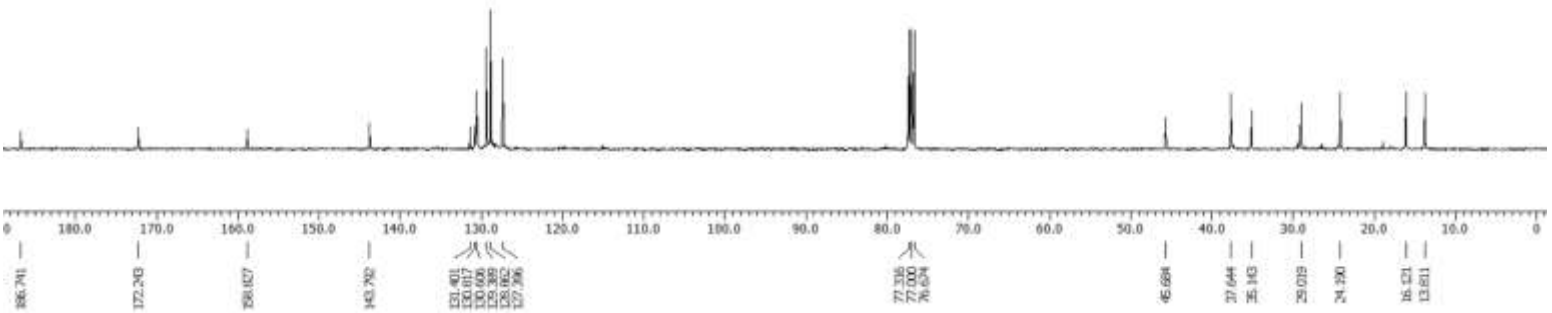


^{13}C NMR spectrum of 2h (100 MHz, $CDCl_3$)



1-methyl-6-phenyl-3-(4-propylphenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 2h

Qualitative Compound Report

Data File	SMT-365.d	**Sample Name**	SMT-365
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	25-11-2023 12:41:27
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

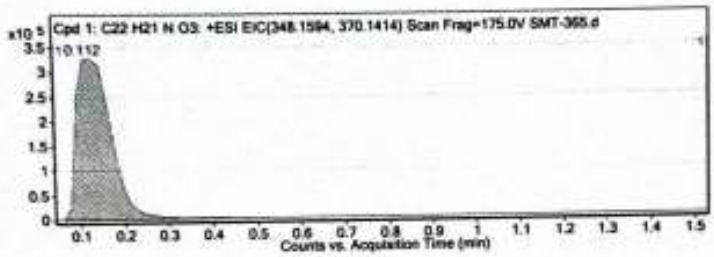
Sample Group **Info.**

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

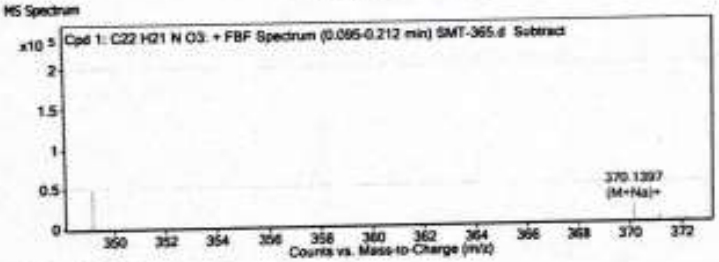
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C22 H21 N O3	0.112	347.1506	191228	C22 H21 N O3	347.1521	-4.51	C22 H21 N O3	C22 H21 N O3

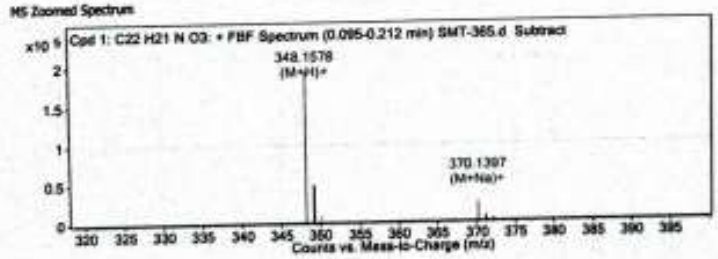
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C22 H21 N O3	348.1578	0.112	Find By Formula	347.1506



MS Spectrum



MS Zoomed Spectrum

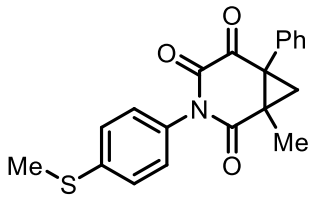


MS Spectrum Peak List

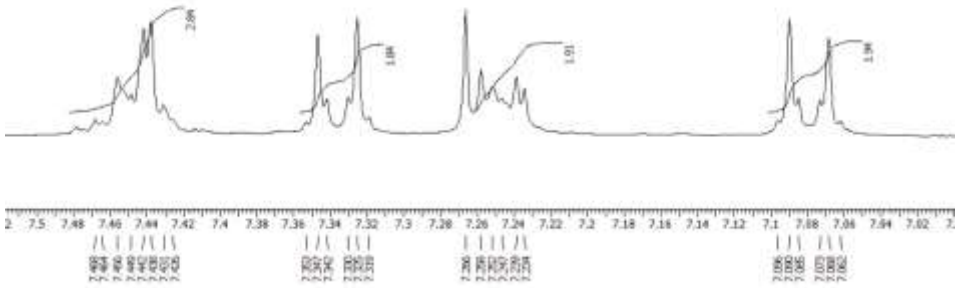
m/z	z	Abund	Formula	Ion
348.1578	1	191227.56	C22H22NO3	(M+H)+
349.1612	1	47687	C22H22NO3	(M+H)+
370.1397	1	22229.53	C22H21NNaO3	(M+Na)+
371.1395	1	5565.53	C22H21NNaO3	(M+Na)+
372.1514	1	3474.86	C22H21NNaO3	(M+Na)+
373.1561	1	947.02	C22H21NNaO3	(M+Na)+

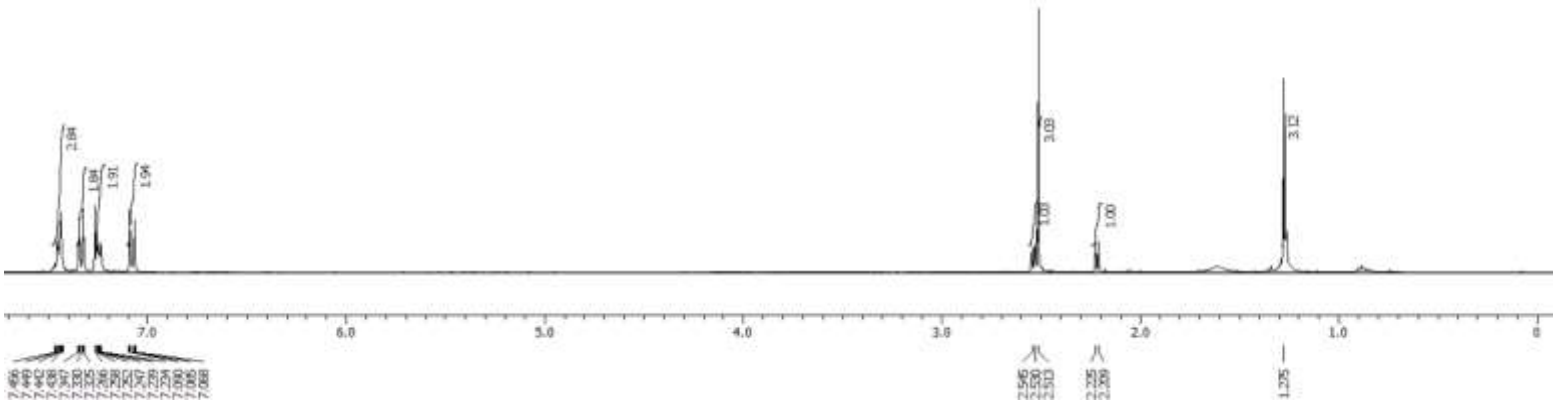
— End Of Report —

^{1}H NMR spectrum of 2i (400 MHz, $CDCl_3$)

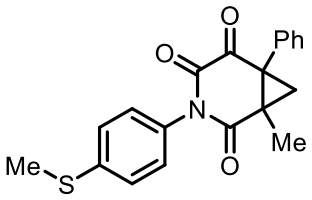


1-methyl-3-(4-(methylthio)phenyl)-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

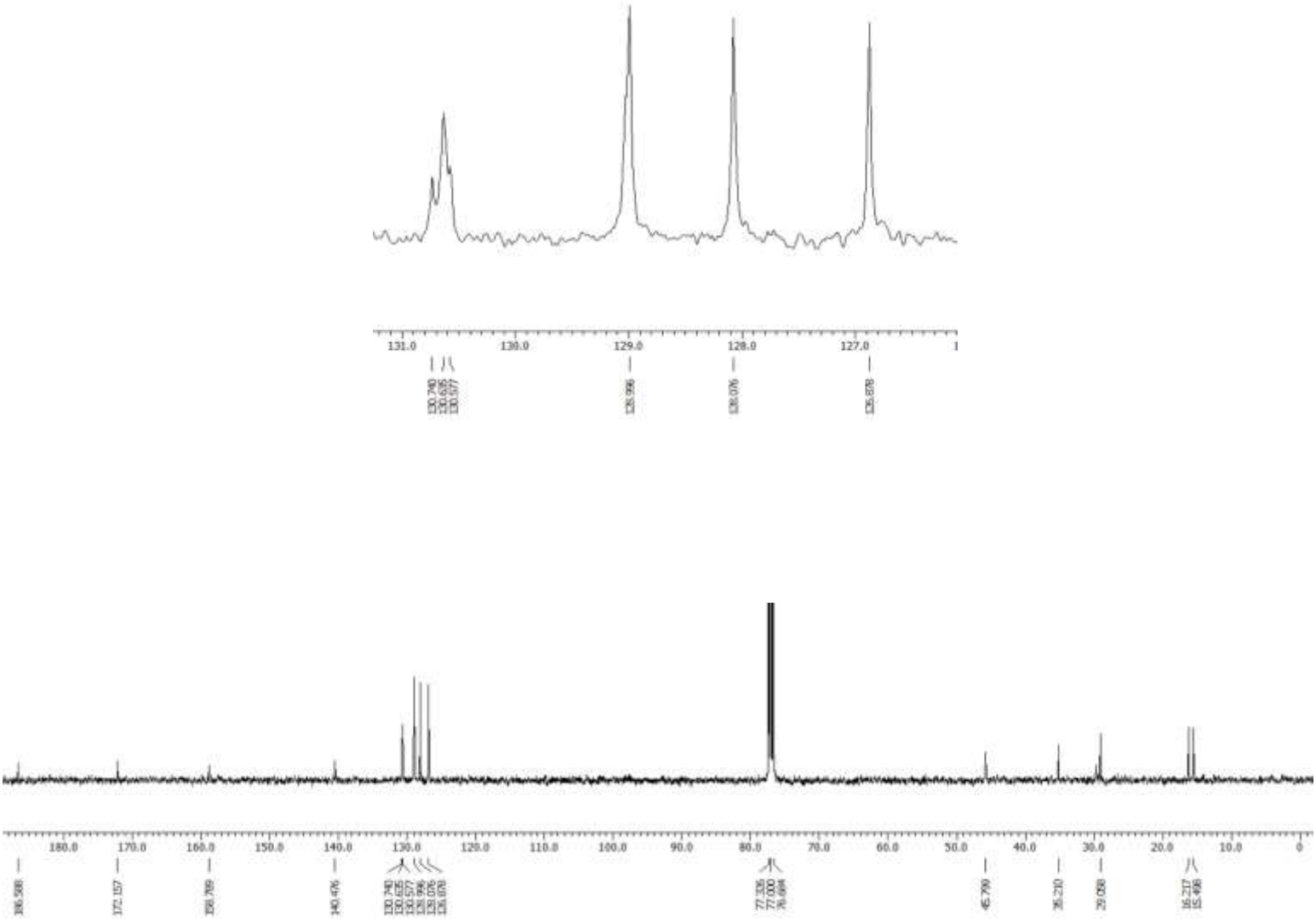




^{13}C NMR spectrum of 2i (100 MHz, $CDCl_3$)

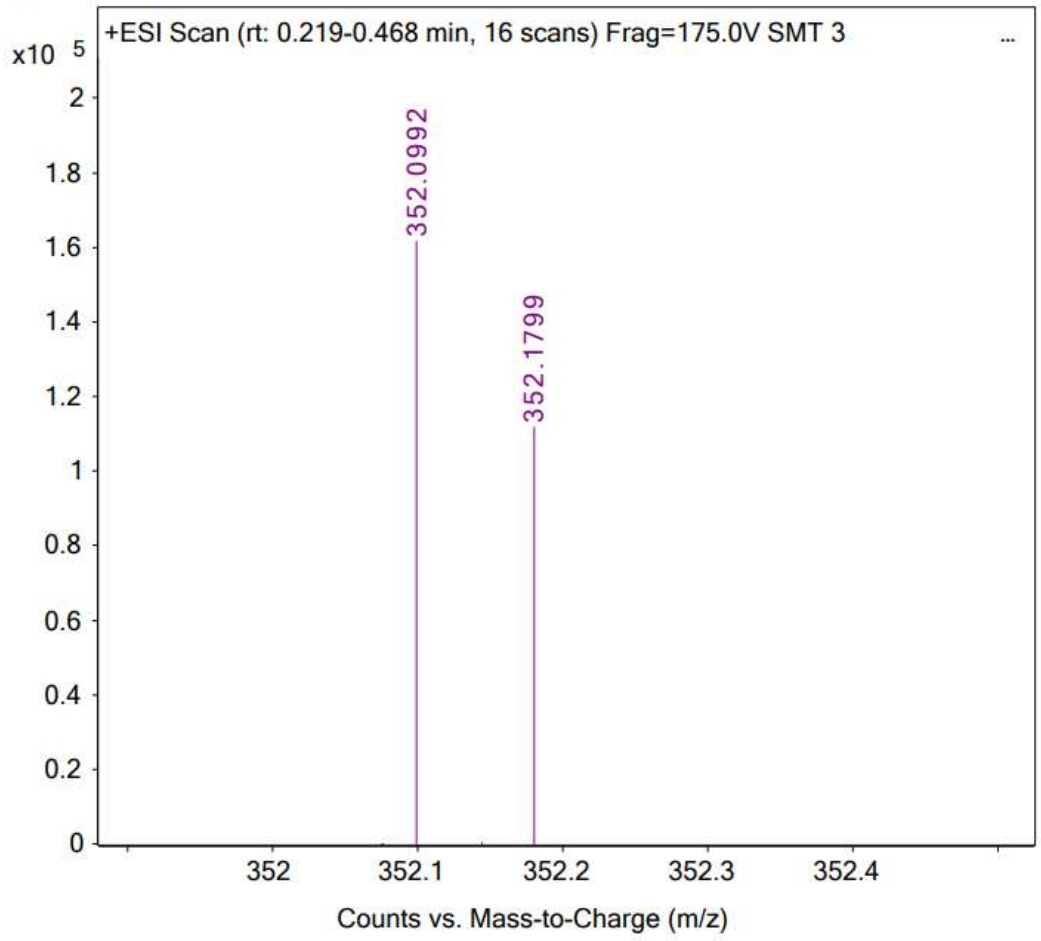


1-methyl-3-(4-(methylthio)phenyl)-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

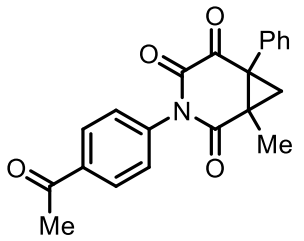


HRMS spectrum of 2i

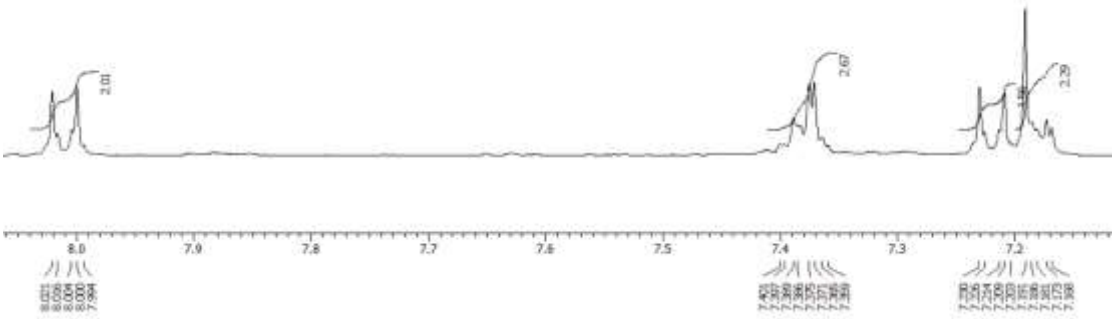
Sample Name	SMT 361	**Position**	P1-B6	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 361.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:42:40 (UTC+05:30)

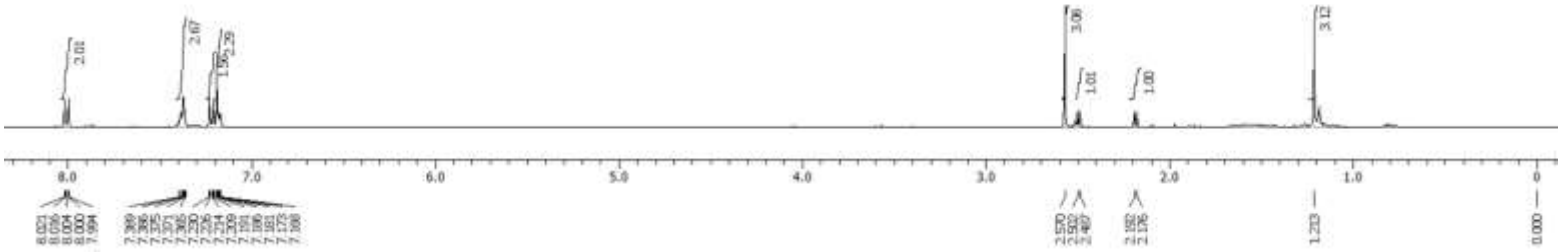


^{1}H NMR spectrum of 2j (400 MHz, $CDCl_3$)

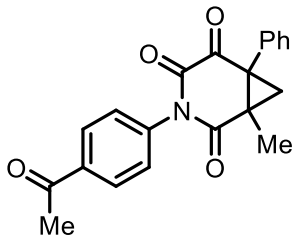


3-(4-acetylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

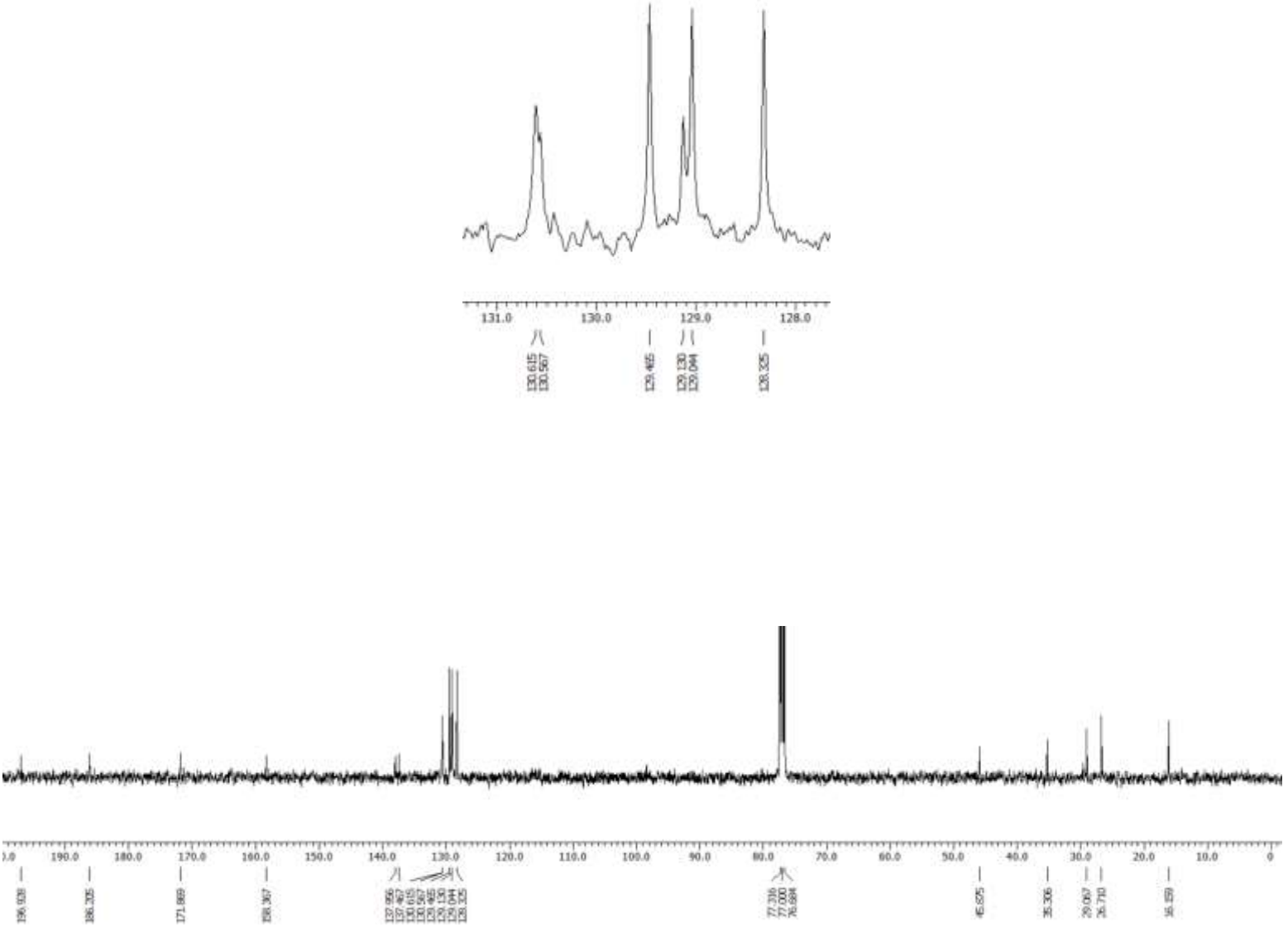




^{13}C NMR spectrum of 2j (100 MHz, $CDCl_3$)

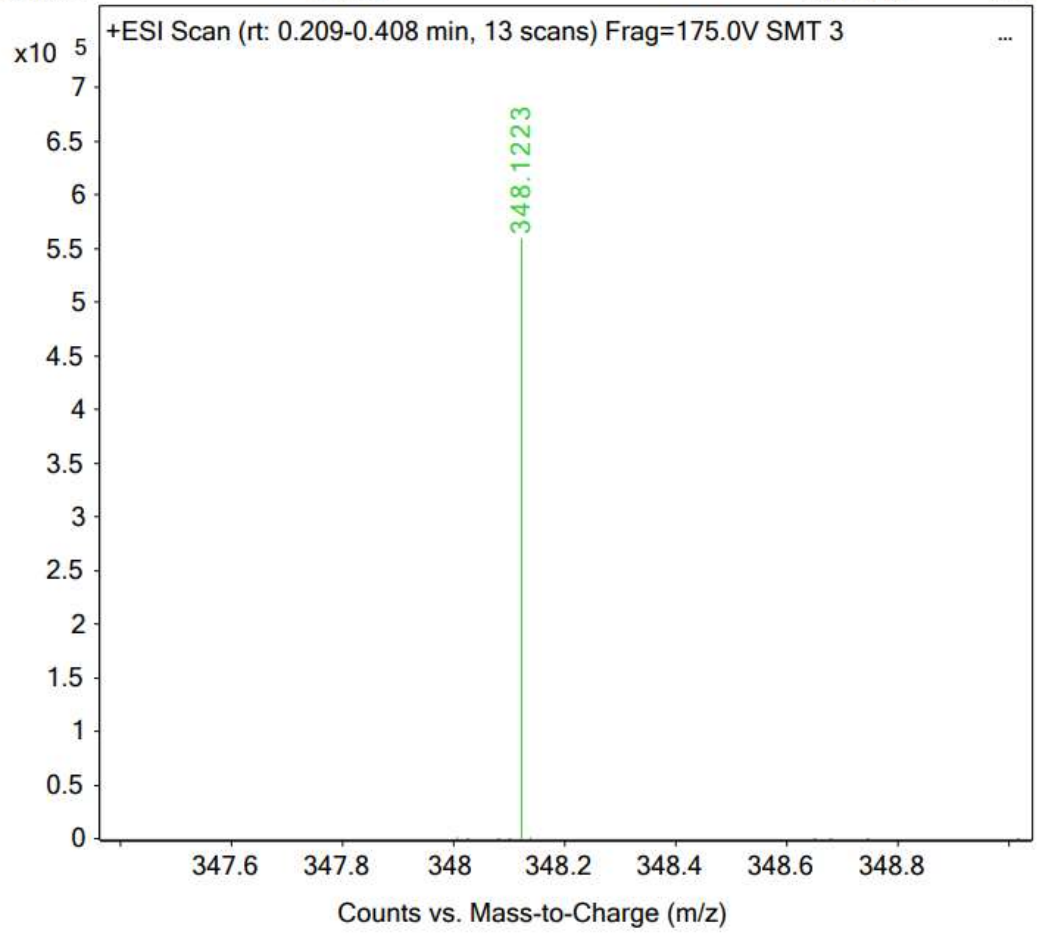


3-(4-acetylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

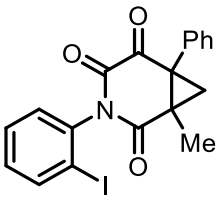


HRMS spectrum of 2j

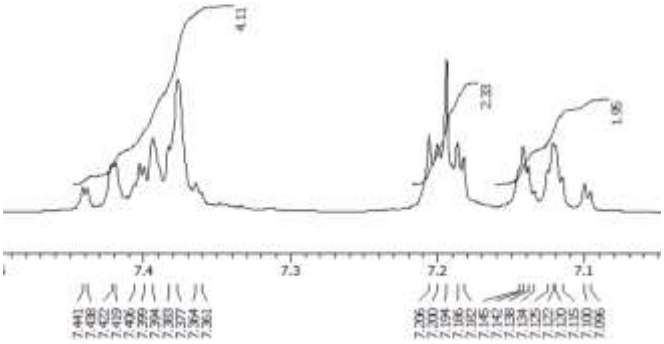
Sample Name	SMT 366	**Position**	P1-B9	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 366.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:54:16 (UTC+05:30)

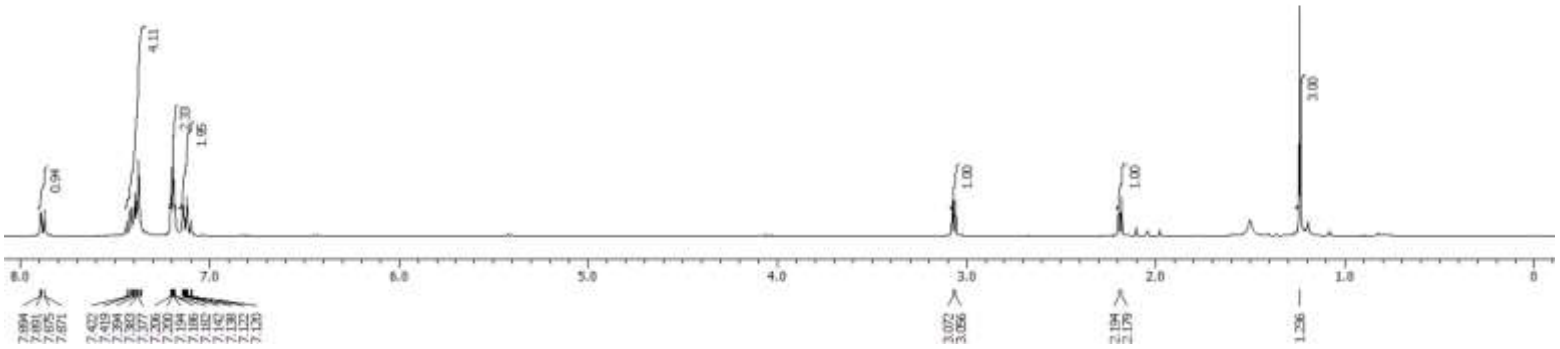


^{1}H NMR spectrum of 2k (400 MHz, $CDCl_3$)

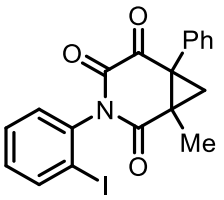


3-(2-iodophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

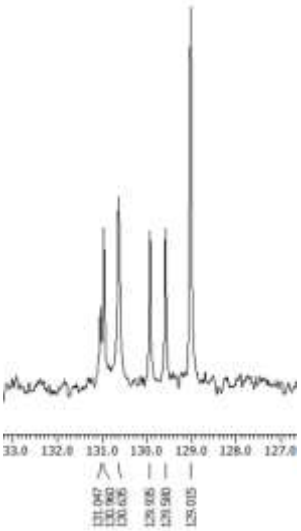


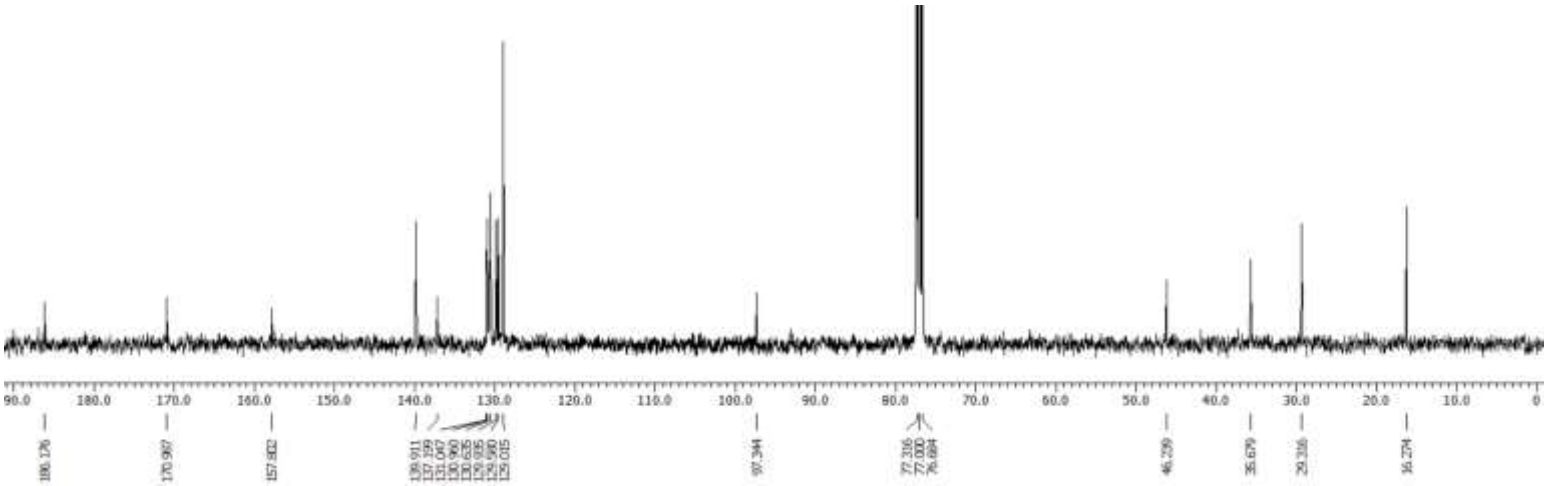


^{13}C NMR spectrum of 2k (100 MHz, $CDCl_3$)



3-(2-iodophenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 2k

Qualitative Compound Report

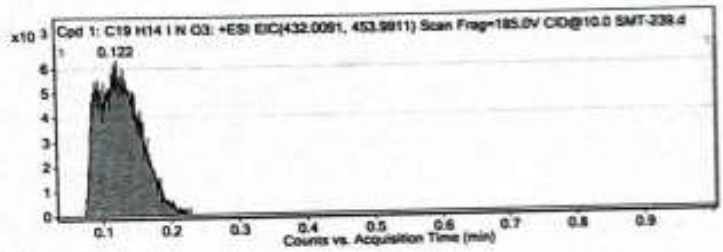
Data File	SMT-239.d	Sample Name	SMT-239
Sample Type	Sample	Position	P1-A6
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	10-04-2023 13:52:20
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

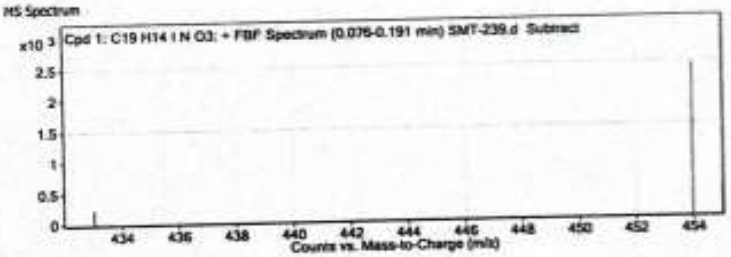
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C19 H14 I N O3	0.122	431.0014	2459	C19 H14 I N O3	431.0018	-0.95	C19 H14 I N O3	C19 H14 I N O3

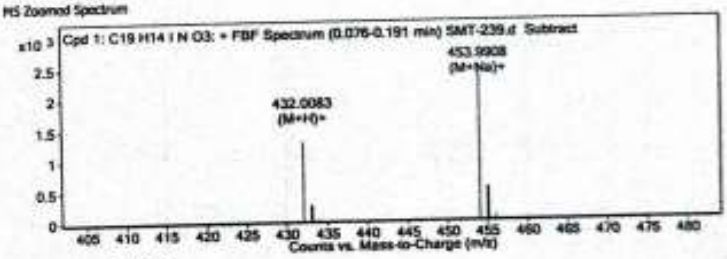
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H14 I N O3	453.9908	0.122	Find By Formula	431.0014



MS Spectrum



MS Zoomed Spectrum

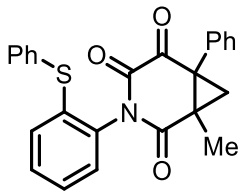


MS Spectrum Peak List

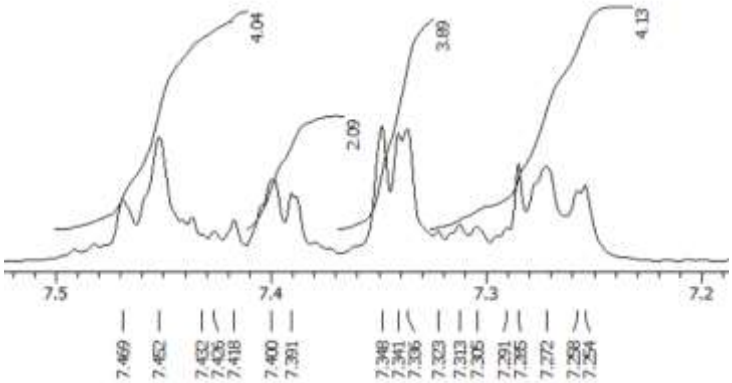
m/z	z	Abund	Formula	Ion
432.0083	1	1290.66	C19H15INO3	(M+H)+
433.0112	1	231.3	C19H15INO3	(M+H)+
453.9908	1	2459.19	C19H14INNaO3	(M+Na)+
454.9945	1	511.43	C19H14INNaO3	(M+Na)+

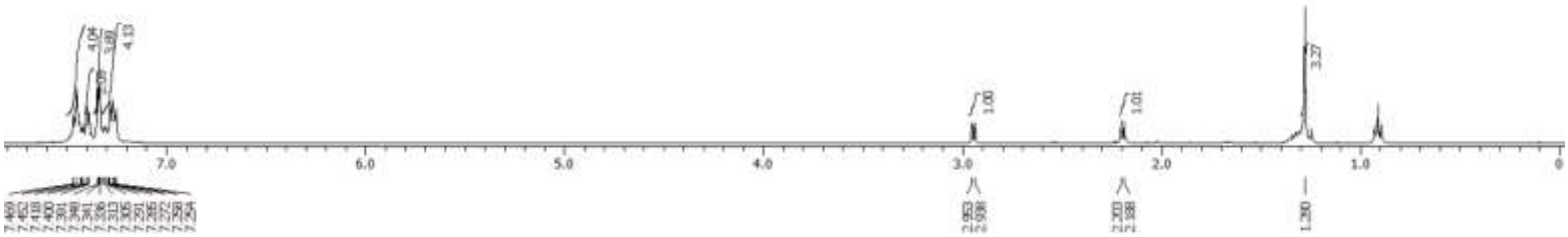
--- End Of Report ---

^{1}H NMR spectrum of 2l (400 MHz, $CDCl_3$)

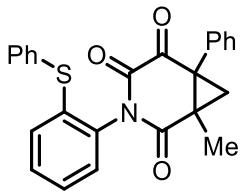


1-methyl-6-phenyl-3-(2-(phenylthio)phenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

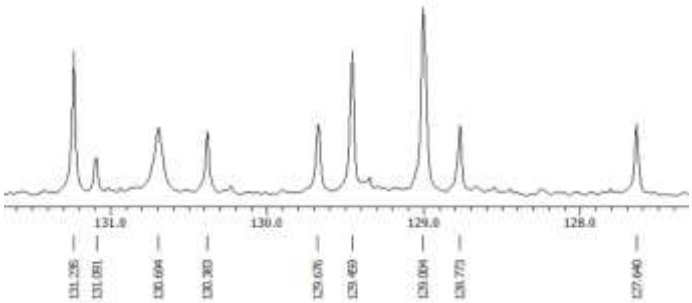


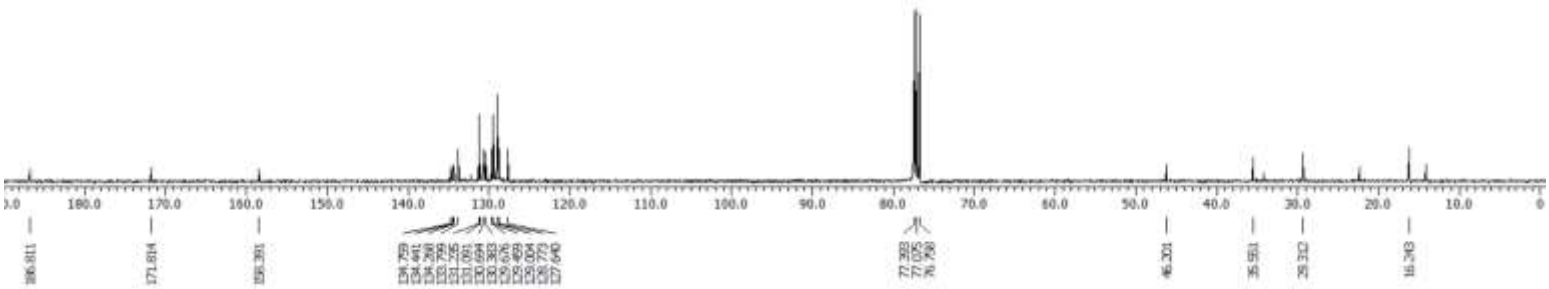


^{13}C NMR spectrum of 2l (100 MHz, $CDCl_3$)



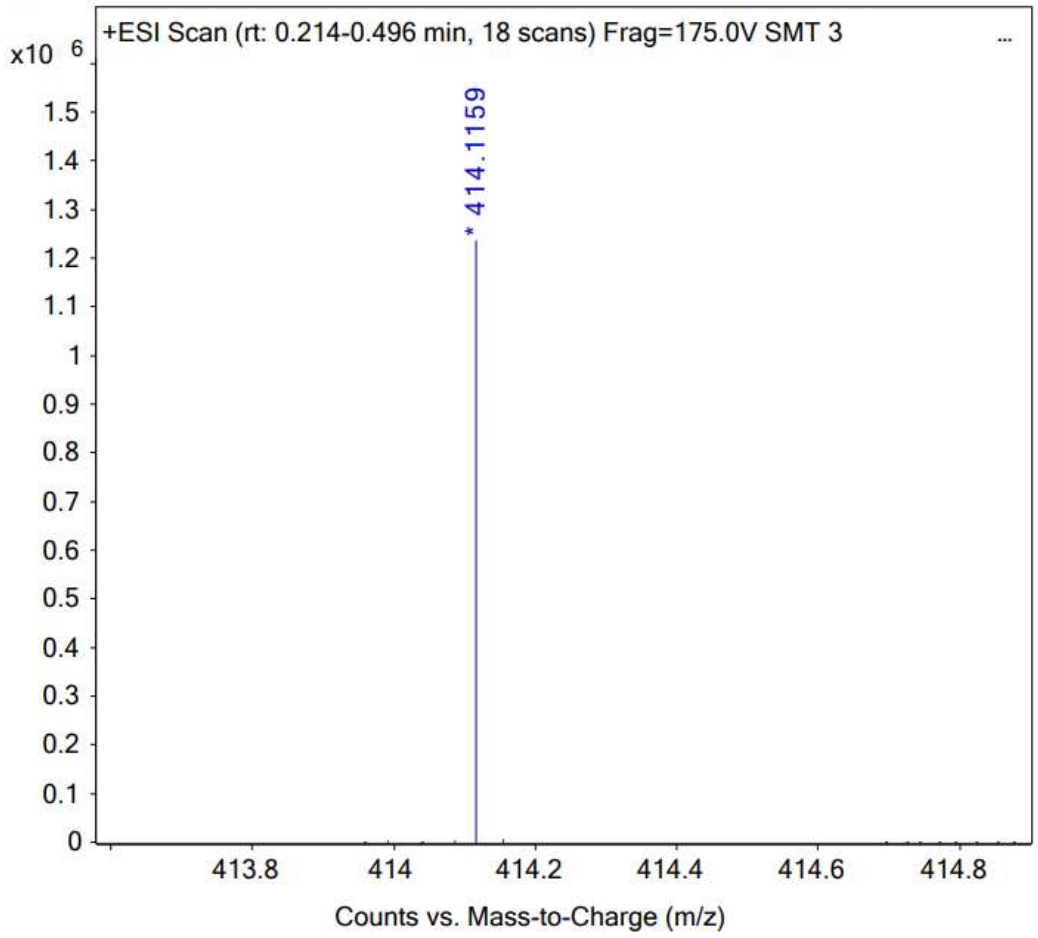
1-methyl-6-phenyl-3-(2-(phenylthio)phenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione



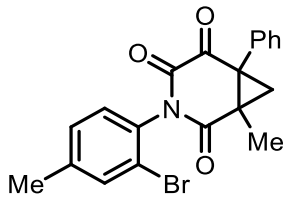


HRMS spectrum of 2l

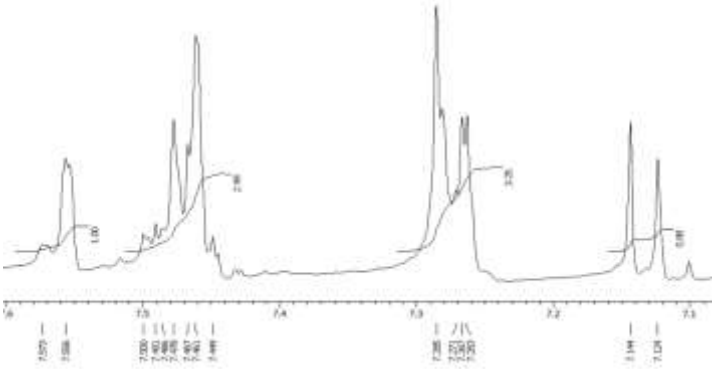
Sample Name	SMT 360	**Position**	P1-A10	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 360.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:15:35 (UTC+05:30)

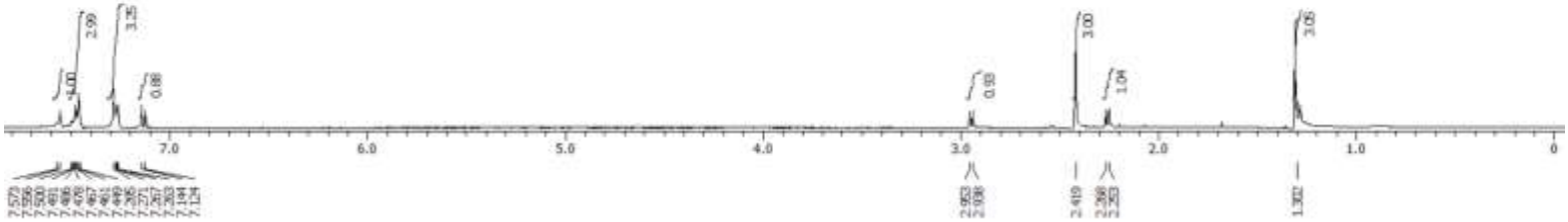


^{1}H NMR spectrum of 2m (400 MHz, $CDCl_3$)

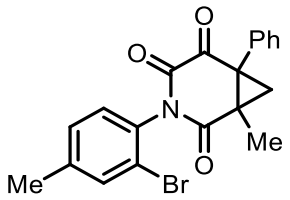


3-(2-bromo-4-methylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

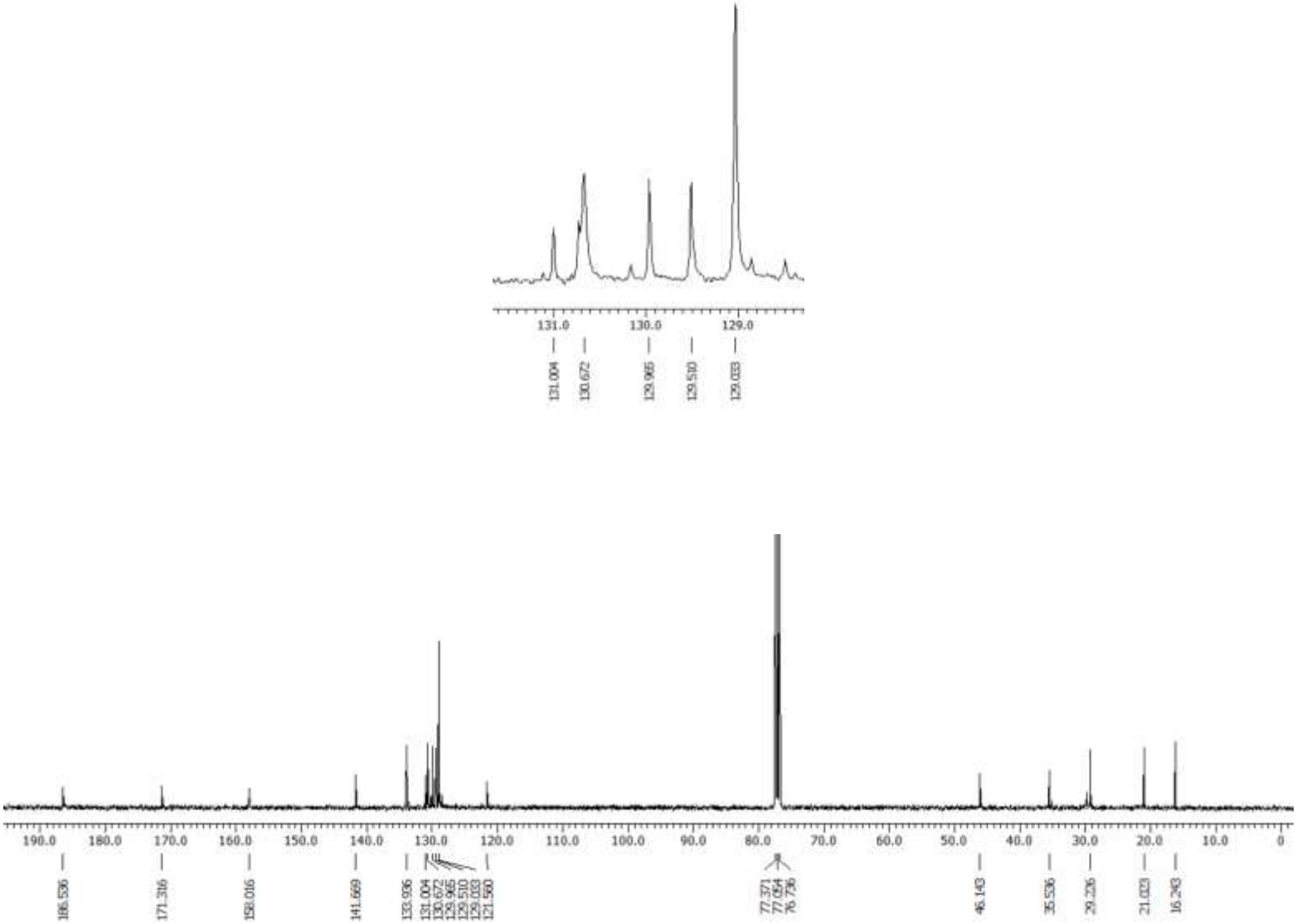




^{13}C NMR spectrum of 2m (100 MHz, $CDCl_3$)



3-(2-bromo-4-methylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2m

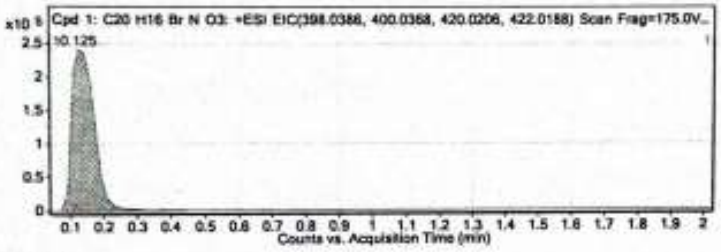
Qualitative Compound Report

Data File	SMT-291.d	Sample Name	SMT-291
Sample Type	Sample	Position	P1-D2
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	09-08-2023 14:18:32
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)		

