Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

Electricity Mediated [3+2]-cycloaddition of *N*-sulfonylcyclopropanes with Olefins via *N*-centered Radical Intermediates: Access to Cyclopentane Analogs

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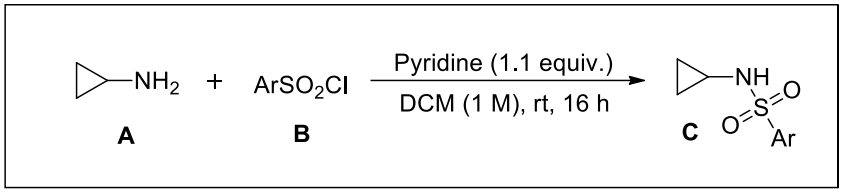
General Remarks

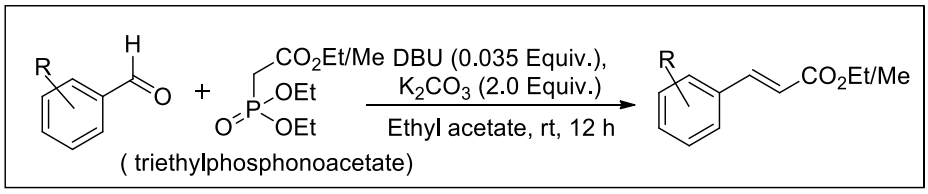
Electrochemical reactions were performed under air at room temperature using IKA Electrasyn 2.0 and DC power supply procured from Keysight technologies limited (Model: E36312A) and GW Instek limited (Model: GPP 3323). Acetonitrile and other solvents were obtained from Merck Life science Private Limited and were used directly without further purification and drying. Reagents like acrylates (spectrochem), acrylonitrile (spectrochem), methylvinyl ketone (TCI), styrene (sigma), diphenyl acrylamides, cyclopropylamine (spectrochem), sulfonyl chlorides (GLR innovations) were procured from various commercially available sources. Electrodes were commercially available from IKA. Cyclic voltammetry experiments were also performed on the CHI1110C instrument. The control of the measurement instrument, the acquisition, and processing of the cyclic voltammetric data was processed with the CH instruments electrochemical analyzer. Yields refer to isolated compounds, estimated to be >95% pure as determined by ^{1}H NMR. Thin-layer chromatography was performed on Merck precoated silica gel 60 F254 aluminum sheets with detection under UV light at 254 nm and charring with the *p*-anisaldehyde solution. Chromatographic purifications were performed with silica gel (230-400 mesh) and melting points were taken on Stuart digital melting point apparatus. Nuclear magnetic resonance (NMR) spectroscopy was performed using JEOL 400 MHz and HRMS was recorded on Waters Xevo G2-XS (Q-TOF) and Agilent Technologies 6530 Accurate- Mass Q-TOF LC/MS. If not otherwise specified, chemical shifts (δ) are provided in ppm and coupling constants are absolute values and are expressed in Hertz. Unless otherwise specified, all the ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$. Chemical shifts of ^{1}H and ^{13}C NMR spectra are expressed in parts per million (ppm) and coupling constant values were given in absolute. The description of the signals includes the following: s = singlet, d = doublet, dd = doublet of doublet, t = triplet, dt = doublet of triplet, q = quartet, br = broad, and m = multiplet.

A) General procedure for preparation of *N*-sulfonylcyclopropylamines. (GP1)[1]



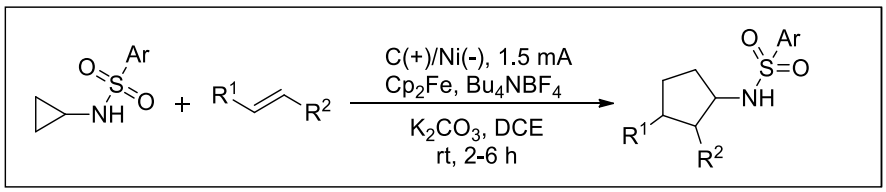
To an oven-dried round bottom flask, cyclopropylamine (1.1 equiv.) was added dichloromethane and the reaction was cooled to 0°C under a nitrogen atmosphere. Further, triethylamine (Et_3N) (1.1 equiv.) was added dropwise, followed by the corresponding arylsulfonyl chloride (1.0 equiv.). The reaction was then brought to room temperature and stirred for 16 h. The reaction solution was quenched with H_2O (10 mL) and further extracted with ethyl acetate (2 X 20 mL). The combined organic layers were washed with brine solution (10 mL) dried over Na_2SO_4 and were further concentrated in vacuo. The crude obtained was purified using silica gel (230-400) column chromatography, where the desired compound was eluted in 20% ethyl acetate in hexane in 80-90% yield.

B) General procedure for preparation of Ethyl/methyl cinnamates. (GP2)[2]



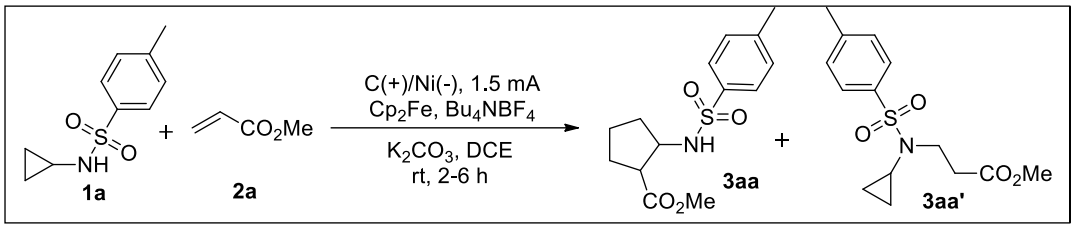
Triethyl phosphonoacetate (1.1 equiv), DBU (0.035 equiv), and finely powdered anhydrous K_2CO_3 (2.0 equiv) were taken in an oven-dried round-bottom flask, and ArCHO (1.0 equiv) was added. The resulting mixture was stirred at room temperature for 4 h. Ethyl acetate was added to the crude mixture, and the solid was filtered off. The solid was washed with ethyl acetate, and the combined filtrate was concentrated in vacuo. The resulting oil was purified using silica gel (mesh size 230-400) column chromatography to give the corresponding alkene (84% yield) (*E*/*Z* = 99:1).

C) Representative procedure for electrochemical [3+2] cycloaddition reaction. (RP1)



An Electrasyn vial/ test tube was equipped with a magnetic stir bar and was added corresponding *N*-sulfonyl cyclopropane (1.0 equiv.), alkene (3.0 equiv.), ferrocene (0.5 equiv.), tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) (2.0 equiv.), potassium carbonate (2.0 equiv.) in dichloroethane solvent (0.04 M). Further, the vial/test tube was purged with an argon balloon for 1-2 minutes and the solution was electrolyzed with carbon anode and nickel cathode at a constant current of 1.5 mA (voltage range of 2.8 V-3.2 V) for 2-6 h at room temperature (25°-30°C). Upon completion (as monitored by TLC), evaporation of solvent gave the crude product. The crude obtained was then purified by silica gel column chromatography (230-400 mesh) and the desired product was eluted at 30% ethyl acetate in hexane.

D) Optimization studies



In an oven-dried undivided reaction flask (10 mL) equipped with a stir bar was added *N*-cyclopropyl-4-methylbenzenesulfonamide (1.0 equiv.), methyl acrylate (3.0 equiv.), base (2.0 equiv.), mediator (0.5 equiv.), electrolyte (2.0 equiv.) and solvent (5 mL). The solution was electrolyzed at a constant current at room temperature under an argon atmosphere for 2-12 h. The solvent was evaporated in vacuo and the crude mixture was purified by silica gel column chromatography using 20-30% ethyl acetate in hexane to get methyl (1*R*,2*R*)-2-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate (**3aa**) in 59-85% isolated yields.

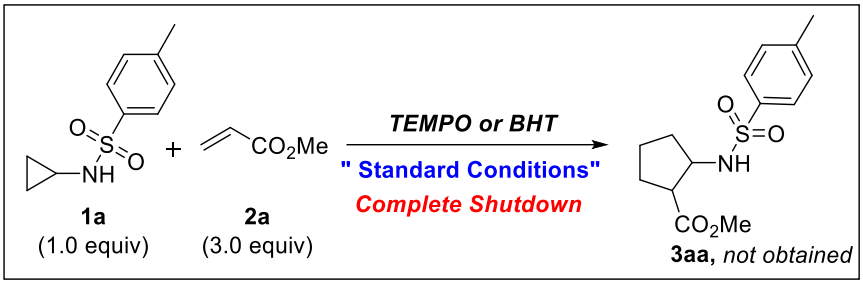
S.No	Electrode	Supporting Electrolyte	Mediator	Base	Current	solvent	Time (h)	% Yield of 3aa
1.	C(+)/C(-)	Bu_4NBF_4	-	-	1.5	CH_3CN	3	N.R.
2.	C(+)/Ni(-)	Bu_4NBF_4	-	K_2CO_3	1.5	CH_3CN	3.5	55 (3aa')
3.	C(+)/Ni(-)	Bu_4NBF_4	-	K_2CO_3	1.5	HFIP	3	N.R.
4.	C(+)/Ni(-)	Bu_4NPF_6	-	K_2CO_3	1.5	CH_3CN	3	c.m.
5.	C(+)/C(-)	Bu_4NBF_4	-	K_2CO_3	1.5	CH_3CN	3	N.R.
6.	C(+)/Ni(-)	Bu_4NOAc	-	K_2CO_3	1.5	CH_3CN	3	N.R.
7.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	CH_3CN: H_2O	4	34
8.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	CH_3CN: H_2O	8	28
9.	C(+)/Ni(-)	Bu_4NPF_6	Cp_2Fe	K_2CO_3	1.5	CH_3CN: H_2O	4	12
10.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	Na_2CO_3	1.5	CH_3CN: H_2O	4	20
11.	C(+)/Cu(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	CH_3CN: H_2O	5	N.R.
12.[a]	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	CH_3CN: H_2O	4	N.R.
13.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	Et_3N	1.5	CH_3CN	5	N.R.
14.	C(+)/Ni(-)	Bu_4NBF_4	-	DBU	1.5	CH_3CN	5	N.R.
15.	**C(+)/Ni(-)**	**Bu_4NBF_4**	**Cp_2Fe**	**K_2CO_3**	**1.5**	**DCE**	**5**	**62**
16.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	Na_2CO_3	1.5	DCE	5	57
17.[b]	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	DCE	5	43
18.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	0.5	DCE	5	38
19.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	2.5-3.0	DCE	5	47
20.	C(+)/Ni(-)	Et_4NOTs	Cp_2Fe	K_2CO_3	1.5	DCE	5	N.R
21.	C(+)/Ni(-)	LiOTf	Cp_2Fe	K_2CO_3	1.5	DCE	5	N.R
22.	C(+)/Ni(-)	Bu_4NPF_6	Cp_2Fe	K_2CO_3	1.5	DCE	5	N.R
23.	C(+)/Pt(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	DCE	5	N.R
24.	C(+)/Cu(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	DCE	5	N.R

25.	Pt(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	DCE	5	N.R
26.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	DMSO	5	N.R
27.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	DMF	5	N.R
28.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	HFIP	5	N.R
29.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	K_2CO_3	1.5	DCE: H_2O	4	42
30.	C(+)/Ni(-)	Bu_4NBF_4	Cp_2Fe	-	1.5	DCE	5	22

All the reactions are performed at room temperature of 25 °C-30 °C [a]Reaction performed without electricity, [b] 0.1M instead of 0.04M.

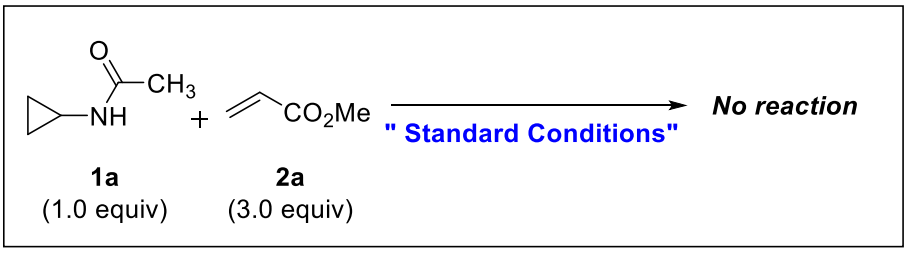
E) Mechanistic Studies

a) **Radical scavenging experiment**



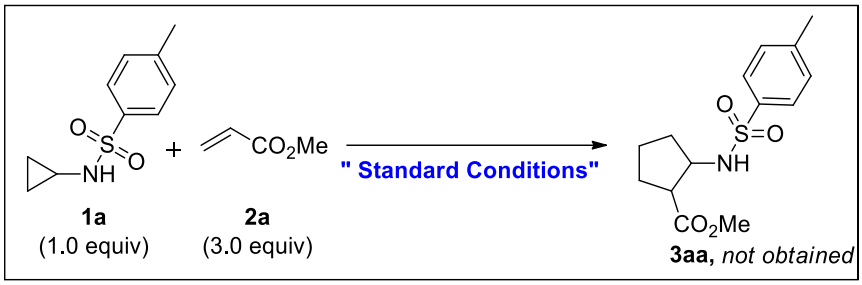
An Electrasyn vial/ test tube was equipped with a magnetic stir bar and was added corresponding *N*-sulfonyl cyclopropane (1.0 equiv.), alkene (3.0 equiv.), ferrocene (0.5 equiv.), tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) (2.0 equiv.), potassium carbonate (2.0 equiv.) in dichloroethane solvent (0.04M). Further, the vial/test tube was purged with an argon balloon for 1-2 minutes and the solution was electrolyzed with carbon anode and nickel cathode at a constant current of 1.5 mA (voltage range of 2.8 V-3.2 V) for 2-6 h at room temperature (25°-30°C). The progress of the reaction was monitored by TLC, which shows that starting material remain unconsumed. This infers that employing TEMPO completely shut down the reaction indicating the possibility of a radical path for the reaction.

b) **Unsuccessful experiment**



An Electrasyn vial/ test tube was equipped with a magnetic stir bar and was added corresponding *N*-acetyl cyclopropane (1.0 equiv.), alkene (3.0 equiv.), ferrocene (0.5 equiv.), tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) (2.0 equiv.), potassium carbonate (2.0 equiv.) in dichloroethane solvent. Further, the vial/test tube was purged with an argon balloon for 1-2 minutes and the solution was electrolyzed with carbon anode and nickel cathode at a constant current of 1.5 mA (voltage range of 3.0 V-4.0 V) for 2-6 h at room temperature (25°-30°C). The progress of the reaction was monitored by TLC, which shows that starting material remain unconsumed. This infers that replacement of tosyl group with acetyl group proved detrimental for the reaction.

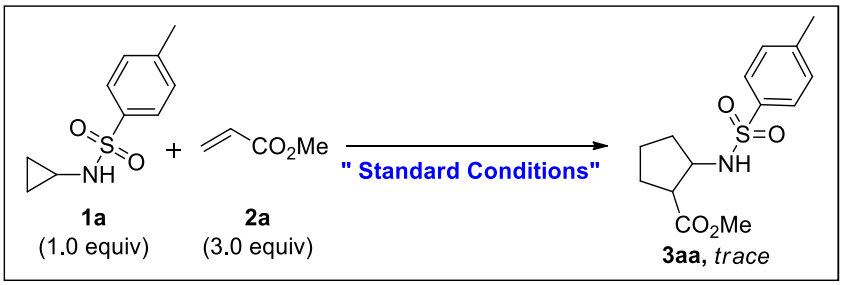
c) **Divided cell experiment**



Case 1: In anodic chamber: A divided cell was equipped with two magnetic stir bars in anodic and cathodic chamber respectively. Further, the anodic chamber was filled with corresponding *N*-tosyl cyclopropane (1.0 equiv.), alkene (3.0 equiv.), ferrocene (0.5 equiv.), tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) (2.0 equiv.), potassium carbonate (2.0 equiv.) in dichloroethane solvent. The cathodic chamber was filled with supporting electrolyte solution and further both the chambers were purged with an argon for 1-2 minutes and the solution was electrolyzed with carbon anode (in anodic chamber) and nickel cathode (in cathodic chamber) at a constant current of +1.5 mA (voltage range of +2.8 V to +3.4 V) for 2-6 h at room temperature (25°-30°C). The progress of the reaction was monitored by TLC, which shows that starting material remain unconsumed. This infers that the cathodic reduction is a key factor in the reaction.

Case 2: In cathodic chamber: A divided cell was equipped with two magnetic stir bars in anodic and cathodic chamber respectively. Further, the cathodic chamber was filled with corresponding *N*-tosyl cyclopropane (1.0 equiv.), alkene (3.0 equiv.), ferrocene (0.5 equiv.), tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) (2.0 equiv.), potassium carbonate (2.0 equiv.) in dichloroethane solvent. The anodic chamber was filled with supporting electrolyte solution and further both the chambers were purged with an argon for 1-2 minutes and the solution was electrolyzed with carbon anode (in anodic chamber) and nickel cathode (in cathodic chamber) at a constant current of -1.5 mA (voltage range of -2.8 V to -3.4 V) for 2-6 h at room temperature (25°-30°C). The progress of the reaction was monitored by TLC, which shows that starting material remain unconsumed. This infers that the reaction gets initiated by the oxidation of cyclopropyl amines.

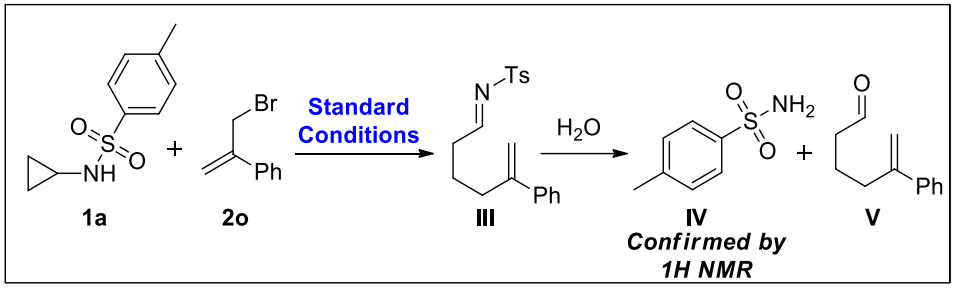
d) **Time based electrolysis**



An Electrasyn vial/ test tube was equipped with a magnetic stir bar and was added corresponding *N*-sulfonyl cyclopropane (1.0 equiv.), alkene (3.0 equiv.), ferrocene (0.5 equiv.), tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) (2.0 equiv.), potassium carbonate (2.0 equiv.) in dichloroethane solvent (0.04M). Further, the vial/test tube was purged with an argon for 1-2 minutes and the solution was electrolyzed with carbon anode and nickel cathode at a constant current of 1.5 mA (voltage range of 2.8 V-3.2 V) for 1 h at room temperature (25°-30°C). The progress of the reaction was monitored by TLC, which shows that starting material remain unconsumed with trace amount of product formation After, that the reaction was stirred overnight without electricity. Again, the progress of the reaction was monitored by TLC, which

indicated that a similar TLC was observed. Further, the reaction mixture was purified through column chromatography and approx. 70% of the starting material was recovered. This indicates that the chain propagation step is absent in this case.

e) **Intermediate detection experiment**



An Electrasyn vial/ test tube was equipped with a magnetic stir bar and was added corresponding *N*-sulfonyl cyclopropane (1.0 equiv.), (3-bromoprop-1-en-2-yl)benzene (3.0 equiv.) (**2o**), ferrocene (0.5 equiv.), tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) (2.0 equiv.), potassium carbonate (2.0 equiv.) in dichloroethane solvent (0.04M). Further, the vial/test tube was purged with an argon balloon for 1-2 minutes and the solution was electrolyzed with carbon anode and nickel cathode at a constant current of 1.5 mA (voltage range of 2.8 V-3.2 V) for 5 h at room temperature (25°-30°C). The progress of the reaction was monitored by TLC, which shows that starting material gets consumed. Further, the reaction mixture was passed through the silica gel column (230-400) at 40% ethylacetate in hexane to remove the supporting electrolyte. Next, the reaction mixture obtained after passing through column was submitted for HRMS. HRMS studies demonstrate the presence of intermediate III and further the purification of reaction mixture delivered the IV (NMR attached at the end). These studies indicate that the reaction follows an anionic pathway.

c) **Cyclic Voltammetry**

Cyclic voltammograms were collected with the three-electrode CHI1110C instrument. The control of the measurement instrument, the acquisition, and processing of the cyclic voltammetric data were performed with the CH instruments electrochemical analyzer. Measurements employed a glassy carbon working electrode, platinum wire counter electrode, and a 3 M KCl silver-silver chloride reference electrode. Samples were prepared with 0.05 mmol of substrate **1a**, 0.05 mmol of substrate **2a**, 0.1 mmol of K_2CO_3, 0.01 mmol of Cp_2Fe dissolved in 5 mL acetonitrile containing 0.1 M Bu_4NBF_4. The scan rate applied was 0.1 V/s. the maximum current (Ip) and potential (Ep) of each substrate was obtained using Origin. All the CV experiments were carried out in nitrogen atmosphere and demonstrated as follows: (a) Blank (black) (b) **2a** (Red) (c) **1a** (Blue) (d) **Cp_2Fe** (Brown) (e) **1a + Cp_2Fe** (Dark blue) (f) **1a + Cp_2Fe + K_2CO_3** (Purple) (g) **1a + 2a** (Pink) (h) **1a + 2a + K_2CO_3** (Green) (i) **1a + 2a + K_2CO_3 + K_2CO_3** (Violet)

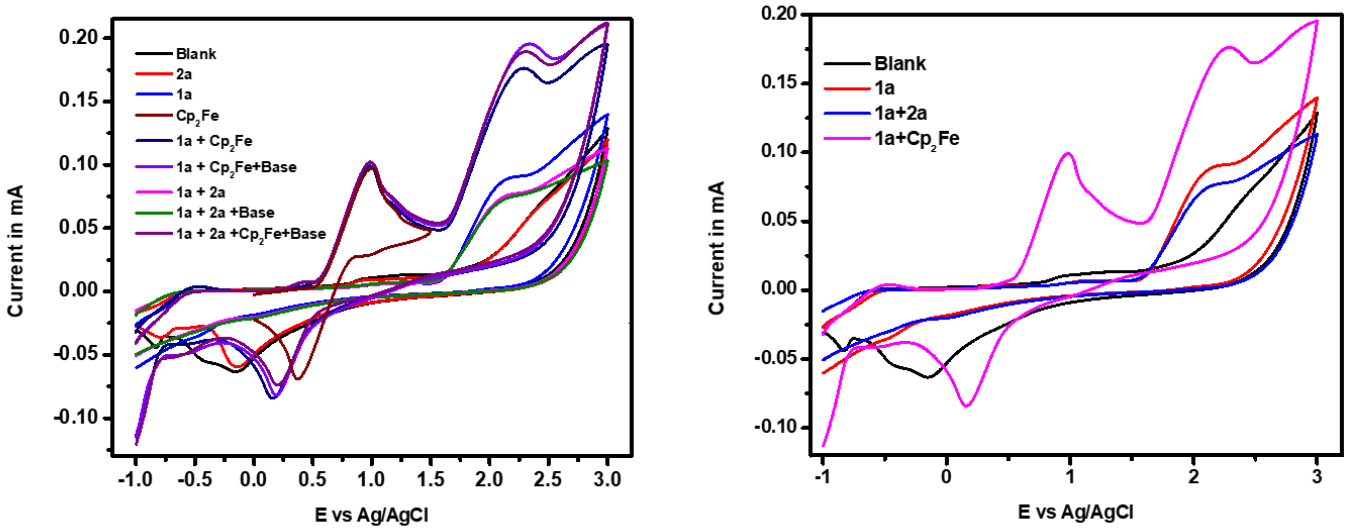
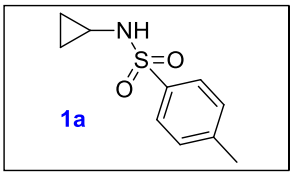


Figure S1: Cyclic Voltammetry experiment

Conclusion: Cyclic Voltammetry experiments indicate the importance of ferrocene and base for the cycloaddition reaction. As demonstrated by the above experiments the introduction of ferrocene enhances the catalytic current making the process more feasible to take place. Although as expected the potential does not shift to the lower region but the electrocatalytic effect led to a huge improvement in the reaction profile. A similar result was observed when the base was added to the same reaction mixture. In conclusion, ferrocene plays a significant role in the generation of *N*-center radical which results in the cycloaddition reaction with acrylate.

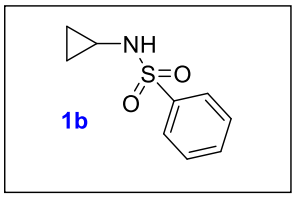
F) Characterization data of Starting materials

a) *N*-cyclopropyl-4-methylbenzenesulfonamide ***(1a)*** [1]



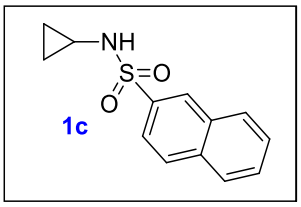
Prepared according to **GP1**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.77 (d, *J* = 8.3 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 5.08 (s, 1H), 2.41 (s, 1H), 2.24 – 2.17 (m, 1H), 0.60 – 0.52 (m, 1H).

b) *N*-cyclopropylbenzenesulfonamide ***(1b)*** [1]



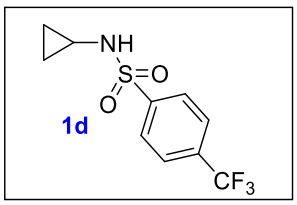
Prepared according to **GP1**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.93 – 7.87 (m, 1H), 7.59 (ddd, *J* = 6.4, 4.2, 1.3 Hz, 1H), 7.55 – 7.49 (m, 1H), 4.94 (s, 1H), 2.27 – 2.20 (m, 1H), 0.62 – 0.56 (m, 1H).

c) *N*-cyclopropylnaphthalene-2-sulfonamide ***(1c)*** [1]



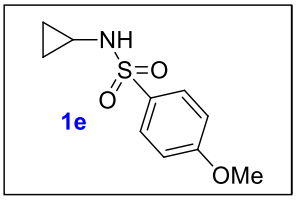
Prepared according to **GP1**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.49 (s, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.86 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.68 – 7.58 (m, 1H), 5.03 (s, 1H), 2.29 – 2.22 (m, 1H), 0.64 – 0.55 (m, 1H).

d) *N*-cyclopropyl-4-(trifluoromethyl)benzenesulfonamide ***(1d)***



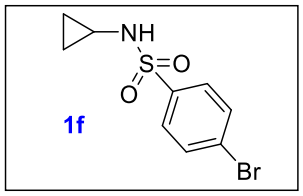
Prepared according to **GP1**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.03 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.3 Hz, 1H), 5.12 (s, 1H), 2.30 – 2.23 (m, 1H), 0.64 – 0.59 (m, 1H).

e) *N*-cyclopropyl-4-methoxybenzenesulfonamide ***(1e)*** [1]



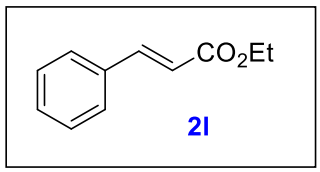
Prepared according to **GP1**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.84 – 7.80 (m, 1H), 7.00 – 6.95 (m, 1H), 4.82 (s, 1H), 3.86 (s, 1H), 2.26 – 2.19 (m, 1H), 0.59 – 0.54 (m, 1H).

f) 4-bromo-*N*-cyclopropylbenzenesulfonamide ***(1f)*** [1]



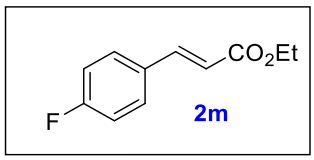
Prepared according to **GP1**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.78 – 7.74 (m, 1H), 7.68 – 7.64 (m, 1H), 4.86 (s, 1H), 2.28 – 2.22 (m, 1H), 0.60 (d, *J* = 5.0 Hz, 1H).

g) Ethyl cinnamate ***(2l)***[2]



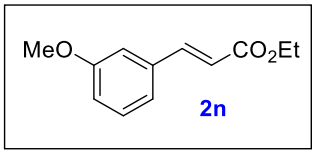
Prepared according to **GP2**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.66 (t, *J* = 11.3 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.40 – 7.34 (m, 1H), 6.43 (d, *J* = 16.0 Hz, 1H), 4.25 (q, *J* = 7.1 Hz, 1H), 1.33 (dd, *J* = 9.5, 4.8 Hz, 1H).

h) (E)-ethyl 3-(4-fluorophenyl)acrylate ***(2m)*** [2]



Prepared according to **GP2**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.62 (d, *J* = 16.0 Hz, 1H), 7.52 – 7.45 (m, 1H), 7.05 (t, *J* = 8.6 Hz, 1H), 6.34 (d, *J* = 16.0 Hz, 1H), 4.24 (q, *J* = 7.2 Hz, 1H), 1.31 (t, *J* = 7.1 Hz, 1H).

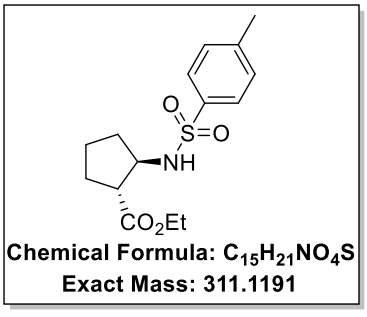
i) *(*E)-ethyl 3-(4-methoxyphenyl)acrylate ***(2n)*** [2]



Prepared according to **GP2**. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.63 (d, *J* = 16.0 Hz, 1H), 7.49 – 7.43 (m, 1H), 6.91 – 6.86 (m, 1H), 6.29 (d, *J* = 16.0 Hz, 1H), 4.23 (q, *J* = 7.1 Hz, 1H), 3.82 (s, 1H), 1.34 – 1.29 (m, 1H).

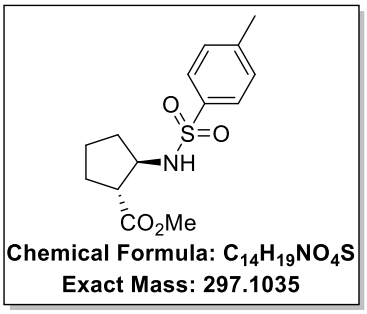
G) Characterization data of Products

a) Ethyl (1*R*,2*R*)-2-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate ***(3aa)***



Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.071 g, 0.708 mmol), **3aa** (0.051 g, 72%). **Reaction time:** 5 h. **Yield:** 72%. **Nature:** oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.74 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 4.80 (d, *J* = 6.0 Hz, 1H), 4.02 (q, *J* = 7.1 Hz, 2H), 3.72-3.64 (m, 1H), 2.61 (dd, *J* = 16.7, 7.7 Hz, 1H), 2.41 (s, 3H), 2.03-1.91 (m, 2H), 1.80-1.63 (m, 2H), 1.50-1.40 (m, 2H), 1.18 (t, *J* = 7.2 Hz, 3H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.2, 143.5, 137.2, 129.7, 127.4, 60.9, 57.8, 50.9, 33.6, 28.0, 22.9, 21.6, 14.2. **HRMS:** [M + H]$^+$ Calculated for $C_{15}H_{22}NO_4S$ 312.1270, found 312.1338.

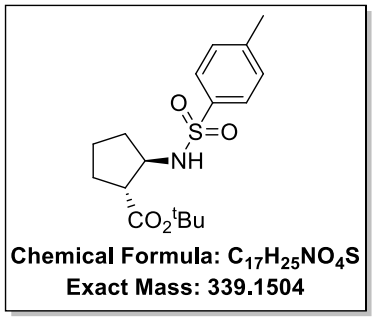
b) Methyl (1*R*,2*R*)-2-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate ***(3ad)***



Chemical Formula: $C_{14}H_{19}NO_4S$
Exact Mass: 297.1035

Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.061 g, 0.708 mmol) **3ad** (0.048 g, 67%). **Reaction time:** 5 h. **Yield:** 72%. **Nature:** oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 4.75 (d, *J* = 5.9 Hz, 1H), 3.73 – 3.65 (m, 1H), 3.57 (s, 3H), 2.63 (dd, *J* = 16.7, 7.8 Hz, 1H), 2.41 (s, 3H), 2.03-1.92 (m, 3H), 1.81 – 1.68 (m, 2H), 1.51 – 1.41 (m, 1H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.6, 143.6, 137.0, 130.0, 129.8, 127.4, 57.9, 52.0, 50.7, 45.1, 34.4, 33.5, 28.0, 22.8, 21.6. **HRMS:** $[M + H]^+$ Calculated for $C_{14}H_{20}NO_4S$ 298.1111, found 298.1113.

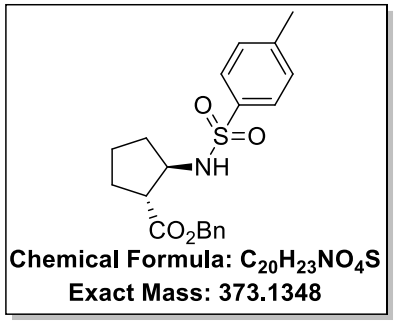
c) *tert*-butyl (1*R*,2*R*)-2-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate ***(3ae)***



Chemical Formula: $C_{17}H_{25}NO_4S$
Exact Mass: 339.1504

Prepared according to **RP1**. **1a** (0.040 g, 0.236 mmol), **2a** (0.090 g, 0.708 mmol), **3ae** (0.041 g, 64%). **Reaction time:** 5 h. **Yield:** 64%. **Nature:** oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.74 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 2H), 4.97 (d, *J* = 5.7 Hz, 1H), 3.66-3.58 (m, 1H), 2.52 (dd, *J* = 16.5, 7.5 Hz, 1H), 2.40 (s, 3H), 1.98-1.84 (m, 2H), 1.68-1.55 (m, 3H), 1.49-1.39 (m, 1H), 1.36 (s, 9H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 173.4, 143.5, 137.2, 129.8, 127.4, 81.0, 57.8, 51.7, 33.6, 28.0, 27.8, 22.9, 21.6. **HRMS:** $[M + Na]^+$ Calculated for $C_{17}H_{25}NO_4SNa$ 362.1402, found 362.1402.

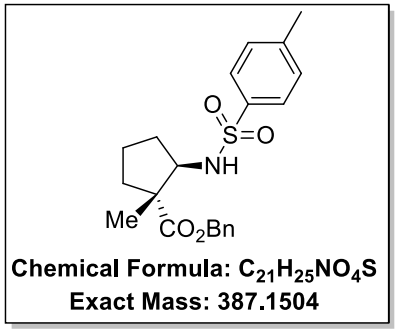
d) Benzyl (1*R*,2*R*)-2-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate ***(3af)***



Chemical Formula: $C_{20}H_{23}NO_4S$
Exact Mass: 373.1348

Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.115 g, 0.708 mmol), **3af** (0.055 g, 63%). **Reaction time:** 5 h. **Yield:** 63%. **Nature:** light yellow liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.35-7.28 (m, 5H), 7.22 (d, *J* = 8.6 Hz, 2H), 5.08-4.96 (m, 3H), 3.80-3.70 (m, 1H), 2.71 (dd, *J* = 16.5, 7.4 Hz, 1H), 2.38 (s, 3H), 2.00-1.91 (m, 2H), 1.81-1.70 (m, 1H), 1.67-1.55 (m, 2H), 1.50-1.40 (m, 1H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.1, 143.5, 137.1, 135.8, 129.7, 128.7, 128.3, 128.2, 127.4, 66.7, 57.8, 50.9, 33.6, 28.2, 22.9, 21.6. **HRMS:** $[M + H]^+$ Calculated for $C_{20}H_{24}NO_4S$ 374.1426, found 374.1426.

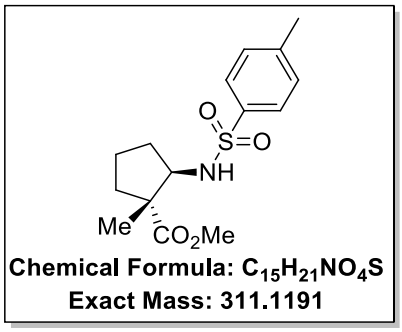
e) Benzyl (1*R*,2*R*)-1-methyl-2-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate ***(3ag)***



Chemical Formula: $C_{21}H_{25}NO_4S$
Exact Mass: 387.1504

Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.124 g, 0.708 mmol), **3ag** (0.061 g, 67%). **Reaction time:** 5.5 h. **Yield:** 67%. **Nature:** white solid. **^{1}H NMR**: δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.37-7.27 (m, 4H), 7.23 (d, *J* = 8.6 Hz, 2H), 5.05-4.91 (m, 3H), 3.8-3.83 (m, 1H), 2.38 (s, 3H), 2.09-1.97 (m, 1H), 1.95-1.84 (m, 1H), 1.65-1.52 (m, 3H), 1.47-1.37 (m, 1H), 1.17 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 176.9, 143.4, 137.4, 129.7, 127.3, 60.0, 52.1, 51.2, 36.1, 31.0, 21.6, 20.2, 17.6. **HRMS:** $[M + H]^+$ Calculated for $C_{21}H_{26}NO_4S$ 388.1583, found 388.1583.

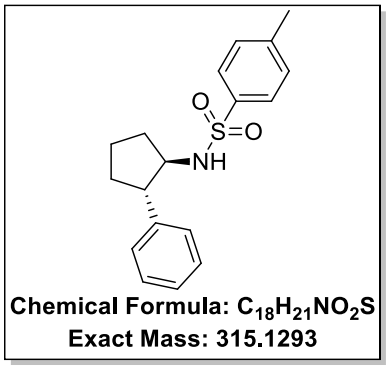
f) Methyl (1*R*,2*R*)-1-methyl-2-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate ***(3ah)***



Chemical Formula: $C_{15}H_{21}NO_4S$
Exact Mass: 311.1191

Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.070 g, 0.708 mmol), **3ah** (0.048 g, 67%). **Reaction time:** 6 h. **Yield:** 67%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 4.79 (t, *J* = 5.7 Hz, 1H), 3.84-3.78 (m, 1H), 3.54 (s, 3H), 2.41 (s, 3H), 2.06-1.96 (m, 1H), 1.96-1.88 (m, 1H), 1.62-1.50 (m, 3H), 1.47-1.37 (m, 1H), 1.14 (s, 3H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 176.2, 143.4, 137.3, 136.0, 129.7, 128.6, 128.2, 128.0, 127.3, 66.7, 60.0, 51.4, 36.2, 31.0, 21.6, 20.3, 17.7. **HRMS:** $[M + H]^+$ Calculated for $C_{15}H_{22}NO_4S$ 312.1270, found 312.1270.

