Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

Electrochemical Access to Benzimidazolone and Quinazolinone Derivatives via *in situ* Generation of Isocyanates

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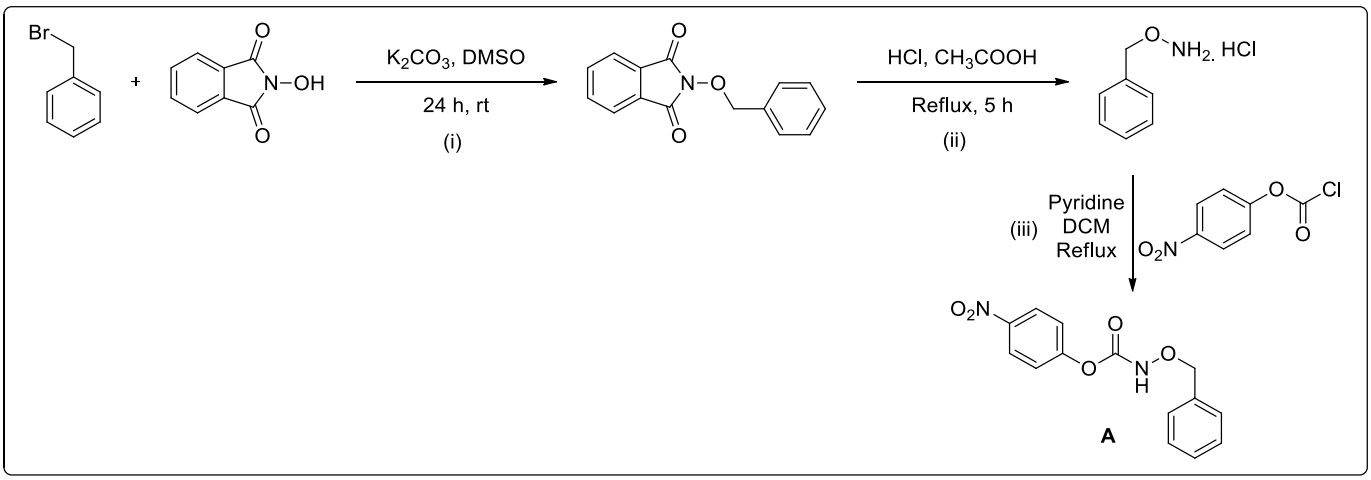
Contents

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). Acetonitrile and other solvents were obtained from Merck Life science Private Limited and were used directly without further purification and drying. Reagents were taken from various commercially available sources. Electrodes were commercially available from IKA. Cyclic voltammetry experiments were also performed on IKA Electrasyn 2.0. 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 *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). 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.

1) General procedure for preparation of 4-nitrophenyl benzyloxycarbamate.[1,2]



(i) To a mixed solution of 2-hydroxyisoindoline-1,3-dione (10.0 mmol, 1.63 g) in DMSO (15 mL) and anhydrous potassium carbonate (8.0 mmol, 1.2 g) benzyl bromide (20.0 mmol, 3.42 g) was added and the resulting mixture was stirred for 24 h at room temperature. After that, 30 mL of cold water was added and the resulting mixture was allowed to stand for 30 minutes. The obtained precipitate was filtered and washed with water (3×5 mL). Then the precipitate was recrystallized from ethanol to give the product *N*-benzyloxyphthalimide as white needle like crystals.

(ii) A mixture of *N*-benzyloxyphthalimide (4.0 mmol, 1.0 g), acetic acid (4 mL) and hydrochloric acid (aq. 37 %) (1.5 mL) was refluxed for 1.5 hours. The reaction mixture was cooled to room temperature and concentrated. Then cold water (10 mL) was added to the solid residue, suspension obtained was adjusted to alkaline by addition of 10% sodium hydroxide solution. The solution formed was subsequently extracted with CH_2Cl_2 (3×15 mL), and the combined organic phases were dried over anhydrous Na_2SO_4 and concentrated to a final volume of 10 mL. Further 6N HCl was added resulting in the formation of white solid compound as Amine hydrochloride (benzyloxy).

(iii) Amine hydrochloride (benzyloxy (A), methoxy-(A)) was suspended in dry dichloromethane (DCM) (200 mL) and pyridine (7.9 g, 10.0 mmol). 4-nitrophenylchloroformate (20.16 g, 10.0 mmol) dissolved in DCM (100 mL) was added dropwise while stirring at room temperature for 45 min. After the addition was completed, the reaction mixture was refluxed for 6 h and then cooled to rt, diluted with DCM (200 mL), washed sequentially with 1N HCl, H_2O, 1M sodium bicarbonate solution, water, and brine. The DCM layer was dried over sodium sulfate and evaporated under vacuum. The crude obtained was further purified by flash chromatography using a mixture of ethyl acetate/hexane.

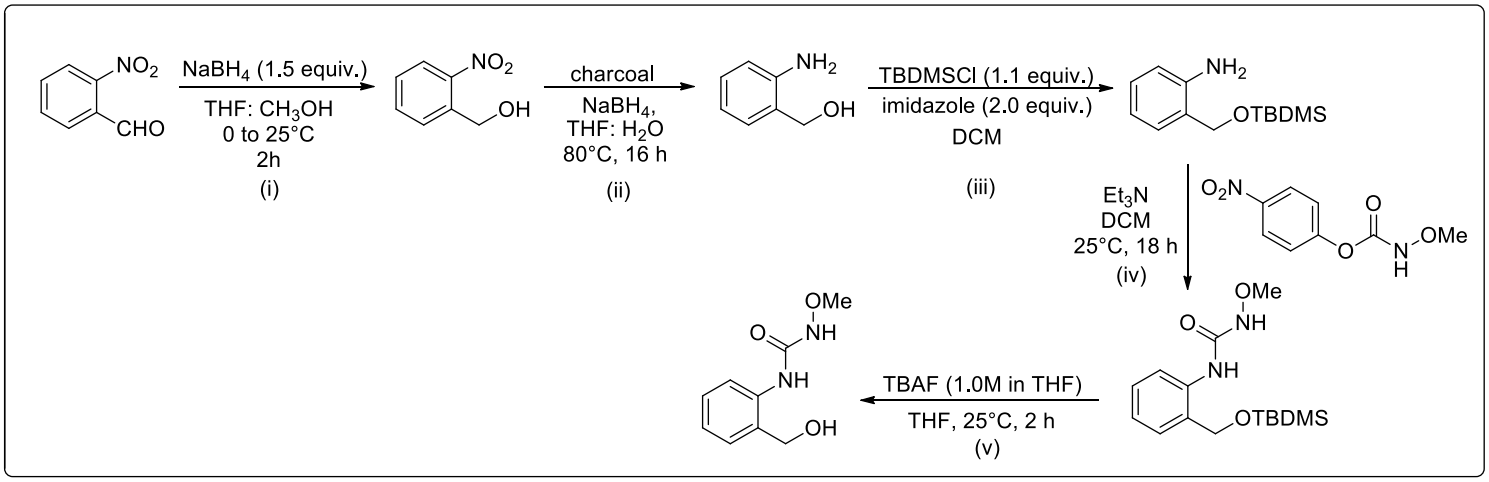
2) General procedure for preparation of 1,1'-(1,2-Phenylene)bis(3-(alkyloxy)urea)(GP 1).

To a solution of 4-nitrophenyl benzyloxycarbamate (2.0 equiv.) in CH_2Cl_2 (20 mL) under air atmosphere was added substituted *o*-phenylene diamine (**a**-**r**) (1.0 equiv.) and triethylamine (1.0-2.0 equiv.). The reaction mixture was stirred at room temperature for 24 hours. After completion, the reaction mixture was quenched with water (15 mL) and the aqueous phase was extracted with CH_2Cl_2 (3 x 15 mL). The combined organic phases were washed with brine, dried over Na_2SO_4, concentrated under reduced pressure and purified by silica gel column chromatography (230-400 mesh) and the desired compound was eluted at 60%-80% ethyl acetate in hexane.

3) General Procedure for Electrochemical Reactions (GP 2)

In an undivided cell (15 mL) equipped with a stirring bar, a mixture of substrates **1a-1r** (1.0 equiv.), nBu_4NBF_4 (2.0 equiv.), Cp_2Fe (0.5 equiv.) and MeCN (5.0 mL) were added. The cell was equipped with graphite as both anode and cathode and performed in an IKA Electrasyn 2.0 and the power supply (Keysight). The reaction mixture was stirred and electrolyzed at a constant current of 3.0 mA at 23 °C for 2-4 h. Upon completion, the solvent was removed directly under reduced pressure to afford the crude product, which was further purified by silica gel column chromatography (230-400 mesh) to afford the desired product.

4) General Procedure for synthesis of 1-(2-(hydroxymethyl)phenyl)-3-methoxyurea (GP 3)



(i) To a mixed solution of 2-nitrobenzaldehyde (6.61 mmol, 1.0 g) in THF: MeOH (10: 8 mL), sodium borohydride (9.92 mmol, 0.375 g) was added slowly to an ice-cold solution in a portion wise manner. Further, the resulting mixture was stirred for 2 h at room temperature. After the completion, 30 mL of cold water followed by brine solution was added. The obtained solution was subsequently extracted with ethyl acetate (3×20 mL), and the combined organic phases were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to obtain the crude product. Further purification by silica gel column chromatography (230-400 mesh) afforded the 2-nitrobenzylalcohol.

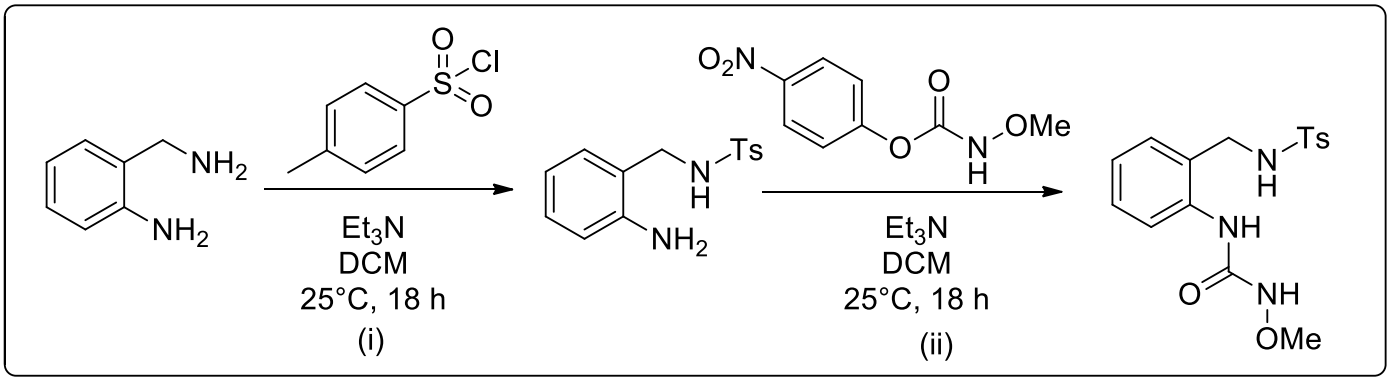
(ii) To a solution of 2-nitrobenzylalcohol (1.0 equiv.) in THF:H_2O (10: 8 mL) under nitrogen atmosphere was added substituted charcoal (6.0 equiv.) and the reaction mixture was stirred at room temperature. After cooling the reaction mixture to 0°C, sodium borohydride (4.0 equiv.) was added in a portion wise manner. The resulting reaction mixture was heated at a temperature of 50°C for 6 hours. After completion, the reaction mixture was filtered through a celite pad and filterate obtained was further washed with 1M NH_4Cl and extracted with ethyl acetate (3X20 mL). The combined organic phases were washed with brine, dried over Na_2SO_4, concentrated under vacuo, purified by silica gel column chromatography (230-400 mesh) and 2-aminobenzyl alcohol was eluted at 60%-80% ethyl acetate in hexane.

(iii) 2-aminobenzyl alcohol (1.0 equiv.) was suspended in CH_2Cl_2 (15 mL) and was added imidazole (2.0 equiv.) and *tert*-butyldimethylsilylchloride (1.1 equiv.). The reaction mixture was stirred at 0°C for 1 h. After completion, the reaction mixture was diluted with 30 mL CH_2Cl_2 and washed with $NaHCO_3$ and brine. Further, it was dried over Na_2SO_4 and after filtration the filtrate obtained was evaporated, purified by silica gel column chromatography (230-400 mesh), eluted at 10%-15% ethyl acetate in hexane to afford the 2-(((tert-butyldimethylsilyl)oxy)methyl)aniline.

(iv) To a solution of 4-nitrophenyl benzyloxycarbamate (1.0 equiv.) in CH_2Cl_2 (20 mL) under air atmosphere was added 2-(((tert-butyldimethylsilyl)oxy)methyl)aniline (1.0 equiv.) and triethylamine (1.2 equiv.). The reaction mixture was stirred at room temperature for 24 hours. After completion, the reaction mixture was quenched with water (15 mL) and the aqueous phase was extracted with CH_2Cl_2 (3 x 15 mL). The combined organic phases were washed with brine, dried over Na_2SO_4, concentrated under reduced pressure and purified by silica gel column chromatography (230-400 mesh) and the desired compound was eluted at 60%-80% ethyl acetate in hexane to afford 1-(2-(((tert-butyldimethylsilyl)oxy)methyl)phenyl)-3-methoxyurea

(v) To a solution of 1-(2-(((tert-butyldimethylsilyl)oxy)methyl)phenyl)-3-methoxyurea (1.0 equiv.) in THF under air atmosphere was added tetrabutyl ammonium fluoride (TBAF, 1.0 M in THF) (2.0 equiv.) under cooling conditions. Further, the reaction mixture was stirred at room temperature for 8 h. After completion, the reaction mixture was added ice cold water (10 mL) and the extracted with CH_2Cl_2 (3X 20 mL). The combined organic layers were washed with water and dried over Na_2SO_4, concentrated under reduced pressure to afford the crude product. The crude obtained was further purified by silica gel column chromatography (230-400 mesh) and the desired product was eluted at 60% ethylacetate in hexane to afford 1-(2-(hydroxymethyl)phenyl)-3-methoxyurea.

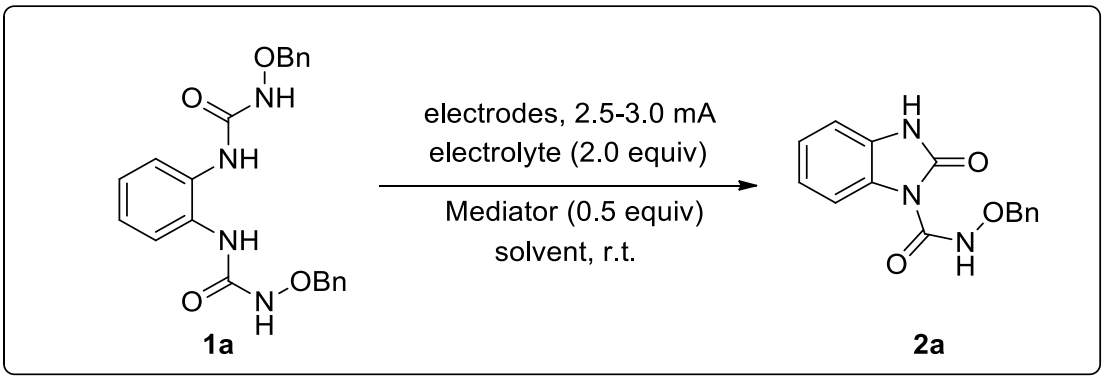
5) General Procedure for synthesis of *N*-(2-(3-methoxyureido)benzyl)-4-methylbenzenesulfonamide (GP 4)



(i) To a solution of 2-aminobenzylamine (1.0 equiv.) in CH_2Cl_2 (20 mL) under air atmosphere was added 2-(((tert-triethylamine (1.2 equiv.). The reaction mixture was stirred at room temperature for 12 hours. After completion, the reaction mixture was quenched with water (15 mL) and the aqueous phase was extracted with CH_2Cl_2 (3 x 15 mL). The combined organic phases were washed with brine, dried over Na_2SO_4, concentrated under reduced pressure and purified by silica gel column chromatography (230-400 mesh) and the desired compound was eluted at 30% ethyl acetate in hexane to afford *N*-(2-aminobenzyl)-4-methylbenzenesulfonamide.

(ii) To a solution of 4-nitrophenyl benzyloxycarbamate (1.0 equiv.) in CH_2Cl_2 (20 mL) under air atmosphere was added *N*-(2-aminobenzyl)-4-methylbenzenesulfonamide (1.0 equiv.) and triethylamine (1.2 equiv.). The reaction mixture was stirred at room temperature for 24 hours. After completion, the reaction mixture was quenched with water (15 mL) and the aqueous phase was extracted with CH_2Cl_2 (3 x 15 mL). The combined organic phases were washed with brine, dried over Na_2SO_4, concentrated under reduced pressure and purified by silica gel column chromatography (230-400 mesh) and the desired compound was eluted at 60%-80% ethyl acetate in hexane to afford *N*-(2-(3-methoxyureido)benzyl)-4-methylbenzenesulfonamide.

6) Optimization studies for synthesis of *N*-methoxy-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide[a]



In an oven-dried undivided reaction flask (10 mL) equipped with a stir bar and electrodes were added 1,1'-(1,2-phenylene)bis(3-(benzyloxy)urea) (**1a**, 0.050 g, 0.12 mmol), electrolyte (2.0 equiv.) and solvent (5 mL). The solution was electrolyzed at a constant current of 2.5- 3.0 mA at room temperature under air for 1.5-3.0 h. The solvent was evaporated in vacuo and the crude mixture was purified by silica gel column chromatography using 60-70% ethyl acetate in hexane to get *N*-methoxy-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide (**2a**) in 40-60% isolated yields.

Table S1: <u>Optimization of reaction conditions</u>

Entry	Solvent	Electrolyte	Electrode	Mediator	Yield (%)[b]
1	CH_3CN	nBu_4NPF_6	C(+)/C(-)	Cp_2Fe	15
2	CH_3CN	nBu_4NBr	C(+)/C(-)	Cp_2Fe	14
3	CH_3CN	nBu_4NClO_4	C(+)/C(-)	Cp_2Fe	17
4	CH_3CN	nEt_4NBF_4	C(+)/C(-)	Cp_2Fe	45
5	CH_3CN	nBu_4NBF_4	C(+)/C(-)	Cp_2Fe	44
6	DCM	nBu_4NBF_4	C(+)/C(-)	Cp_2Fe	n.r.
7	MeOH	nBu_4NBF_4	C(+)/C(-)	Cp_2Fe	n.r.
8	DMF	nBu_4NBF_4	C(+)/C(-)	Cp_2Fe	n.r.
9	**$CH_3CN:H_2O$ (4.5:0.5)**	**nBu_4NBF_4**	**C(+)/C(-)**	**Cp_2Fe**	**60**
10	$CH_3CN:H_2O$ (4.5:0.5)	nBu_4NBF_4	C(+)/C(-)	TEMPO	58
11	$CH_3CN:H_2O$ (4.5:0.5)	nBu_4NBF_4	Pt(+)/C(-)	Cp_2Fe	n.r.
12	$CH_3CN:H_2O$ (4.5:0.5)	nBu_4NBF_4	C(+)/Pt(-)	Cp_2Fe	56

13[c]	$CH_3CN:H_2O$ (4.5:0.5)	nBu_4NBF_4	C(+)/C(-)	Cp_2Fe	Trace
14[d]	$CH_3CN:H_2O$ (4.5:0.5)	nBu_4NBF_4	C(+)/C(-)	Cp_2Fe	24
15[e]	$CH_3CN:H_2O$ (4.5:0.5)	nBu_4NBF_4	C(+)/C(-)	Cp_2Fe	n.r.
16	$CH_3CN:H_2O$ (4.5:0.5)	nBu_4NBF_4	C(+)/C(-)	-	n.r.
17[f], [g], [h]	$CH_3CN:H_2O$ (4.5:0.5)	nBu_4NBF_4	C(+)/C(-)	Cp_2Fe	n.r.