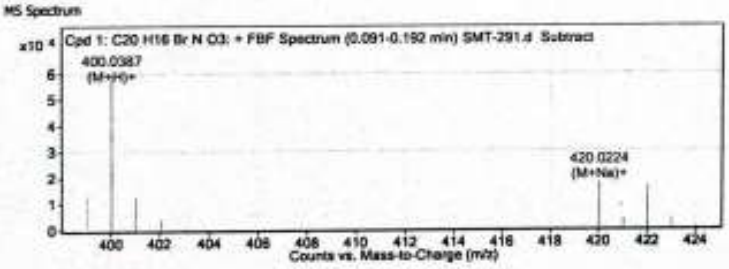
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H16 Br N O3	0.125	397.0331	58652	C20 H16 Br N O3	397.0314	4.34	C20 H16 Br N O3	C20 H16 Br N O3

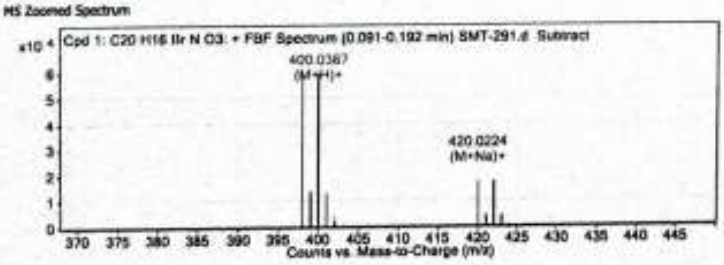
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H16 Br N O3	400.0387	0.125	Find By Formula	397.0331



MS Spectrum



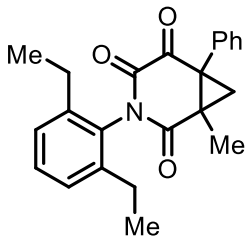
MS Zoomed Spectrum



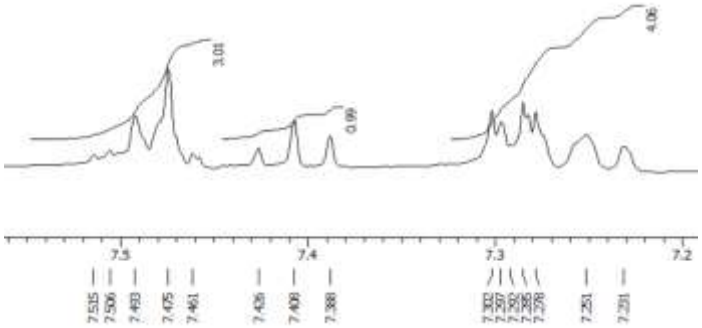
MS Spectrum Peak List

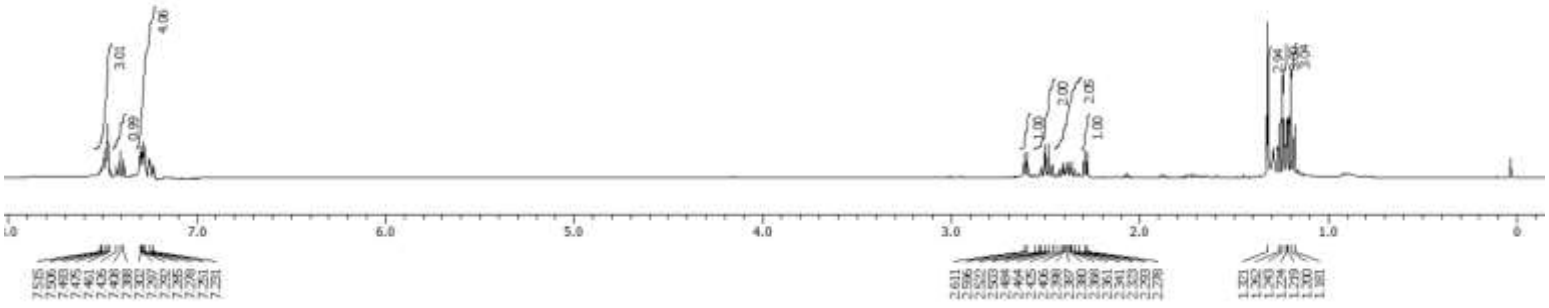
m/z	z	Abund	Formula	Ion
398.04	1	58728.86	C20H17BrNO3	(M+H)+
399.0429	1	12843.39	C20H17BrNO3	(M+H)+
400.0387	1	58652.48	C20H17BrNO3	(M+H)+
401.0417	1	12783.69	C20H17BrNO3	(M+H)+
402.0472	1	4070.92	C20H17BrNO3	(M+H)+
403.0522	1	860.16	C20H17BrNO3	(M+H)+
420.0224	1	17402.69	C20H16BrNNaO3	(M+Na)+
421.0264	1	3901.49	C20H16BrNNaO3	(M+Na)+
422.0207	1	16613.83	C20H16BrNNaO3	(M+Na)+
423.0235	1	3922.7	C20H16BrNNaO3	(M+Na)+
424.0274	1	781.98	C20H16BrNNaO3	(M+Na)+

^{1}H NMR spectrum of 2n (400 MHz, $CDCl_3$)

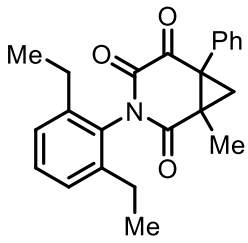


3-(2,6-diethylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

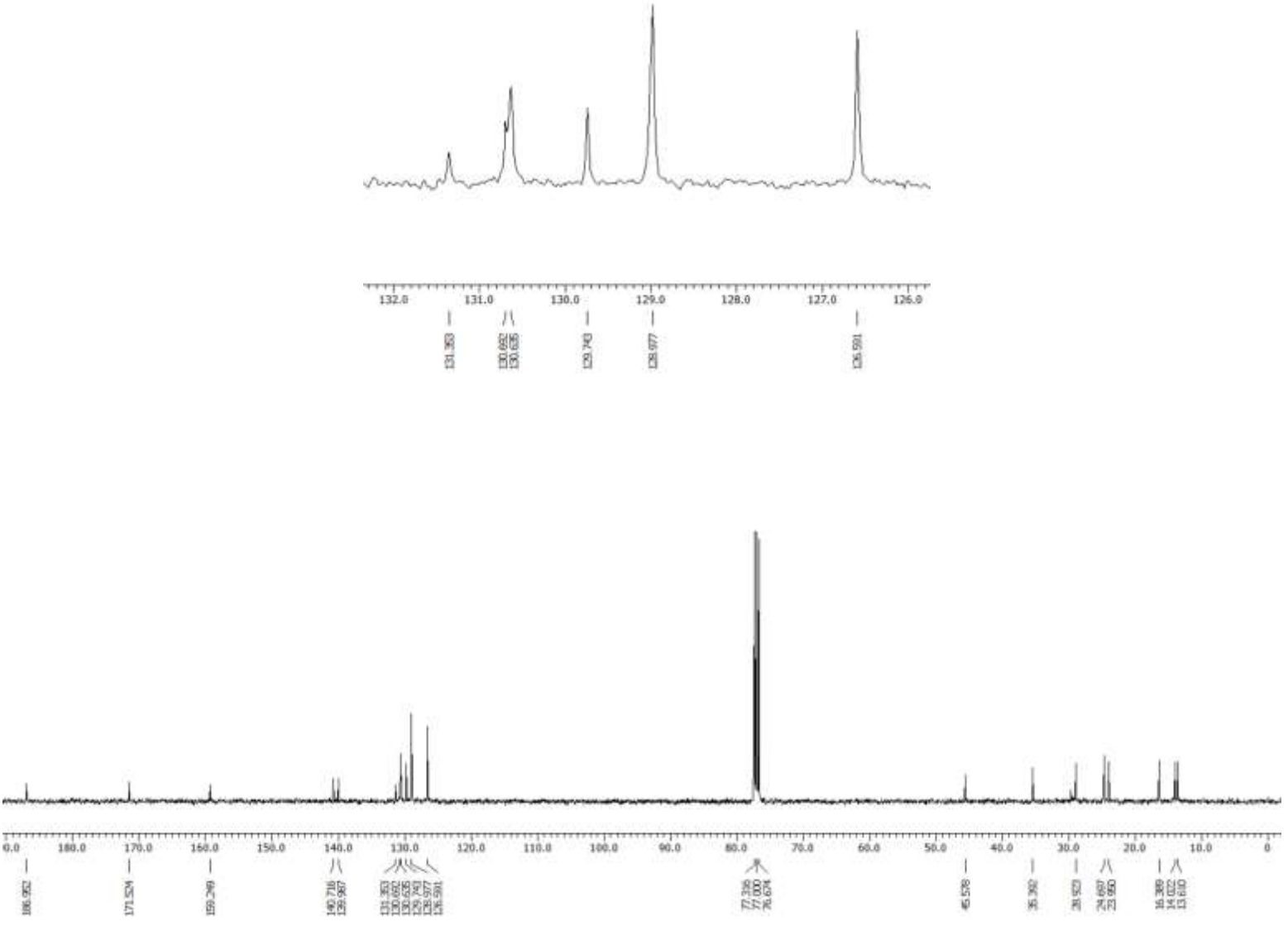




^{13}C NMR spectrum of 2n (100 MHz, $CDCl_3$)



3-(2,6-diethylphenyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2n

Qualitative Compound Report

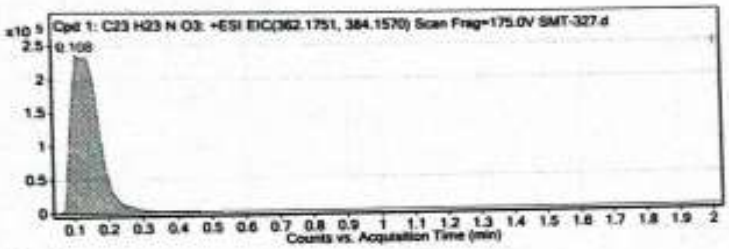
Data File	SMT-327.d	**Sample Name**	SMT-327
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	11-10-2023 14:24:18
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

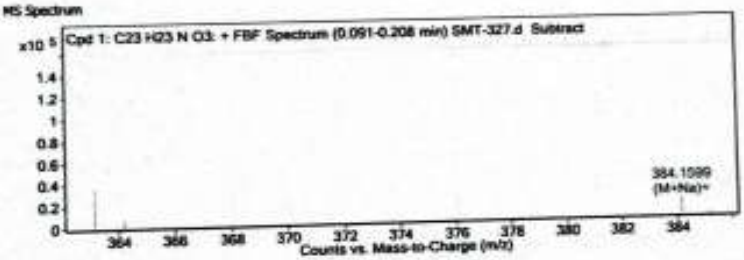
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C23 H23 N O3	0.108	361.1698	140472	C23 H23 N O3	361.1678	5.6	C23 H23 N O3	C23 H23 N O3

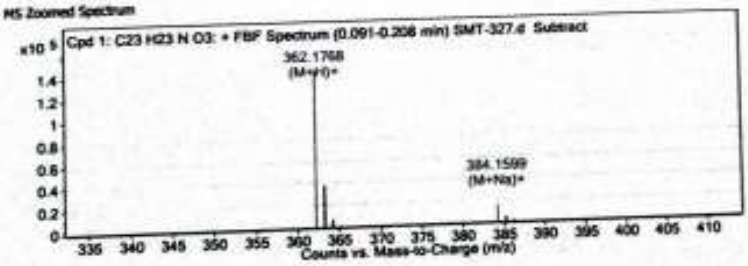
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C23 H23 N O3	362.1768	0.108	Find By Formula	361.1698



MS Spectrum



MS Zoomed Spectrum

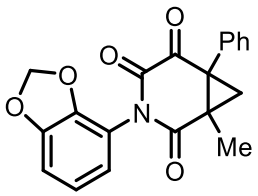


MS Spectrum Peak List

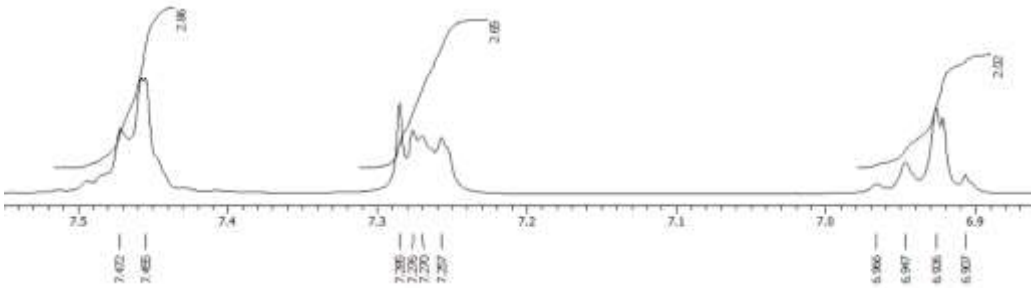
m/z	z	Abund	Formula	Ion
362.1768	1	140471.73	C23H24NO3	(M+H)+
363.1801	1	35844.18	C23H24NO3	(M+H)+
364.1859	1	7459.89	C23H24NO3	(M+H)+
365.1917	1	1485.31	C23H24NO3	(M+H)+
384.1599	1	15211.84	C23H23NNaO3	(M+Na)+
385.1637	1	3989.82	C23H23NNaO3	(M+Na)+
386.1661	1	937.49	C23H23NNaO3	(M+Na)+

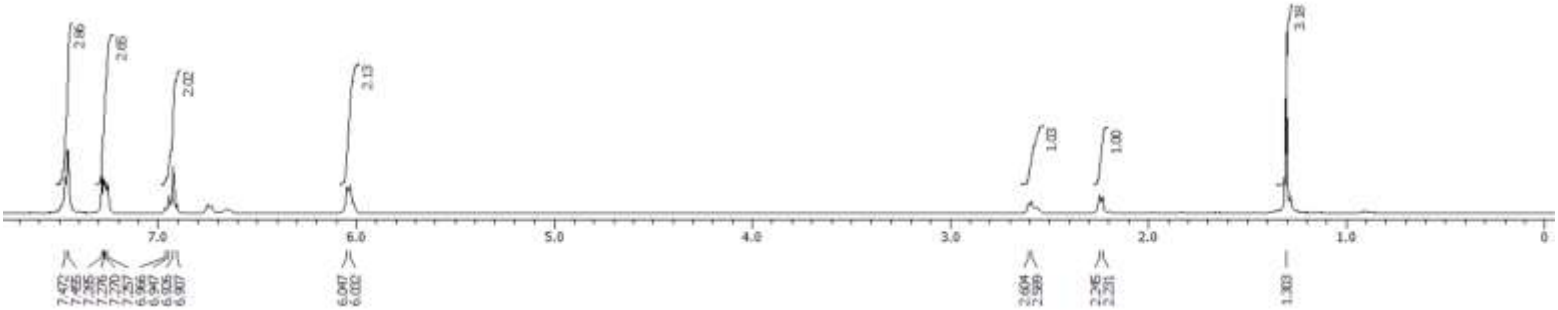
--- End Of Report ---

^{1}H NMR spectrum of 2o (400 MHz, $CDCl_3$)

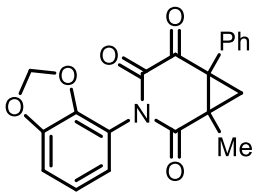


3-(benzo[*d*][1,3]dioxol-4-yl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

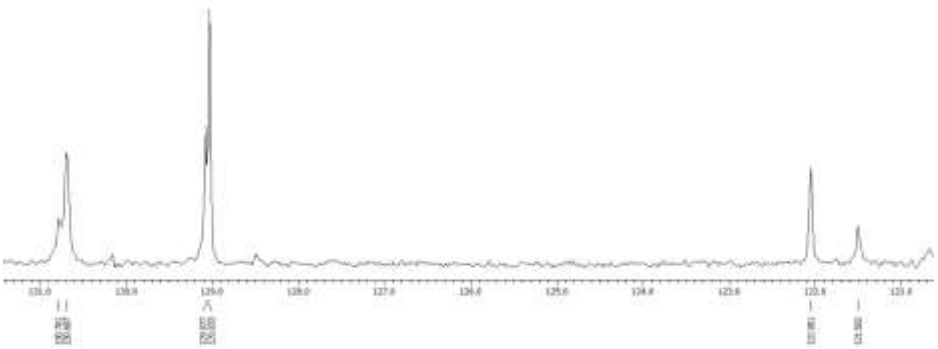


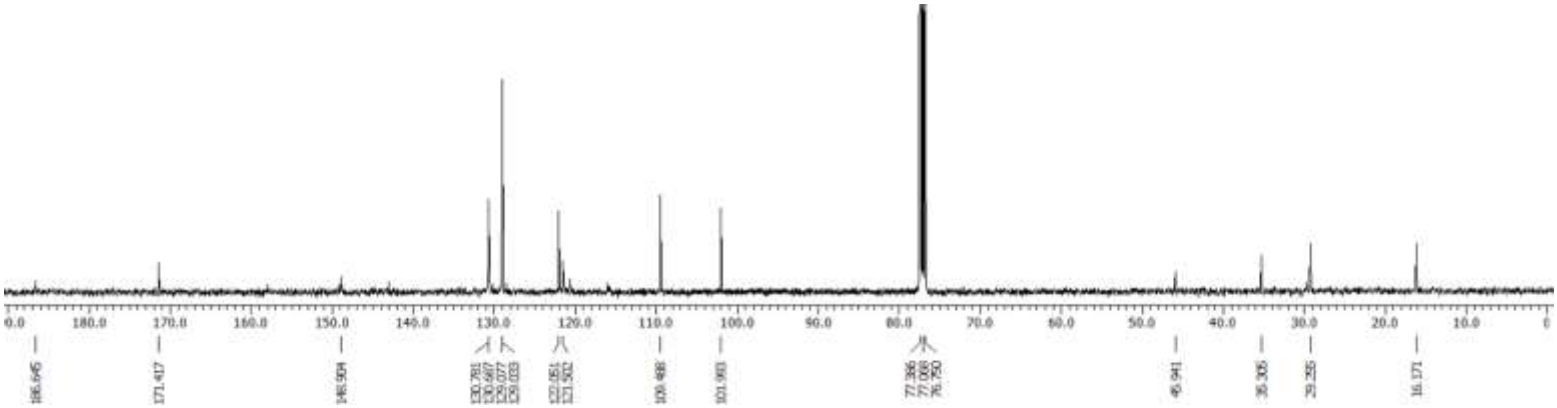


^{13}C NMR spectrum of 2o (100 MHz, $CDCl_3$)



3-(benzo[*d*][1,3]dioxol-4-yl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 2o

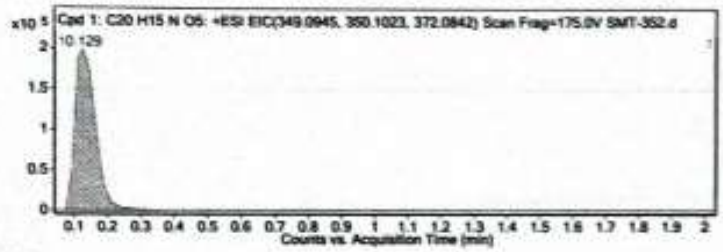
Qualitative Compound Report

Data File	SMT-352.d	Sample Name	SMT-352
Sample Type	Sample	Position	P1-C1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	09-11-2023 14:11:12
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)		

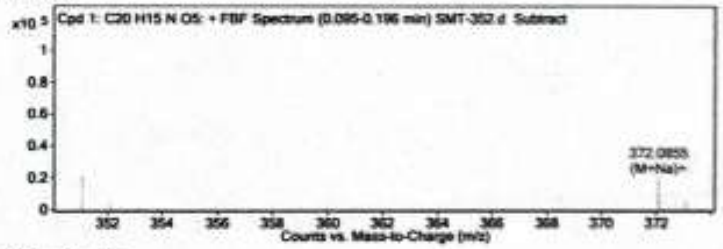
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H15 N O5	0.129	349.0951	96035	C20 H15 N O5	349.095	0.22	C20 H15 N O5	C20 H15 N O5

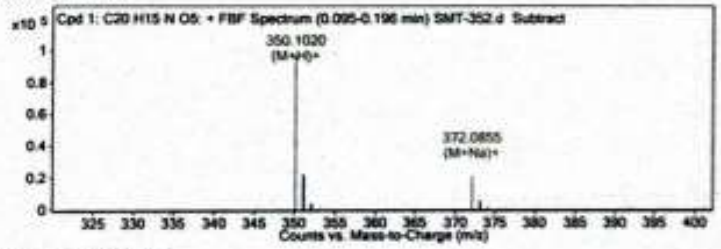
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H15 N O5	350.102	0.129	Find By Formula	349.0951



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
350.102	1	96035.33	C20H16NO5	(M+H)+
351.1053	1	20963.48	C20H16NO5	(M+H)+
352.1081	1	3973.8	C20H16NO5	(M+H)+
353.1065	1	713.54	C20H16NO5	(M+H)+
372.0855	1	20288.39	C20H15NNaO5	(M+Na)+
373.09	1	5335.91	C20H15NNaO5	(M+Na)+
374.0996	1	1122.35	C20H15NNaO5	(M+Na)+

--- End Of Report ---

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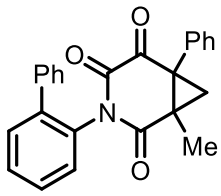
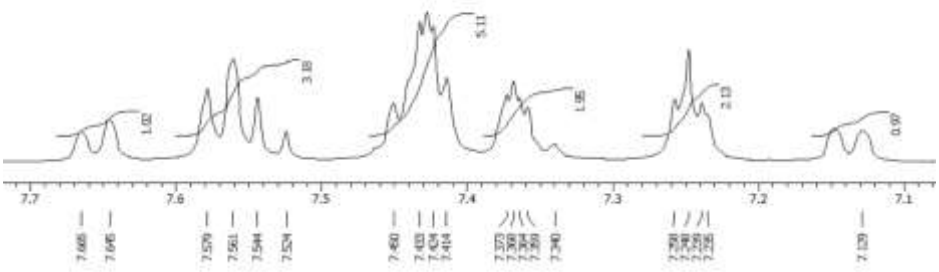
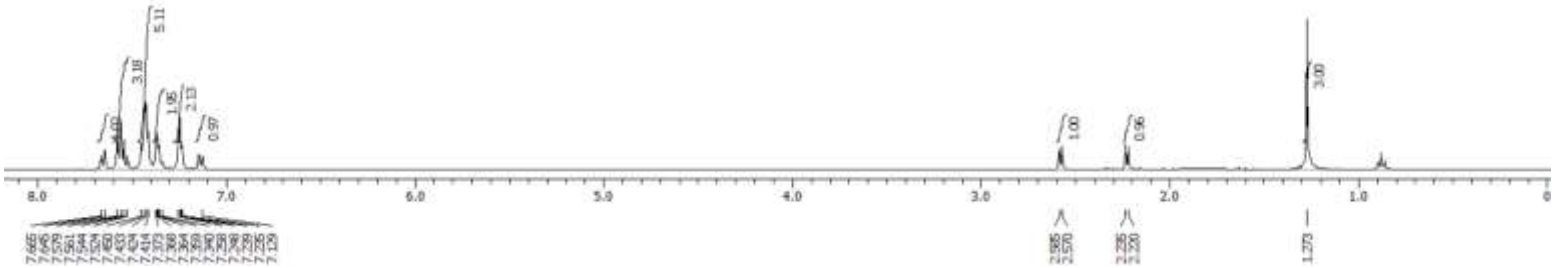
^{1}H NMR spectrum of 2p (400 MHz, $CDCl_3$)

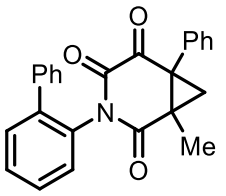


3-([1,1'-biphenyl]-2-yl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

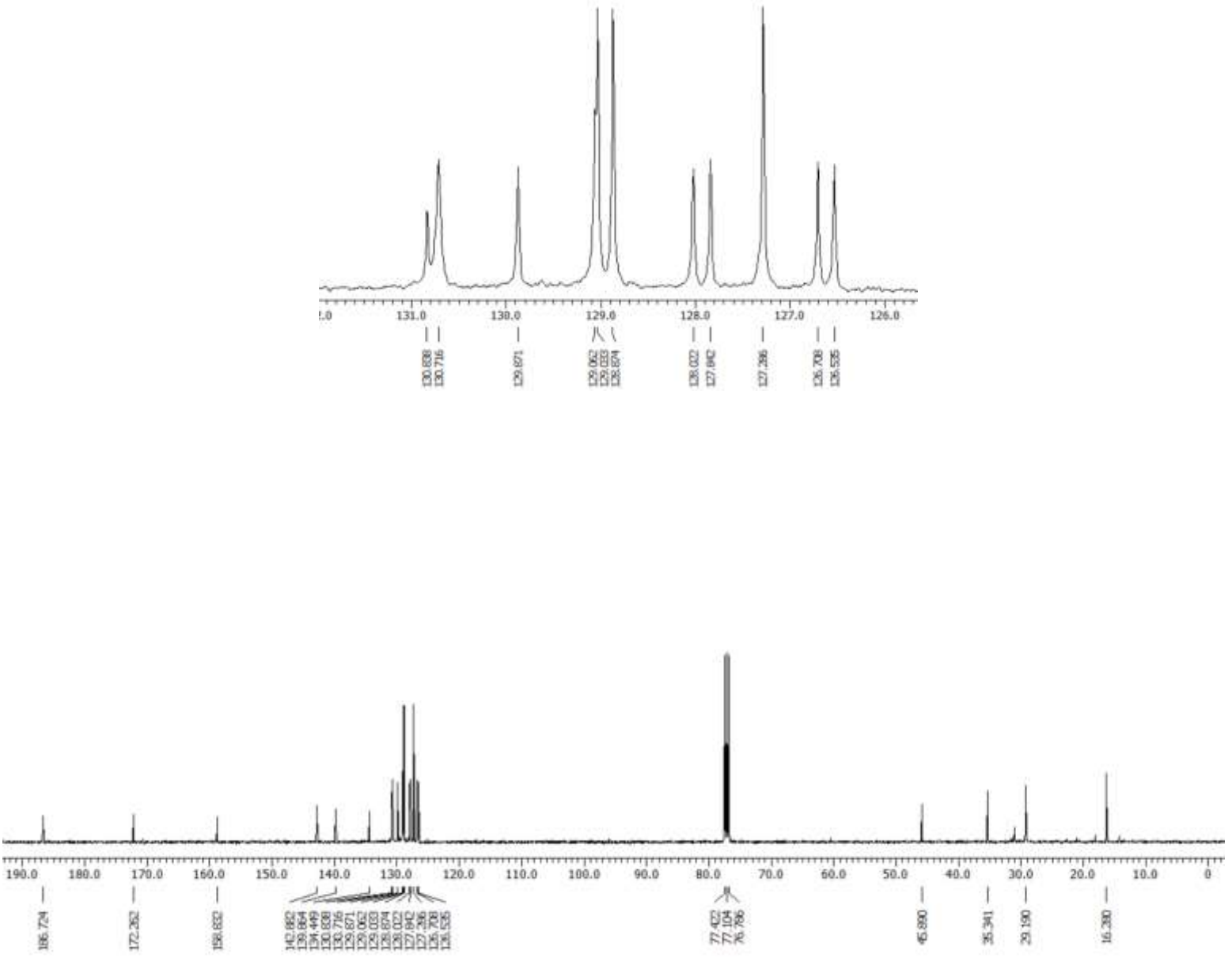




^{13}C NMR spectrum of 2p (400 MHz, $CDCl_3$)



3-([1,1'-biphenyl]-2-yl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2p

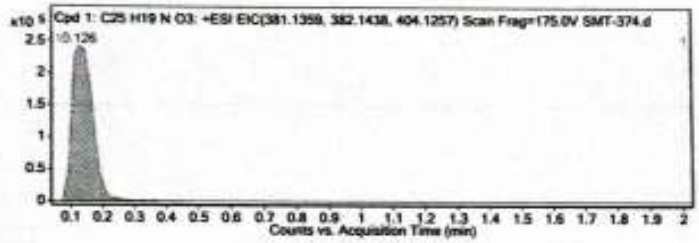
Qualitative Compound Report

Data File	SMT-374.d	Sample Name	SMT-374
Sample Type	Sample	Position	P1-A1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	08-12-2023 12:07:16
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)		

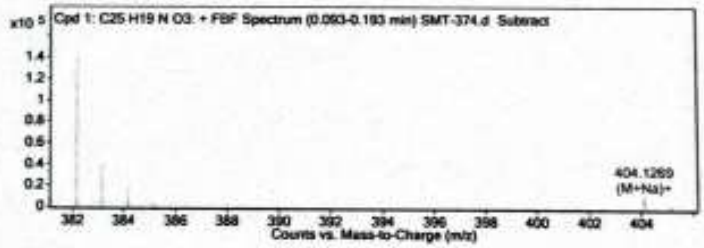
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C25 H19 N O3	0.126	381.1376	12049	C25 H19 N O3	381.1365	2.93	C25 H19 N O3	C25 H19 N O3

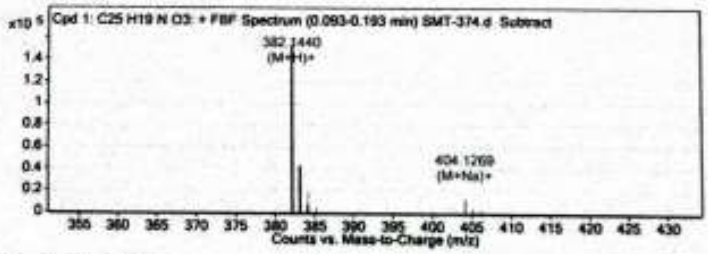
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C25 H19 N O3	404.1269	0.126	Find By Formula	381.1376



MS Spectrum



MS Zoomed Spectrum

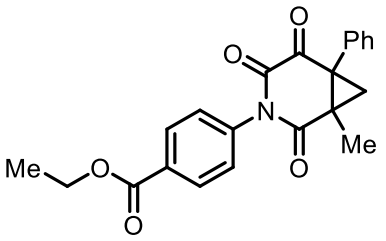


MS Spectrum Peak List

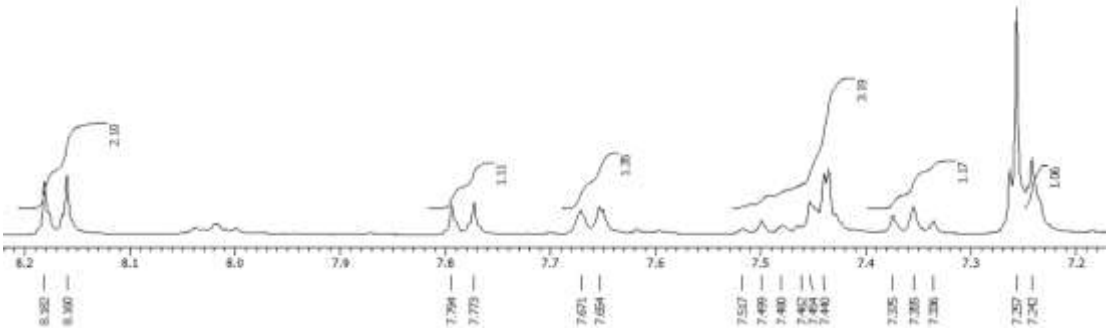
m/z	z	Abund	Formula	Ion
381.1446	1	341.26	C25H19NO3	M+·
382.144	1	141119.53	C25H20NO3	(M+H)+
383.1473	1	39744.75	C25H20NO3	(M+H)+
384.0567	1	18175.52	C25H20NO3	(M+H)+
385.1619	1	4514.32	C25H20NO3	(M+H)+
404.1269	1	12049.43	C25H19NNaO3	(M+Na)+
405.1308	1	3778.33	C25H19NNaO3	(M+Na)+
406.1425	1	1127.72	C25H19NNaO3	(M+Na)+

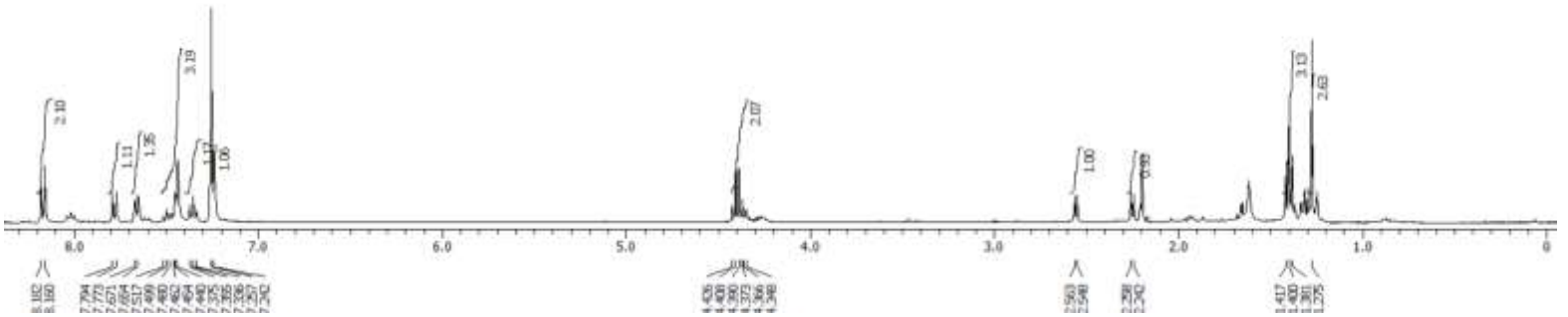
--- End Of Report ---

^{1}H NMR spectrum of 2q (400 MHz, $CDCl_3$)

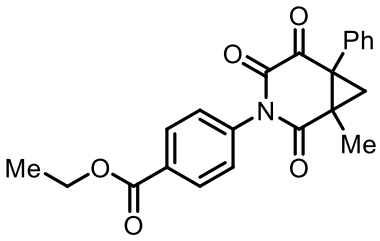


ethyl 4-(1-methyl-2,4,5-trioxo-6-phenyl-3-azabicyclo[4.1.0]heptan-3-yl)benzoate

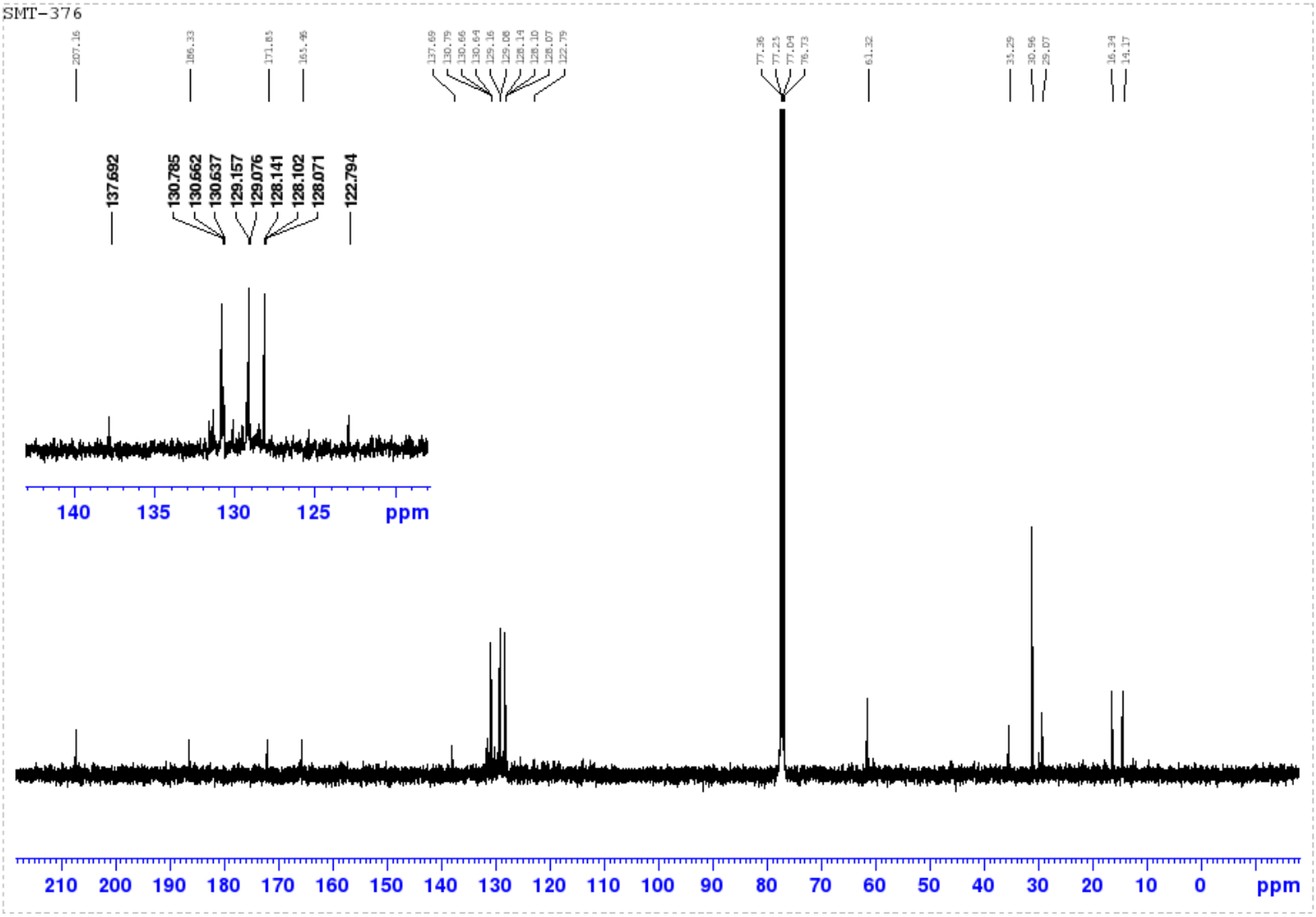




^{13}C NMR spectrum of 2q (100 MHz, $CDCl_3$)

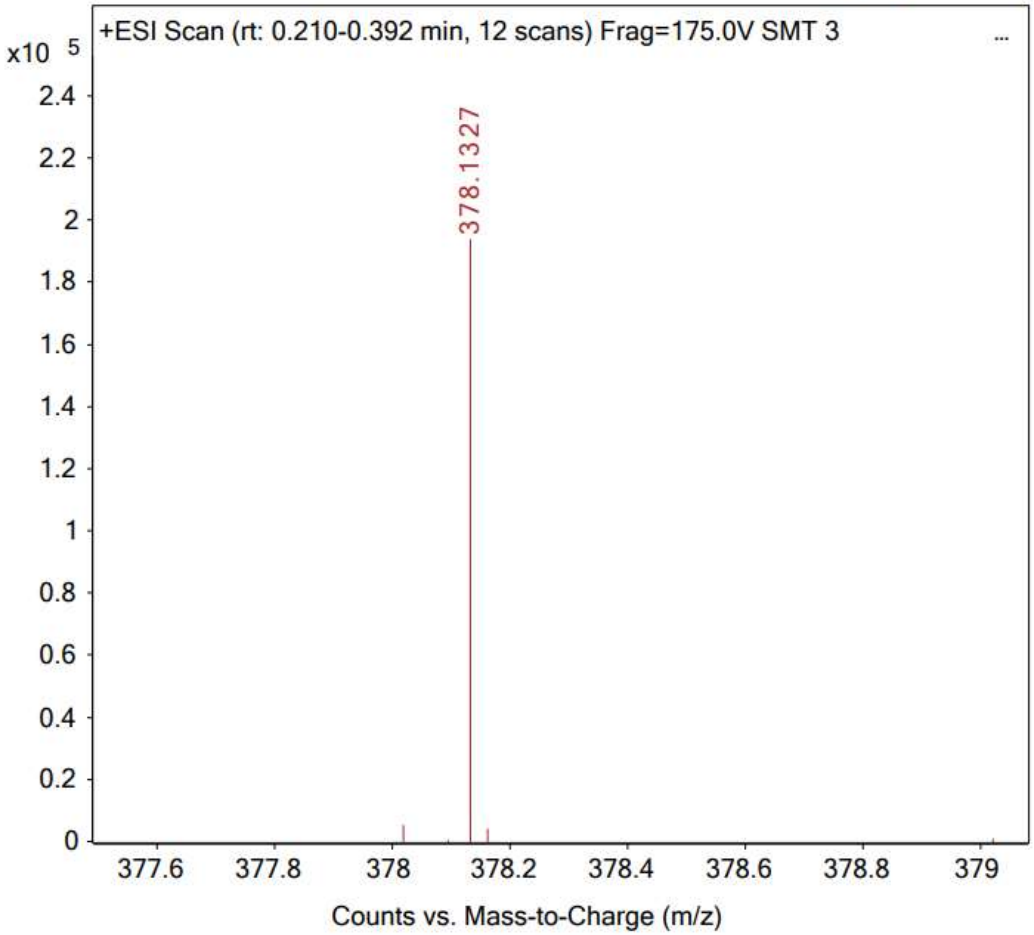


ethyl 4-(1-methyl-2,4,5-trioxo-6-phenyl-3-azabicyclo[4.1.0]heptan-3-yl)benzoate

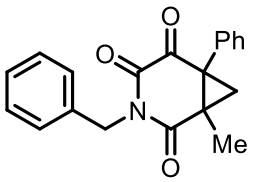


HRMS spectrum of 2q

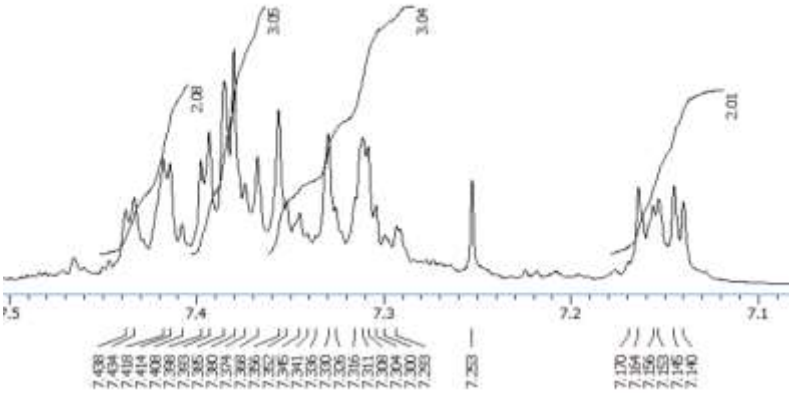
Sample Name	SMT 362	**Position**	P1-A2	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 362.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 11:44:42 (UTC+05:30)

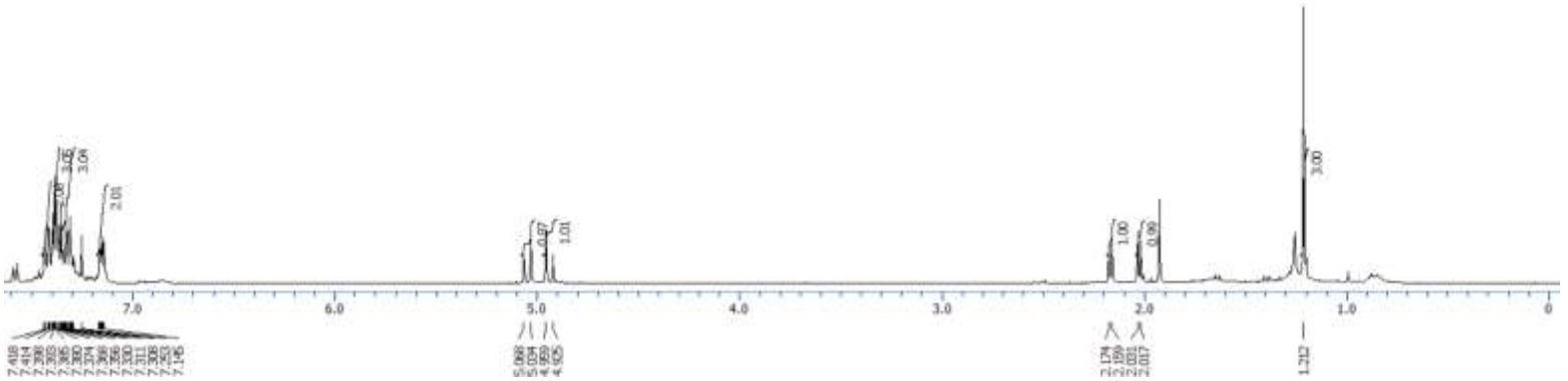


^{1}H NMR spectrum of 2r (400 MHz, $CDCl_3$)

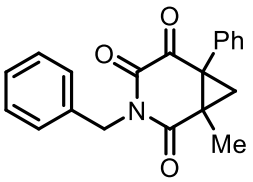


3-benzyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

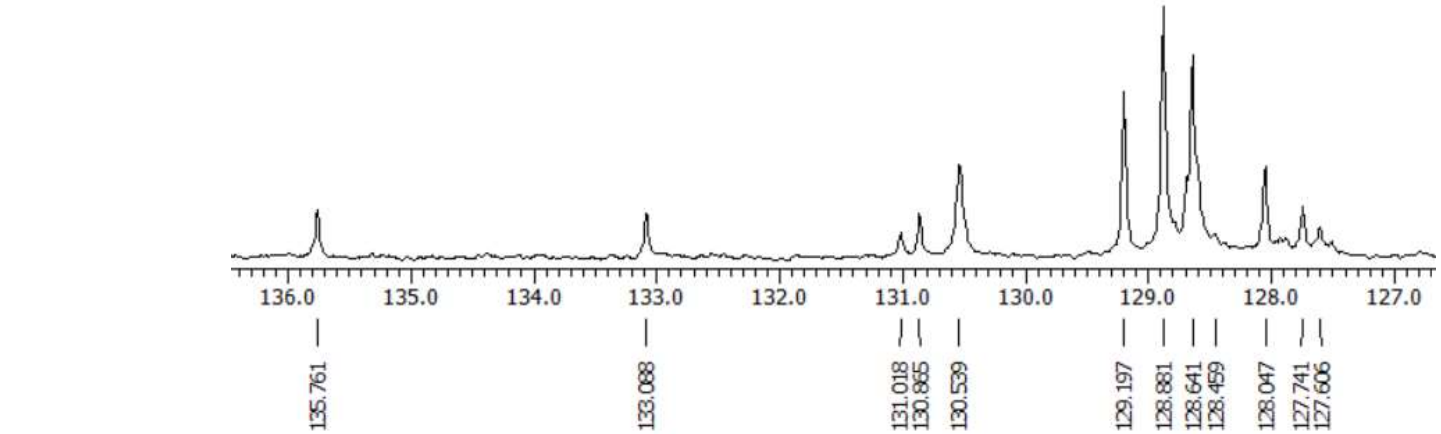


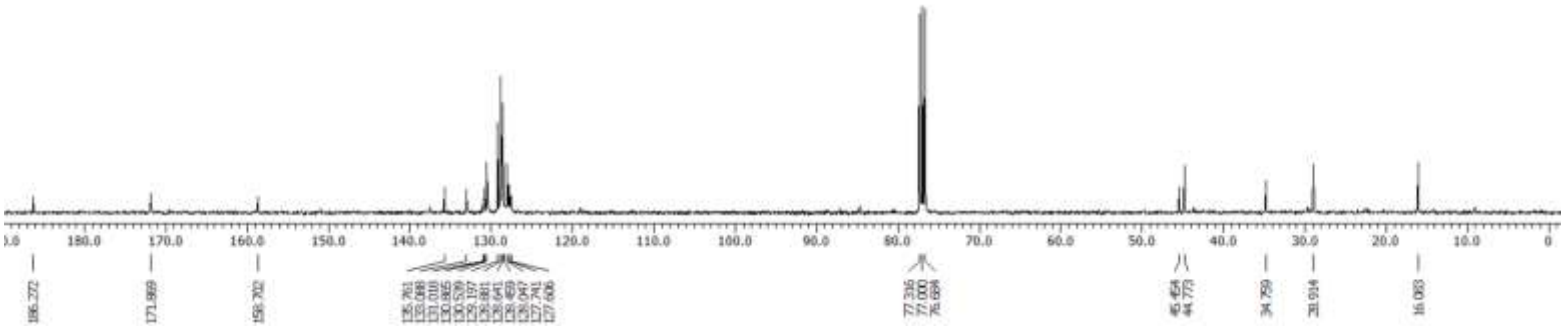


^{13}C NMR spectrum of 2r (100 MHz, $CDCl_3$)



3-benzyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 2r

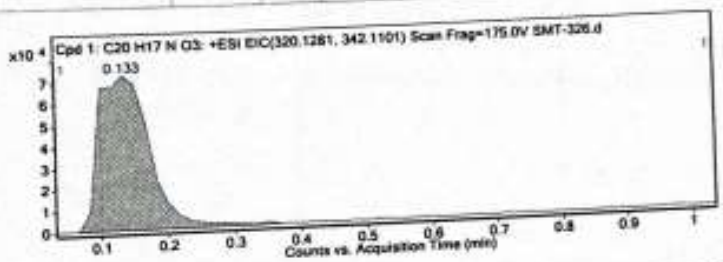
Qualitative Compound Report

Data File	SMT-326.d	**Sample Name**	SMT-326
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	16-09-2023 13:15:26
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)		