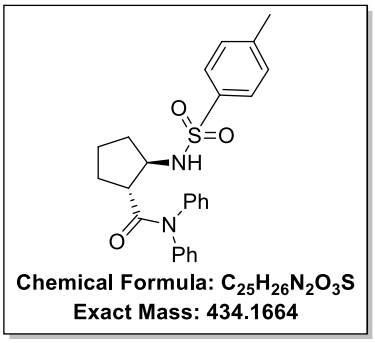
g) 4-methyl-*N*-((1*R*,2*S*)-2-phenylcyclopentyl)benzenesulfonamide ***(3ai)***



Chemical Formula: $C_{18}H_{21}NO_2S$
Exact Mass: 315.1293

Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.124 g, 0.708 mmol), **3ai** (0.048 g, 66%). **Reaction time:** 5.5 h. **Yield:** 66%. **Nature:** Oily Liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.46 (d, *J* = 8.3 Hz, 2H), 7.17-7.12 (m, 3H), 7.10 (d, *J* = 8.6 Hz, 2H), 7.00-6.94 (m, 2H), 4.71 (d, *J* = 6.3 Hz, 1H), 3.50-3.40 (m, 1H), 2.73 (dd, *J* = 18.0, 9.8 Hz, 1H), 2.37 (s, 3H), 2.19-2.08 (m, 1H), 2.07-1.78 (m, 2H), 1.74 (d, *J* = 31.8 Hz, 2H), 1.60-1.52 (dd, *J* = 23.3, 8.5 Hz, 2H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 143.0, 141.6, 137.1, 129.5, 128.6, 127.3, 127.1, 126.7, 61.4, 52.5, 33.3, 32.3, 22.2, 21.6. **HRMS:** $[M + H]^+$ Calculated for $C_{18}H_{22}NO_2S$ 316.1371, found 316.1371.

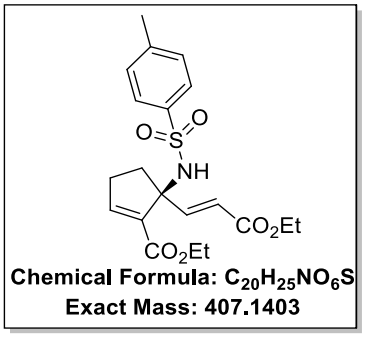
h) (1*R*,2*R*)-2-(4-methylphenylsulfonamido)-*N*,*N*-diphenylcyclopentanecarboxamide ***(3aj)***



Chemical Formula: $C_{25}H_{26}N_2O_3S$
Exact Mass: 434.1664

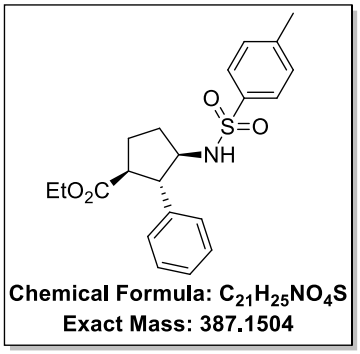
Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.158 g, 0.708 mmol), **3aj** (0.069 g, 58%). **Reaction time:** 3 h. **Yield:** 58%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.44 – 7.29 (m, 1H), 7.20 – 7.14 (m, 1H), 4.28 (d, *J* = 6.8 Hz, 1H), 4.06 – 3.97 (m, 1H), 2.80 (dd, *J* = 15.7, 8.4 Hz, 1H), 2.41 (s, 3H), 1.95 – 1.85 (m, 1H), 1.80-1.76 (m, 2H), 1.69 – 1.58 (m, 1H), 1.30 – 1.20 (m, 2H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.7, 143.7, 143.5, 142.9, 137.1, 129.8, 129.8, 129.1, 128.9, 128.0, 127.4, 126.8, 126.5, 126.2, 58.4, 50.3, 34.0, 30.7, 23.6, 21.7. **HRMS:** $[M + H]^+$ Calculated for $C_{25}H_{27}N_2O_3S$ 435.1742, found 435.1742.

i) Ethyl (*S*,*E*)-5-(3-ethoxy-3-oxoprop-1-en-1-yl)-5-((4-methylphenyl)sulfonamido)cyclopent-1-ene-1-carboxylate ***(3ak)***



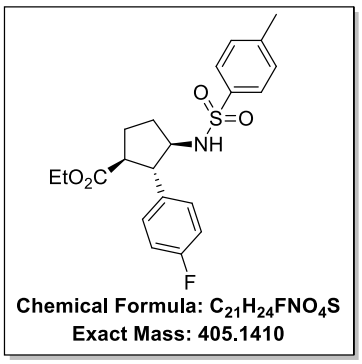
Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.124 g, 0.708 mmol), **3ak** (0.055 g, 58%). **Reaction time:** 3 h. **Yield:** 58%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.82 (d, *J* = 14.4 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.00 (q, *J* = 2.4 Hz, 1H), 5.50 (s, 1H), 5.24 (d, *J* = 14.5 Hz, 1H), 4.13 (q, *J* = 7.1 Hz, 2H), 4.04-3.93 (m, 2H), 2.61-2.55 (m, 1H), 2.50-2.45 (m, 1H), 2.41 (s, 3H), 2.23-2.21 (m, 1H), 1.94-1.88 (m, 1H), 1.24 (t, *J* = 7.2 Hz, 3H), 1.16 (t, *J* = 7.1 Hz, 3H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 167.4, 163.0, 148.5, 144.6, 136.1, 134.0, 129.9, 127.7, 99.3, 62.8, 60.6, 60.2, 31.2, 28.0, 21.7, 14.4, 14.1. **HRMS:** $[M + H]^+$ Calculated for $C_{20}H_{26}NO_6S$ 408.1481, found 408.1481.

j) Ethyl (1*S*,2*S*,3*R*)-3-((4-methylphenyl)sulfonamido)-2-phenylcyclopentane-1-carboxylate ***(3al)***



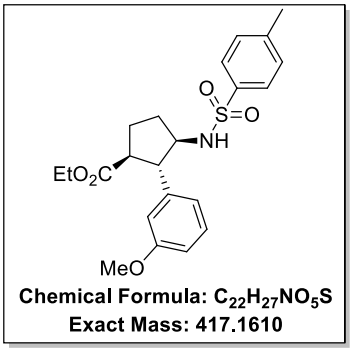
Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.124 g, 0.708 mmol), **3al** (0.054 g, 60%). **Reaction time:** 4 h. **Yield:** 60%. **Nature:** Transparent liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.45 (d, *J* = 8.3 Hz, 2H), 7.17-7.09 (m, 5H), 6.94 (dd, *J* = 7.5, 2.0 Hz, 2H), 4.77 (d, *J* = 6.9 Hz, 1H), 4.02 (q, *J* = 7.1 Hz, 2H), 3.63-3.59 (m, 1H), 3.07-3.05 (m, 1H), 2.80-2.78 (m, 1H), 2.37 (s, 3H), 2.20-2.18 (m, 1H), 2.07-1.99 (m, 2H), 1.72-1.63 (m, 1H), 1.11 (t, *J* = 7.2 Hz, 3H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 175.1, 143.1, 139.5, 137.2, 129.7, 129.6, 129.1, 128.7, 128.4, 127.5, 127.1, 127.0, 61.0, 60.9, 58.2, 55.2, 51.7, 49.5, 46.4, 32.6, 27.1, 21.6, 14.2. **HRMS:** $[M + H]^+$ Calculated for $C_{21}H_{26}NO_4S$ 388.1582, found 388.1582.

k) (1*S*,2*S*,3*R*)-ethyl 2-(4-fluorophenyl)-3-(4-methylphenylsulfonamido)cyclopentanecarboxylate ***(3am)***



Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.137 g, 0.708 mmol), **3am** (0.055 g, 58%). **Reaction time:** 4.5 h. **Yield:** 58%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.45 (d, *J* = 8.3 Hz, 2H), 7.11 (d, *J* = 8.1 Hz, 2H), 6.91-6.86 (m, 2H), 6.80 (t, *J* = 8.7 Hz, 2H), 4.57 (d, *J* = 7.4 Hz, 1H), 4.02 (q, *J* = 7.1 Hz, 2H), 3.61-3.56 (m, 1H), 3.03 (t, *J* = 9.6 Hz, 1H), 2.74-2.73 (m, 1H), 2.39 (s, 3H), 2.21-2.20 (m, 1H), 2.18-2.07 (m, 1H), 2.04-1.90 (m, 1H), 1.70-1.67 (m, 1H), 1.11 (t, *J* = 7.1 Hz, 3H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.8, 143.4, 137.1, 135.1, 129.5, 129.0, 128.9, 127.0, 115.6, 115.4, 61.1, 60.9, 54.6, 49.5, 32.5, 26.8, 21.6, 14.2. **HRMS:** $[M + H]^+$ Calculated for $C_{21}H_{25}NO_4FS$ 406.1488, found 406.1488.

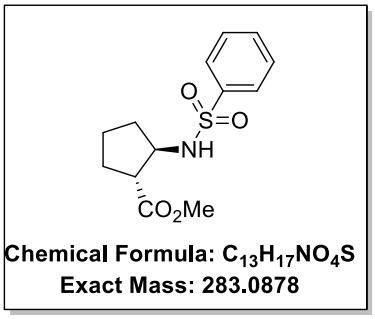
l) Ethyl (1*S*,2*S*,3*R*)-2-(3-methoxyphenyl)-3-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate ***(3an)***



Chemical Formula: $C_{22}H_{27}NO_5S$
Exact Mass: 417.1610

Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.146 g, 0.708 mmol), **3an** (0.056 g, 58%). **Reaction time:** 4 h. **Yield:** 58%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.44 (d, *J* = 8.3 Hz, 2H), 7.08 (dd, *J* = 7.9, 5.9 Hz, 3H), 6.71-6.70 (m, 1H), 6.55 (d, *J* = 7.6 Hz, 1H), 6.44-6.42 (m, 1H), 4.90 (d, *J* = 6.9 Hz, 1H), 4.02 (q, *J* = 7.2 Hz, 2H), 3.68 (s, 3H), 3.58-3.56 (m, 1H), 3.05 (t, *J* = 9.3 Hz, 1H), 2.79-2.77 (m, 1H), 2.36 (s, 3H), 2.19-2.18 (m, 1H), 2.06-2.04 (m, 3H), 1.72-1.66 (m, 1H), 1.11 (t, *J* = 7.1 Hz, 3H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 175.1, 159.8, 143.1, 141.2, 137.1, 129.7, 129.5, 127.0, 119.9, 112.9, 112.7, 61.1, 60.9, 55.2, 55.1, 49.3, 32.6, 27.1, 21.6, 14.2. **HRMS:** $[M + H]^+$ Calculated for $C_{22}H_{28}NO_5S$ 418.1688, found 418.1688.

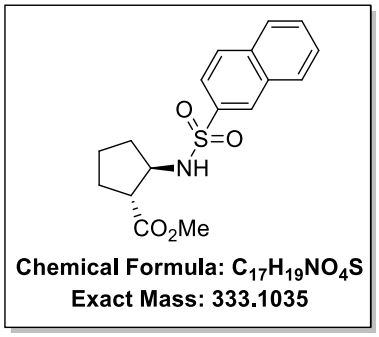
m) Methyl (1*R*,2*R*)-2-(phenylsulfonamido)cyclopentane-1-carboxylate ***(3ba)***



Chemical Formula: $C_{13}H_{17}NO_4S$
Exact Mass: 283.0878

Prepared according to **RP1**. **1a** (0.040 g, 0.205 mmol), **2a** (0.053 g, 0.615 mmol), **3ba** (0.026 g, 46%). **Reaction time:** 4 h. **Yield:** 46%. **Nature:** transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.88-7.84 (m, 2H), 7.59-7.55 (m, 1H), 7.54-7.47 (m, 2H), 5.06 (d, *J* = 6.2 Hz, 1H), 3.77-3.70 (m, 1H), 3.54 (s, 3H), 2.63 (dd, *J* = 16.7, 7.7 Hz, 1H), 2.00-1.93 (m, 2H), 1.78-1.71 (m, 1H), 1.65-1.58 (m, 2H), 1.50-1.42 (m, 1H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.6, 140.1, 132.8, 129.2, 127.3, 57.9, 52.0, 50.7, 33.7, 28.1, 22.9. **HRMS:** $[M + H]^+$ Calculated for $C_{13}H_{17}NO_4SNa$ 306.0776, found 306.0776.

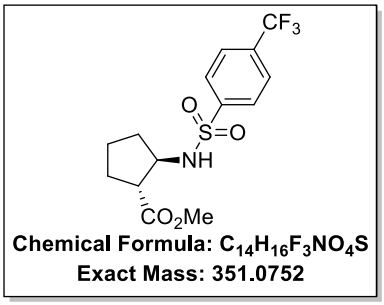
n) Methyl (1*R*,2*R*)-2-(naphthalene-2-sulfonamido)cyclopentane-1-carboxylate ***(3ca)***



Chemical Formula: $C_{17}H_{19}NO_4S$
Exact Mass: 333.1035

Prepared according to **RP1**. **1a** (0.050 g, 0.205 mmol), **2a** (0.053 g, 0.615 mmol), **3ac** (0.042 g, 62%). **Reaction time:** 4 h. **Yield:** 62%. **Nature:** oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.45 (s, 1H), 7.96 (dd, *J* = 8.1, 5.3 Hz, 2H), 7.89 (d, *J* = 8.9 Hz, 1H), 7.83 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.65-7.56 (m, 2H), 5.16 (d, *J* = 6.6 Hz, 1H), 3.83-3.76 (m, 1H), 3.42 (s, 3H), 2.64 (dd, *J* = 16.6, 7.6 Hz, 1H), 1.96 (d, *J* = 53.5 Hz, 2H), 1.76-1.69 (m, 1H), 1.66-1.51 (s, 2H), 1.53-1.42 (m, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.6, 137.0, 134.9, 132.2, 129.5, 129.4, 128.9, 128.8, 128.0, 127.6, 122.5, 57.9, 51.9, 50.8, 33.7, 28.2. **HRMS:** $[M + H]^+$ Calculated for $C_{17}H_{20}NO_4S$ 334.1118, found 334.1118.

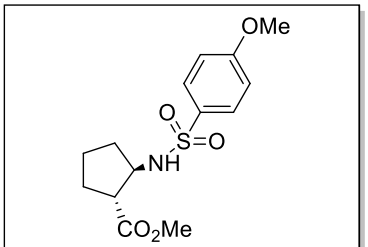
o) Methyl (1*R*,2*R*)-2-((4-(trifluoromethyl)phenyl)sulfonamido)cyclopentane-1-carboxylate ***(3da)***



Chemical Formula: $C_{14}H_{16}F_3NO_4S$
Exact Mass: 351.0752

Prepared according to **RP1**. **1a** (0.054 g, 0.205 mmol), **2a** (0.053 g, 0.615 mmol), **3ad** (0.043 g, 61%). **Reaction time:** 8 h. **Yield:** 61%. **Nature:** Oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.00 (d, *J* = 8.3 Hz, 2H), 7.77 (d, *J* = 8.3 Hz, 2H), 5.15 (d, *J* = 6.6 Hz, 1H), 3.82-3.74 (m, 1H), 3.54 (s, 3H), 2.67-2.59 (m, 1H), 2.07-1.93 (m, 2H), 1.79-1.72 (m, 3H), 1.48-1.44 (m, 1H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.5, 143.9, 127.9, 126.3, 126.3, 126.3, 126.2, 124.7, 122.0, 57.9, 52.0, 50.7, 33.7, 29.8, 28.3, 22.8. **HRMS:** $[M + H]^+$ Calculated for $C_{14}H_{17}NO_4SF_3$ 352.0830, found 352.0830.

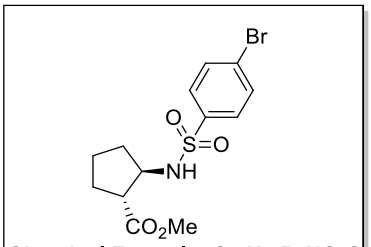
p) Ethyl (1*R*,2*R*)-2-((4-methylphenyl)sulfonamido)cyclopentane-1-carboxylate ***(3ea)***



Chemical Formula: $C_{14}H_{19}NO_5S$
Exact Mass: 313.0984

Prepared according to **RP1**. **1a** (0.047 g, 0.205 mmol), **2a** (0.053 g, 0.615 mmol), **3ea** (0.043 g, 68%). **Reaction time:** 5 h. **Yield:** 68%. **Nature:** Yellow oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.79 (d, *J* = 9.0 Hz, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 5.08 (d, *J* = 6.3 Hz, 1H), 3.85 (s, 3H), 3.73-3.65 (m, 1H), 3.57 (s, 3H), 2.64 (dd, *J* = 16.6, 7.6 Hz, 1H), 2.02-1.90 (m, 2H), 1.75-1.52 (m, 2H), 1.50-1.38 (m, 1H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.8, 163.0, 131.7, 129.5, 114.3, 57.8, 55.7, 52.0, 50.7, 33.6, 28.2, 22.9. **HRMS:** $[M + H]^+$ Calculated for $C_{14}H_{20}NO_5S$ 314.1062, found 314.1062.

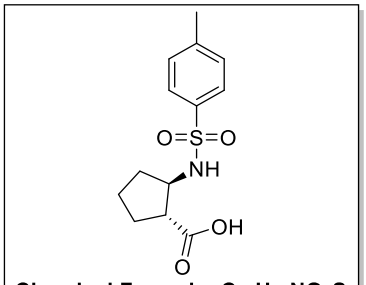
q) Methyl (1*R*,2*R*)-2-((4-bromophenyl)sulfonamido)cyclopentane-1-carboxylate ***(3fa)***



Chemical Formula: $C_{13}H_{16}BrNO_4S$
Exact Mass: 360.9983

Prepared according to **RP1**. **1a** (0.056 g, 0.205 mmol), **2a** (0.053 g, 0.615 mmol), **3fa** (0.058 g, 62%). **Reaction time:** 6 h. **Yield:** 62%. **Nature:** Light yellow oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.75 – 7.70 (m, 2H), 7.66-7.61 (m, 2H), 5.15 (d, *J* = 6.6 Hz, 1H), 3.78-3.69 (m, 1H), 3.57 (s, 3H), 2.66-2.60 (m, 1H), 2.00-1.98 (m, 2H), 1.97-1.71 (m, 1H), 1.69-1.48 (m, 2H), 1.46-1.42 (m, 1H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 174.6, 139.3, 132.4, 128.9, 127.7, 57.9, 52.1, 50.7, 33.6, 28.3, 22.9. **HRMS:** $[M + H]^+$ Calculated for $C_{13}H_{17}NO_4SBr$ 362.0062, found 362.0062.

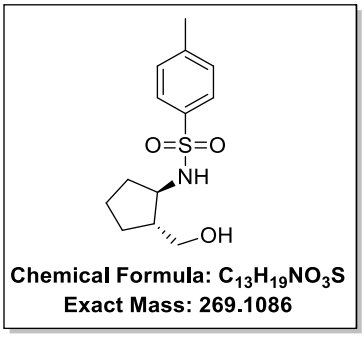
r) *N*-((1*R*,2*R*)-2-(hydroxymethyl)cyclopentyl)-4-methylbenzenesulfonamide ***(3ada)***



Chemical Formula: $C_{13}H_{17}NO_4S$
Exact Mass: 283.0878

Prepared according to **RP1**. **3ad** (0.030 g, 0.100 mmol), **3ada** (0.025 g, 86%). **Reaction time:** 3 h. **Yield:** 86%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.75 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 5.13 (d, *J* = 5.7 Hz, 1H), 3.80 – 3.73 (m, 1H), 2.74-2.68 (m, 1H), 2.40 (s, 3H), 2.05-2.00 (m, 2H), 1.98-1.92 (m, 1H), 1.82-1.62 (m, 2H), 1.49-1.42 (m, 1H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 179.5, 143.7, 136.9, 129.8, 127.4, 57.6, 50.7, 33.5, 28.3, 23.0, 21.7. **HRMS:** $[M + H]^+$ Calculated for $C_{13}H_{18}NO_4S$ 284.0957, found 284.0957.

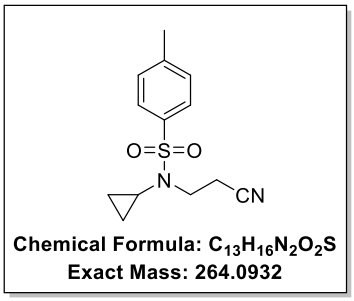
s) *N*-((1*R*,2*R*)-2-(hydroxymethyl)cyclopentyl)-4-methylbenzenesulfonamide ***(3adb)***



Chemical Formula: $C_{13}H_{19}NO_3S$
Exact Mass: 269.1086

Prepared according to **RP1**. **3ad** (0.030 g, 0.100 mmol), **3adb** (0.022 g, 81%). **Reaction time:** 4 h. **Yield:** 81%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.76 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 5.18 (d, *J* = 6.5 Hz, 1H), 3.67 (dd, *J* = 11.0, 5.0 Hz, 1H), 3.48 (dd, *J* = 11.0, 6.8 Hz, 1H), 3.29-3.20 (m, 1H), 2.41 (s, 3H), 2.12 (s, 1H), 1.90-1.78 (m, 1H), 1.77-1.68 (m, 2H), 1.66-1.54 (m, 1H), 1.54-1.41 (m, 1H), 1.40-1.30 (m, 1H), 1.29-1.18 (m, 1H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 143.5, 137.4, 129.8, 127.2, 64.5, 57.9, 48.4, 33.1, 26.1, 22.0, 21.6. **HRMS:** $[M + H]^+$ Calculated for $C_{13}H_{20}NO_3S$ 270.1164, found 270.1164.

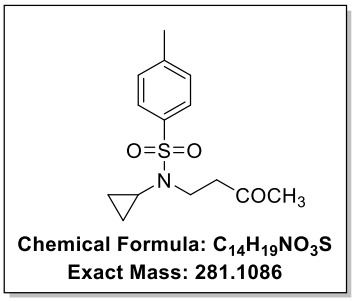
t) *N*-(2-cyanoethyl)-*N*-cyclopropyl-4-methylbenzenesulfonamide ***(3ab')***



Chemical Formula: $C_{13}H_{16}N_2O_2S$
Exact Mass: 264.0932

Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.037 g, 0.708 mmol), **3an** (0.056 g, 77%). **Reaction time:** 4 h. **Yield:** 58%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.72 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 7.9 Hz, 2H), 3.42 (t, *J* = 7.0 Hz, 2H), 2.72 (t, *J* = 6.9 Hz, 2H), 2.09 (tt, *J* = 6.9, 3.6 Hz, 1H), 0.88 (d, *J* = 16.1 Hz, 2H), 0.72 (d, *J* = 19.7 Hz, 2H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 144.3, 134.4, 129.9, 127.9, 118.0, 47.5, 31.6, 21.7, 18.9, 7.9. **HRMS:** $[M + H]^+$ Calculated for $C_{13}H_{20}NO_3S$ 265.0972, found 265.1011.

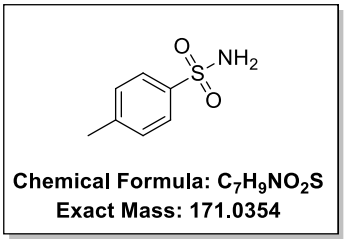
u) *N*-(2-cyanoethyl)-*N*-cyclopropyl-4-methylbenzenesulfonamide ***(3ac')***



Chemical Formula: $C_{14}H_{19}NO_3S$
Exact Mass: 281.1086

Prepared according to **RP1**. **1a** (0.050 g, 0.236 mmol), **2a** (0.049 g, 0.708 mmol), **3an** (0.055 g, 83%). **Reaction time:** 4 h. **Yield:** 58%. **Nature:** Transparent oily liquid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 3.39-3.33 (m, 2H), 2.85-2.78 (m, 2H), 2.40 (s, 3H), 2.12 (s, 3H), 1.97-1.92 (m, 1H), 0.82-0.76 (m, 2H), 0.67-0.61 (m, 2H).**^{13}C NMR (101 MHz, $CDCl_3$)**: δ 207.1, 143.7, 134.8, 129.7, 127.8, 46.3, 43.3, 31.4, 30.4, 21.6, 7.6.

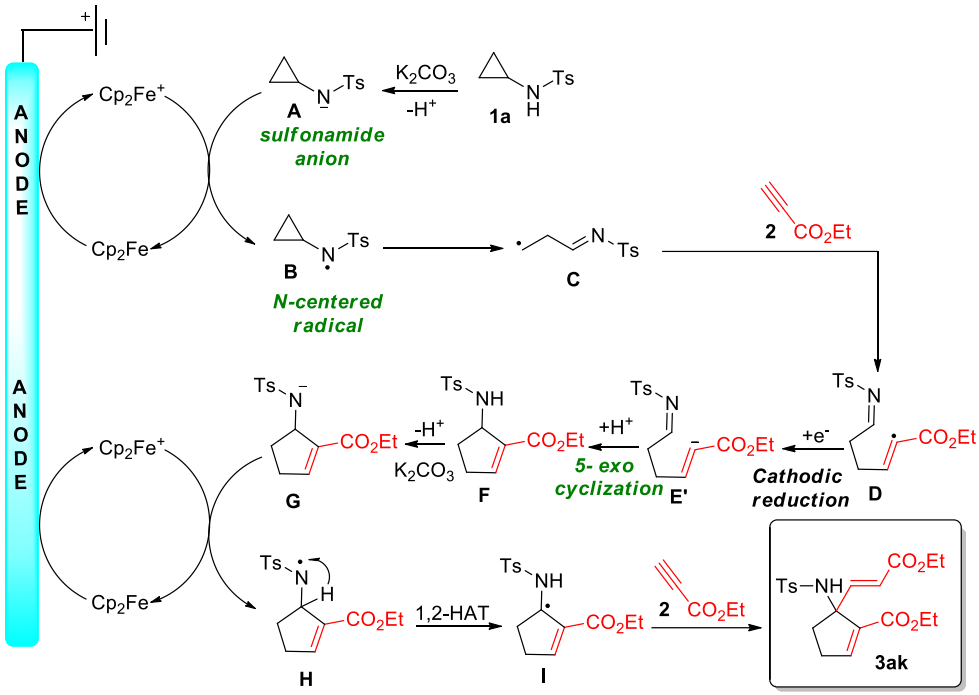
v) 4-methylbenzenesulfonamide ***(IV)***



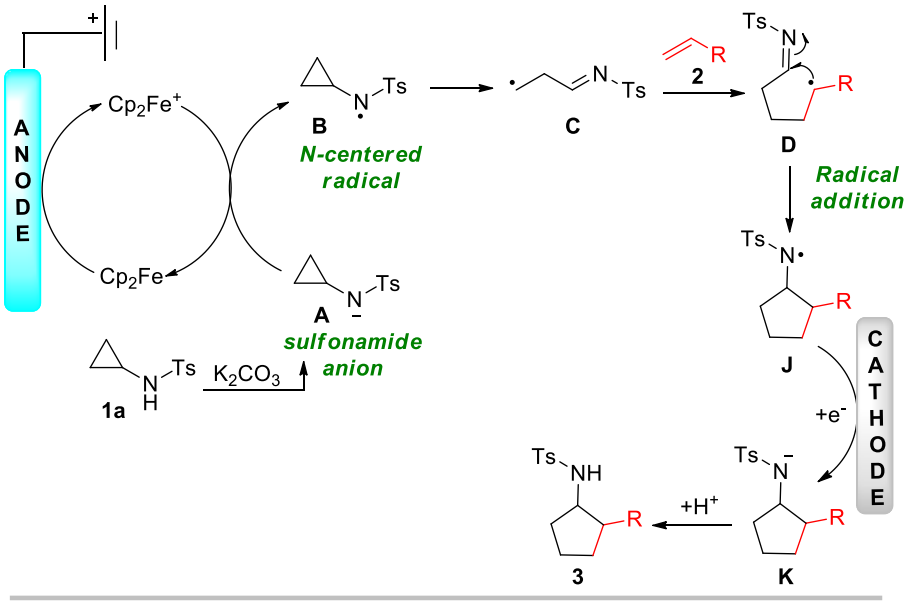
Chemical Formula: $C_7H_9NO_2S$
Exact Mass: 171.0354

Nature: white solid. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.80 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 4.87 (s, 2H), 2.42 (s, 3H).

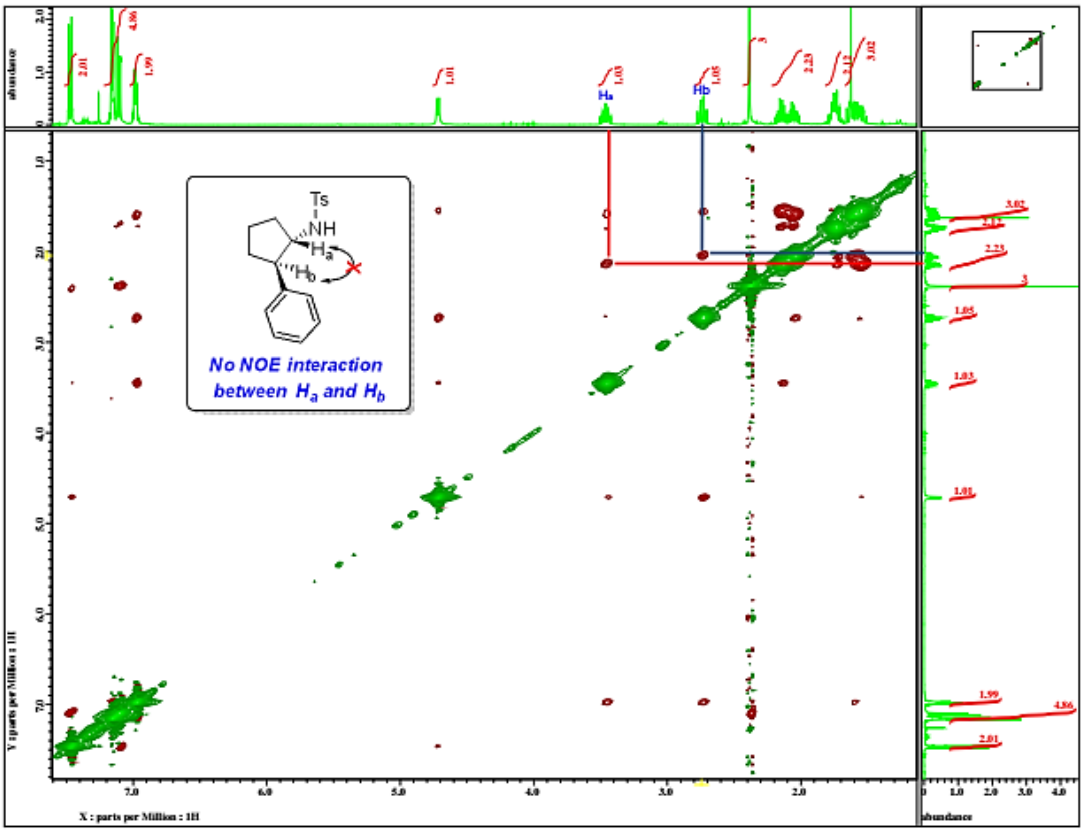
H) Mechanism for formation of 3ak



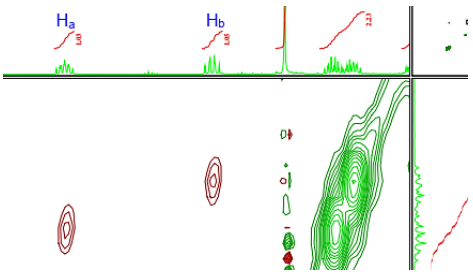
I) Alternate mechanism for the protocol



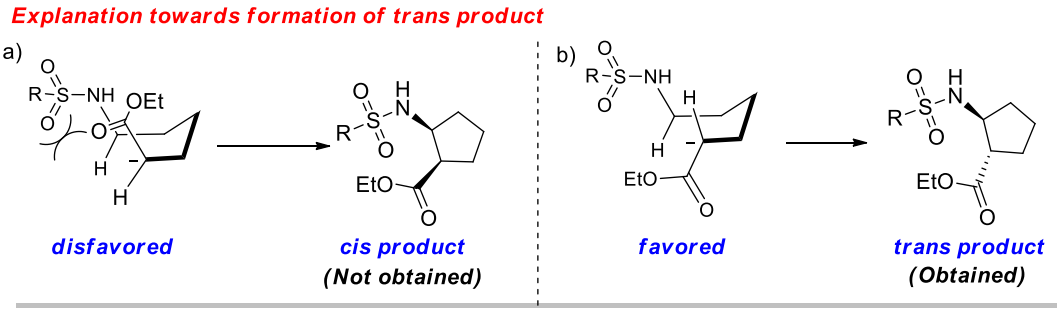
J) NOESY Experiment



Zoomed Version



Conclusion: NOESY experiments reveals that there is no interaction Ha and Hb. This confirms the *trans* product



As described by Aggarwal et al, the reason for the diastereoselective formation of products could be the steric repulsion between the N-sulfonyl imine and the ester group which disfavors the cis product in comparison to the trans where the molecule do not suffer any steric repulsion.

K) Single Crystal data of 3ag and 3al

For the determination of X-ray crystal structures of **3ag** and **3al** a single crystal was selected and mounted with paratone oil on a glass fiber using gum. The data was collected at 293K on a CMOS based Bruker D8 Venture PHOTON 100 diffractometer equipped with an INCOATEC micro-focus source with graphite monochromatic Mo Kα radiation (λ = 0.71073 Å) operation at 50 kV and 30 mA. For the integration of diffraction profiles SAINT program[3] was used. Absorption correction was done applying SADABS program.[4] The crystal structure was solved by SIR 92[5] and refined by full matrix least square method using SHELXL-97[6] WinGX system, Ver 1.70.01.[7] All the non-hydrogen atoms in the structure were located the Fourier map and refined anisotropically. The hydrogen atoms were fixed by HFIX in their ideal positions and refined using riding model with isotropic thermal parameters. The crystal structure (excluding structure factor) has been deposited to Cambridge Crystallographic Data Centre and allocated deposition number**: 3ag: CCDC 2115609**, **3al: CCDC 2145541.**

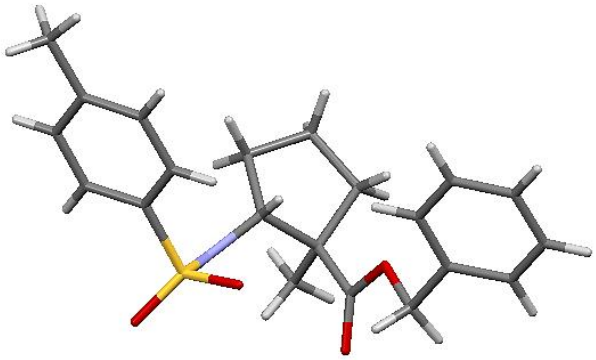


Figure S1: X-ray crystal structure of **3ag**

CCDC No.	CCDC 2115609
Formula	C21 H25 N O4 S
Formula weight	387.48
Crystal System	Monoclinic
Space group	P21/n
a, b, c (Å)	13.4901(9) 9.8844(7) 15.6641(11)
α, β, γ (°)	90 104.766(2) 90
V (Å^3)	2019.7(2)
Z	4
Calculated Density (g/cm^3)	1.274
Absorption coefficient (mm^{-1})	0.186
F(000)	824
Crystal Size (mm^3)	0.05 x 0.23 x 0.36
Theta range for data collection:	2.3^o to 26.4°
Data set	-16: 16 ; -12: 12 ; -19: 19

Reflection	70148
Independent refl.	[R(int) = 0.066]
data [I > 2σ(I)]	3433
R indices (all data)	R = 0.0461, wR_2 = 0.1201
S	1.05
Min. and Max. Resd. Dens. (e/Å^3)	-0.27 and 0.32

Table S1: Selected bond lengths [Å] of 3ag

Atoms	Bond lengths [Å]	Atoms	Bond lengths [Å]
S1 -O1	1.4301(16)	C19 -C20	1.373(4)
S1 -O2	1.4301(17)	C1 -H1A	0.9300
S1 -N1	1.6103(15)	C2 -H2	0.9300
S1 -C7	1.7690(17)	C4 -H4A	0.9600
O3 -C13	1.193(2)	C4 -H4B	0.9600
O4 -C13	1.328(2)	C4 -H4C	0.9600
O4 -C14	1.456(2)	C5 -H5	0.9300
N1 -C8	1.459(2)	C6 -H6	0.9300
C1 -C2	1.377(3)	C8 -H8	0.9800
C1 -C7	1.375(3)	C9 -H9A	0.9700
N1 -H1	0.8600	C9 -H9B	0.9700
C00A -C8	1.552(2)	C10 -H10A	0.9700
C00A -C12	1.522(3)	C10 -H10B	0.9700
C00A -C13	1.514(2)	C11 -H11A	0.9700
C00A -C11	1.539(3)	C11 -H11B	0.9700
C2 -C3	1.376(3)	C12 -H12A	0.9600
C3 -C5	1.386(3)	C12 -H12B	0.9600
C3 -C4	1.512(3)	C12 -H12C	0.9600
C5 -C6	1.378(3)	C14 -H14A	0.9700
C6 -C7	1.389(3)	C14 -H14B	0.9700
C8 -C9	1.534(3)	C16 -H16	0.9300
C9 -C10	1.516(3)	C17 -H17	0.9300
C10 -C11	1.527(3)	C18 -H18	0.9300
C14 -C15	1.496(3)	C19 -H19	0.9300
C15 -C20	1.384(3)	C20 -H20	0.9300
C15 -C16	1.377(3)		
C16 -C17	1.378(4)		
C17 -C18	1.370(4)		
C18 -C19	1.366(4)		