[a] Unless otherwise stated all the reactions were performed at a constant current of 3.0 mA at room temperature, [b] isolated yields, [c] constant current = 5 mA, [d] constant current =1.5-2.0 mA, [e] without electricity, n.r = no reaction was observed**.** [f] Without electricity in the presence of NaH (0.5 equiv.). [g] Without electricity in the presence of NaOH (0.5 equiv.). [h] Without electricity in the presence of K_2CO_3 (0.5 equiv.). CH_3CN employed has been dried according to literature procedure.

7) Mechanistic studies

a. Cyclic Voltammetry

Cyclic voltammograms were collected with IKA Potentiostat. Samples were prepared with 0.05 mmol of substrate, 0.01 mmol of Cp_2Fe, dissolved in 5 mL of 0.1 M Bu_4NBF_4 in acetonitrile. Measurements employed a glassy carbon working electrode, platinum plate counter electrode and a 3 M KCl silver-silver chloride reference electrode. The scan rate applied was 0.05 V/s. Maximum current (I_p) of each substrate was obtained using Origin and the potential ($E_{p/2}$) was determined at half of this value ($I_{p/2}$). All the CV experiments were carried out in N_2 atmosphere and demonstrated as follows: (a) Fc/Fc^+ (black) (b) 0.01M Cp_2Fe, 0.01M **1c** (red) (c) 0.01M Cp_2Fe, 0.01M **1c**, 0.01M NaOH (blue) (d) 0.01M **1c** (pink). From CV, concluson can be drawn that Cp_2Fe acts as an mediator to furnish the desired oxidation of substrate **1c** at lower potential. Moreover, addition of base enhances the current density making the process more favorable.

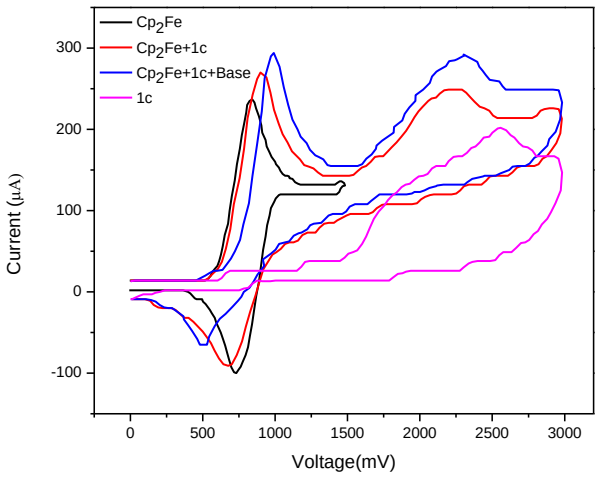
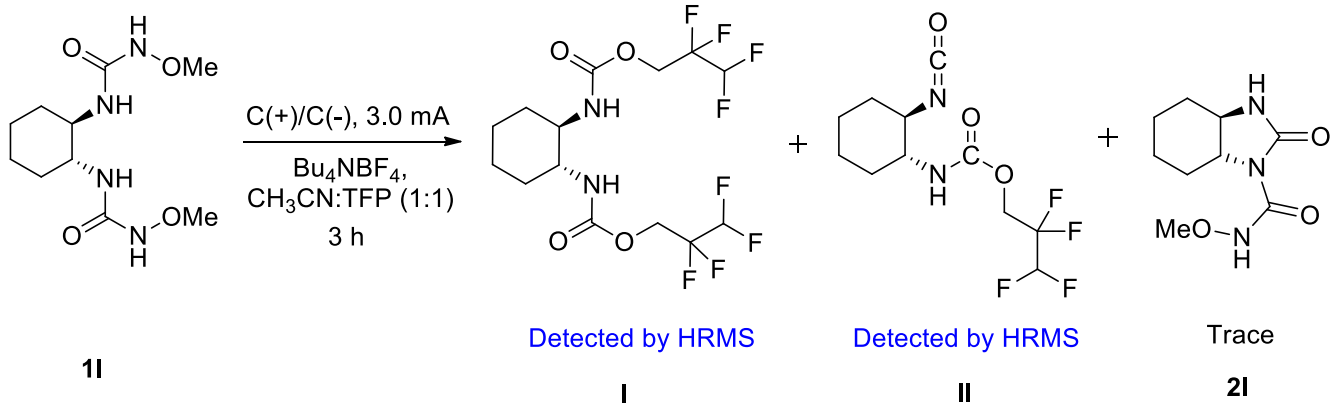


Figure S1: Cyclic voltammetry experiment. $E_{p/2}$ for Cp_2Fe = (0.77 V+ 0.74V)/2 = 0.75 V v/s Ag/AgCl (3M KCl)

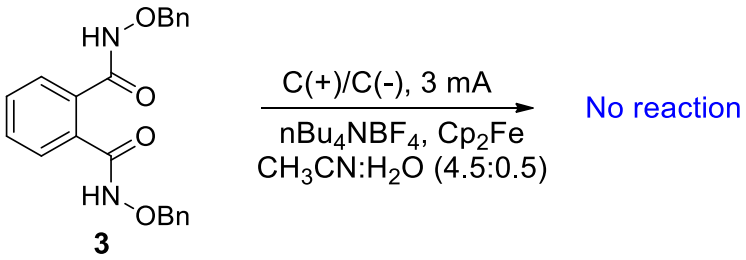
b. Intermediate trap experiment[3]



1l **I** **II** **2l**

In an undivided cell (15 mL) equipped with a stirring bar, a mixture of substrates **1l** (1.0 equiv.), Bu_4NBF_4 (2.0 equiv.), Cp_2Fe (0.5 equiv.) and MeCN (2.5 mL) were added. Furthermore, stoichiometric amount of 1,1,2,2 tetrafluoroisopropanol (2.5 mL) was added as trapping agent. The cell was equipped with graphite as both anode and cathode and performed in an IKA Electrasyn 2.0. The reaction mixture was stirred and electrolyzed at a constant current of 3.0 mA at 23 °C for 3.0 h. Upon completion, the solvent was removed directly under reduced pressure to afford the crude product, which was further filtered by silica gel column chromatography (230-400 mesh) to remove Bu_4NBF_4. Further the filtrate was concentrated under vacuo to afford adduct (**I**) and (**II**) which was detected by HRMS.

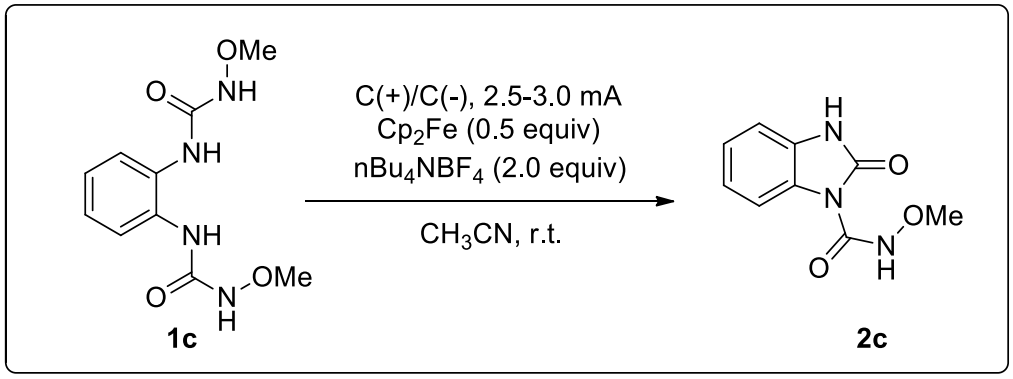
c) Unsuccessful experiment



3

In an undivided cell (15 mL) equipped with a stirring bar, a mixture of substrates **3** (1.0 equiv.), Bu_4NBF_4 (2.0 equiv.), Cp_2Fe (0.5 equiv.) and CH_3CN: H_2O (4.5: 0.5) was added. The cell was equipped with graphite as both anode and cathode and the reaction was performed in an IKA Electrasyn 2.0. The reaction mixture was stirred and electrolyzed at a constant current of 3.0 mA at 23 °C for 3 h. The progress of the reaction was monitored using TLC which shows that the starting material remain unreacted confirming the absence of *in situ* isocyanate generation.

8) Procedure for electrochemical gram scale synthesis



In an oven-dried two neck round bottom flask (100 mL) equipped with a stir bar and electrodes, were added 1,1'-(1,2-phenylene)bis(3-methoxyurea) (**1c**, 3.93 mmol, 1.0 g), Bu_4NBF_4 (2.0 equiv.) and MeCN (20 mL). The solution was electrolyzed at a constant current of 2.5- 3.0 mA at room temperature under air for 5.0 h. The solvent was evaporated in vacuo and the crude mixture was purified by silica gel column chromatography using 60-70% ethyl acetate in hexane to get *N*-methoxy-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide (**2c**) in 51% isolated yields.

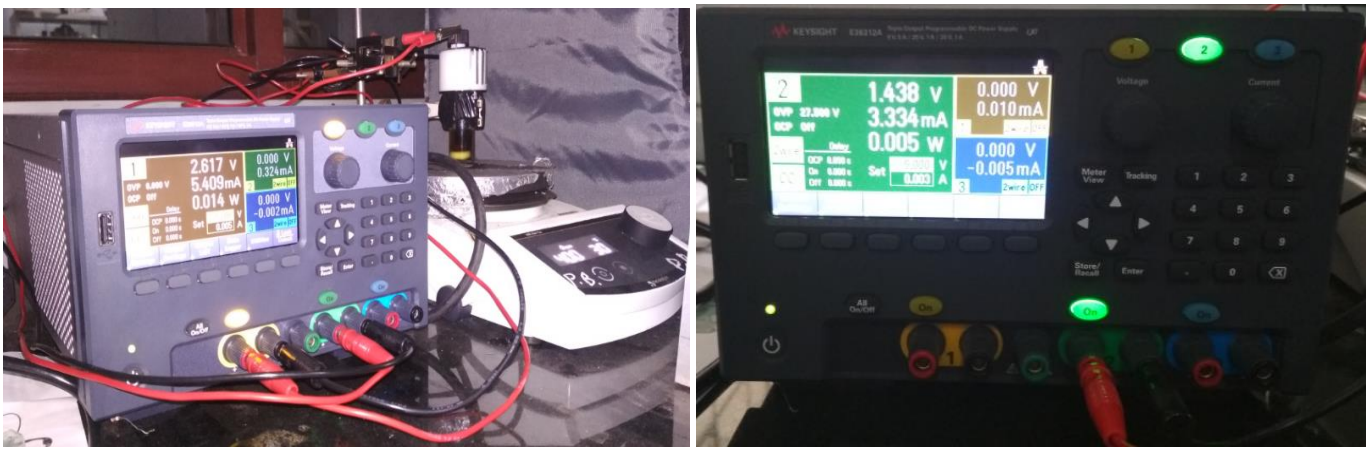
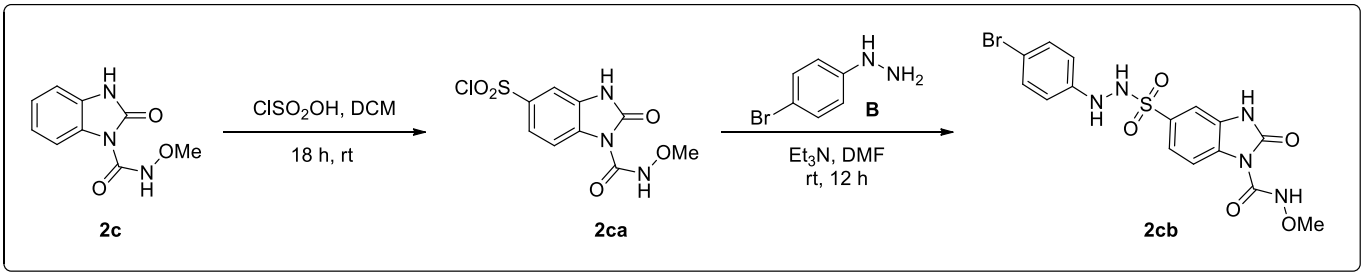


Figure S2: Electrochemical set up for gram scale electrolysis

9) Procedure for synthetic application[4]



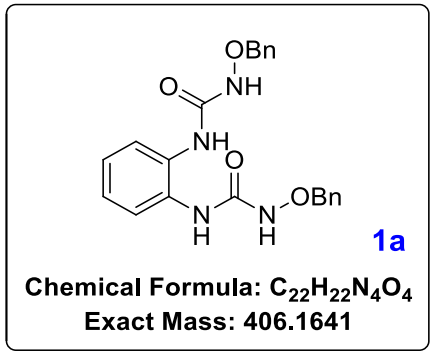
1) Chlorosulfonic acid (0.5 mL) wa**s** added slowly to *N*-methoxy-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide (**2c**, 0.050 g, 0.24 mmol) at room temperature, and the reaction mixture was stirred at room temperature for 18 h. The resulting mixture was added to ice with NaCl(s) carefully and extracted with ethyl acetate. The organic layer was dried over Na_2SO_4 and concentrated in vacuo to give the desired product **2ca**, which was used directly for the next step (0.040 g, 55%).

2) 4-bromophenylhydrazine (0.2 mmol, 2.0 equiv) was added to **2ca** (0.13 mmol, 1.0 equiv) at room temperature, and the reaction mixture was stirred at room temperature for 12 h. Formation of the product was monitored using TLC. After the completion of the reaction, the reaction mixture was added water (10 mL) and was extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4 and concentrated in vacuo to give desired product**,** which was purified by washing with 40% ether in pentane to get 5-((2-(4-bromophenyl)hydrazinyl)sulfonyl)-*N*-methoxy-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide **2cb** (0.049g, 84%).

10) Characterization data

i) Characterization data of the starting materials

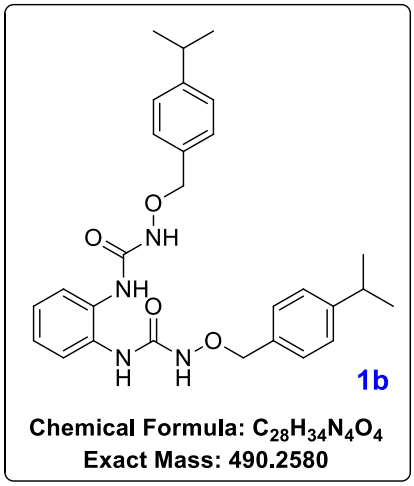
1,1'-(1,2-phenylene)bis(3-(benzyloxy)urea) *(1a)*



Chemical Formula: $C_{22}H_{22}N_4O_4$
Exact Mass: 406.1641

Prepared according to **GP1**, **a** (0.236 g, 2.18 mmol), **A[1]** (1.26 g, 4.37 mmol), **1a** (0.50 g, 56%). **Reaction time:** 22 h. **Yield:** 56%. **Nature:** White solid. **Melting Point:** 157°C**.** **^{1}H-NMR** (400 MHz): δ 7.99 (s, 2H), 7.47-7.29 (m, 12H), 7.20-7.14 (m, 2H), 7.26 (s, 2H), 4.87 (s, 4H).**^{13}C-NMR** (100 MHz): δ158.1, 135.3, 130.1, 129.7, 129.3, 129.1, 126.4, 125.4, 79.3. **FTIR (neat):** 1690, 1475, 1336, 904. 727,649 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{22}H_{23}N_4O_4$ 407.1719, found 407.1720.

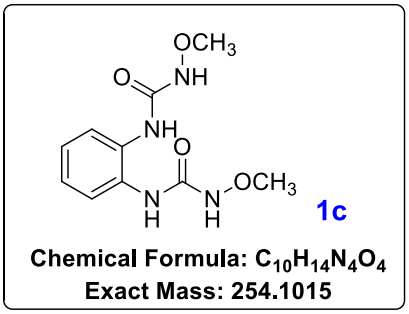
1,1'-(1,2-Phenylene)bis(3-((4-isopropylbenzyl)oxy)urea) *(1b)*



Chemical Formula: $C_{28}H_{34}N_4O_4$
Exact Mass: 490.2580

Prepared according to **GP1**, **b** (0.050 g, 0.46 mmol), **A[3]** (0.305 g, 0.924 mmol), **1b** (0.126 g, 62%). **Reaction time:** 21 h. **Yield:** 62%. **Nature:** White solid. **Melting Point:** 142°C. **^{1}H-NMR** (400 MHz): δ 7.94 (s, 2H), 7.36 (d, 4H, J= 8.07 Hz), 7.28-7.22 (m, 6H), 7.16-7.10 (m, 2H), 7.02 (s, 2H), 7.06 (s, 1H), 4.83 (s, 4H), 2.97-2.88 (m, 2H), 1.26 (s, 6H), 1.24 (s, 6H). **^{13}C-NMR** (100 MHz): δ158.1, 150.3, 132.8, 130.2, 129.9, 127.2, 126.3, 125.3, 79.2, 34.3, 24.3. **FTIR (neat):** 3406, 3151, 2957, 1662, 1598, 1546, 1510, 1482, 1278, 1075, 960, 809, 745, 714, 603 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{28}H_{35}N_4O_4$ 491.2658, found 491.2651.