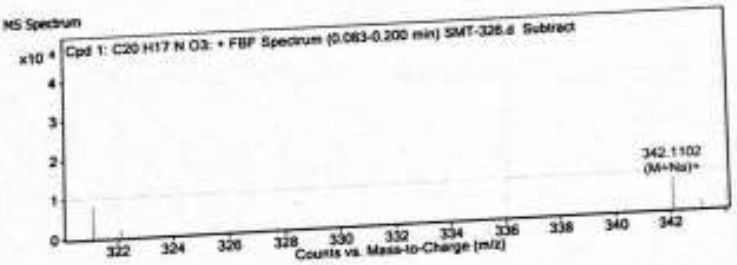
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H17 N O3	0.133	319.1211	38436	C20 H17 N O3	319.1208	0.72	C20 H17 N O3	C20 H17 N O3

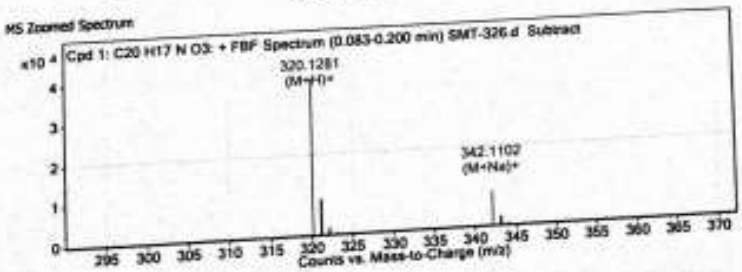
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H17 N O3	320.1281	0.133	Find By Formula	319.1211



MS Spectrum



MS Zoomed Spectrum

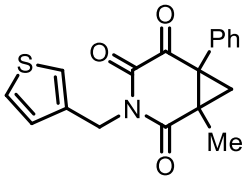


MS Spectrum Peak List

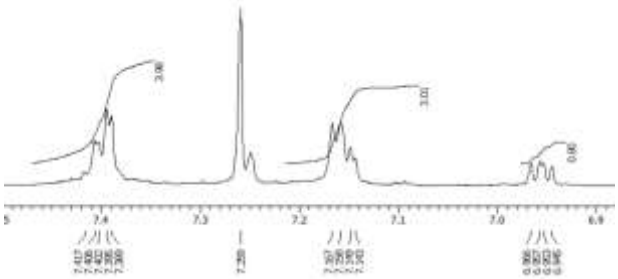
m/z	z	Abund	Formula	Ion
320.1281	1	38436.3	C20H18NO3	(M+H)+
321.1316	1	8497.19	C20H18NO3	(M+H)+
322.1378	1	1755.03	C20H18NO3	(M+H)+
323.1414	1	448.67	C20H18NO3	(M+H)+
342.1102	1	8318.78	C20H17NNaO3	(M+Na)+
343.1146	1	2138.4	C20H17NNaO3	(M+Na)+
344.114	1	301.63	C20H17NNaO3	(M+Na)+

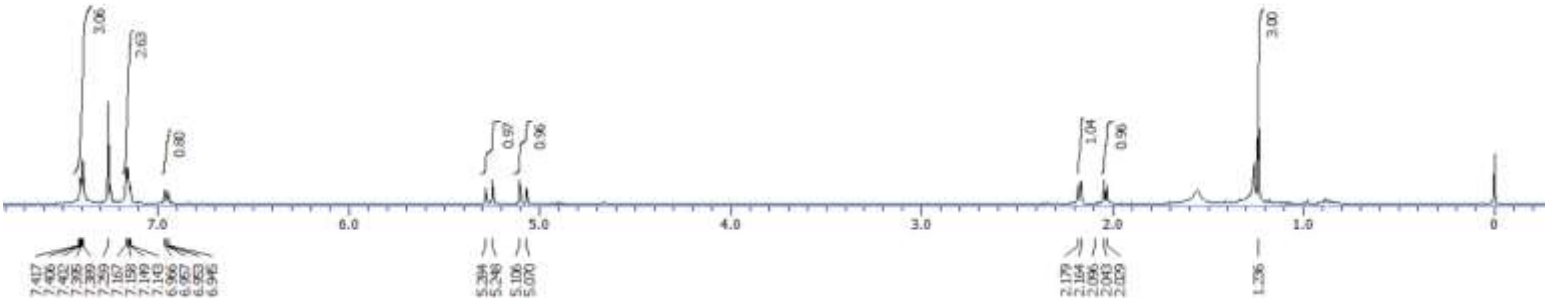
--- End Of Report ---

^{1}H NMR spectrum of 2s (400 MHz, $CDCl_3$)

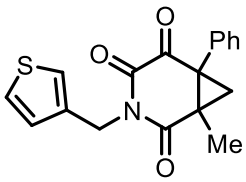


1-methyl-6-phenyl-3-(thiophen-3-ylmethyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

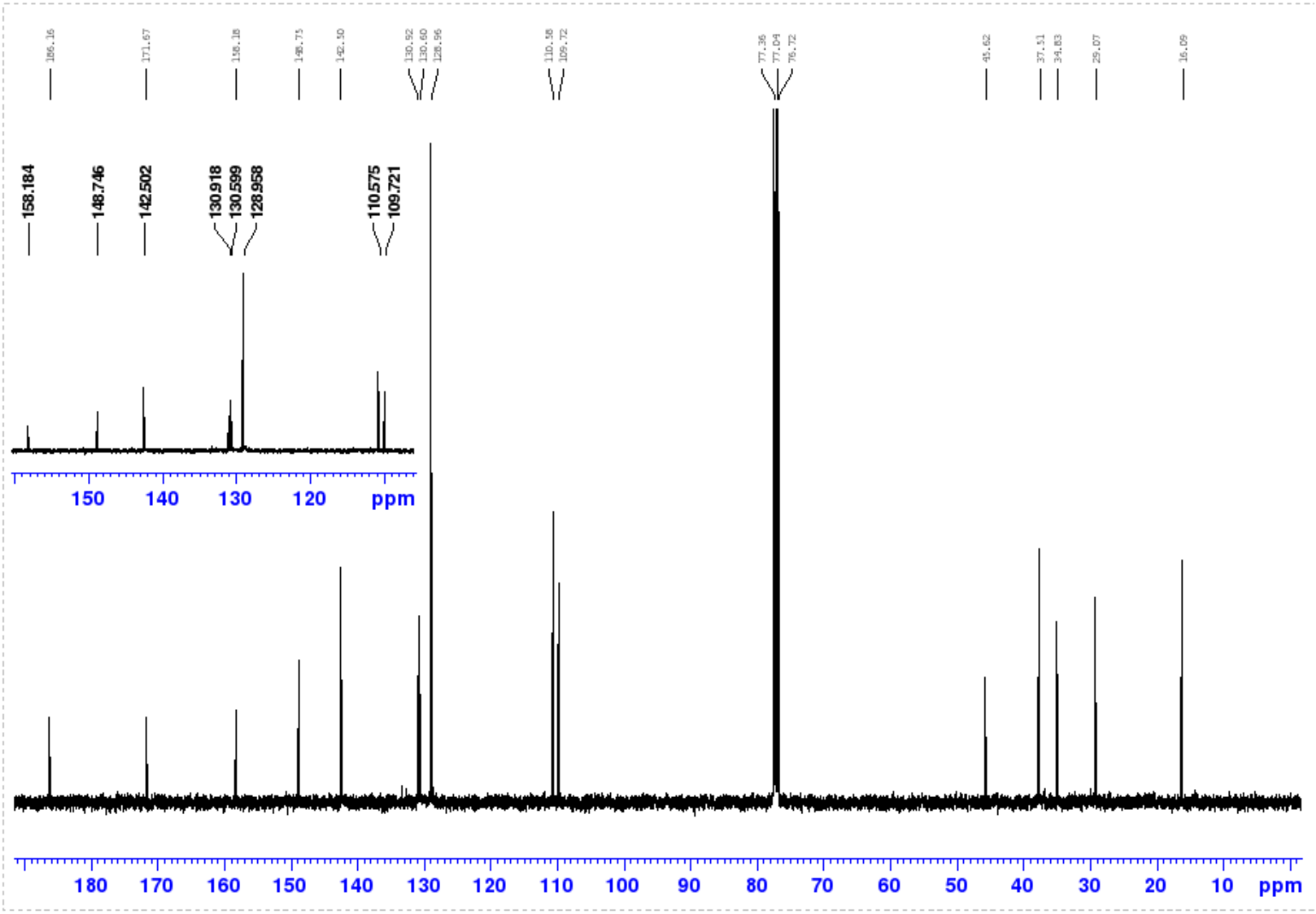




^{13}C NMR spectrum of 2s (100 MHz, $CDCl_3$)



1-methyl-6-phenyl-3-(thiophen-3-ylmethyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2s

Qualitative Compound Report

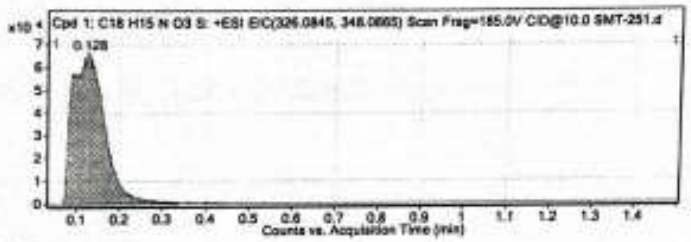
Data File	SMT-251.d	Sample Name	SMT-251
Sample Type	Sample	Position	P1-B8
Instrument Name	Instrument 1	User Name	
Acq Method	HS Scan.m	Acquired Time	22-05-2023 14:52:49
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

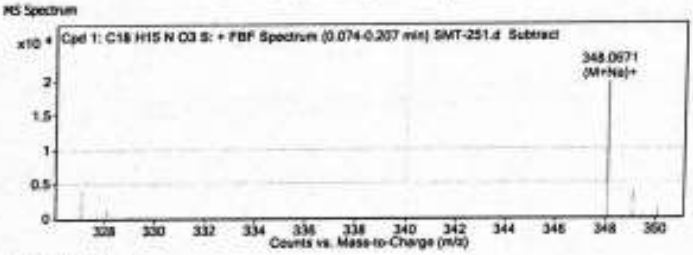
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	HFG Formula	DB Formula
Cpd 1: C18 H15 N O3 S	0.128	325.0778	21176	C18 H15 N O3 S	325.0773	1.61	C18 H15 N O3 S	C18 H15 N O3 S

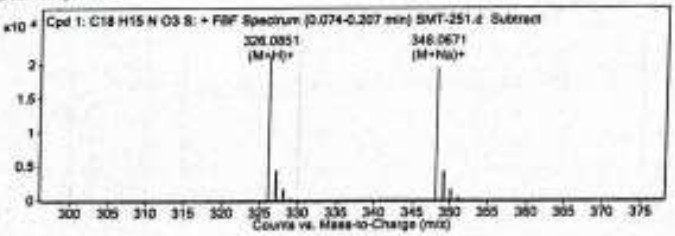
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H15 N O3 S	326.0851	0.128	Find By Formula	325.0778



MS Spectrum



MS Zoomed Spectrum

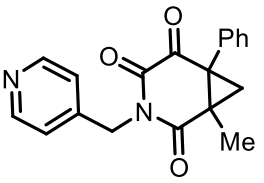


MS Spectrum Peak List

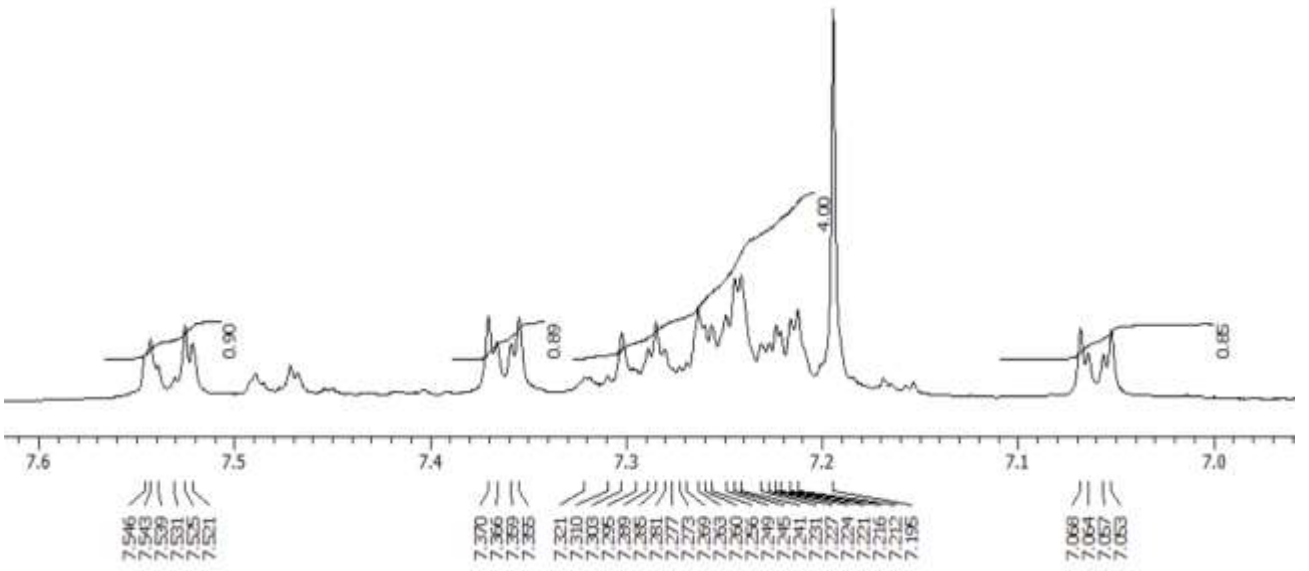
m/z	z	Abund	Formula	Ion
326.0851	1	21175.79	C18H16NO3S	(M+H)+
327.0879	1	4072.82	C18H16NO3S	(M+H)+
328.0846	1	1352.05	C18H16NO3S	(M+H)+
329.0864	1	211.24	C18H16NO3S	(M+H)+
348.0671	1	19646.03	C18H15NNaO3S	(M+Na)+
349.0699	1	3813.65	C18H15NNaO3S	(M+Na)+
350.0673	1	1202.58	C18H15NNaO3S	(M+Na)+
351.0691	1	186.7	C18H15NNaO3S	(M+Na)+

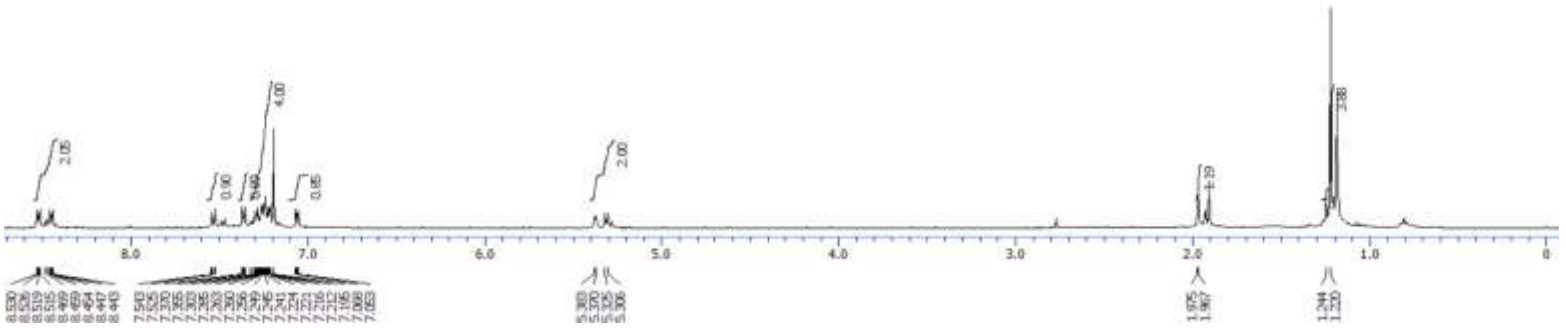
— End Of Report —

^{1}H NMR spectrum of 2t (400 MHz, $CDCl_3$)

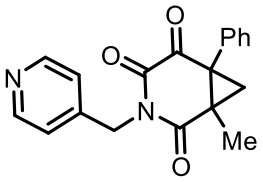


1-methyl-6-phenyl-3-(pyridin-4-ylmethyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

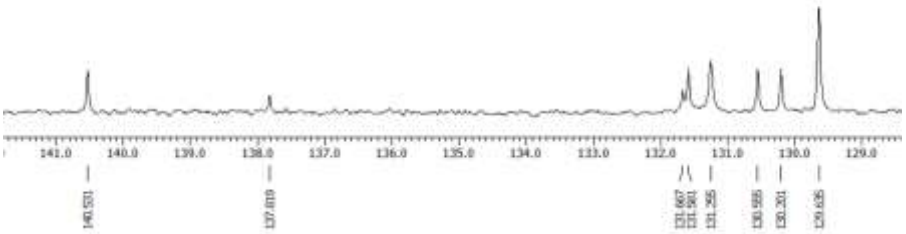


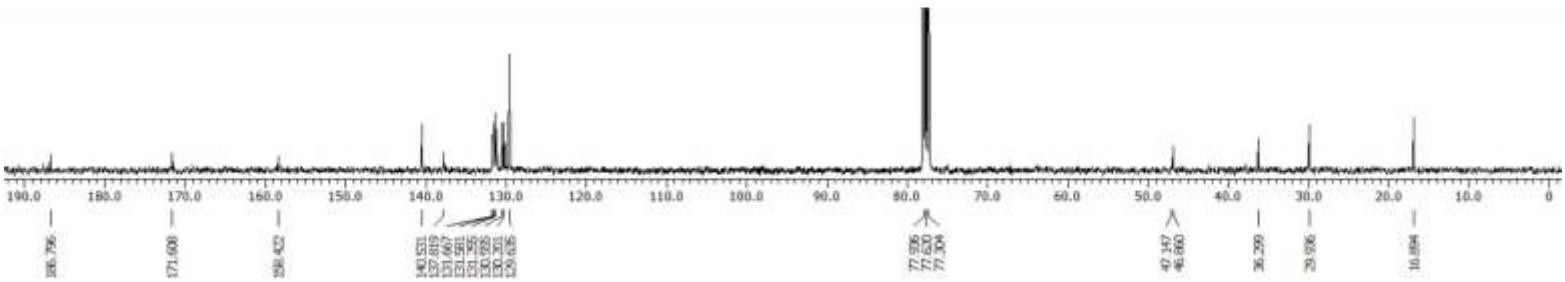


^{13}C NMR spectrum of 2t (100 MHz, $CDCl_3$)

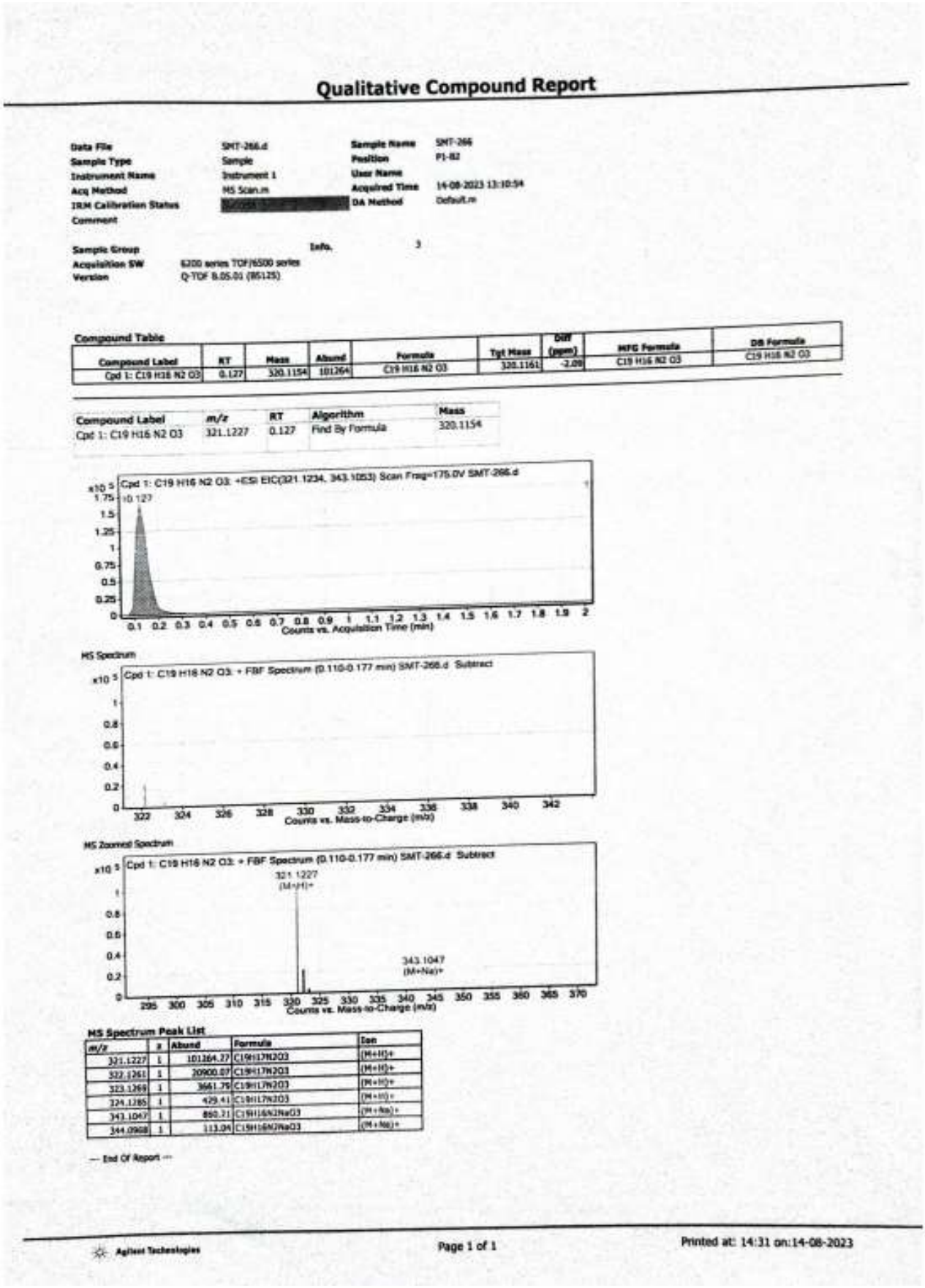


1-methyl-6-phenyl-3-(pyridin-4-ylmethyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 2t



Qualitative Compound Report

Data File SMT-266.d
Sample Type Sample
Instrument Name Instrument 1
Acq Method MS Scan.m
IRM Calibration Status [redacted]
Comment

Sample Name SMT-266
Position P1-B2
User Name
Acquired Time 14-08-2023 13:10:54
DA Method Default.m

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: C19 H16 N2 O3	0.127	320.1154	101364	C19 H16 N2 O3	320.1161	-2.08	C19 H16 N2 O3	C19 H16 N2 O3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H16 N2 O3	321.1227	0.127	Find By Formula	320.1154

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
321.1227	1	101364.27	C19H17N2O3	(M+H)+
322.1261	1	20900.07	C19H17N2O3	(M+H)+
323.1269	1	3661.75	C19H17N2O3	(M+H)+
324.1285	1	429.41	C19H17N2O3	(M+H)+
343.1047	1	860.71	C19H16N2NaO3	(M+Na)+
344.0968	1	113.04	C19H16N2NaO3	(M+Na)+

--- End Of Report ---

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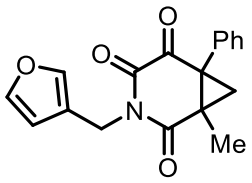
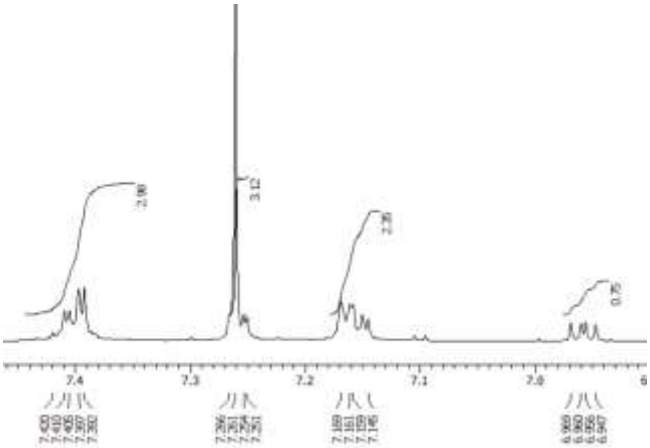
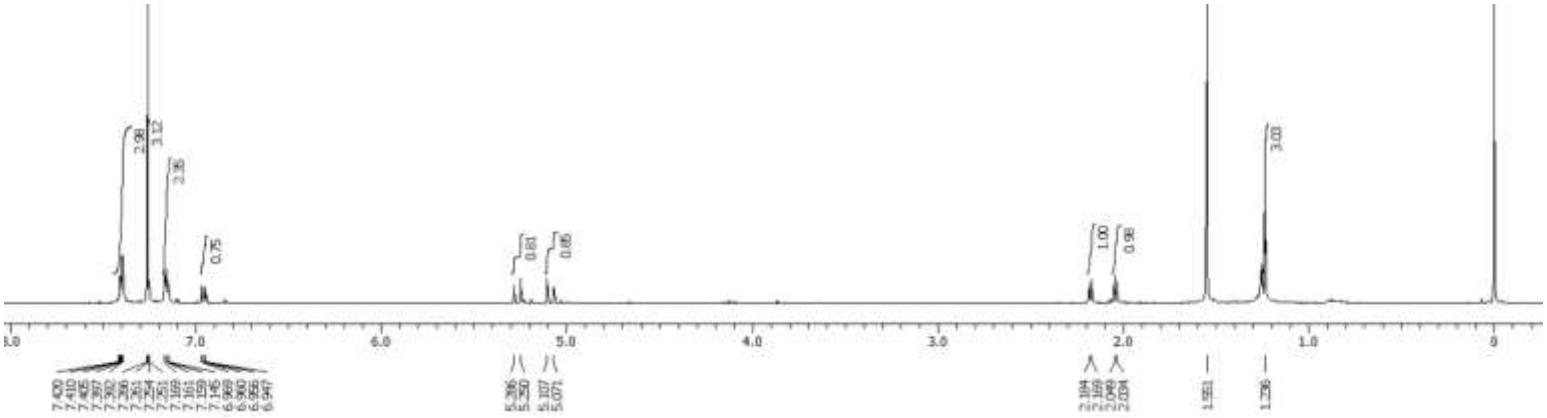
^{1}H NMR spectrum of 2u (400 MHz, $CDCl_3$)

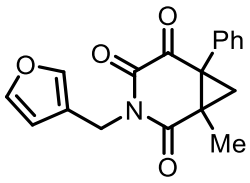


3-(furan-3-ylmethyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

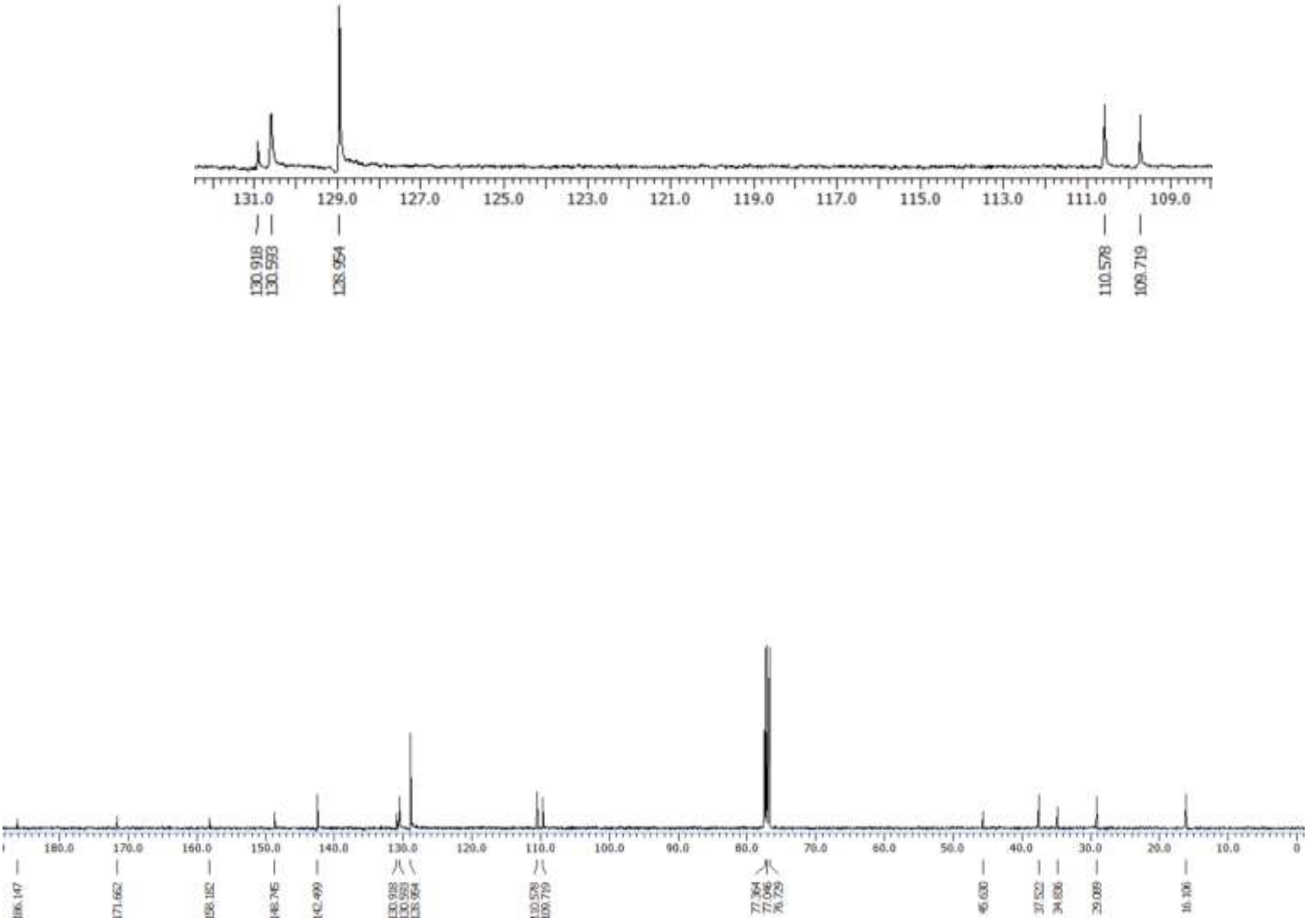




^{13}C NMR spectrum of 2u (100 MHz, $CDCl_3$)



3-(furan-3-ylmethyl)-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2u

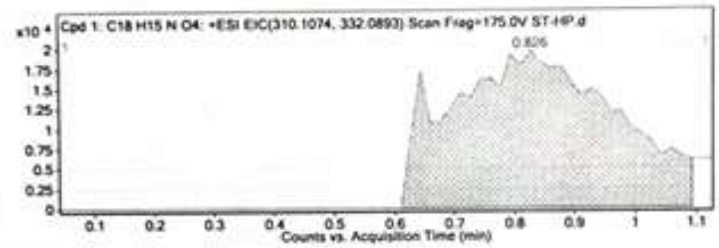
Qualitative Compound Report

Data File	ST-HP.d	**Sample Name**	ST-HP
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	11-05-2024 12:51:32
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)		

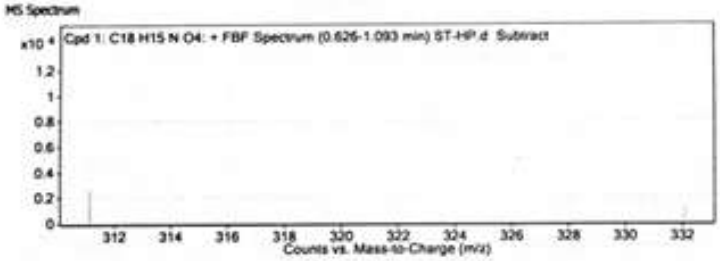
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C18 H15 N O4	0.826	309.1015	11735	C18 H15 N O4	309.1001	4.37	C18 H15 N O4	C18 H15 N O4

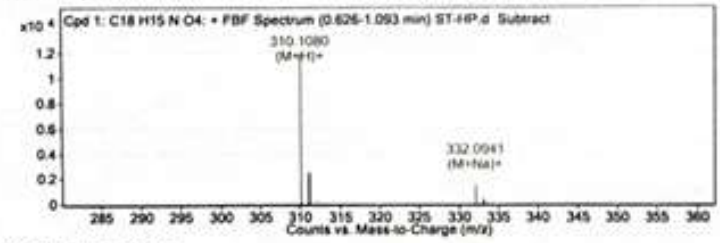
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H15 N O4	310.108	0.826	Find By Formula	309.1015



MS Spectrum



MS Zoomed Spectrum

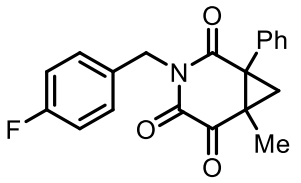


MS Spectrum Peak List

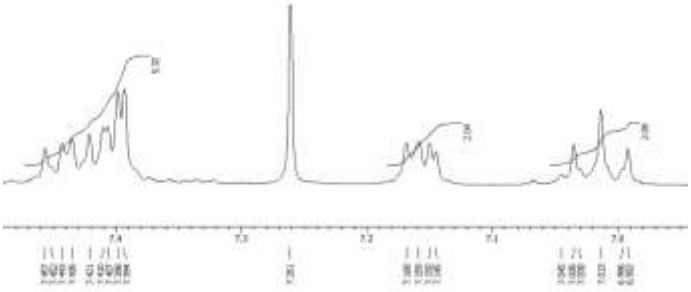
m/z	z	Abund	Formula	Ion
310.108	1	11734.58	C18H16NO4	(M+H)+
311.1121	1	2620.15	C18H16NO4	(M+H)+
332.0941	1	1336.19	C18H15NNaO4	(M+Na)+
333.1021	1	495.89	C18H15NNaO4	(M+Na)+

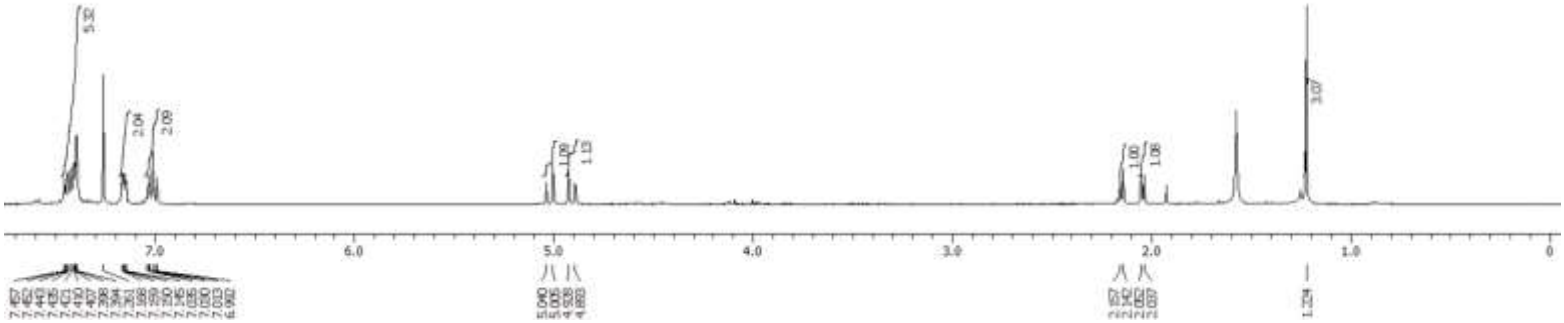
— End Of Report —

^{1}H NMR spectrum of 2v (400 MHz, $CDCl_3$)

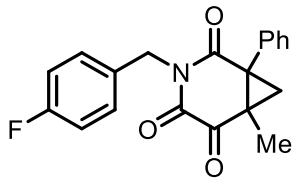


3-(4-fluorobenzyl)-6-methyl-1-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

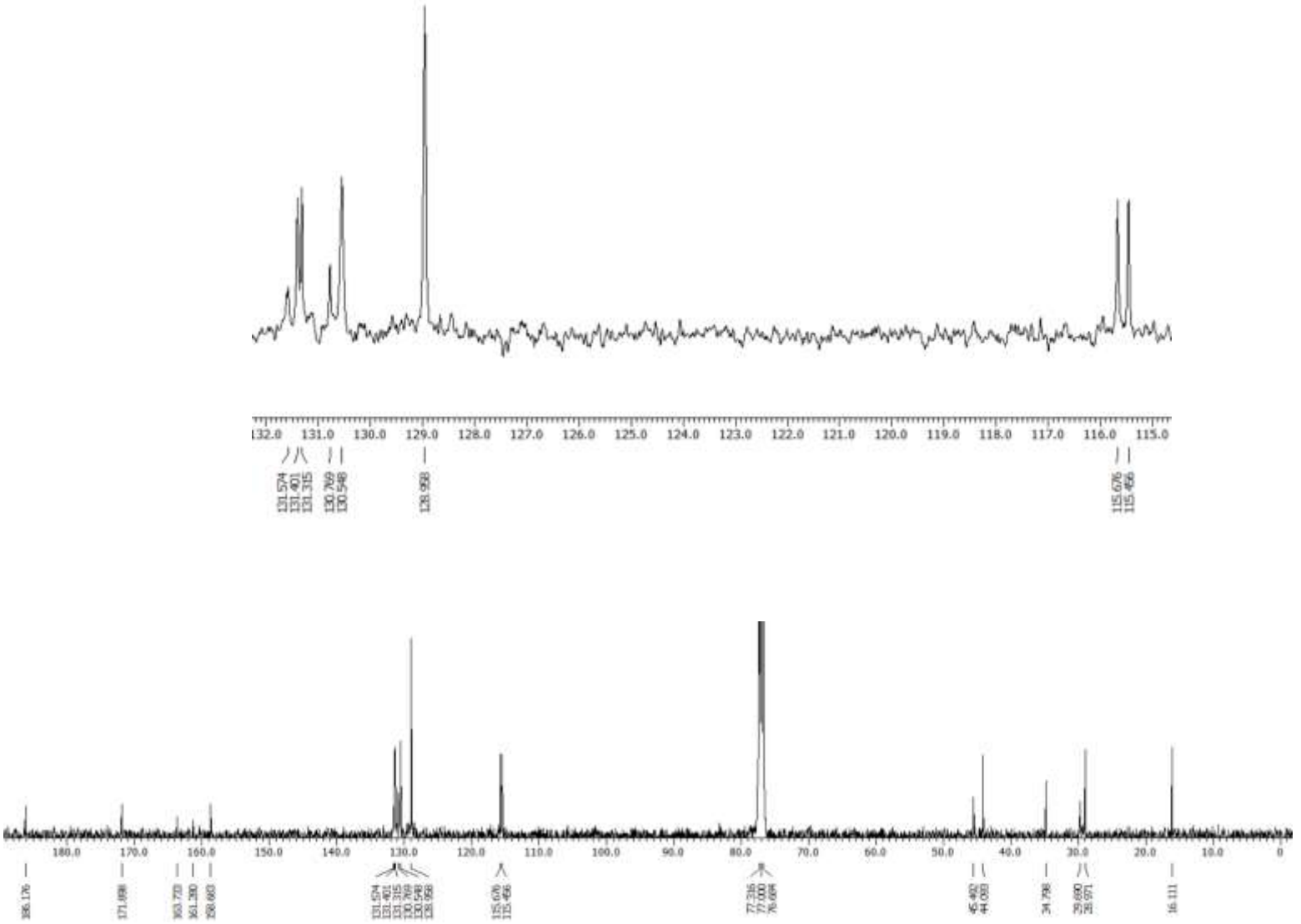




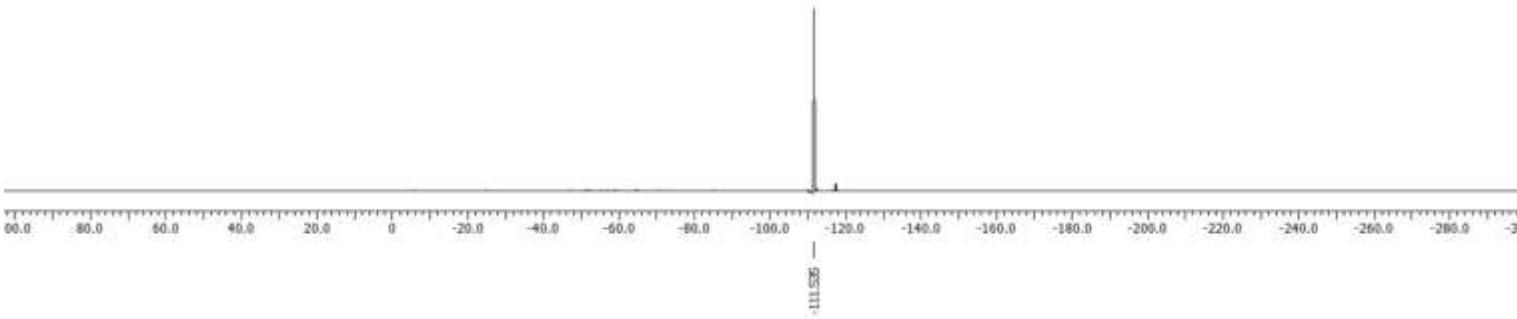
^{13}C NMR spectrum of 2v (100 MHz, $CDCl_3$)



3-(4-fluorobenzyl)-6-methyl-1-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



^{19}F NMR spectrum of 2v (376 MHz, CDCl3)



HRMS spectrum of 2v

Qualitative Compound Report

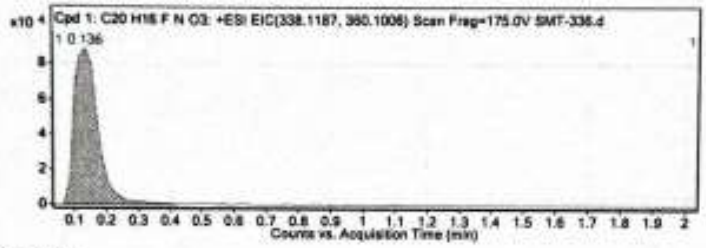
Data File	SMT-336.d	**Sample Name**	SMT-336
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	09-10-2023 13:07:50
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

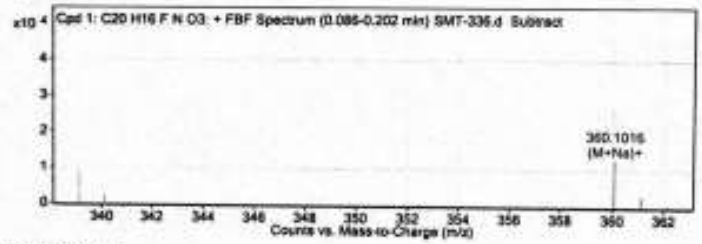
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H16 F N O3	0.136	337.1103	13000	C20 H16 F N O3	337.1114	-3.24	C20 H16 F N O3	C20 H16 F N O3

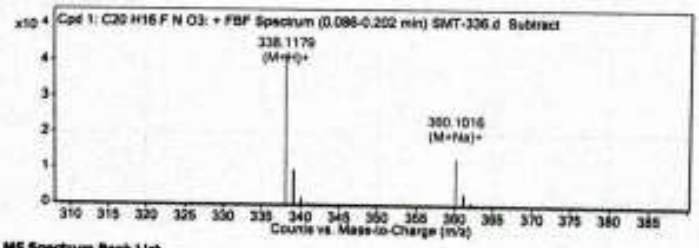
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H16 F N O3	360.1016	0.136	Find By Formula	337.1103



MS Spectrum



MS Zoomed Spectrum

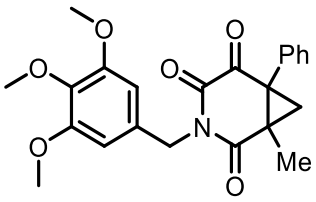


MS Spectrum Peak List

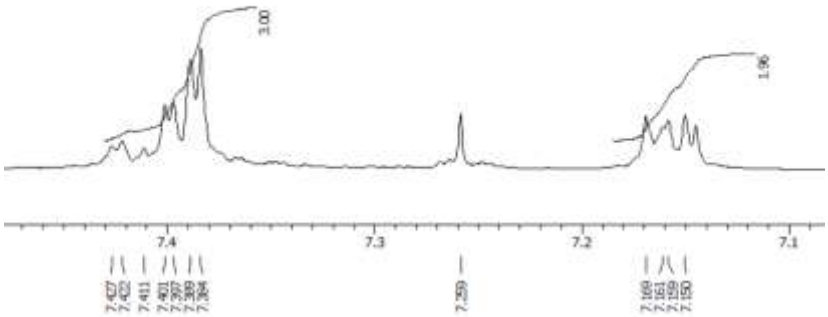
m/z	z	Abund	Formula	Ion
338.1179	1	40890.29	C20H17FNO3	(M+H)+
339.1211	1	9365.87	C20H17FNO3	(M+H)+
340.1045	1	2473.36	C20H17FNO3	(M+H)+
341.1051	1	377.79	C20H17FNO3	(M+H)+
360.1016	1	12999.96	C20H16FNNaO3	(M+Na)+
361.1067	1	3045.46	C20H16FNNaO3	(M+Na)+
362.1113	1	526.55	C20H16FNNaO3	(M+Na)+
363.108	1	92.41	C20H16FNNaO3	(M+Na)+

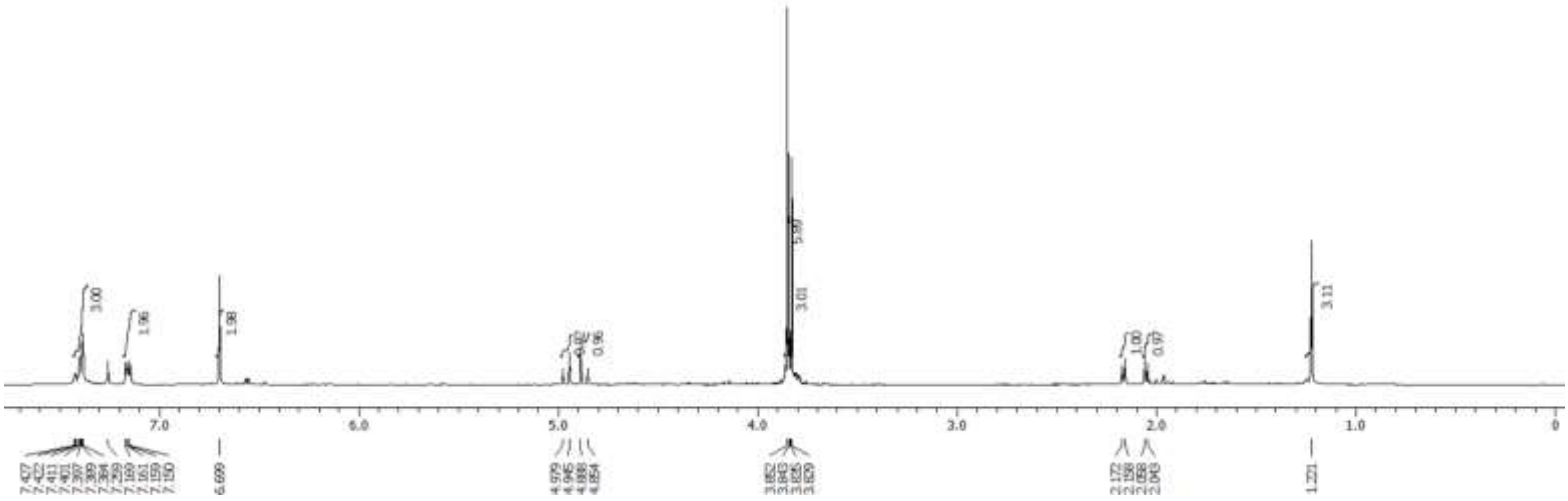
--- End Of Report ---

^{1}H NMR spectrum of 2w (400 MHz, $CDCl_3$)

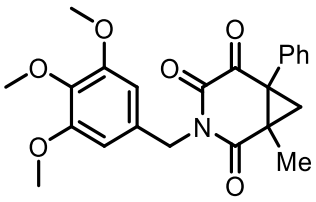


1-methyl-6-phenyl-3-(3,4,5-trimethoxybenzyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