Table S2: Selected bond angles [º] of 3ag

Atoms	Bond angles[º]	Atoms	Bond angles[º]
O1 -S1 -O2	120.44(10)	N1 -C8 -C9	114.76(15)
O1 -S1 -N1	107.68(8)	C8 -C9 -C10	105.53(16)
O1 -S1 -C7	107.11(9)	C9 -C10 -C11	106.52(17)
O2 -S1 -N1	105.93(9)	C00A -C11 -C10	105.97(17)
O2 -S1 -C7	107.39(9)	O3 -C13 -C00A	124.38(17)
N1 -S1 -C7	107.74(8)	O3 -C13 -O4	122.49(16)
C13 -O4 -C14	115.95(14)	O4 -C13 -C00A	113.10(15)
S1 -N1 -C8	121.57(12)	O4 -C14 -C15	107.32(15)
C2 -C1 -C7	120.04(18)	C14 -C15 -C16	120.51(17)
C8 -N1 -H1	119.00	C16 -C15 -C20	118.77(19)
S1 -N1 -H1	119.00	C14 -C15 -C20	120.69(18)
C8 -C00A -C12	112.01(15)	C15 -C16 -C17	120.7(2)
C8 -C00A -C11	100.43(14)	C16 -C17 -C18	119.7(2)
C11 -C00A -C13	114.20(15)	C17 -C18 -C19	120.4(3)
C12 -C00A -C13	109.40(15)	C18 -C19 -C20	120.1(3)
C11 -C00A -C12	112.02(15)	C15 -C20 -C19	120.4(2)
C8 -C00A -C13	108.51(13)	C2 -C1 -H1A	120.00
C1 -C2 -C3	121.5(2)	C7 -C1 -H1A	120.00
C2 -C3 -C4	121.6(2)	C1 -C2 -H2	119.00
C2 -C3 -C5	118.12(19)	C3 -C2 -H2	119.00
C4 -C3 -C5	120.27(19)	C3 -C4 -H4A	109.00
C3 -C5 -C6	121.19(19)	C3 -C4 -H4B	109.00
C5 -C6 -C7	119.69(19)	C3 -C4 -H4C	109.00
S1 -C7 -C6	119.66(14)	H4A -C4 -H4B	110.00
C1 -C7 -C6	119.48(16)	H4A -C4 -H4C	109.00
S1 -C7 -C1	120.86(13)	H4B -C4 -H4C	109.00
C00A -C8 -C9	103.29(14)	C3 -C5 -H5	119.00
N1 -C8 -C00A	113.74(14)	C6 -C5 -H5	119.00
C5 -C6 -H6	120.00	C00A -C12 -H12B	109.00
C7 -C6 -H6	120.00	C00A -C12 -H12C	109.00
N1 -C8 -H8	108.00	H12A -C12 -H12B	109.00
C00A -C8 -H8	108.00	H12A -C12 -H12C	109.00
C9 -C8 -H8	108.00	H12B -C12 -H12C	109.00
C8 -C9 -H9A	111.00	O4 -C14 -H14A	110.00
C8 -C9 -H9B	111.00	O4 -C14 -H14B	110.00
C10 -C9 -H9A	111.00	C15 -C14 -H14A	110.00
C10 -C9 -H9B	111.00	C15 -C14 -H14B	110.00
H9A -C9 -H9B	109.00	H14A -C14 -H14B	109.00
C9 -C10 -H10A	110.00	C15 -C16 -H16	120.00
C9 -C10 -H10B	110.00	C17 -C16 -H16	120.00
C11 -C10 -H10A	110.00	C16 -C17 -H17	120.00
C11 -C10 -H10B	110.00	C18 -C17 -H17	120.00
H10A -C10 -H10B	109.00	C17 -C18 -H18	120.00
C00A -C11 -H11A	111.00	C19 -C18 -H18	120.00
C00A -C11 -H11B	111.00	C18 -C19 -H19	120.00
C10 -C11 -H11A	111.00	C20 -C19 -H19	120.00
C10 -C11 -H11B	111.00	C15 -C20 -H20	120.00
H11A -C11 -H11B	109.00	C19 -C20 -H20	120.00
C00A -C12 -H12A	109.00		

Table S3: Selected hydrogen bonding geometry [Å, º] for a compound 3ag

D--H.. A	D..H	H..A	D..A	D--H..A
N1 -- H1 .. O3	0.8600	2.3000	2.880(2)	125.00
C1 -- H1A .. O1	0.9300	2.5300	2.880(2)	105.00
C8 -- H8 .. O1	0.9800	2.5600	2.964(2)	105.00
C11 -- H11A .. O4	0.9700	2.3800	2.811(2)	106.00

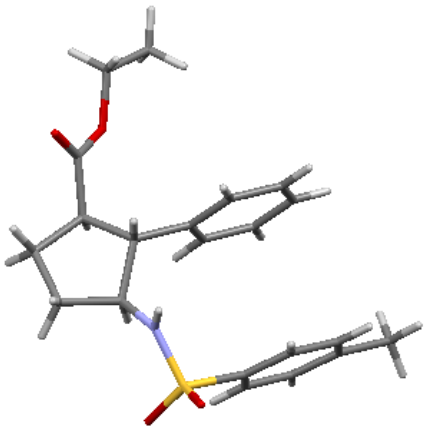


Figure S1: X-ray crystal structure of **3al**

CCDC No.	CCDC 2145541
Formula	C21 H25 N O4 S
Formula weight	387.48
Crystal System	Monoclinic
Space group	P21/n
a, b, c (Å)	15.4139(12) 8.4945(6) 17.2042(15)
α, β, γ (°)	90 112.732(2) 90
V ($Å^3$)	2077.6(3)
Z	4
Calculated Density (g/cm^3)	1.239
Absorption coefficient (mm^{-1})	0.181
F(000)	824
Crystal Size (mm^3)	0.28 x 0.29 x 0.31
Theta range for data collection:	2.6º to 25.7°

Data set	-18: 18 ; -10: 10 ; -20: 21
Reflection	28113
Independent refl.	[R(int) = 0.063]
data [I > 2σ(I)]	2816
R indices (all data)	R = 0.0503, wR_2 = 0.1393
S	1.03
Min. and Max. Resd. Dens. (e/Å^3)	-0.25 and 0.28

Table S1: Selected bond lengths [Å] of 3al

Atoms	Bond lengths [Å]	Atoms	Bond lengths [Å]
S1 -O3	1.4331(18)	C18 -C19	1.377(5)
S1 -O4	1.426(2)	C1 -H1	0.9300
S1 -N101	1.600(2)	C025 -H02A	0.9600
S1 -C20	1.763(2)	C025 -H02B	0.9600
O1 -C12	1.205(4)	C025 -H02C	0.9600
O2 -C12	1.314(3)	C2 -H2	0.9300
O2 -C13	1.443(4)	C3 -H3	0.9300
N101 -C8	1.453(3)	C4 -H4	0.9300
N101 -H101	0.8600	C5 -H5	0.9300
C1 -C3	1.347(6)	C7 -H7	0.9800
C1 -C2	1.356(6)	C8 -H8	0.9800
C025 -C18	1.508(4)	C9 -H9A	0.9700
C2 -C4	1.399(5)	C9 -H9B	0.9700
C3 -C5	1.379(4)	C10 -H10A	0.9700
C4 -C6	1.370(4)	C10 -H10B	0.9700
C5 -C6	1.375(4)	C11 -H11	0.9800
C6 -C7	1.509(3)	C13 -H13A	0.9700
C7 -C11	1.545(4)	C13 -H13B	0.9700
C7 -C8	1.534(4)	C14 -H14A	0.9600
C8 -C9	1.534(4)	C14 -H14B	0.9600
C9 -C10	1.508(4)	C14 -H14C	0.9600
C10 -C11	1.534(4)	C15 -H15	0.9300
C11 -C12	1.491(4)	C16 -H16	0.9300
C13 -C14	1.375(6)	C17 -H17	0.9300
C15 -C20	1.372(4)	C19 -H19	0.9300
C15 -C19	1.383(4)		
C16 -C17	1.376(4)		
C16 -C20	1.378(4)		
C17 -C18	1.376(4)		

Table S2: Selected bond angles [º] of 3al

Atoms	Bond angles[º]	Atoms	Bond angles[º]
O3 -S1 -O4	119.83(12)	C10 -C11 -C12	114.9(2)
O3 -S1 -N101	105.54(11)	O2 -C12 -C11	111.7(2)
O3 -S1 -C20	108.31(11)	O1 -C12 -C11	124.6(3)
O4 -S1 -N101	108.51(11)	O1 -C12 -O2	123.7(3)
O4 -S1 -C20	107.14(12)	O2 -C13 -C14	110.5(3)
N101 -S1 -C20	106.86(12)	C19 -C15 -C20	119.6(3)
C12 -O2 -C13	117.5(2)	C17 -C16 -C20	119.6(3)
S1 -N101 -C8	123.03(18)	C16 -C17 -C18	121.6(3)
C8 -N101 -H101	118.00	C17 -C18 -C19	117.8(3)
S1 -N101 -H101	119.00	C025 -C18 -C17	120.4(3)
C2 -C1 -C3	119.4(3)	C025 -C18 -C19	121.8(3)
C1 -C2 -C4	120.6(4)	C15 -C19 -C18	121.5(3)
C1 -C3 -C5	120.3(4)	C15 -C20 -C16	119.9(2)
C2 -C4 -C6	120.6(3)	S1 -C20 -C15	119.9(2)
C3 -C5 -C6	122.0(3)	S1 -C20 -C16	120.2(2)
C4 -C6 -C7	120.9(2)	C2 -C1 -H1	120.00
C5 -C6 -C7	122.1(2)	C3 -C1 -H1	120.00
C4 -C6 -C5	117.1(2)	C18 -C025 -H02A	109.00
C8 -C7 -C11	101.96(19)	C18 -C025 -H02B	109.00
C6 -C7 -C8	115.7(2)	C18 -C025 -H02C	109.00
C6 -C7 -C11	115.9(2)	H02A -C025 -H02B	109.00
C7 -C8 -C9	103.9(2)	H02A -C025 -H02C	109.00
N101 -C8 -C7	113.0(2)	H02B -C025 -H02C	109.00
N101 -C8 -C9	112.9(2)	C1 -C2 -H2	120.00
C8 -C9 -C10	106.2(2)	C4 -C2 -H2	120.00
C9 -C10 -C11	107.1(2)	C1 -C3 -H3	120.00
C7 -C11 -C12	109.9(2)	C5 -C3 -H3	120.00
C7 -C11 -C10	104.5(2)	C2 -C4 -H4	120.00
C6 -C4 -H4	120.00	C10 -C11 -H11	109.00
C3 -C5 -H5	119.00	C12 -C11 -H11	109.00
C6 -C5 -H5	119.00	O2 -C13 -H13A	110.00
C6 -C7 -H7	108.00	O2 -C13 -H13B	110.00
C8 -C7 -H7	108.00	C14 -C13 -H13A	110.00
C11 -C7 -H7	108.00	C14 -C13 -H13B	110.00
N101 -C8 -H8	109.00	H13A -C13 -H13B	108.00
C7 -C8 -H8	109.00	C13 -C14 -H14A	109.00
C9 -C8 -H8	109.00	C13 -C14 -H14B	109.00
C8 -C9 -H9A	110.00	C13 -C14 -H14C	109.00
C8 -C9 -H9B	111.00	H14A -C14 -H14B	109.00
C10 -C9 -H9A	111.00	H14A -C14 -H14C	110.00
C10 -C9 -H9B	111.00	H14B -C14 -H14C	109.00
H9A -C9 -H9B	109.00	C19 -C15 -H15	120.00
C9 -C10 -H10A	110.00	C20 -C15 -H15	120.00
C9 -C10 -H10B	110.00	C17 -C16 -H16	120.00
C11 -C10 -H10A	110.00	C20 -C16 -H16	120.00
C11 -C10 -H10B	110.00	C16 -C17 -H17	119.00
H10A -C10 -H10B	109.00	C18 -C17 -H17	119.00
C7 -C11 -H11	109.00	C15 -C19 -H19	119.00

Table S3: Selected hydrogen bonding geometry [Å, º] for a compound 3al

D--H.. A	D..H	H..A	D..A	D--H..A
N101 -- H101 .. O1	0.8600	2.1200	2.950(3)	162.00
C10 -- H10A .. O1	0.9700	2.5100	2.924(4)	105.00
C11 -- H11 .. O3	0.9800	2.5300	3.218(3)	128.00
C16 -- H16 .. O4	0.9300	2.5300	2.900(3)	104.00

References

1. D. H. White, A. Noble, K. L. Booker-Milburn, and V. K. Aggarwal, *Org. Lett.* 2021, 23, 3038.
2. R. Kumar and P. Banerjee, *J. Org. Chem*., 2021, 86, 16104.
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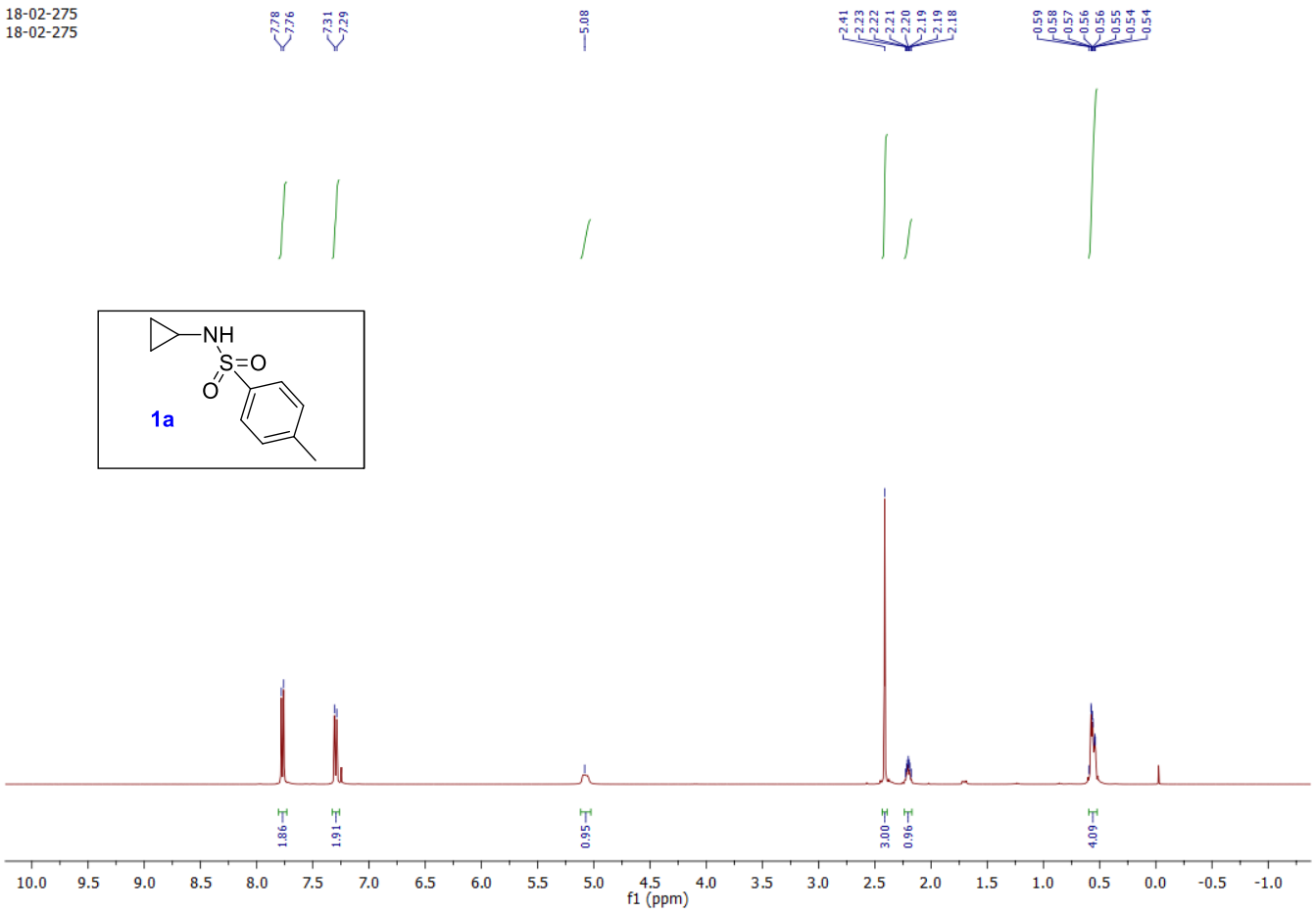
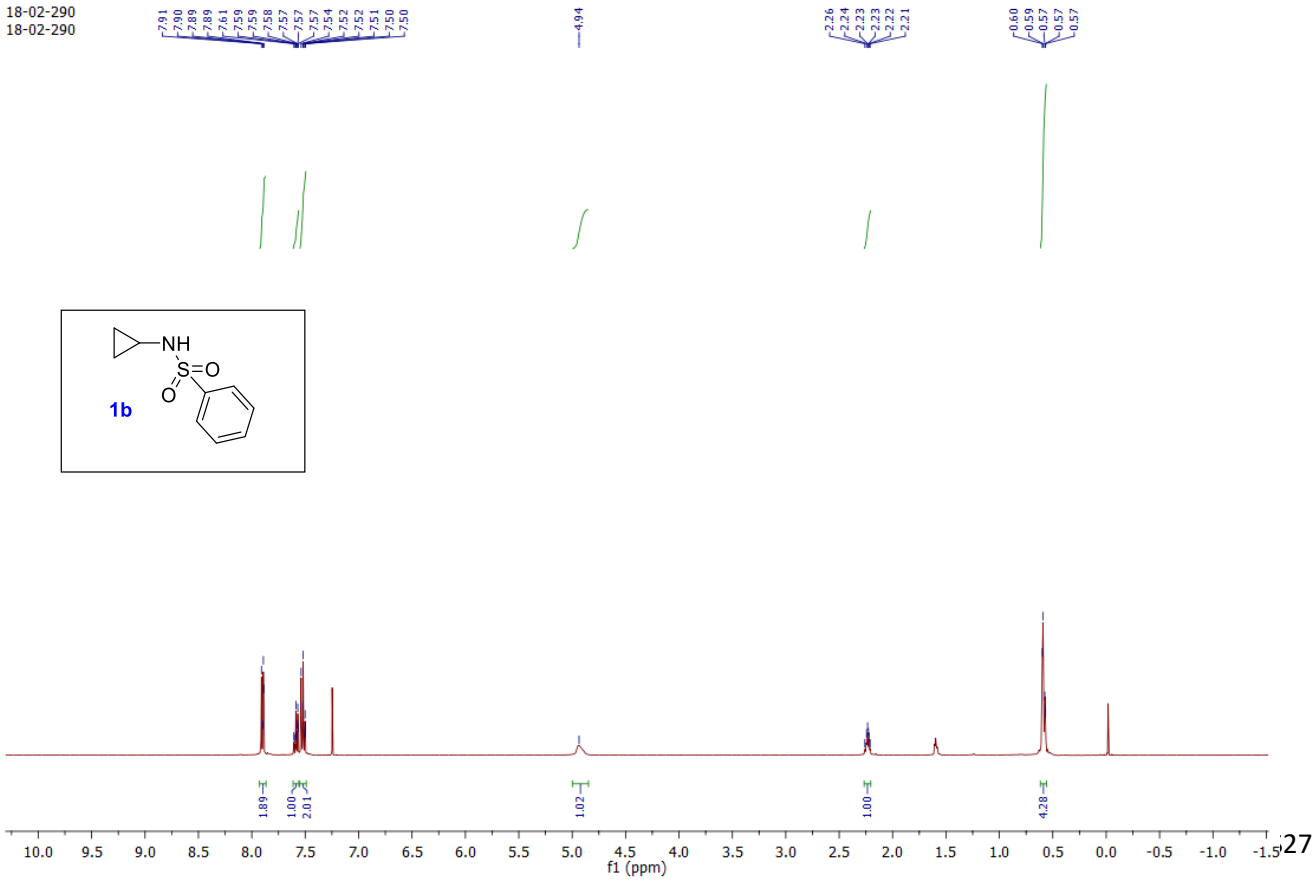
5. A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, *J. Appl. Cryst.*, 1993, 26, 343.
6. Sheldrick, G. M. SHELXL-97, Program for Crystal Structure Solution and Refinement, University of Göttingen, Göttingen, Germany 1997.
7. L. J. Farrugia, *J. Appl. Cryst.* 1999, 32, 837.
8. CCDC 2115609 and CCDC 2145541 contains supplementary crystallographic data for the compounds 3ag and 3al respectively.