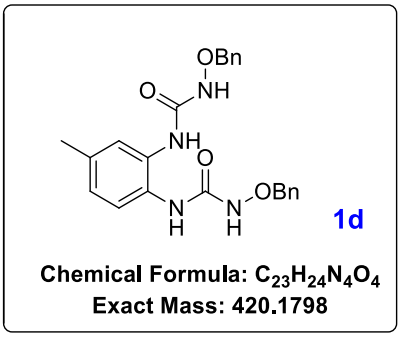
1,1'-(1,2-Phenylene)bis(3-methoxyurea) ***(1c)***



Chemical Formula: $C_{10}H_{14}N_4O_4$
Exact Mass: 254.1015

Prepared according to **GP1**, **c** (0.050 g, 0.46 mmol), **A²** (0.196 g, 0.92 mmol), **1c** (0.060 g, 51%). **Reaction time:** 22 h. **Yield:** 51%. **Nature:** White solid. **Melting Point:** 146°C. **^{1}H-NMR** (400 MHz): δ 8.15 (s, 2H), 7.50-7.47 (m, 2H), 7.24-7.20 (m, 6H), 3.80 (s, 6H). **^{13}C-NMR** (100 MHz): δ157.9, 131.4, 130.1, 125.4, 125.0, 120.8, 108.9, 64.4. **FTIR (neat):** 3259, 1665, 1595, 1533, 1289, 969, 746 cm^{-1}. **HRMS (ESI, Q-TOF)** ***m/z*****:** [M + Na]$^+$ Calculated for $C_{10}H_{14}N_4O_4Na$ 277.0913, found 277.0895.

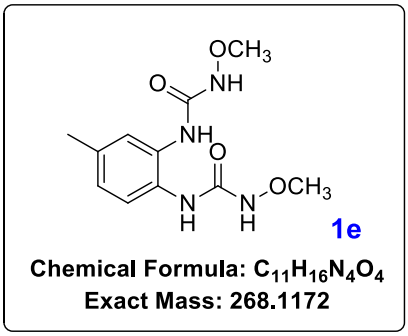
1,1'-(4-Methyl-1,2-phenylene)bis(3-(benzyloxy)urea) ***(1d)***



Chemical Formula: $C_{23}H_{24}N_4O_4$
Exact Mass: 420.1798

Prepared according to **GP1**, **d** (0.080 g, 0.65 mmol), **A¹** (0.376 g, 1.30 mmol), **1d** (0.160 g, 58%). **Reaction time:** 24 h. **Yield:** 58%. **Nature:** White solid. **Melting Point:** 150.2°C**. ^{1}H-NMR** (400 MHz): δ 7.97 (s, 1H), 7.85 (s, 1H), 7.43-7.36 (m, 11H), 7.15 (d, 2H, J=8.48 Hz), 7.08 (d, 2H, J=3.49 Hz), 6.96 (d, 1H, J= 8.80 Hz), 4.85 (s, 4H), 2.30 (s, 3H).**^{13}C-NMR** (100 MHz): δ158.4, 158.2, 136.6, 135.4, 130.2, 129.6, 129.2, 129.0, 127.3, 127.0, 125.6, 125.4, 79.25, 21.29. **FTIR (neat):** 3174, 1655, 1524, 1322, 1089, 967, 730, 691 cm^{-1}. **HRMS (ESI, Q-TOF)** ***m/z*****:** [M + H]$^+$ Calculated for $C_{23}H_{25}N_4O_4$ 421.1876, found 421.1869.

1,1'-(4-Methyl-1,2-phenylene)bis(3-methoxyurea) ***(1e)***

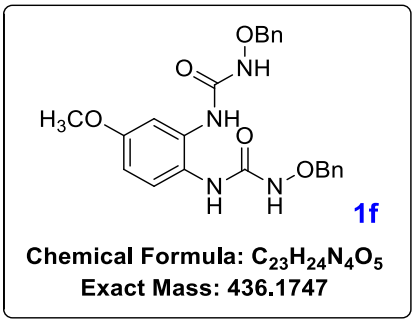


Chemical Formula: $C_{11}H_{16}N_4O_4$
Exact Mass: 268.1172

Prepared according to **GP1**, **e** (0.050 g, 0.40 mmol), **A²** (0.173 g, 0.81 mmol), **1e** (0.056 g, 53%). **Reaction time:** 21 h. **Yield:** 53%. **Nature:** White solid. **Melting Point:** 148°C. **^{1}H-NMR** (400 MHz): δ 10.48 (s, 1H), 9.72 (d, 2H, J= 15.79 Hz), 8.77 (s, 1H), 7.33 (s, 1H), 6.97 (s, 1H), 6.77 (m, 1H), 3.66 (s, 6H), 2.29 (s, 3H).**^{13}C-NMR** (100 MHz): δ158.1, 157.8, 155.9, 134.4, 131.4, 128.6, 125.5, 121.3, 109.5, 108.6, 64.3, 21.5, 21.0. **FTIR (neat):** 3172, 1656, 1597, 1524, 1331, 1078, 729, 693, 470 cm^{-1}.

HRMS (ESI, Q-TOF) ***m/z*****:** [M + H]$^+$ Calculated for $C_{11}H_{17}N_4O_4$ 269.1250, found 269.1242.

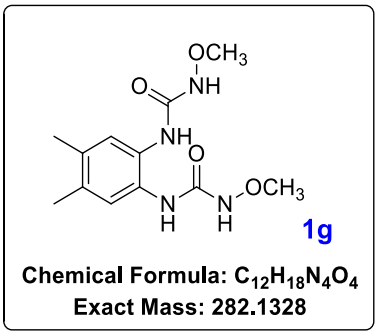
1,1'-(4-Methoxy-1,2-phenylene)bis(3-(benzyloxy)urea) ***(1f)***



Chemical Formula: $C_{23}H_{24}N_4O_5$
Exact Mass: 436.1747

Prepared according to **GP1**, **f** (0.050 g, 0.36 mmol), **A[1]** (0.208 g, 0.723 mmol), **1f** (0.080 g, 51%). **Reaction time:** 22 h. **Yield:** 51%. **Nature:** White solid. **Melting Point:** 138°C. **^{1}H-NMR** (400 MHz): δ 8.08 (s, 1H), 7.58 (s, 1H) 7.43-7.34 (m, 11H), 7.07-7.04 (m, 2H), 7.03-7.01 (m, 1H), 6.69-6.65 (dd, 1H, J= 2.95 Hz, J= 6.04 Hz), 4.85 (s, 2H), 4.83 (s, 2H), 3.76 (s, 3H).**^{13}C-NMR** (100 MHz): δ158.5, 158.4, 157.8, 135.4, 135.3, 132.5, 129.7, 129.4, 129.3, 129.19, 129.10, 127.0, 121.8, 112.0, 109.5, 79.3, 55.9. **FTIR (neat):** 3171, 1656, 1523, 1274, 1205, 1165, 1089, 1042, 730, 693 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_{23}H_{25}N_4O_5$ 437.1825, found 437.1817.

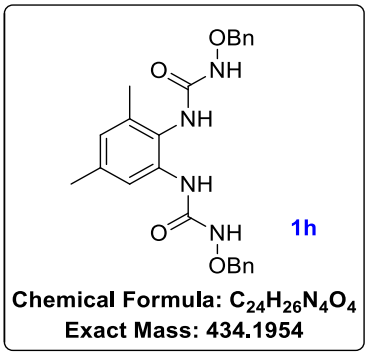
1,1'-(4,5-dimethyl-1,2-phenylene)bis(3-methoxyurea) ***(1g)***



Chemical Formula: $C_{12}H_{18}N_4O_4$
Exact Mass: 282.1328

Prepared according to **GP1**, **g** (0.050 g, 0.36 mmol), **A[2]** (0.155 g, 0.73 mmol), **1g** (0.065 g, 44%). **Reaction time:** 24 h. **Yield:** 44%. **Nature:** White solid. **Melting Point:** 149°C. **^{1}H-NMR** (400 MHz): δ 9.67 (s, 2H), 8.70 (s, 2H), 7.25 (s, 2H), 3.64 (s, 6H), 2.21 (s, 6H). **^{13}C-NMR** (100 MHz): δ158.4, 133.3, 129.3, 126.7, 64.7, 19.8. **FTIR (neat):** 2946, 2834, 1704, 1655, 1449, 1413, 1368, 1231, 1018 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_{12}H_{19}N_4O_4$ 283.1406, found 283.1400.

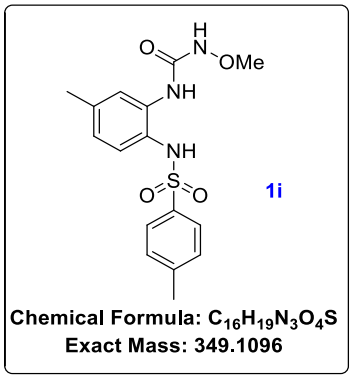
1,1'-(3,5-Dimethyl-1,2-phenylene)bis(3-(benzyloxy)urea) ***(1h)***



Chemical Formula: $C_{24}H_{26}N_4O_4$
Exact Mass: 434.1954

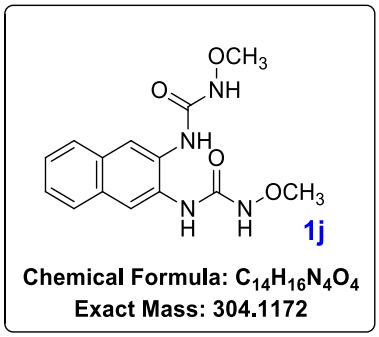
Prepared according to **GP1**, **h** (0.050 g, 0.367 mmol), **A[1]** (0.211 g, 0.734 mmol), **1h** (0.072 g, 45%). **Reaction time:** 20 h. **Yield:** 45%. **Nature:** White solid. **Melting Point:** 144°C. **^{1}H-NMR** (400 MHz): δ 8.09 (s, 1H), 7.44 -7.34 (m, 10H), 7.31 (s, 1H), 7.23 (s, 1H), 7.12 (s, 2H), 6.85 (s, 1H), 4.85 (d, 4H, J= 4.16 Hz), 2.28 (s, 3H), 2.12 (s, 3H). **^{13}C-NMR** (100 MHz): δ158.3, 158.0, 137.6, 135.4, 135.2, 135.2, 132.9, 129.7, 129.6, 129.3, 129.2, 129.1, 129.0, 128.5, 124.9, 123.0, 79.3, 79.1, 21.4, 18.5. **FTIR (neat):** 3324, 3199, 1651, 1542, 1512, 1363, 1301, 1090, 969, 798, 727, 693, 629 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_{24}H_{27}N_4O_4$ 435.2032, found 435.2034.

N*-(2-(3-methoxyureido)-4-methylphenyl)-4-methylbenzenesulfonamide *(1i)



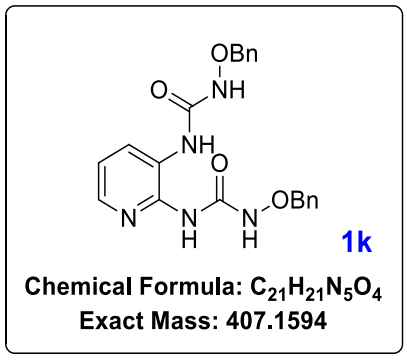
Prepared according to **GP1**, **i** (0.050 g, 0.180 mmol), **A[1]** (0.038 g, 0.180 mmol), **1i** (0.045 g, 67%). **Reaction time:** 24 h. **Yield:** 67%. **Nature:** White solid. **^{1}H-NMR** (400 MHz): δ 8.35 (s, 1H), 7.62 (s, 1H), 7.57 (d, 2H, J=8.92 Hz), 7.26-7.19 (m, 4H), 6.75 (m, 1H), 6.64 (s, 1H), 6.59 (d, 1H, J= 8.92 Hz), 3.82 (s, 3H), 2.42 (s, 3H), 2.31 (s, 3H). **^{13}C-NMR** (100 MHz): δ157.4, 144.0, 139.0, 135.6, 134.2, 129.6, 128.2, 127.5, 125.5, 123.7, 123.3, 65.0, 21.7, 21.3. **FTIR (neat):** 2956, 2925, 2855, 1675, 1593, 1539, 1328, 1159, 1091 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H] $^+$ Calculated for $C_{16}H_{20}N_3O_4S$ 350.1175, found 350.1169.

1,1'-(naphthalene-2,3-diyl)bis(3-methoxyurea) *(1j)*



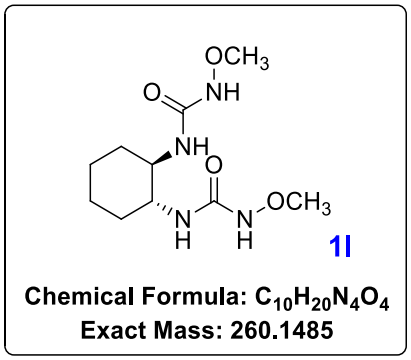
Prepared according to **GP1**, **j** (0.080 g, 0.50 mmol), **A[2]** (0.214 g, 1.01 mmol), **1j** (0.056 g, 36%). **Reaction time:** 24 h. **Yield:** 36%. **Nature:** White solid. **Melting Point:** 140°C. **^{1}H-NMR** (400 MHz): δ10.81 (s, 1H), 9.85 (s, 1H), 8.93 (s, 1H), 8.02 (s, 1H), 7.85-7.77 (m, 2H), 7.45-7.40 (m, 1H), 7.32-7.25 (m, 2H), 3.67 (s, 3H). **^{13}C-NMR** (100 MHz): 158.1, 131.5, 130.9, 130.9, 129.7, 127.4, 127.3, 125.9, 123.8, 122.3, 104.1, 64.5 . **FTIR (neat):** 2250, 2125, 1661, 1024, 821, 758 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + Na] $^+$ Calculated for $C_{14}H_{17}N_4O_4Na$ 327.1069, found 327.1051.

1,1'-(Pyridine-2,3-diyl)bis(3-(benzyloxy)urea) *(1k)*



Prepared according to **GP1**, **k** (0.050 g, 0.45 mmol), **A[1]** (0.264 g, 0.91 mmol), **1k** (0.090 g, 48%). **Reaction time:** 24 h. **Yield:** 48%. **Nature:** White solid. **Melting Point:** 163°C. **^{1}H-NMR** (400 MHz): δ 8.18 (s, 1H), 8.10-8.04 (m, 1H), 8.01 (s, 1H), 7.45-7.32 (m, 10H), 7.13-7.07 (m, 1H), 4.91 (s, 2H), 4.88 (s, 2H).**^{13}C-NMR** (100 MHz): δ157.8, 129.6, 129.4, 129.1, 128.9, 79.3, 79.2. **FTIR (neat):** 3183, 1666, 1503, 1432, 1306, 1094, 958, 733, 693 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H] $^+$ Calculated for $C_{21}H_{22}N_5O_4$ 408.1672, found 408.1664.

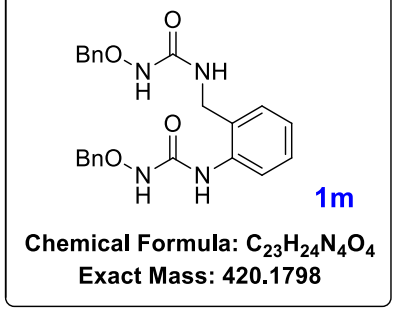
1,1'-(Cyclohexane-1,2-diyl)bis(3-methoxyurea) ***(1l)***



Chemical Formula: $C_{10}H_{20}N_4O_4$
Exact Mass: 260.1485

Prepared according to **GP1**, **l** (0.050 g, 0.43 mmol), **A²** (0.185 g, 0.87 mmol), **1l** (0.060 g, 53%). **Reaction time:** 20 h. **Yield:** 53%. **Nature:** White solid. **Melting Point:** 113°C. **^{1}H-NMR** (400 MHz): δ 6.99 (s, 2H), 6.00 (s, 2H), 3.70 (s, 6H), 3.59 (s, 2H), 2.13-2.04 (m, 2H), 1.82-1.75 (m, 2H), 1.40-1.24 (m, 4H). **^{13}C-NMR** (100 MHz): δ160.4, 64.7, 54.3, 33.1, 25.1. **FTIR (neat):** 3208, 2936, 1656, 1539, 744 cm^{-1}. **HRMS (ESI, Q-TOF)** ***m/z*:** $[M + H]^+$ Calculated for $C_{10}H_{21}N_4O_4$ 261.1563, found 261.1543.

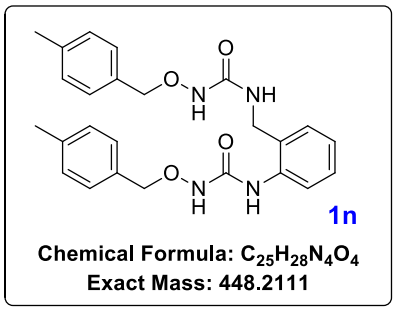
1-(benzyloxy)-3-(2-((3-benzyloxyureido)methyl)phenyl)urea ***(1m)***



Chemical Formula: $C_{23}H_{24}N_4O_4$
Exact Mass: 420.1798

Prepared according to **GP1**, **m** (0.050 g, 0.40 mmol), **A¹** (0.235 g, 0.81 mmol), **1m** (0.093 g, 54%). **Reaction time:** 18 h. **Yield:** 54%. **Nature:** White solid. **Melting Point:** 126°C. **^{1}H-NMR** (400 MHz): δ 8.87 (s, 1H), 7.69 (d, 1H, J= 8.17 Hz), 7.46-7.41 (m, 2H), 7.40-7.27 (m, 9H), 7.17-7.07 (m, 2H), 7.06 (s, 1H), 6.90 (s, 1H), 6.13 (m, 1H), 4.93 (s, 2H), 4.76 (s, 2H), 4.25(d, 2H, J= 6.69 Hz). **^{13}C-NMR** (100 MHz): δ160.5, 136.0, 135.9, 135.4, 130.5, 130.2, 129.7, 129.5, 129.3, 129.1, 129.0, 129.0, 128.9, 125.3, 124.7, 79.1, 79.0, 40.5. **FTIR (neat):** 3081, 2949, 1798, 1728, 1650, 1470, 156, 1260, 1135, 1047, 1019, 998, 779, 625 cm^{-1}. **HRMS (ESI, Q-TOF)** ***m/z*:** $[M + H]^+$ Calculated for $C_{23}H_{25}N_4O_4$ 421.1876, found 421.1871.

1-(2-((3-(4-methylbenzyloxyureido)methyl)phenyl)-3-((4-methylbenzyl)oxy)urea ***(1n)***

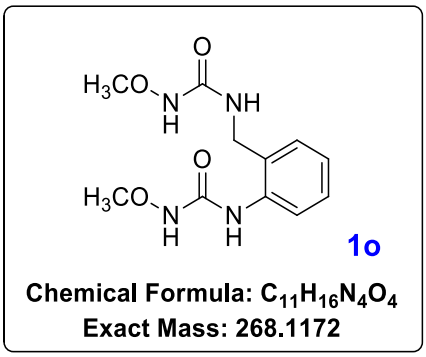


Chemical Formula: $C_{25}H_{28}N_4O_4$
Exact Mass: 448.2111

Prepared according to **GP1**, **n** (0.050 g, 0.40 mmol), **A⁵** (0.247 g, 0.81 mmol), **1n** (0.096 g, 52%). **Reaction time:** 19 h. **Yield:** 52%. **Nature:** White solid. **Melting Point:** 127°C. **^{1}H-NMR** (400 MHz): δ 8.83 (s, 1H), 7.69 (d, 1H, J= 8.08 Hz), 7.34-7.26 (m, 3H), 7.24-7.07 (m, 8H), 7.00 (s, 1H), 6.85 (s, 1H), 6.13-6.08 (m, 1H), 4.88 (s, 1H), 4.72 (s, 1H), 4.23 (d, 2H, J= 6.45 Hz), 2.35 (s, 6H).**^{13}C-NMR** (100 MHz): δ160.6, 158.3, 139.2, 138.9, 133.0, 130.4, 130.2, 129.8, 129.6, 125.2, 124.6, 79.0, 78.9, 40.5, 21.65, 21.61. **FTIR (neat):** 3214,

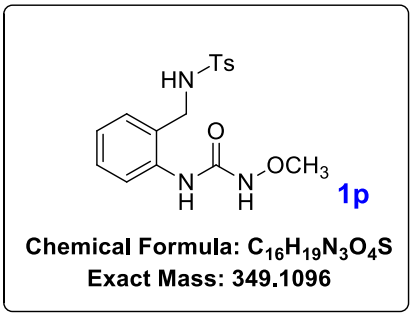
1707, 1602, 1474, 1419, 1326, 1202, 1130, 1099, 1039, 803, 744, 610 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z***: [M + H]$^+$ Calculated for $C_{19}H_{29}N_4O_4$ 449.2189, found 449.2173.