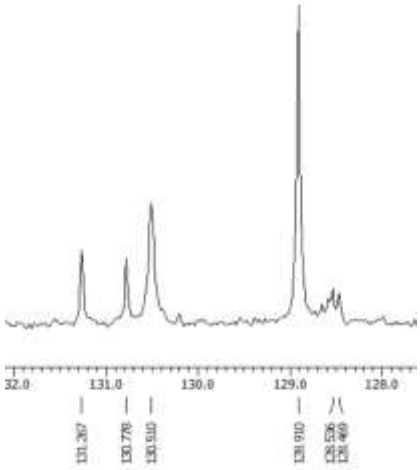


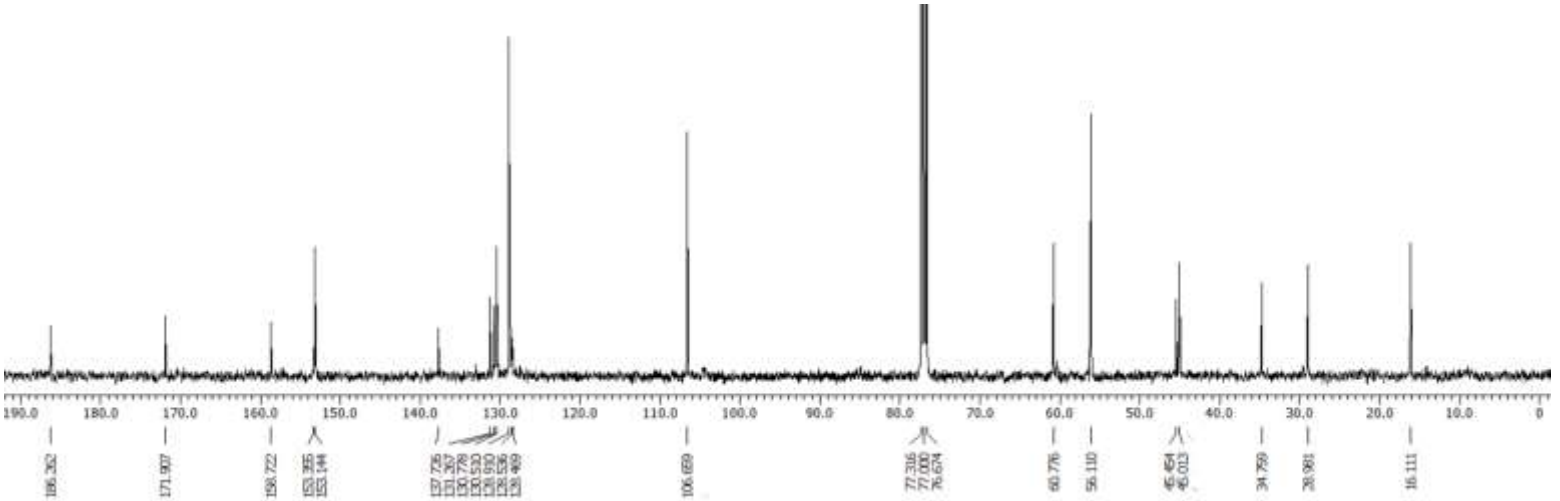


^{13}C NMR spectrum of 2w (100 MHz, $CDCl_3$)



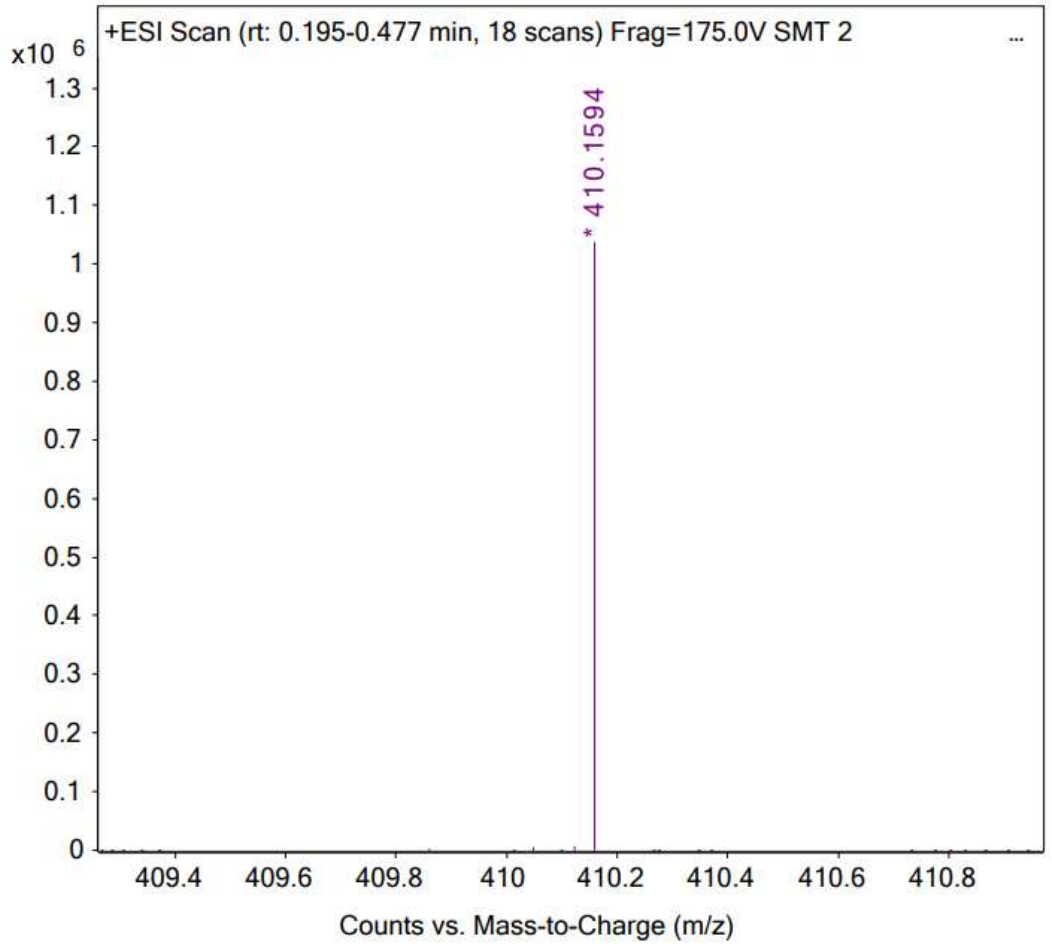
1-methyl-6-phenyl-3-(3,4,5-trimethoxybenzyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione



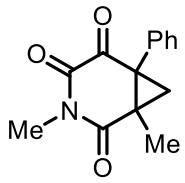


HRMS spectrum of 2w

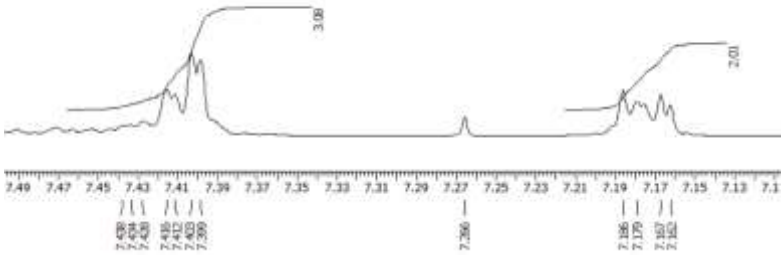
Sample Name	SMT 286	**Position**	P1-B10	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 286.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:58:07 (UTC+05:30)

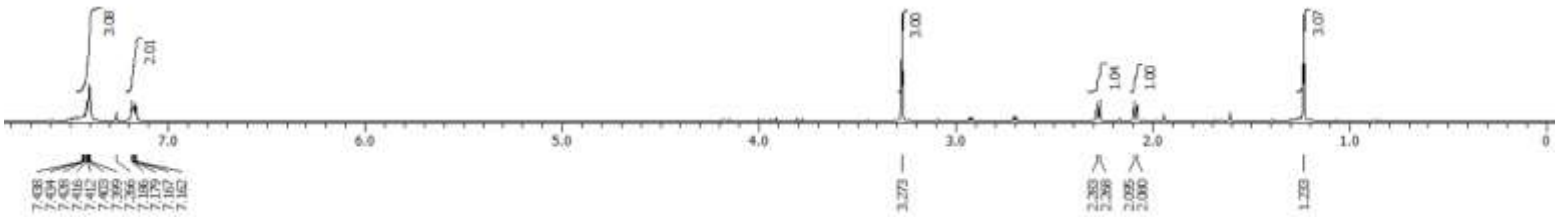


^{1}H NMR spectrum of 2x (400 MHz, $CDCl_3$)

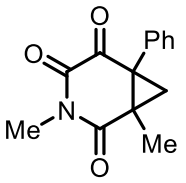


1,3-dimethyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

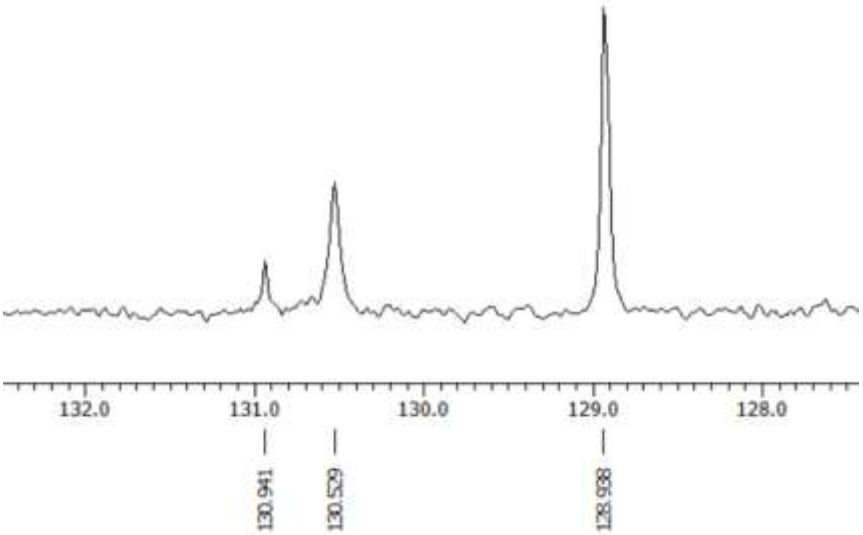


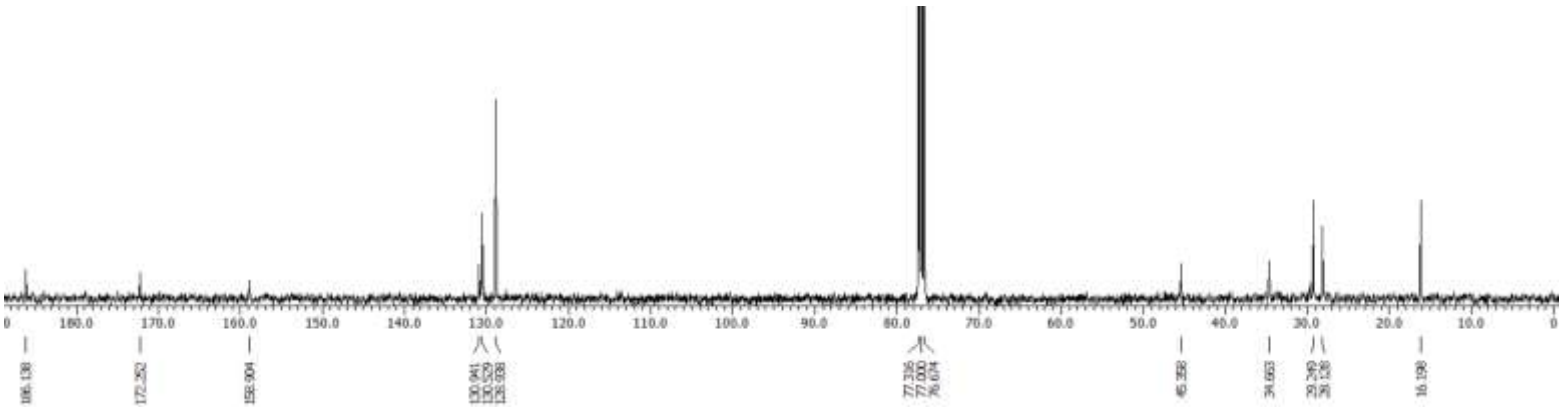


^{13}C NMR spectrum of 2x (100 MHz, $CDCl_3$)

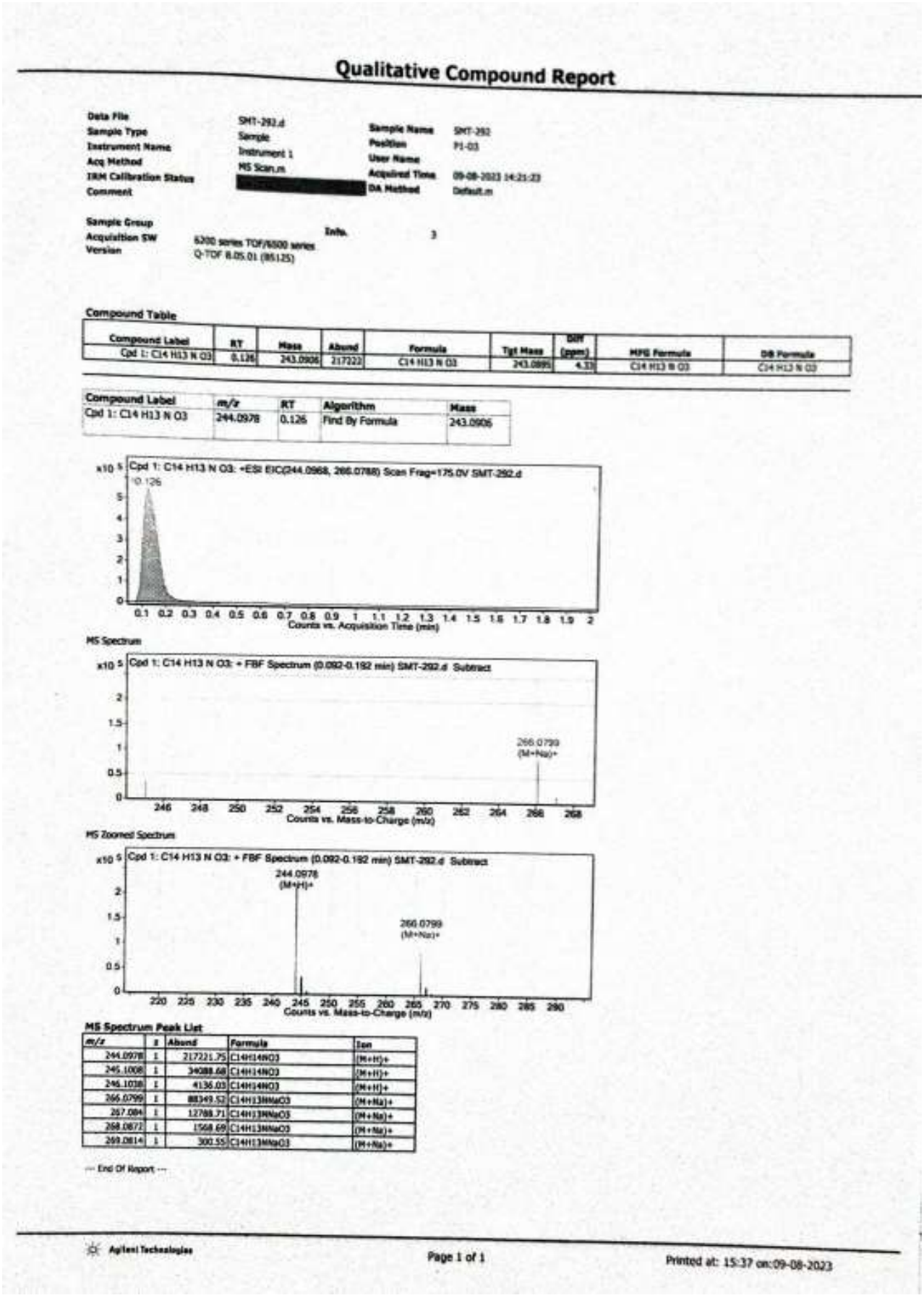


1,3-dimethyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 2x



Qualitative Compound Report

Data File SMT-292.d
Sample Type Sample
Instrument Name Instrument 1
Acq Method MS Scan.m
IRM Calibration Status [redacted]
Comment

Sample Name SMT-292
Position P1-D3
User Name
Acquired Time 09-08-2023 14:21:23
DA Method Default.m

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

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	DiffM (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H13 N O3	0.126	243.0906	217221	C14 H13 N O3	243.0895	4.33	C14 H13 N O3	C14 H13 N O3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C14 H13 N O3	244.0978	0.126	Find By Formula	243.0906

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
244.0978	1	217221.75	C14H14NO3	(M+H)+
245.1008	1	34088.68	C14H14NO3	(M+H)+
246.1038	1	4136.03	C14H14NO3	(M+H)+
266.0799	1	88349.52	C14H13NNaO3	(M+Na)+
267.084	1	12788.71	C14H13NNaO3	(M+Na)+
268.0872	1	1568.69	C14H13NNaO3	(M+Na)+
269.0814	1	300.55	C14H13NNaO3	(M+Na)+

--- End Of Report ---

Agilent Technologies

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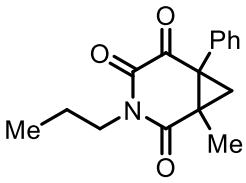
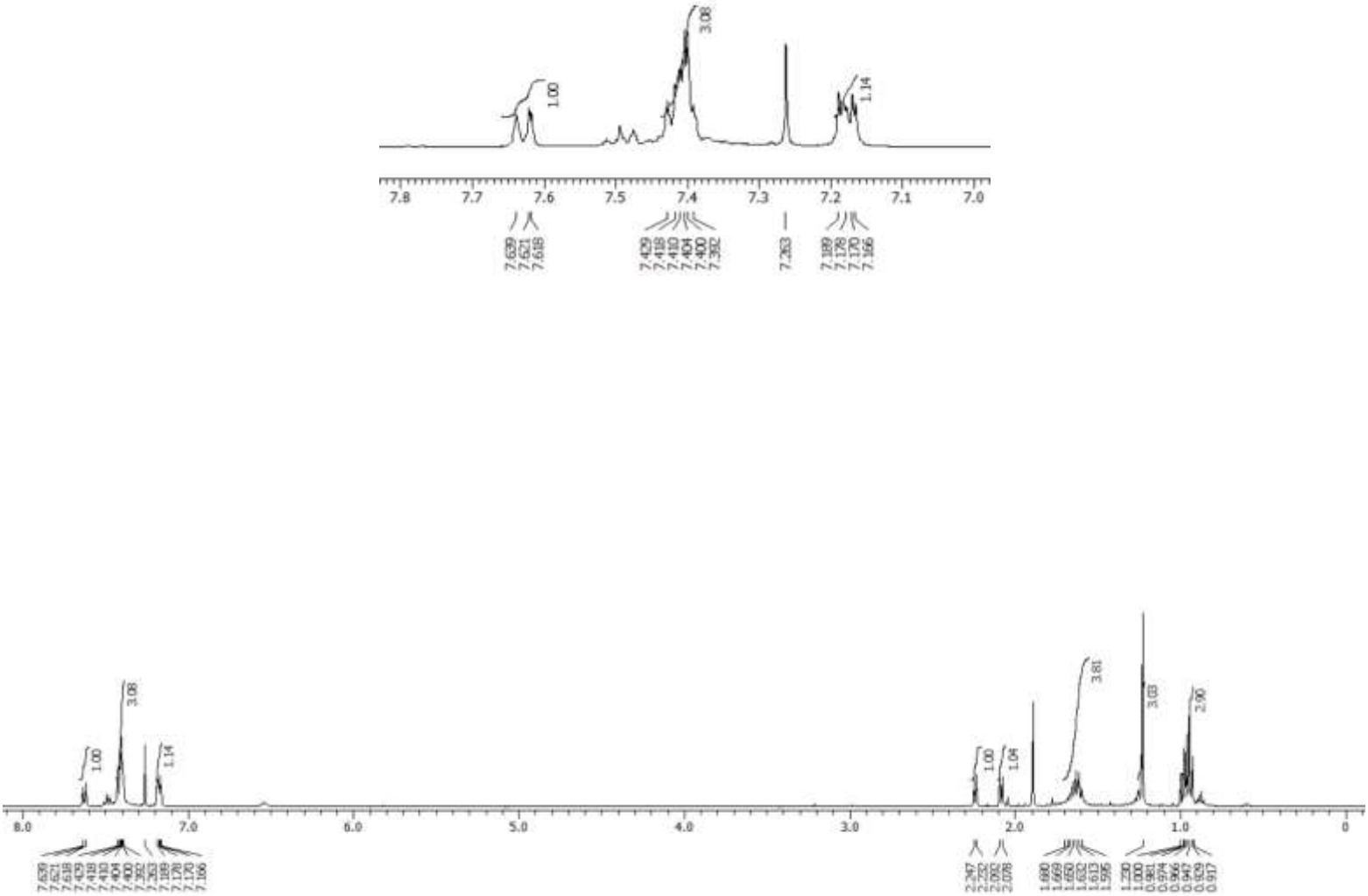
Printed at: 15:37 on:09-08-2023

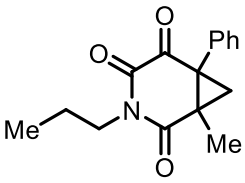
^{1}H NMR spectrum of 2y (400 MHz, $CDCl_3$)



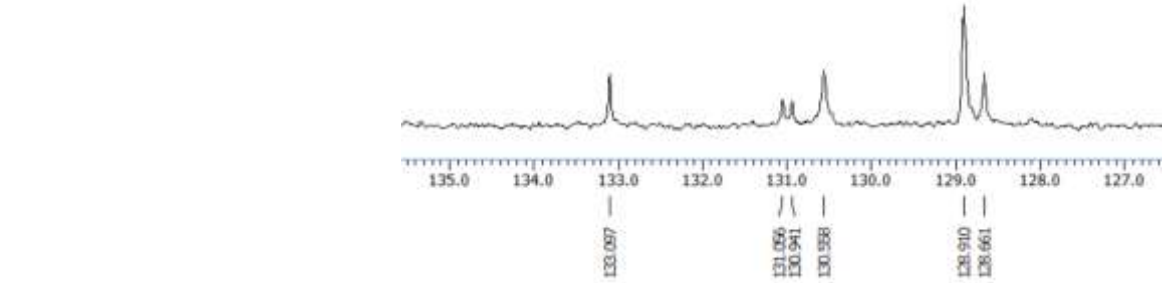
1-methyl-6-phenyl-3-propyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

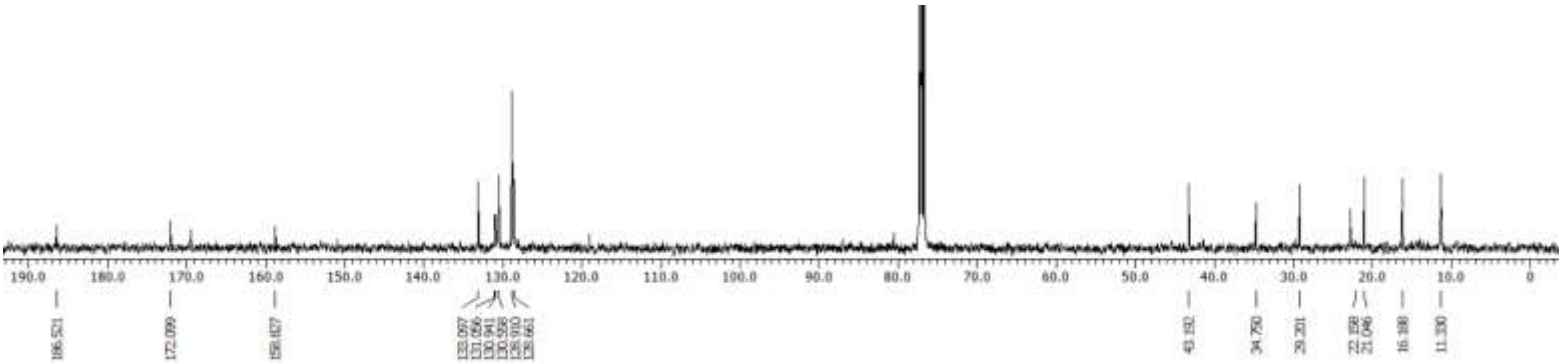


^{13}C NMR spectrum of 2y (100 MHz, $CDCl_3$)



1-methyl-6-phenyl-3-propyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 2y

Qualitative Compound Report

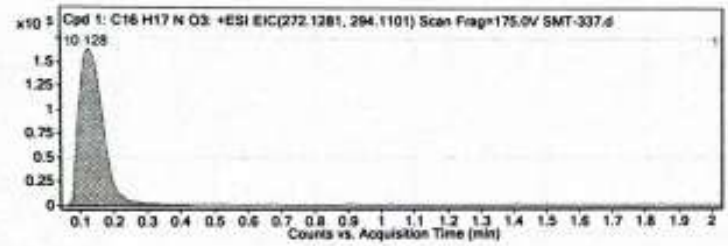
Data File	SMT-337.d	**Sample Name**	SMT-337
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	04-10-2023 13:07:59
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

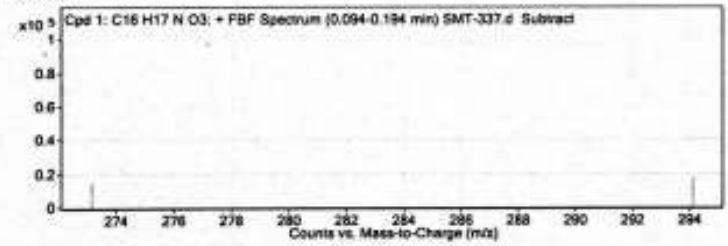
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C16 H17 N O3	0.128	271.1224	90017	C16 H17 N O3	271.1208	5.74	C16 H17 N O3	C16 H17 N O3

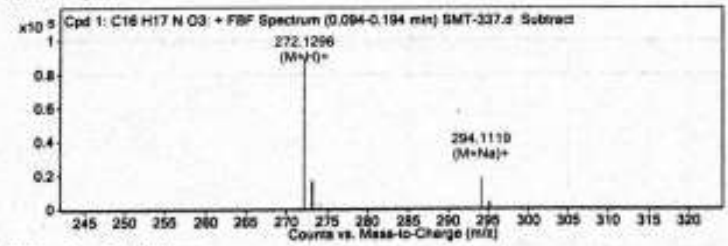
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C16 H17 N O3	272.1296	0.128	Find By Formula	271.1224



MS Spectrum



MS Zoomed Spectrum

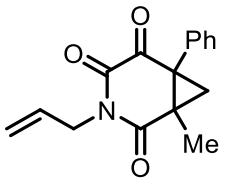


MS Spectrum Peak List

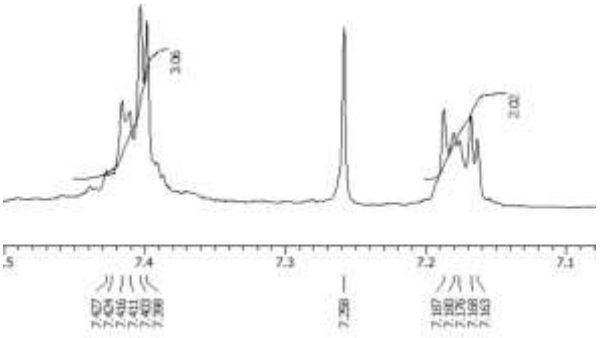
m/z	z	Abund	Formula	Ion
272.1296	1	90017.44	C16H18NO3	(M+H)+
273.133	1	15761.02	C16H18NO3	(M+H)+
294.1119	1	17787.05	C16H17NNaO3	(M+Na)+
295.1156	1	3542.04	C16H17NNaO3	(M+Na)+

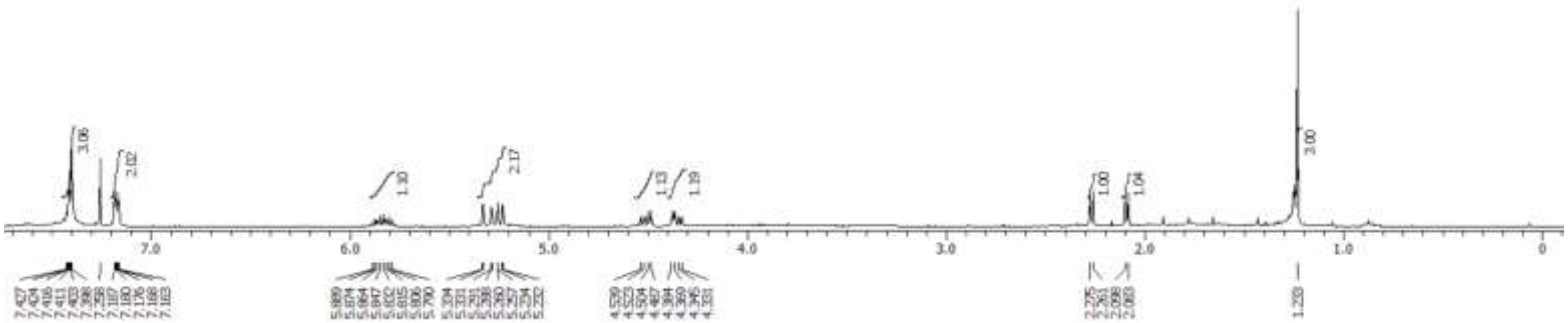
--- End Of Report ---

^{1}H NMR spectrum of 2z (400 MHz, $CDCl_3$)

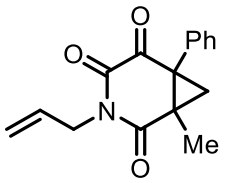


3-allyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

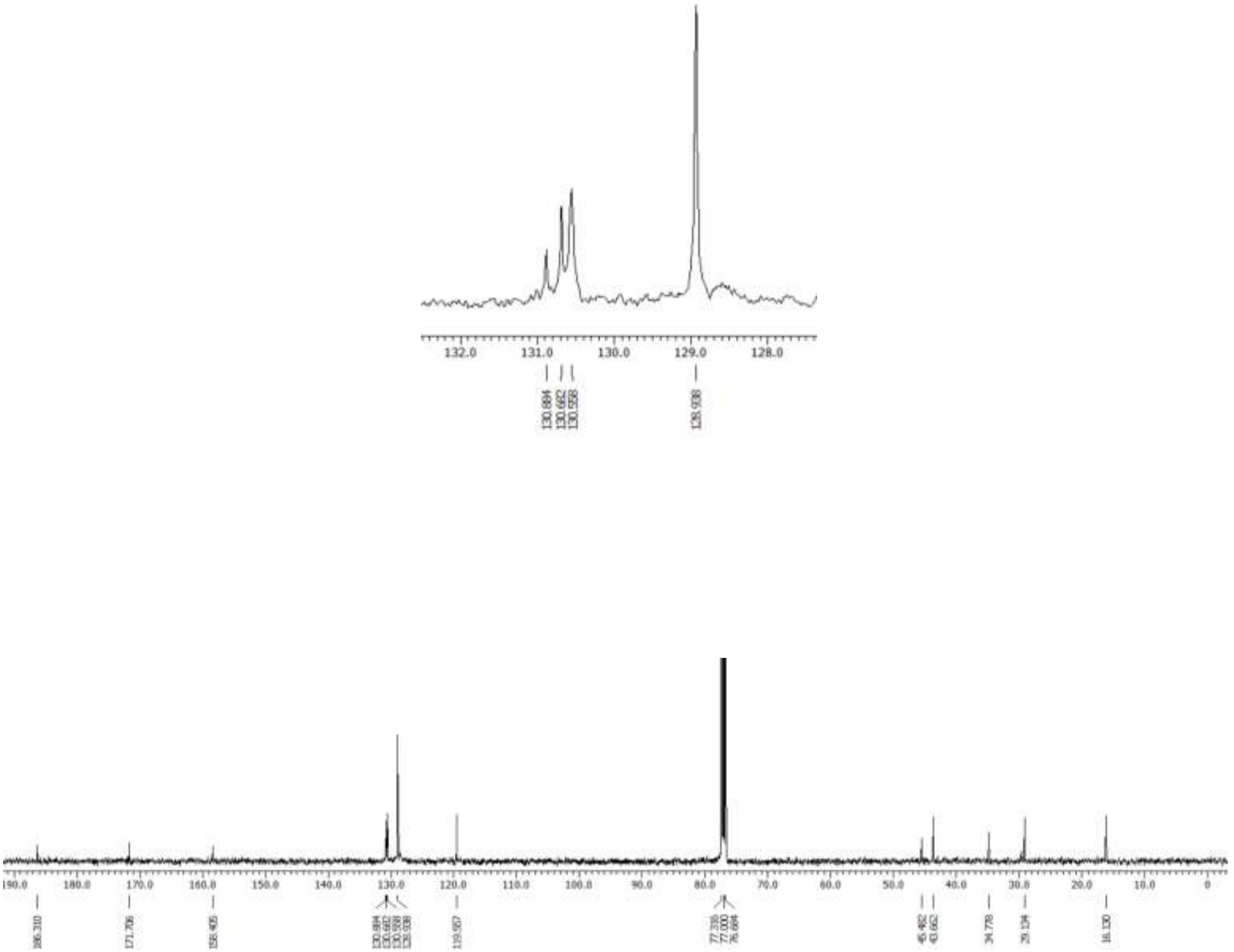




^{13}C NMR spectrum of 2z (100 MHz, $CDCl_3$)

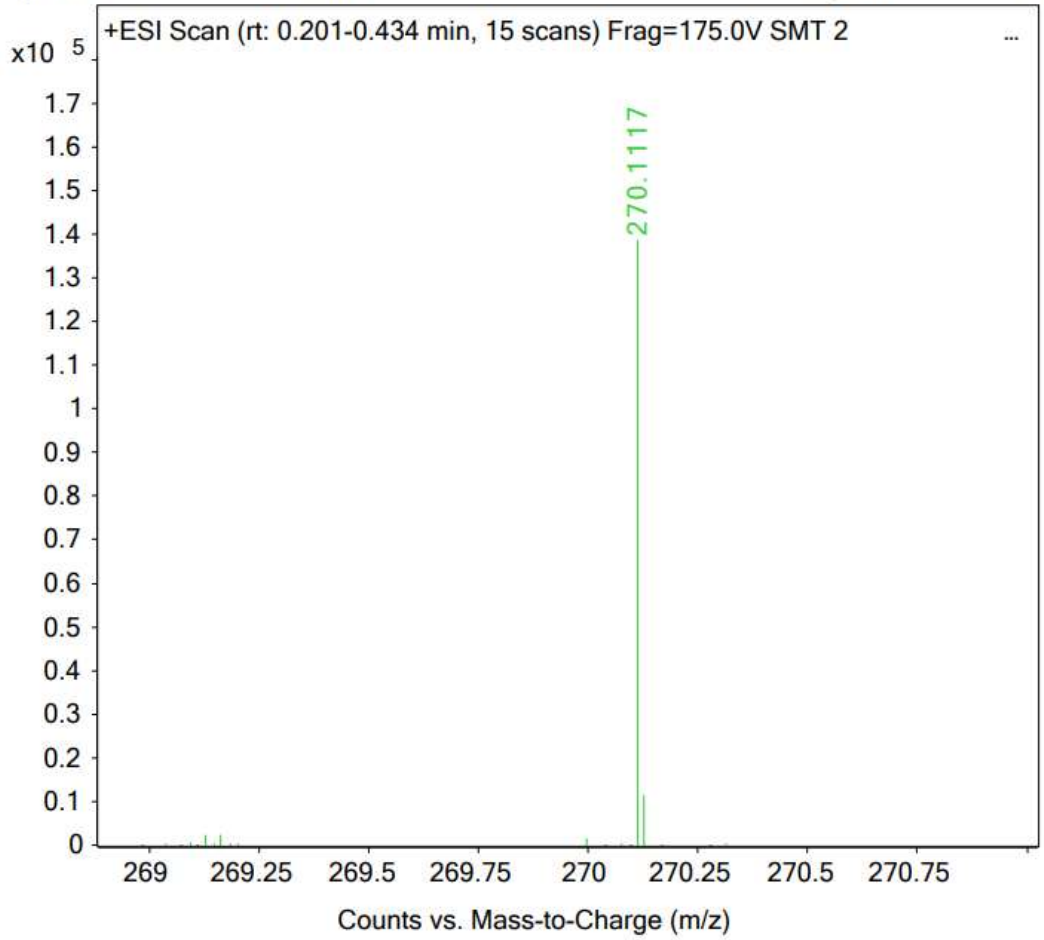


3-allyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

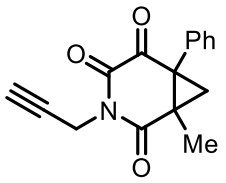


HRMS spectrum of 2z

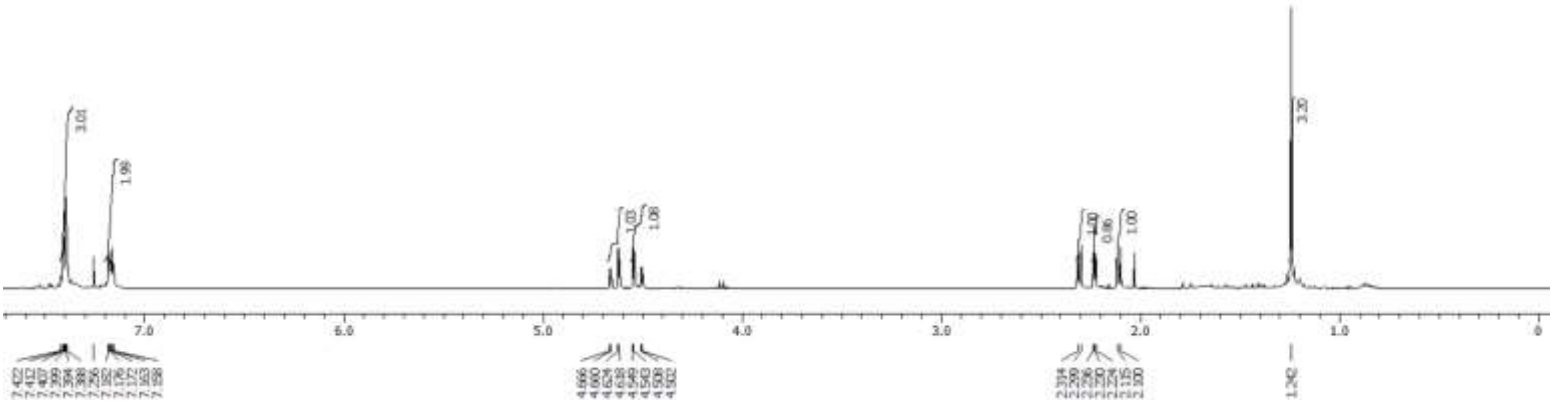
Sample Name	SMT 293	**Position**	P1-A11	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 293.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:19:28 (UTC+05:30)



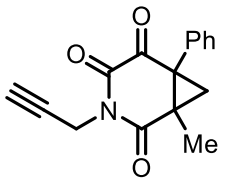
^{1}H NMR spectrum of 2aa (400 MHz, $CDCl_3$)



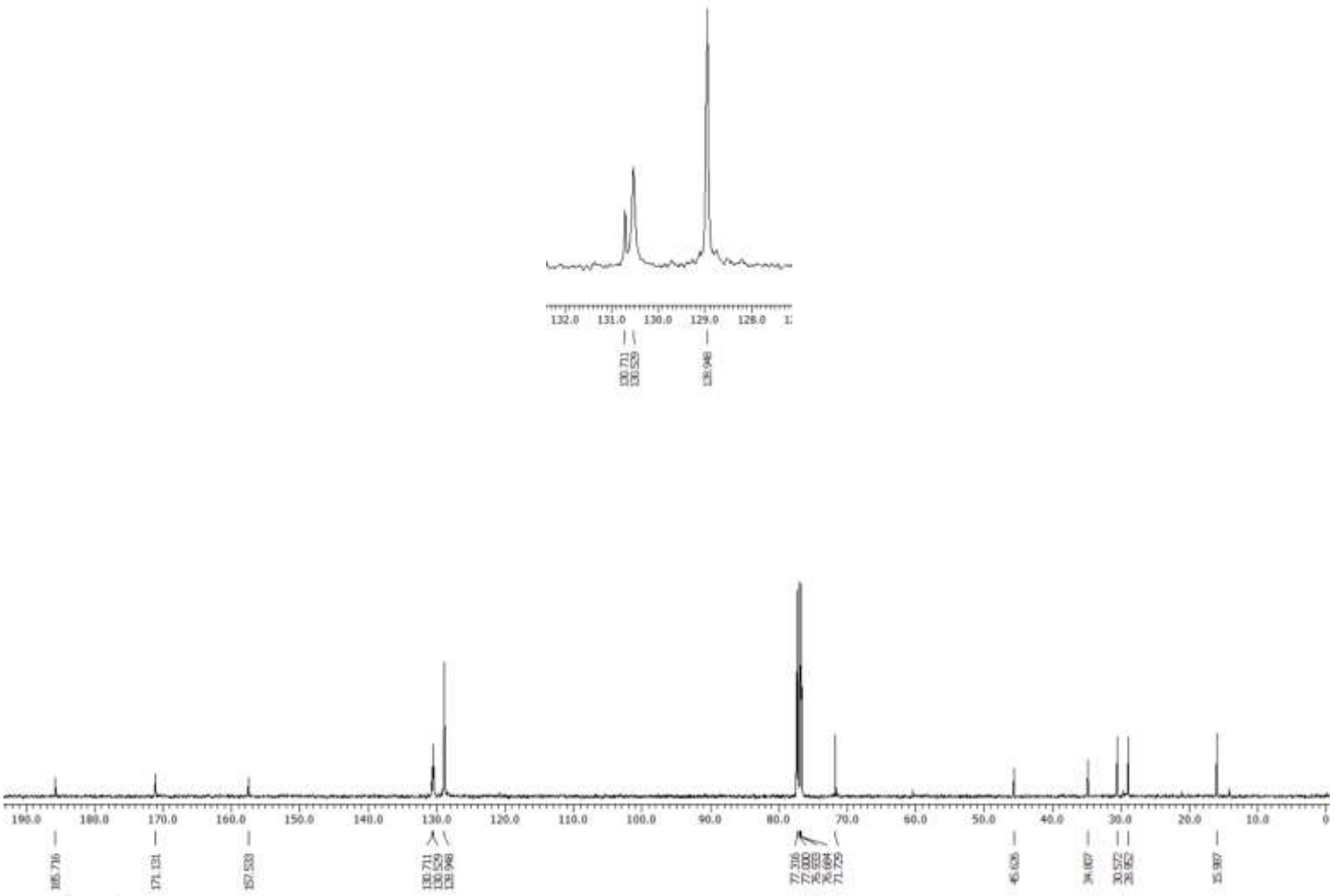
1-methyl-6-phenyl-3-(prop-2-yn-1-yl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione



^{13}C NMR spectrum of 2aa (100 MHz, $CDCl_3$)



1-methyl-6-phenyl-3-(prop-2-yn-1-yl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2aa

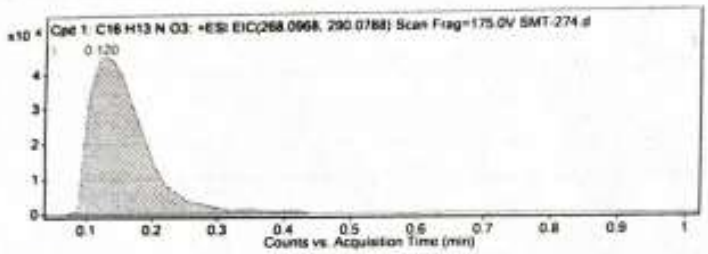
Qualitative Compound Report

Data File	SMT-274.d	**Sample Name**	SMT-274
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	24-02-2024 12:31:31
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	1
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

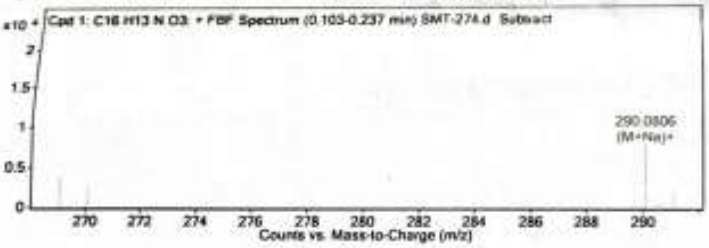
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C16 H13 N O3	0.12	267.0892	7720	C16 H13 N O3	267.0895	-1.28	C16 H13 N O3	C16 H13 N O3

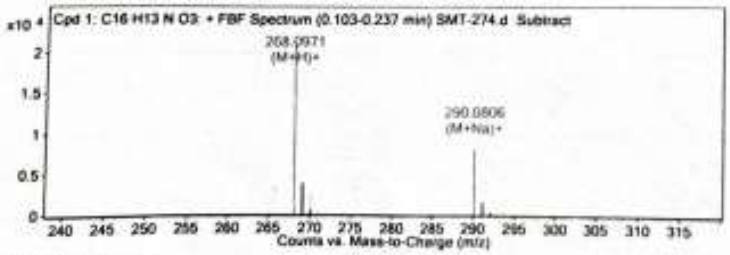
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C16 H13 N O3	290.0806	0.12	Find By Formula	267.0892



MS Spectrum



MS Zoomed Spectrum

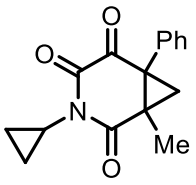


MS Spectrum Peak List

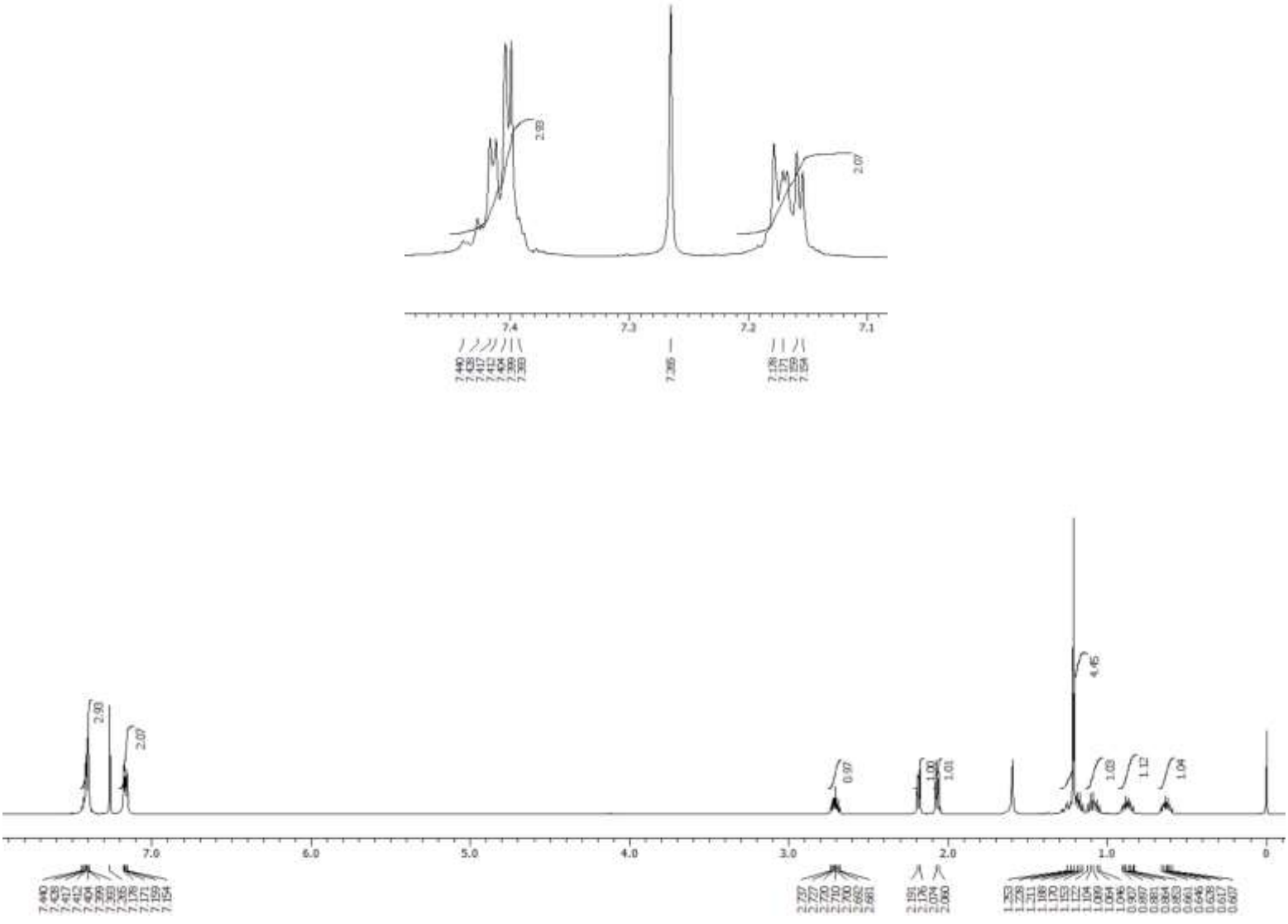
m/z	z	Abund	Formula	Ion
268.0971	1	19404.28	C16H14NO3	(M+H)+
269.0992	1	3859.24	C16H14NO3	(M+H)+
270.087	1	2420.91	C16H14NO3	(M+H)+
290.0806	1	7719.63	C16H13NNaO3	(M+Na)+
291.086	1	1756.64	C16H13NNaO3	(M+Na)+
292.09	1	349.7	C16H13NNaO3	(M+Na)+

--- End Of Report ---

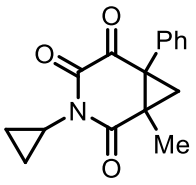
^{1}H NMR spectrum of 2ab (400 MHz, $CDCl_3$)