L) ^{1}H NMR of the Starting materials

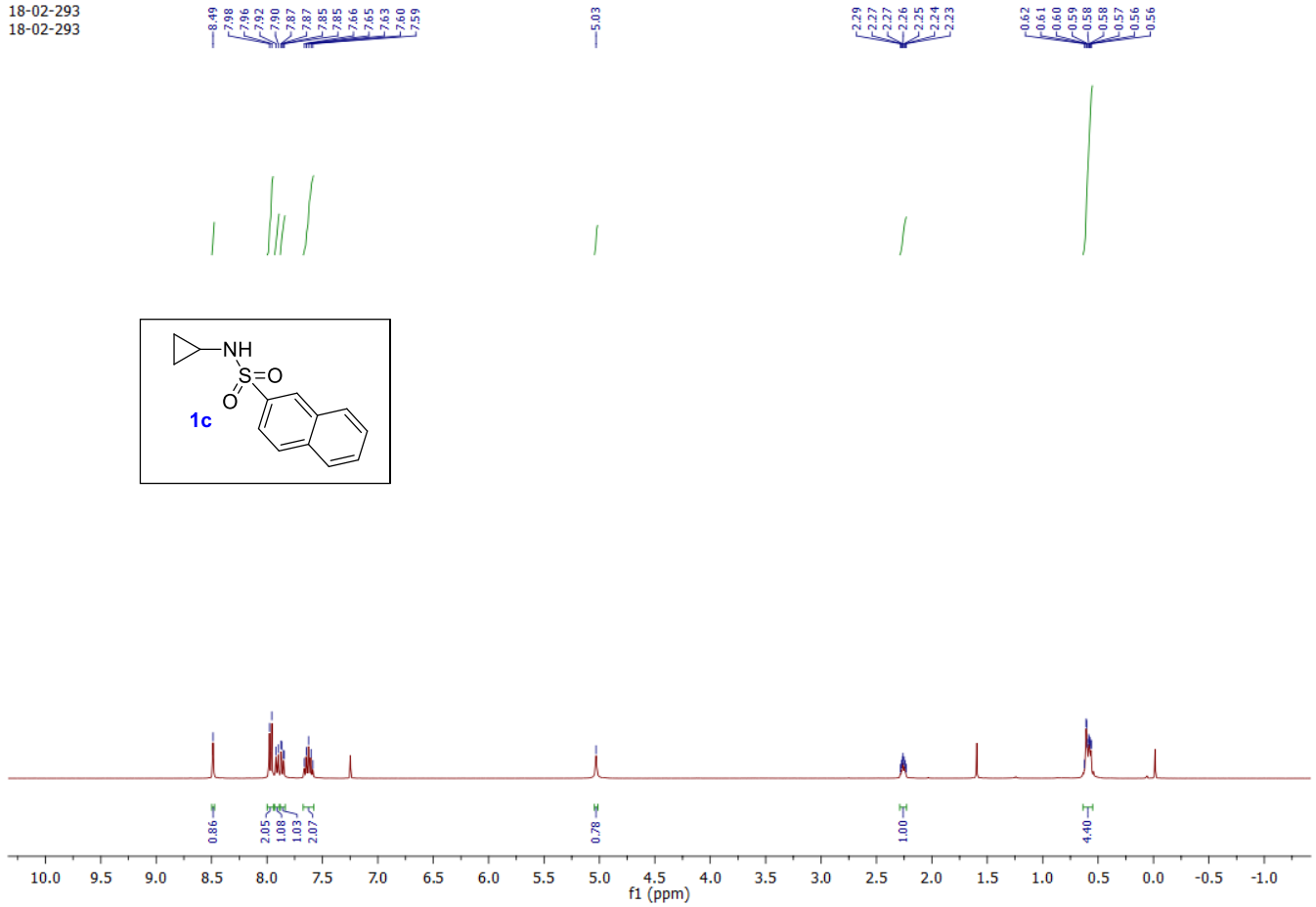
^{1}H NMR ($CDCl_3$, 400 MHz) of 1a



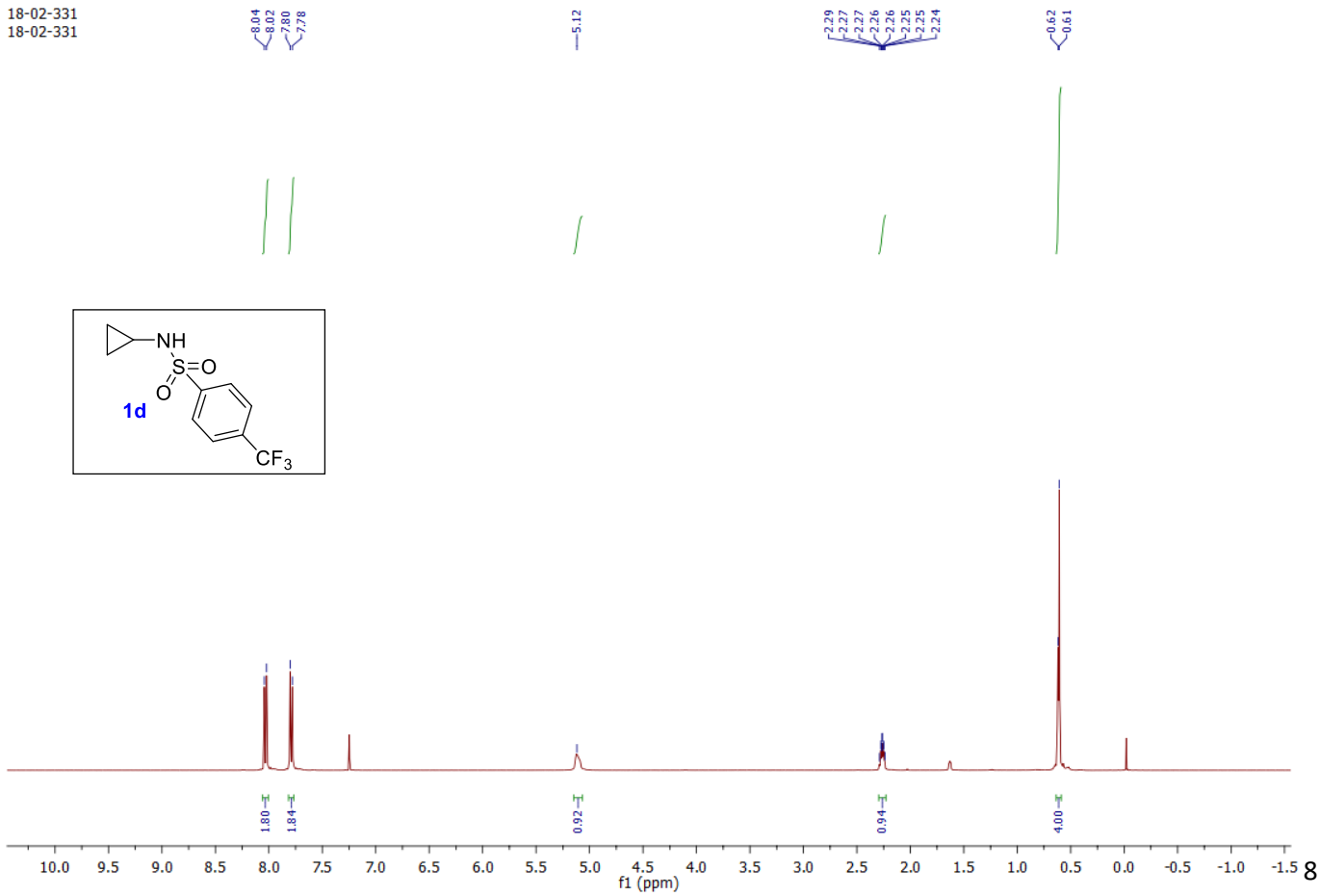
^{1}H NMR ($CDCl_3$, 400 MHz) of 1b



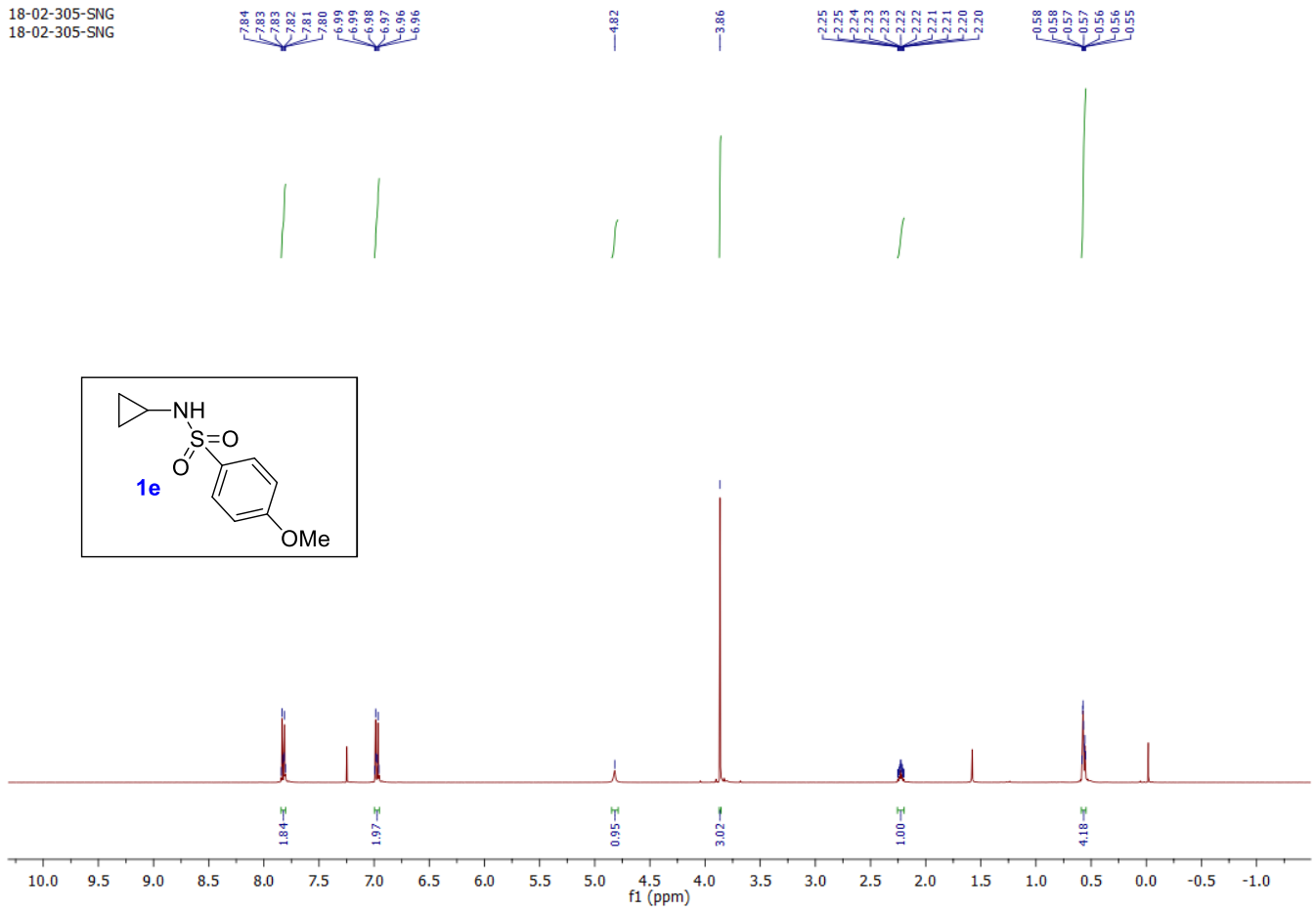
^{1}H NMR ($CDCl_3$, 400 MHz) of 1c



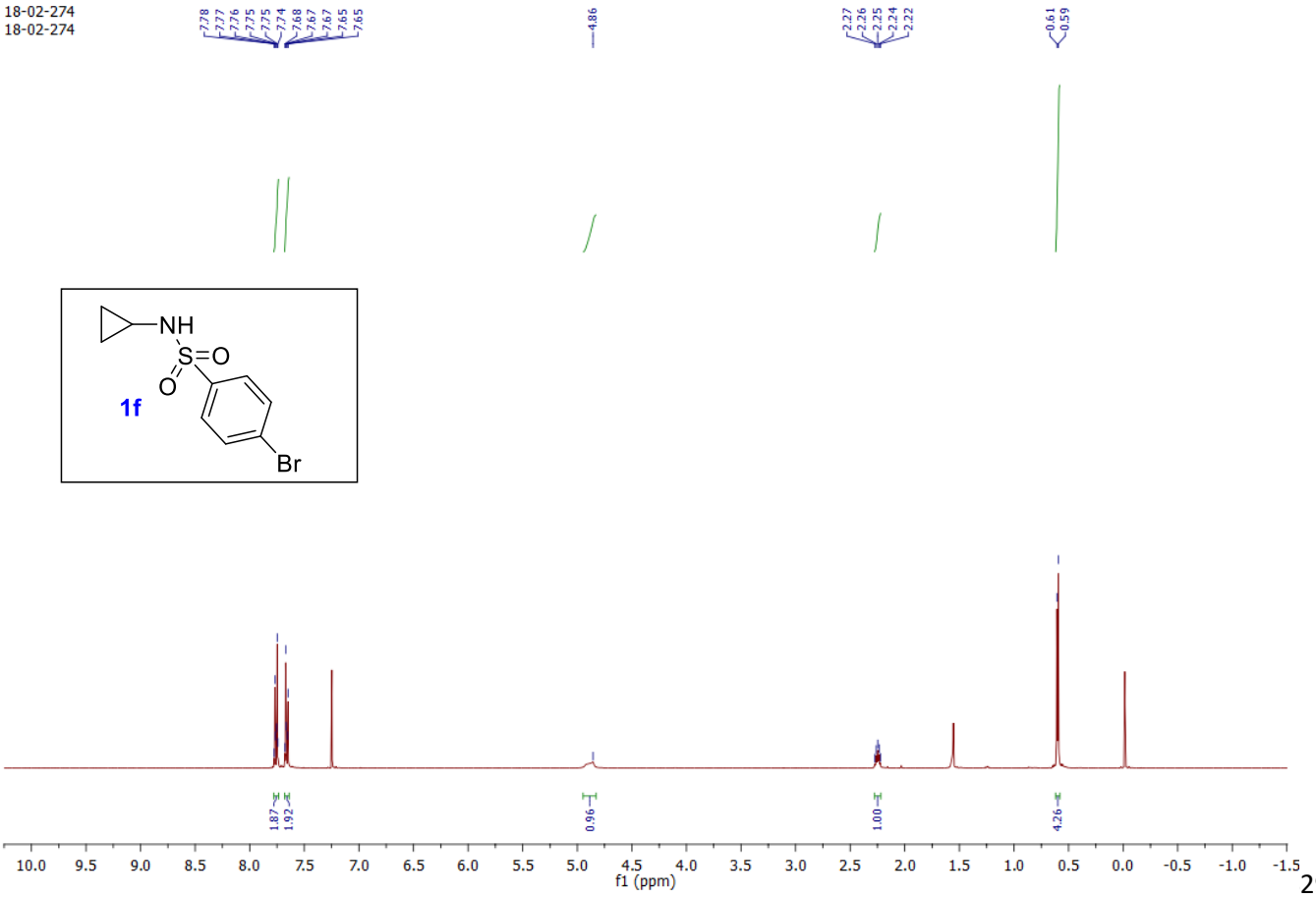
^{1}H NMR ($CDCl_3$, 400 MHz) of 1d



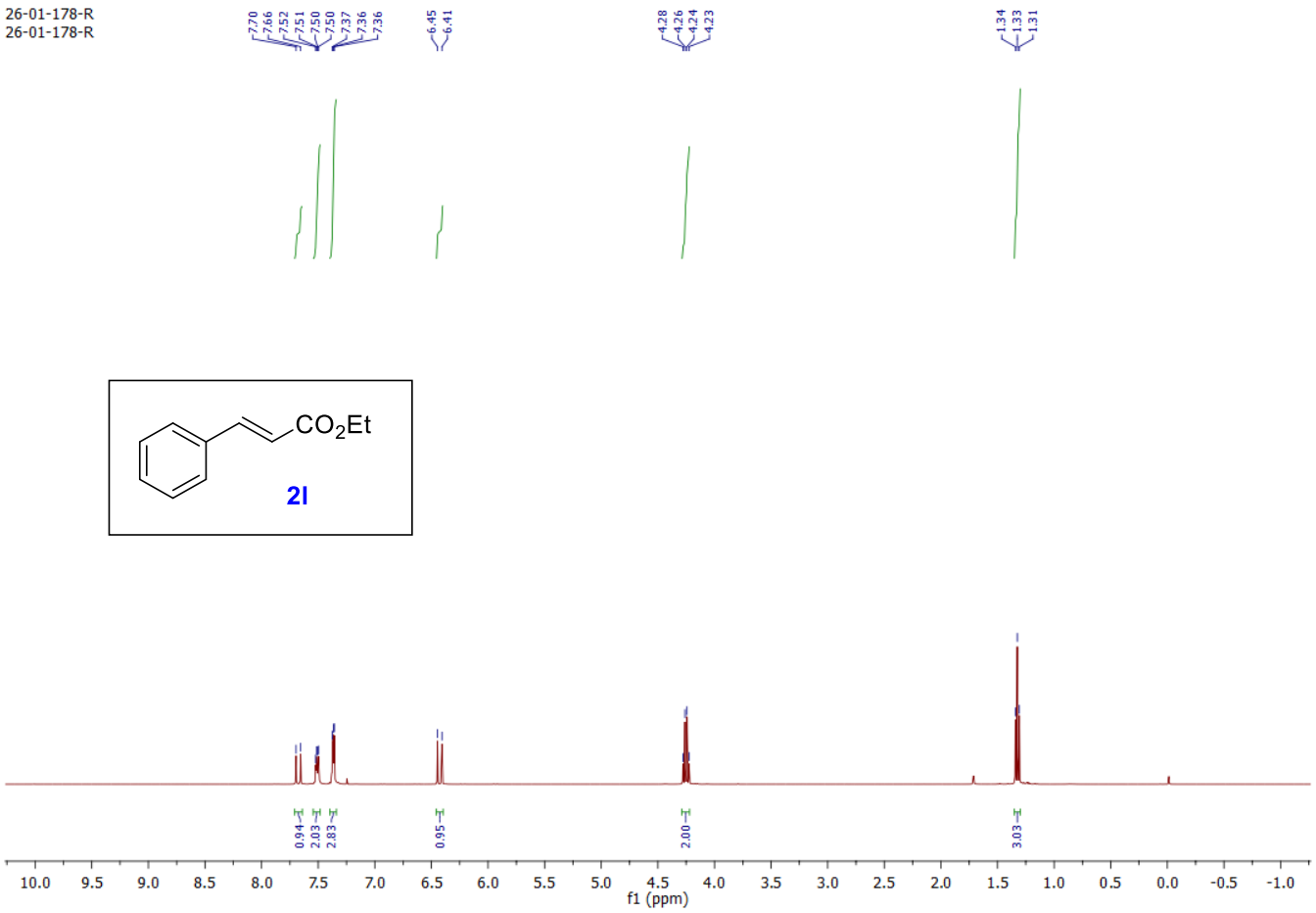
^{1}H NMR ($CDCl_3$, 400 MHz) of 1e



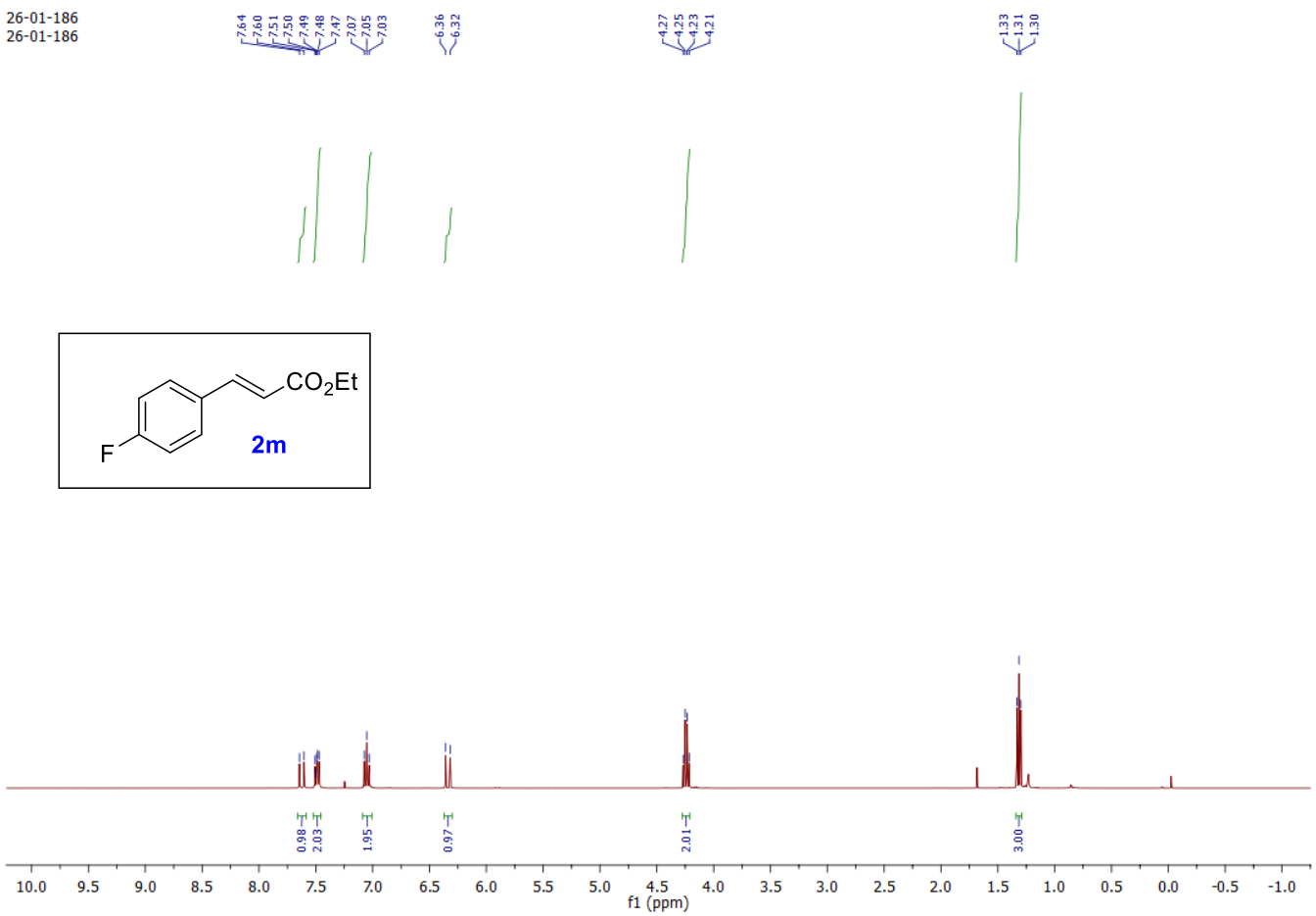
^{1}H NMR ($CDCl_3$, 400 MHz) of 1f



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



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



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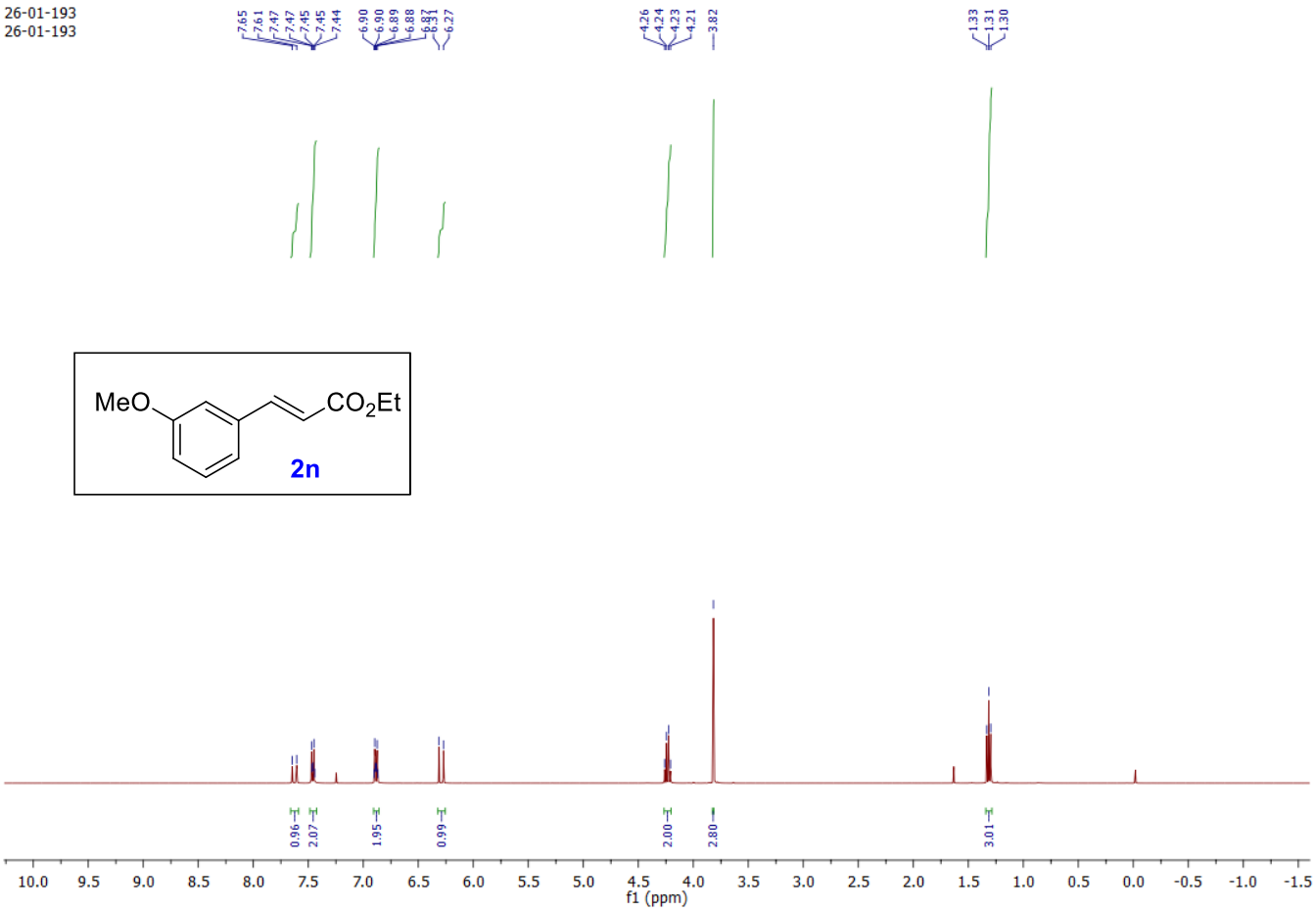
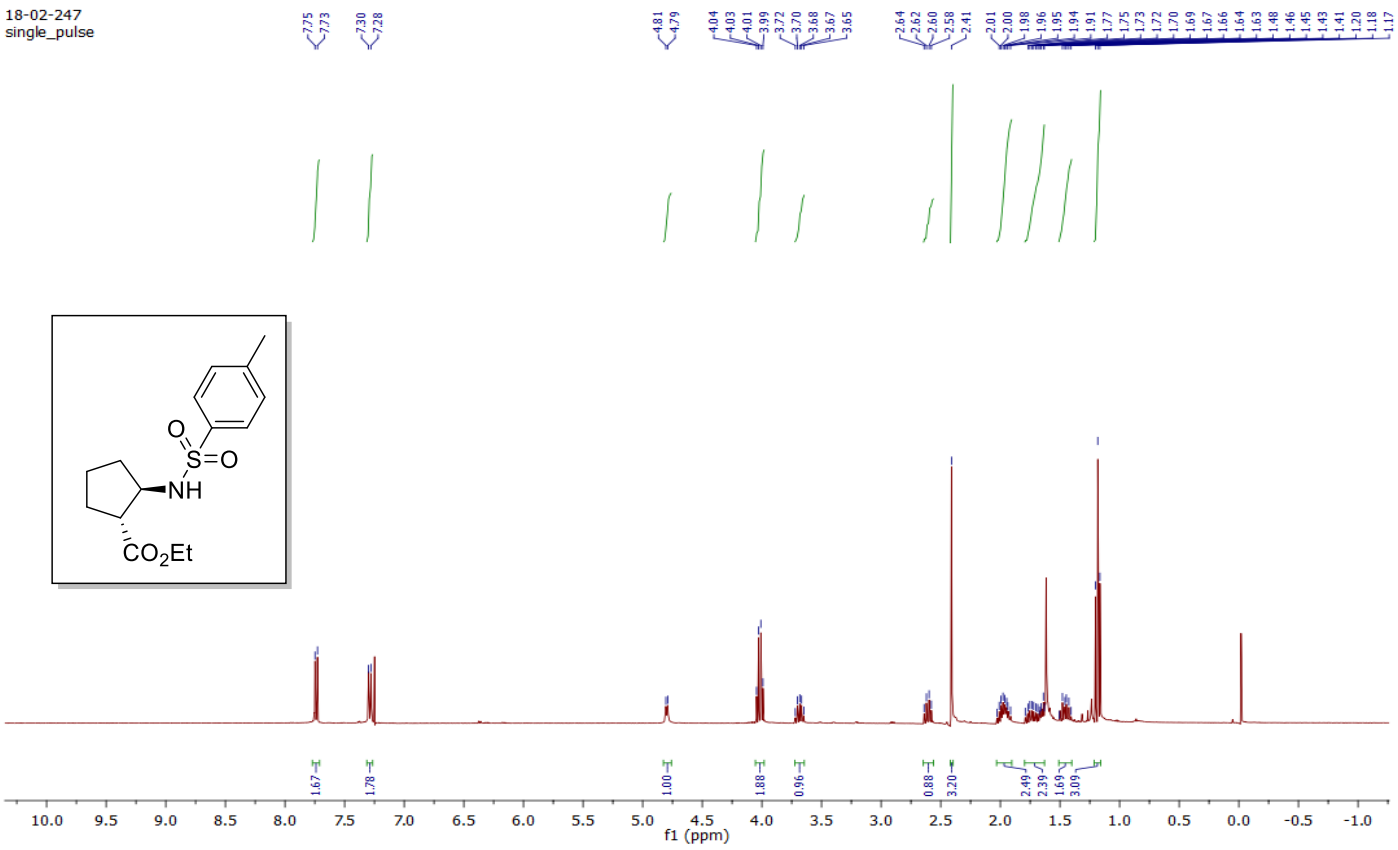
^{1}H NMR ($CDCl_3$, 400 MHz) of 2n

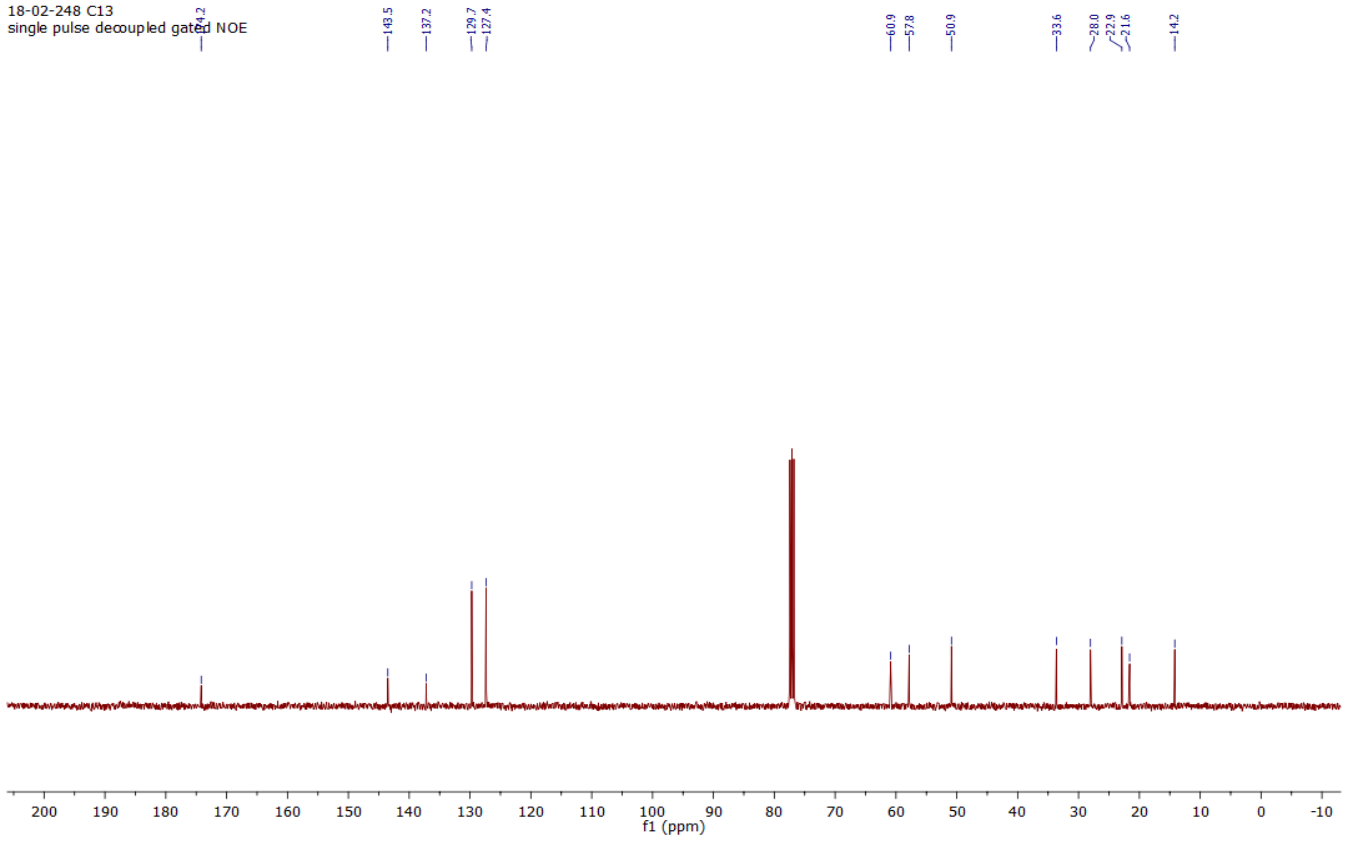


M) NMR and HRMS of the Products

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3aa



HRMS of 3aa

Elemental Composition Report

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-15 H: 0-100 N: 0-1 O: 0-4 S: 0-1

Sample Name : 230821_18-02-248 IITRPR XEVO G2-XS QTOF
Test Name :
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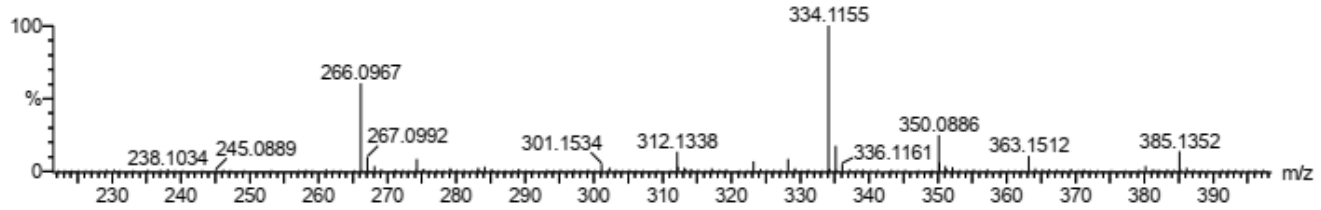
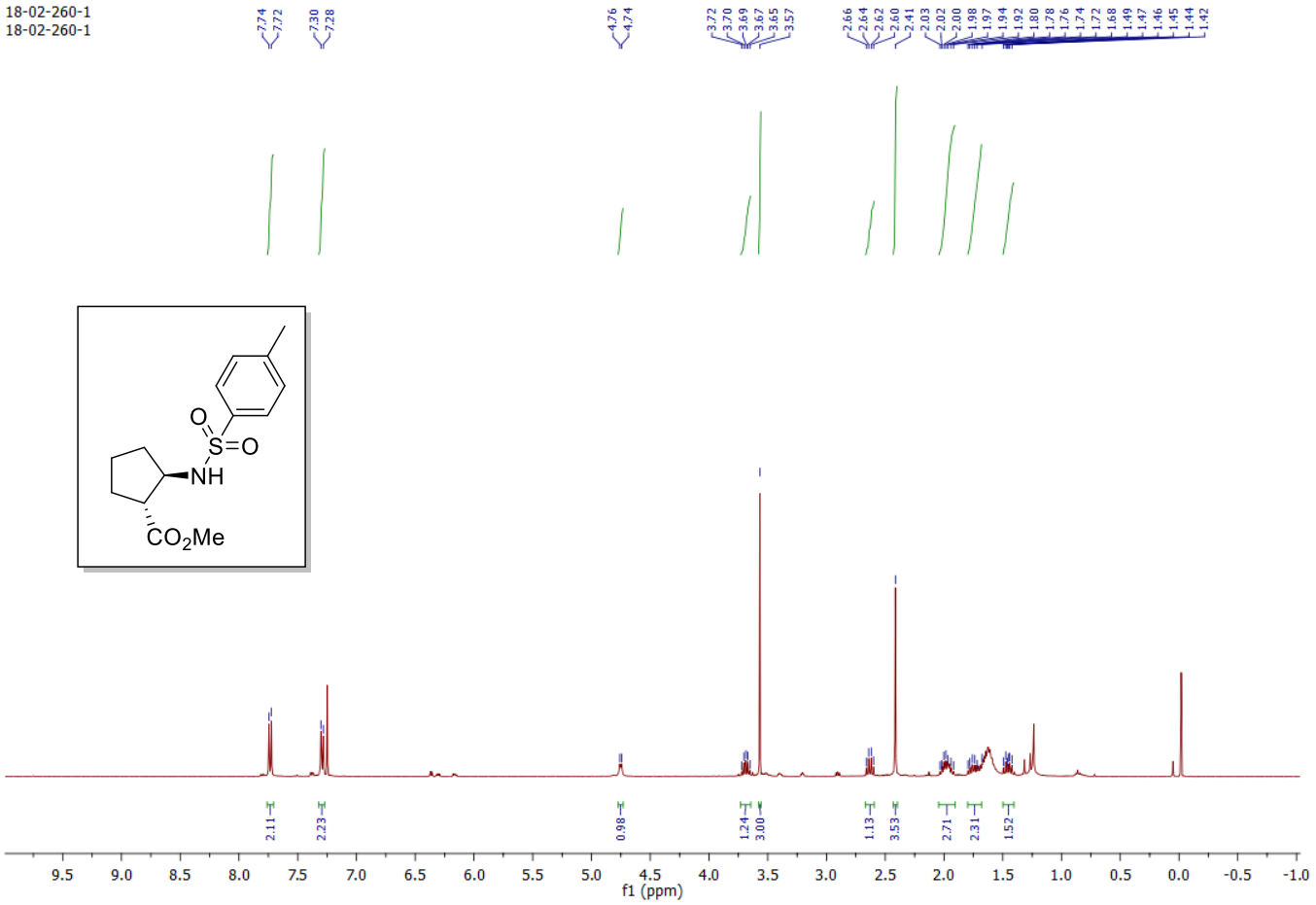
4.03e+006

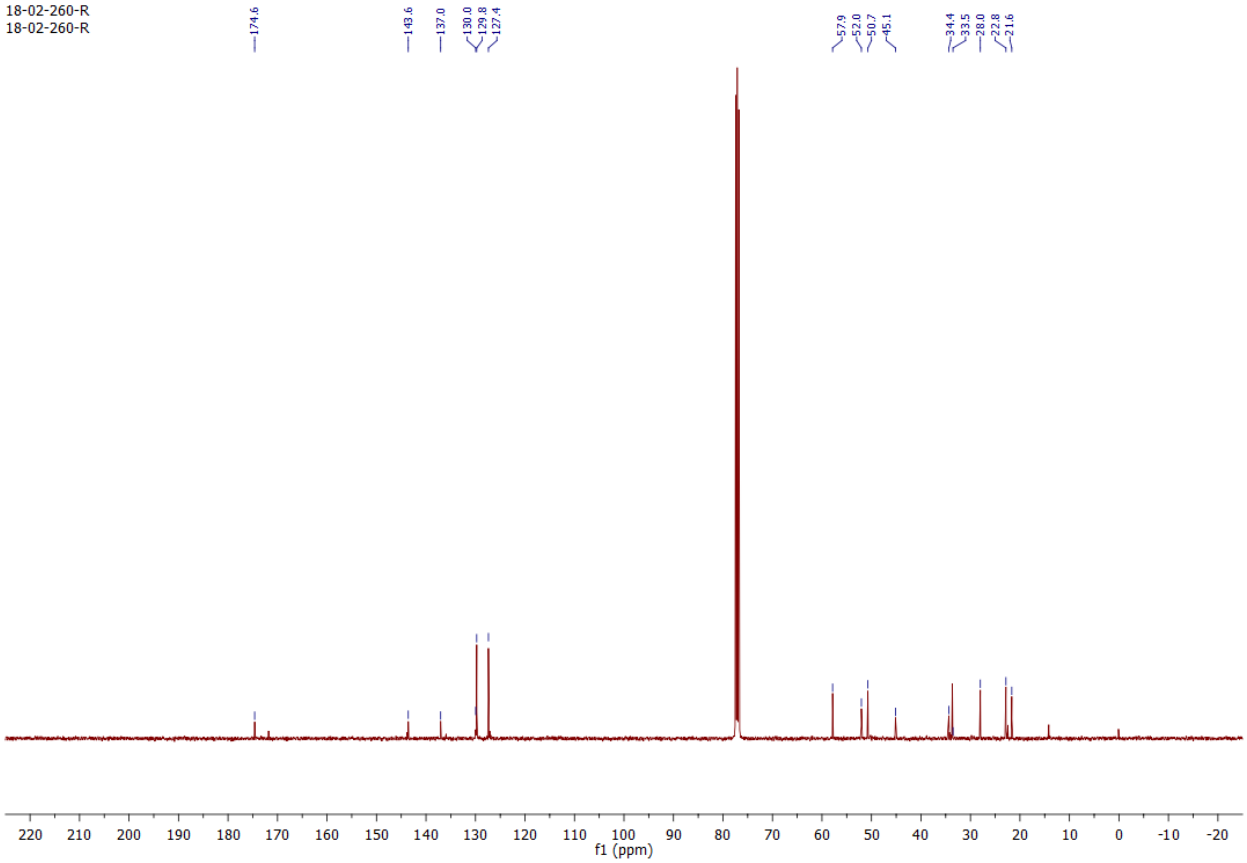


Minimum:				-1.5				
Maximum:		2.0	300.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.1338	312.1270	6.8	21.8	5.5	839.2	n/a	n/a	C15 H22 N O4 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ad



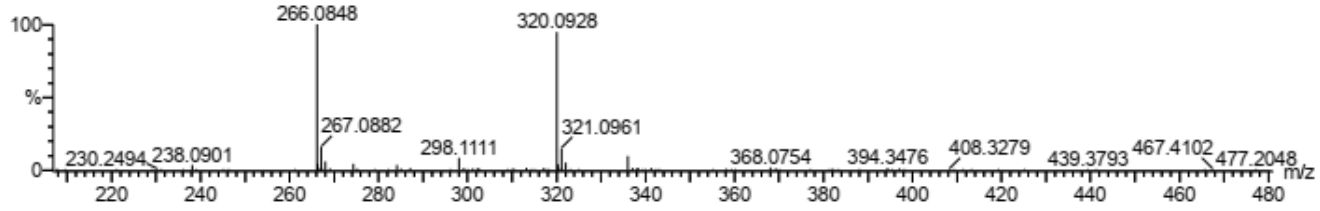
Elemental Composition Report

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

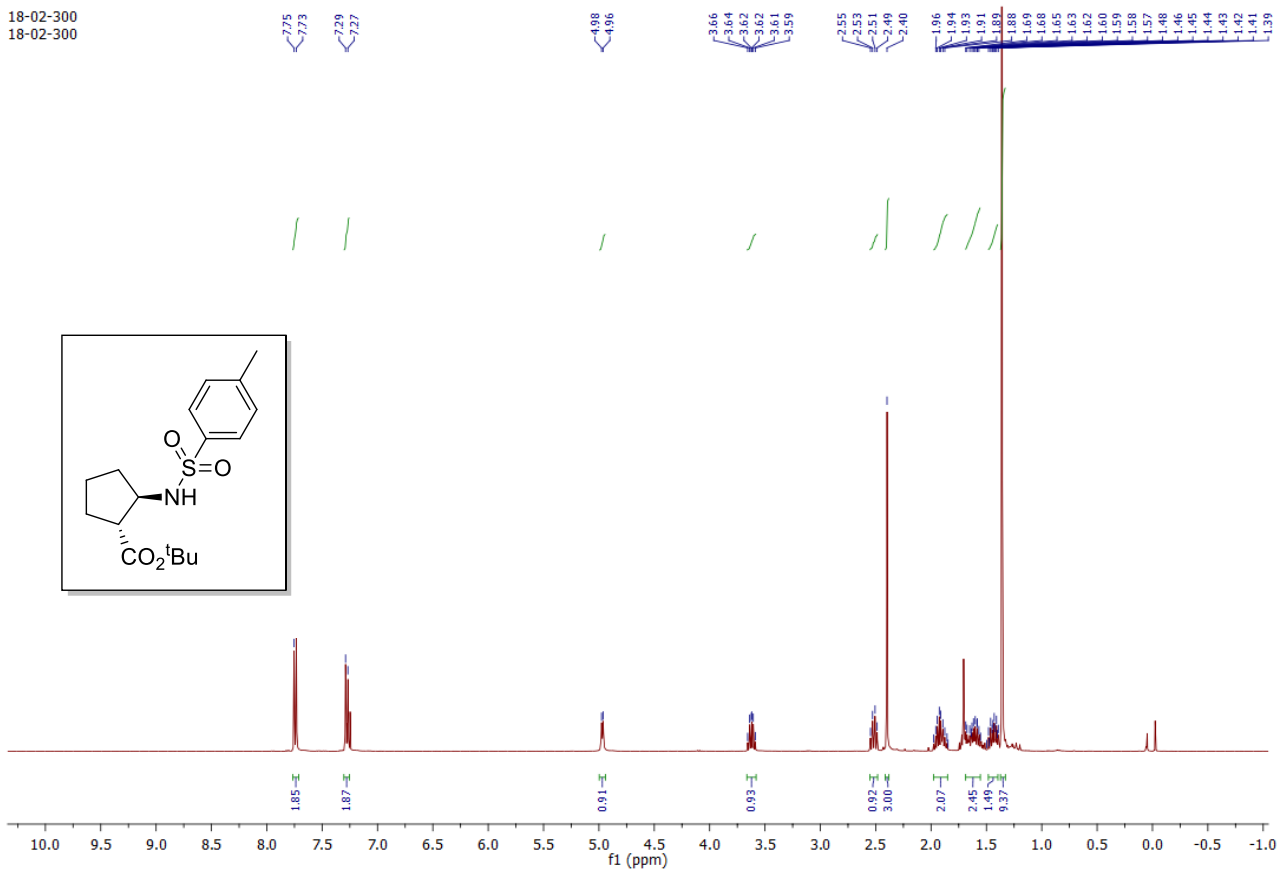
Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 14-14 H: 0-100 N: 0-1 O: 4-4 S: 0-1

Sample Name : 160921_18-02-260-IR IITRPR XEVO G2-XS QTOF
Test Name :
160921_18-02-260-IR 10 (0.232) 1: TOF MS ES+
4.78e+007

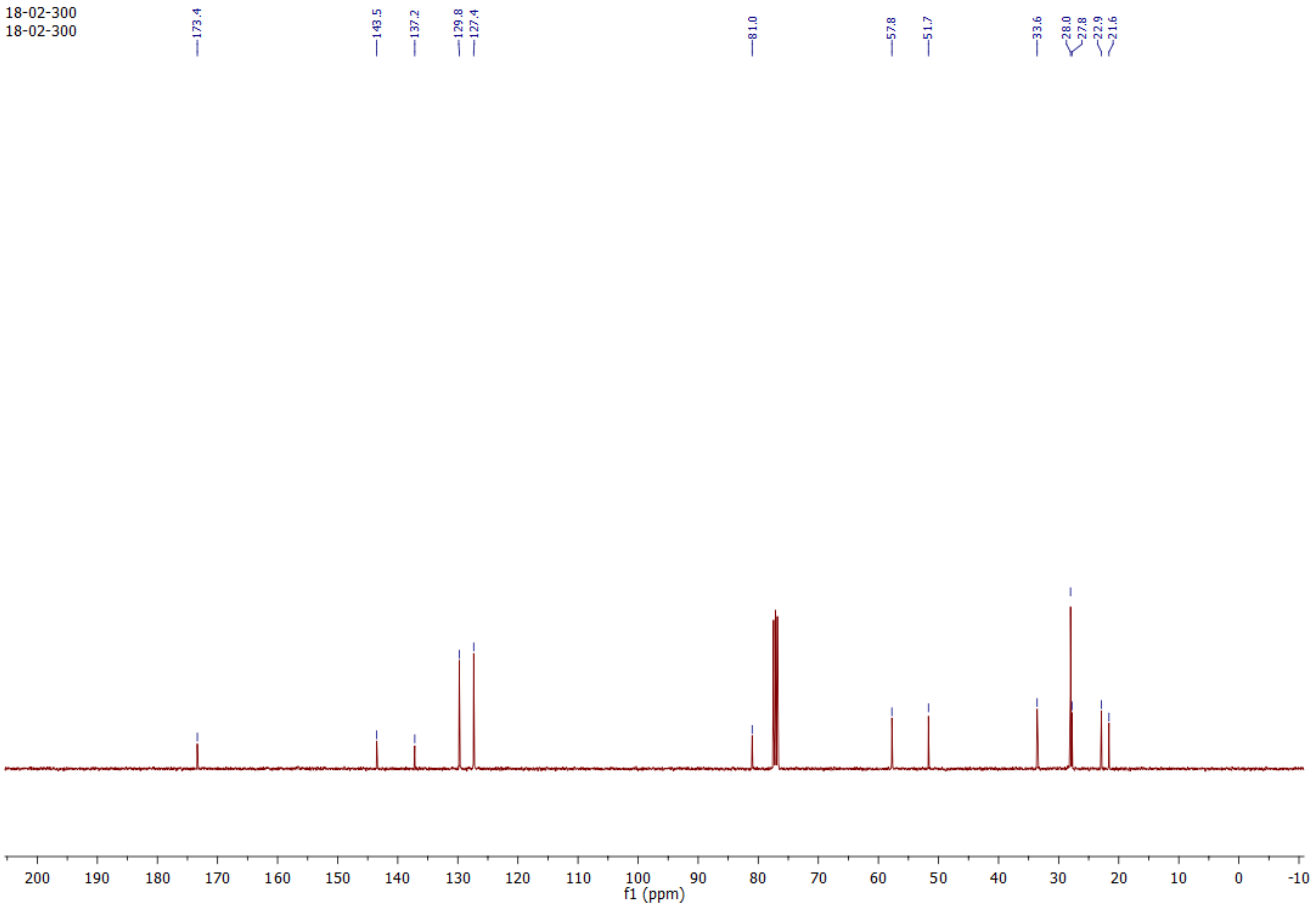


Minimum:				-1.5				
Maximum:		2.0	300.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
298.1111	298.1113	-0.2	-0.7	5.5	1771.3	n/a	n/a	C14 H20 N O4 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ae



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
645 formula(e) evaluated with 9 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 10-25 H: 1-30 N: 1-3 O: 1-5 S: 0-2 Cl: 0-2 Na: 0-1

Sample Name : 18_02_300 IITRPR XEVO G2-XS QTOF
Test Name :
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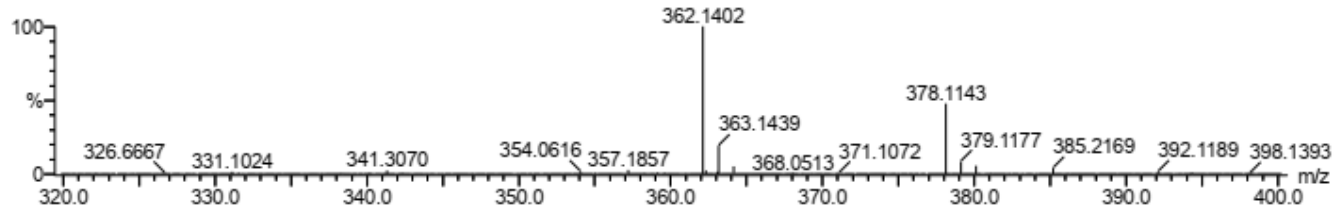
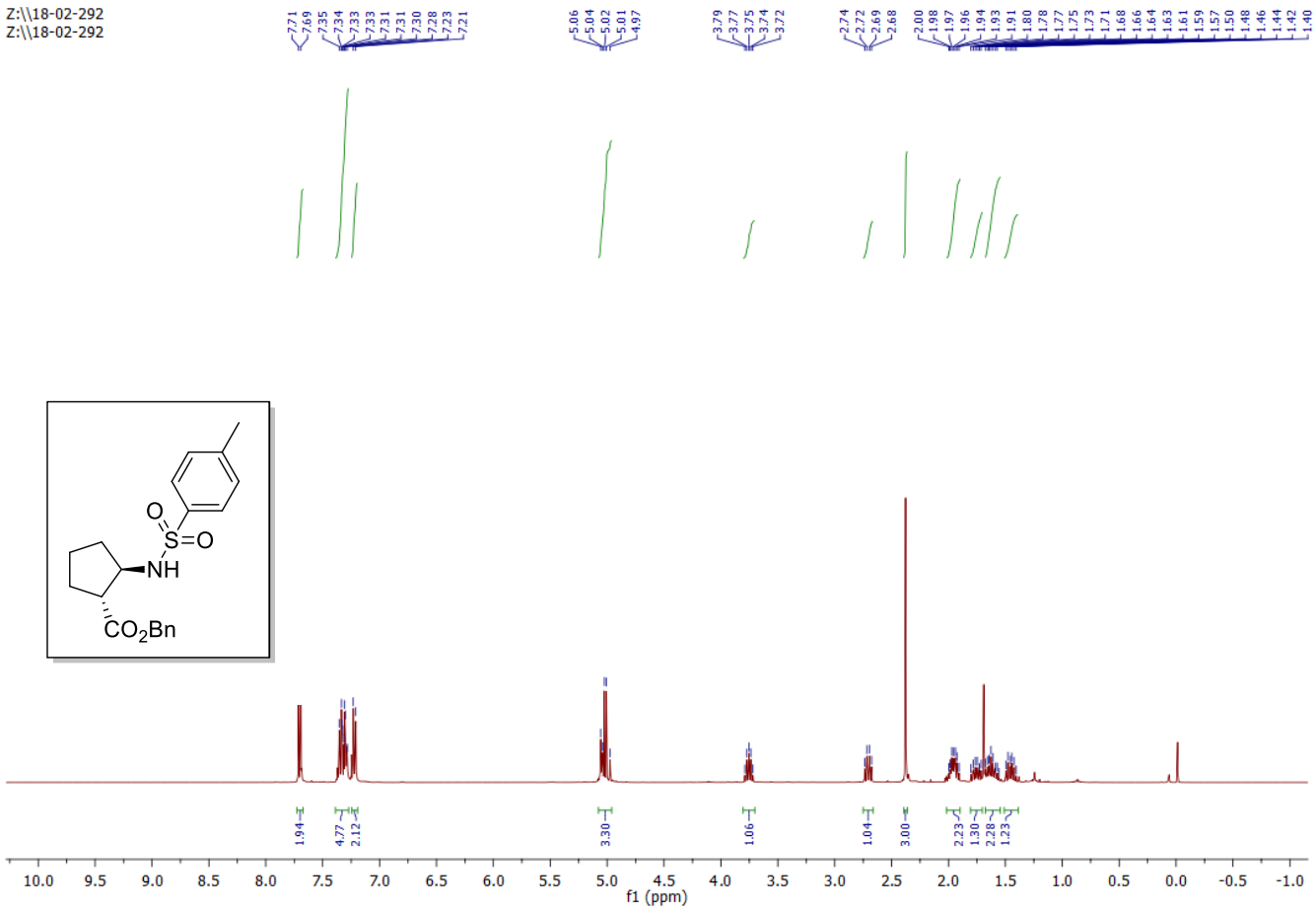
5.17e+006

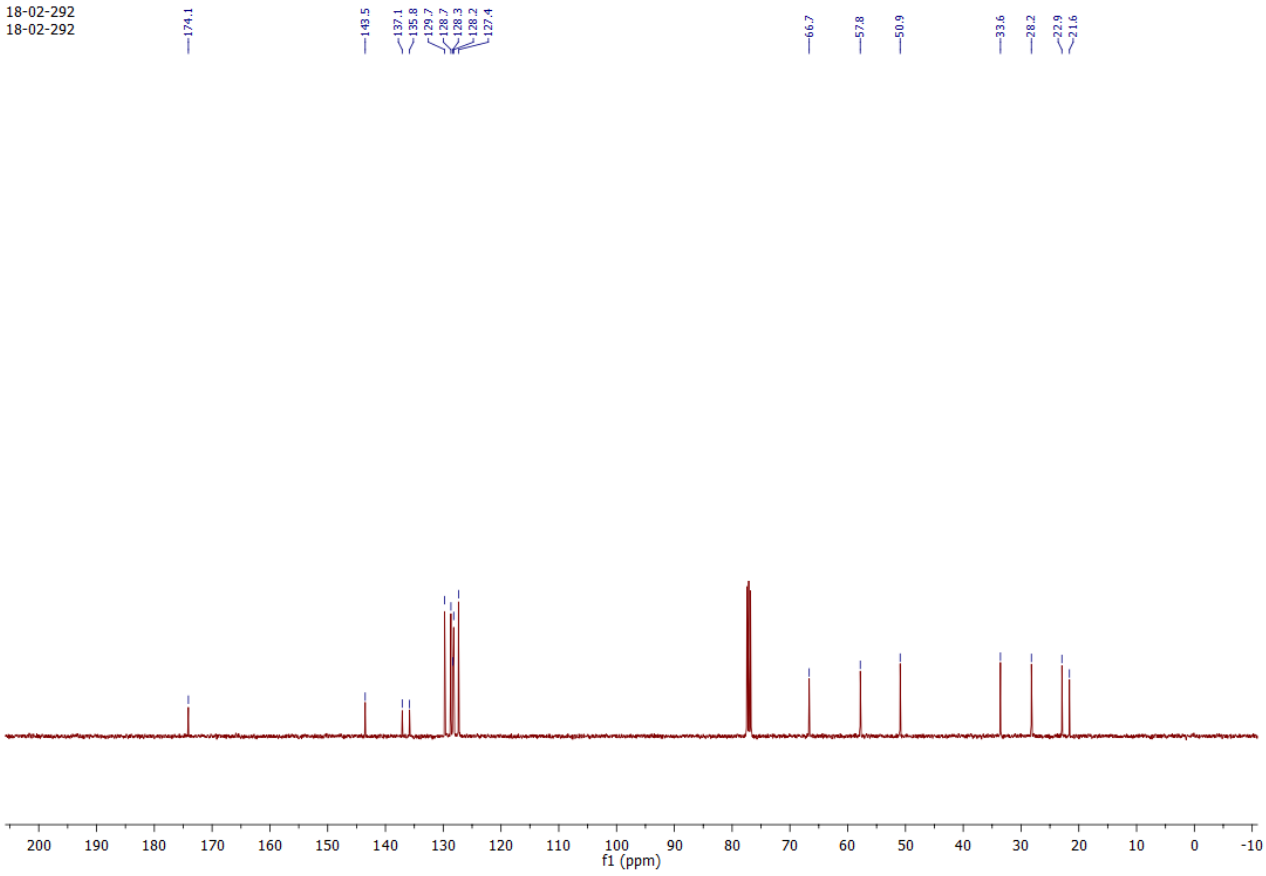


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
362.1402	362.1402	0.0	0.0	5.5	1468.2	n/a	n/a	C17 H25 N O4 S Na