1-(methoxy)-3-(2-((3-methoxyureido)methyl)phenyl)urea *(1o)*



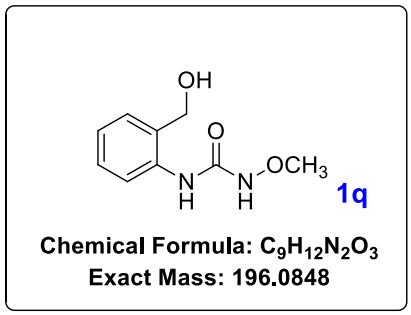
Prepared according to **GP1**, **o** (0.050 g, 0.40 mmol), **A²** (0.173 g, 0.81 mmol), **1o** (0.053 g, 53%). **Reaction time:** 18 h. **Yield:** 53%. **Nature:** White solid. **Melting Point:** 137°C. **^{1}H-NMR** (400 MHz): δ 9.13 (s, 1H), 7.81 (d, 1H, J=8.48 Hz), 7.33 (t, 1H), 7.28-7.26 (m, 1H), 7.23 (s, 1H), 7.15-7.10 (m, 1H), 7.05 (s, 1H), 6.28-6.23 (m, 1H), 4.39 (d, 2H, J=6.66 Hz), 3.82 (s, 3H), 3.67 (s, 3H). **^{13}C-NMR** (100 MHz): δ160.6, 158.5, 136.1, 130.6, 130.0, 129.2, 125.2, 124.7, 65.3, 64.7, 40.6. **FTIR (neat):** 3207, 1661, 1592, 1531, 1324, 1289, 1158, 1056, 744 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z***: [M + H]$^+$ Calculated for $C_{11}H_{17}N_4O_4$ 269.1250, found 269.1242.

N*-(2-(3-methoxyureido)benzyl)-4-methylbenzenesulfonamide *(1p)



Prepared according to **GP4**, **p** (0.100 g, 0.36 mmol), **A²** (0.076 g, 0.36 mmol), **1p** (0.067 g, 53%). **Reaction time:** 20 h. **Yield:** 47%. **Nature:** White solid. **Melting Point:** 107°C. **^{1}H-NMR** (400 MHz): δ 8.34 (s, 1H), 7.87 (d, 1H, J= 8.74 Hz), 7.76 (d, 2H, J= 8.12 Hz), 7.37-7.30 (m, 3H), 7.15 (s, 1H), 7.09-7.02 (m, 2H), 4.73 (m, 1H), 4.05 (d, 2H, J= 6.93 Hz), 3.87 (s, 3H), 2.46 (s, 3H).**^{13}C-NMR** (100 MHz): δ130.4, 130.0, 129.7, 127.4, 124.6, 123.1, 65.1, 45.8. **FTIR (neat):** 3226, 1676, 1590, 1530, 1453, 1323, 1158, 1091, 905, 728 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z***: [M + H]$^+$ Calculated for $C_{16}H_{20}N_3O_4S$ 350.1175, found 350.1178.

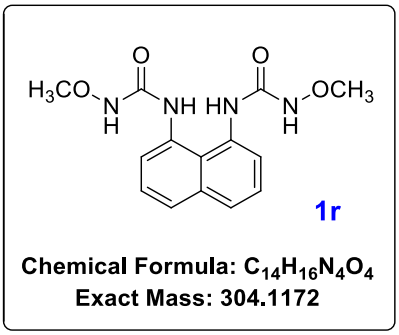
1-(2-(hydroxymethyl)phenyl)-3-methoxyurea *(1q)*



Chemical Formula: $C_9H_{12}N_2O_3$
Exact Mass: 196.0848

Prepared according to **GP3**, **q** (1.5 g, 0.36 mmol), **TBAF** (4.8 ml, 4.83 mmol), **1q** (0.9 g, 63%). **Reaction time:** 31 h. **Yield:** 63%. **Nature:** white solid. **Melting Point:** 115°C. **^{1}H-NMR** (400 MHz): δ 8.89 (s, 1H), 8.01 (d, 1H, J= 9.51 Hz), 7.34 (t, 1H, J= 8.78 Hz), 7.23-7.18 (m, 2H), 7.08 (t, 1H, J= 7.83 Hz), 4.74 (s, 2H), 3.81 (s, 3H).**^{13}C-NMR** (100 MHz): δ157.9, 137.4, 129.8, 129.6, 129.2, 124.2, 122.1, 65.1, 64.8. **FTIR (neat):** 3295, 3219, 2929, 2873, 1652, 1589, 1540, 1454, 1326, 1002, 946, 752 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z***: $[M + Na]^+$ Calculated for $C_9H_{12}N_2O_3Na$ 219.0746, found 219.0728.

1,1'-(naphthalene-1,8-diyl)bis(3-methoxyurea) *(1r)*

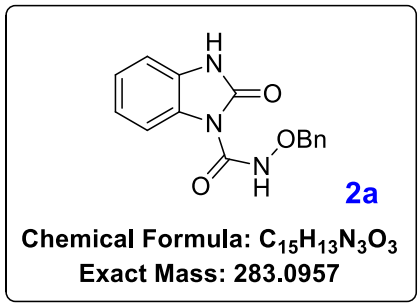


Chemical Formula: $C_{14}H_{16}N_4O_4$
Exact Mass: 304.1172

Prepared according to **GP1**, **r** (0.050 g, 0.31 mmol), **A^2** (0.134 g, 0.63 mmol), **1r** (0.055 g, 57%). **Reaction time:** 20 h. **Yield:** 57%. **Nature:** White solid. **Melting Point:** 298°C. **^{1}H-NMR** (400 MHz): δ 10.08 (s, 2H), 9.73 (d, 2H, J= 27.16 Hz), 7.83-7.68 (m, 2H), 7.44 (s, 1H), 7.25-7.05 (m, 3H), 6.50 (s, 1H), 3.66 (s, 3H), 3.34 (s, 3H). **^{13}C-NMR** (100 MHz): δ158.9, 150.9, 138.5, 136.4, 135.0, 134.9, 128.9, 126.3, 123.6, 122.7, 118.5, 114.5, 104.9, 64.8. **FTIR (neat):** 3270, 1649, 1564, 1379, 1094, 772 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{14}H_{17}N_4O_4$ 305.1250, found 305.1233.

ii) Characterization data of products

N-(benzyloxy)-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide *(2a)*

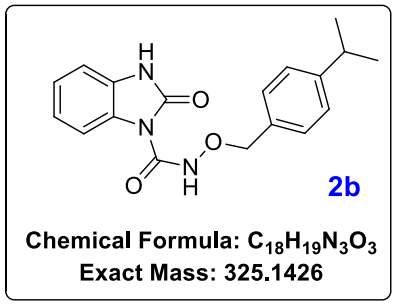


2a

Chemical Formula: $C_{15}H_{13}N_3O_3$
Exact Mass: 283.0957

Prepared according to **GP2, 1a** (0.050 g, 0.123 mmol), **2a** (0.043 g, 60%). **Reaction time:** 3.0 h. **Yield:** 60%. **Nature:** White solid. **Melting Point:** 196°C**.** **^{1}H-NMR** (400 MHz): δ 10.86 (s, 1H), 8.20-8.16 (m, 1H), 7.49-7.45 (m, 2H), 7.36-7.18 (m, 3H), 7.05-7.02 (m, 1H), 7.01 (s, 1H), 5.05 (s, 4H). **^{13}C-NMR** (100 MHz): δ153.5, 151.8, 136.3, 129.9, 129.5, 129.4, 129.3, 127.8, 124.7, 122.7, 114.7, 110.5, 78.6. **FTIR (neat):** 3237, 1690, 1475, 1336, 904, 727, 649 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_{15}H_{14}N_3O_3$ 284.1035, found 284.1028.

N-((4-isopropylbenzyl)oxy)-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide *(2b)*

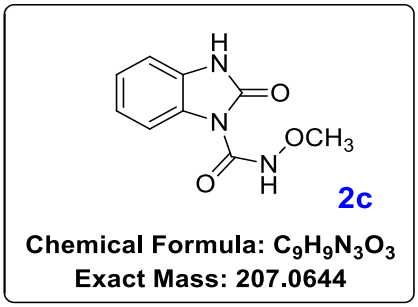


2b

Chemical Formula: $C_{18}H_{19}N_3O_3$
Exact Mass: 325.1426

Prepared according to **GP2, 1b** (0.050 g, 0.101mmol), **2b** (0.036 g, 57%). **Reaction time:** 3.0 h. **Yield:** 57%. **Nature:** White solid. **Melting Point:** 199°C. **^{1}H-NMR** (400 MHz): δ 10.86 (s, 1H), 8.21-8.16 (m, 1H), 8.07 (s, 1H), 7.40 (d, 2H, J=8.49 Hz), 7.26 (s, 1H), 7.54-7.23 (m, 1H), 7.06-7.01 (m, 1H), 5.02 (s, 2H), 2.96-2.88 (m, 1H), 1.26 (s, 3H), 1.24 (s, 3H).**^{13}C-NMR** (100 MHz): δ153.2, 151.4, 149.7, 132.4, 129.5, 127.2, 127.2, 126.8, 124.3, 123.3, 115.4, 109.4, 79.0, 34.0, 24.0. **FTIR (neat):** 3251, 2955, 1746, 1689, 1470, 1332, 1170, 1093, 1060, 1016, 930, 842, 809, 752, 655 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_{18}H_{20}N_3O_3$ 326.1505, found 326.1492.

N*-methoxy-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide *(2c)

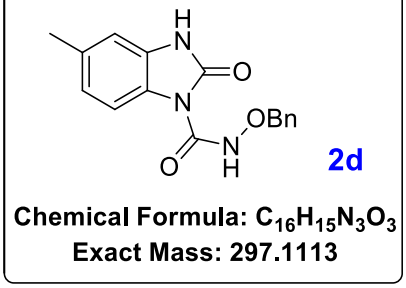


2c

Chemical Formula: $C_9H_9N_3O_3$
Exact Mass: 207.0644

Prepared according to **GP2, 1c** (0.050 g, 0.196 mmol), **2c** (0.036 g, 60%). **Reaction time:** 2.3 h. **Yield:** 60%. **Nature:** White solid. **Melting Point:** 153°C. **^{1}H-NMR** (400 MHz): δ 11.60 (s, 1H), 11.15 (s, 1H), 7.90 (d, 1H, J= 8.07 Hz), 7.19-7.04 (m, 3H), 3.74 (s, 3H). **^{13}C-NMR** (100 MHz): δ153.5, 151.6, 129.5, 127.8, 124.6, 122.6, 114.7, 110.4, 64.8. **FTIR (neat):** 3212, 1753, 1686, 1493, 1368, 1338, 1175, 1137, 1055, 937, 610 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_9H_{10}N_3O_3$ 208.0722, found 208.0709.

N*-(benzyloxy)-5-methyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide *(2d)

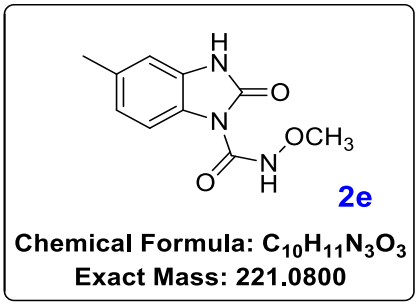


2d

Chemical Formula: $C_{16}H_{15}N_3O_3$
Exact Mass: 297.1113

Prepared according to **GP2, 1d** (0.050 g, 0.118 mmol), **2d** (0.056 g, 80%). **Reaction time:** 2.3 h. **Yield:** 80%. **Nature:** White solid. **Melting Point:** 199°C**. ^{1}H-NMR** (400 MHz): δ 10.88 (s, 1H), 10.83 (s, 1H), 8.03-8.00 (m, 2H), 7.75 (s, 2H), 7.49-7.45 (m, 4H), 7.43-7.34 (m, 6H), 7.01 (s, 1H), 6.99 (s, 1H), 6.91 (d, 1H, J=8.23 Hz), 6.84 (s, 1H), 5.05 (s, 4H), 2.41 (s, 3H), 2.38 (s, 3H). **^{13}C-NMR** (100 MHz): δ153.7, 151.8, 136.4, 134.1, 131.9, 129.9, 129.6, 129.4, 129.3, 127.9, 127.2, 125.6, 125.2, 123.3, 115.2, 114.5, 110.9, 110.2, 78.6, 22.1, 21.9. **FTIR (neat):** 3237, 1754, 1687, 1475, 1335, 1191, 1136, 1107, 1062, 800, 739, 696, 662, 618, 432 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_{16}H_{16}N_3O_3$ 298.1192, found 298.1185.

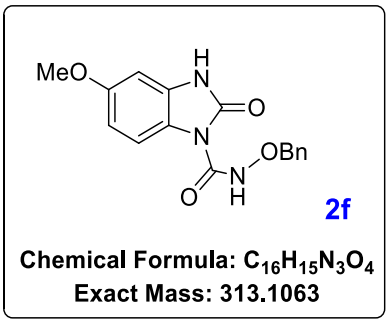
_N_-methoxy-5-methyl-2-oxo-2,3-dihydro-1_H_-benzo[_d_]imidazole-1-carboxamide _(2e)_



Chemical Formula: $C_{10}H_{11}N_3O_3$
Exact Mass: 221.0800

Prepared according to **GP2, 1e** (0.050 g, 0.186 mmol), **2e** (0.046 g, 78%). **Reaction time:** 2.2 h. **Yield:** 78%. **Nature:** White solid. **Melting Point:** 153°C. **^{1}H-NMR** (400 MHz): δ 10.91 (s, 1H), 10.86 (s, 1H), 8.4 (d, 2H, J= 15.7 Hz), 7.96 (s, 1H), 7.93 (s, 1H), 6.97-6.87 (m, 3H), 6.83 (s, 1H), 3.85 (s, 6H), 2.35 (s, 3H), 2.33 (s, 3H). **^{13}C-NMR** (100 MHz): δ153.7, 151.9, 151.8, 134.7, 133.5, 127.6, 127.5, 125.2, 124.2, 116.0, 115.3, 110.2, 109.4, 65.3, 21.9, 21.7. **FTIR (neat):** 3260, 1736, 1685, 1479, 1340, 1192, 1136, 1108, 1075, 933, 800, 708, 659 cm^{-1}. **HRMS (ESI, Q-TOF) _m/z_:** [M + H]$^+$ Calculated for $C_{10}H_{12}N_3O_3$ 222.0879, found 222.0866.

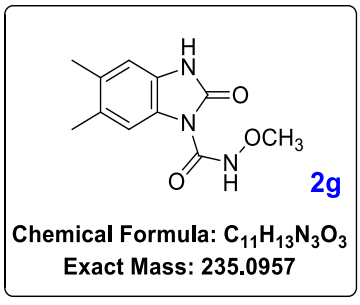
_N_-(benzyloxy)-5-methoxy-2-oxo-2,3-dihydro-1_H_-benzo[_d_]imidazole-1-carboxamide _(2f)_



Chemical Formula: $C_{16}H_{15}N_3O_4$
Exact Mass: 313.1063

Prepared according to **GP2, 1f** (0.050 g, 0.115 mmol), **2f** (0.025 g, 70%). **Reaction time:** 2.2 h. **Yield:** 70%. **Nature:** light orange solid. **Melting Point:** 205°C.**^{1}H-NMR** (400 MHz): δ 10.91 (s, 1H), 10.70 (s, 1H), 8.04 (d, 1H, J=9.37 Hz), 7.83 (d, 1H, J= 2.25 Hz), 7.49-7.45 (m, 4H), 7.43-7.30 (m, 8H), 6.92 (d, 1H, J= 8.66 Hz), 6.61 (d, 1H, J= 2.27 Hz), 5.04 (d, 4H, J=2.03 Hz), 3.84 (s, 3H), 3.81 (s, 3H).**^{13}C-NMR** (100 MHz): δ129.4, 129.0, 128.8, 128.1, 111.4, 109.9, 101.3, 79.2, 56.2. **FTIR (neat):** 3242, 2916, 1758, 1666, 1479, 1336, 1140, 1062, 741, 696, 620 cm^{-1}. **HRMS (ESI, Q-TOF) _m/z_:** [M + H]$^+$ Calculated for $C_{16}H_{16}N_3O_4$ 314.1141, found 314.1120.

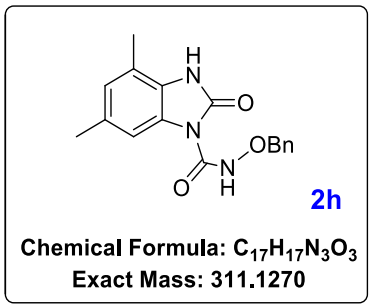
_N_-methoxy-5,6-dimethyl-2-oxo-2,3-dihydro-1_H_-benzo[_d_]imidazole-1-carboxamide _(2g)_



Chemical Formula: $C_{11}H_{13}N_3O_3$
Exact Mass: 235.0957

Prepared according to **GP2, 1g** (0.040 g, 0.098 mmol), **2g** (0.029 g, 87%). **Reaction time:** 2.2 h. **Yield:** 87%. **Nature:** White solid. **Melting Point:** 158°C. **^{1}H-NMR** (400 MHz): δ 11.48 (s, 1H), 11.16 (s, 1H), 7.73 (s, 1H), 6.89 (s, 1H), 3.77 (s, 3H), 2.26 (s, 6H). **^{13}C-NMR** (100 MHz): δ152.6, 150.7, 131.6, 129.4, 126.4, 124.8, 114.6, 110.3, 63.8, 19.5, 19.3. **FTIR (neat):** 2918, 1741, 1684, 1486, 1340, 1294, 1060, 933, 750 cm^{-1}. **HRMS (ESI, Q-TOF) _m/z_:** [M + H]$^+$ Calculated for $C_{11}H_{14}N_3O_3$ 236.1032, found 236.1032.