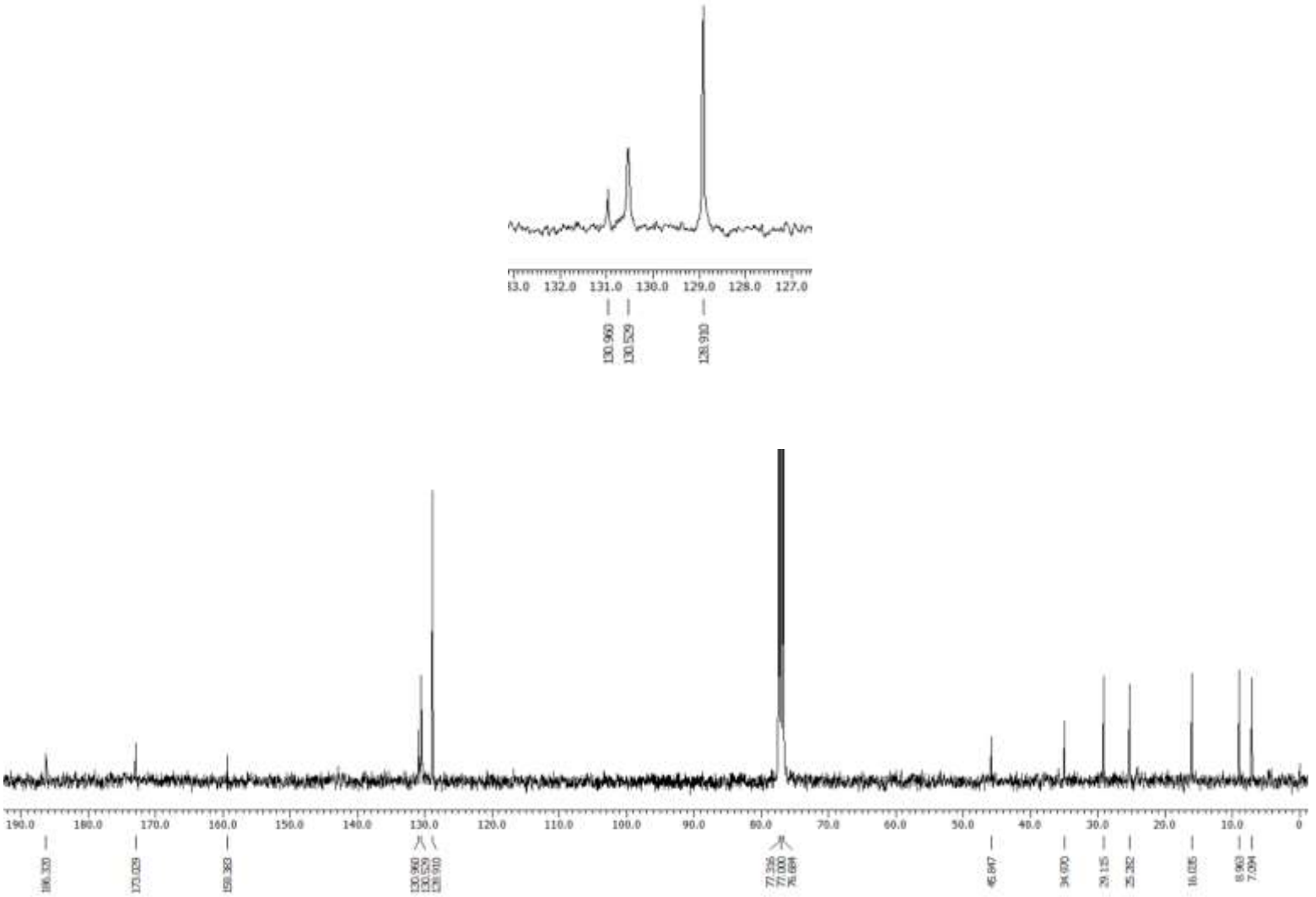
3-cyclopropyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



^{13}C NMR spectrum of 2ab (100 MHz, $CDCl_3$)



3-cyclopropyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2ab

Qualitative Compound Report

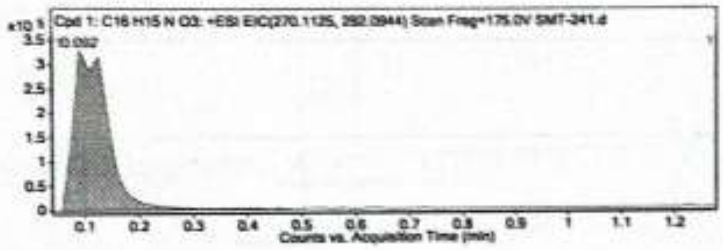
Data File	SMT-241.d	Sample Name	SMT-241
Sample Type	Sample	Position	P1-B4
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	22-07-2023 13:03:11
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

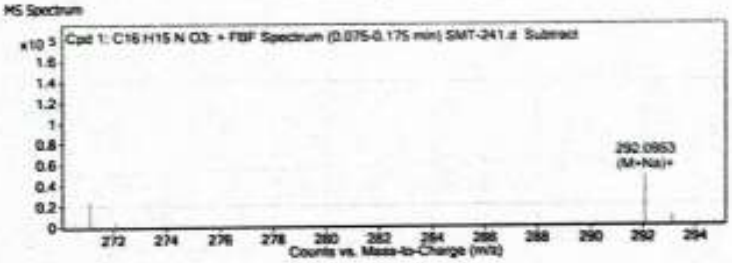
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFE Formula	DB Formula
Cpd 1: C16 H15 N O3	0.092	269.106	146165	C16 H15 N O3	269.1052	3.04	C16 H15 N O3	C16 H11 N O3

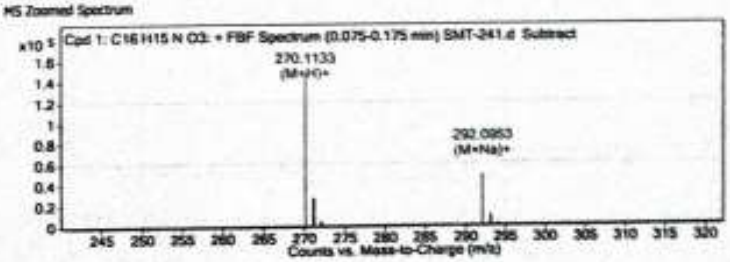
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C16 H15 N O3	270.1133	0.092	Find By Formula	269.106



MS Spectrum



MS Zoomed Spectrum

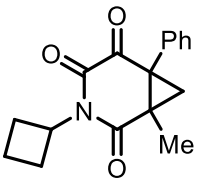


MS Spectrum Peak List

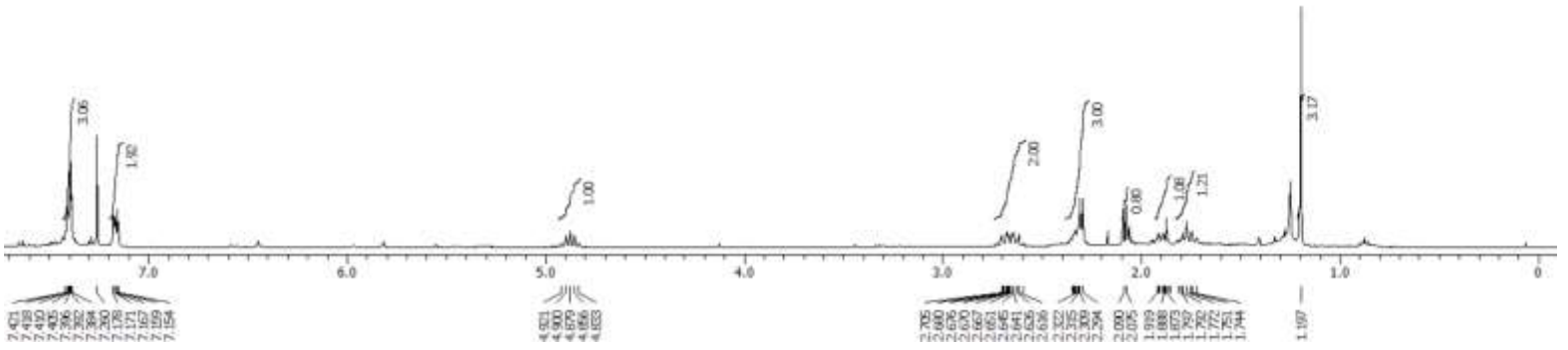
m/z	z	Abund	Formula	Ion
270.1133	1	146165.22	C16H16NO3	(M+H)+
271.1164	1	25012.88	C16H16NO3	(M+H)+
272.1196	1	3277.24	C16H16NO3	(M+H)+
292.0953	1	48354.04	C16H15NNaO3	(M+Na)+
293.0986	1	8668.77	C16H15NNaO3	(M+Na)+
294.102	1	1351.5	C16H15NNaO3	(M+Na)+
295.105	1	262	C16H15NNaO3	(M+Na)+

--- End Of Report ---

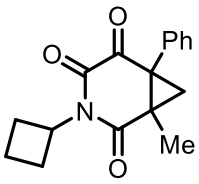
^{1}H NMR spectrum of 2ac (400 MHz, $CDCl_3$)



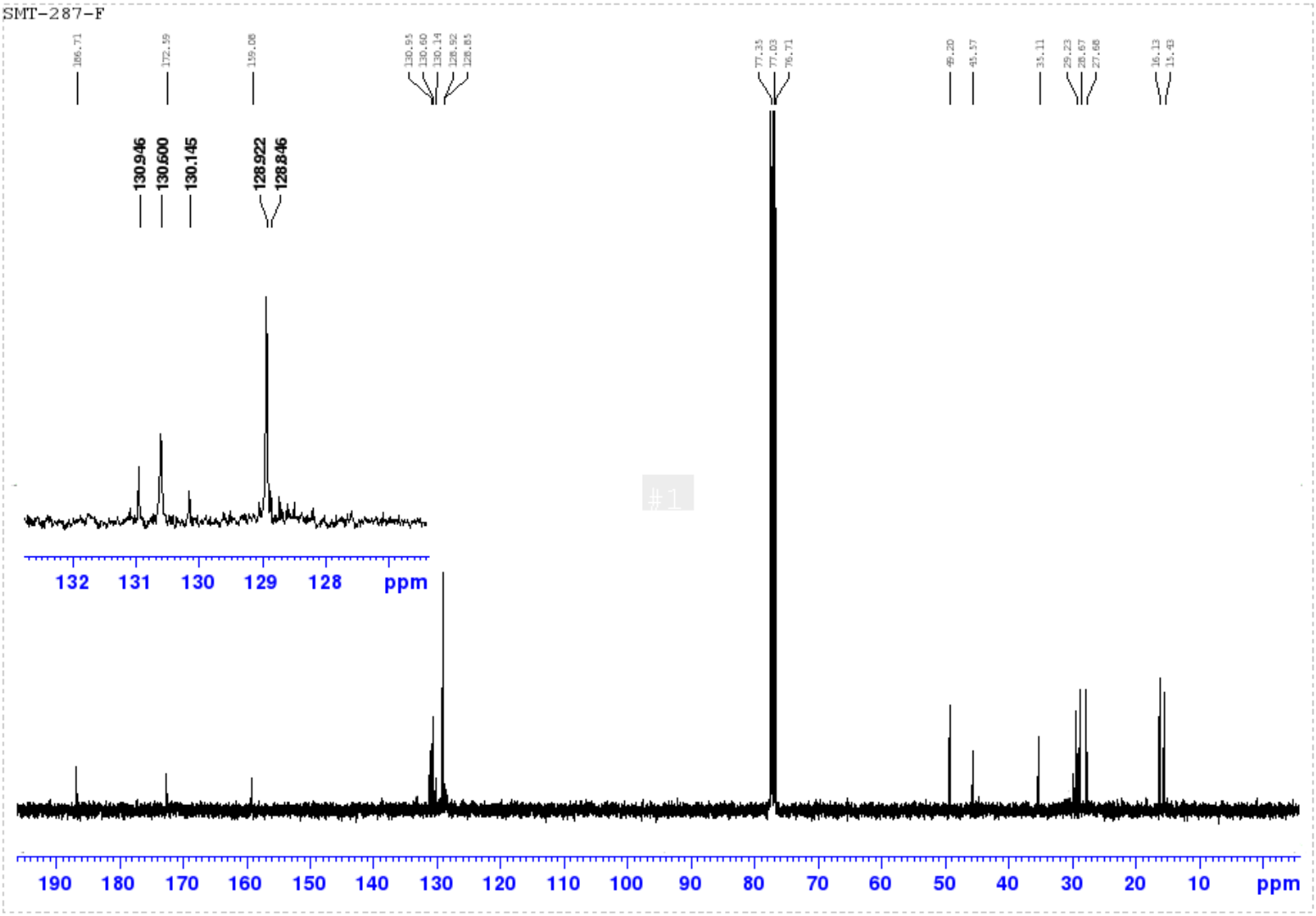
3-cyclobutyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



^{13}C NMR spectrum of 2ac (100 MHz, $CDCl_3$)



3-cyclobutyl-1-methyl-6-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 2ac

Qualitative Compound Report

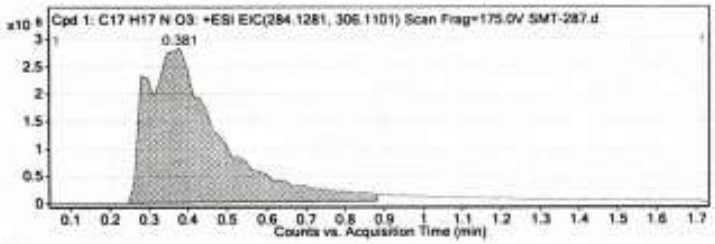
Data File	SMT-287.d	**Sample Name**	SMT-287
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	02-05-2024 14:06:04
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

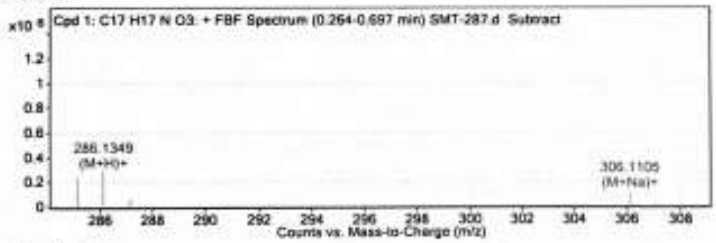
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H17 N O3	0.381	283.1214	116974	C17 H17 N O3	283.1208	2.13	C17 H17 N O3	C17 H17 N O3

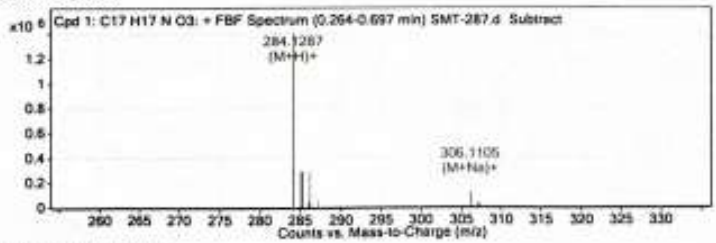
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H17 N O3	306.1105	0.381	Find By Formula	283.1214



MS Spectrum



MS Zoomed Spectrum

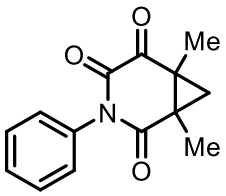


MS Spectrum Peak List

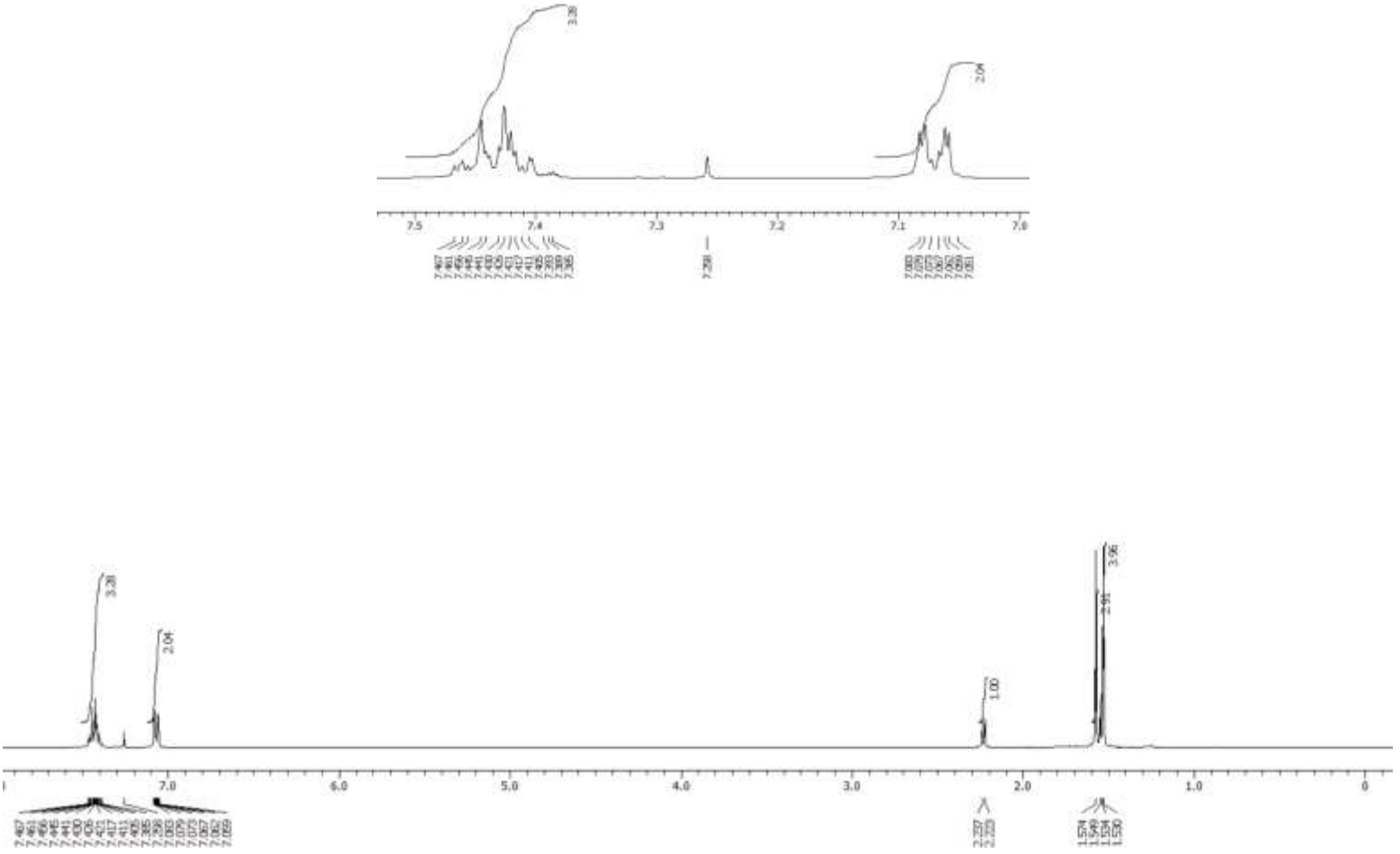
m/z	z	Abund	Formula	Ion
284.1287	1	1207303	C17H18NO3	(M+H)+
285.1319	1	235527.08	C17H18NO3	(M+H)+
286.1349	1	285519.47	C17H18NO3	(M+H)+
287.1377	1	58143.21	C17H18NO3	(M+H)+
288.1389	1	6946.44	C17H18NO3	(M+H)+
306.1105	1	116974.35	C17H17NNaO3	(M+Na)+
307.1138	1	21103.47	C17H17NNaO3	(M+Na)+
308.1196	1	3689.51	C17H17NNaO3	(M+Na)+
309.117	1	113.18	C17H17NNaO3	(M+Na)+

--- End Of Report ---

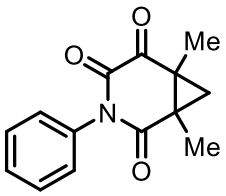
^{1}H NMR spectrum of 4a (400 MHz, $CDCl_3$)



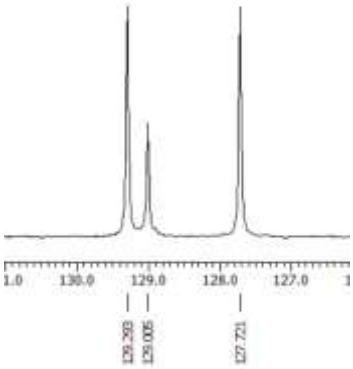
1,6-dimethyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

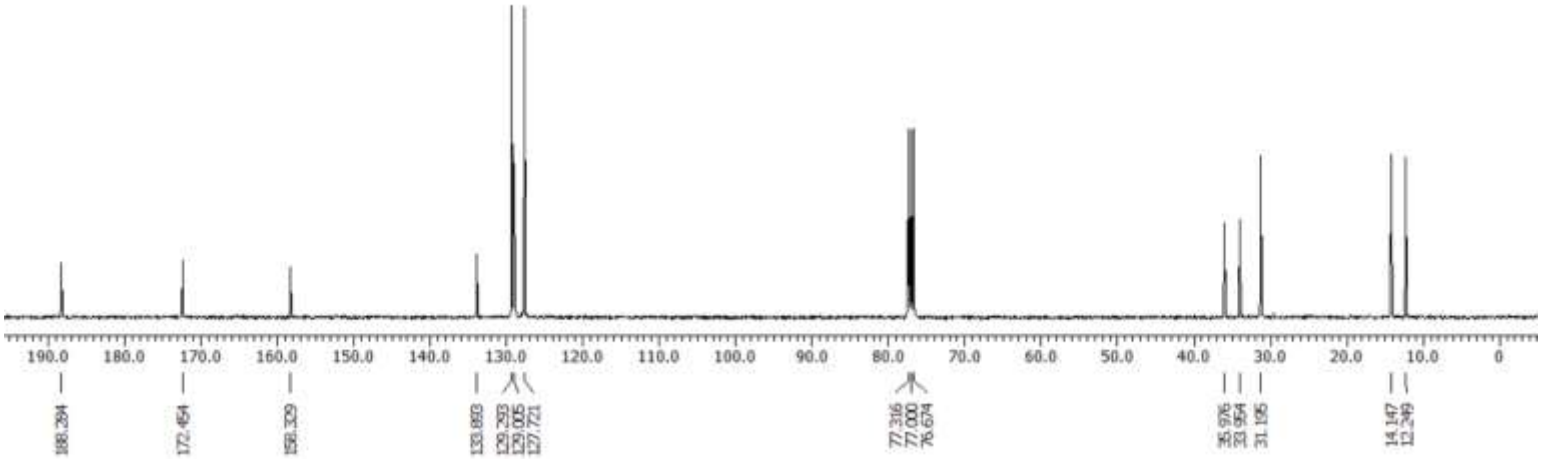


^{13}C NMR spectrum of 4a (100 MHz, $CDCl_3$)



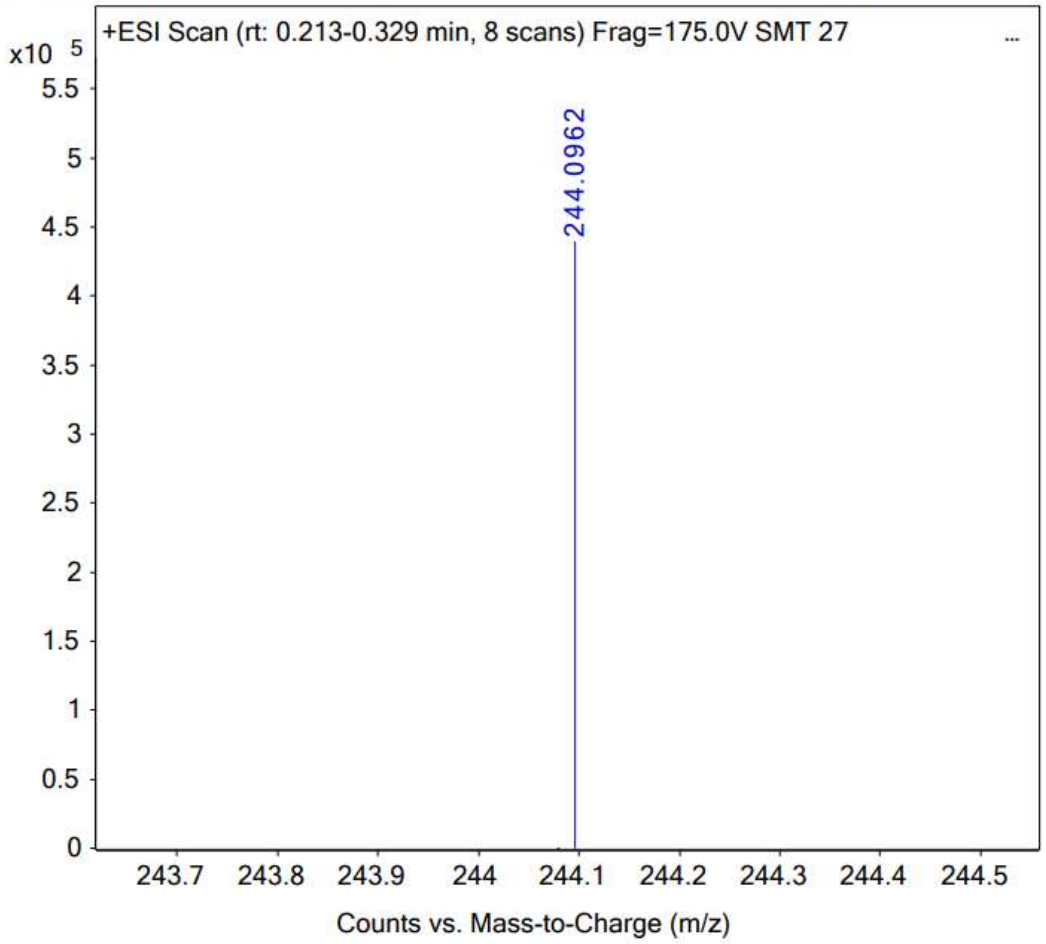
1,6-dimethyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



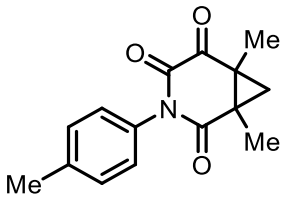


HRMS spectrum of 4a

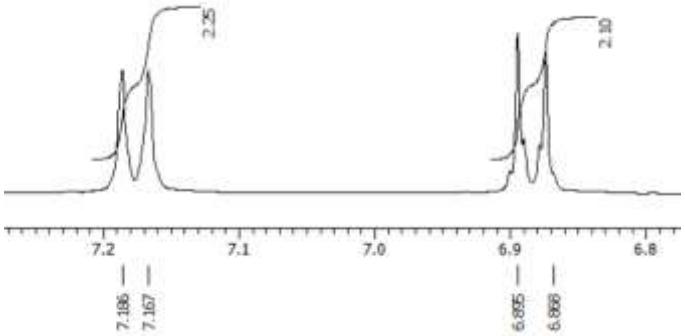
Sample Name	SMT 279	**Position**	P1-C2	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 279.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 13:09:43 (UTC+05:30)

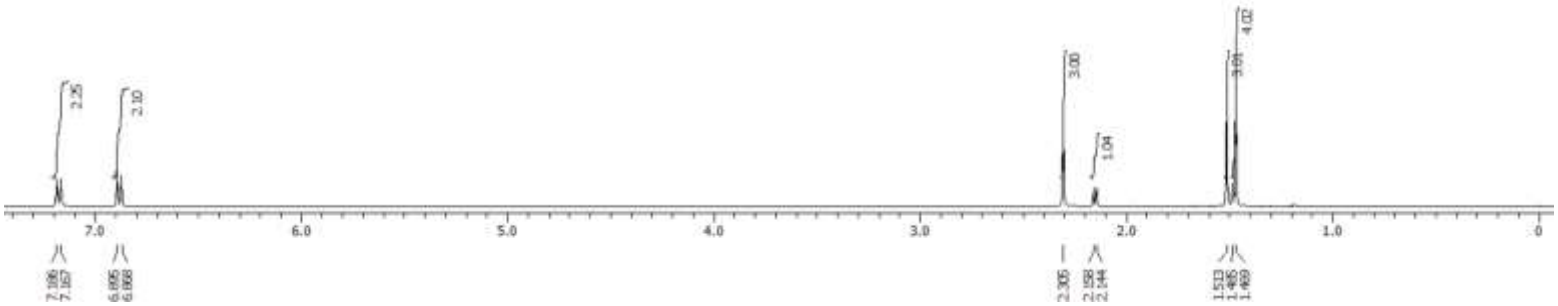


^{1}H NMR spectrum of 4b (400 MHz, $CDCl_3$)

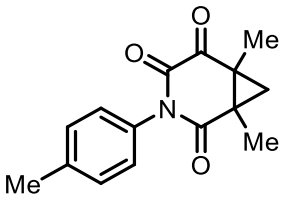


1,6-dimethyl-3-(*p*-tolyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

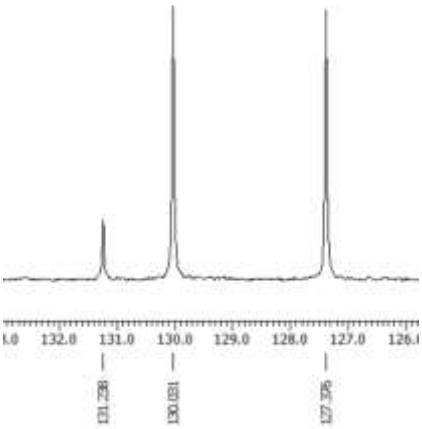


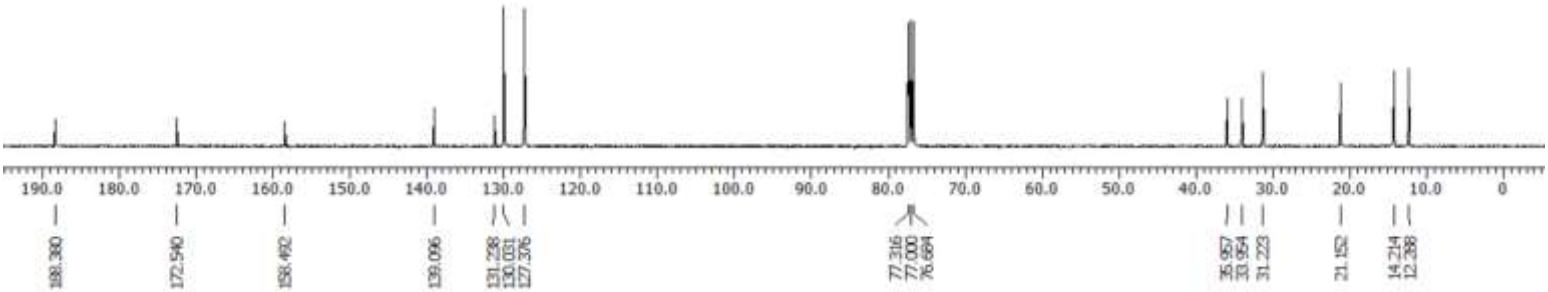


^{13}C NMR spectrum of 4b (100 MHz, $CDCl_3$)



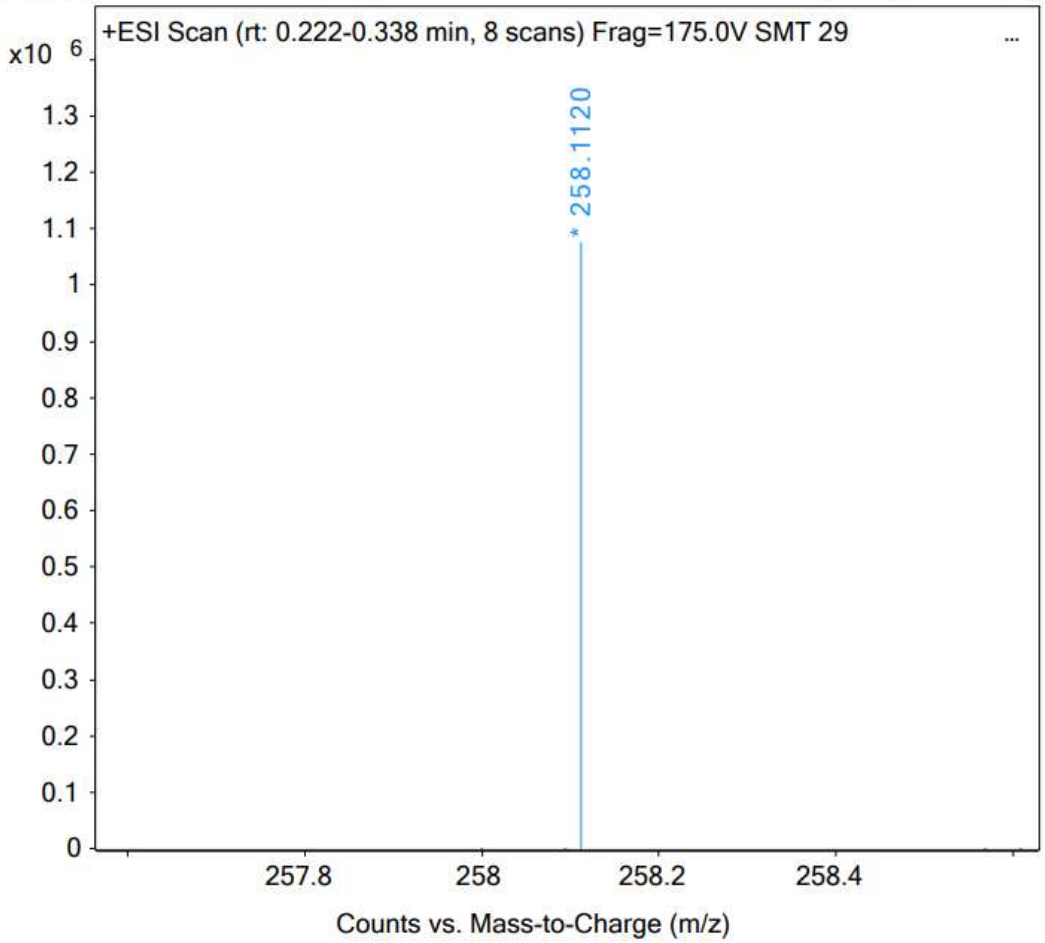
1,6-dimethyl-3-(*p*-tolyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione



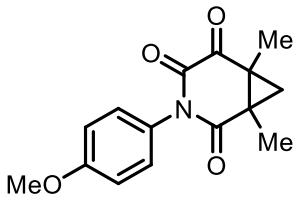


HRMS spectrum of 4b

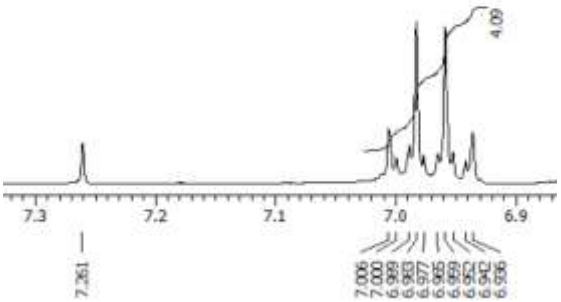
Sample Name	SMT 294	**Position**	P1-A3	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 294.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 11:48:37 (UTC+05:30)

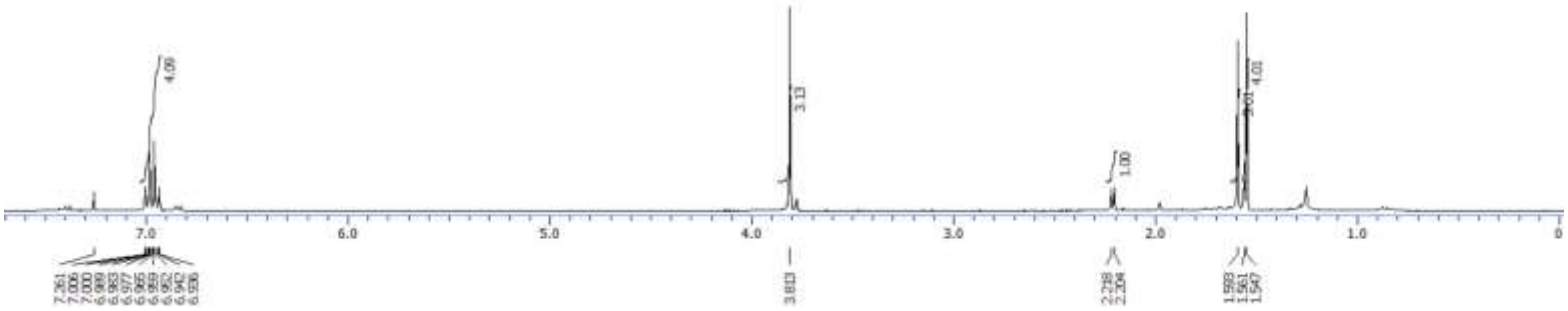


^{1}H NMR spectrum of 4c (400 MHz, $CDCl_3$)

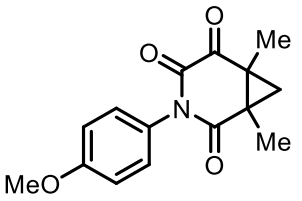


3-(4-methoxyphenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

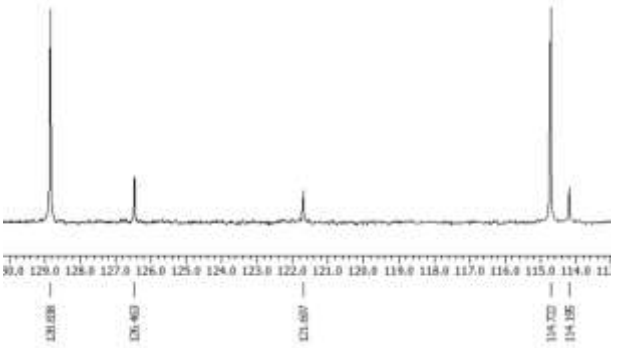


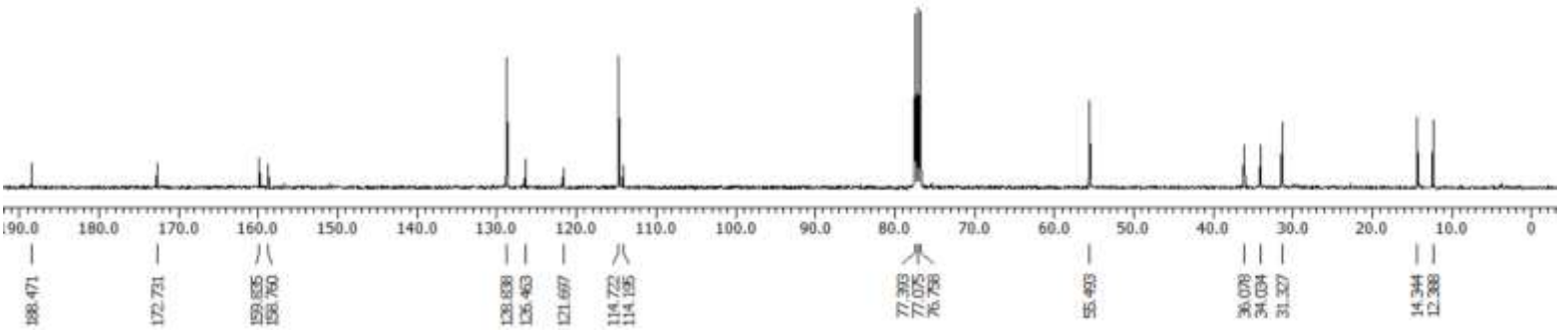


^{13}C NMR spectrum of 4c (100 MHz, $CDCl_3$)



3-(4-methoxyphenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 4c

Qualitative Compound Report

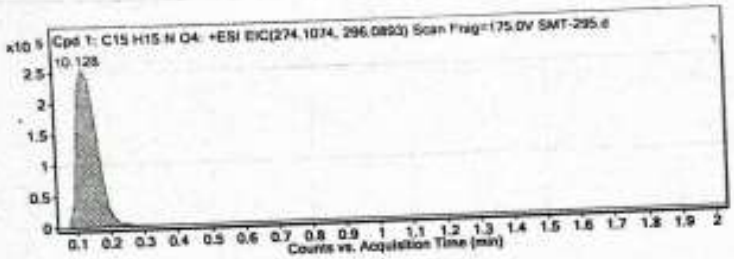
Data File	SMT-295.d	Sample Name	SMT-295
Sample Type	Sample	Position	P1-C2
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	14-08-2023 13:34:56
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

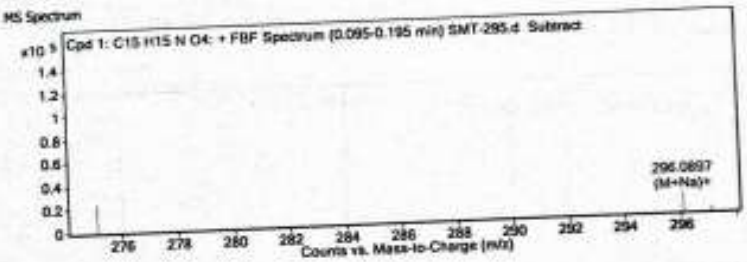
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	DiM (ppm)	MFG Formula	DB Formula
Cpd 1: C15 H15 N O4	0.128	273.1004	16528	C15 H15 N O4	273.1001	1.02	C15 H15 N O4	C15 H15 N O4

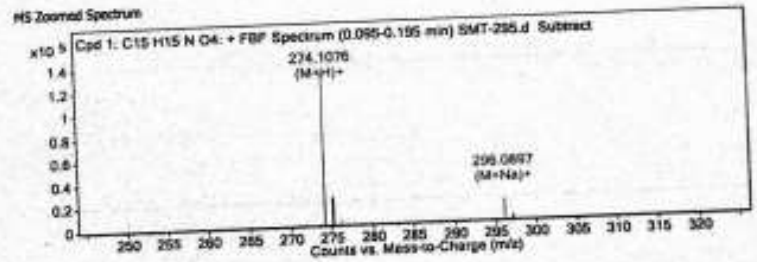
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C15 H15 N O4	296.0897	0.128	Find By Formula	273.1004



MS Spectrum



MS Zoomed Spectrum

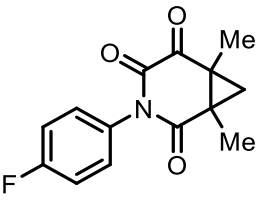


MS Spectrum Peak List

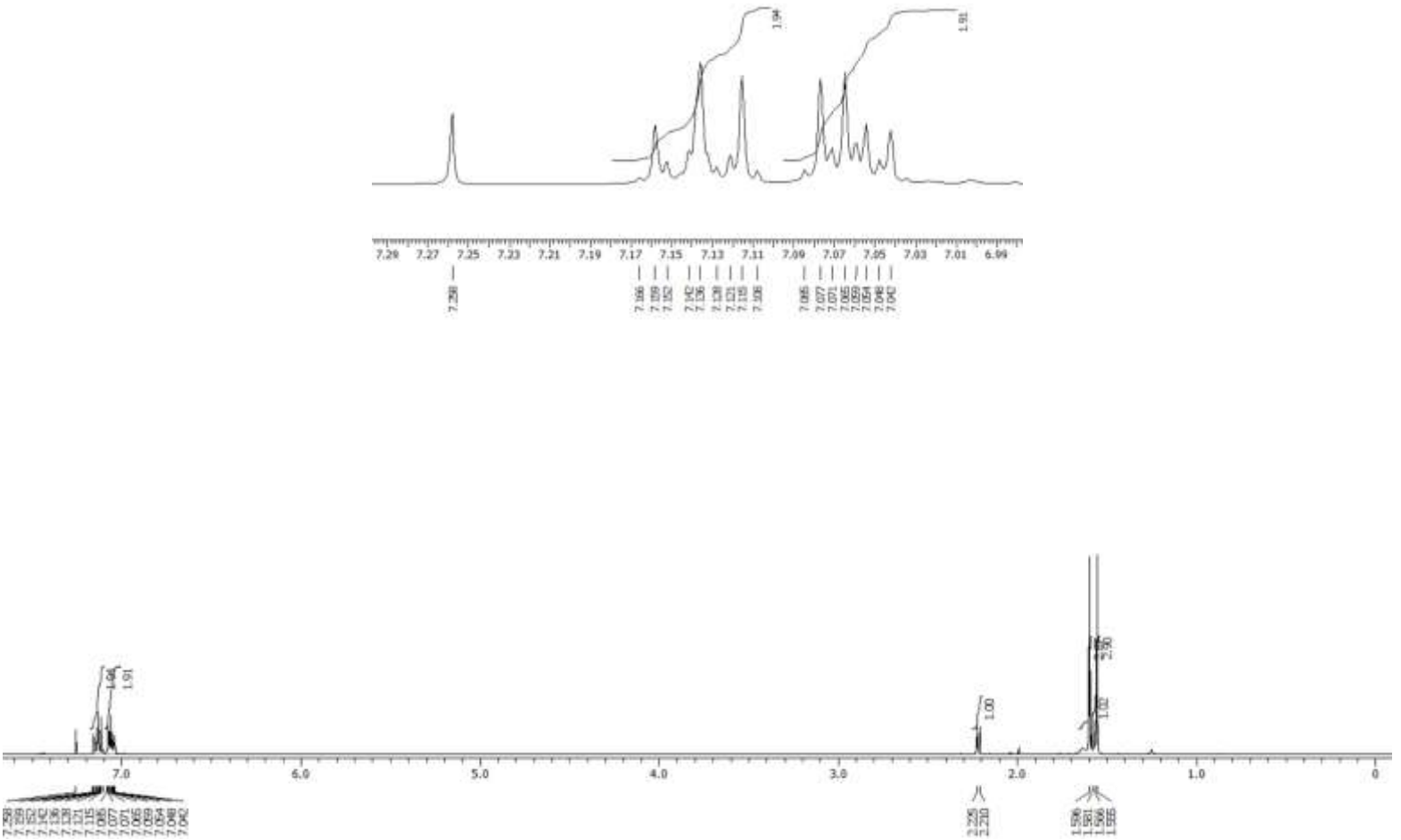
m/z	z	Abund	Formula	Ion
274.1076	1	130911.44	C15H16NO4	(M+H)+
275.1111	1	23930.31	C15H16NO4	(M+H)+
296.0897	1	16527.8	C15H15NNaO4	(M+Na)+
297.0923	1	3652.39	C15H15NNaO4	(M+Na)+
298.0991	1	941.86	C15H15NNaO4	(M+Na)+

--- End Of Report ---

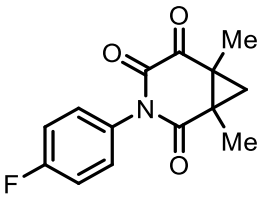
^{1}H NMR spectrum of 4d (400 MHz, $CDCl_3$)



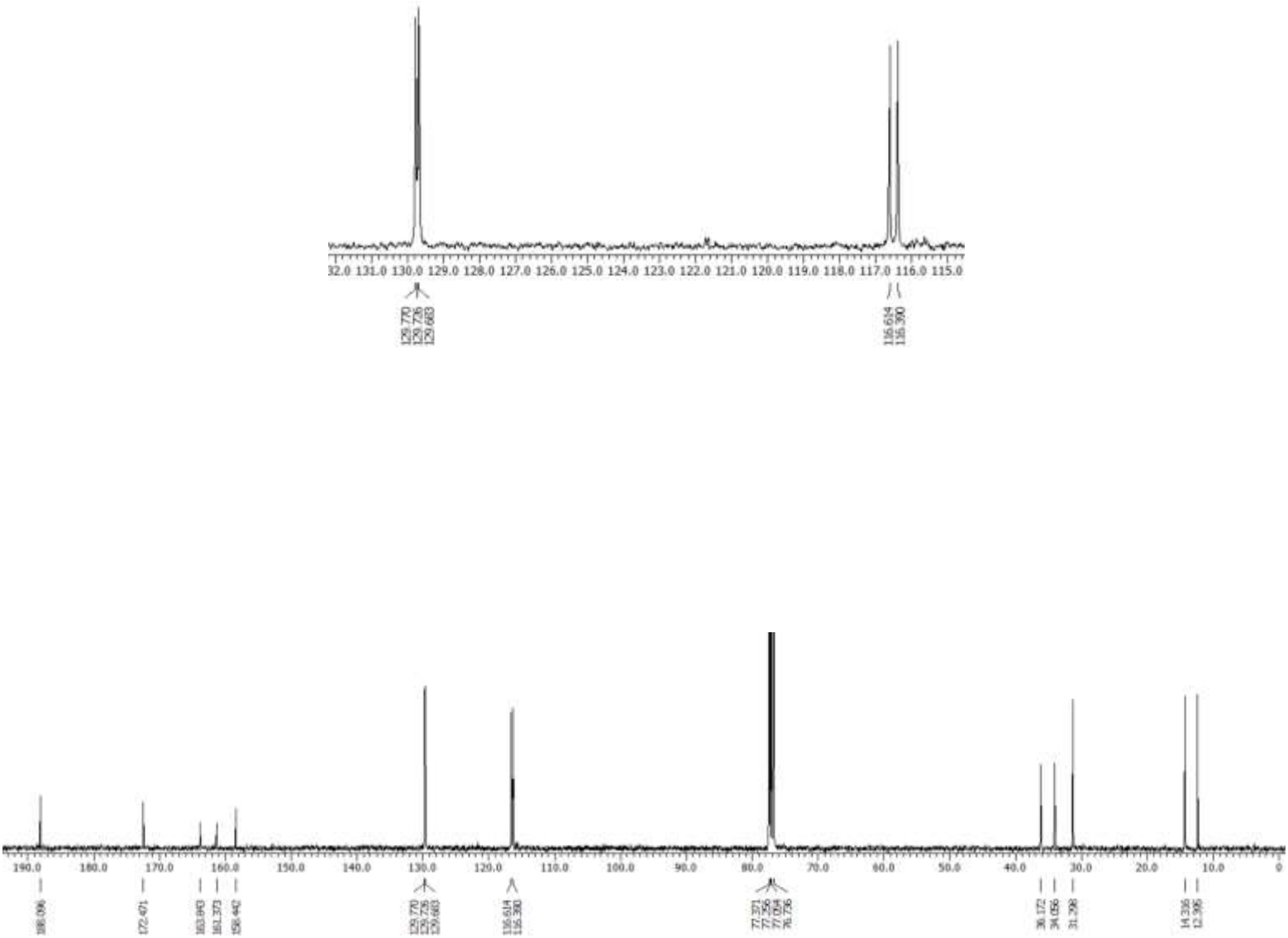
3-(4-fluorophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