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3af



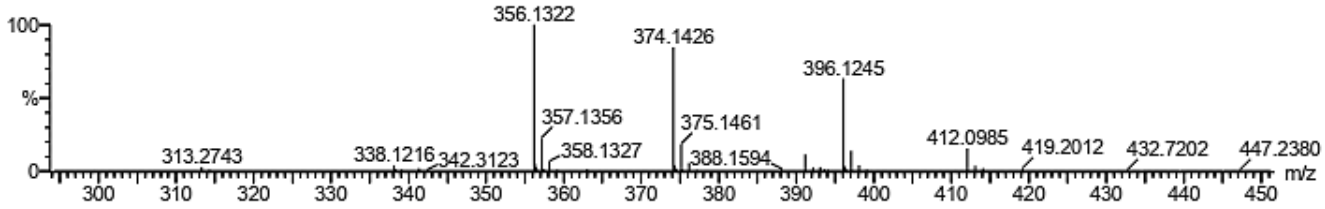
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

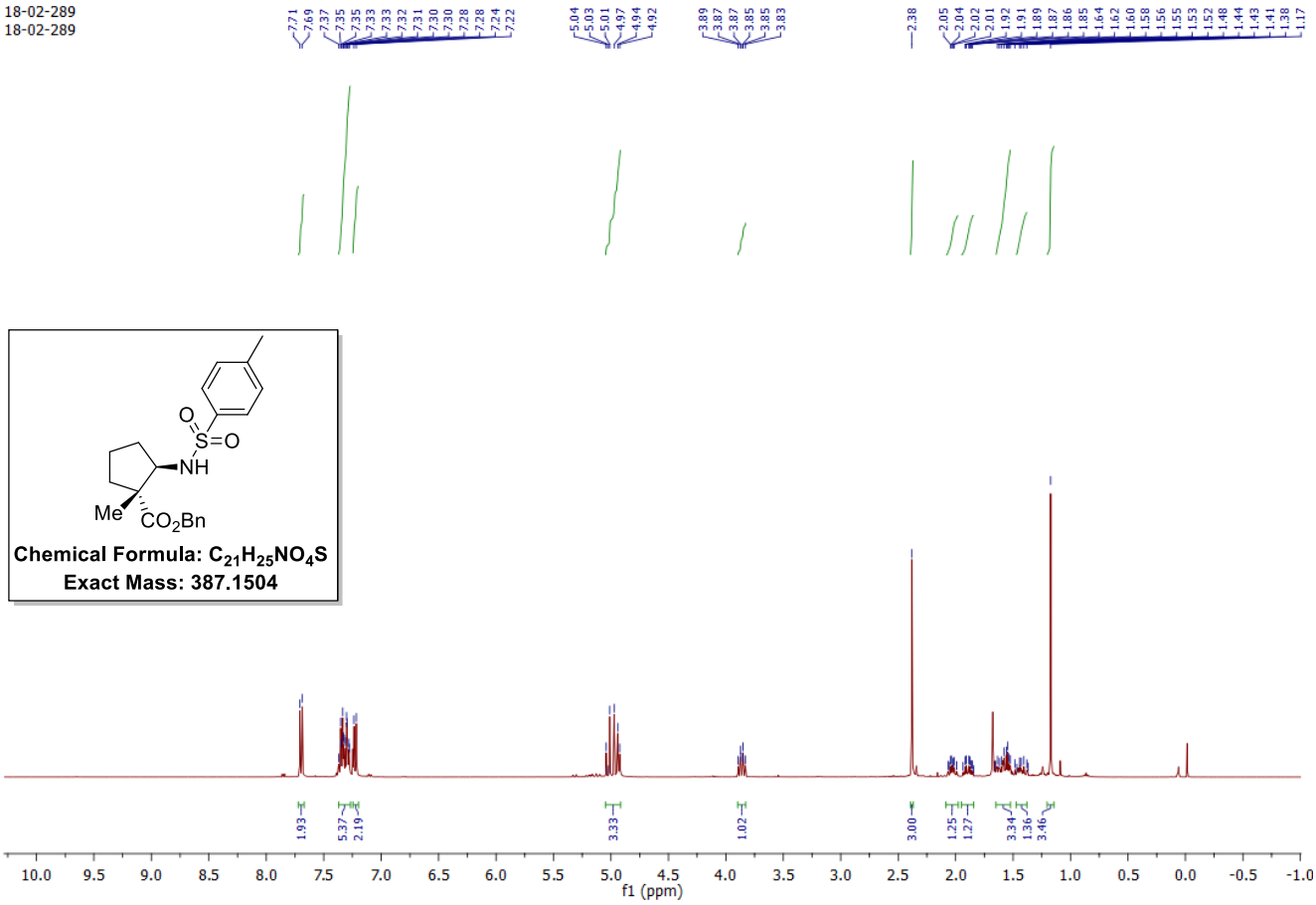
Monoisotopic Mass, Even Electron Ions
2833 formula(e) evaluated with 23 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-6 F: 0-3 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_292 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_292 13 (0.294) 1: TOF MS ES+
1.74e+007

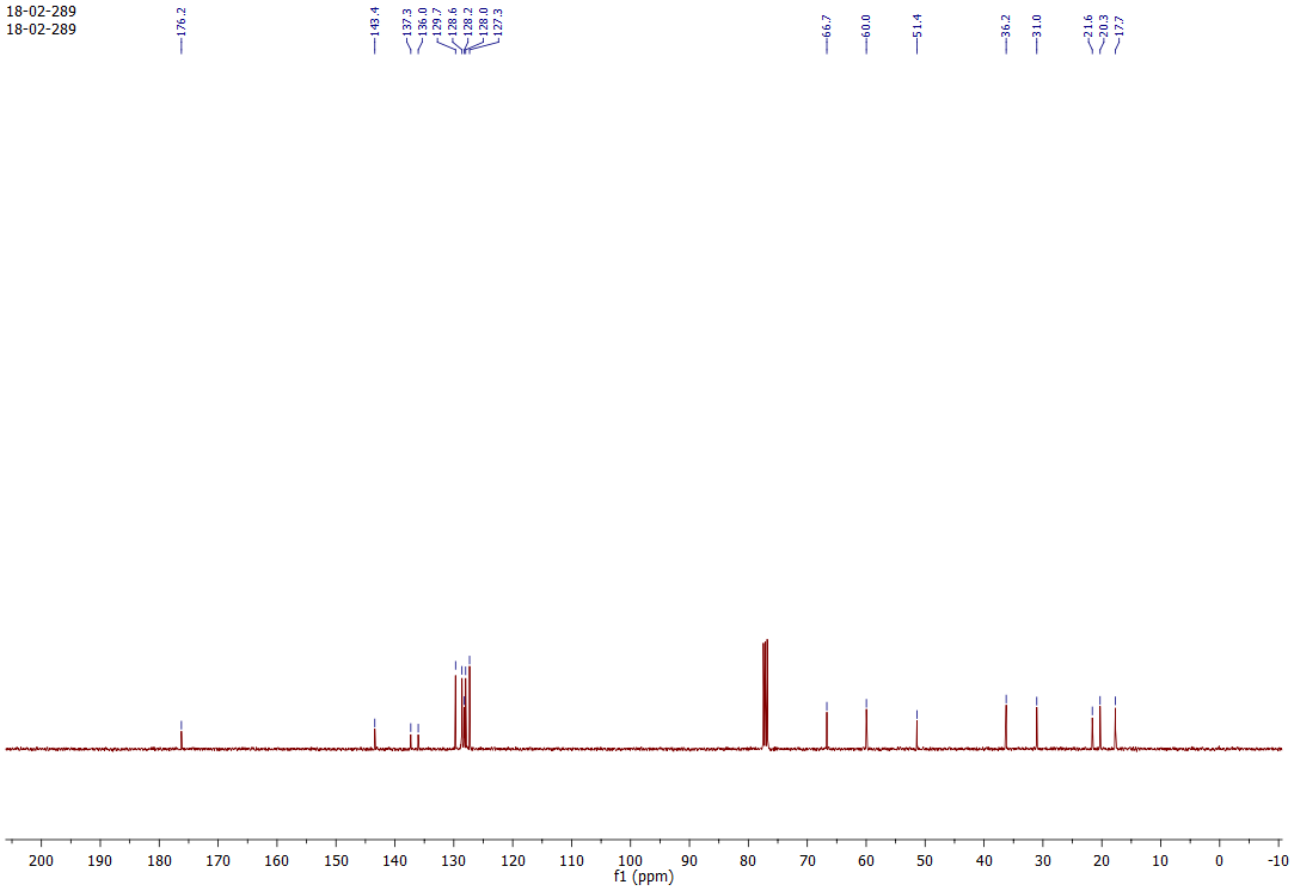


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
374.1426	374.1426	0.0	0.0	9.5	1551.7	n/a	n/a	C20 H24 N O4 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ag



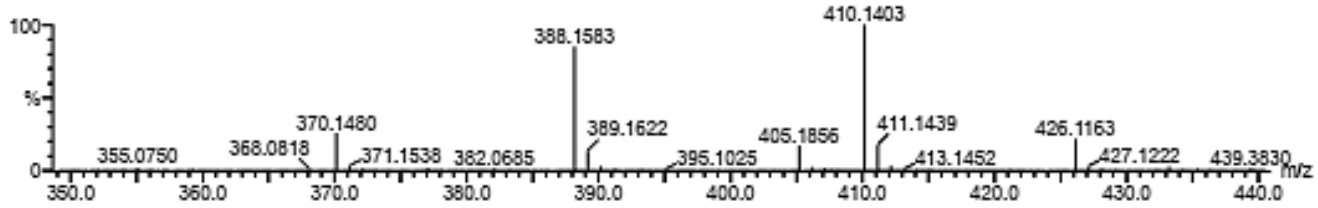
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

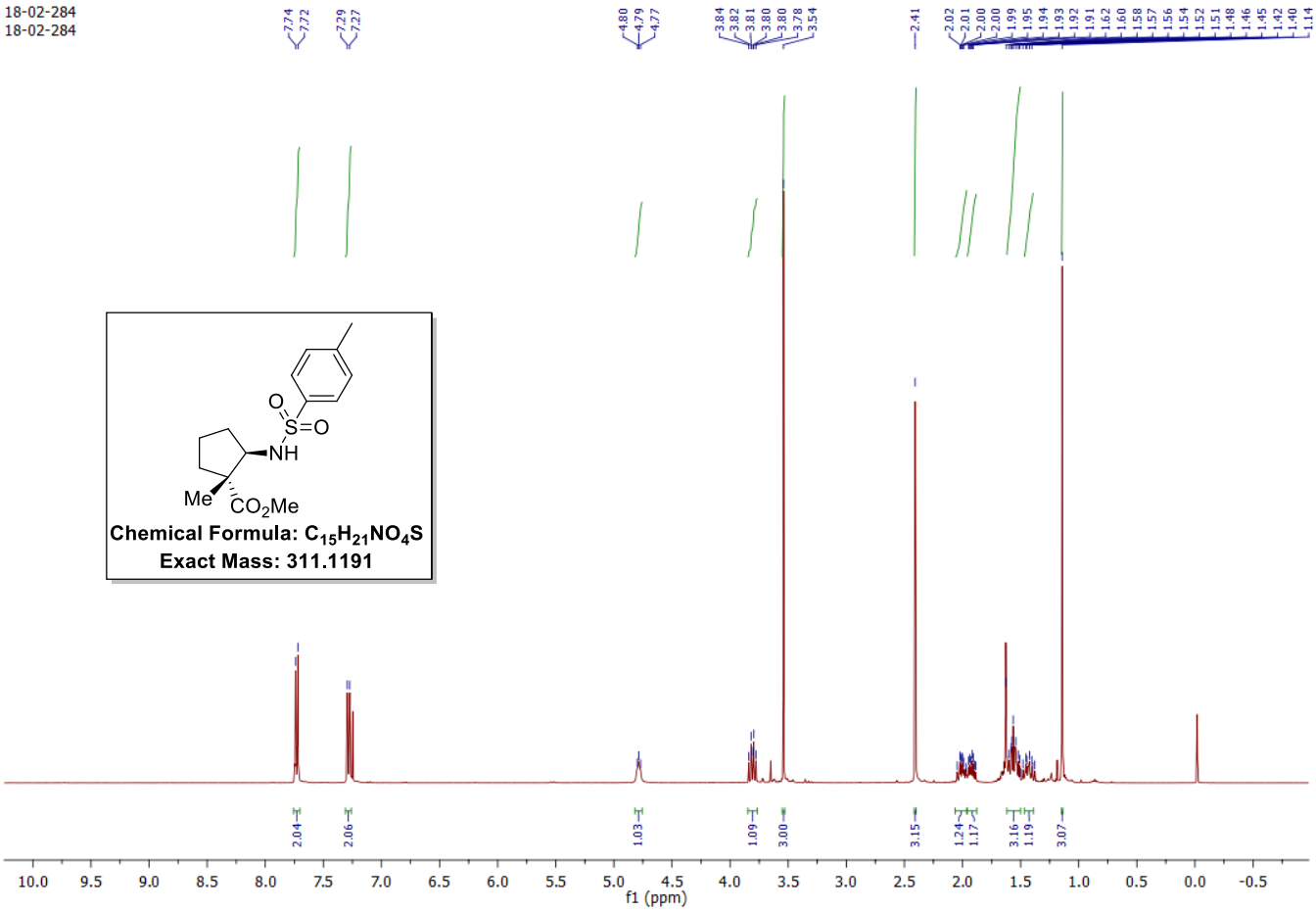
Monoisotopic Mass, Even Electron Ions
641 formula(e) evaluated with 6 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 10-25 H: 1-30 N: 1-3 O: 1-5 Na: 0-1 S: 0-2 Cl: 0-2

Sample Name : 18_02_289 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_289 46 (0.978) 1: TOF MS ES+
9.31e+005

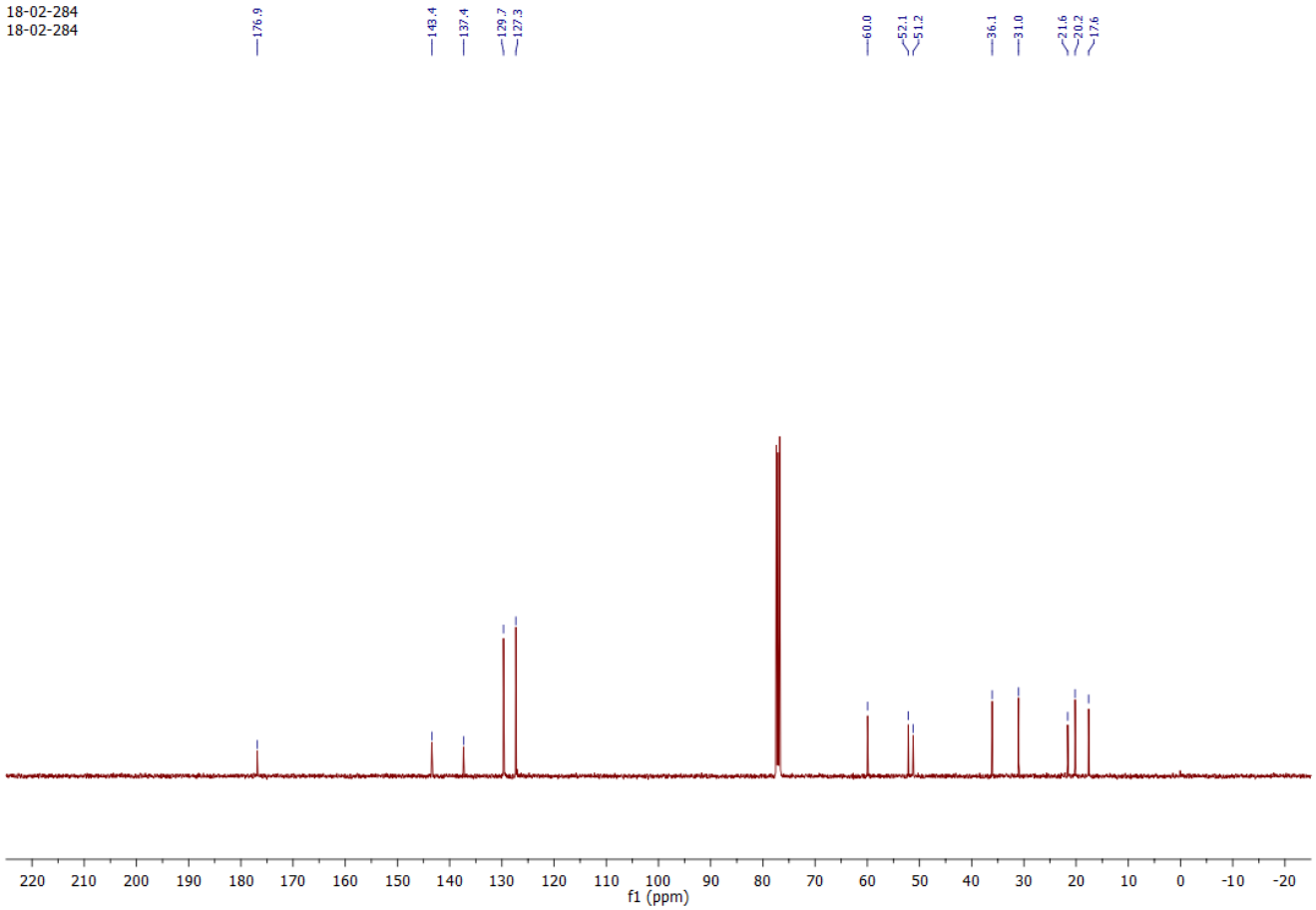


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
388.1583	388.1583	0.0	0.0	9.5	1112.1	n/a	n/a	C21 H26 N O4 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ah



HRMS of 3ah

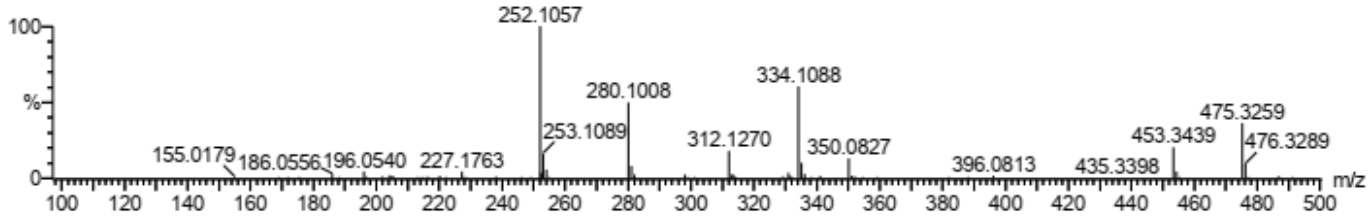
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

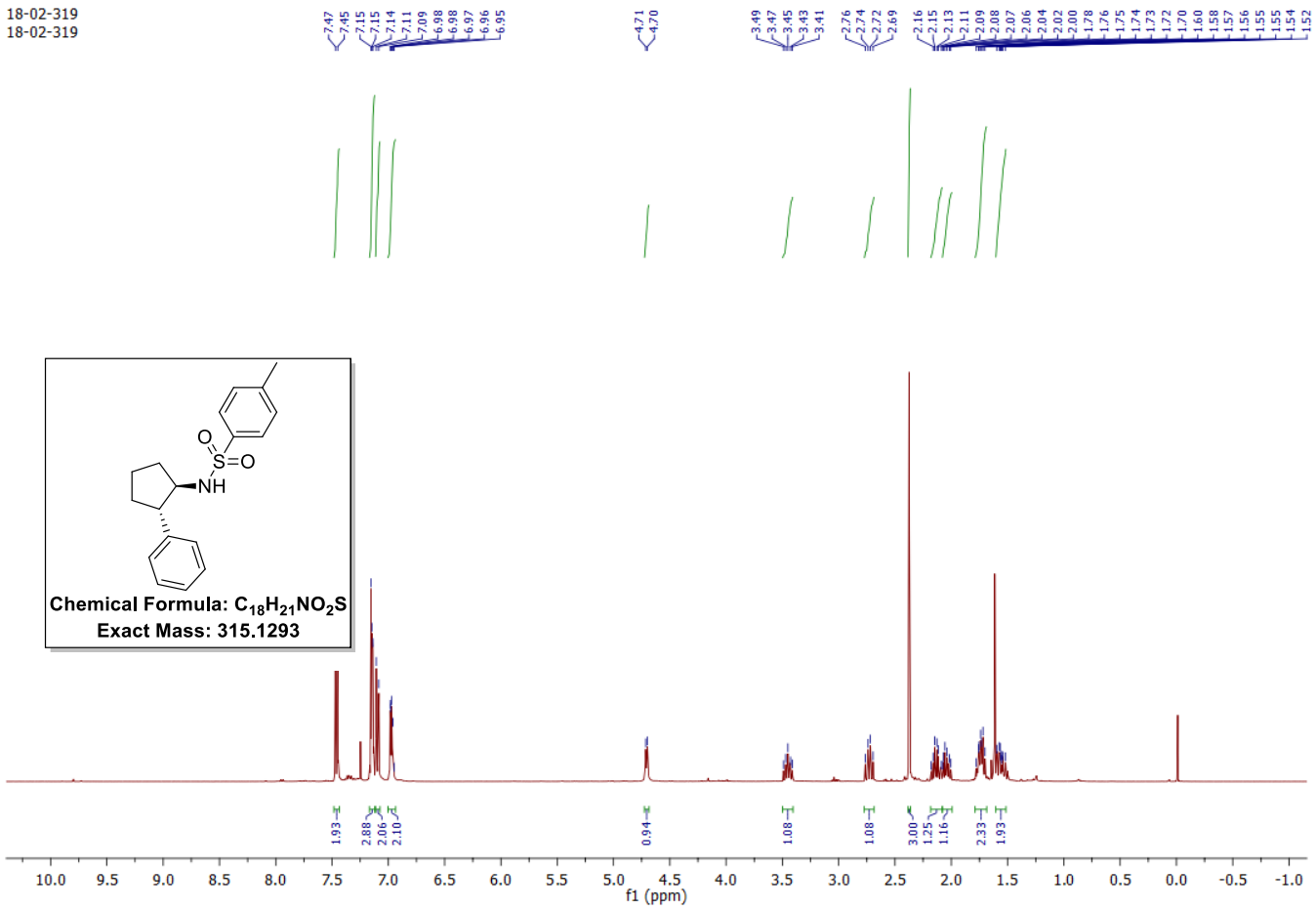
Monoisotopic Mass, Even Electron Ions
280 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 10-25 H: 1-30 N: 1-3 O: 1-5 S: 0-2 Cl: 0-2

Sample Name : 18_02_284 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_284 30 (0.639) 1: TOF MS ES+
5.30e+006

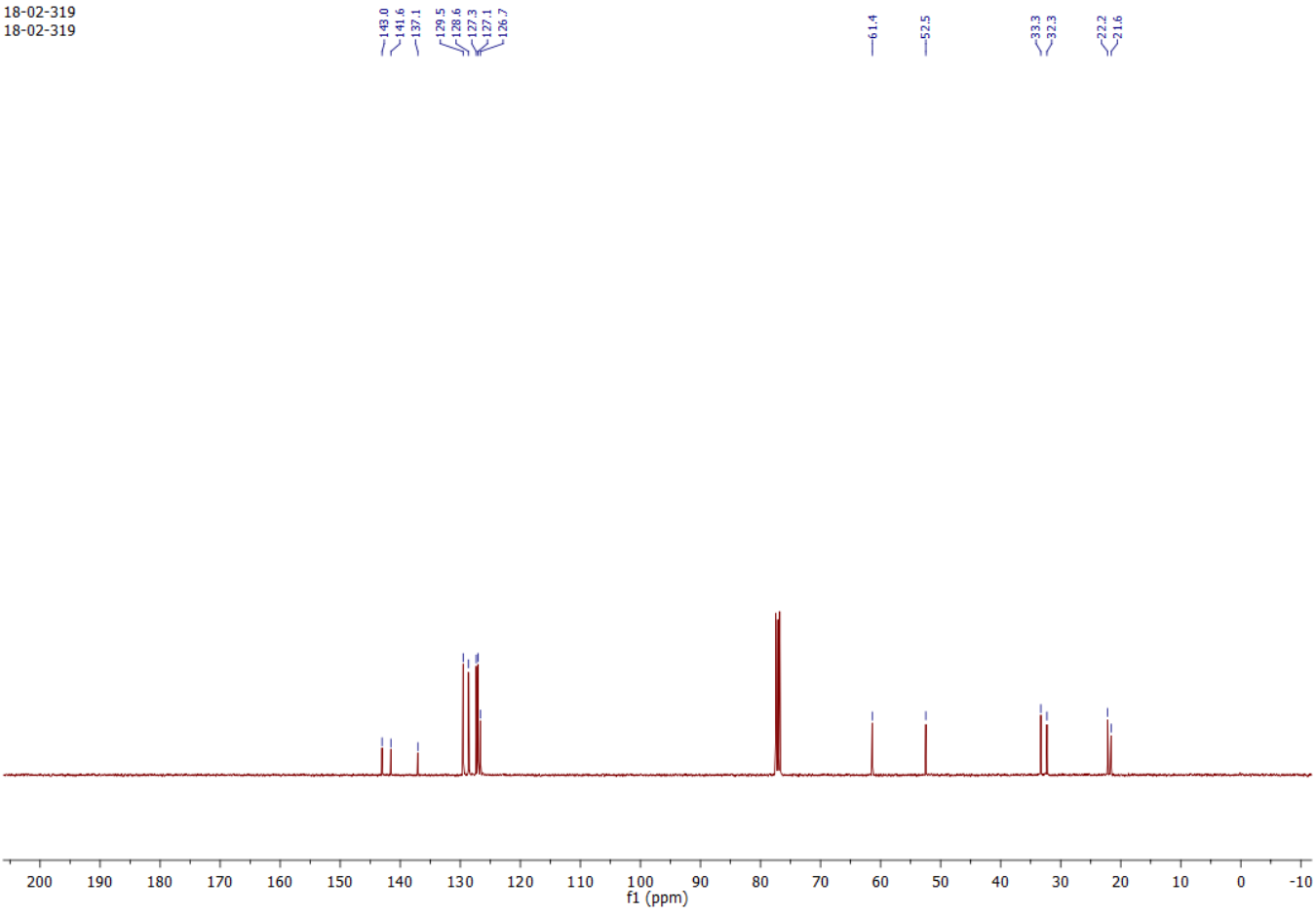


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.1270	312.1270	0.0	0.0	5.5	1394.0	n/a	n/a	C15 H22 N O4 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ai



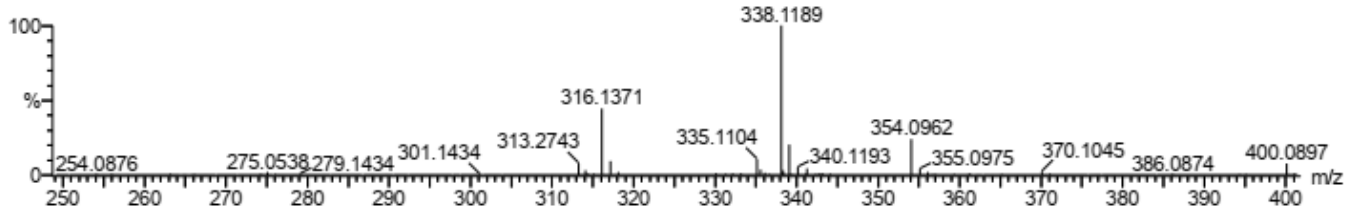
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

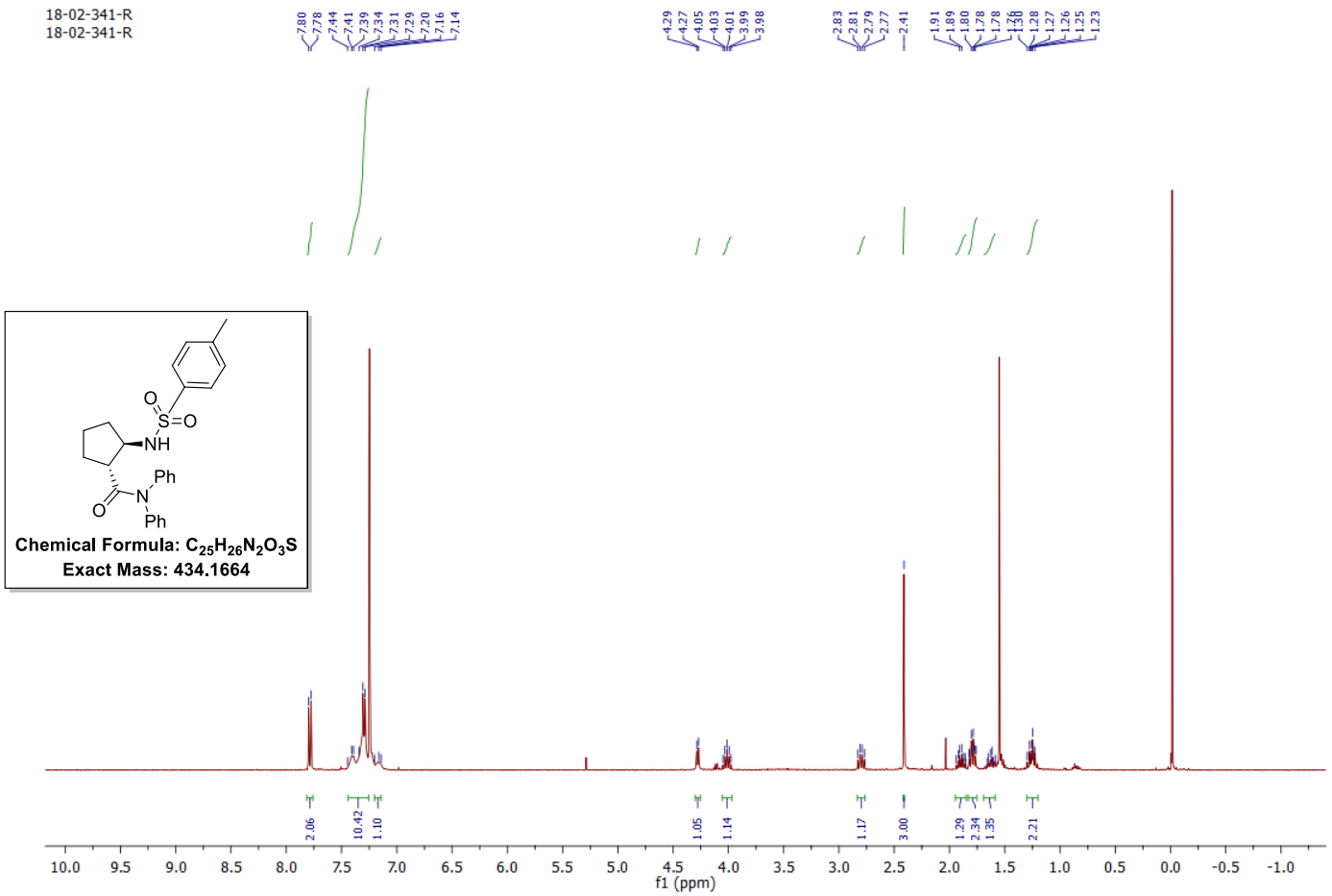
Monoisotopic Mass, Even Electron Ions
666 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-6 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_319 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_319 16 (0.356) 1: TOF MS ES+
5.34e+006

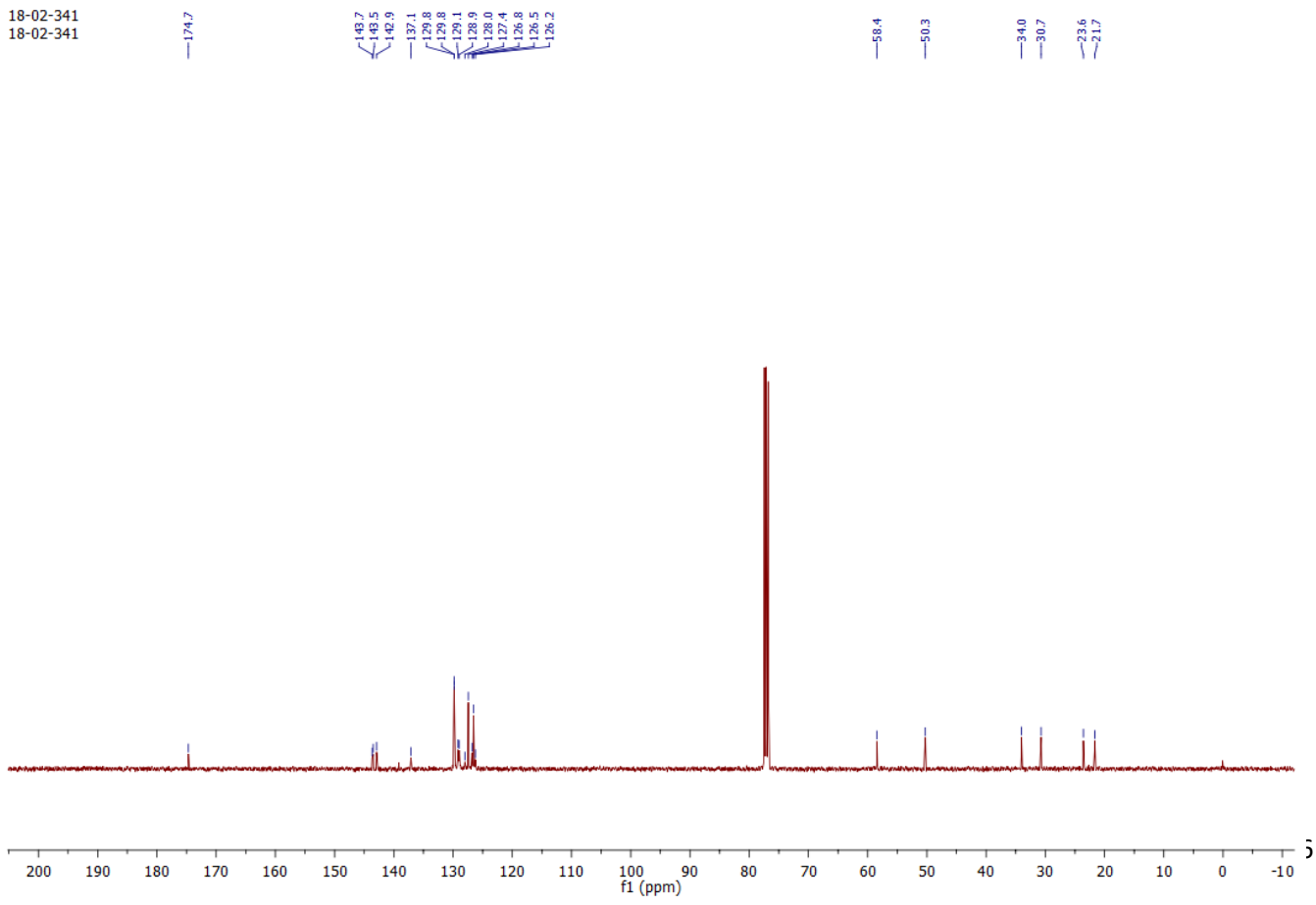


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
316.1371	316.1371	0.0	0.0	8.5	1493.1	n/a	n/a	C18 H22 N O2 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3aj



HRMS of 3aj

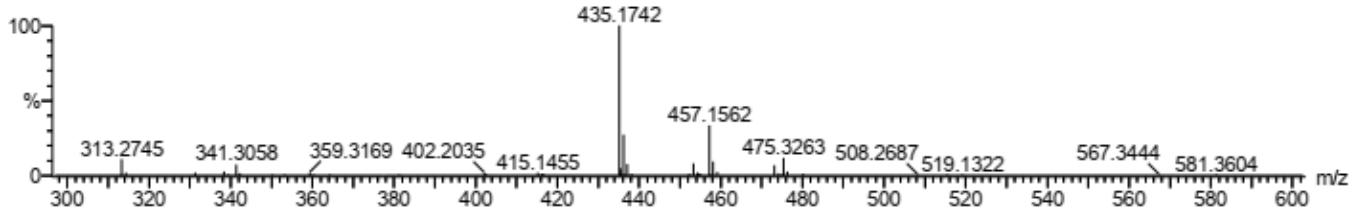
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

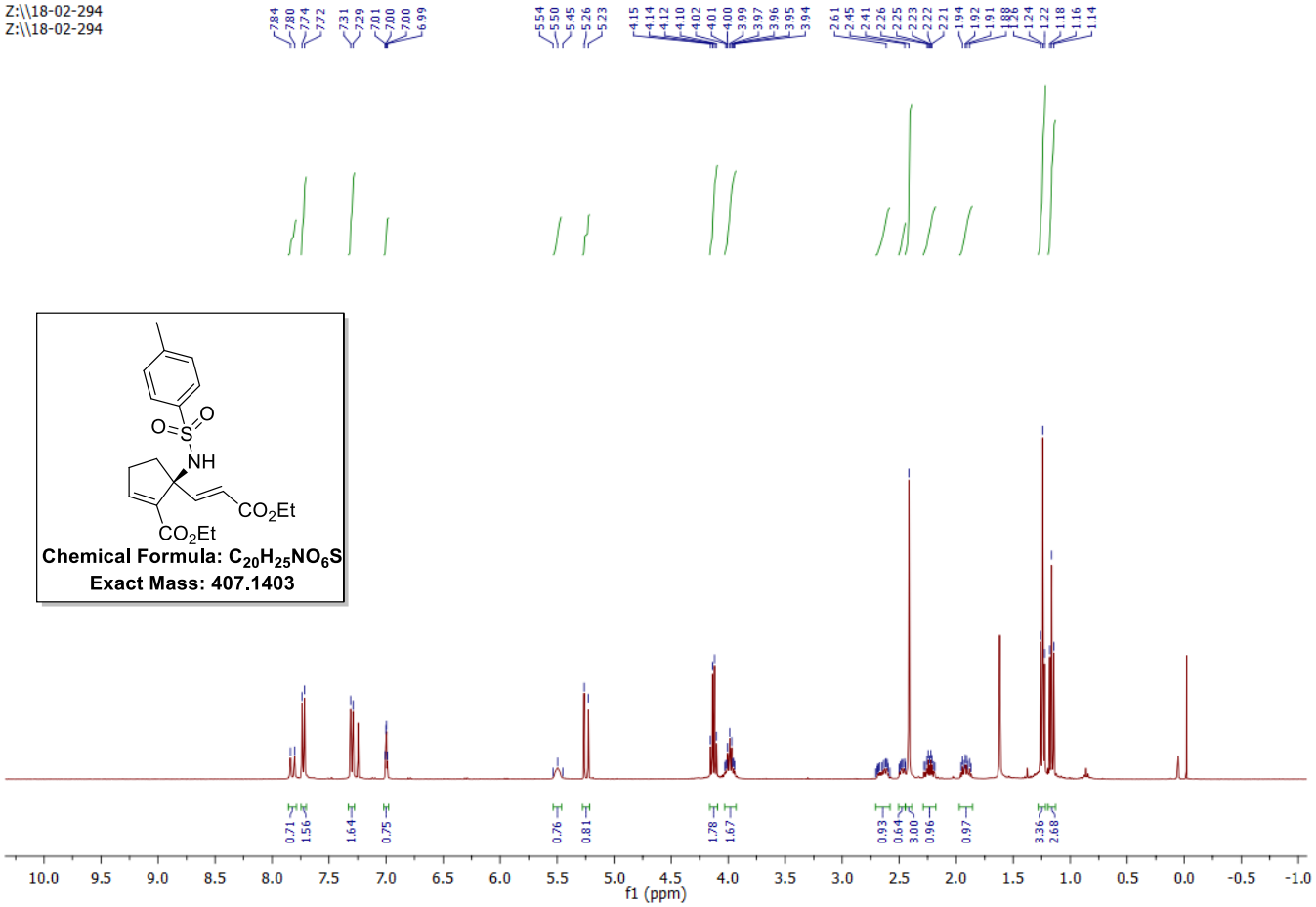
Monoisotopic Mass, Even Electron Ions
3110 formula(e) evaluated with 10 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-6 F: 0-3 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_341 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_341 10 (0.232) 1: TOF MS ES+
1.16e+007