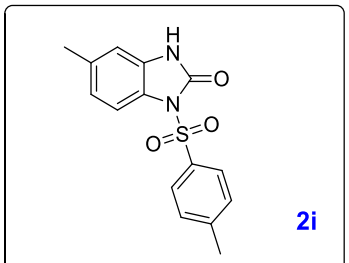
N*-(benzyloxy)-4,6-dimethyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide *(2h)



Chemical Formula: $C_{17}H_{17}N_3O_3$
Exact Mass: 311.1270

Prepared according to **GP2, 1h** (0.050 g, 0.115 mmol), **2h** (0.040 g, 59%). **Reaction time:** 2.3 h. **Yield:** 59%. **Nature:** White solid. **Melting Point:** 203°C.**^{1}H-NMR** (400 MHz): δ 10.88 (s, 1H), 8.22 (s, 1H), 7.85 (s, 1H), 7.49-7.44 (m, 2H), 7.42-7.35 (m, 3H), 6.83 (s, 1H), 5.05 (s, 2H), 2.37 (s, 3H), 2.25 (s, 3H).**^{13}C-NMR** (100 MHz): δ153.7, 151.9, 135.4, 133.4, 129.5, 129.1, 128.9, 127.2, 126.5, 124.1, 118.7, 113.6, 79.2, 21.8, 16.3. **FTIR (neat):** 2920, 1731, 1691, 1483, 1359, 1213, 1101, 1045, 738, 698 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{17}H_{18}N_3O_3$ 312.1348, found 312.1335.

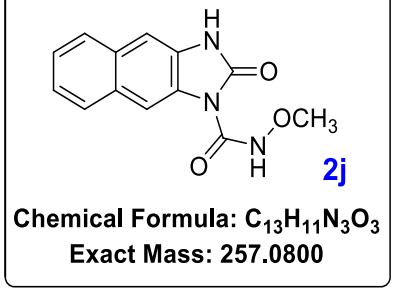
5-methyl-1-tosyl-1*H*-benzo[*d*]imidazol-2(3*H*)-one *(2i)*



Chemical Formula: $C_{15}H_{14}N_2O_3S$
Exact Mass: 302.0725

Prepared according to **GP2, 1i** (0.050 g, 0.143 mmol), **2i** (0.029 g, 68%). **Reaction time:** 2.1 h. **Yield:** 68%. **Nature:** White solid. **^{1}H-NMR** (400 MHz): δ7.91 (d, 2H, J= 8.68 Hz), 7.70 (d, 1H, J= 8.38 Hz), 7.39 (d, 2H, J= 8.21 Hz), 6.96 (d, 1H, J= 8.42 Hz), 6.83 (s, 1H), 2.41 (s, 3H), 2.34 (s, 3H).**^{13}C-NMR** (100 MHz): δ148.4, 137.0, 132.0, 129.7, 114.8, 112.3, 99.9, 22.3. **FTIR (neat):** 2918, 1696, 1600, 1403, 1356, 1172, 1028, 756, 541 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{17}H_{18}N_3O_3$ 303.0803, found 303.0784.

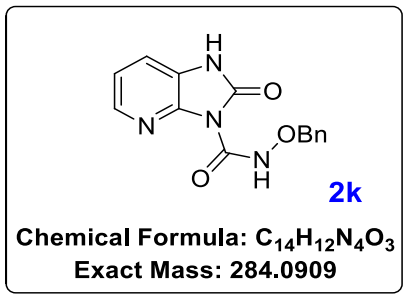
N*-methoxy-2-oxo-2,3-dihydro-1*H*-naphtho[2,3-*d*]imidazole-1-carboxamide *(2j)



Chemical Formula: $C_{13}H_{11}N_3O_3$
Exact Mass: 257.0800

Prepared according to **GP2, 1j** (0.050 g, 0.164 mmol), **2j** (0.028 g, 66%). **Reaction time:** 3.0 h. **Yield:** 66%. **Nature:** White solid. **Melting Point:** 158°C. **^{1}H-NMR** (400 MHz): δ 8.36 (s, 1H), 7.96-7.87 (m, 2H), 7.46 (s, 1H), 7.44-7.35 (m, 2H), 7.30-7.25 (m, 1H), 3.76 (s, 3H). **^{13}C-NMR** (100 MHz): δ153.9, 151.2, 130.8, 129.7, 128.5, 128.2, 127.4, 125.5, 124.7, 111.1, 105.4, 64.4. **FTIR (neat):** 3264, 1739, 1687, 1467, 1312, 1139, 1051, 854, 738, 705 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{13}H_{12}N_3O_3$ 258.0879, found 258.0860.

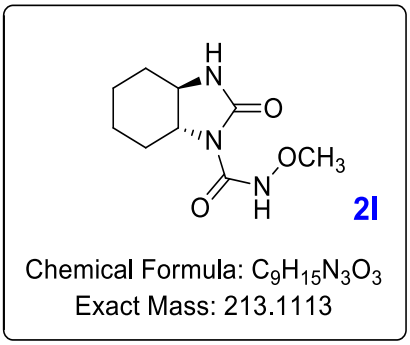
N*-(benzyloxy)-2-oxo-1*H*-imidazo[4,5-*b*]pyridine-3(2*H*)-carboxamide *(2k)



Chemical Formula: $C_{14}H_{12}N_4O_3$
Exact Mass: 284.0909

Prepared according to **GP2, 1k** (0.050 g, 0.122 mmol), **2k** (0.031 g, 44%). **Reaction time:** 4.0 h. **Yield:** 44%. **Nature:** White solid. **Melting Point:** 153°C. **^{1}H-NMR** (400 MHz): δ 10.74 (s, 1H), 8.37-8.34 (s, 1H), 8.18-8.15 (s, 1H), 7.50-7.44 (m, 2H), 7.43-7.34 (m, 4H), 7.19-7.14 (m, 1H), 5.05 (s, 2H). **^{13}C-NMR** (100 MHz): δ152.4, 151.1, 143.0, 142.9, 135.0, 129.5, 129.3, 129.0, 122.9, 122.2, 119.1, 79.4, 34.0, 24.0. **FTIR (neat):** 2916, 1736, 1711, 1615, 1477, 1352, 1247, 1176, 1134, 1078, 976, 912, 764 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_{14}H_{13}N_4O_3$ 285.0988, found 285.0977.

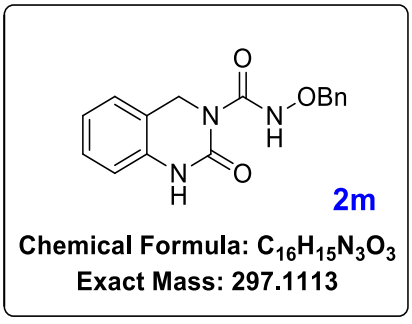
rac*-*N*-methoxy-2-oxooctahydro-1*H*-benzo[*d*]imidazole-1-carboxamide *(2l)



Chemical Formula: $C_9H_{15}N_3O_3$
Exact Mass: 213.1113

Prepared according to **GP2, 1l** (0.050 g, 0.192 mmol), **2l** (0.037 g, 61%). **Reaction time:** 3.2 h. **Yield:** 61%. **Nature:** White solid. **Melting Point:** 158°C. **^{1}H-NMR** (400 MHz): δ 10.3 (s, 1H), 4.87 (s, 1H), 3.78 (s, 3H), 3.50-3.42 (m, 1H), 3.20-3.13 (m, 1H), 2.91-2.79 (m, 1H), 2.50-1.94 (m, 1H), 1.91-1.78 (m, 2H), 1.51-1.35 (m, 4H). **^{13}C-NMR** (100 MHz): δ160.3, 155.5, 65.0, 63.6, 59.0, 29.7, 29.6, 24.4, 24.2. **FTIR (neat):** 3282, 2949, 1727, 1677, 1484, 1356, 1309, 1252, 1164, 1113, 1098, 1043, 951, 854, 618 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_9H_{16}N_3O_3$ 214.1192, found 214.1182.

N*-(benzyloxy)-2-oxo-1,2-dihydroquinazoline-3(4*H*)-carboxamide *(2m)

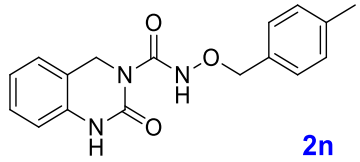


Chemical Formula: $C_{16}H_{15}N_3O_3$
Exact Mass: 297.1113

Prepared according to **GP2, 1m** (0.050 g, 0.118 mmol), **2m** (0.042 g, 60%). **Reaction time:** 2.3 h. **Yield:** 60%. **Nature:** White solid. **Melting Point:** 168°C. **^{1}H-NMR** (400 MHz): δ 11.01 (s, 1H), 7.45-7.28 (m, 5H), 7.25-7.17 (m, 2H), 7.06 (t, 1H), 6.89 (s, 1H), 6.70 (d, 1H, J= 7.97 Hz), 4.98 (s, 2H), 4.95 (s, 2H).**^{13}C-NMR** (100 MHz): δ155.2, 153.7, 135.7, 135.1, 129.4, 128.9, 128.8, 126.5, 124.0, 118.6, 113.9, 78.8, 44.9. **FTIR**

(neat): 2921, 1679, 1602, 1456, 1326, 1223, 1145, 1103, 1027, 746, 726, 695, 597 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{16}H_{16}N_3O_3$ 298.1192, found 298.1188.

_N_-((4-methylbenzyl)oxy)-2-oxo-1,2-dihydroquinazoline-3(4*H*)-carboxamide *(2n)*

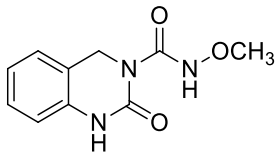


2n

Chemical Formula: $C_{17}H_{17}N_3O_3$
Exact Mass: 311.1270

Prepared according to **GP2, 1n** (0.050 g, 0.111 mmol), **2n** (0.042 g, 59%). **Reaction time:** 2.3 h. **Yield:** 59%. **Nature:** White solid. **Melting Point:** 152°C**. ^{1}H-NMR** (400 MHz): δ 10.99 (s, 1H), 7.32 (d, 2H, J=7.70 Hz), 7.24-7.15 (m, 4H), 7.08-7.03 (m, 2H), 6.69 (d, 1H, J= 8.34 Hz), 4.98 (s, 2H),4.91 (s, 2H), 2.34 (s, 3H).**^{13}C-NMR** (100 MHz): δ155.1, 153.8, 138.8, 135.1, 132.7, 129.58, 129.53, 128.9, 126.5, 124.0, 118.6, 113.9, 78.7, 44.9, 24.0. **FTIR (neat):** 3214, 1707, 1602, 1474, 1419, 1326, 1202, 1130, 1099, 1039, 803, 744, 610 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{17}H_{18}N_3O_3$ 312.1348, found 312.1335.

_N_-methoxy-2-oxo-1,2-dihydroquinazoline-3(4*H*)-carboxamide *(2o)*

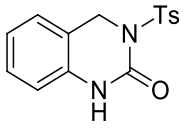


2o

Chemical Formula: $C_{10}H_{11}N_3O_3$
Exact Mass: 221.0800

Prepared according to **GP2, 1o** (0.050 g, 0.186 mmol), **2o** (0.034 g, 57%). **Reaction time:** 2.2 h. **Yield:** 57%. **Nature:** White solid. **Melting Point:** 159°C. **^{1}H-NMR** (400 MHz): δ 11.10 (s, 1H), 7.32-7.26 (m, 1H), 7.25-7.17 (m, 2H), 7.06 (t, 1H), 6.76 (d, 1H, J= 8.25 Hz), 4.98 (s, 2H), 3.81 (s, 3H).**^{13}C-NMR** (100 MHz): δ155.3, 153.9, 135.1, 128.9, 126.5, 124.0, 118.6, 114.0, 64.9, 44.9. **FTIR (neat):** 3221, 2923, 1709, 1672, 1601, 1401, 1308, 1252, 1220, 1143, 1099, 943, 872, 758, 581 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{10}H_{12}N_3O_3$ 222.0879, found 222.0865.

3-tosyl-3,4-dihydroquinazolin-2(1*H*)-one *(2p)*



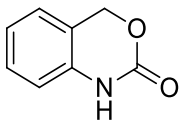
2p

Chemical Formula: $C_{15}H_{14}N_2O_3S$
Exact Mass: 302.0725

Prepared according to **GP2, 1p** (0.050 g, 0.143 mmol), **2p** (0.041 g, 95%). **Reaction time:** 0.5 h. **Yield:** 95%. **Nature:** White solid. **Melting Point:** 152°C**. ^{1}H-NMR** (400 MHz): δ 7.96 (d, 2H, J= 8.54 Hz), 7.33 (d, 2H, J= 8.24 Hz), 7.24-7.17 (m, 3H), 7.05 (t, 1H, J= 7.58 Hz), 6.69 (d, 1H, J= 7.90 Hz), 5.00 (s, 2H), 2.43 (s, 3H).**^{13}C-NMR** (100 MHz):

δ145.0, 135.7, 135.3, 129.5, 128.9, 128.7, 126.1, 123.5, 118.3, 114.1, 47.07, 21.7. **FTIR (neat):** 3102, 1717, 1604, 1499, 1466, 1413, 1295, 1262, 1056, 760 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{15}H_{14}N_2O_3S$ 303.0803, found 303.0799.

1H-benzo[d][1,3]oxazin-2(4*H*)-one *(2q)*

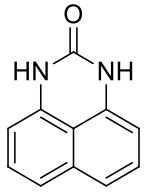


2q

Chemical Formula: $C_8H_7NO_2$
Exact Mass: 149.0477

Prepared according to **GP2, 1q** (0.050 g, 0.255 mmol), **2q** (0.034 g, 89%). **Reaction time:** 1.0 h. **Yield:** 89%. **Nature:** White solid. **Melting Point:** 152°C**.** **^{1}H-NMR** (400 MHz): δ 7.33-7.27 (m, 1H), 7.16-7.04 (m, 2H), 6.78 (d, 1H, J= 7.88 Hz), 5.31 (s, 2H).**^{13}C-NMR** (100 MHz): δ129.3, 124.4, 123.5, 113.8, 68.7. **FTIR (neat):** 2922, 1696, 1600, 1499, 1455, 1355, 1214, 1170, 1027, 961 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_8H_8NO_2$ 150.0555, found 150.0550.

1*H*-perimidin-2(3*H*)-one *(2r')*



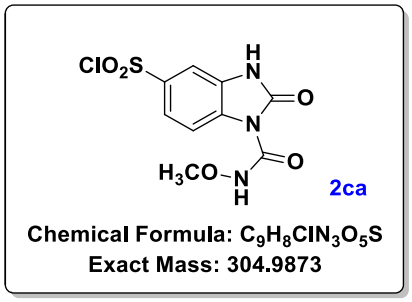
2r'

Chemical Formula: $C_{11}H_8N_2O$
Exact Mass: 184.0637

Prepared according to **GP2, 1r** (0.050 g, 0.164 mmol), **2r** (0.047 g, 57%). **Reaction time:** 2.3 h. **Yield:** 57%. **Nature:** White solid. **Melting Point:** 295°C. **^{1}H-NMR** (400 MHz): δ 10.0 (s, 2H), 7.20 (t, 2H), 7.10 (d, 2H, J= 7.89 Hz), 6.50 (d, 2H, J= 7.89Hz). **^{13}C-NMR** (100 MHz): δ150.9, 138.5, 135.0, 128.8, 118.4, 114.5, 104.8, 80.1, 79.8, 79.4. **FTIR (neat):** 3229, 1714, 1665, 1611, 1470, 1379, 1265, 1166, 1094, 988, 814, 771, 754, 531, 456 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** $[M + H]^+$ Calculated for $C_{11}H_9N_2O$ 185.0715, found 185.0705.

iii) Characterization data of derivatives

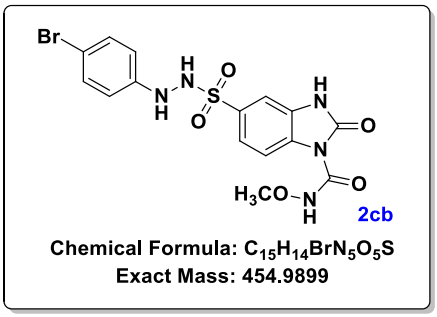
1-(Methoxycarbamoyl)-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-sulfonyl chloride *(2ca)*



Chemical Formula: $C_9H_8ClN_3O_5S$
Exact Mass: 304.9873

Prepared according to **7**, **2c** (0.050 g, 0.24 mmol), **ClSO$_2$OH** (0.5 ml), **2ca** (0.040 g, 55%). **Reaction time:** 18 h. **Yield:** 55%. **Nature:** light orange solid. **Melting Point:** 298°C. **^{1}H-NMR** (400 MHz): δ 11.69 (s, 1H), 11.16 (s, 1H), 8.18 (s, 1H), 7.44 (d, 1H, J= 8.45 Hz), 6.98 (d, 1H, J= 8.79 Hz). **^{13}C-NMR** (100 MHz): δ153.8, 151.5, 129.3, 126.7, 122.2, 112.3, 109.0, 64.7. **FTIR (neat):** 3270, 1649, 1564, 1379, 1094, 772 cm^{-1}. **HRMS (ESI, Q-TOF) *m/z*:** [M + H]$^+$ Calculated for $C_9H_9N_3O_5SCl$ 305.9951, found 305.9935.

5-((2-(4-Bromophenyl)hydrazinyl)sulfonyl)-*N*-methoxy-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-1-carboxamide *(2cb)*



Chemical Formula: $C_{15}H_{14}BrN_5O_5S$
Exact Mass: 454.9899

Prepared according to **7**, **2ca** (0.040 g, 0.31 mmol), **B** (0.134 g, 0.63 mmol), **2cb** (0.049 g, 84%). **Reaction time:** 12 h. **Yield:** 57%. **Nature:** light yellow solid. **Melting Point:** 350°C. **^{1}H-NMR** (400 MHz): δ 11.22 (s, 1H), 9.54 (s, 1H), 8.35 (s, 1H), 7.73 (s, 1H), 7.62 (d, 1H, J= 7.98 Hz), 7.22 (d, 3H, J= 8.36 Hz), 6.73 (d, 2H, J= 9.71 Hz), 3.75 (s, 3H). **HRMS (ESI, Q-TOF) *m/z*:** [M - H]$^-$ Calculated for $C_{15}H_{13}N_5O_5SBr$ 453.9821, found 453.9819.