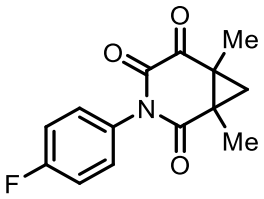
^{13}C NMR spectrum of 4d (100 MHz, $CDCl_3$)



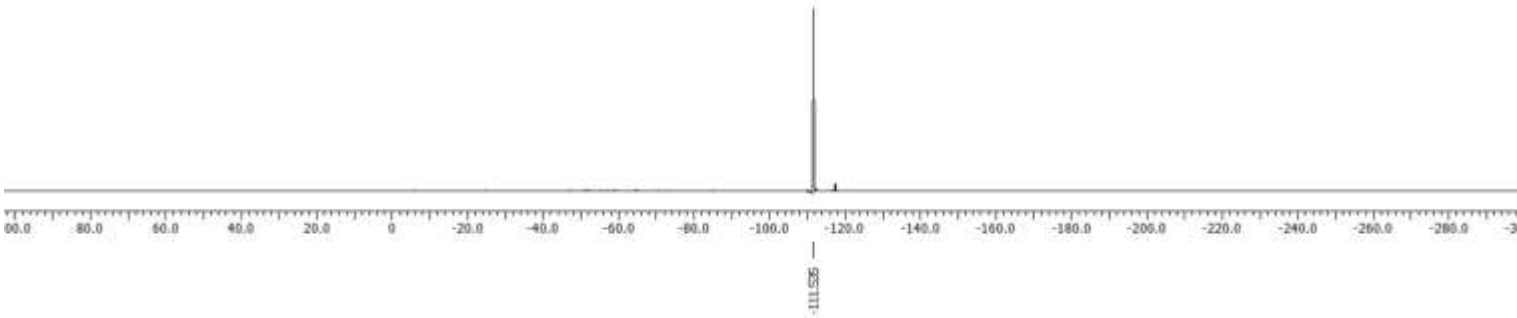
3-(4-fluorophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



^{19}F NMR spectrum of 4d (MHz, $CDCl_3$)

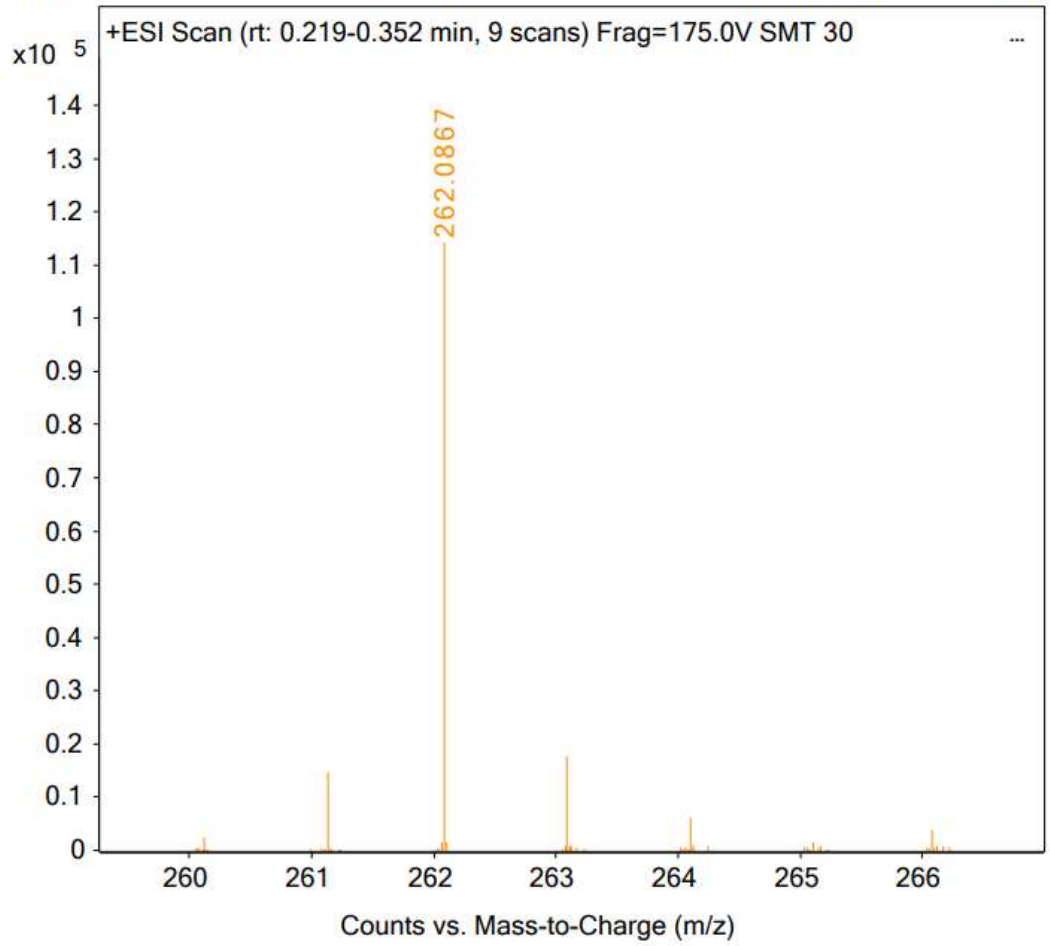


3-(4-fluorophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

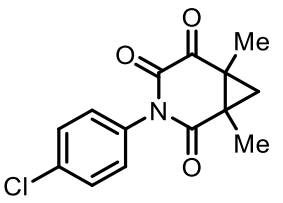


HRMS spectrum of 4d

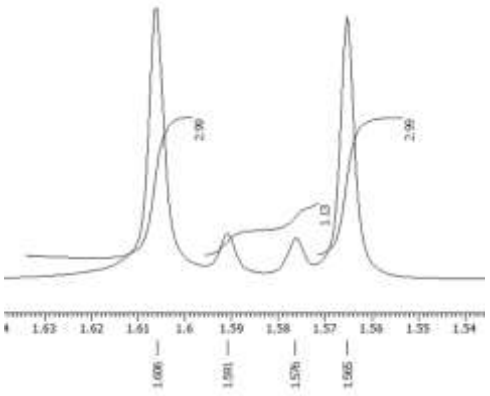
Sample Name	SMT 307	**Position**	P1-A4	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 307.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 11:52:31 (UTC+05:30)

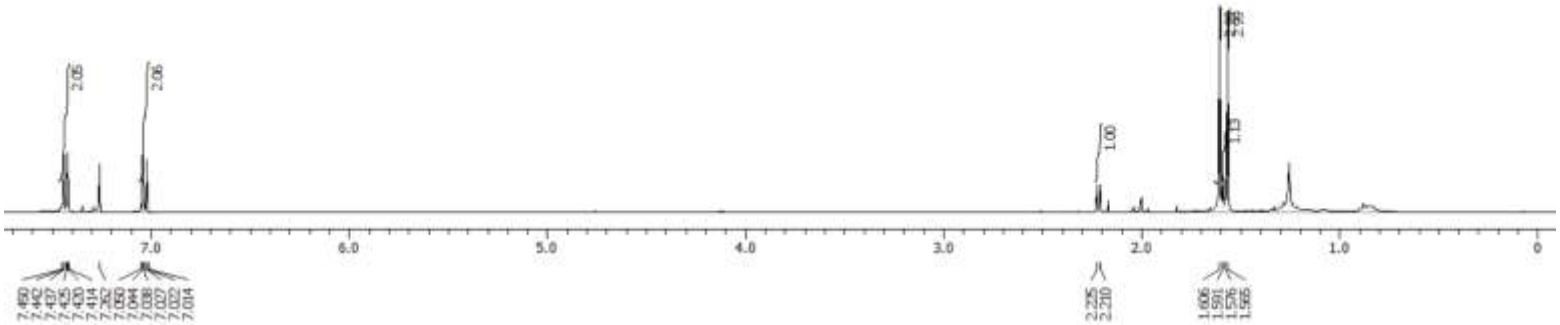


^{1}H NMR spectrum of 4e (400 MHz, $CDCl_3$)

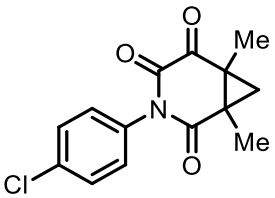


3-(4-chlorophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

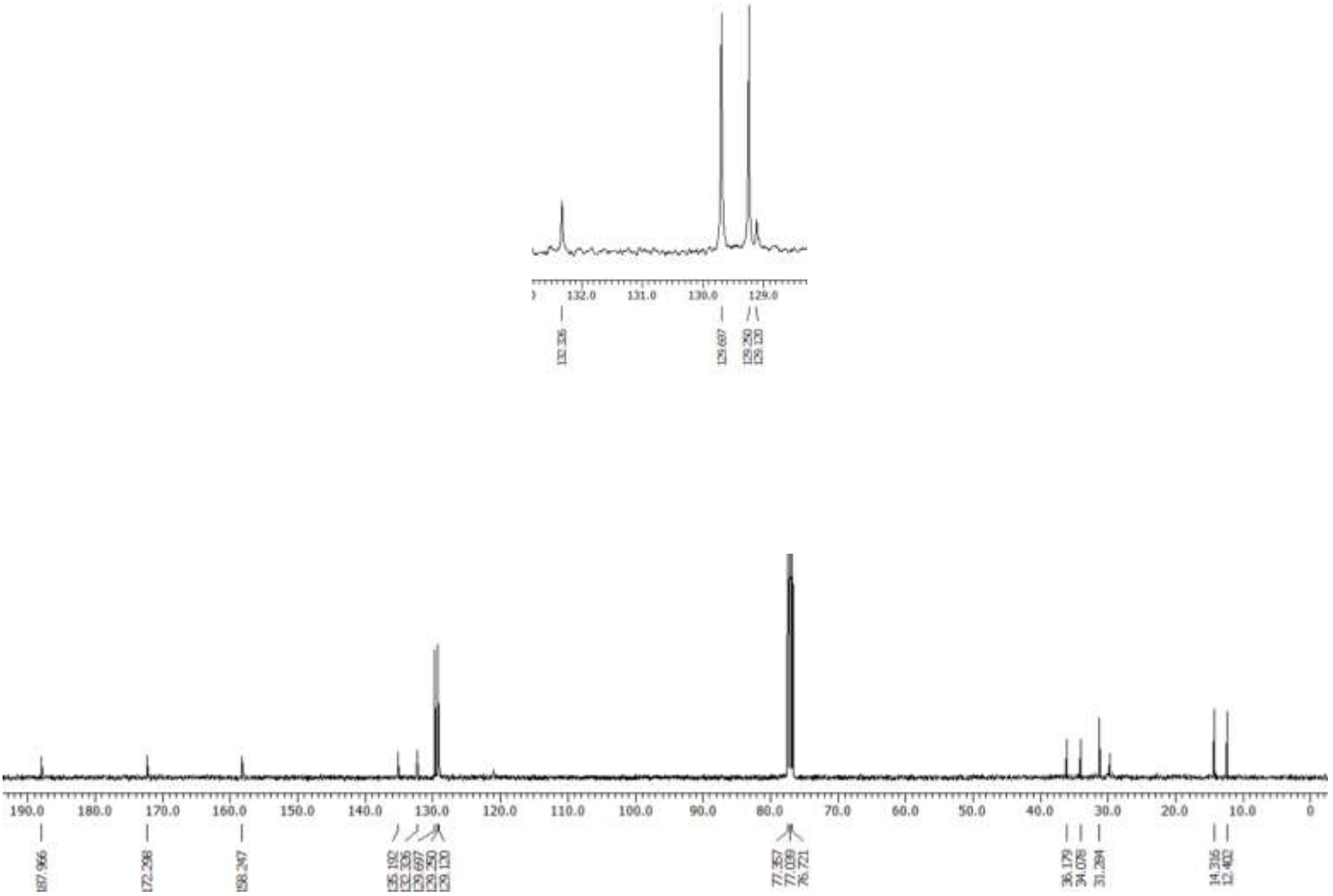




^{13}C NMR spectrum of 4e (100 MHz, $CDCl_3$)



3-(4-chlorophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 4e

Qualitative Compound Report

Data File	SMT-308.d	**Sample Name**	SMT-308
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	23-08-2023 13:45:12
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

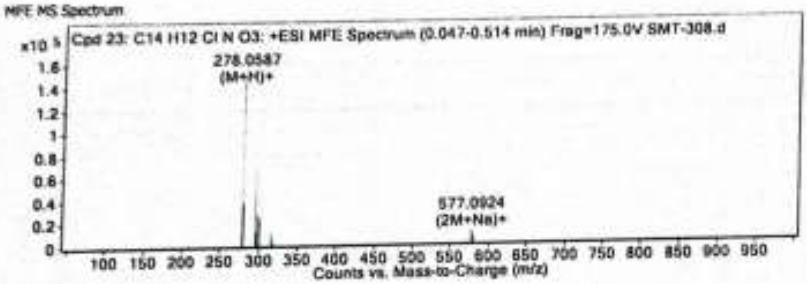
Sample Group		**Info.**	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

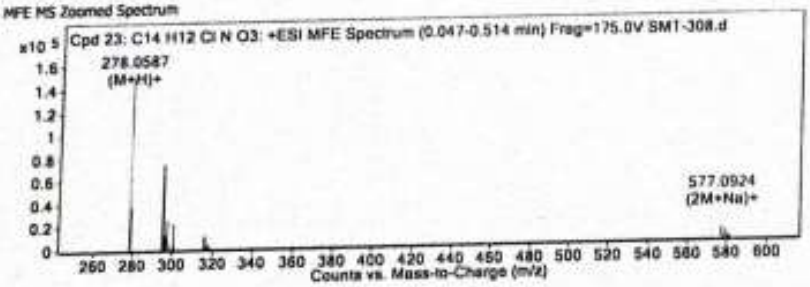
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 23: C14 H12 Cl N O3	0.127	277.0513	C14 H12 Cl N O3	C14 H12 Cl N O3	-2.54	C14 H12 Cl N O3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 23: C14 H12 Cl N O3	278.0587	0.127	Find by Molecular Feature	277.0513

MFE MS Spectrum



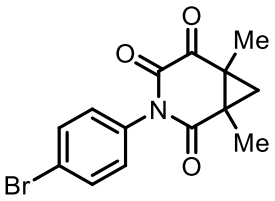
MFE MS Zoomed Spectrum



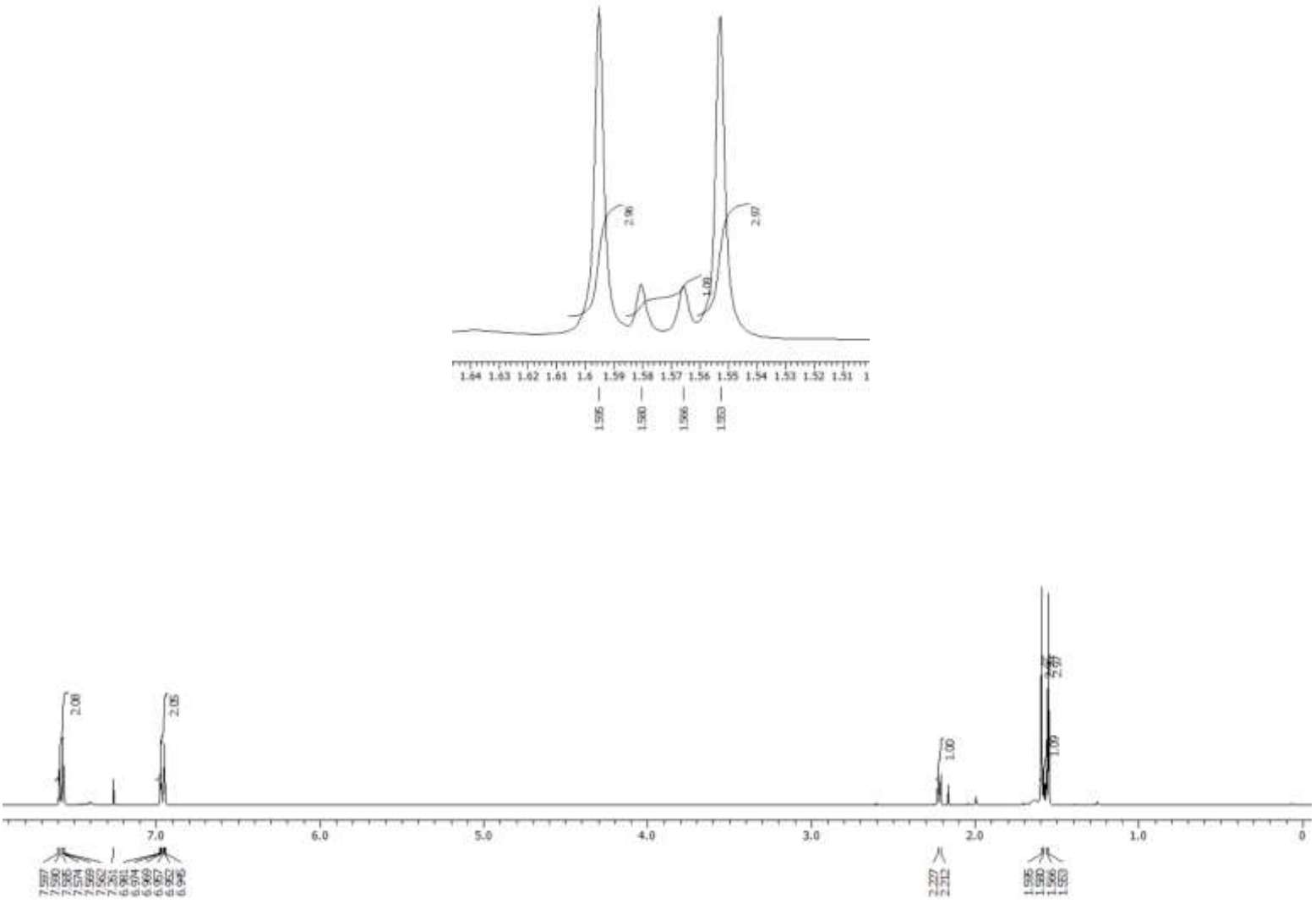
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
278.0587	1	148156.91		(M+H)+
279.0634	1	37340.95		(M+H)+
295.0852	1	70381.17	C14 H16 Cl N2 O3	(M+NH4)+
296.087	1	12641.83	C14 H16 Cl N2 O3	(M+NH4)+
297.0829	1	26971.41	C14 H16 Cl N2 O3	(M+NH4)+
298.0853	1	5620.01	C14 H16 Cl N2 O3	(M+NH4)+
299.0902	1	723.27	C14 H16 Cl N2 O3	(M+NH4)+
300.0406	1	23512.27		(M+Na)+
301.0435	1	3353.12		(M+Na)+
316.0146	1	10270.66	C14 H12 Cl K N O3	(M+K)+
317.0182	1	1736.83	C14 H12 Cl K N O3	(M+K)+
318.0169	1	4382.6	C14 H12 Cl K N O3	(M+K)+
319.0227	1	921.47	C14 H12 Cl K N O3	(M+K)+
572.1319	1	701.37		(2M+NH4)+
577.0924	1	10346.55	C28 H24 Cl2 N2 Na O6	(2M+Na)+

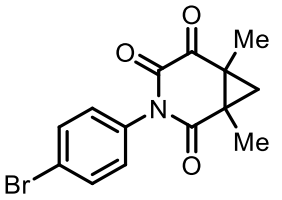
^{1}H NMR spectrum of 4f (400 MHz, $CDCl_3$)



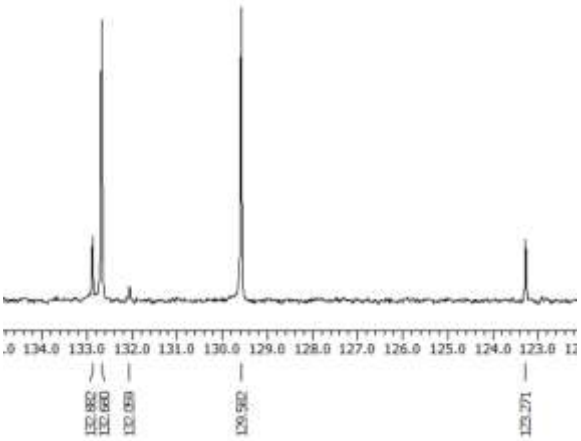
3-(4-bromophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

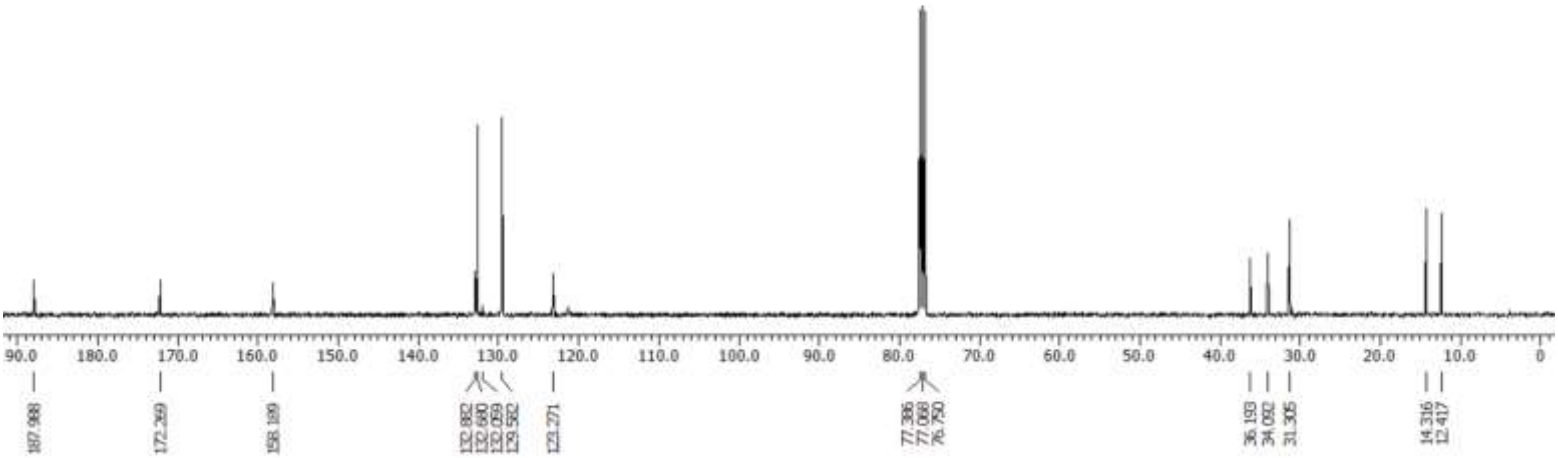


^{13}C NMR spectrum of 4f (100 MHz, $CDCl_3$)



3-(4-bromophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 4f

Qualitative Compound Report

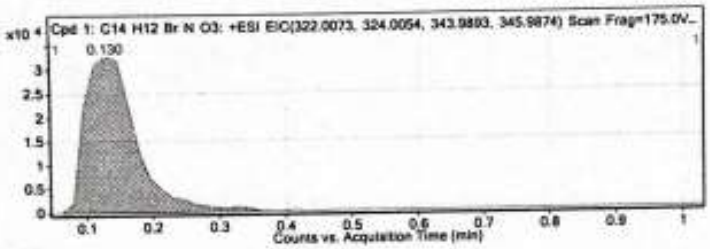
Data File	SMT-328.d	**Sample Name**	SMT-328
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	16-09-2023 13:19:52
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

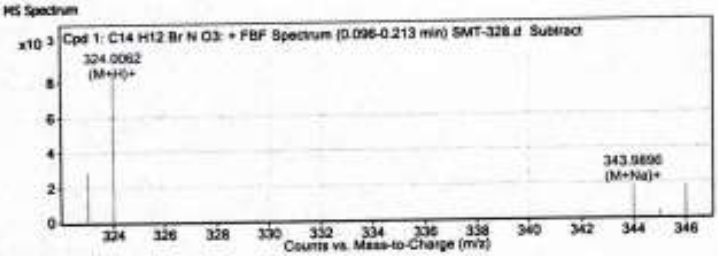
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H12 Br N O3	0.13	321.0006	1825	C14 H12 Br N O3	321.0001	1.83	C14 H12 Br N O3	C14 H12 Br N O3

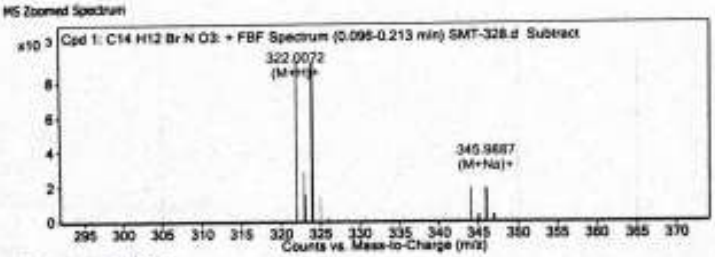
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C14 H12 Br N O3	345.9887	0.13	Find By Formula	321.0006



MS Spectrum



MS Zoomed Spectrum

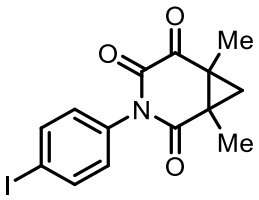


MS Spectrum Peak List

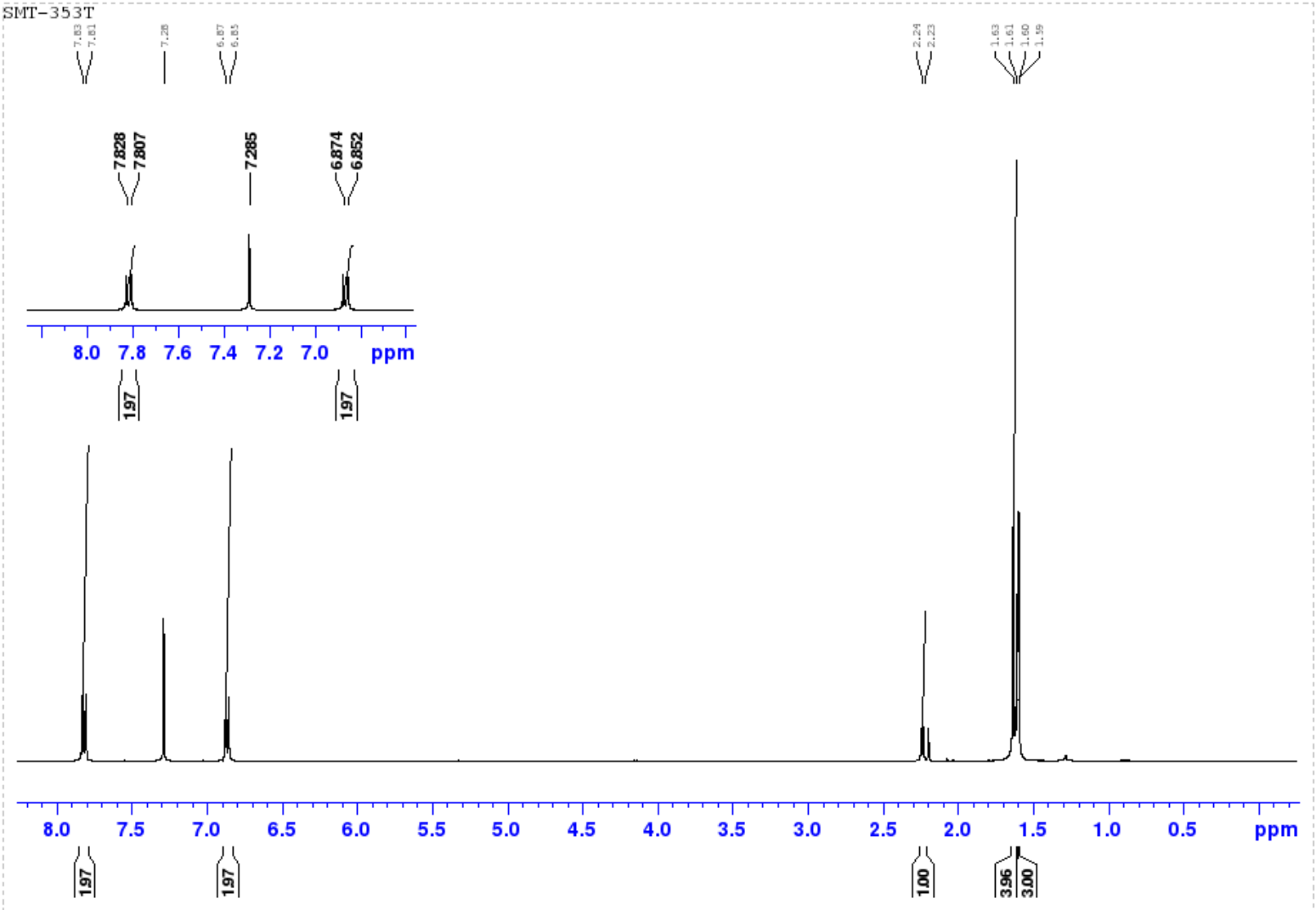
m/z	z	Abund	Formula	Ion
322.0072	1	8521.02	C14H13BrNO3	(M+H)+
323.0129	1	2839.49	C14H13BrNO3	(M+H)+
324.0062	1	8467.97	C14H13BrNO3	(M+H)+
343.9896	1	1785.15	C14H12BrNNaO3	(M+Na)+
344.9913	1	302.24	C14H12BrNNaO3	(M+Na)+
345.9887	1	1825.28	C14H12BrNNaO3	(M+Na)+
346.9895	1	390.57	C14H12BrNNaO3	(M+Na)+

--- End Of Report ---

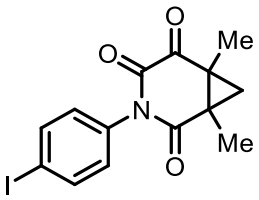
^{1}H NMR spectrum of 4g (400 MHz, $CDCl_3$)



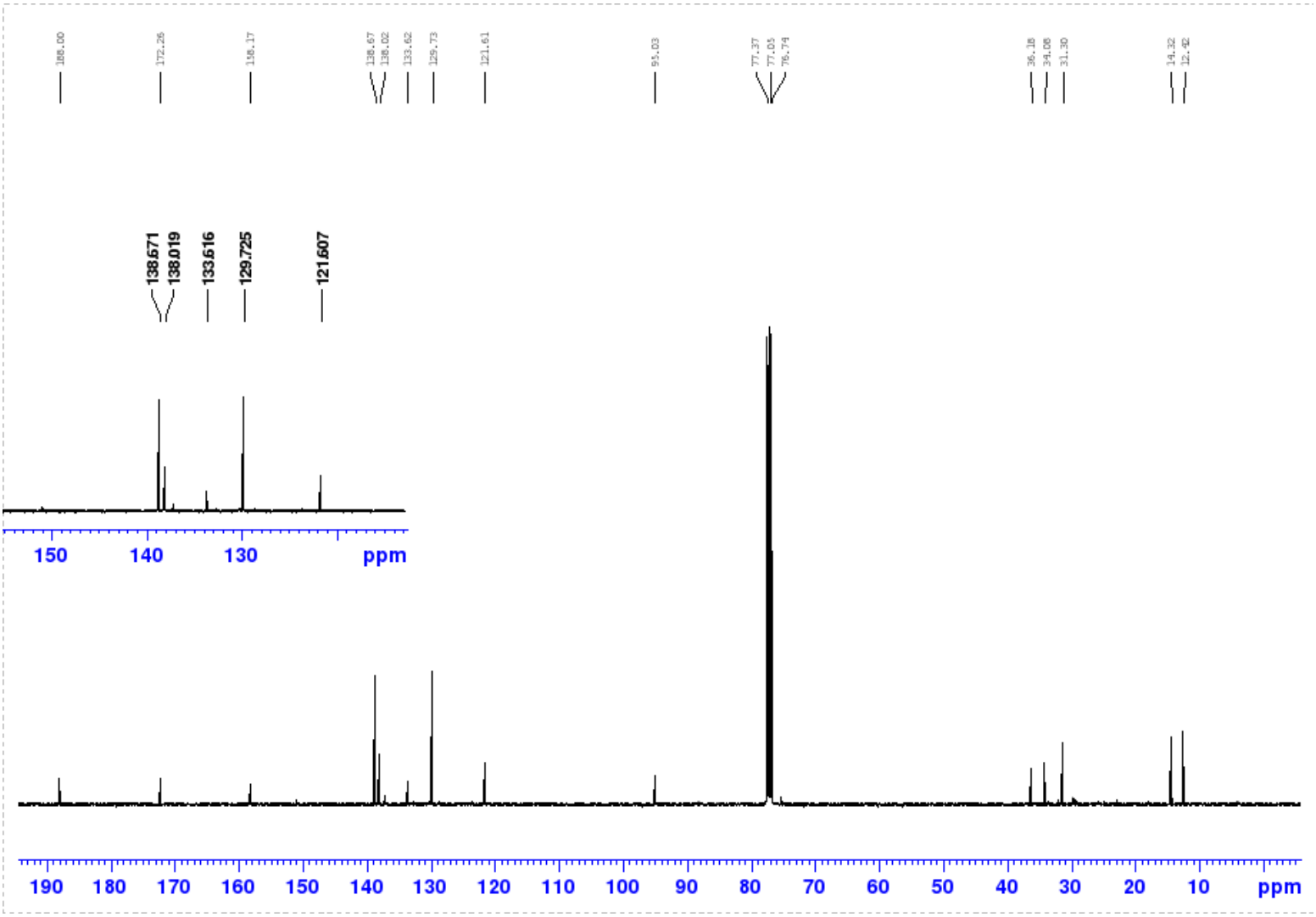
3-(4-iodophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



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



3-(4-iodophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 4g

Qualitative Compound Report

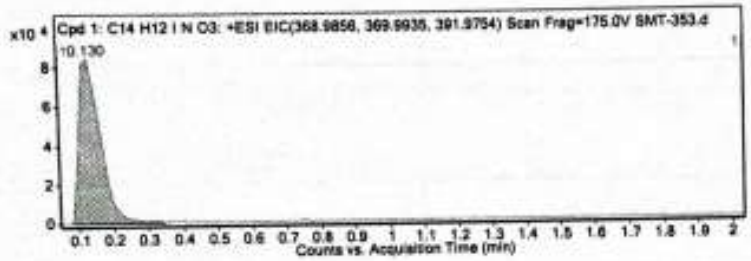
Data File	SMT-353.d	**Sample Name**	SMT-353
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	09-11-2023 14:15:05
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

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

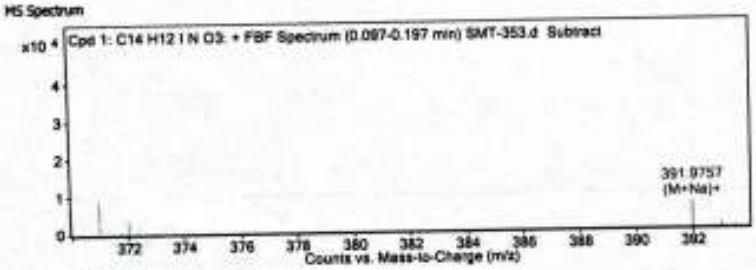
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H12 I N O3	0.13	368.9869	7382	C14 H12 I N O3	368.9862	2.06	C14 H12 I N O3	C14 H12 I N O3

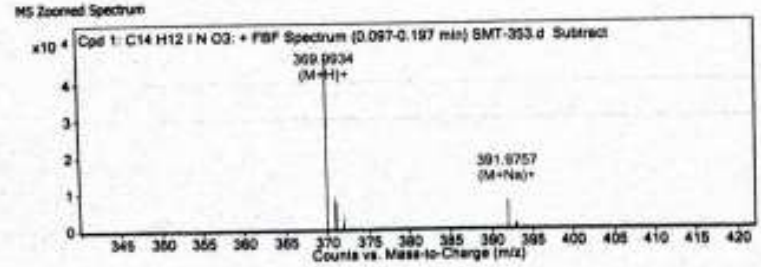
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C14 H12 I N O3	391.9757	0.13	Find By Formula	368.9869



MS Spectrum



MS Zoomed Spectrum

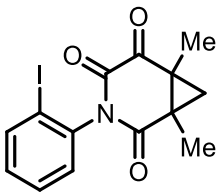


MS Spectrum Peak List

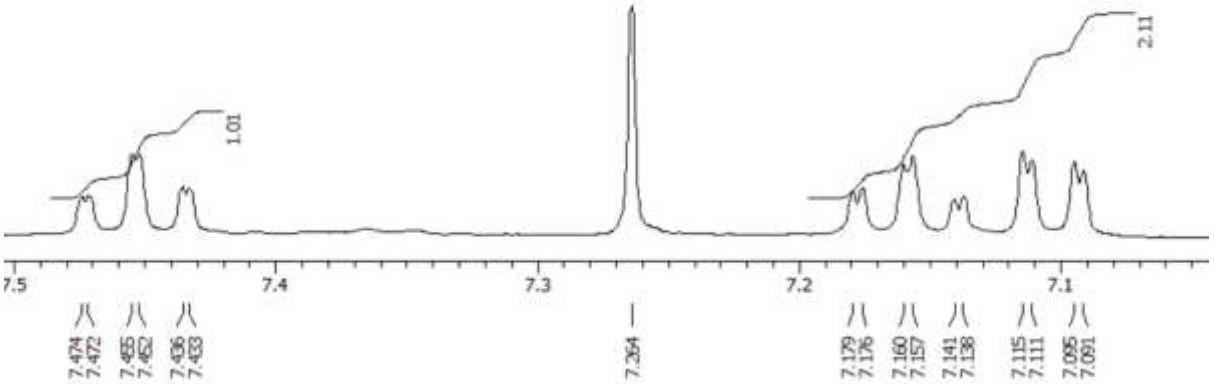
m/z	z	Abund	Formula	Ion
369.9934	1	41965.15	C14H13INO3	(M+H)+
370.998	1	9985.35	C14H13INO3	(M+H)+
372.0069	1	3598.11	C14H13INO3	(M+H)+
373.0125	1	991.35	C14H13INO3	(M+H)+
391.9757	1	7382.03	C14H12INNaO3	(M+Na)+
392.9784	1	994	C14H12INNaO3	(M+Na)+
393.9847	1	401.13	C14H12INNaO3	(M+Na)+

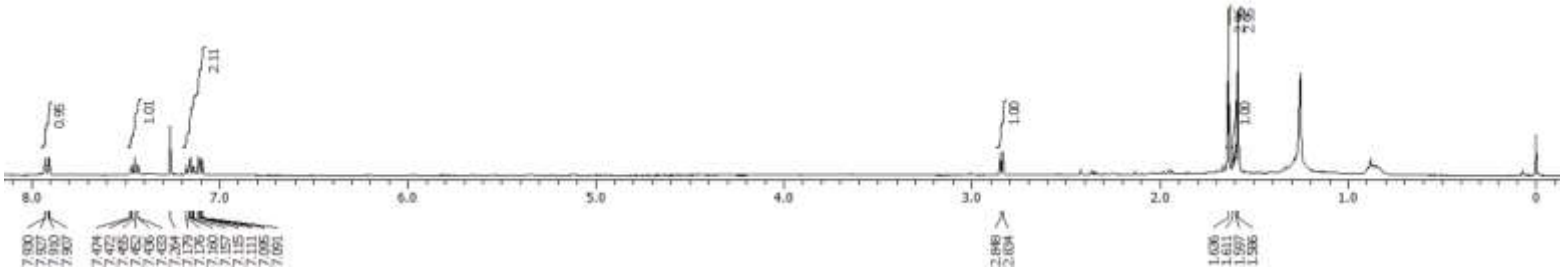
--- End Of Report ---

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

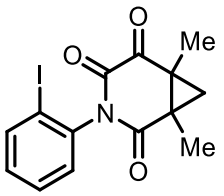


3-(2-iodophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

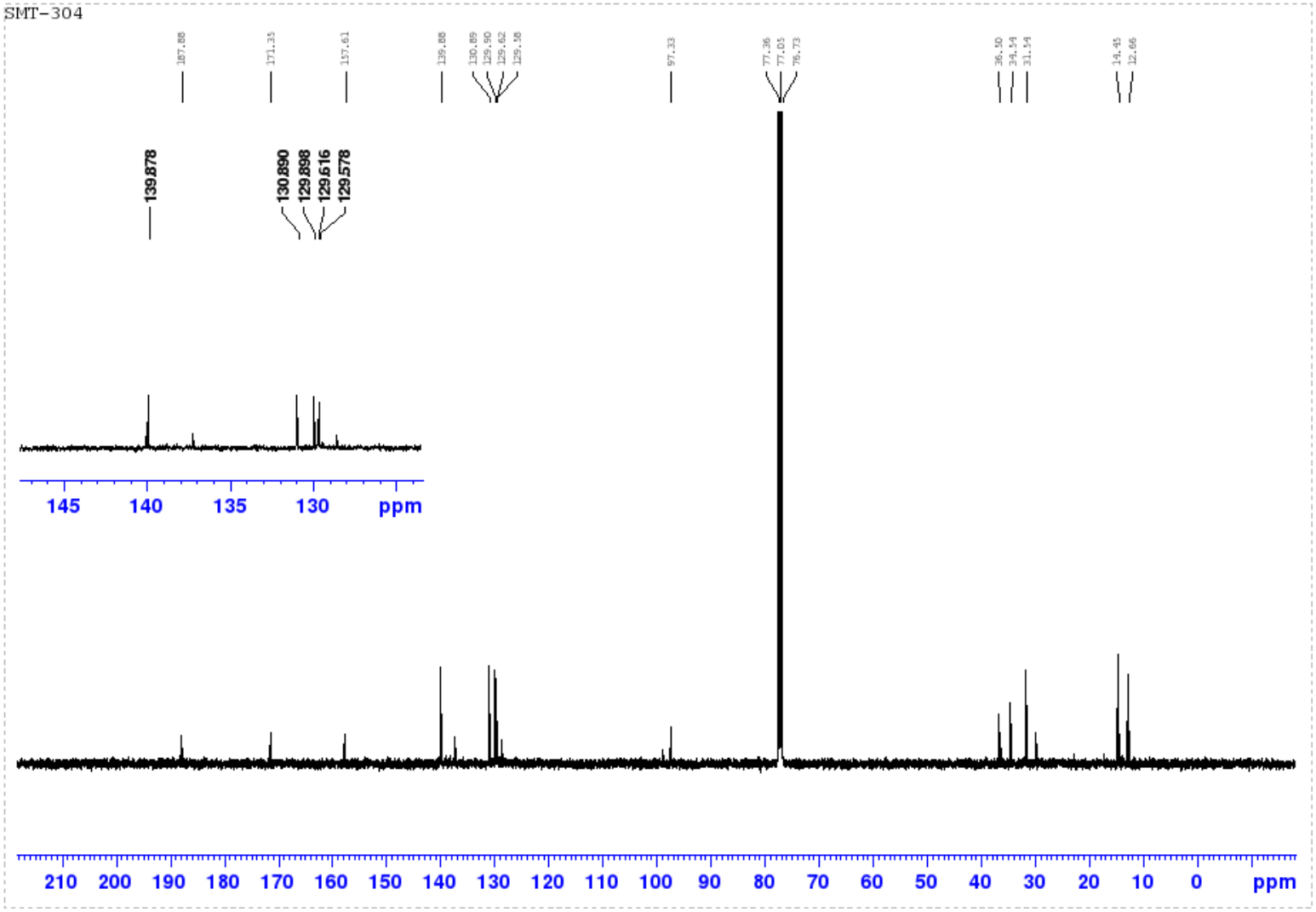




^{13}C NMR spectrum of 4h (100 MHz, $CDCl_3$)



3-(2-iodophenyl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



HRMS spectrum of 4h

Qualitative Compound Report

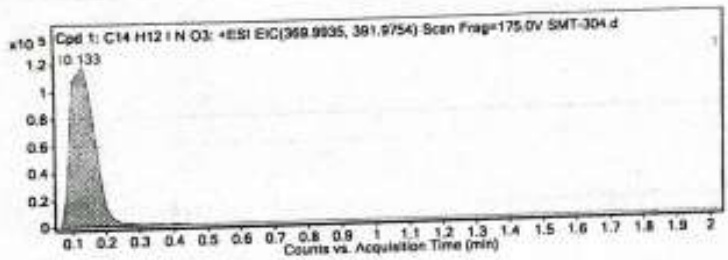
Data File	SMT-304.d	Sample Name	SMT-304
Sample Type	Sample	Position	P1-A5
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	17-08-2023 12:59:00
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

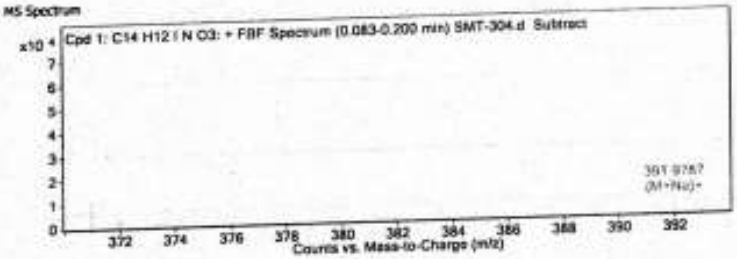
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H12 I N O3	0.133	368.9878	64517	C14 H12 I N O3	368.9862	4.47	C14 H12 I N O3	C14 H12 I N O3

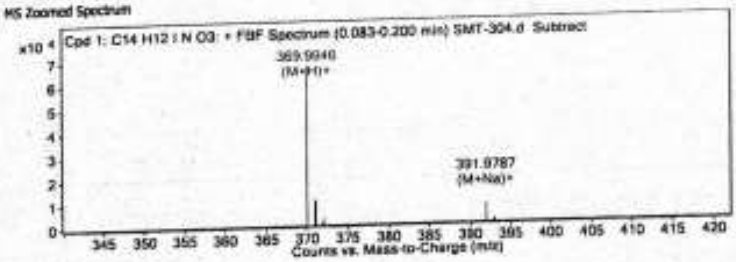
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C14 H12 I N O3	369.9946	0.133	Find By Formula	368.9878



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
369.9946	1	64517.24	C14H13INO3	(M+H)+
370.9978	1	10397.83	C14H13INO3	(M+H)+
371.0069	1	3402.96	C14H13INO3	(M+H)+
373.0123	1	517.55	C14H13INO3	(M+H)+
391.9787	1	7187.47	C14H12INaO3	(M+Na)+
392.981	1	1207.37	C14H12INaO3	(M+Na)+
393.9873	1	555.94	C14H12INaO3	(M+Na)+

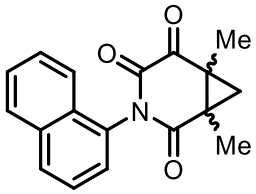
--- End Of Report ---

Agilent Technologies

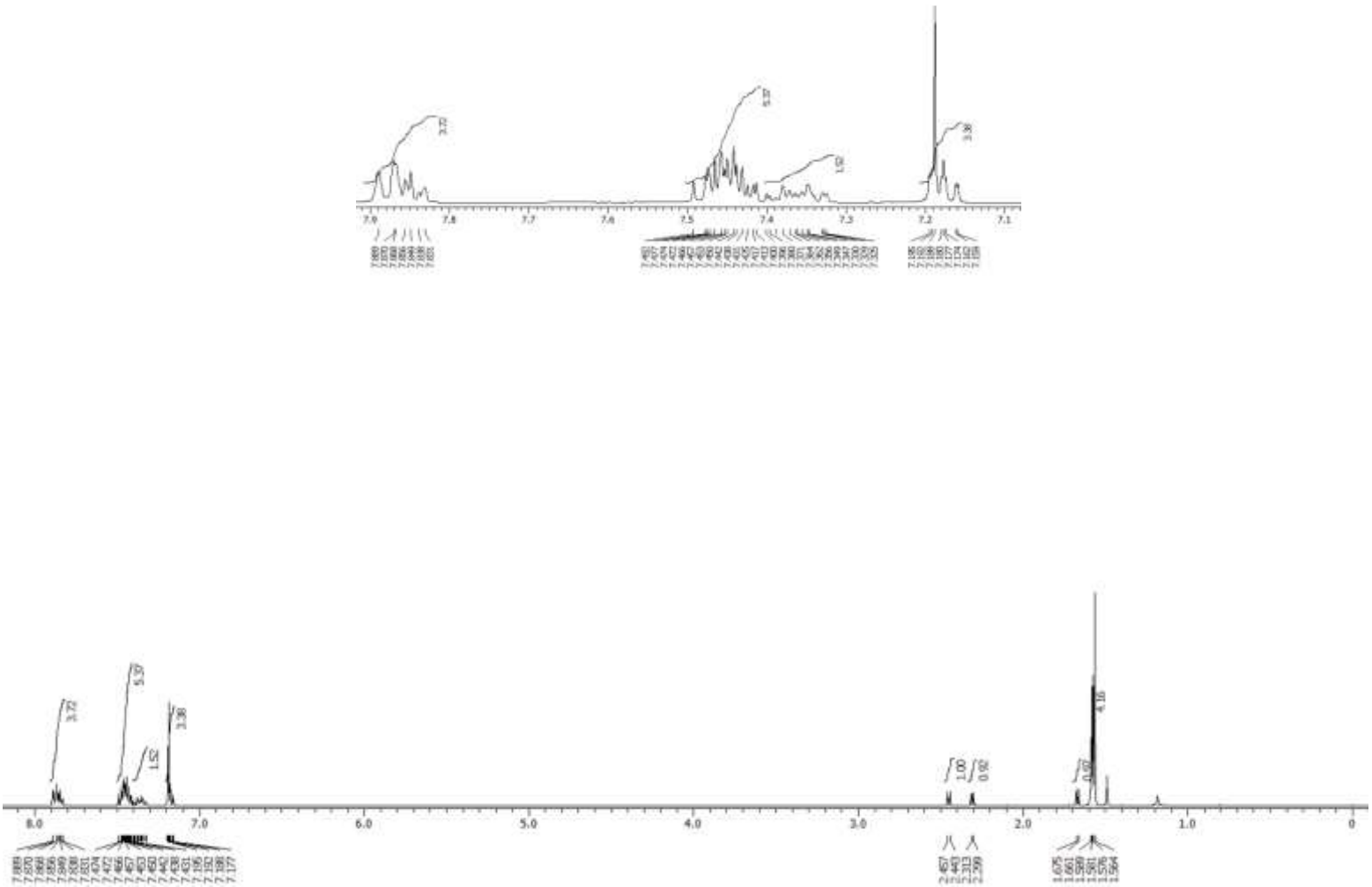
Page 1 of 1

Printed at: 15:08 on 17-08-2023

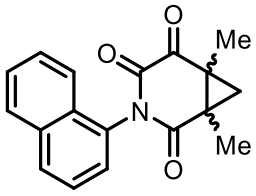
^{1}H NMR spectrum of 4i (400 MHz, $CDCl_3$)