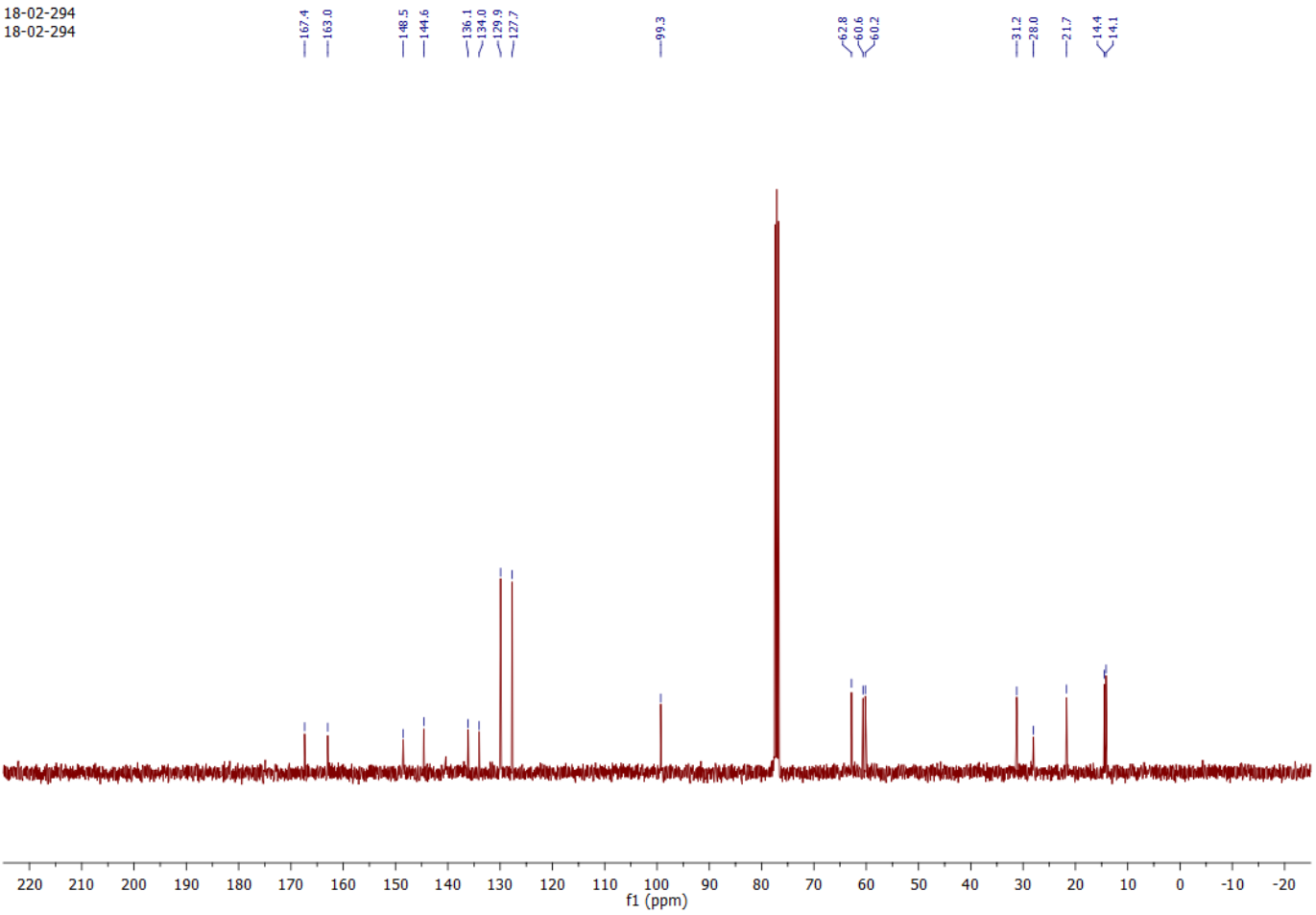


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
435.1742	435.1742	0.0	0.0	13.5	1368.9	n/a	n/a	C25 H27 N2 O3 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ak



HRMS of 3ak

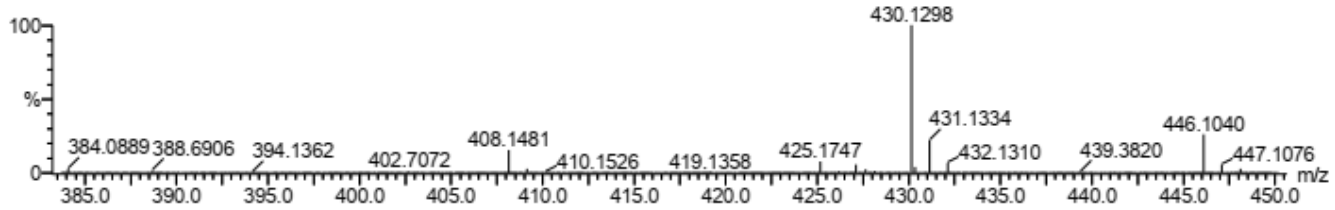
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

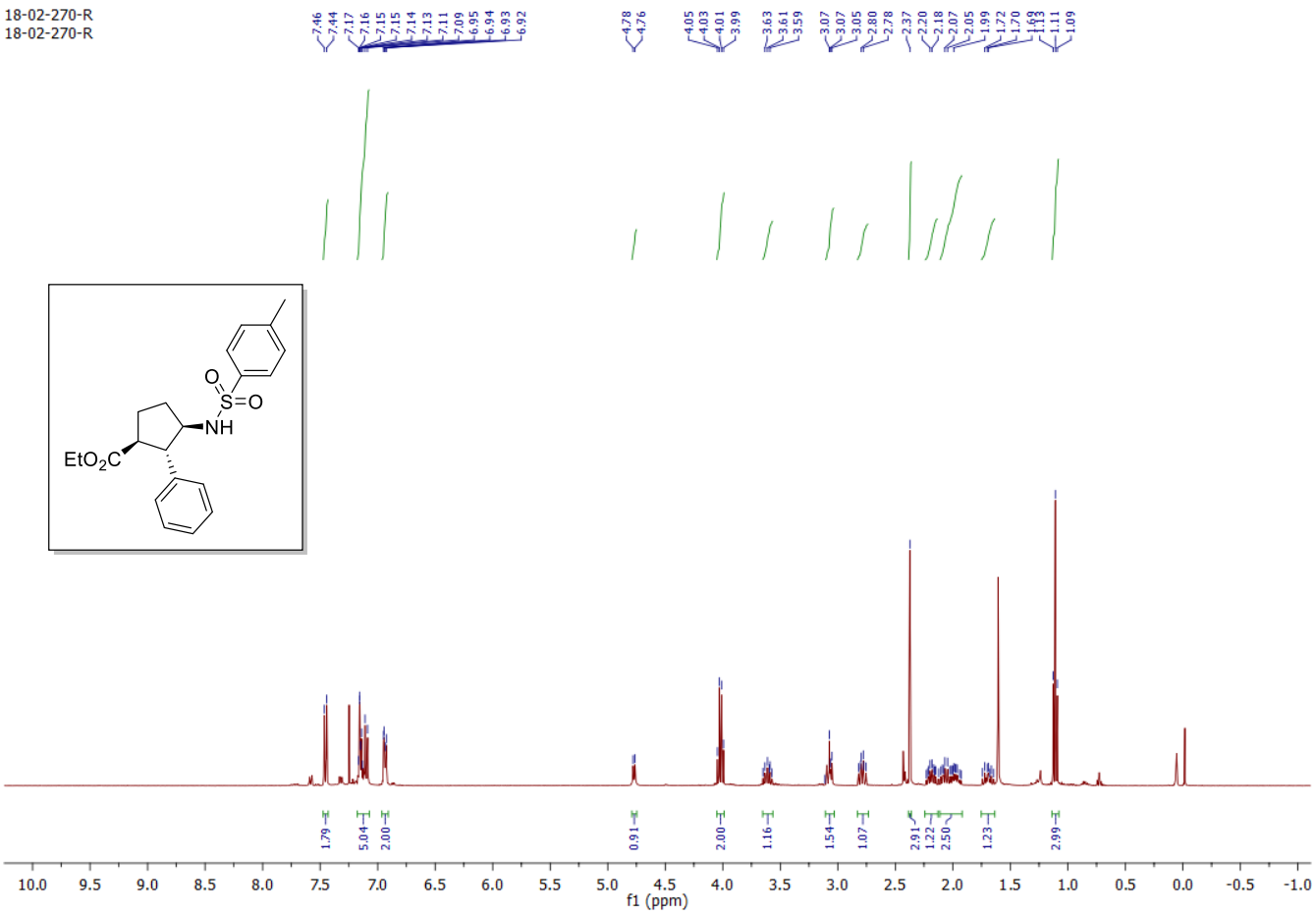
Monoisotopic Mass, Even Electron Ions
793 formula(e) evaluated with 8 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-6 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_294 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_294 12 (0.265) 1: TOF MS ES+
6.38e+006

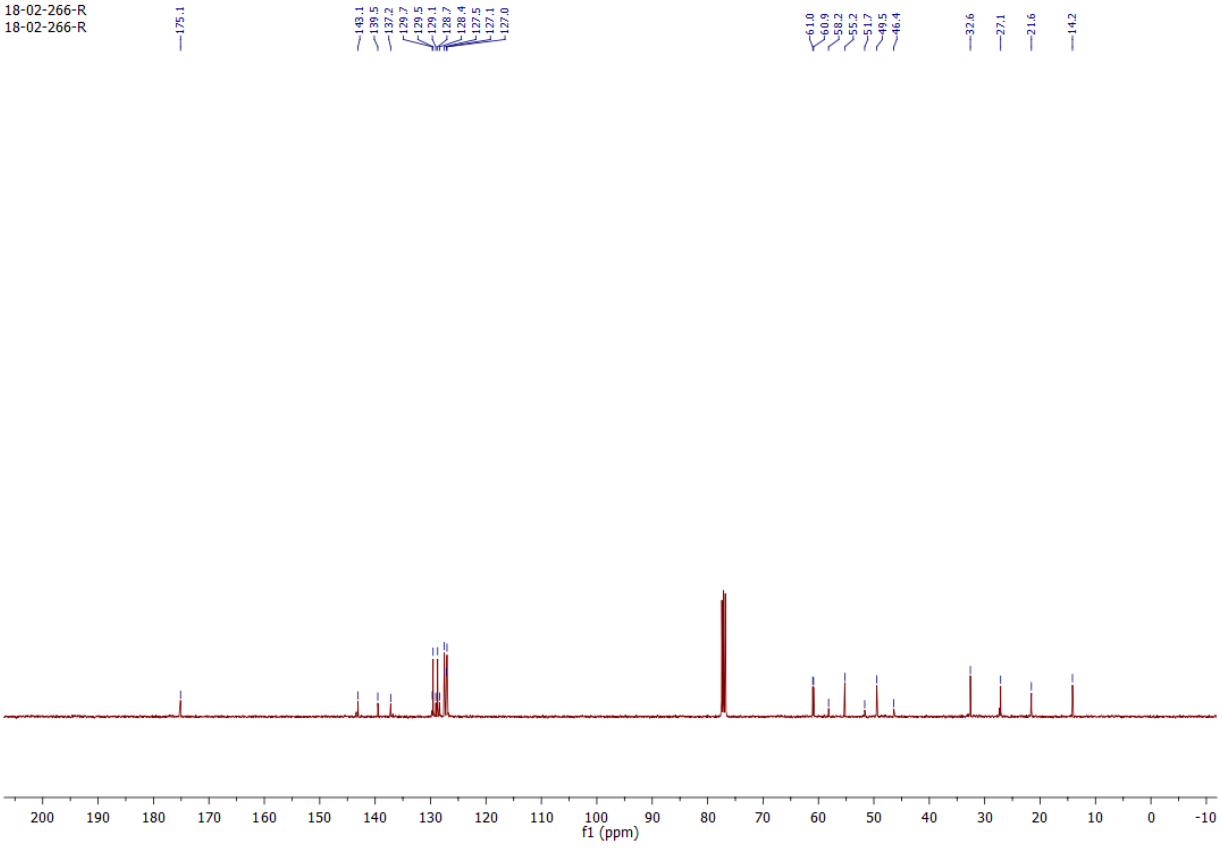


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
408.1481	408.1481	0.0	0.0	8.5	1268.7	n/a	n/a	C20 H26 N O6 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3al



HRMS of 3al

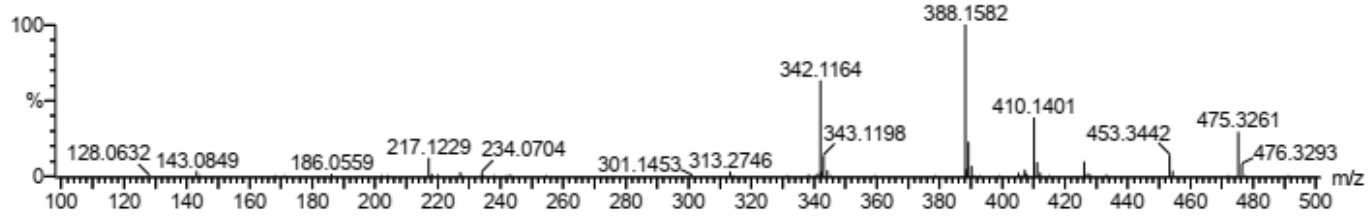
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

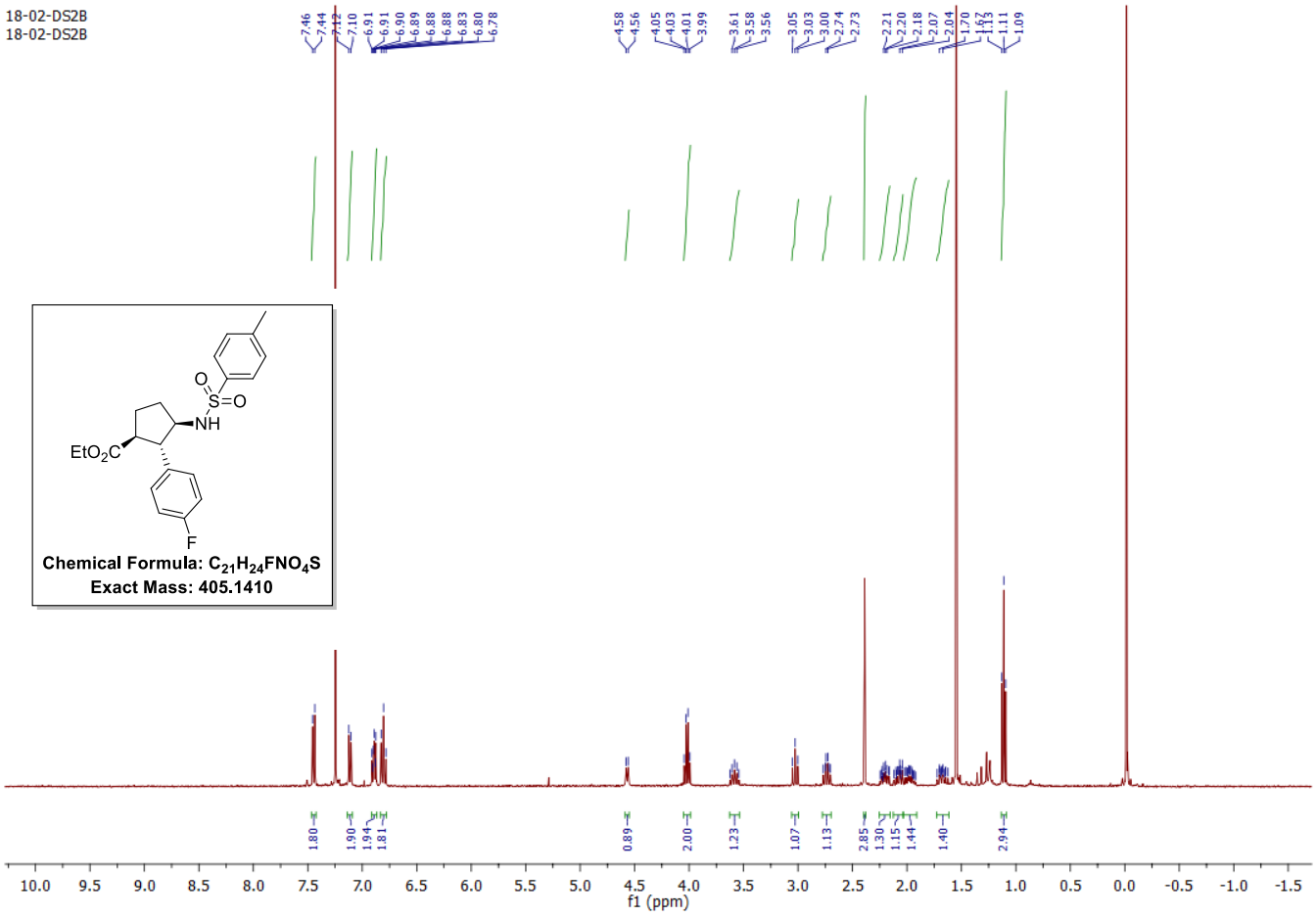
Monoisotopic Mass, Even Electron Ions
317 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 10-25 H: 1-30 N: 1-3 O: 1-5 S: 0-2 Cl: 0-2

Sample Name : 18_02_266 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_266 25 (0.543) 1: TOF MS ES+
9.39e+006

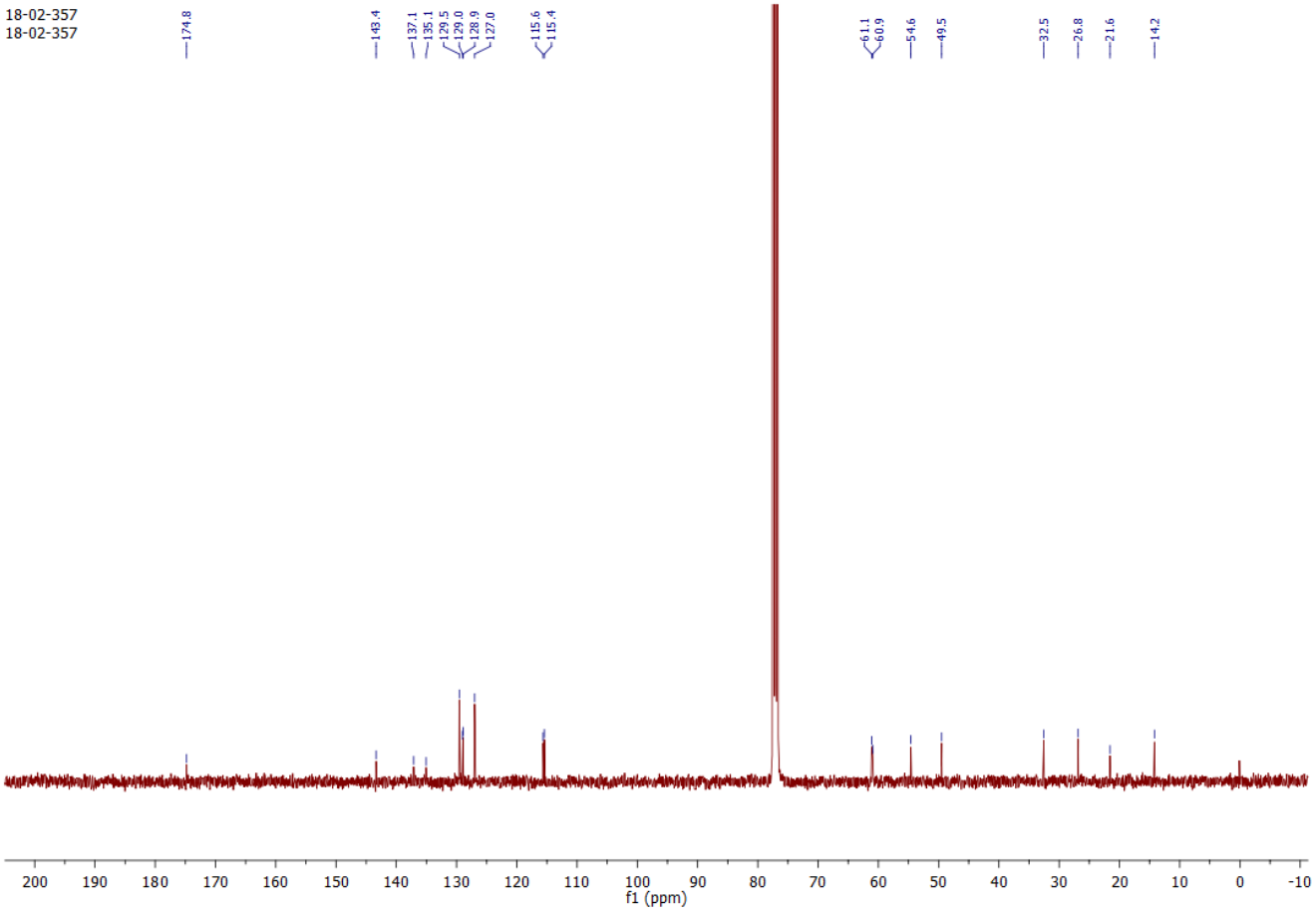


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
388.1582	388.1583	-0.1	-0.3	9.5	1466.6	n/a	n/a	C21 H26 N O4 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3am



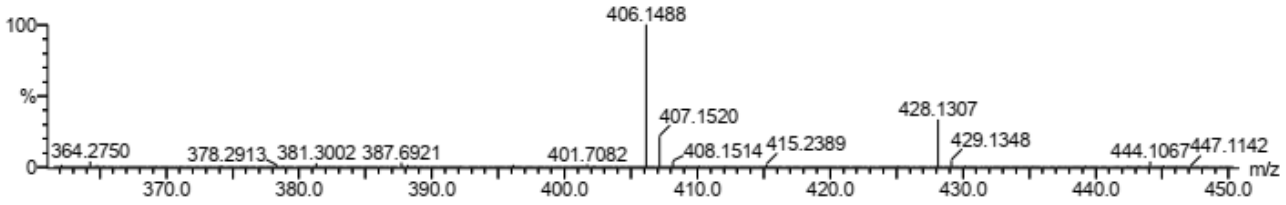
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

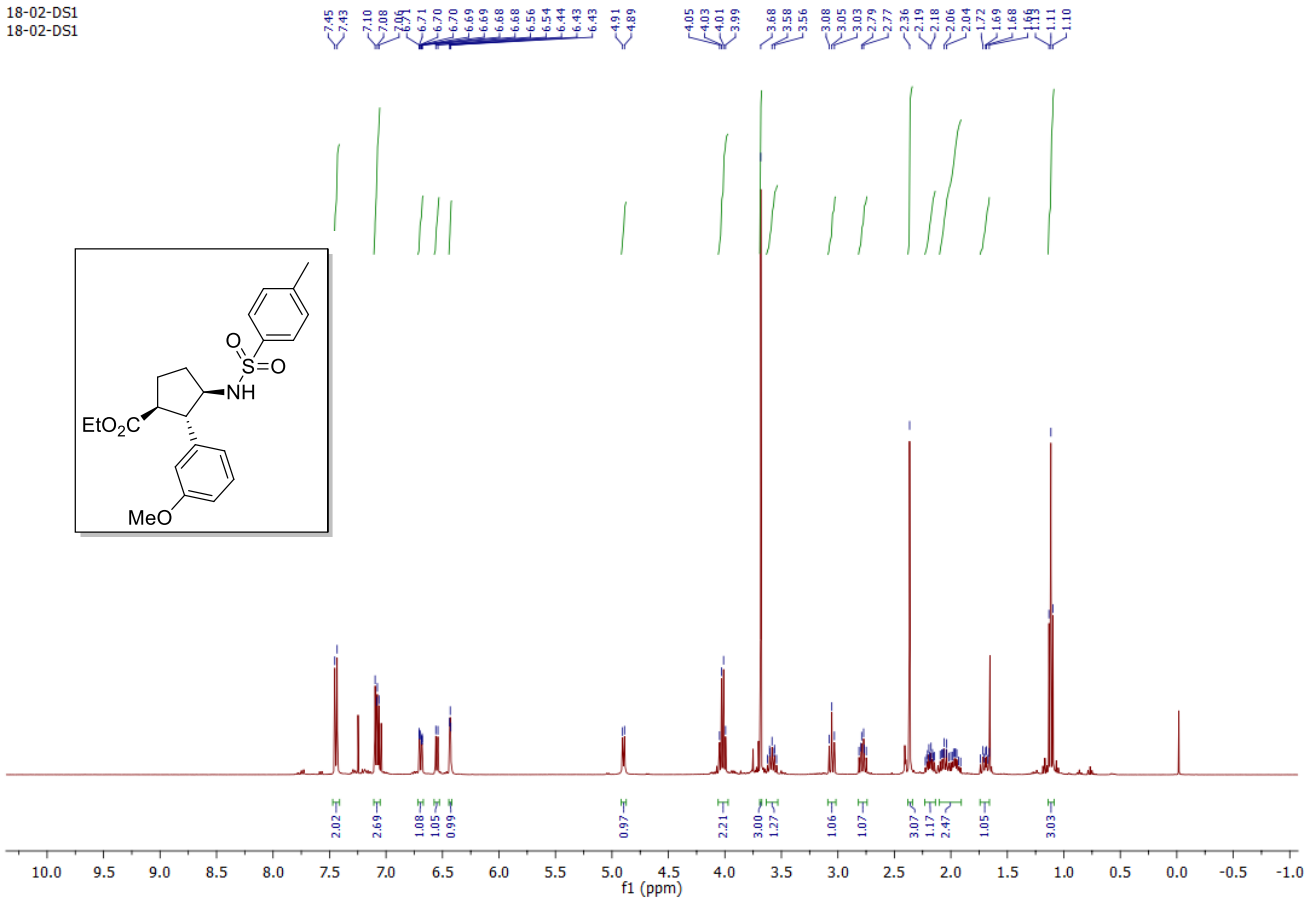
Monoisotopic Mass, Even Electron Ions
3025 formula(e) evaluated with 27 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-6 F: 0-3 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_357 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_357 11 (0.249) 1: TOF MS ES+
1.81e+006

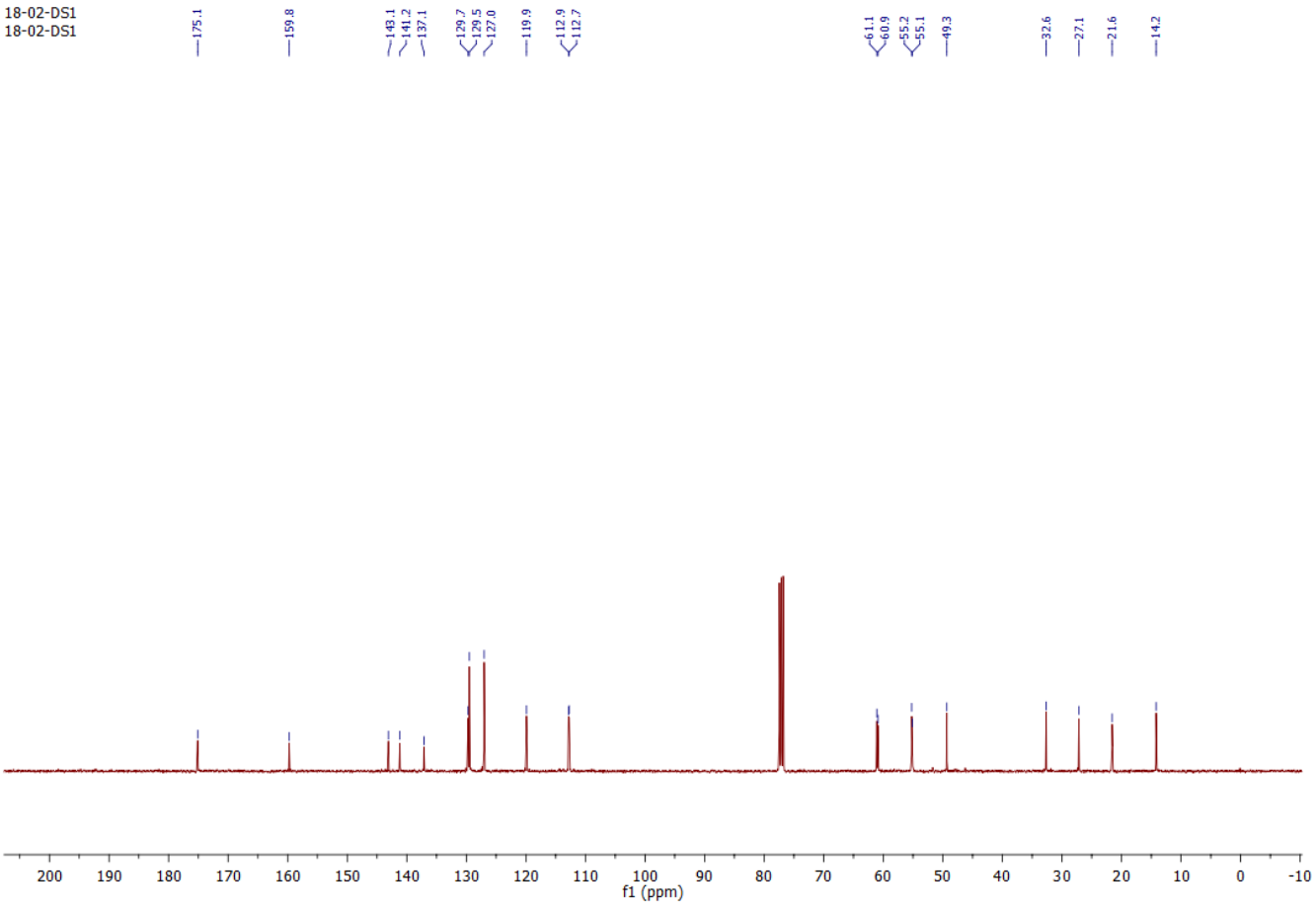


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
406.1488	406.1488	0.0	0.0	9.5	1260.5	n/a	n/a	C21 H25 N O4 F S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3an



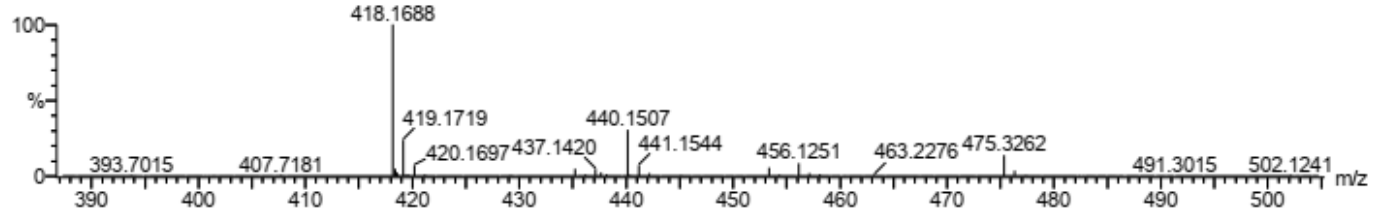
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

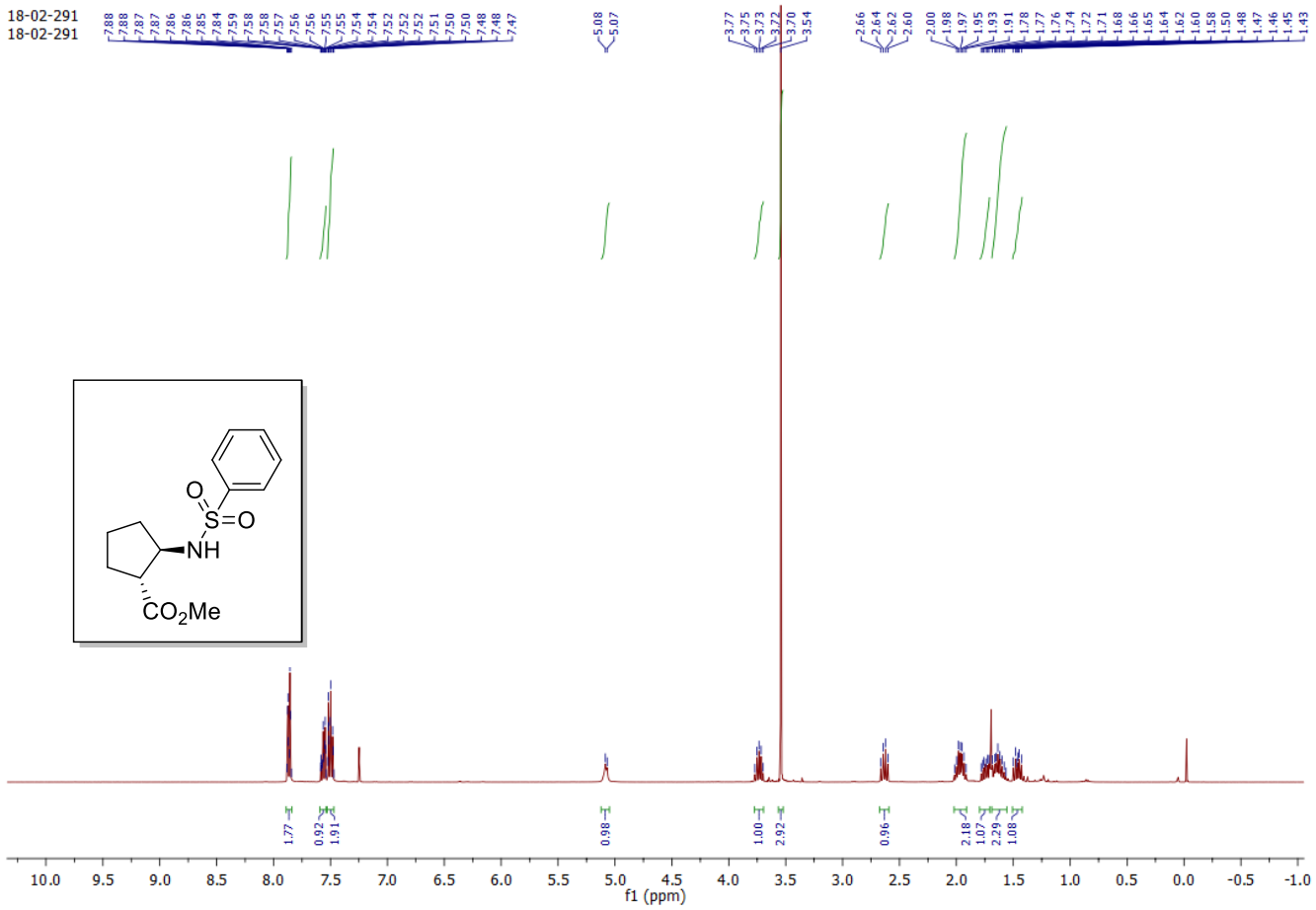
Monoisotopic Mass, Even Electron Ions
3058 formula(e) evaluated with 15 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-6 F: 0-3 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_356 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_356 19 (0.418) 1: TOF MS ES+
1.55e+007

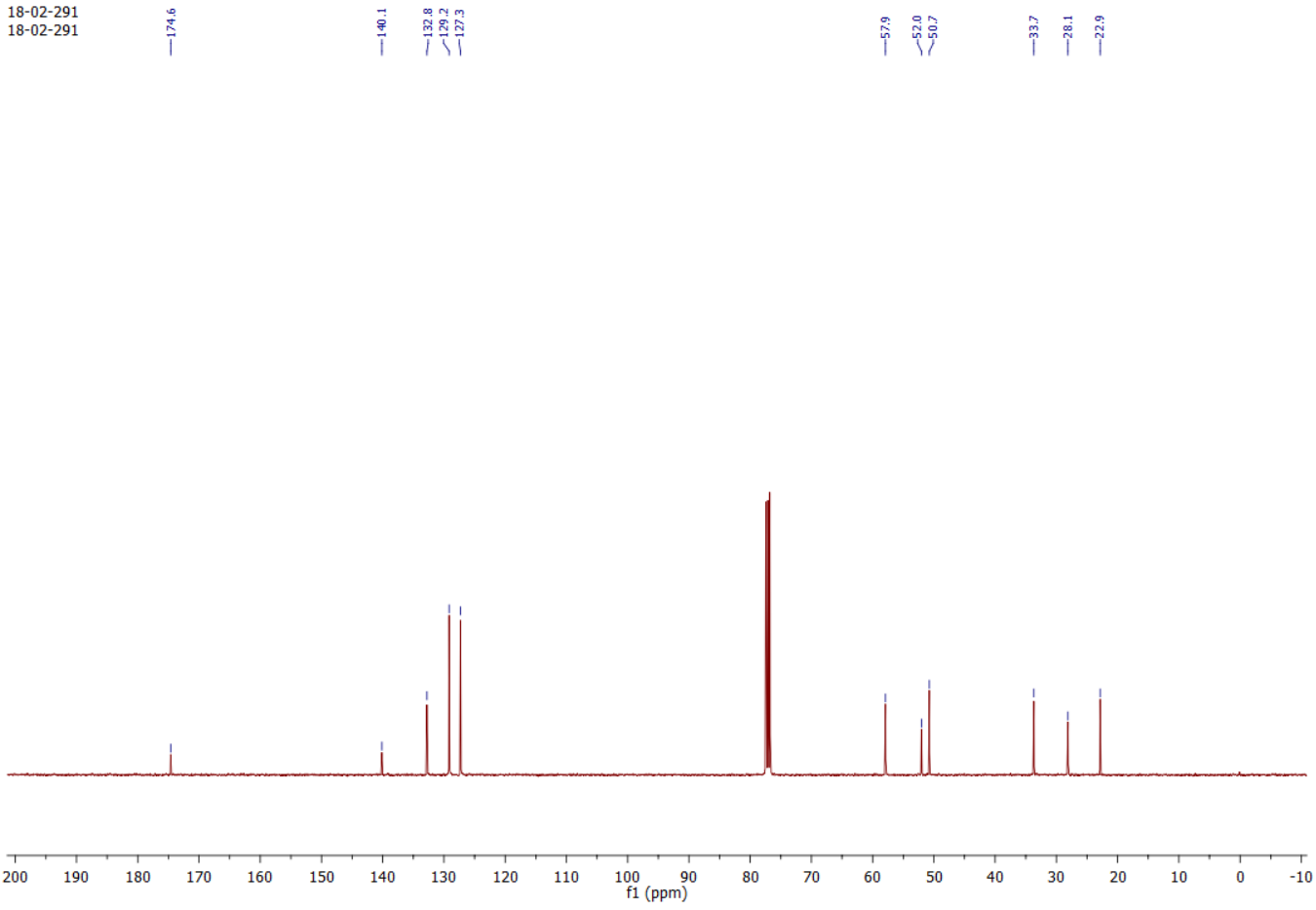


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
418.1688	418.1688	0.0	0.0	9.5	1451.6	n/a	n/a	C22 H28 N O5 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ba