11) Single-crystal X-Ray data of 2m and 2a

For the determination of X-ray crystal structures of **2a** and **2m** 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[5] was used. Absorption correction was done applying SADABS program.[6] The crystal structure was solved by SIR 92[7] and refined by full matrix least square method using SHELXL-97[8] WinGX system, Ver 1.70.01.[9] 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**: 2a: CCDC 1983427 and 2m: CCDC 1965927**.[10]

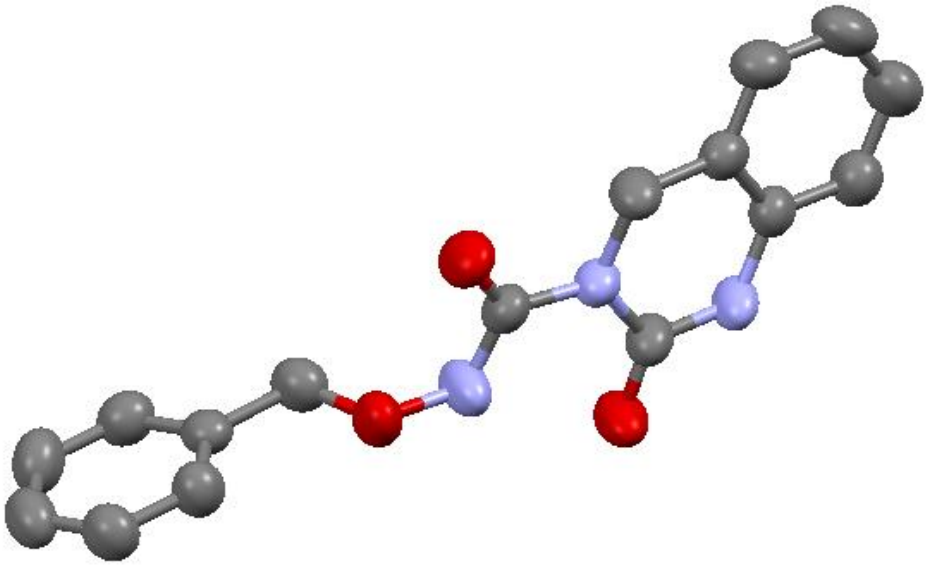


Figure S3: X-ray crystal structure of **2m**

CCDC No.	CCDC 1965927
Formula	C16 H15 N3 O3
Formula weight	297.31
Crystal System	Monoclinic
Space group	P21/c
a, b, c (Å)	10.300(5) 13.359(5) 10.747(5)
α, β, γ (°)	90 103.880(5) 90
V (Å^3)	1435.6(11)
Z	4
Calculated Density (g/cm^3)	1.376

Absorption coefficient (mm^{-1})	0.097
F(000)	624
Crystal Size (mm^3)	0.20 x 0.32 x 0.40
Theta range for data collection:	2.5^o to 27.3°
Data set	-13: 13 ; -17: 17 ; -13: 11
Reflection	19165
Independent refl.	[R(int) = 0.086]
data [$I > 2\sigma(I)$]	1859
R indices (all data)	$R = 0.0520$, $wR_2 = 0.1679$
S	1.03
Min. and Max. Resd. Dens. ($e/Å^3$)	-0.15 and 0.22

Table S2: Selected bond lengths [Å] of 2m

Atoms	Bond lengths [Å]	Atoms	Bond lengths [Å]
O001-C9	1.215(3)	C11-C16	1.386(4)
O002-N03	1.396(3)	C11-C12	1.380(3)
O002-C10	1.424(3)	C12-C13	1.374(3)
N02-C7	1.475(3)	C13-C14	1.382(3)
N02-C8	1.390(3)	C14-C15	1.367(3)
N02-C9	1.406(3)	C15-C16	1.368(4)
N01-C1	1.397(3)	C2-H2	0.9300
N01-C8	1.350(3)	C3-H3	0.9300
N03-C9	1.330(3)	C4-H4	0.9300
C1-C2	1.387(3)	C5-H5	0.9300
C1-C6	1.382(3)	C7-H7A	0.9700
C2-C3	1.379(4)	C7-H7B	0.9700
N01-H01	0.8600	C10-H10A	0.9700
C3-C4	1.380(4)	C10-H10B	0.9700
N03-H03	0.8600	C11-H11	0.9300
C4-C5	1.380(3)	C13-H13	0.9300
C5-C6	1.382(3)	C14-H14	0.9300
C6-C7	1.494(3)	C15-H15	0.9300
C10-C12	1.497(3)	C16-H16	0.9300

Table S3: Selected bond angles [º] of 2m

Atoms	Bond angles[º]	Atoms	Bond angles[º]
N03-O002-C10	108.98(16)	C12-C11-C16	120.3(2)
C7-N02 -C8	123.28(17)	C10-C12-C11	122.99(19)
C7-N02-C9	113.13(15)	C10-C12-C13	118.60(18)
C8-N02-C9	123.37(17)	C11-C12-C13	118.41(19)
C1-N01-C8	126.44(17)	C12-C13-C14	121.13(19)
O002-N03-C9	117.57(18)	C13-C14-C15	120.1(2)
N01-C1-C2	120.85(19)	C14-C15-C16	119.6(2)
N01-C1-C6	118.20(18)	C11-C16-C15	120.5(2)
C2-C1-C6	120.95(19)	C1-C2-H2	120.00
C1-C2-C3	119.5(2)	C3-C2-H2	120.00
C1-N01-H01	117.00	C2-C3-H3	120.00
C8-N01-H01	117.00	C4-C3-H3	120.00
C2-C3-C4	120.2(2)	C3-C4-H4	120.00
O002-N03-H03	121.00	C5-C4-H4	120.00
C9-N03-H03	121.00	C4-C5-H5	120.00
C3-C4-C5	119.8(3)	C6-C5-H5	120.00
C4-C5-C6	121.0(2)	N02-C7-H7A	109.00
C1-C6-C7	120.48(18)	N02-C7-H7B	109.00
C5-C6-C7	120.83(19)	C6-C7-H7A	109.00
C1-C6-C5	118.65(19)	C6-C7-H7B	109.00
N02-C7-C6	113.41(16)	H7A-C7-H7B	108.00
N02-C8-N01	116.24(18)	O002-C10-H10A	110.00
O003-C8-N02	123.41(19)	O002-C10-H10B	110.00
O003-C8 -N01	120.35(19)	C12-C10-H10A	110.00
O001-C9-N03	123.3(2)	C12-C10-H10B	110.00
N02-C9-N03	116.68(18)	H10A-C10-H10B	108.00
O001-C9-N02	119.99(19)	C12-C11-H11	120.00
O002-C10-C12	110.14(17)	C16-C11-H11	120.00
C12-C13-H13	119.00	C14-C15-H15	120.00
C14-C13-H13	119.00	C16-C15-H15	120.00
C13-C14-H14	120.00	C11-C16-H16	120.00
C15-C14-H14	120.00	C15-C16-H16	120.00

Table S4: Selected hydrogen bonding geometry [Å, º] for a compound 2m

D--H.. A	D..H	H..A	D..A	D--H..A
N01 - H01 . O001	0.8600	1.9800	2.839(3)	173.00

N03 - H03 . O003	0.8600	1.9000	2.545(3)	131.00
C11 - H11 . O002	0.9300	2.4200	2.751(3)	101.00

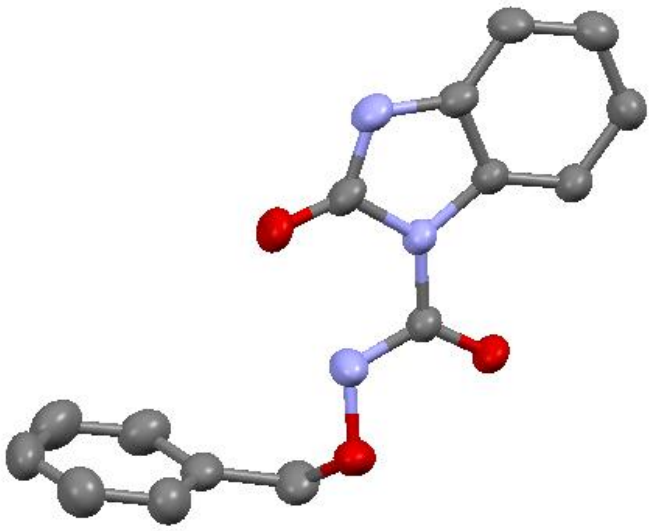


Figure S4: X-ray crystal structure of **2a**

CCDC No.	CCDC 1983427
Formula	C15 H13 N3 O3
Formula weight	283.28
Crystal System	Triclinic
Space group	P1 (No. 1)
a, b, c (Å)	5.0971(6) 5.3649(7) 12.3429(16)
α, β, γ (°)	99.966(5) 96.111(4) 90.897(4)
V ($Å^3$)	330.34(7)
Z	1
Calculated Density (g/cm^3)	1.424
Absorption coefficient (mm^{-1})	0.102
F(000)	148
Crystal Size (mm^3)	0.27 x 0.28 x 0.30
Theta range for data collection:	3.4^o to 29.6°
Data set	-7: 7 ; -7: 7 ; -17: 17

Reflection	4129
Independent refl.	[R(int) = 0.061]
data [I > 2σ(I)]	2328
R indices (all data)	R = 0.0722, wR_2 = 0.2059
S	1.07
Min. and Max. Resd. Dens. (e/Å^3)	-0.64 and 0.57

Table S5: Selected bond lengths [Å] of 2a

Atoms	Bond lengths [Å]	Atoms	Bond lengths [Å]
O1-C2	1.212(5)	C6-C9	1.368(6)
O2-N1	1.400(5)	C7-C8	1.404(7)
O2-C5	1.449(6)	C8-C9	1.396(7)
O3-C14	1.229(6)	C10-C11	1.392(10)
N1-C2	1.338(5)	C11-C13	1.375(9)
N2-C2	1.410(5)	C12-C15	1.390(8)
N2-C6	1.416(5)	C12-C13	1.359(9)
N2-C14	1.413(6)	C1-H1A	0.9300
N3-C4	1.379(6)	C5-H5A	0.9700
N3-C14	1.356(6)	C5-H5B	0.9700
C1-C4	1.394(6)	C7-H7	0.9300
C1-C7	1.379(7)	C8-H8	0.9300
N1-H1	0.8600	C9-H9	0.9300
C3-C5	1.502(7)	C10-H10	0.9300
C3-C15	1.386(8)	C11-H11	0.9300
C3-C10	1.393(7)	C12-H12	0.9300
N3-H3	0.8600	C13-H13	0.9300
C4-C6	1.398(5)	C15-H15	0.9300

Table S6: Selected bond angles [º] of 2a

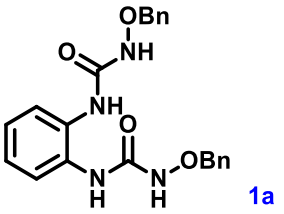
Atoms	Bond angles[º]	Atoms	Bond angles[º]
N1-O2-C5	109.1(3)	C10-C11-C13	120.4(6)
O2-N1-C2	115.1(4)	C13-C12-C15	119.8(6)
C2-N2-C6	124.4(3)	C11-C13-C12	120.3(6)
C2-N2-C14	126.2(3)	O3-C14-N3	128.7(4)
C6-N2-C14	109.4(3)	N2-C14-N3	105.5(4)
C4-N3-C14	111.5(4)	O3-C14-N2	125.8(4)
C4-C1-C7	117.5(4)	C3-C15-C12	121.4(5)
C2-N1-H1	122.00	C4-C1-H1A	121.00
O2-N1-H1	123.00	C7-C1-H1A	121.00

O1-C2-N2	121.5(4)	O2-C5-H5A	109.00
O1-C2-N1	125.0(4)	O2-C5-H5B	109.00
N1-C2-N2	113.5(3)	C3-C5-H5A	109.00
C5-C3-C15	120.9(4)	C3-C5-H5B	109.00
C10-C3-C15	118.0(5)	H5A-C5-H5B	108.00
C5-C3-C10	121.1(5)	C1-C7-H7	119.00
C4-N3-H3	124.00	C8-C7-H7	119.00
C14-N3-H3	124.00	C7-C8-H8	120.00
N3-C4-C6	108.1(4)	C9-C8-H8	120.00
C1-C4-C6	120.8(4)	C6-C9-H9	121.00
N3-C4-C1	131.1(4)	C8-C9-H9	121.00
O2-C5-C3	112.7(4)	C3-C10-H10	120.00
C4-C6-C9	121.9(4)	C11-C10-H10	120.00
N2-C6-C4	105.5(3)	C10-C11-H11	120.00
N2-C6-C9	132.6(3)	C13-C11-H11	120.00
C1-C7-C8	121.5(4)	C13-C12-H12	120.00
C7-C8-C9	120.6(5)	C15-C12-H12	120.00
C6-C9-C8	117.7(4)	C11-C13-H13	120.00
C3-C10-C11	120.1(5)	C12-C13-H13	120.00
C3-C15-H15	119.00	C12-C15-H15	120.00

Table S7: Selected hydrogen bonding geometry [Å, º] for a compound 2a

D--H.. A	**D..H**	**H..A**	**D..A**	**D--H..A**
N1 -- H1 .. O3	0.8600	1.9800	2.632(5)	132.00
N3 -- H3 .. O1	0.8600	2.1700	2.911(5)	144.00
N3 -- H3 .. O2	0.8600	2.4700	3.215(5)	146.00
C5 -- H5A .. O3	0.9700	2.5500	3.322(6)	137.00
C9 -- H9 .. O1	0.9300	2.4100	2.929(6)	115.00

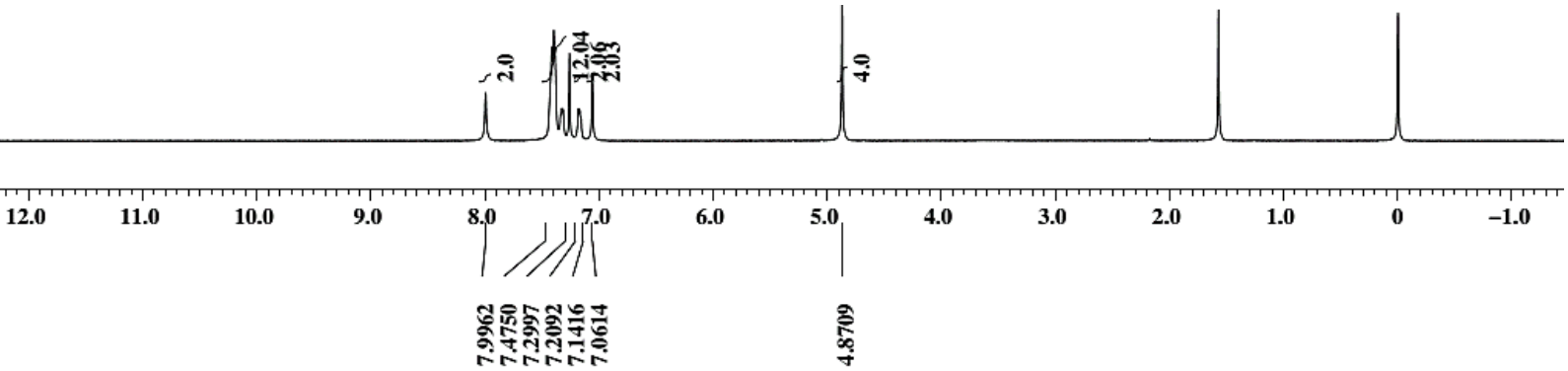
12) NMR, FTIR and HRMS of the compounds



1a

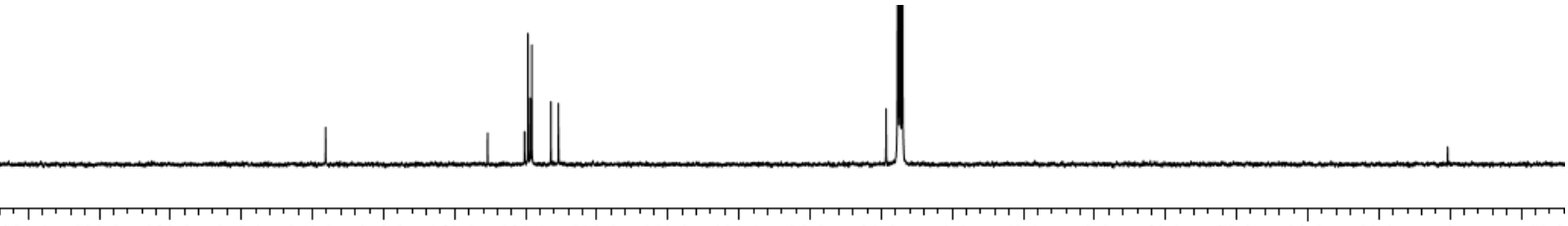
Chemical Formula: $C_{22}H_{22}N_4O_4$
Exact Mass: 406.1641

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



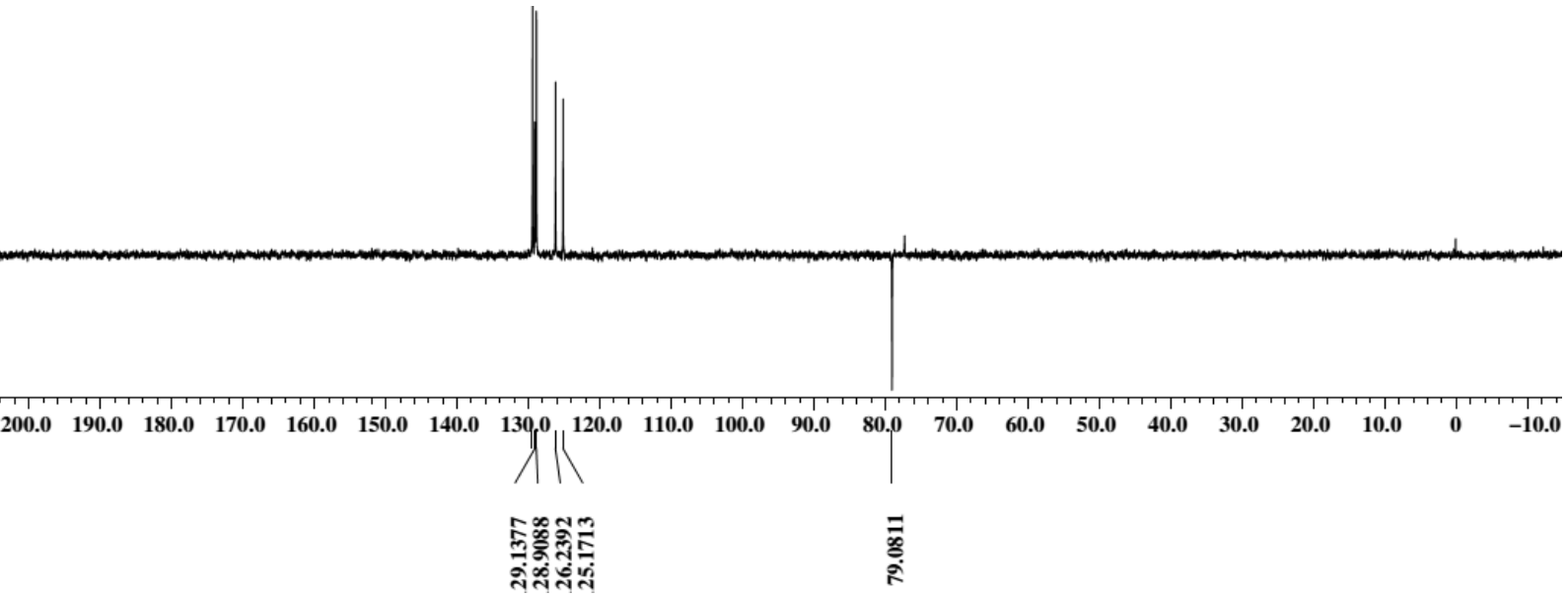
7.9962
7.4750
7.2997
7.2092
7.1416
7.0614
4.8709