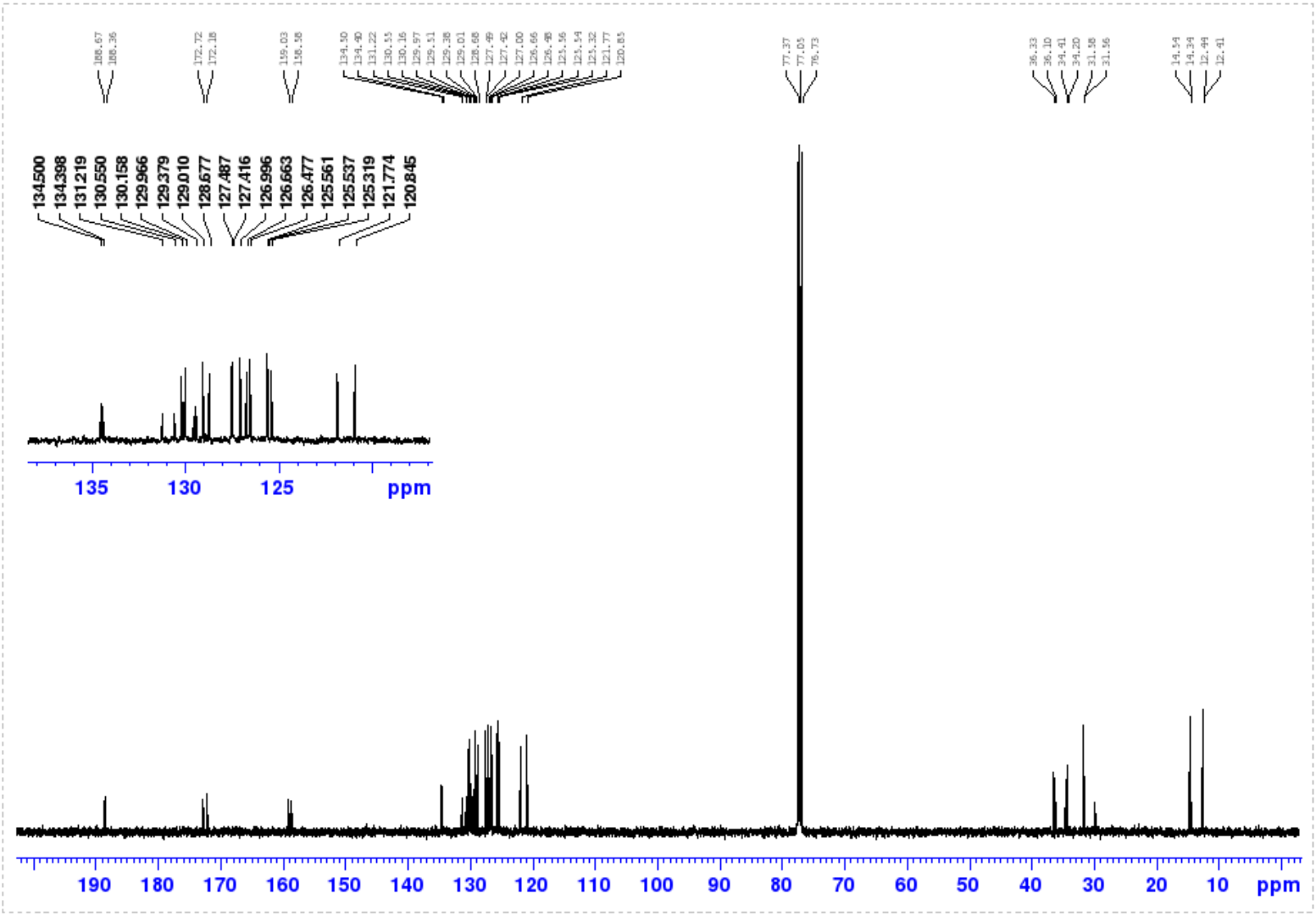
1,6-dimethyl-3-(naphthalen-1-yl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (*dr* 1:1)



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



1,6-dimethyl-3-(naphthalen-1-yl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione (*dr* 1:1)



HRMS spectrum of 4i

Qualitative Compound Report

Data File	SMT-317.d	Sample Name	SMT-317
Sample Type	Sample	Position	P1-B1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	08-11-2023 14:40:20
DA Calibration Status	[redacted]	DA Method	Default.m
Comment			

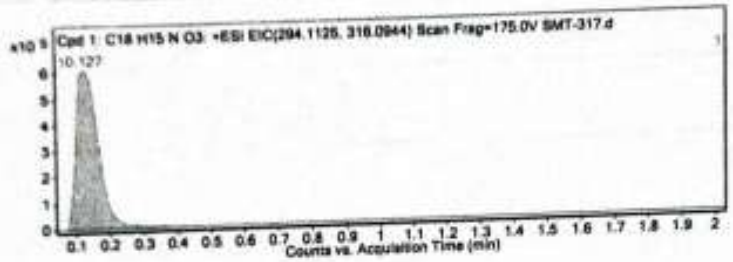
Sample Group: Info. 3

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

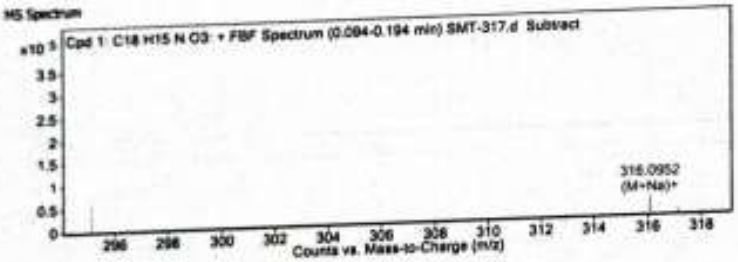
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C18 H15 N O3	0.127	293.1058	336310	C18 H15 N O3	293.1052	1.97	C18 H15 N O3	C18 H15 N O3

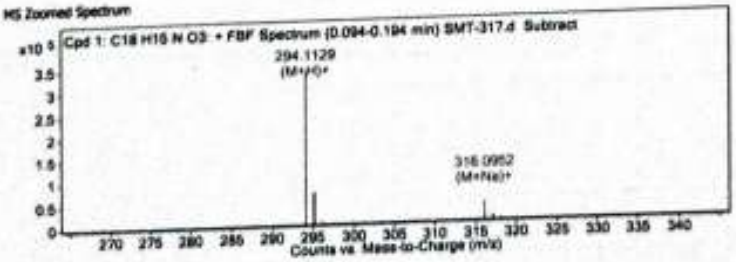
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H15 N O3	294.1129	0.127	Find By Formula	293.1058



MS Spectrum



MS Zoomed Spectrum

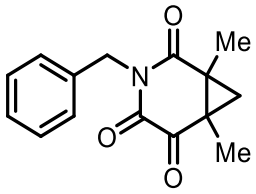


MS Spectrum Peak List

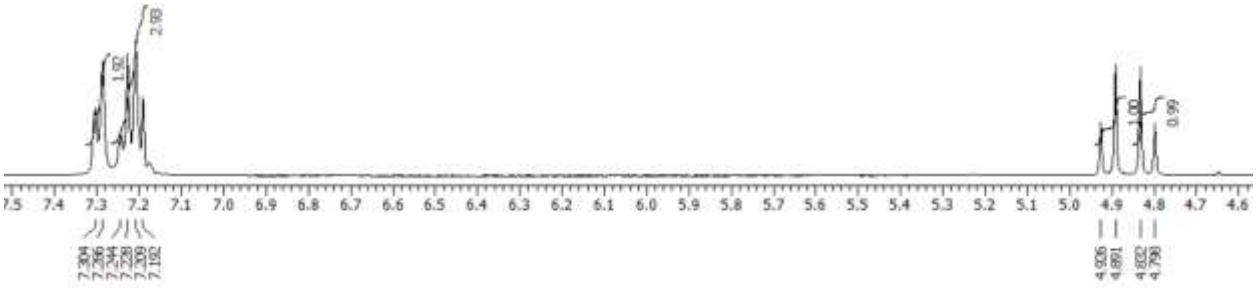
m/z	z	Abund	Formula	Ion
294.1129	1	336309.97	C18H16NO3	(M+H)+
295.116	1	66659.52	C18H16NO3	(M+H)+
316.0952	1	38880.66	C18H15NNaO3	(M+Na)+
317.0934	1	9616.48	C18H15NNaO3	(M+Na)+
318.1081	1	2617.96	C18H15NNaO3	(M+Na)+
319.1103	1	483.31	C18H15NNaO3	(M+Na)+

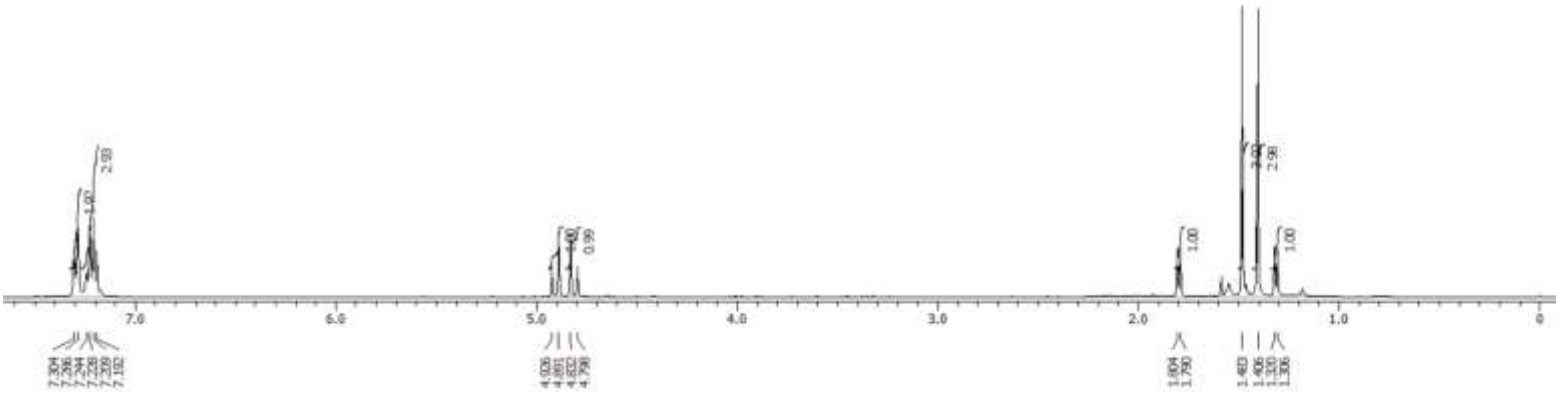
--- End Of Report ---

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

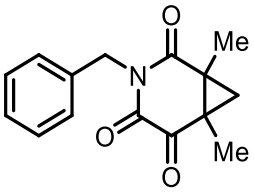


3-benzyl-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

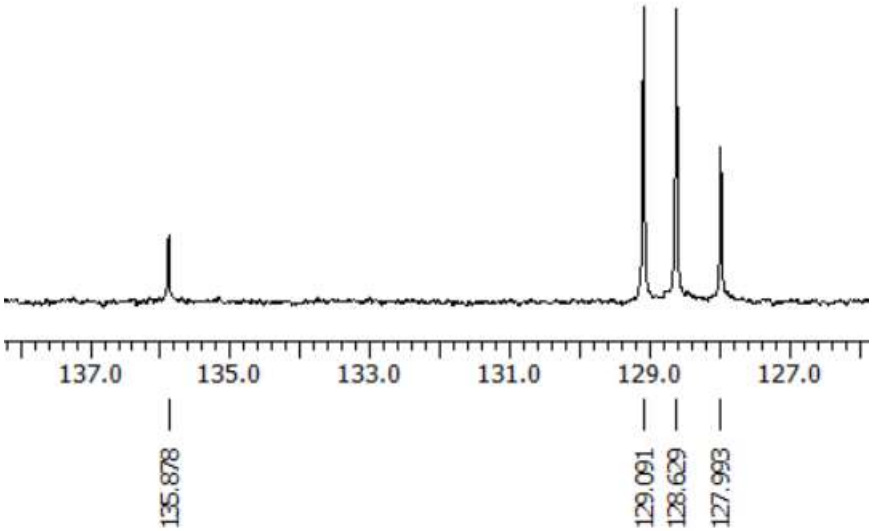


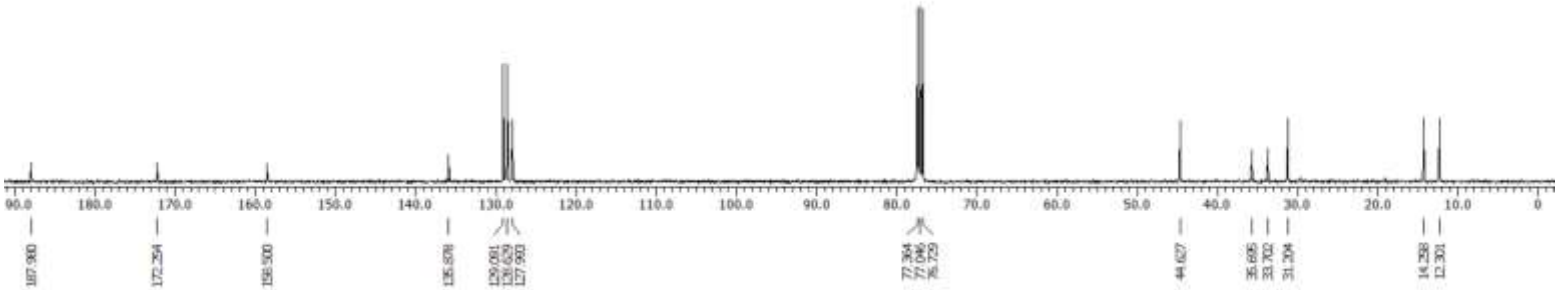


^{13}C NMR spectrum of 4j (100 MHz, $CDCl_3$)



3-benzyl-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 4j

Qualitative Compound Report

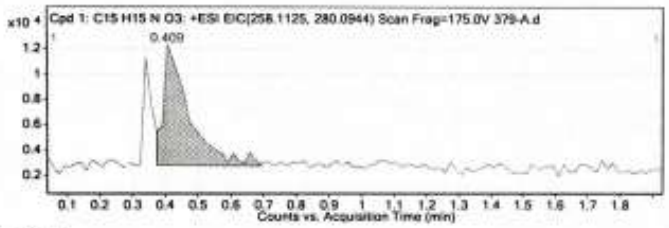
Data File	379-A.d	**Sample Name**	379-A
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	03-05-2024 13:39:48
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

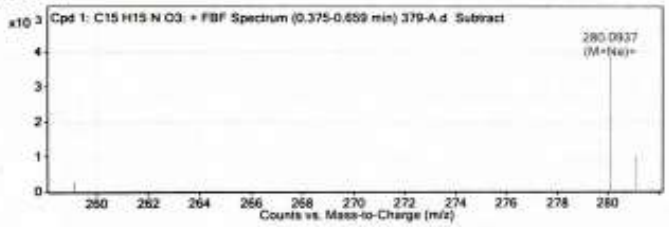
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C15 H15 N O3	0.409	257.1067	4004	C15 H15 N O3	257.1052	5.93	C15 H15 N O3	C15 H15 N O3

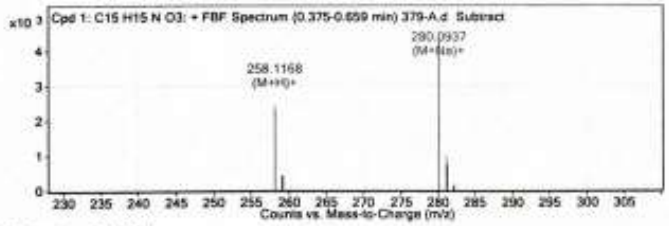
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C15 H15 N O3	280.0937	0.409	Find By Formula	257.1067



MS Spectrum



MS Zoomed Spectrum

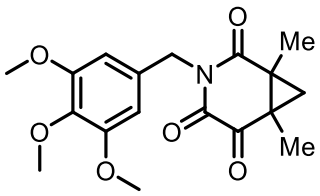


MS Spectrum Peak List

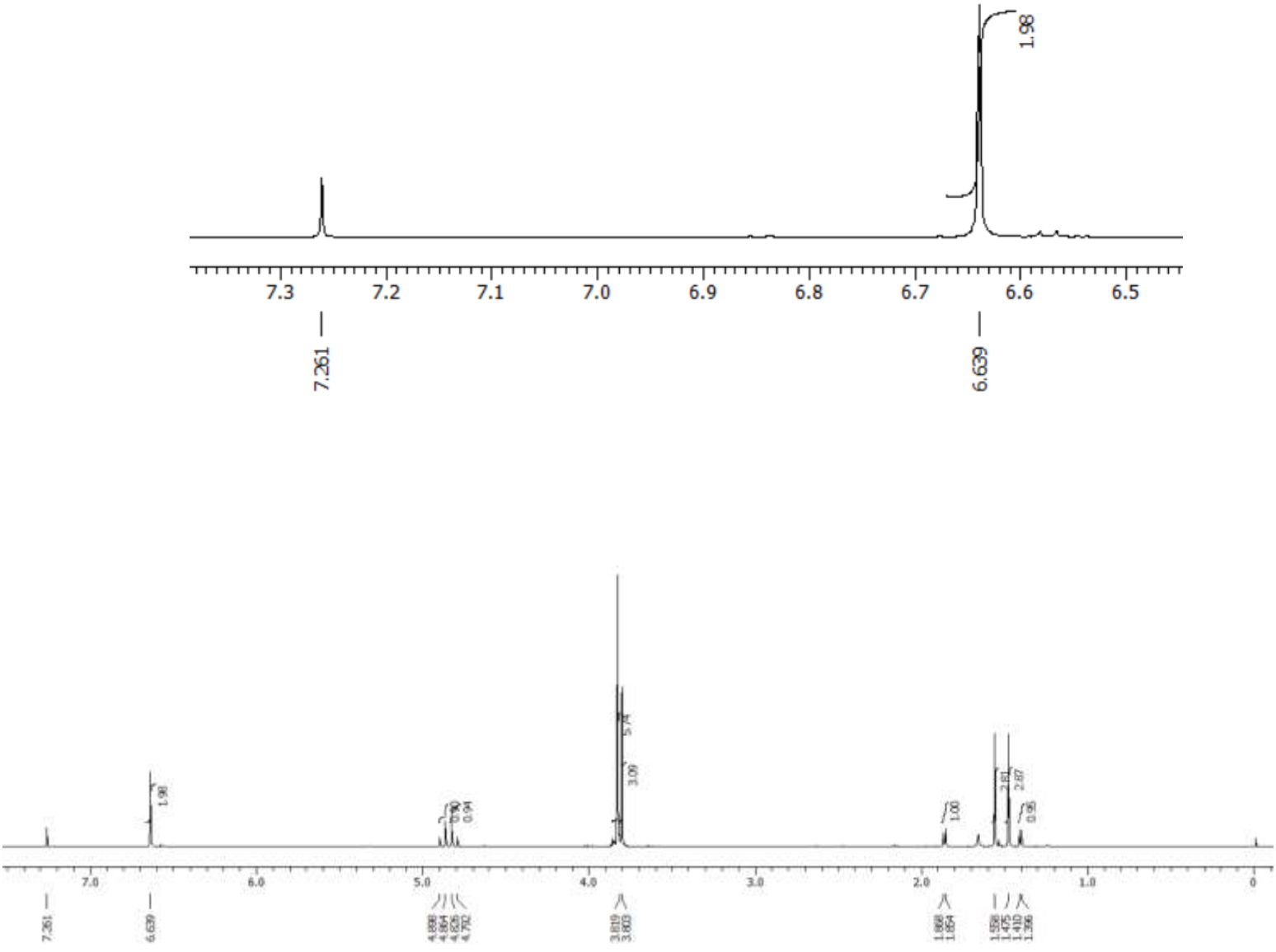
m/z	z	Abund	Formula	Ion
258.1168	1	2451.67	C15H16NO3	(M+H)+
259.1193	1	296.24	C15H16NO3	(M+H)+
280.0937	1	4003.77	C15H15NNaO3	(M+Na)+
281.0996	1	990.11	C15H15NNaO3	(M+Na)+
282.1063	1	204.34	C15H15NNaO3	(M+Na)+

--- End Of Report ---

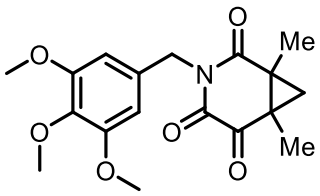
^{1}H NMR spectrum of 4k (400 MHz, $CDCl_3$)



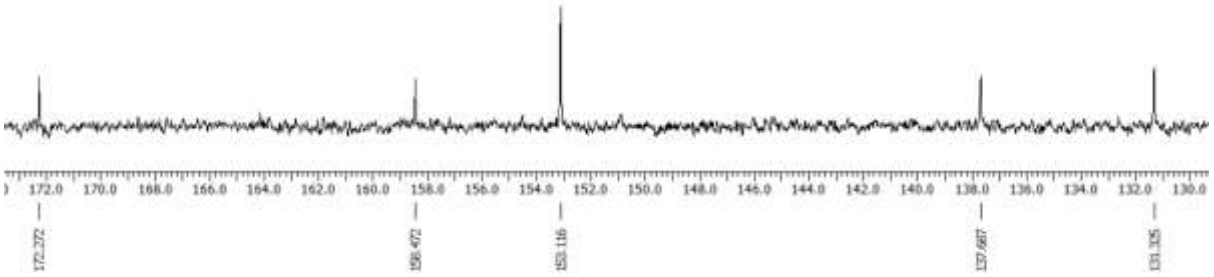
1,6-dimethyl-3-(3,4,5-trimethoxybenzyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

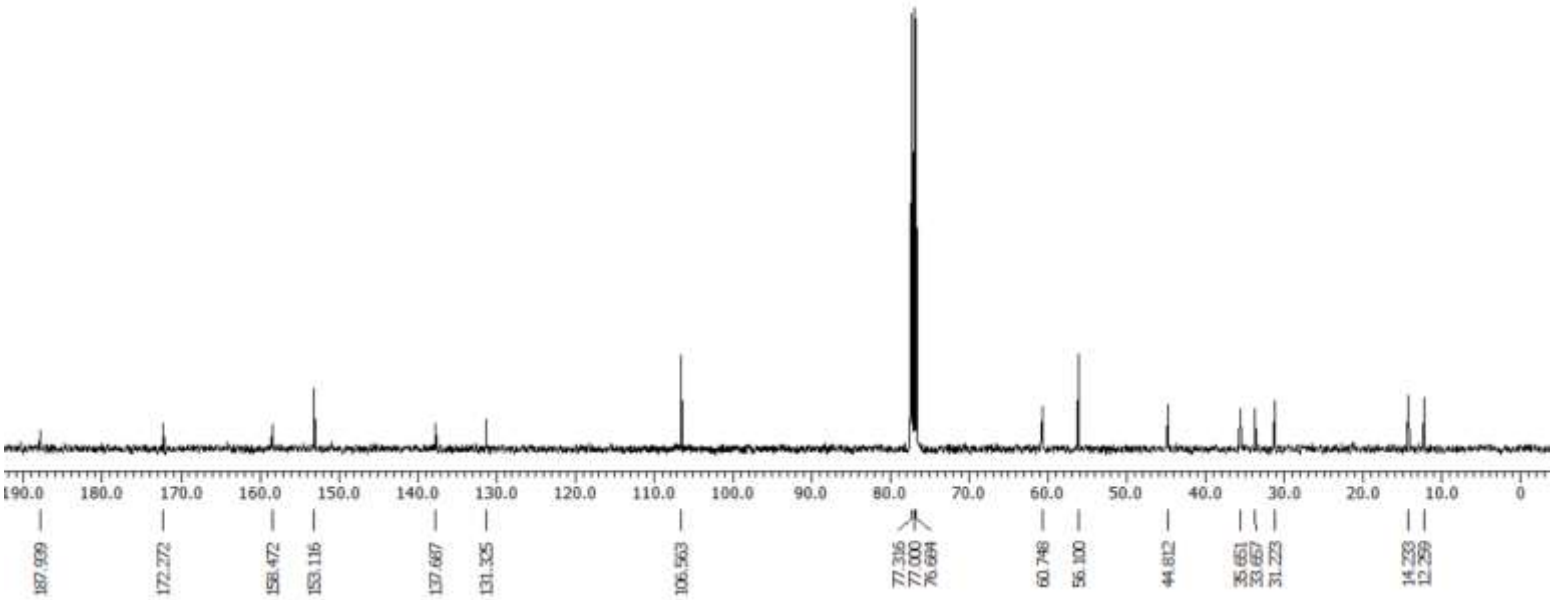


^{13}C NMR spectrum of 4k (100 MHz, $CDCl_3$)



1,6-dimethyl-3-(3,4,5-trimethoxybenzyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 4k

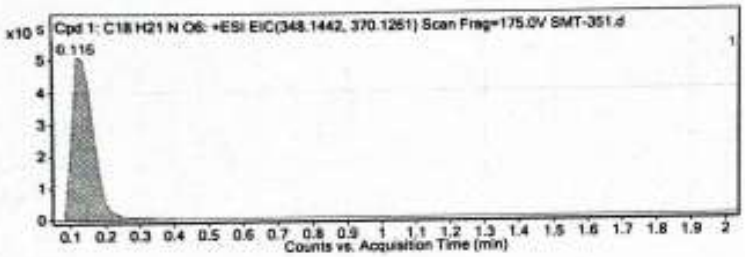
Qualitative Compound Report

Data File	SMT-351.d	Sample Name	SMT-351
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	08-11-2023 14:44:10
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)		

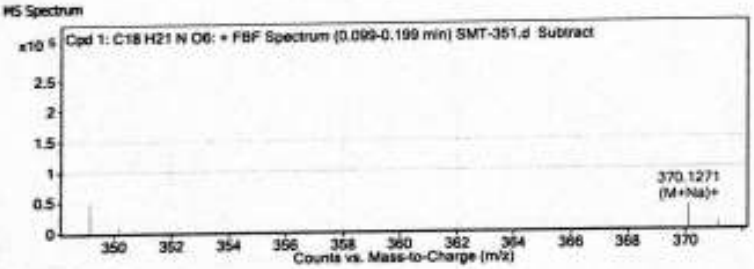
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C18 H21 N O6	0.116	347.137	256176	C18 H21 N O6	347.1369	0.47	C18 H21 N O6	C18 H21 N O6

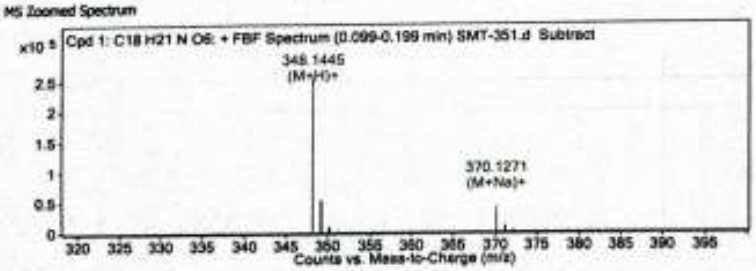
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H21 N O6	348.1445	0.116	Find By Formula	347.137



MS Spectrum



MS Zoomed Spectrum

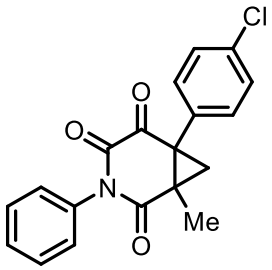


MS Spectrum Peak List

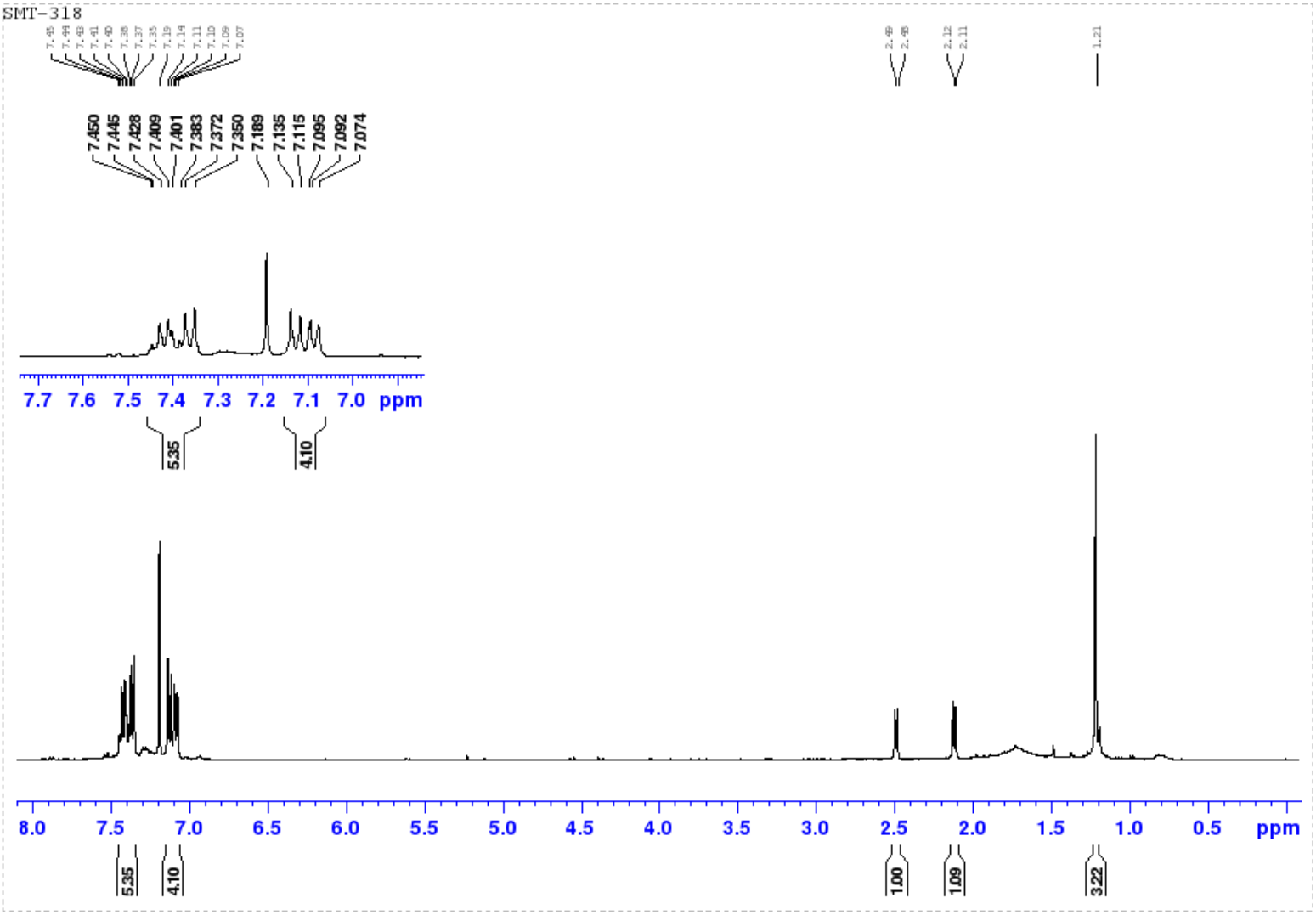
m/z	z	Abund	Formula	Ion
348.1445	1	256176.03	C18H22NO6	(M+H)+
349.1477	1	50212.76	C18H22NO6	(M+H)+
350.1501	1	8633.46	C18H22NO6	(M+H)+
351.1503	1	1313.11	C18H22NO6	(M+H)+
370.1271	1	38554.06	C18H21NNaO6	(M+Na)+
371.1317	1	9704.82	C18H21NNaO6	(M+Na)+
372.179	1	3355.55	C18H21NNaO6	(M+Na)+

--- End Of Report ---

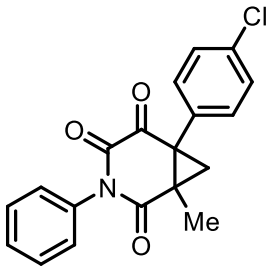
^{1}H NMR spectrum of 5a (400 MHz, $CDCl_3$)



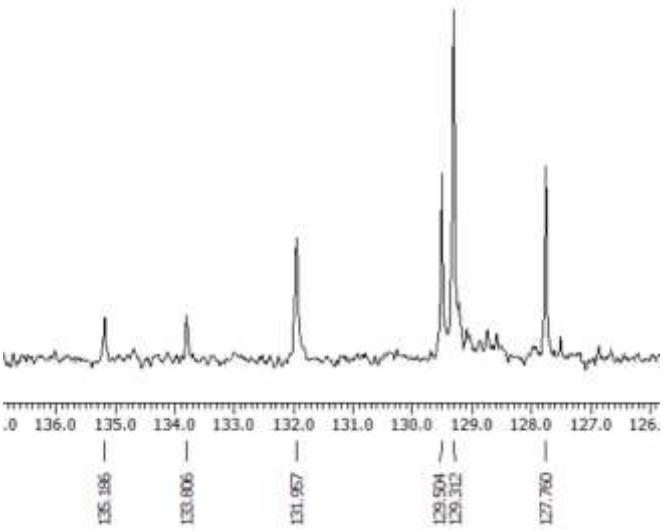
6-(4-chlorophenyl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

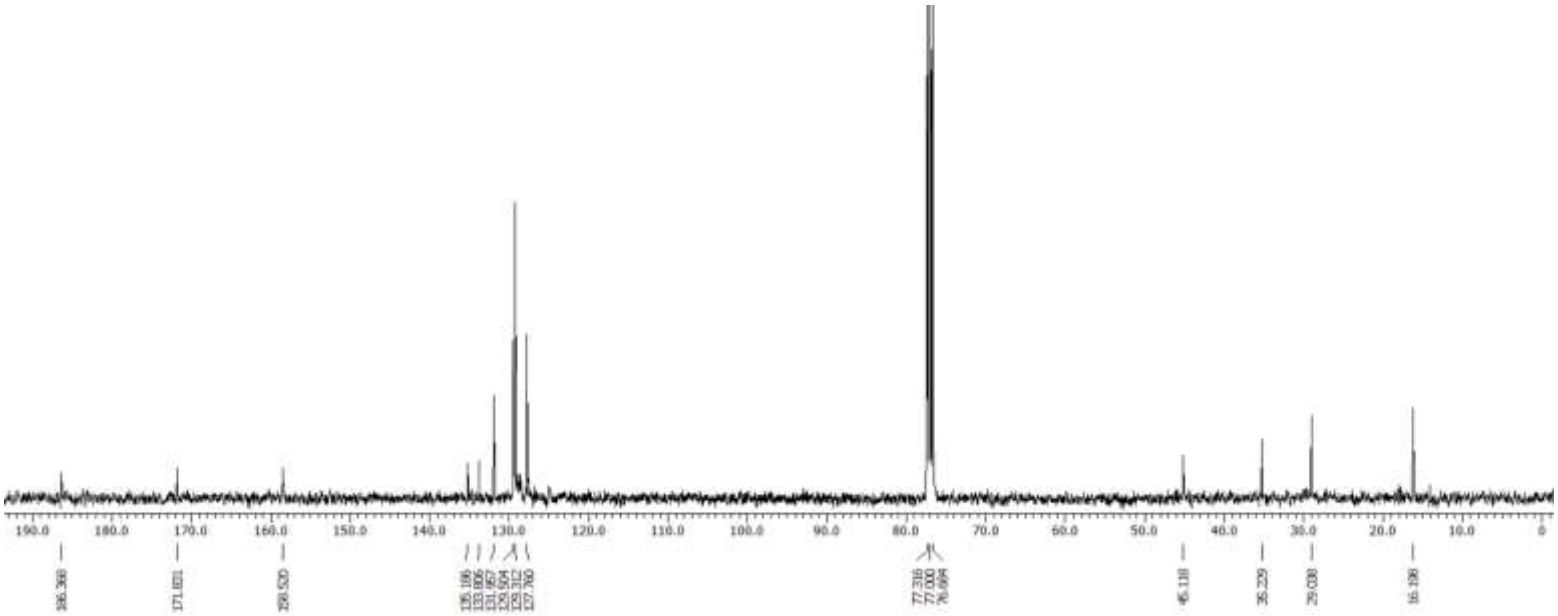


^{13}C NMR spectrum of 5a (100 MHz, $CDCl_3$)



6-(4-chlorophenyl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione





HRMS spectrum of 5a

Qualitative Compound Report

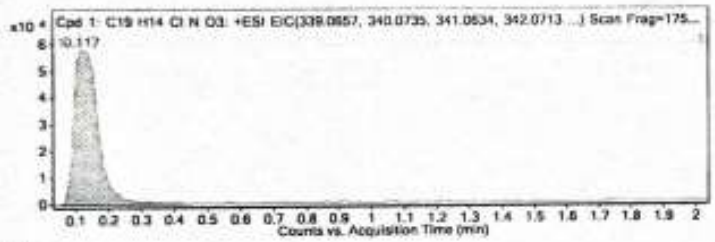
Data File	SMT-318.d	Sample Name	SMT-318
Sample Type	Sample	Position	P1-B3
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	11-09-2023 13:36:47
IRM Calibration Status	[redacted]	DA Method	Default.m
Comment			

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

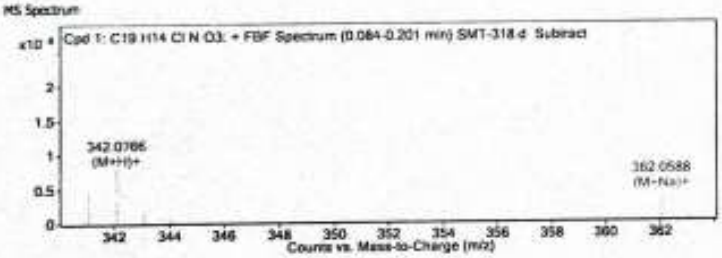
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C19 H14 Cl N O3	0.117	339.0694	21820	C19 H14 Cl N O3	339.0662	9.48	C19 H14 Cl N O3	[illegible]

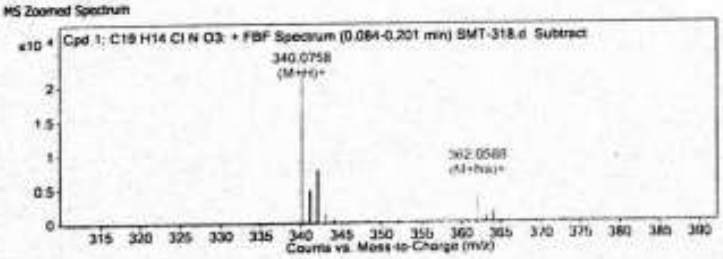
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H14 Cl N O3	340.0758	0.117	Find By Formula	339.0694



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
340.0758	1	21820.17	C19H15ClNO3	(M+H)+
341.0793	1	4239.5	C19H15ClNO3	(M+H)+
342.0766	1	7910.84	C19H15ClNO3	(M+H)+
343.0786	1	1786.13	C19H15ClNO3	(M+H)+
344.082	1	620.25	C19H15ClNO3	(M+H)+
362.0588	1	3979.56	C19H14ClNNaO3	(M+Na)+
363.0622	1	965.11	C19H14ClNNaO3	(M+Na)+
364.0576	1	1360.5	C19H14ClNNaO3	(M+Na)+

--- End Of Report ---

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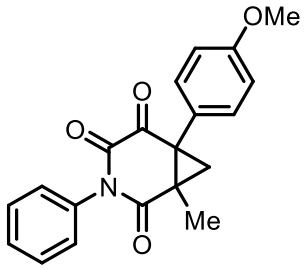
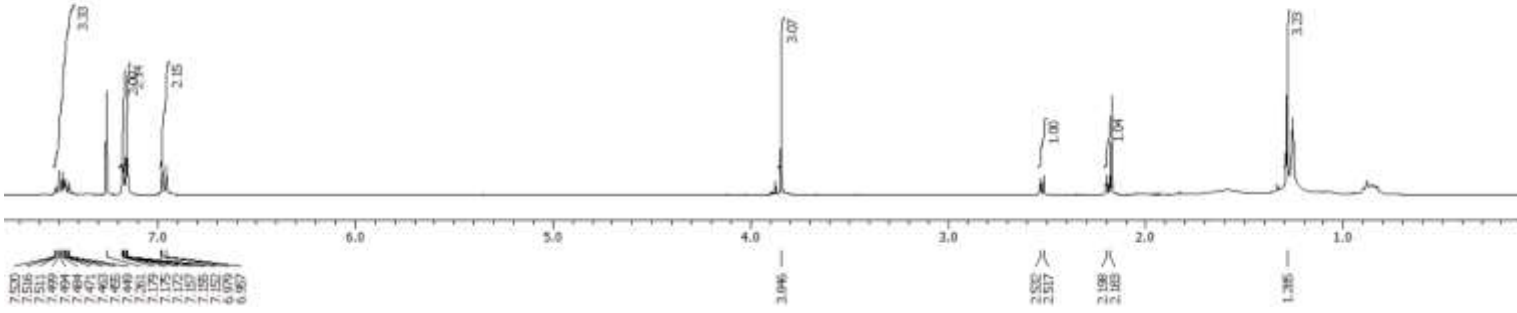
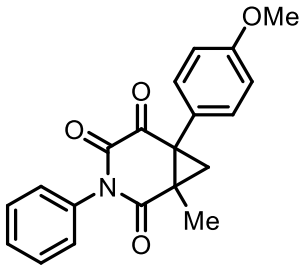
^{1}H NMR spectrum of 5b (400 MHz, $CDCl_3$)



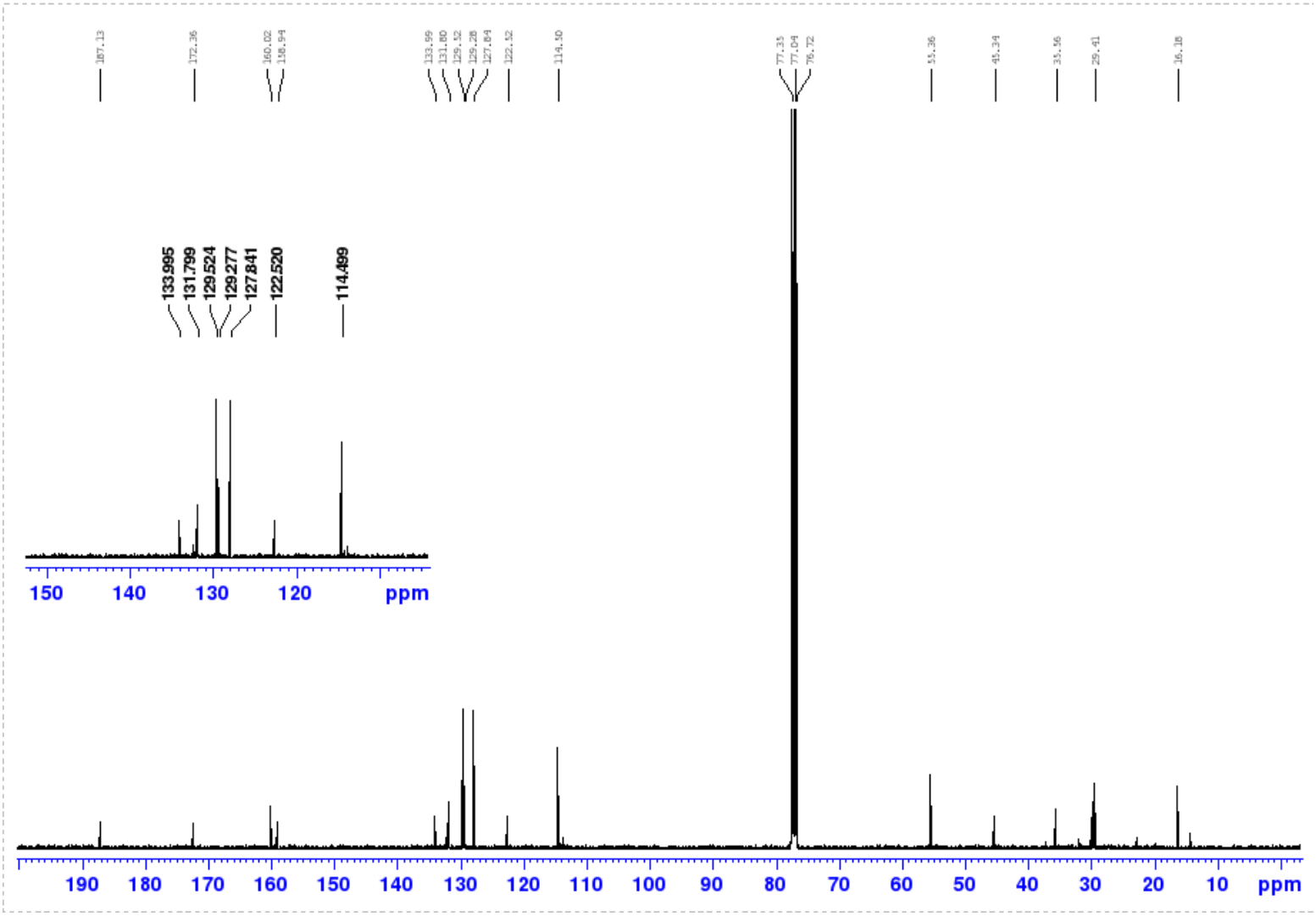
6-(4-methoxyphenyl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione



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

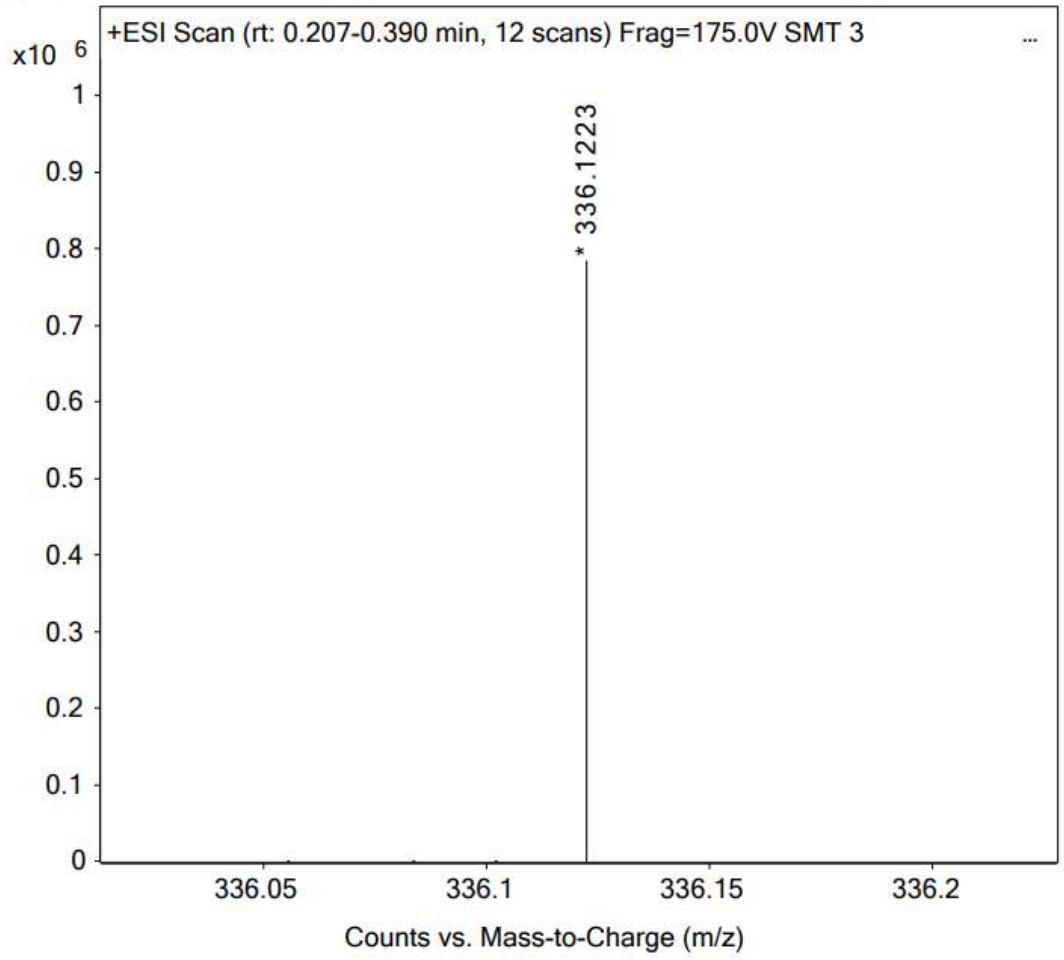


6-(4-methoxyphenyl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

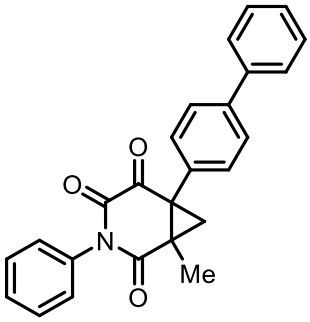


HRMS spectrum of 5b

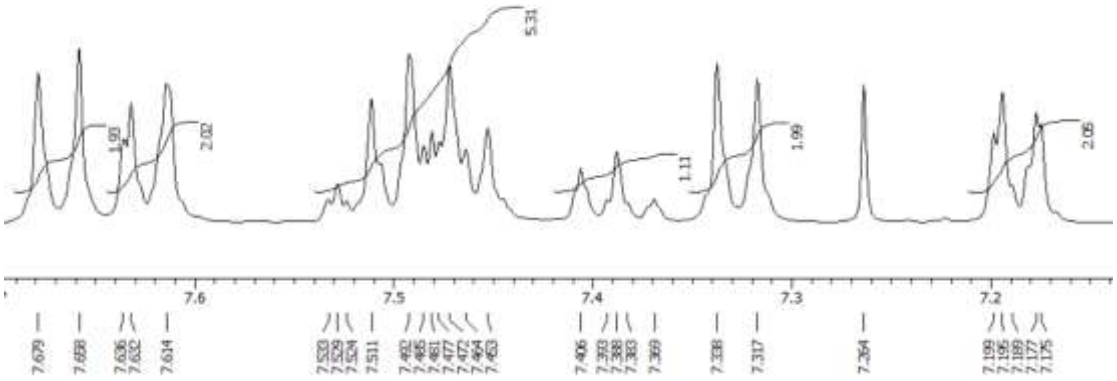
Sample Name	SMT 325	**Position**	P1-A1	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 325.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 10:53:36 (UTC+05:30)