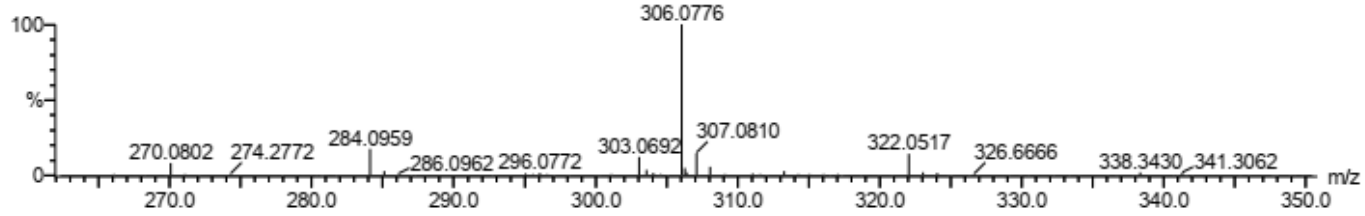
Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

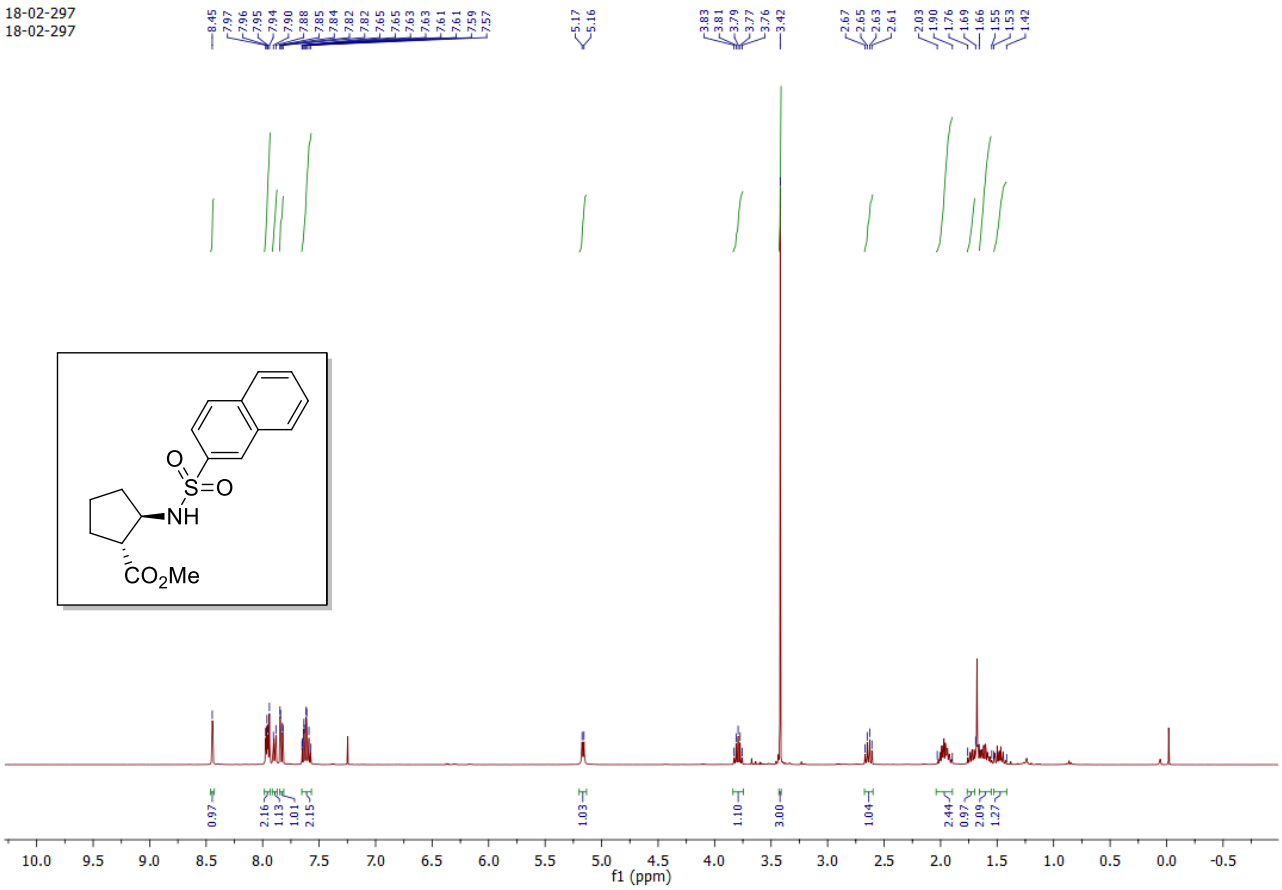
Monoisotopic Mass, Even Electron Ions
117 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 13-13 H: 1-30 N: 1-3 O: 1-5 Na: 1-1 S: 0-2 Cl: 0-2

Sample Name : 18_02_291 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_291 12 (0.265) 1: TOF MS ES+
1.28e+007

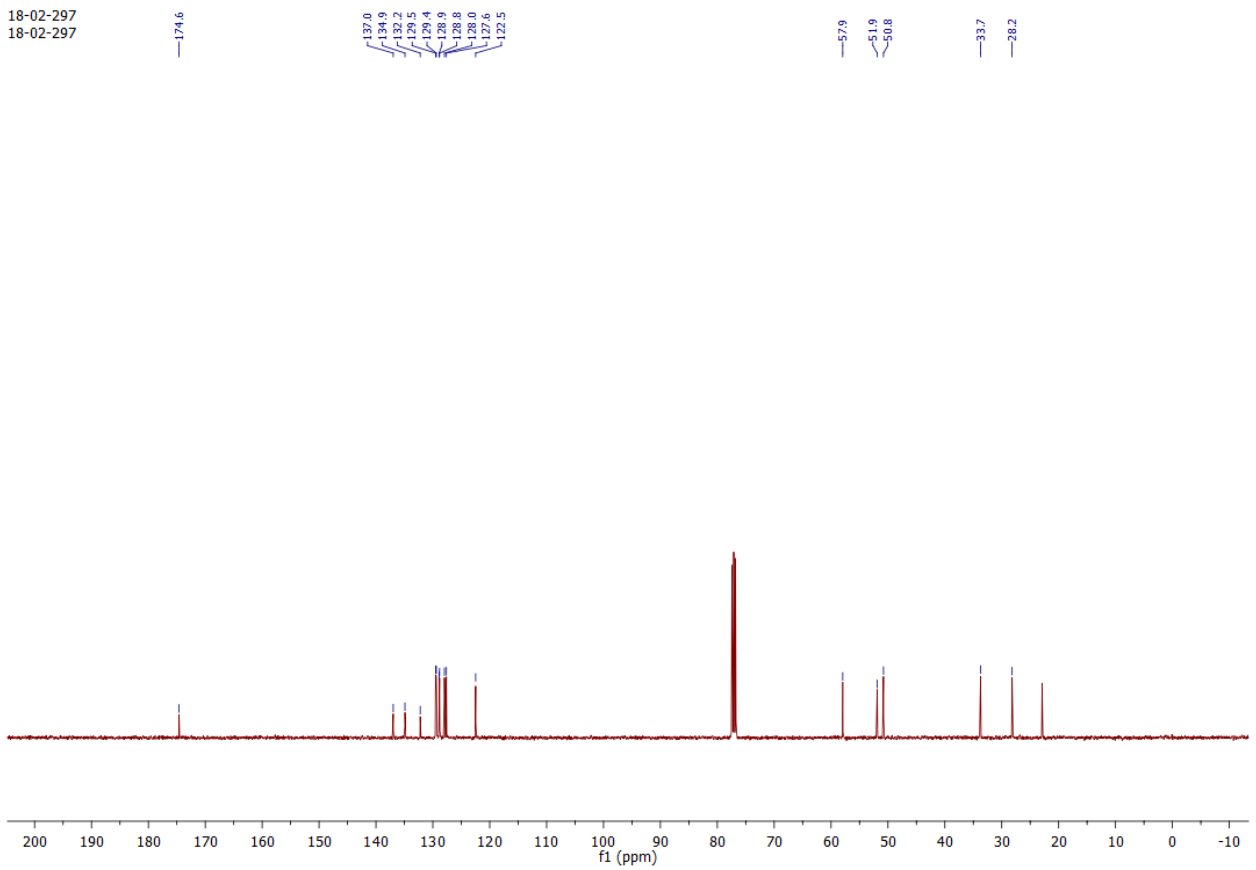


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
306.0776	306.0776	0.0	0.0	5.5	1730.4	n/a	n/a	C13 H17 N O4 Na S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ca



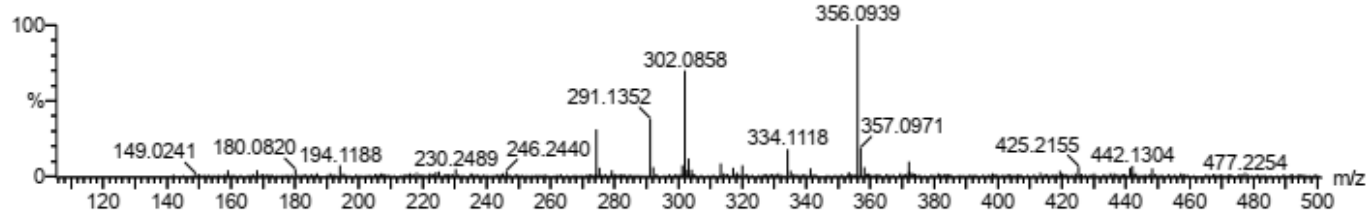
Elemental Composition Report

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

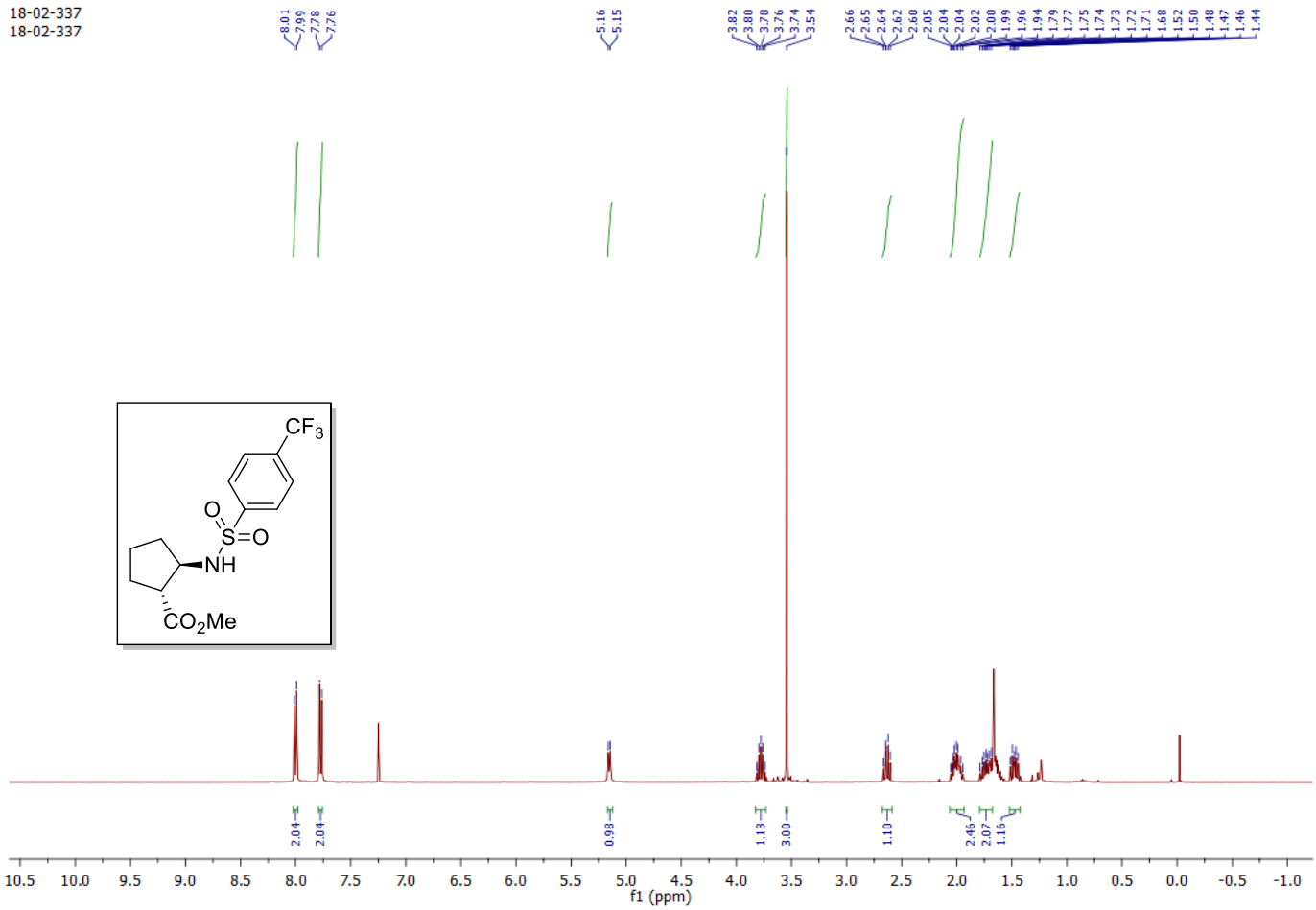
Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 17-17 H: 0-300 N: 0-1 O: 0-6 S: 1-1

Sample Name : 121035_18-02-297 IITRPR XEVO G2-XS QTOF
Test Name :
121035_18-02-297 34 (0.729) 1: TOF MS ES+
3.14e+006

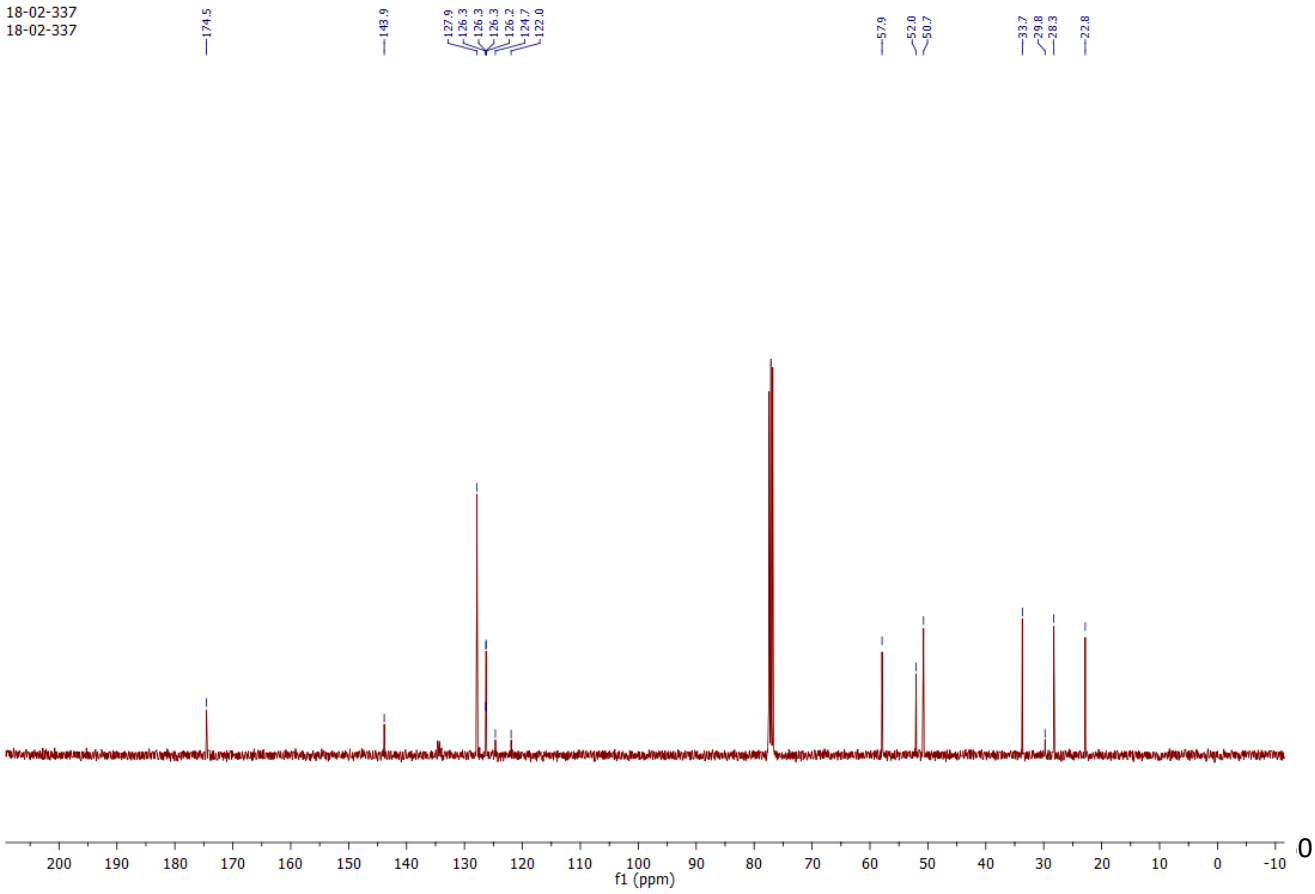


Minimum:				-1.5				
Maximum:		2.0	300.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
334.1118	334.1113	0.5	1.5	8.5	1365.1	n/a	n/a	C17 H20 N O4 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3da



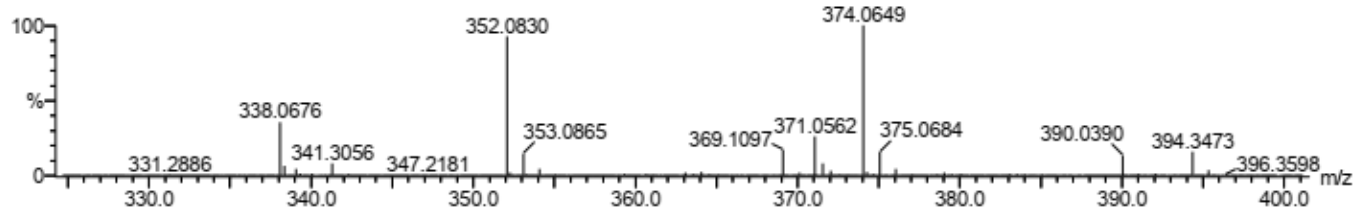
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

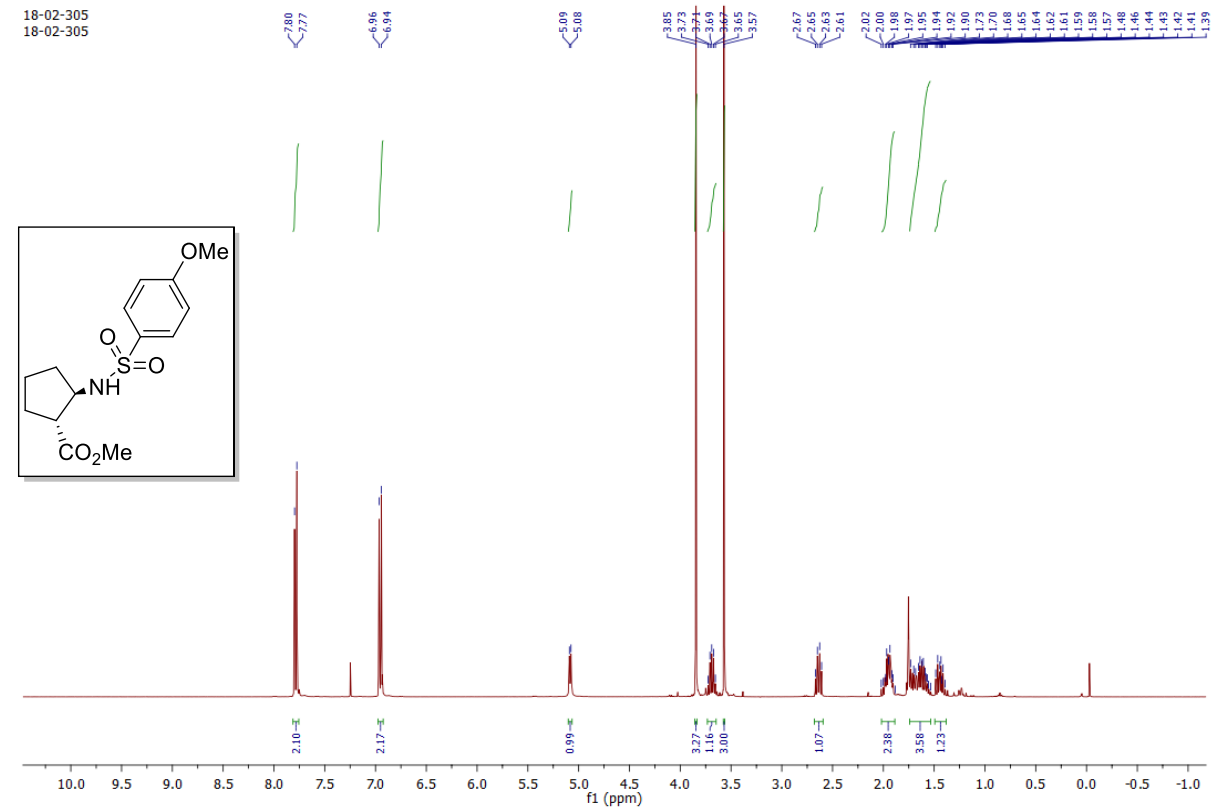
Monoisotopic Mass, Even Electron Ions
1184 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 14-14 H: 1-30 N: 1-3 O: 1-6 S: 0-2 Cl: 0-2 Br: 0-1 F: 0-3

Sample Name : 18_02_337 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_337 13 (0.294) 1: TOF MS ES+
5.12e+006

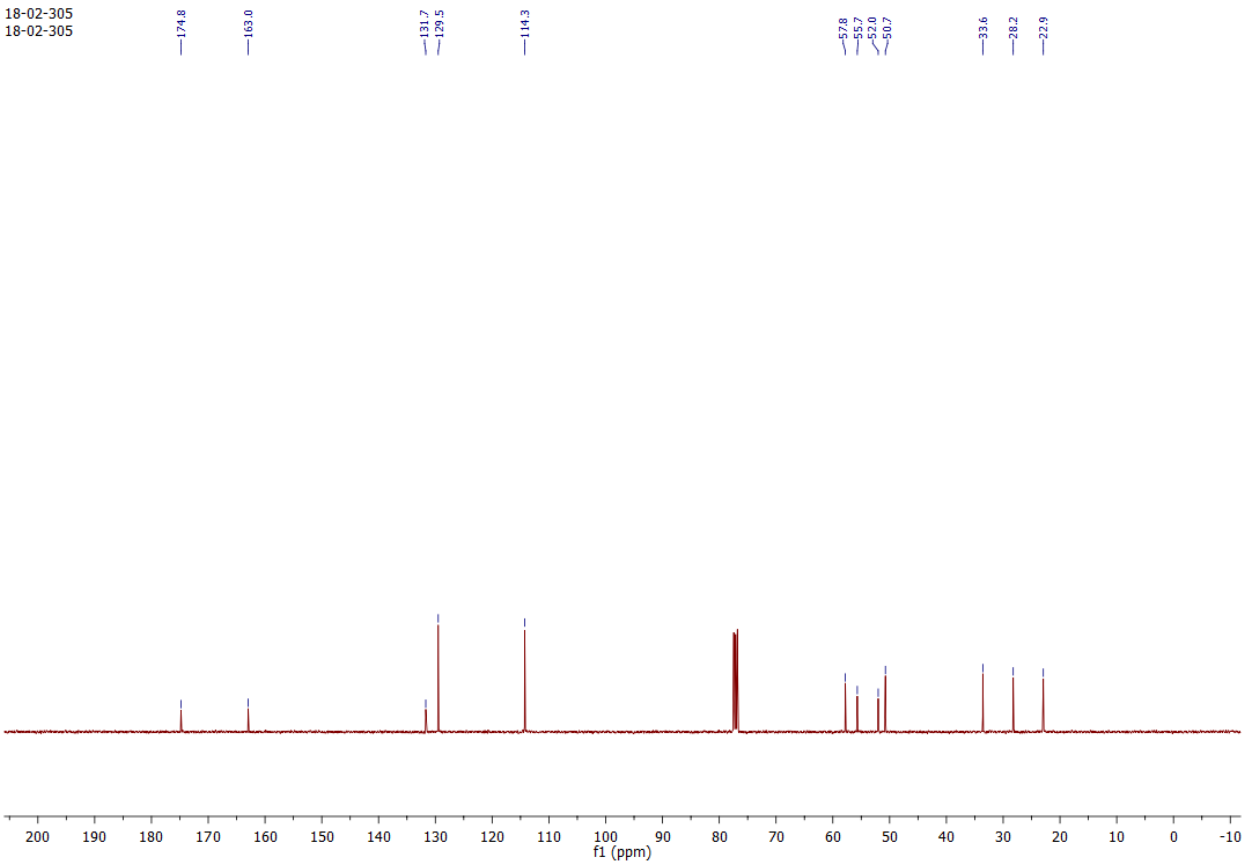


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
352.0830	352.0830	0.0	0.0	5.5	1398.7	n/a	n/a	C14 H17 N O4 S F3

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



^{13}C NMR ($CDCl_3$, 400 MHz) of 3ea

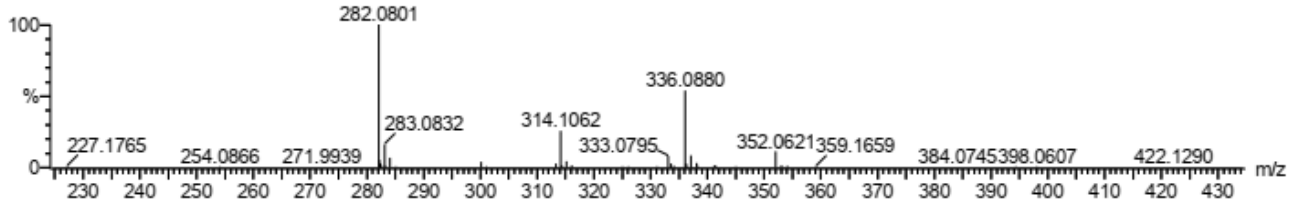


Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

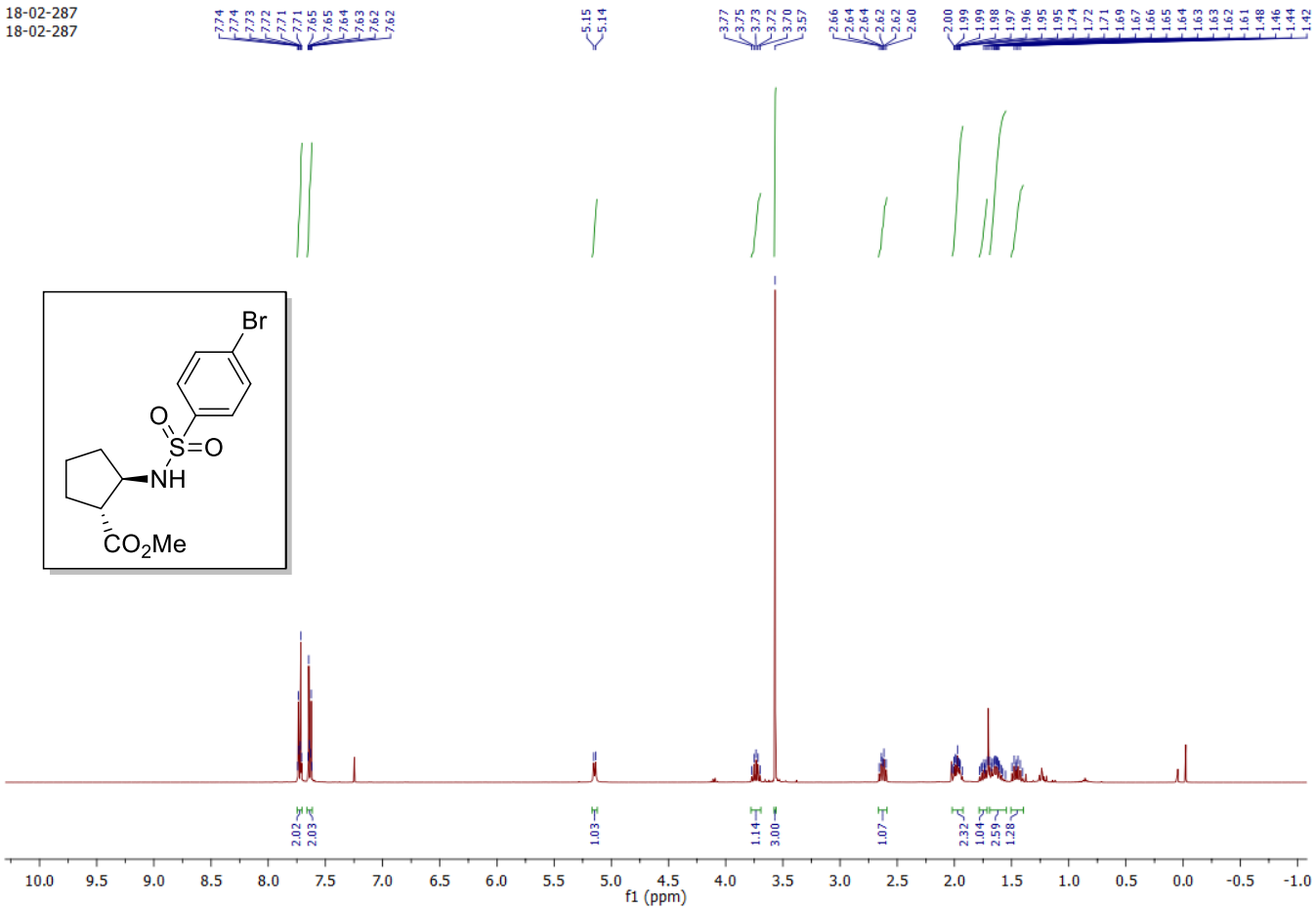
Monoisotopic Mass, Even Electron Ions
332 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-5 S: 0-2 Cl: 0-2

Sample Name : 18_02_305 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_305 16 (0.356) 1: TOF MS ES+
1.77e+007

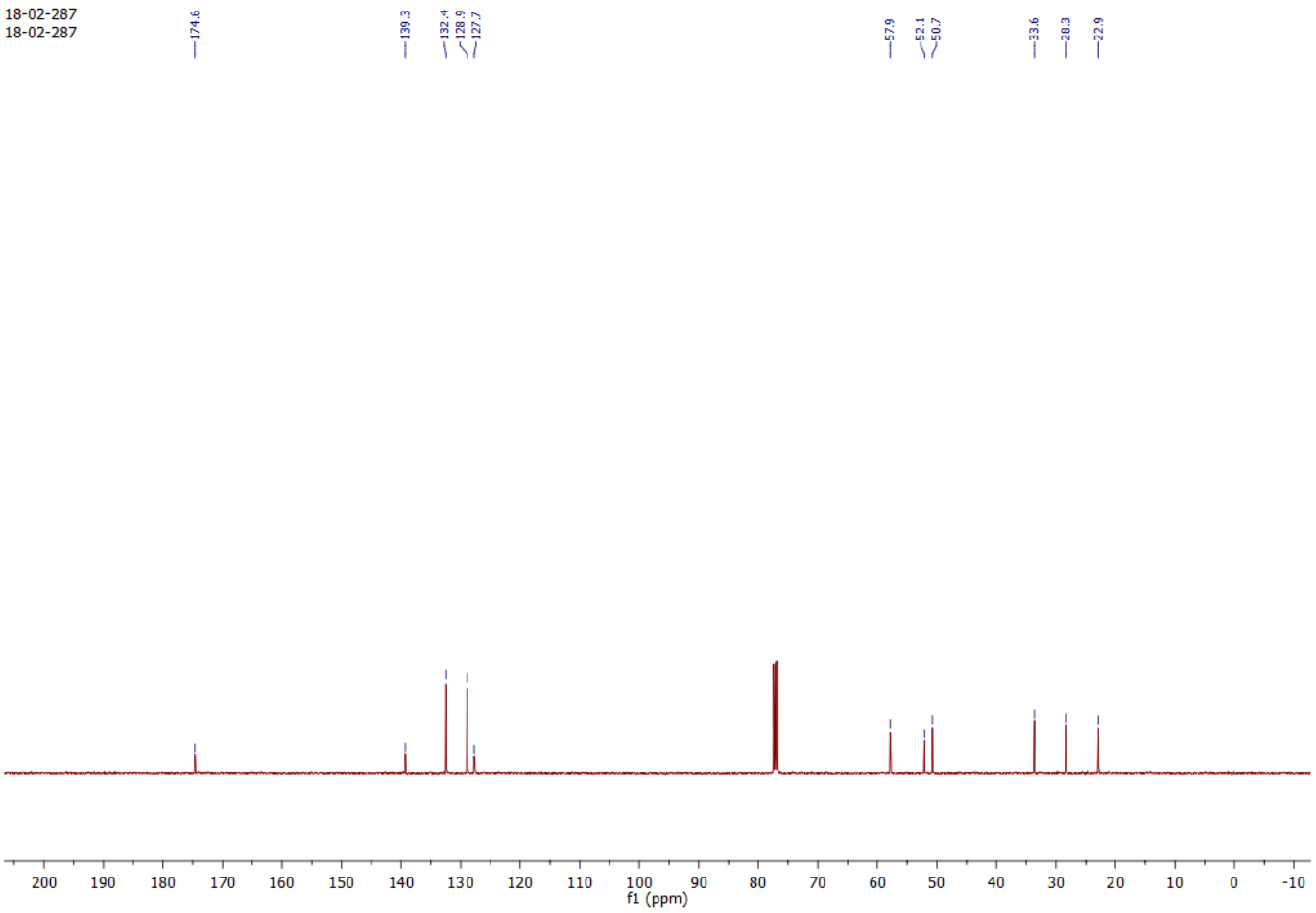


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
314.1062	314.1062	0.0	0.0	5.5	1600.2	n/a	n/a	C14 H20 N O5 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3fa



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

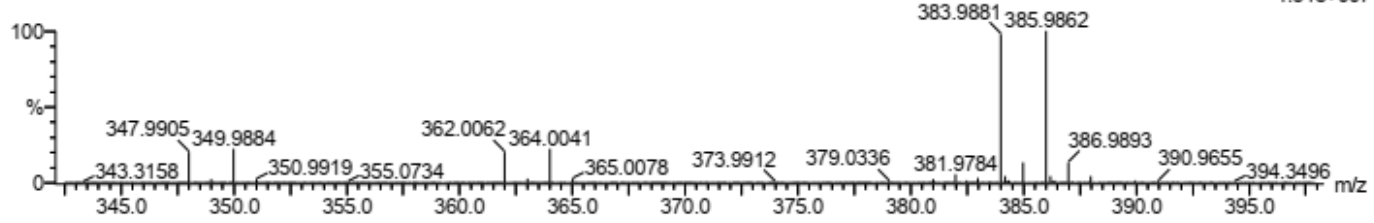
Monoisotopic Mass, Even Electron Ions
650 formula(e) evaluated with 10 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-5 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_287
Test Name :
12012022_18_02_287 4 (0.107)