^{13}C-NMR ($CDCl_3$, 100 MHz) of 1a



158.1607
130.1862
129.7095
129.3853
129.1565
126.4868
125.4189
79.3383

^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1a



HRMS of 1a

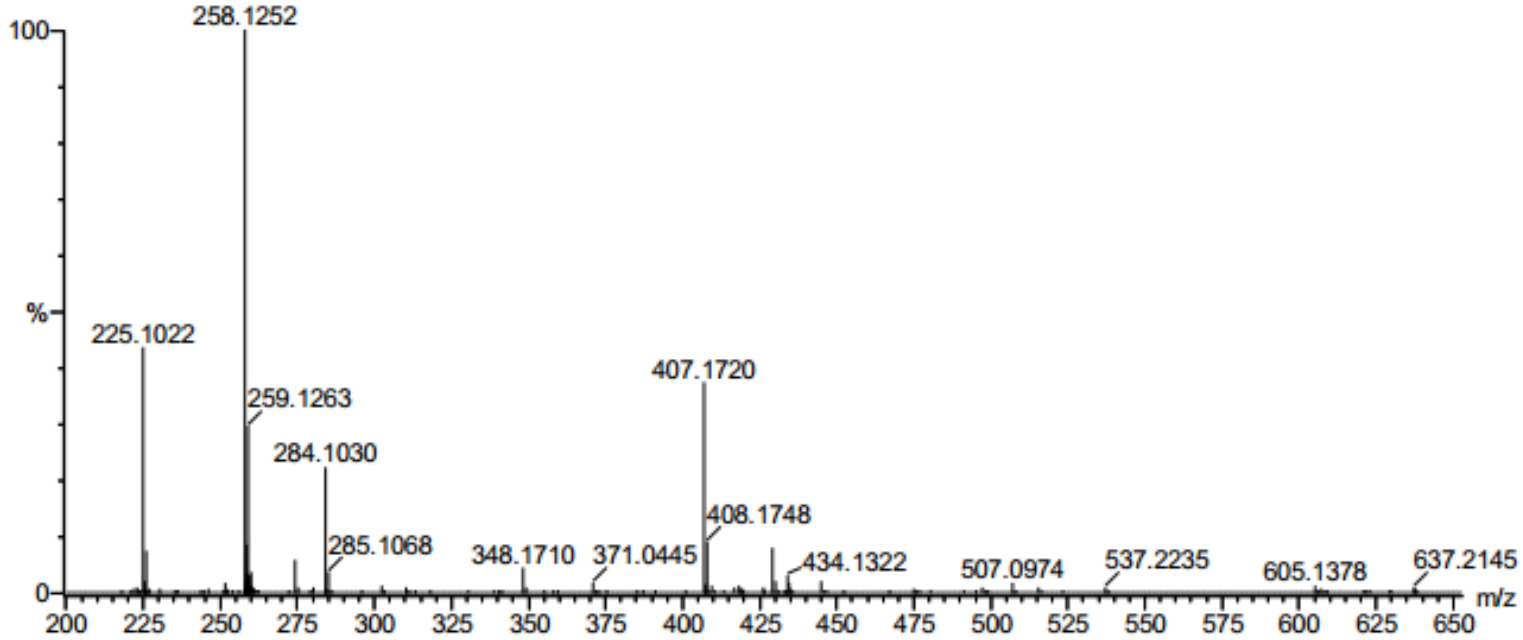
Elemental Composition Report

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 = 3

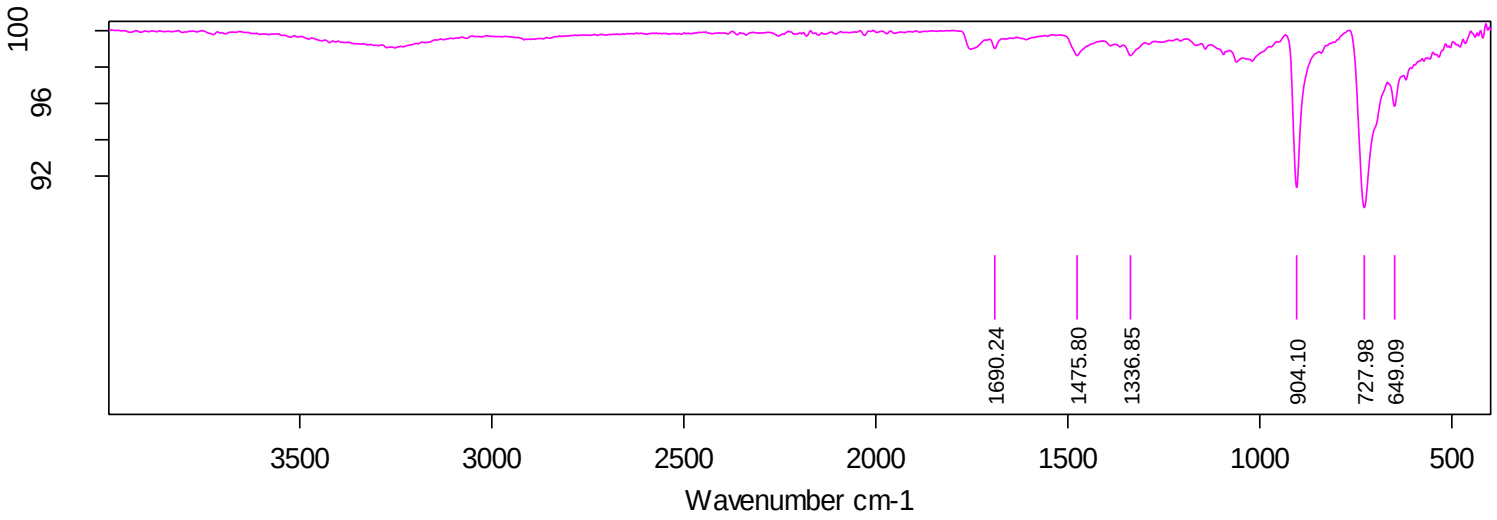
Monoisotopic Mass, Even Electron Ions
101 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-25 H: 5-25 N: 0-5 O: 1-4 Cu: 0-2

Sample Name : 18-01-281 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
280819-18-01-281- 17 (0.174) AM2 (Ar,22000.0,0.00,0.00); Cm (17:20) 1: TOF MS ES+
3.77e+007



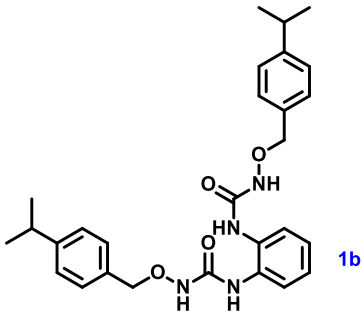
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
407.1720	407.1719	0.1	0.2	13.5	699.5	n/a	n/a	C22 H23 N4 O4

FTIR of 1a



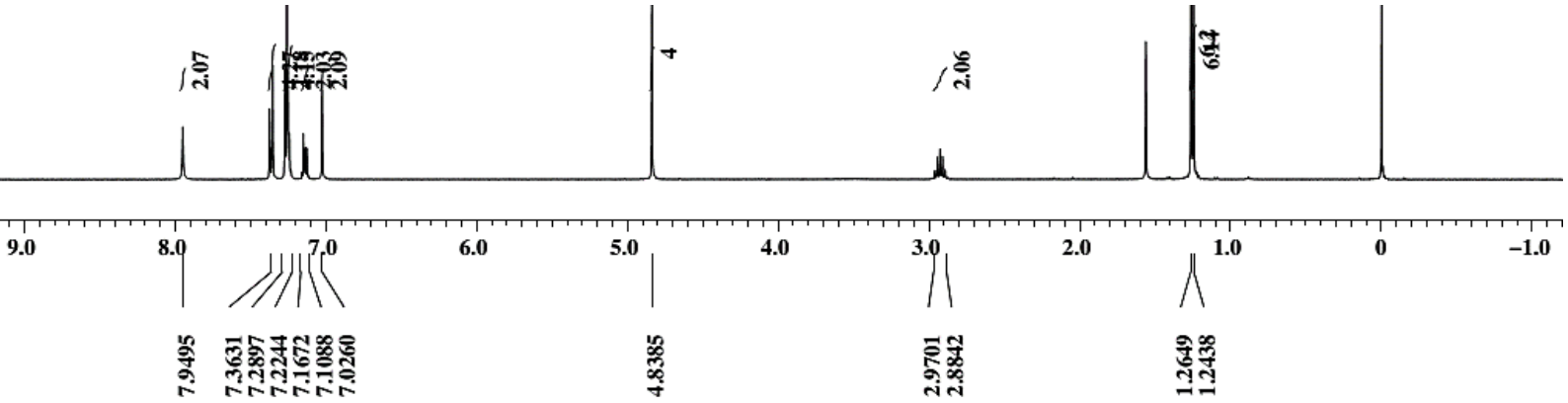
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-397.0	18-01-397	Instrument type and / or accessory	2/4/2020

Wavenumber cm-1	Transmittance [%]
3997.524564	1.000340
3996.095345	1.000353
3994.666126	1.000359
3993.236908	1.000347
3991.807689	1.000322
3990.378470	1.000295
3988.949252	1.000278
3987.520033	1.000269
3986.090814	1.000252
3984.661596	1.000214
3983.232377	1.000163
3981.803159	1.000119
3980.373940	1.000098
3978.944721	1.000101
3977.515503	1.000117
3976.086284	1.000137
3974.657065	1.000155
3973.227847	1.000163
3971.798628	1.000150
3970.369409	1.000108
3968.940191	1.000043

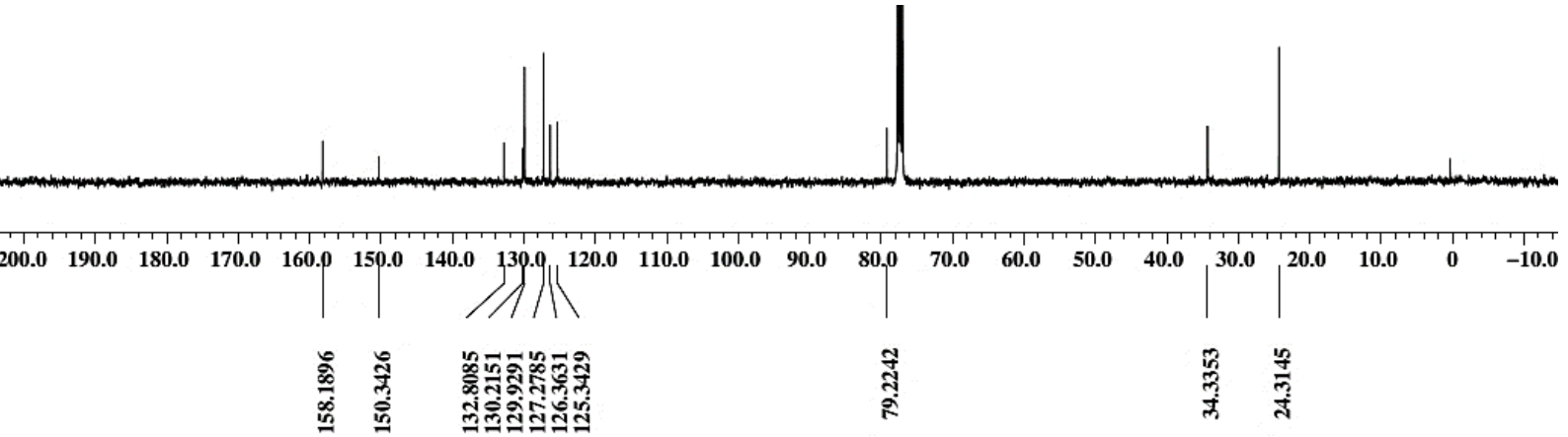


Chemical Formula: $C_{28}H_{34}N_4O_4$
Exact Mass: 490.2580

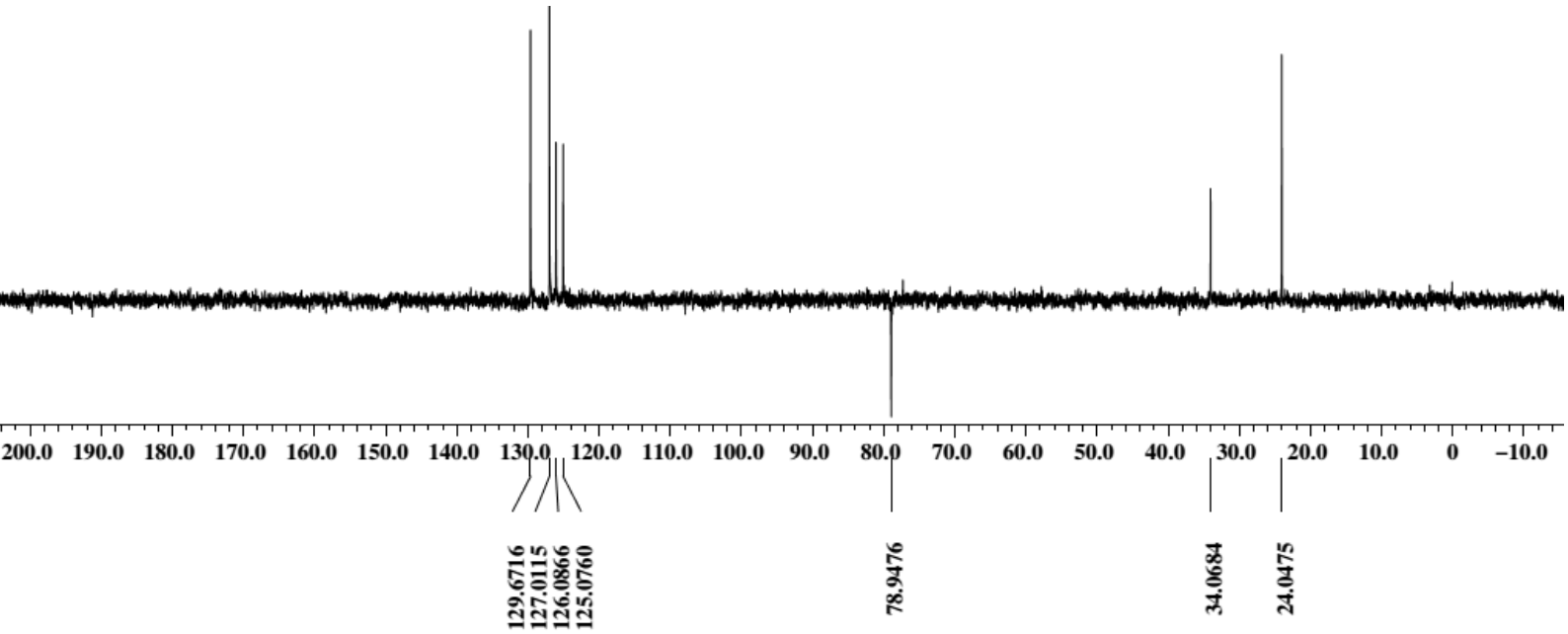
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1b



^{13}C-NMR ($CDCl_3$, 100 MHz) of 1b



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1b



HRMS of 1b

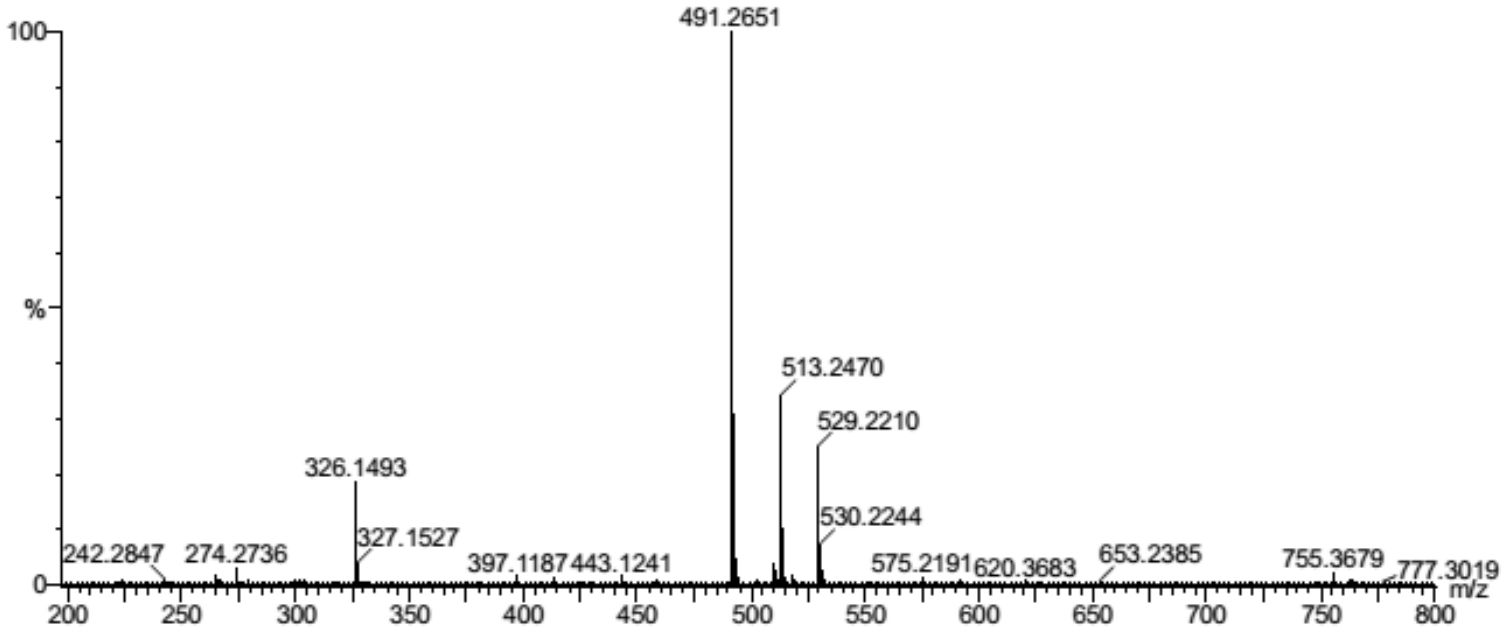
Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