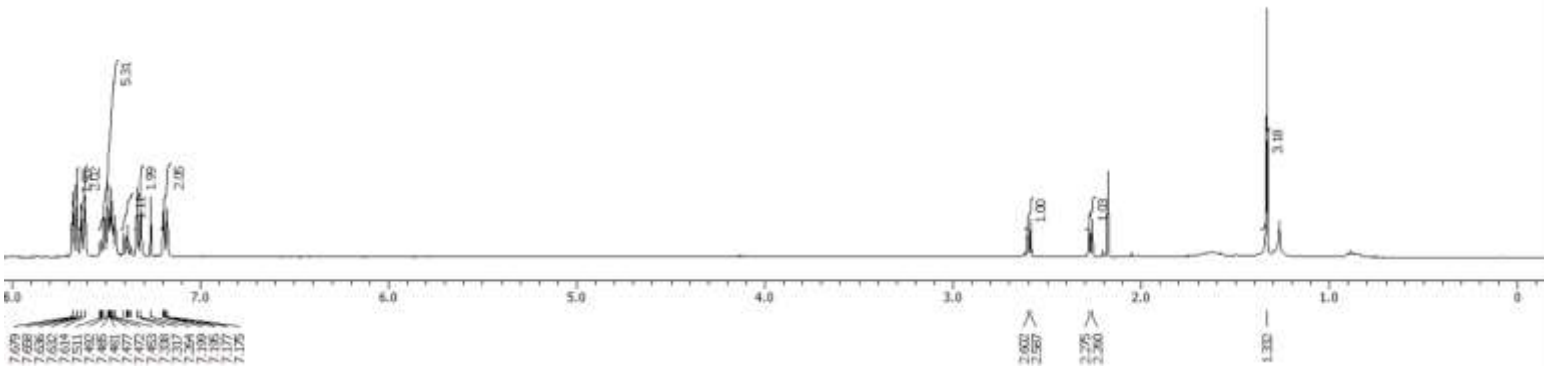


^{1}H NMR spectrum of 5c (400 MHz, $CDCl_3$)

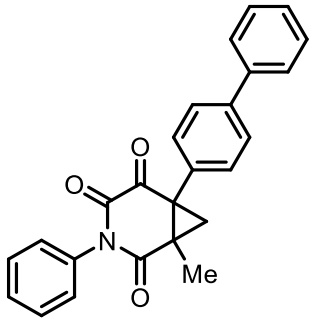


6-([1,1'-biphenyl]-4-yl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

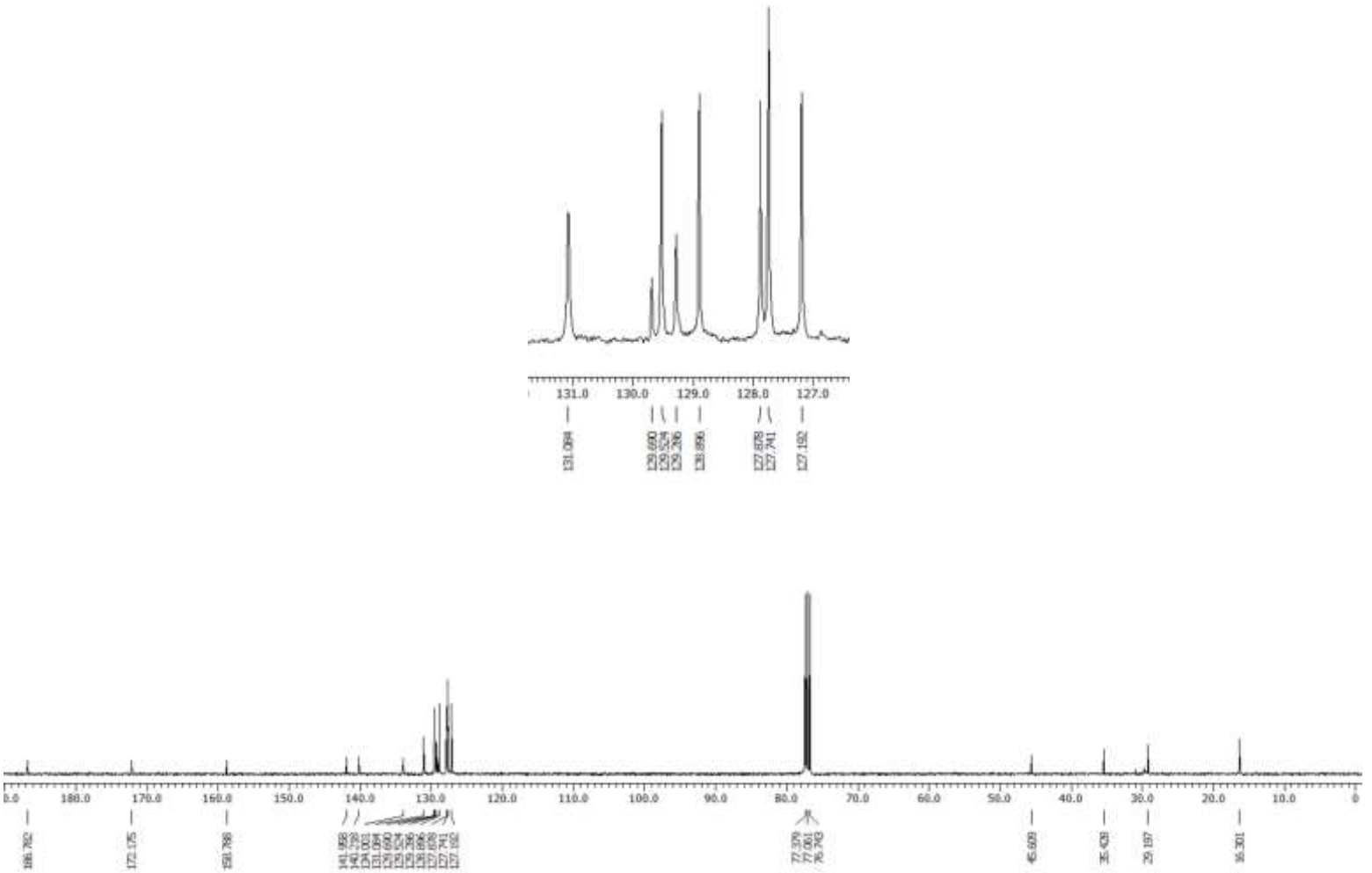




^{13}C NMR spectrum of 5c (100 MHz, $CDCl_3$)

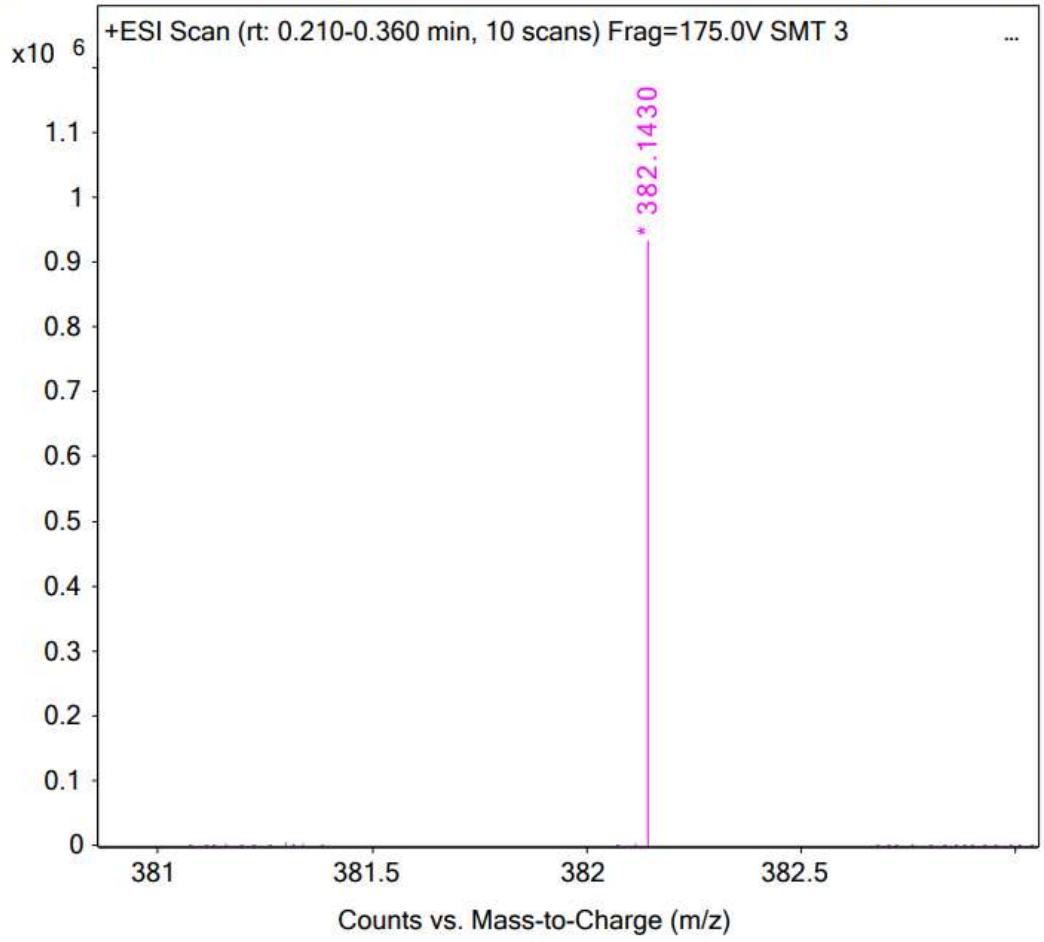


6-([1,1'-biphenyl]-4-yl)-1-methyl-3-phenyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

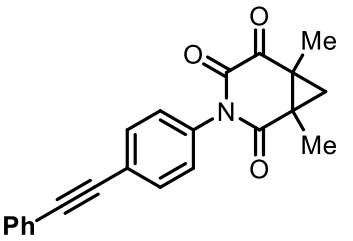


HRMS spectrum of 5c

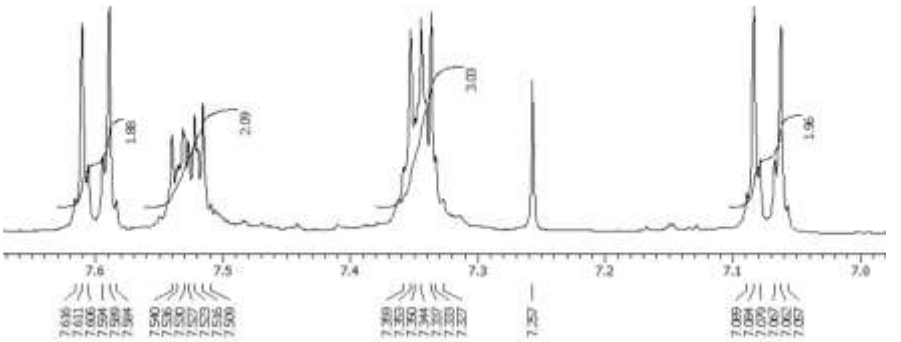
Sample Name	SMT 324	**Position**	P1-A9	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 324.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:11:44 (UTC+05:30)

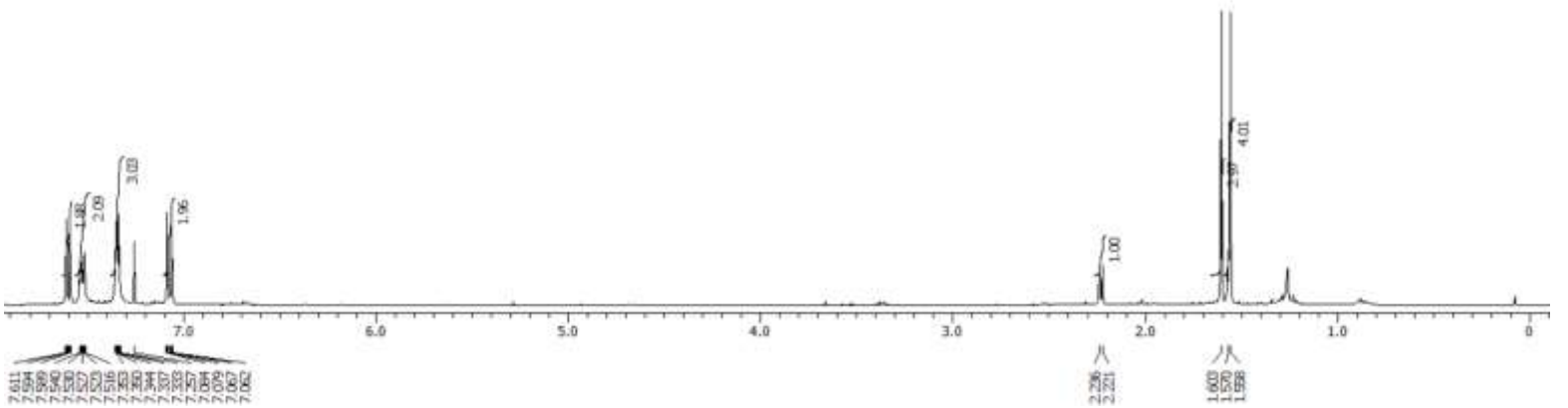


^{1}H NMR spectrum of 6 (400 MHz, $CDCl_3$)

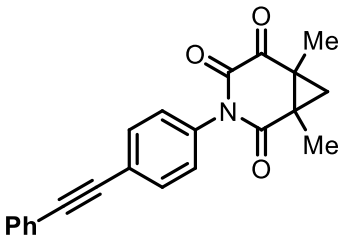


1,6-dimethyl-3-(4-(phenylethynyl)phenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione

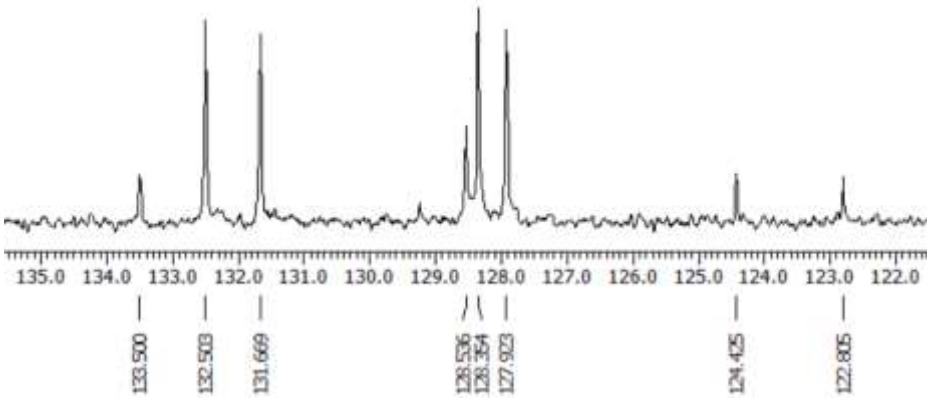


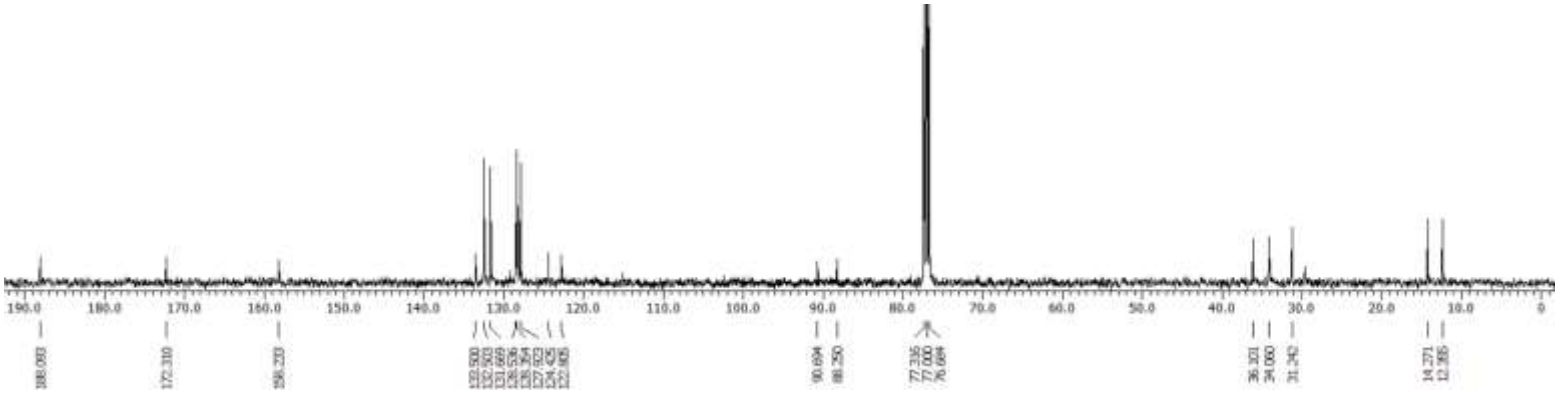


^{13}C NMR spectrum of 6 (100 MHz, $CDCl_3$)



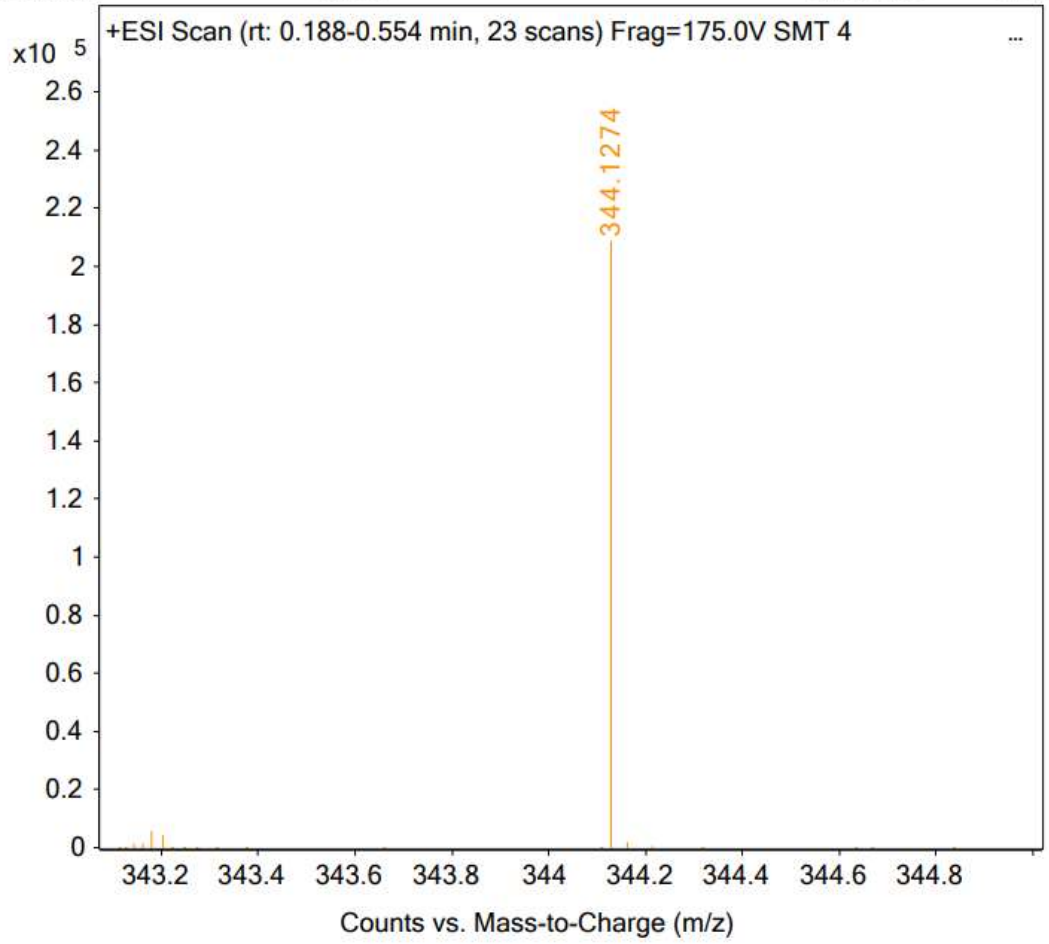
1,6-dimethyl-3-(4-(phenylethynyl)phenyl)-3-azabicyclo[4.1.0]heptane-2,4,5-trione



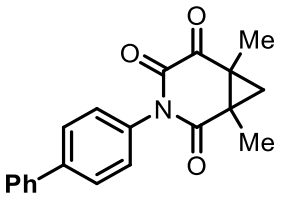


HRMS spectrum of 6

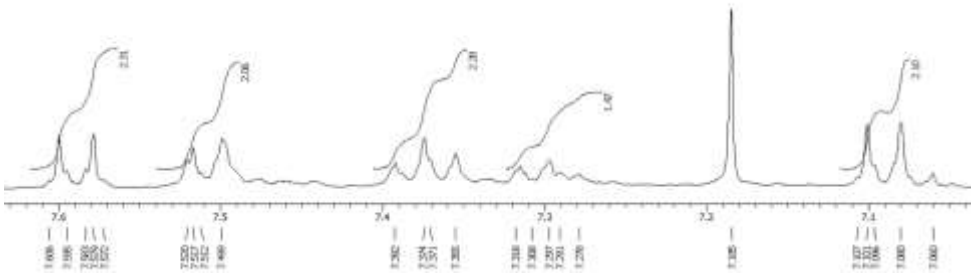
Sample Name	SMT 481	**Position**	P1-C6	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 481.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 13:25:12 (UTC+05:30)

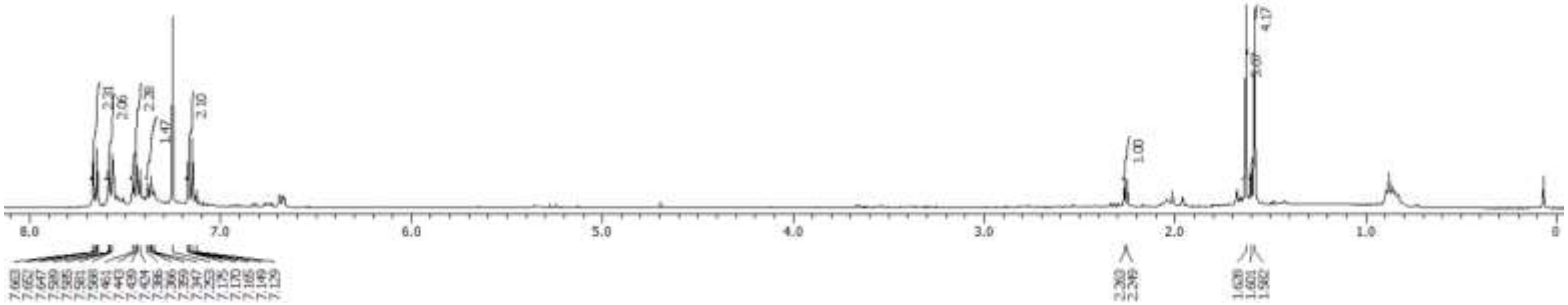


^{1}H NMR spectrum of 7 (400 MHz, $CDCl_3$)

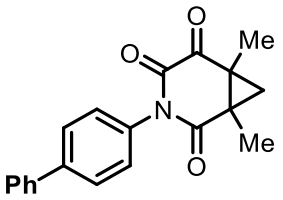


3-([1,1'-biphenyl]-4-yl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

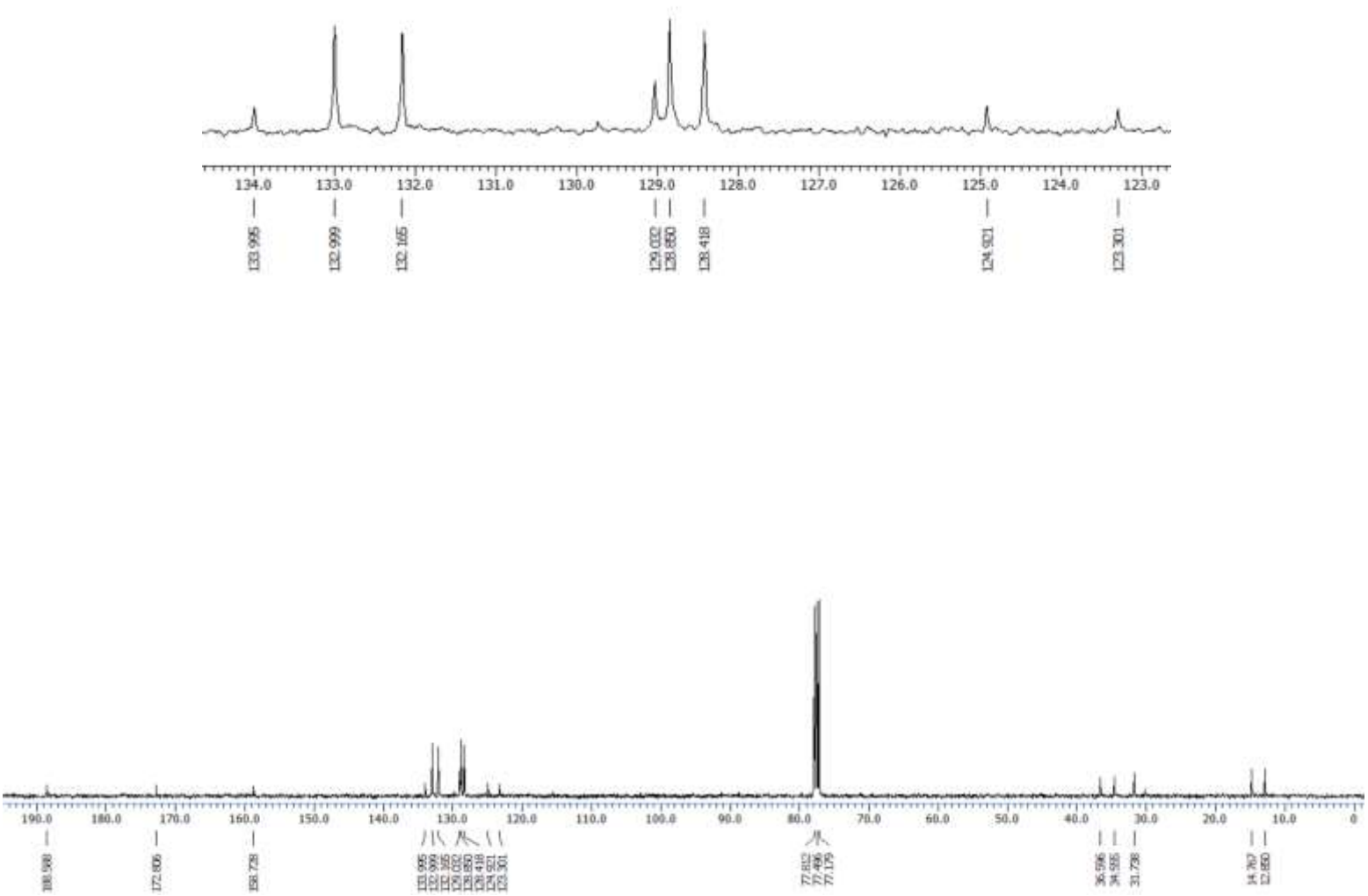




^{13}C NMR spectrum of 7 (100 MHz, $CDCl_3$)

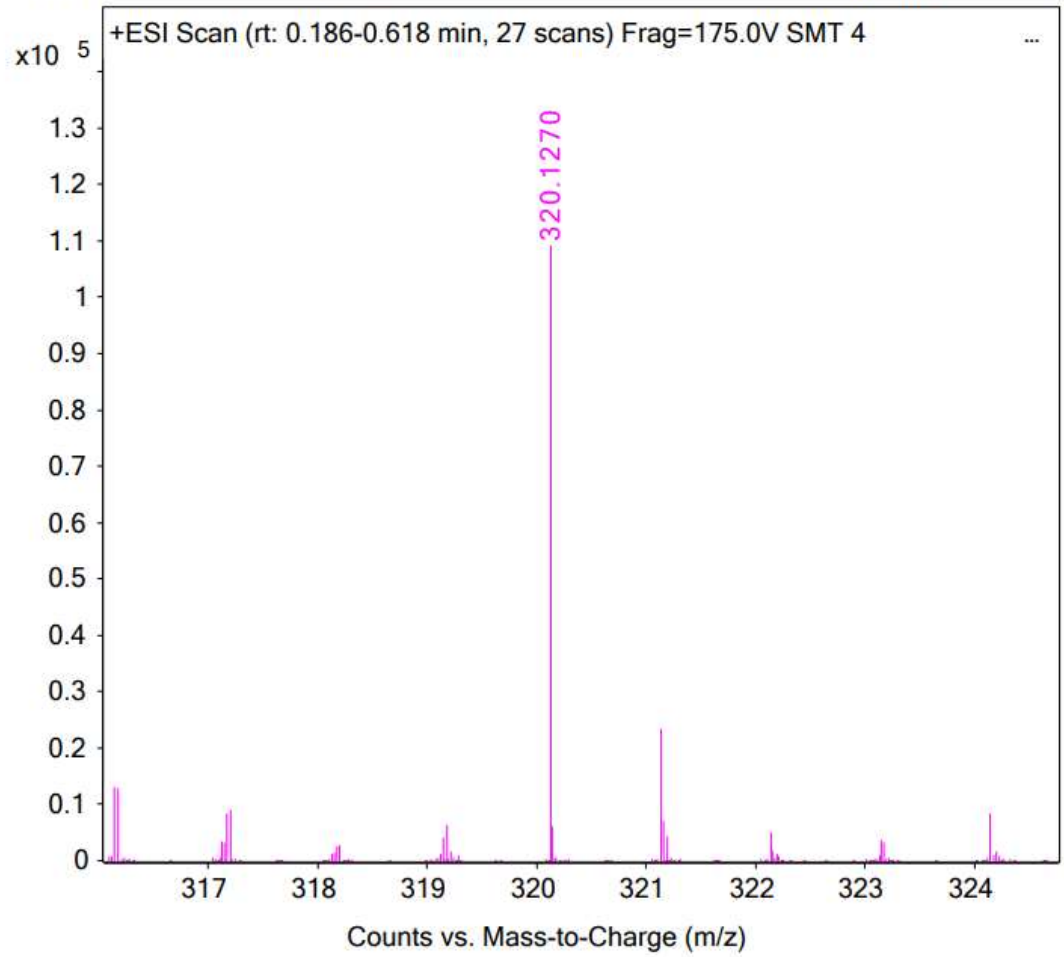


3-([1,1'-biphenyl]-4-yl)-1,6-dimethyl-3-azabicyclo[4.1.0]heptane-2,4,5-trione

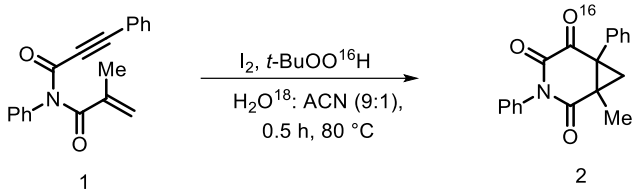


HRMS spectrum of 7

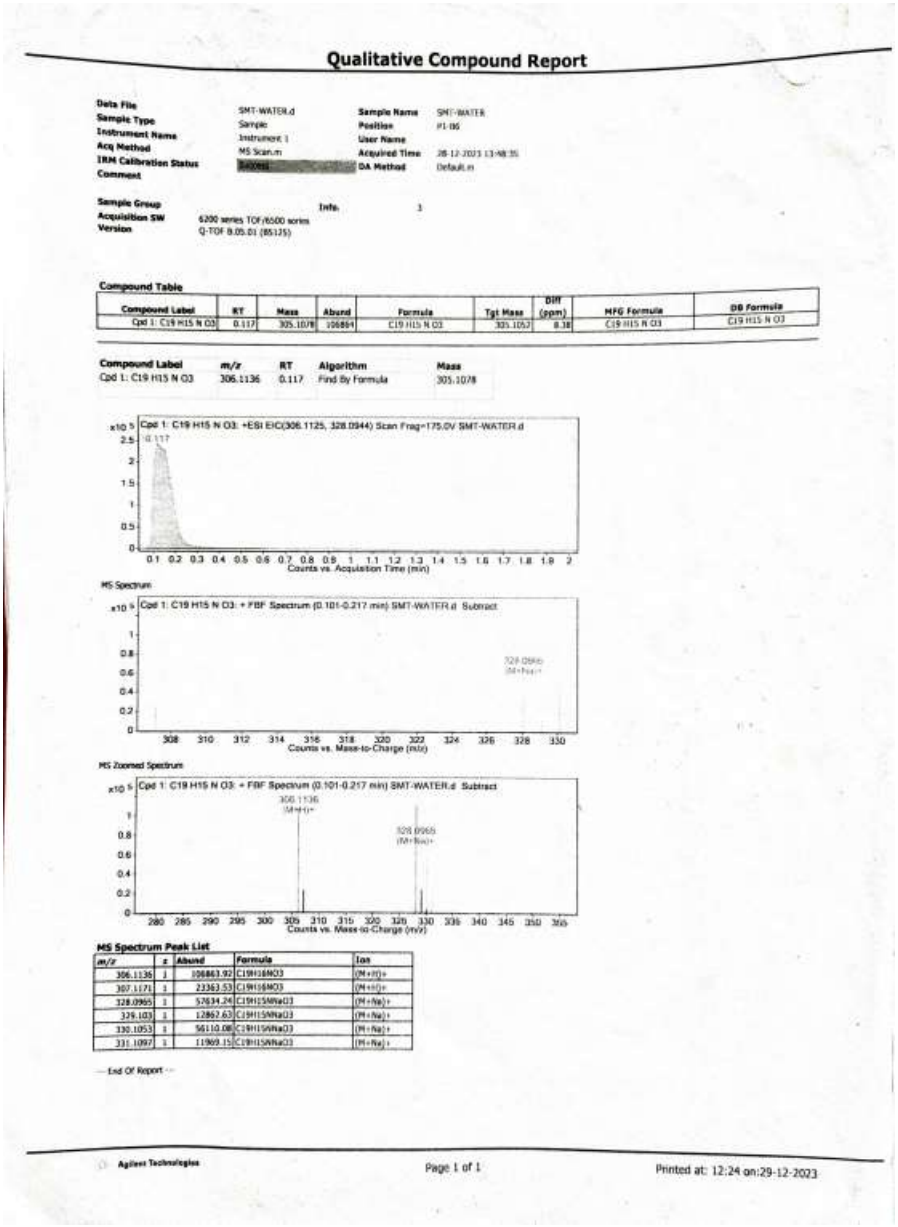
Sample Name	SMT 482	**Position**	P1-A8	**Instrument Name**	BIOQTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SMT 482.d
ACQ Method	Pos_100ACN.m	**Comment**		**Acquired Time**	27-04-2024 12:07:53 (UTC+05:30)



(10) Isotopic study:



Molecular Formula	Molecular weight	Molecular mass found
$C_{19}H_{15}NO_2O^{16}$	305.1078	306.1136



Qualitative Compound Report

Data File SMT-WATER.d
Sample Type Sample
Instrument Name Instrument 1
Acq Method MS Scan.m
IRM Calibration Status Success
Comment
Sample Name SMT-WATER
Position P1-B6
User Name
Acquired Time 28 12 2023 13:48:35
DA Method Default.m

Sample Group Info. 1
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: C19 H15 N O3	0.117	305.1078	106864	C19 H15 N O3	305.1052	8.38	C19 H15 N O3	C19 H15 N O3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H15 N O3	306.1136	0.117	Find By Formula	305.1078

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
306.1136	1	106863.92	C19H16NO3	(M+H)+
307.1171	1	23363.53	C19H16NO3	(M+H)+
328.0965	1	57634.24	C19H15NNaO3	(M+Na)+
329.103	1	12862.63	C19H15NNaO3	(M+Na)+
330.1053	1	56110.08	C19H15NNaO3	(M+Na)+
331.1097	1	11909.15	C19H15NNaO3	(M+Na)+

End Of Report

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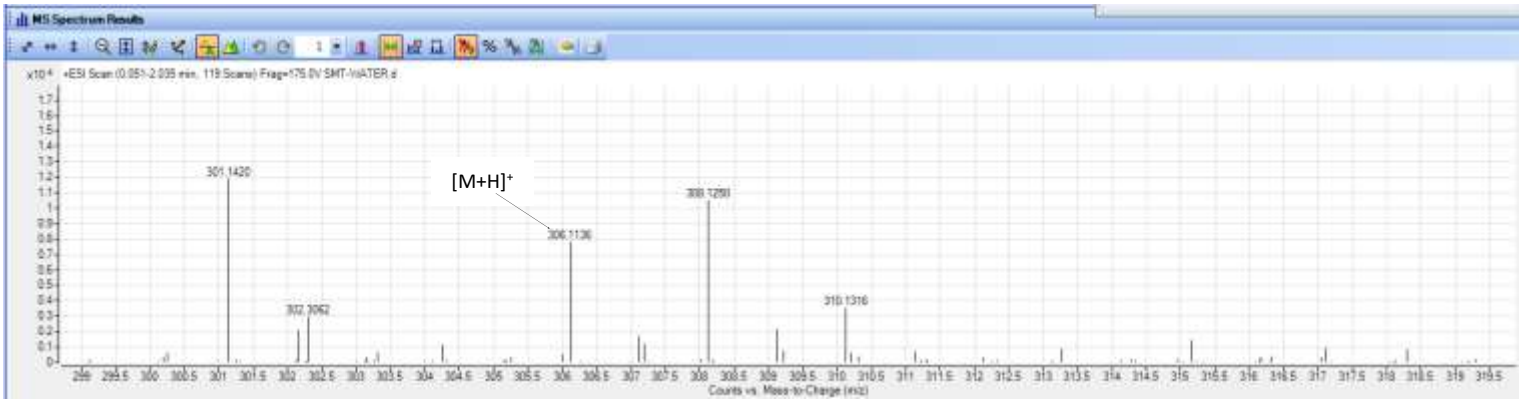
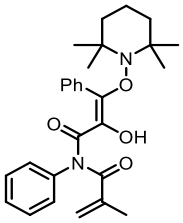


Figure S5: Mass spectrum

(11) Intermediate Adduct Data:

1) HRMS Data of TEMPO adduct:

Structure of TEMPO Adduct	Molecular Formula	Molecular weight	Molecular mass found
	$C_{28}H_{34}N_2O_4$	462.2526	463.2597

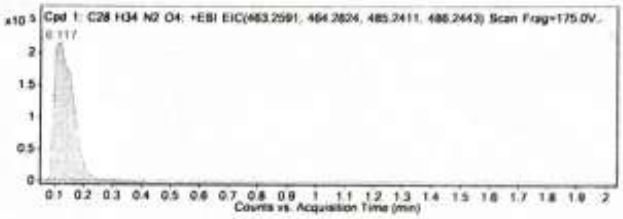
Qualitative Compound Report

Data File	SMT-TEMPO.d	Sample Name	SMT-TEMPO
Sample Type	Sample	Position	P1-B9
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	28.12.2023 13:40:55
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 (B5175)		

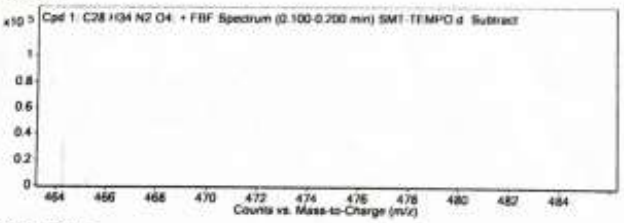
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C28 H34 N2 O4	0.117	462.2526	103329	C28 H34 N2 O4	462.2519	1.64	C28 H34 N2 O4	C28 H34 N2 O4

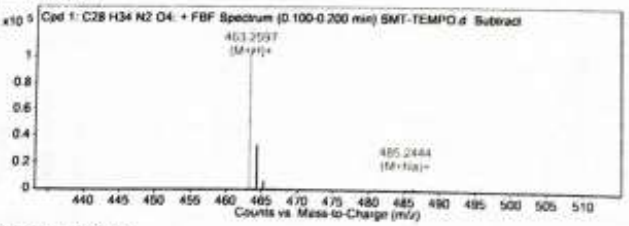
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C28 H34 N2 O4	463.2597	0.117	Find By Formula	462.2526



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
463.2597	1	103329.14	C28H35N2O4	(M+H)+
464.263	1	32288.25	C28H35N2O4	(M+H)+
465.2691	1	5909.44	C28H35N2O4	(M+H)+
466.2668	1	642.05	C28H35N2O4	(M+H)+
485.2444	1	1680.43	C28H34N2NaO4	(M+Na)+
486.2526	1	49.89	C28H34N2NaO4	(M+Na)+

--- End Of Report ---

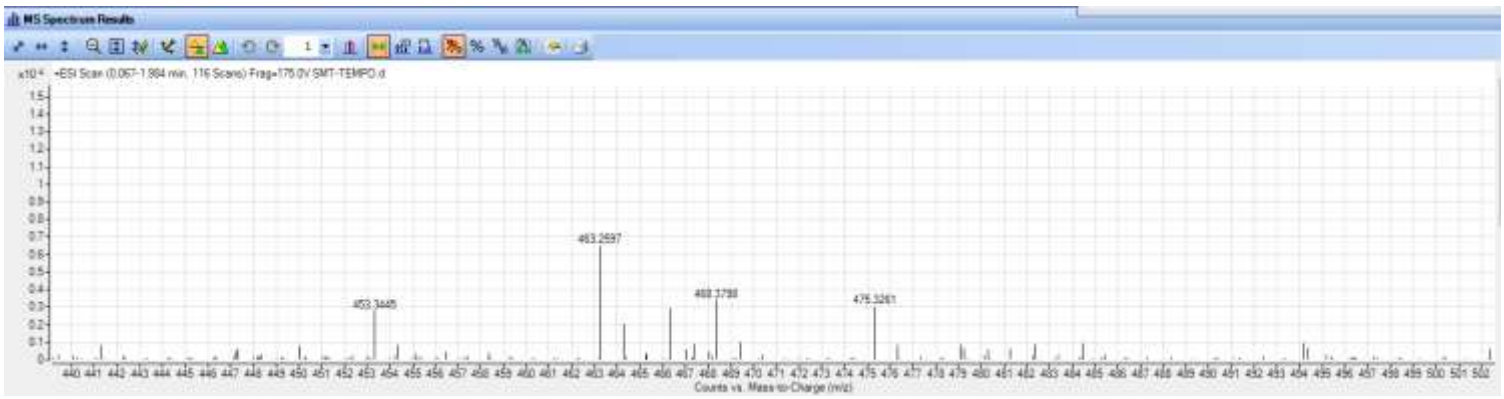
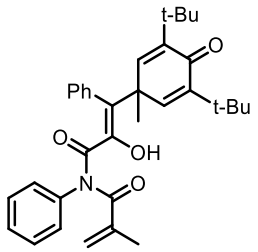


Figure S6: Mass spectrum of TEMPO adduct

2) HRMS Data of BHT adduct:

Compound	Molecular Formula	Molecular weight	Molecular mass found
	$C_{34}H_{39}NO_4$	525.2902	526.2976

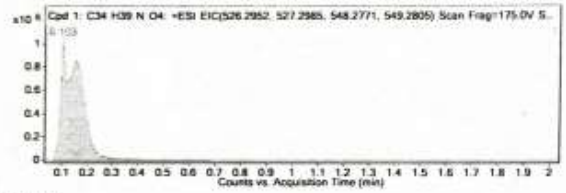
Qualitative Compound Report

Data File	SMT-BHT.d	Sample Name	SMT-BHT
Sample Type	Sample	Position	P1-B5
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	28-12-2023 13:44:45
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)		

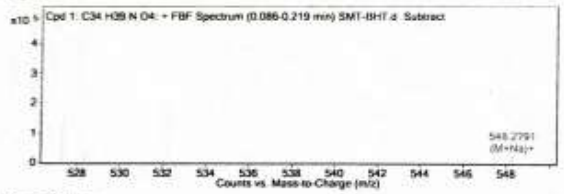
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C34 H39 N O4	0.103	525.2902	27800	C34 H39 N O4	525.2879	4.45	C34 H39 N O4	C34 H39 N O4

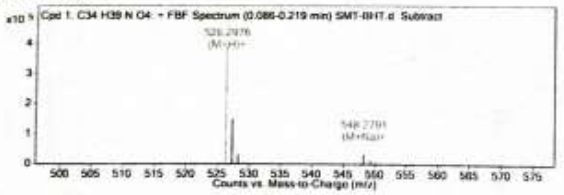
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C34 H39 N O4	548.2791	0.103	Find By Formula	525.2902



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
526.2976	1	394556.88	C34H40NO4	(M+H)+
527.3008	1	142982.61	C34H40NO4	(M+H)+
528.3037	1	28356.84	C34H40NO4	(M+H)+
529.3085	1	4353.88	C34H40NO4	(M+H)+
548.2791	1	27800.47	C34H39NNaO4	(M+Na)+
549.2822	1	10087.07	C34H39NNaO4	(M+Na)+
550.2877	1	2477.24	C34H39NNaO4	(M+Na)+

— End Of Report —

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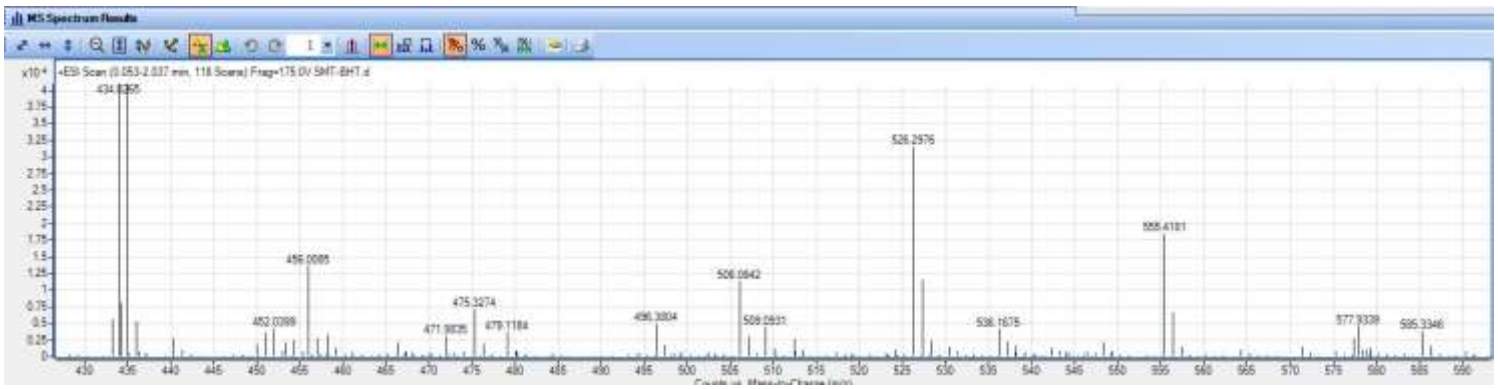

Figure S7: Mass Spectrum of BHT adduct

(12) References:

1) K. L. Vikse, M. P. Woods and J. S. McIndoe, *Organometallics*, 2010, **29**, 6615.

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