IITRPR

XEVO G2-XS QTOF

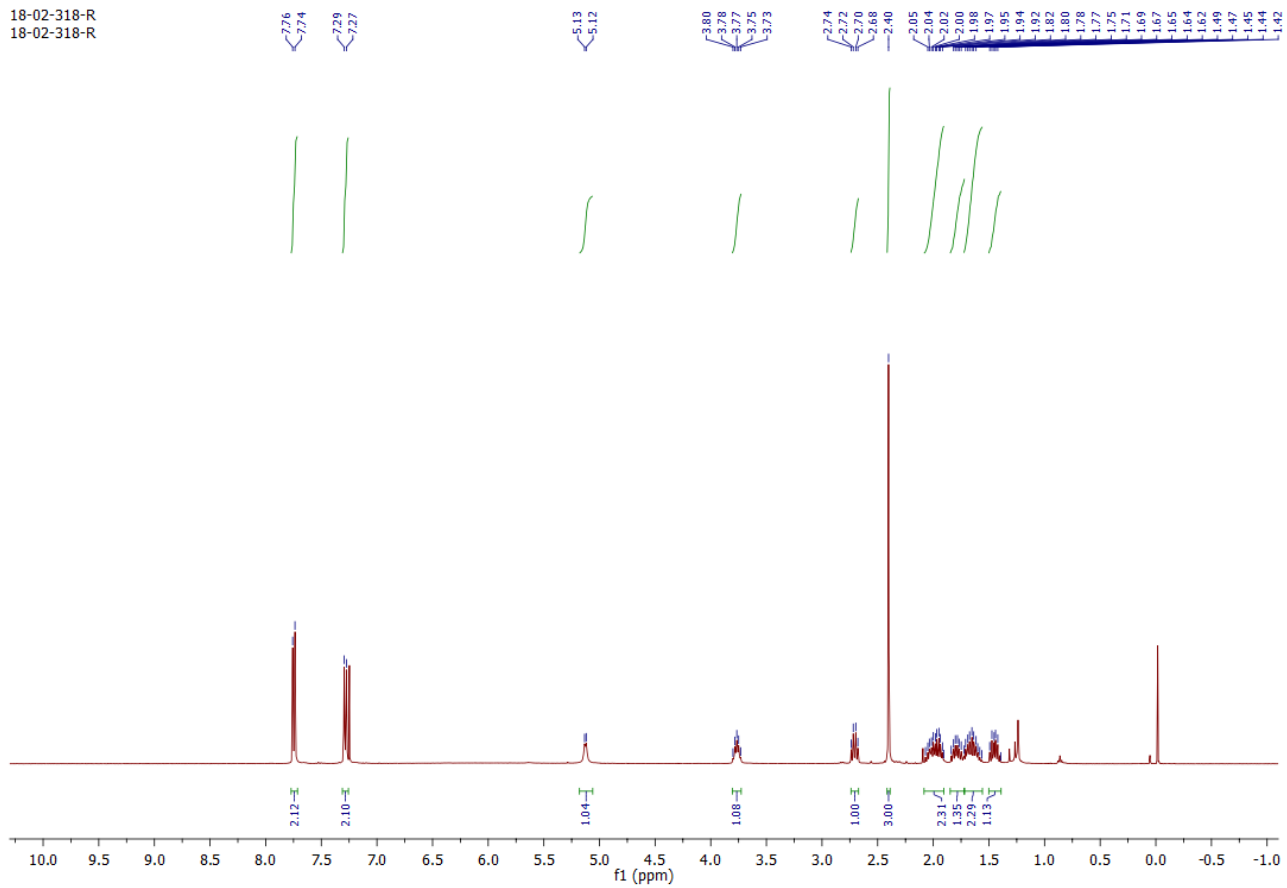
1: TOF MS ES+
1.31e+007



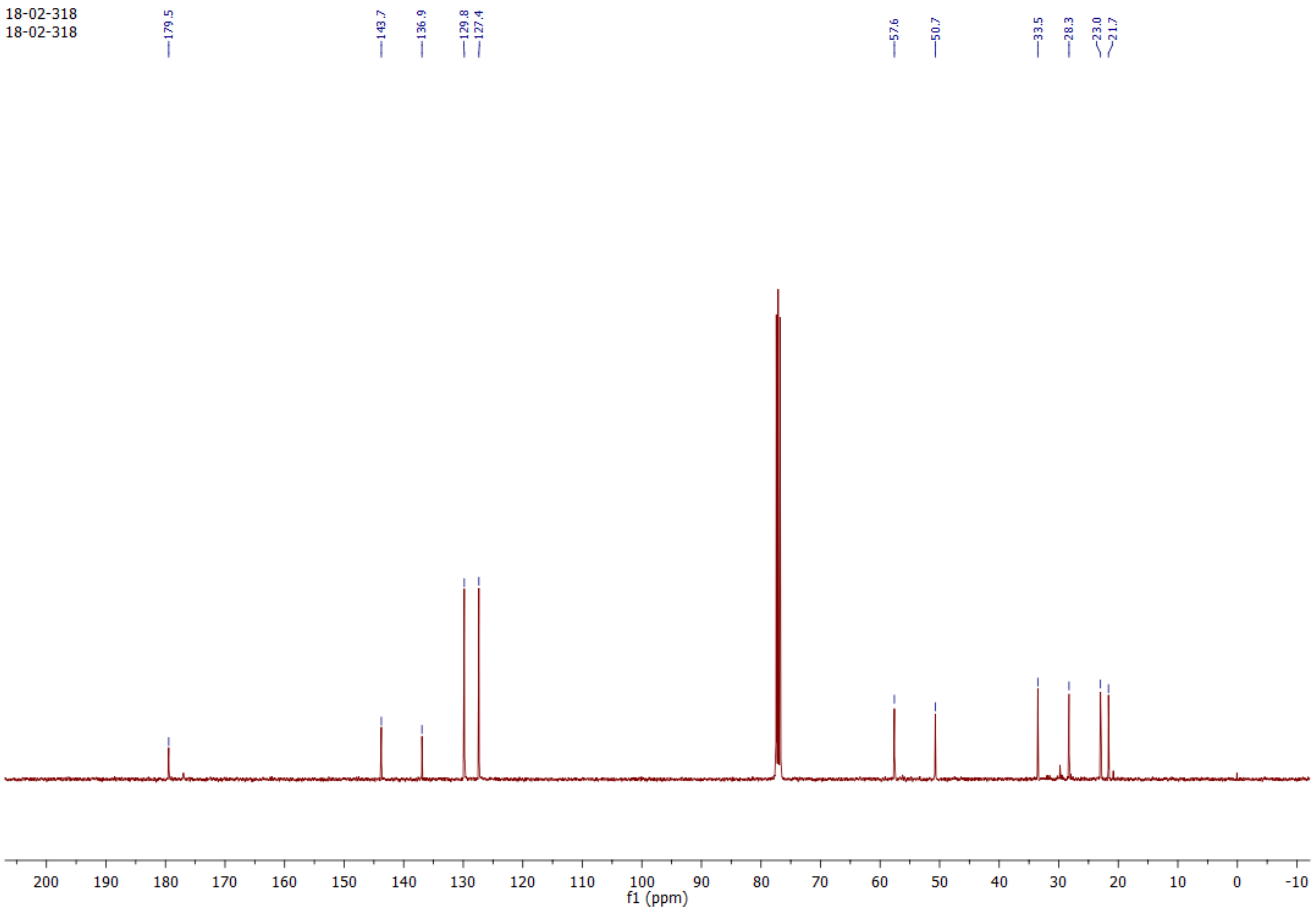
Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
362.0062	362.0062	0.0	0.0	5.5	1392.6	n/a	n/a	C13 H17 N O4 S Br

L) NMR and HRMS of derivatives

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ada



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

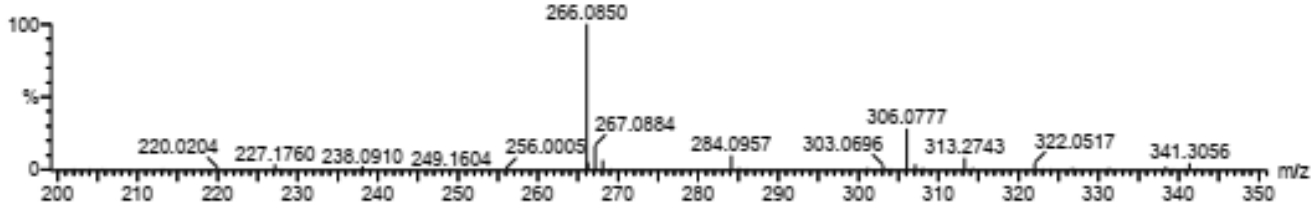
Monoisotopic Mass, Even Electron Ions
578 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-6 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_318
Test Name :
12012022_18_02_318 21 (0.452)

IITRPR

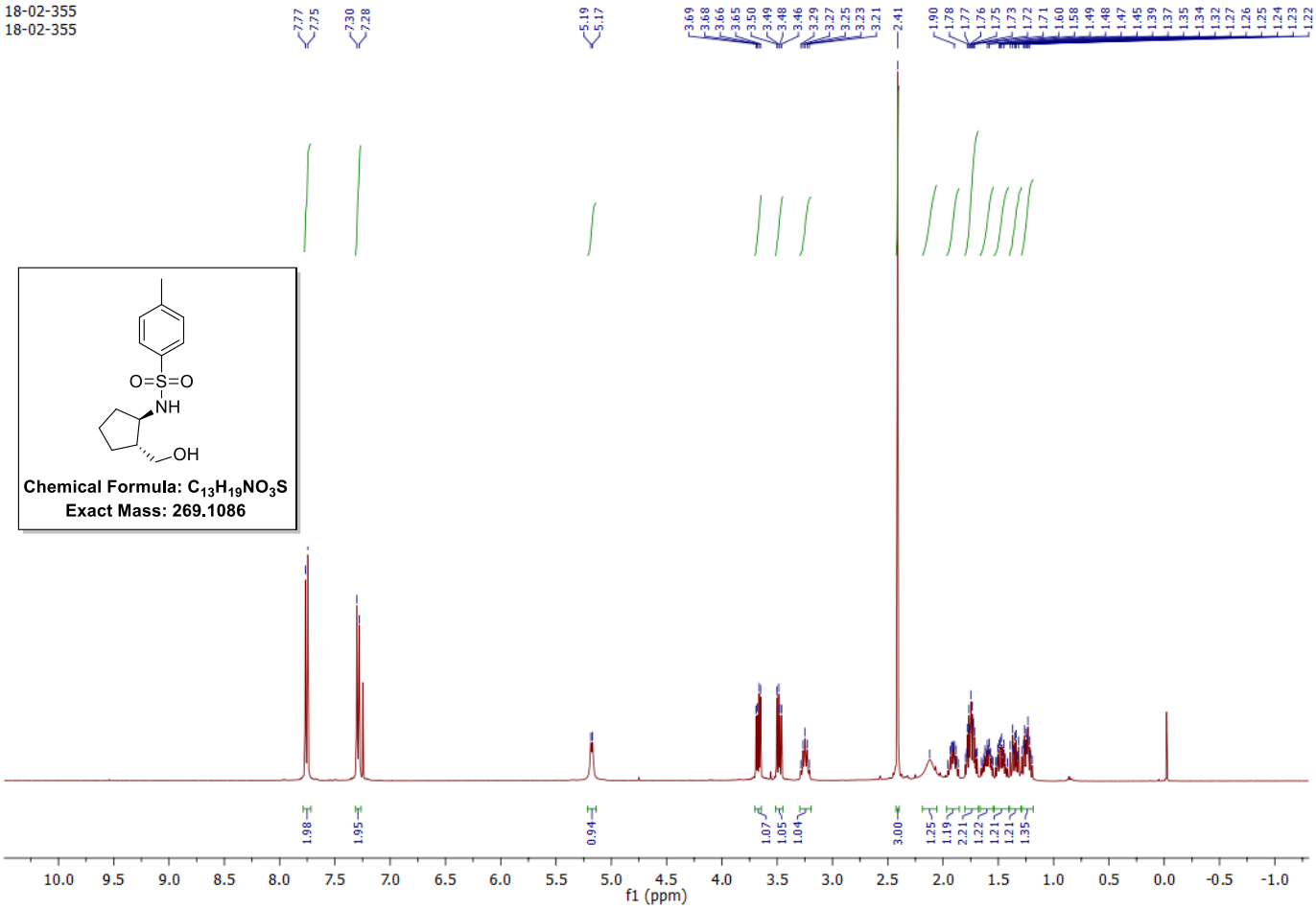
XEVO G2-XS QTOF

1: TOF MS ES+
6.24e+006

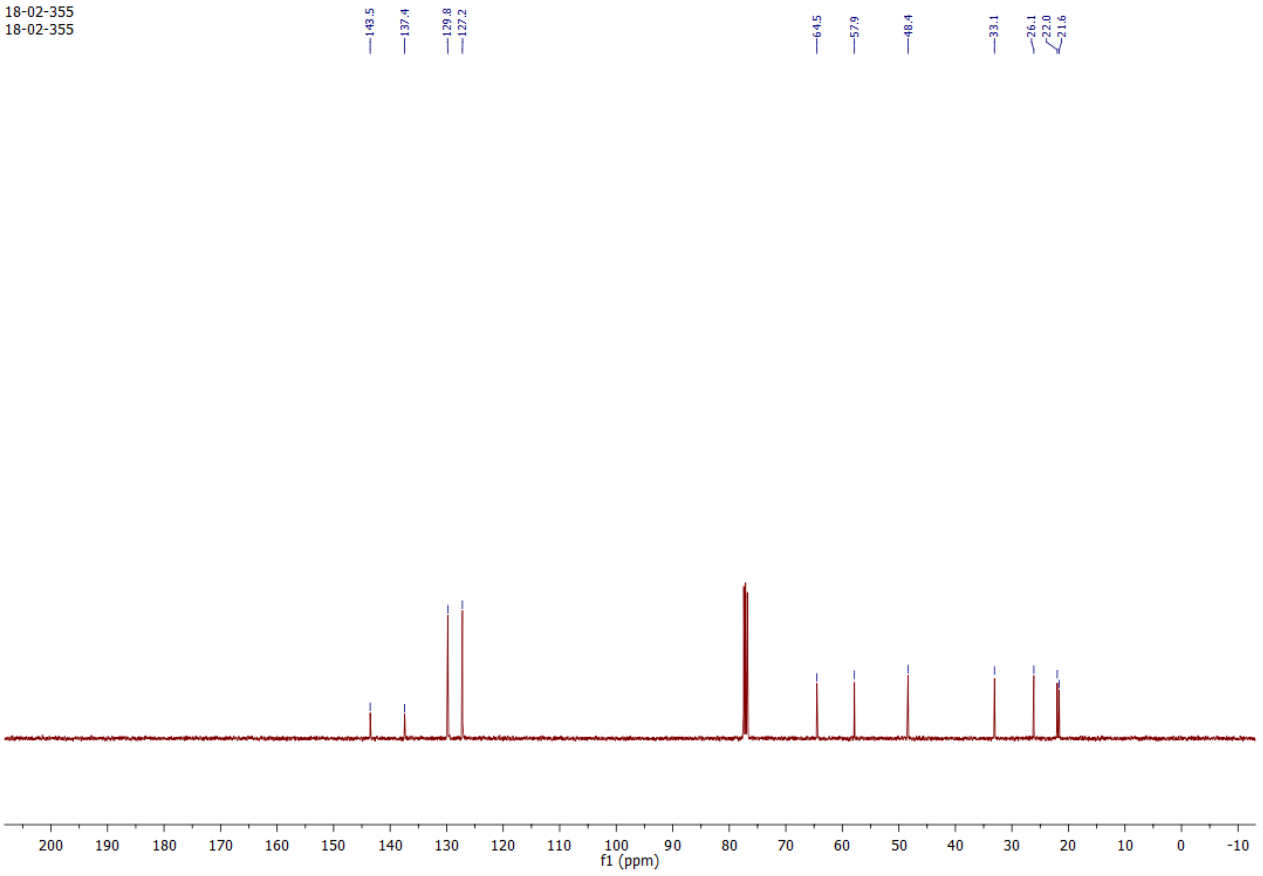


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
284.0957	284.0957	0.0	0.0	5.5	1313.8	n/a	n/a	C13 H18 N O4 S

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



^{13}C NMR ($CDCl_3$, 101 MHz) of 3adb



HRMS of 3abb

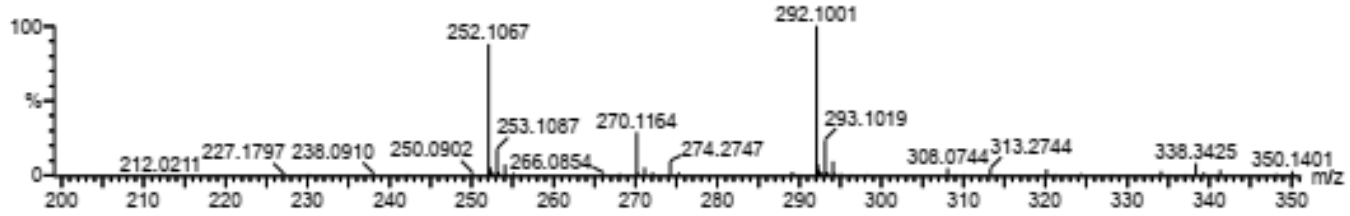
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

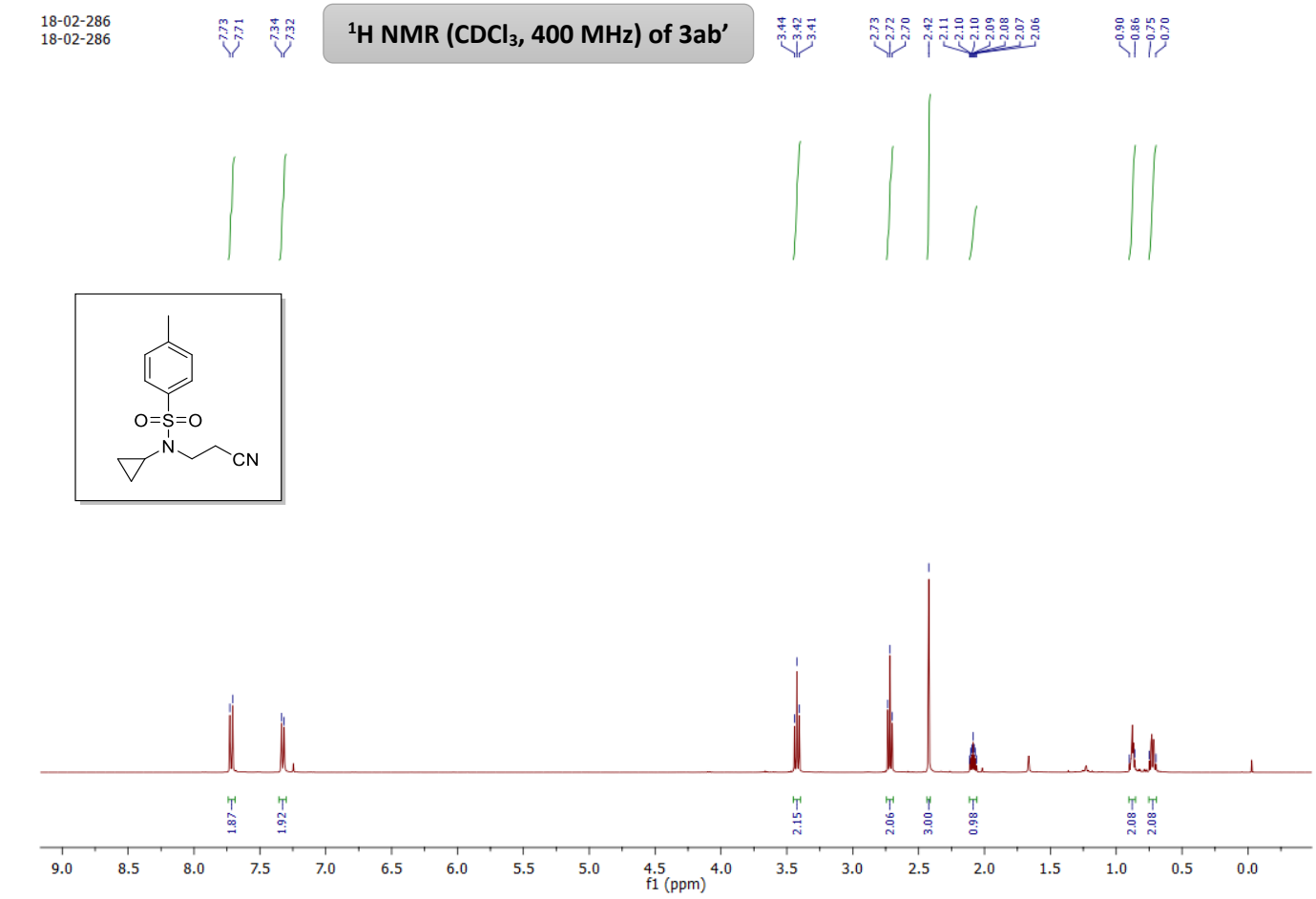
Monoisotopic Mass, Even Electron Ions
1586 formula(e) evaluated with 8 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-30 H: 1-30 N: 1-3 O: 1-6 F: 0-3 S: 0-2 Cl: 0-2 Br: 0-1

Sample Name : 18_02_355 IITRPR XEVO G2-XS QTOF
Test Name :
12012022_18_02_355 5 (0.124) 1: TOF MS ES+
2.77e+007

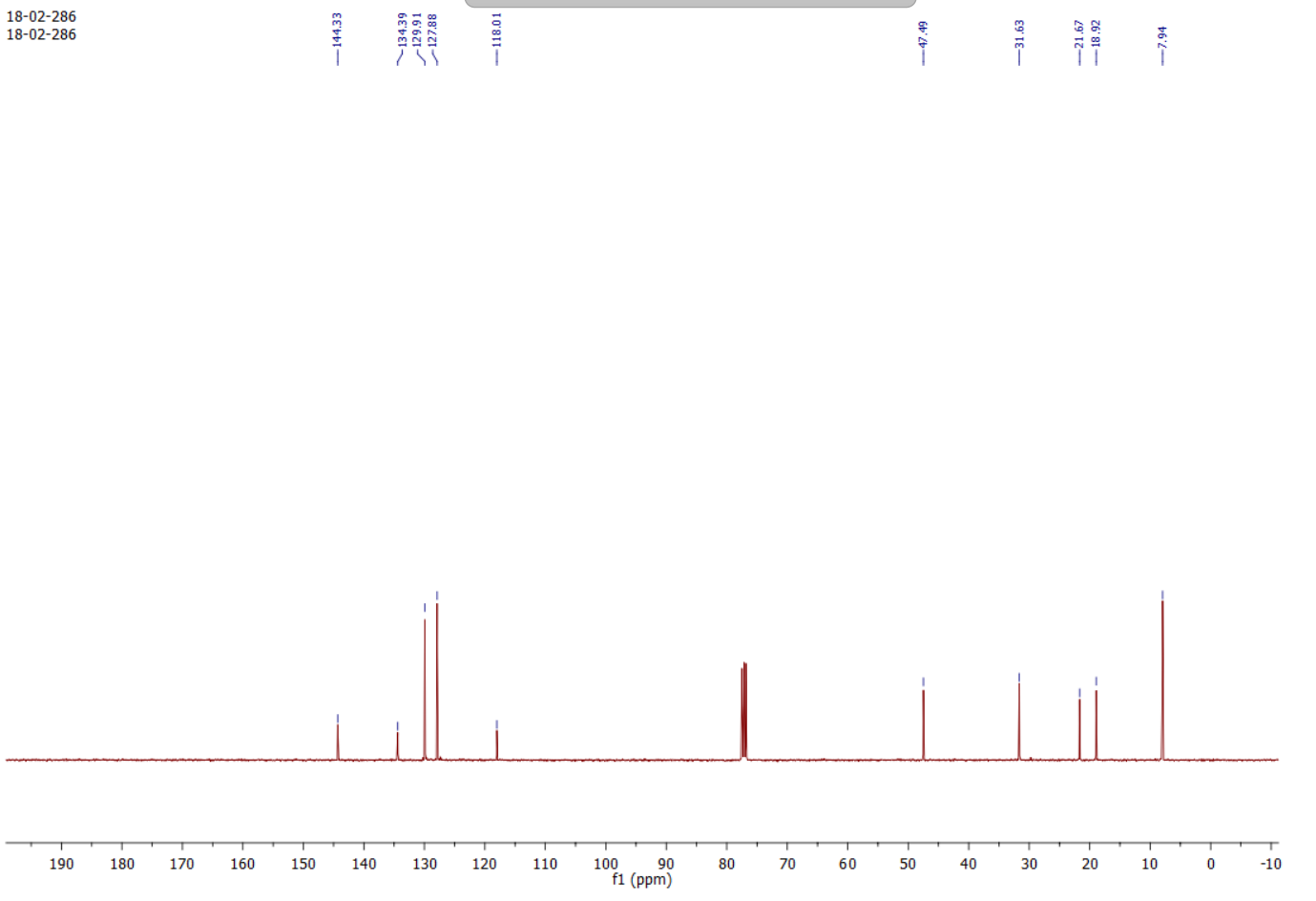


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
270.1164	270.1164	0.0	0.0	4.5	1930.0	n/a	n/a	C13 H20 N O3 S

N) NMR and HRMS of Michael adducts



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ab'



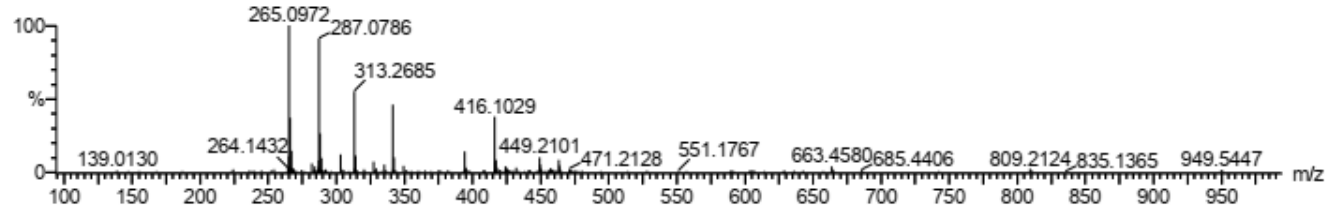
Elemental Composition Report

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

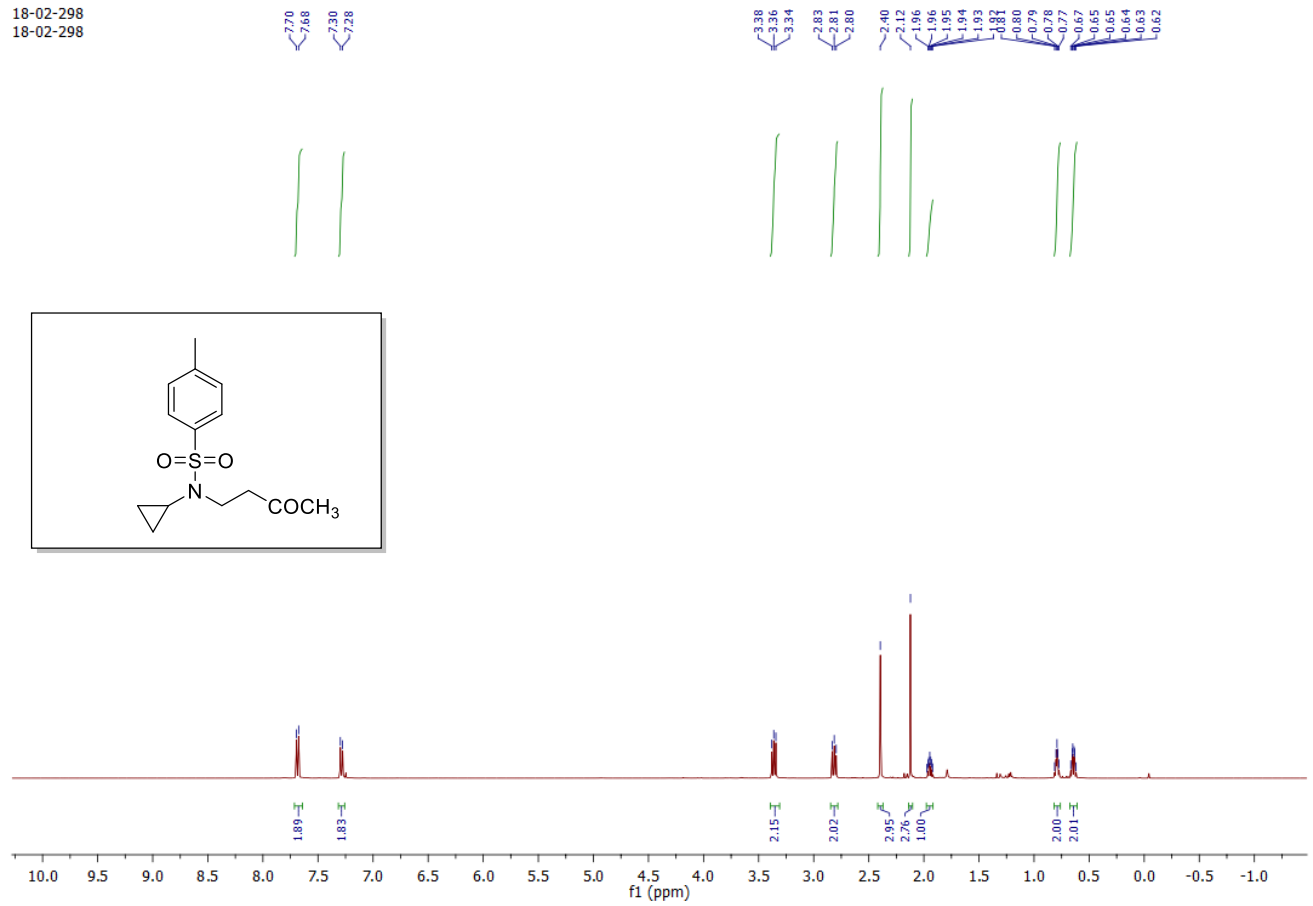
Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 13-13 H: 0-300 N: 1-2 O: 1-2 S: 1-1

Sample Name : 201021_18-02-286 IITRPR XEVO G2-XS QTOF
Test Name :
201021_18-02-286 7 (0.169) 1: TOF MS ES+
2.63e+007

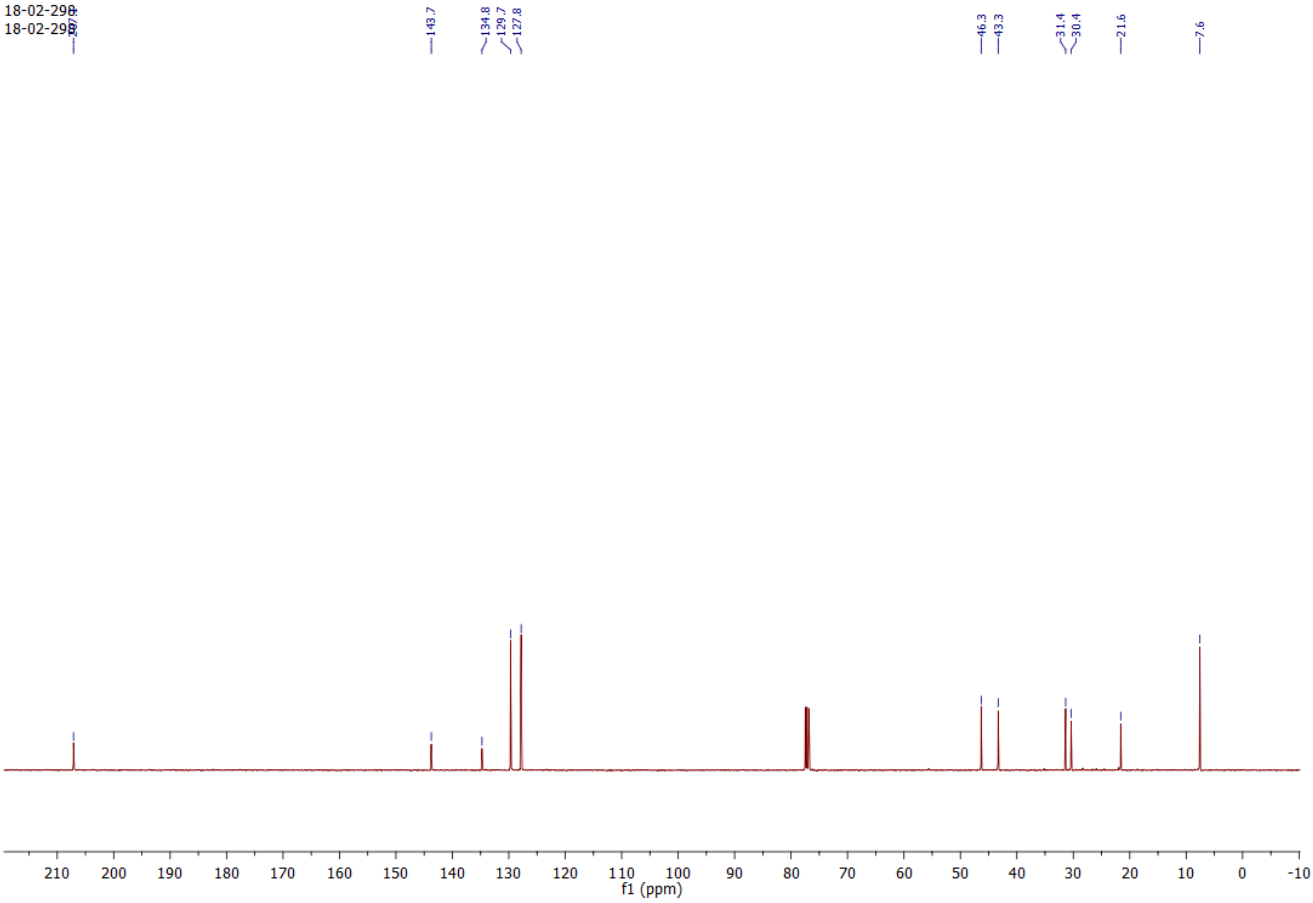


Minimum:				-1.5				
Maximum:		2.0	300.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
265.0972	265.1011	-3.9	-14.7	6.5	2367.7	n/a	n/a	C13 H17 N2 O2 S

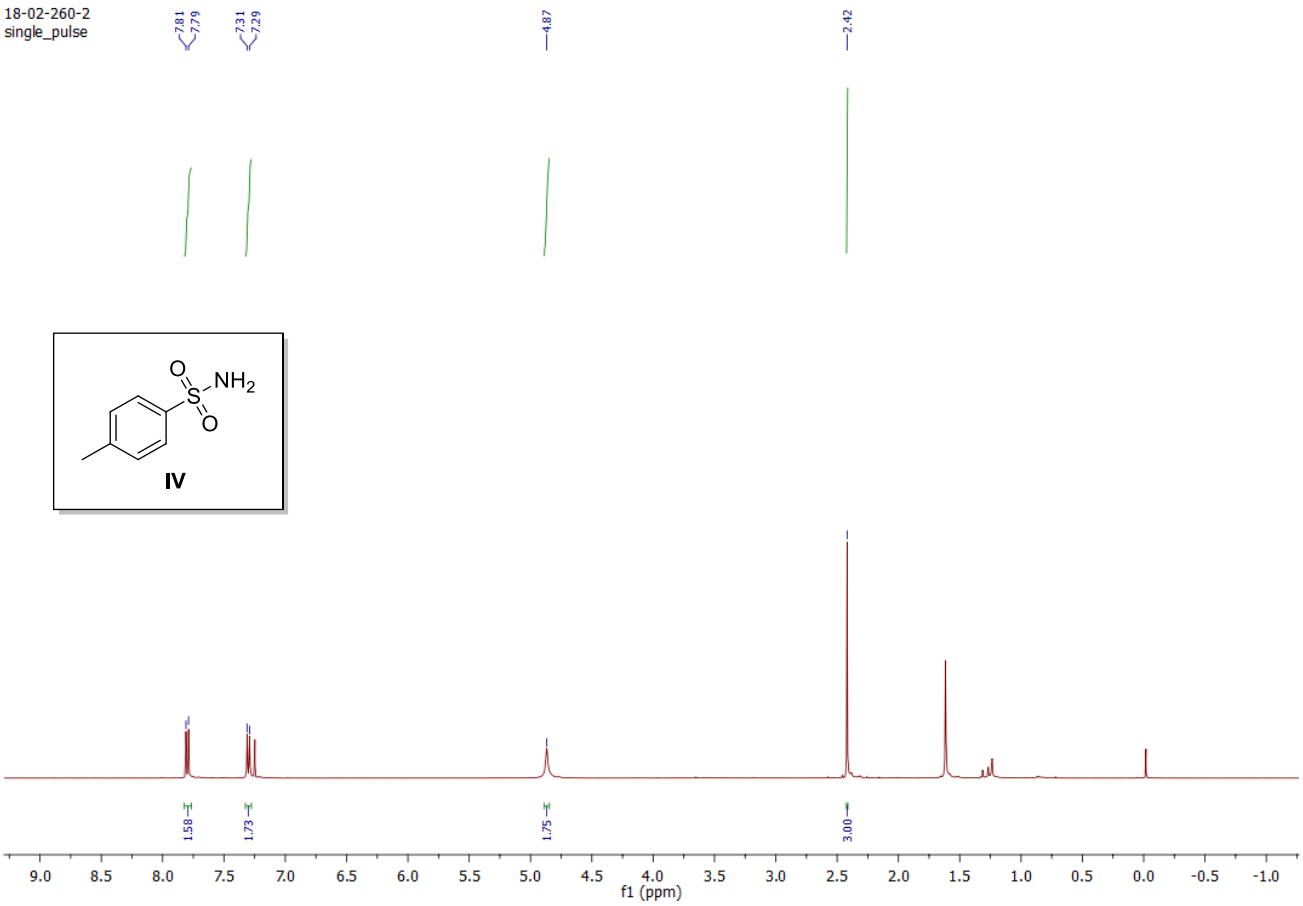
^{1}H NMR ($CDCl_3$, 400 MHz) of 3ac'



^{13}C NMR ($CDCl_3$, 101 MHz) of 3ac'



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



HRMS of "III"

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

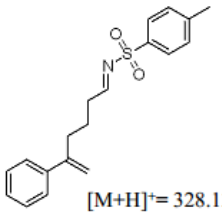
Monoisotopic Mass, Even Electron Ions
145 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-2 O: 0-4 S: 1-1 Br: 0-4

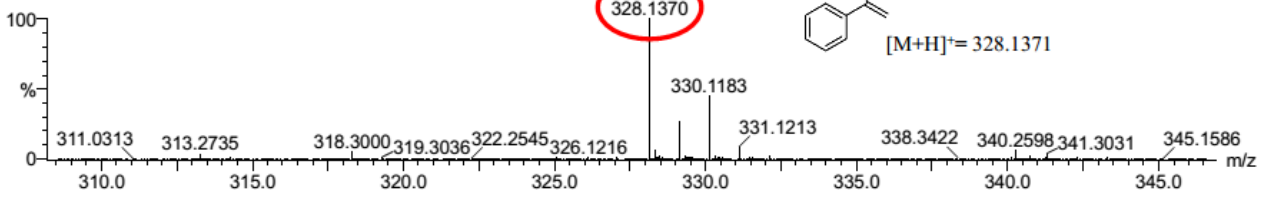
Sample Name : 18_02_372
Test Name :
03032022_18_02_372 6 (0.141)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
1.71e+008





Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
328.1370	328.1371	-0.1	-0.3	9.5	1783.2	n/a	n/a	C19 H22 N O2 S

HRMS of "F"

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

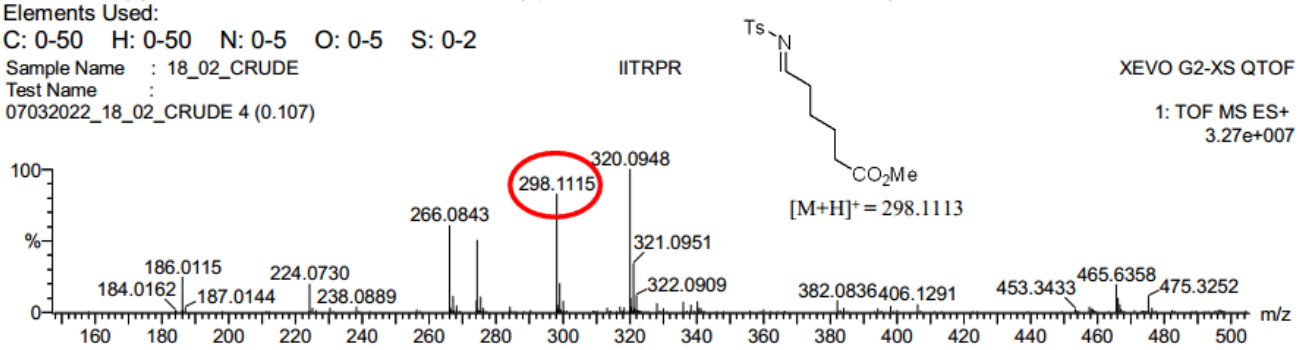
Monoisotopic Mass, Even Electron Ions
370 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-5 O: 0-5 S: 0-2

Sample Name : 18_02_CRUDE
Test Name :
07032022_18_02_CRUDE 4 (0.107)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
3.27e+007



Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
298.1115	298.1113	0.2	0.7	5.5	2029.7	n/a	n/a	C14 H20 N O4 S