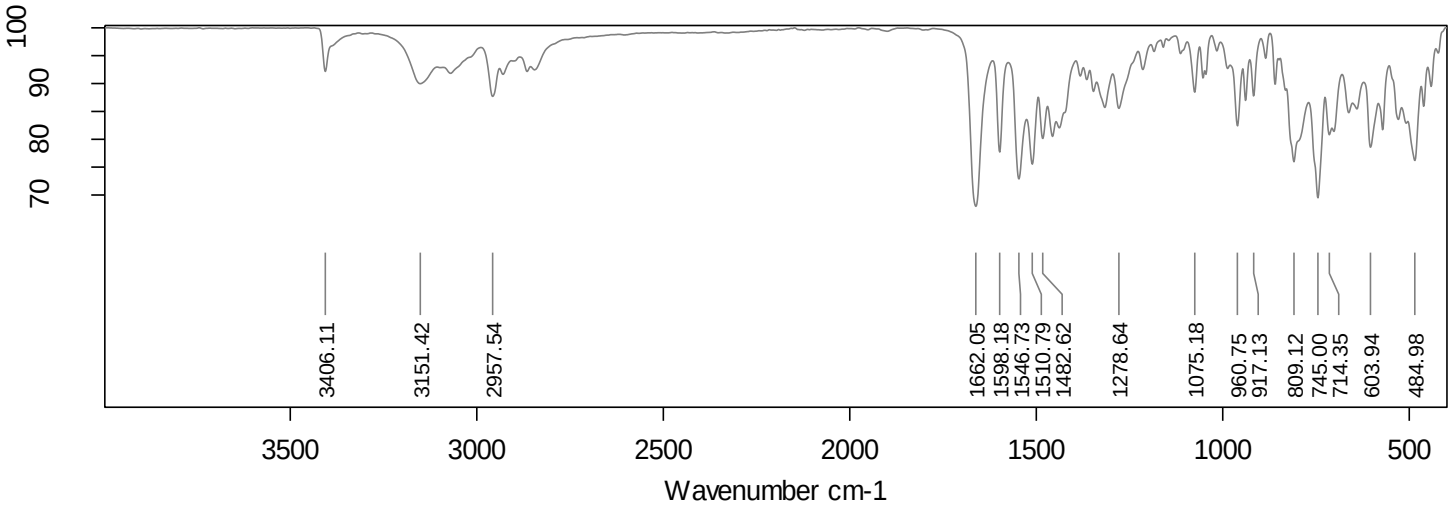
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 11-35 N: 0-5 O: 1-4

Sample Name : 18-01-339 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
051119-18-01-339 18 (0.183) AM2 (Ar,22000.0,0.00,0.00); Cm (18:20) 1: TOF MS ES+
1.17e+007



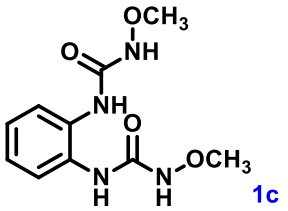
Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
491.2651	491.2658	-0.7	-1.4	13.5	620.2	n/a	n/a	C28 H35 N4 O4

FTIR of 1b



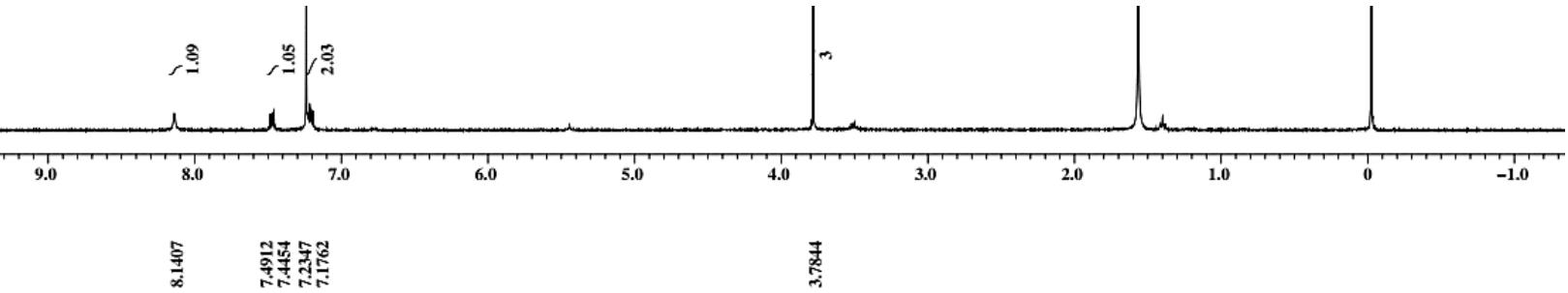
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-339.0	18-01-339	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	0.999675
3996.073013	0.999782
3994.643803	0.999879
3993.214592	0.999953
3991.785381	0.999994
3990.356171	1.000000
3988.926960	0.999974
3987.497749	0.999926
3986.068539	0.999868
3984.639328	0.999810
3983.210117	0.999758
3981.780907	0.999713
3980.351696	0.999672
3978.922485	0.999637
3977.493275	0.999612
3976.064064	0.999599
3974.634853	0.999588
3973.205643	0.999568
3971.776432	0.999532
3970.347221	0.999489
3968.918011	0.999453



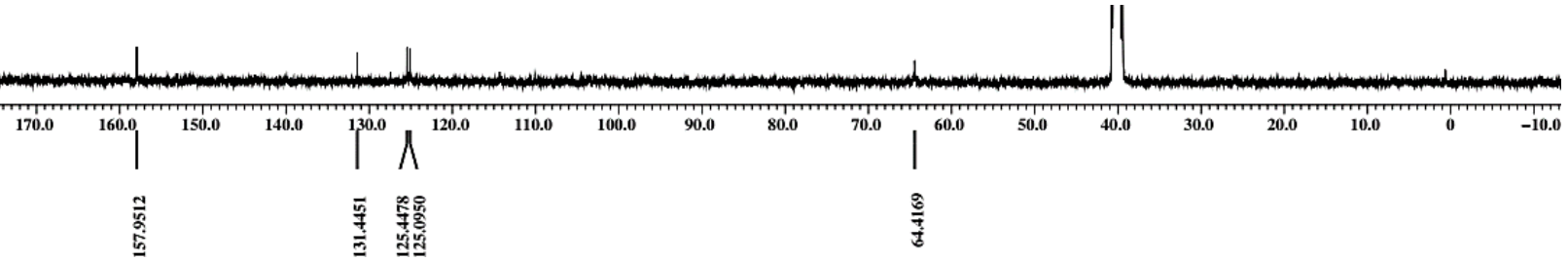
Chemical Formula: $C_{10}H_{14}N_4O_4$
Exact Mass: 254.1015

1H-NMR ($CDCl_3$, 400 MHz) of 1c



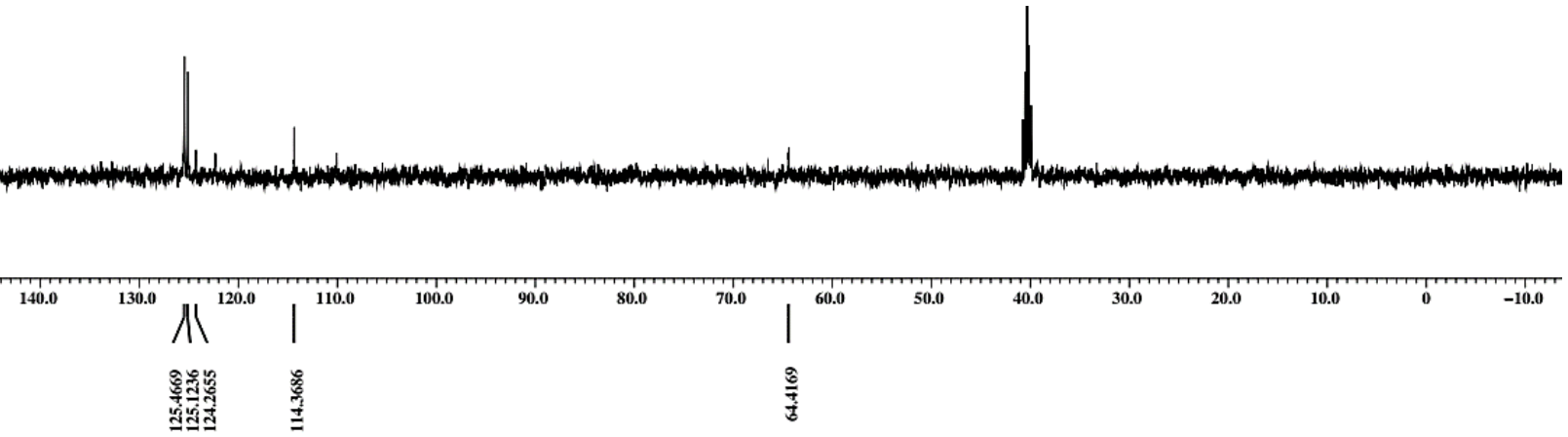
8.1407
7.4912
7.4454
7.2347
7.1762
3.7844

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



157.9512
131.4451
125.4478
125.0950
64.4169

^{13}C-DEPT (DMSO-d6, 100 MHz) of 1c



HRMS of 1c

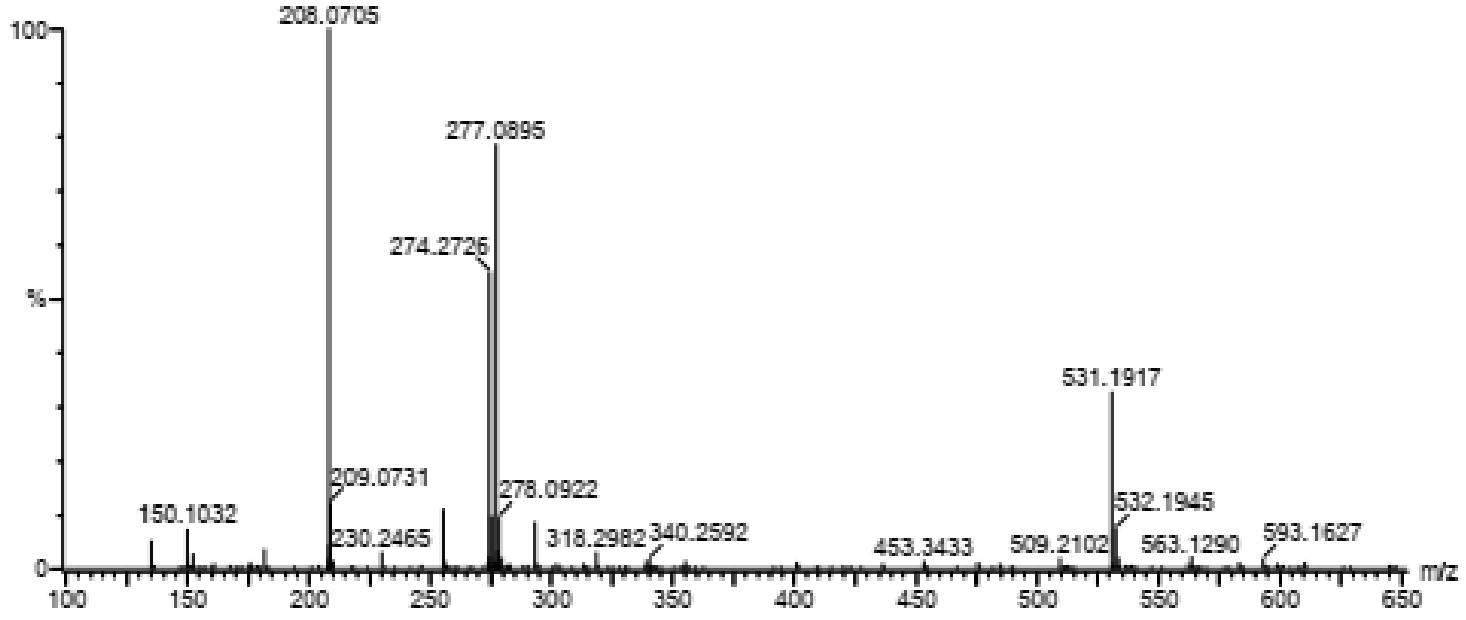
Elemental Composition Report

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 = 3

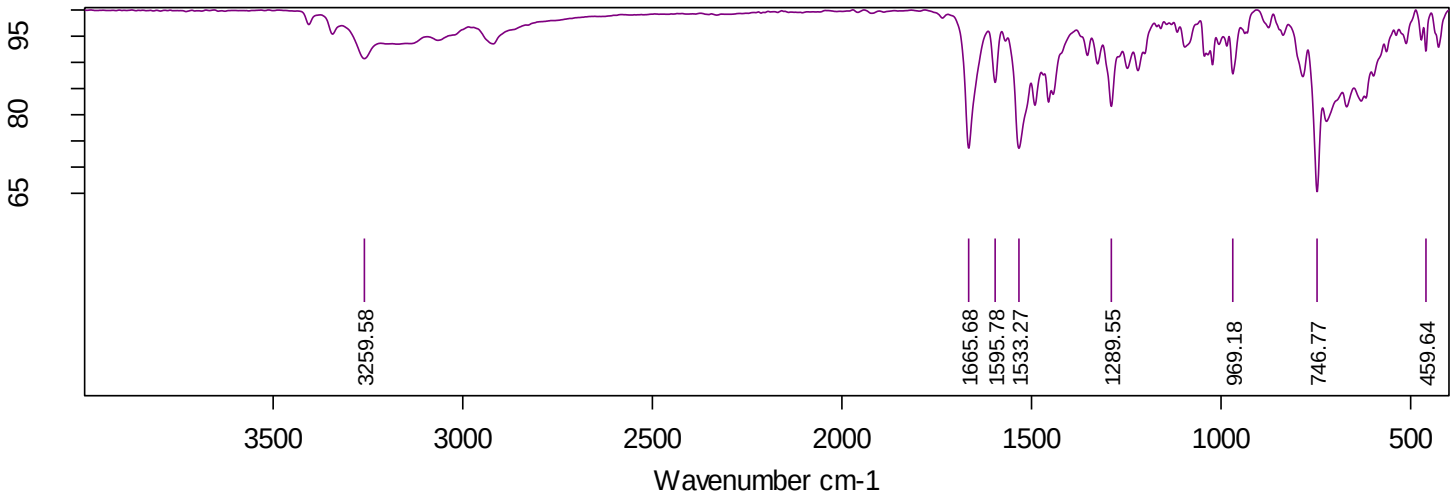
Monoisotopic Mass, Even Electron Ions
99 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 7-30 N: 0-4 O: 1-5 Na: 0-1

Sample Name : 18-01-367 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
281119-18-01-367- 17 (0.174) AM2 (Ar,22000.0,0.00,0.00); Cm (17:20) 1: TOF MS ES+
2.21e+007



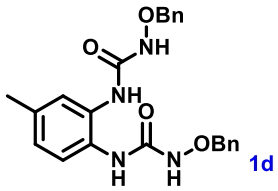
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
277.0895	277.0913	-1.8	-6.5	5.5	891.9	n/a	n/a	C10 H14 N4 O4 Na

FTIR of 1c



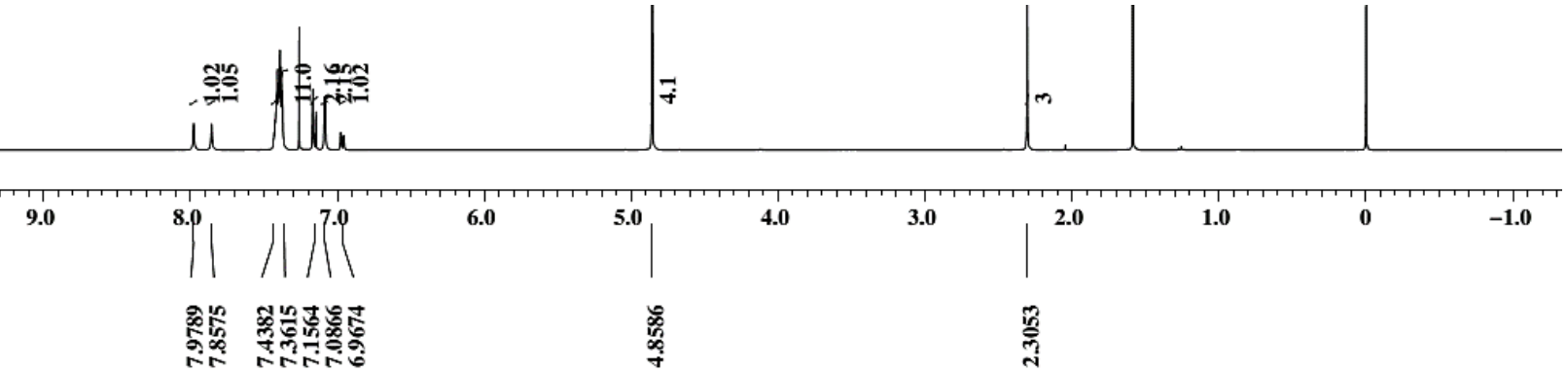
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-303.0	18-01-303	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	0.999918
3996.073013	0.999762
3994.643803	0.999611
3993.214592	0.999482
3991.785381	0.999403
3990.356171	0.999396
3988.926960	0.999459
3987.497749	0.999572
3986.068539	0.999705
3984.639328	0.999833
3983.210117	0.999936
3981.780907	0.999997
3980.351696	1.000000
3978.922485	0.999939
3977.493275	0.999820
3976.064064	0.999660
3974.634853	0.999489
3973.205643	0.999335
3971.776432	0.999217
3970.347221	0.999138
3968.918011	0.999096

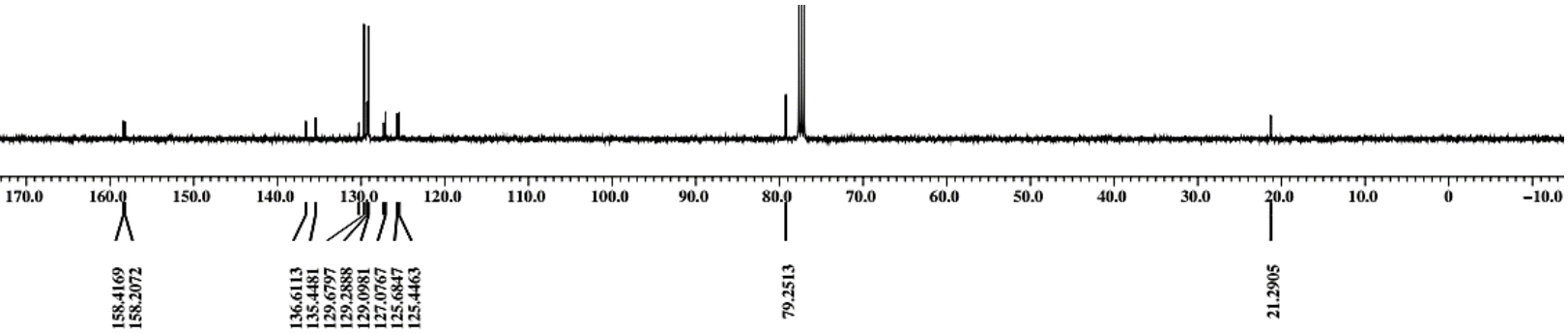


Chemical Formula: $C_{23}H_{24}N_4O_4$
Exact Mass: 420.1798

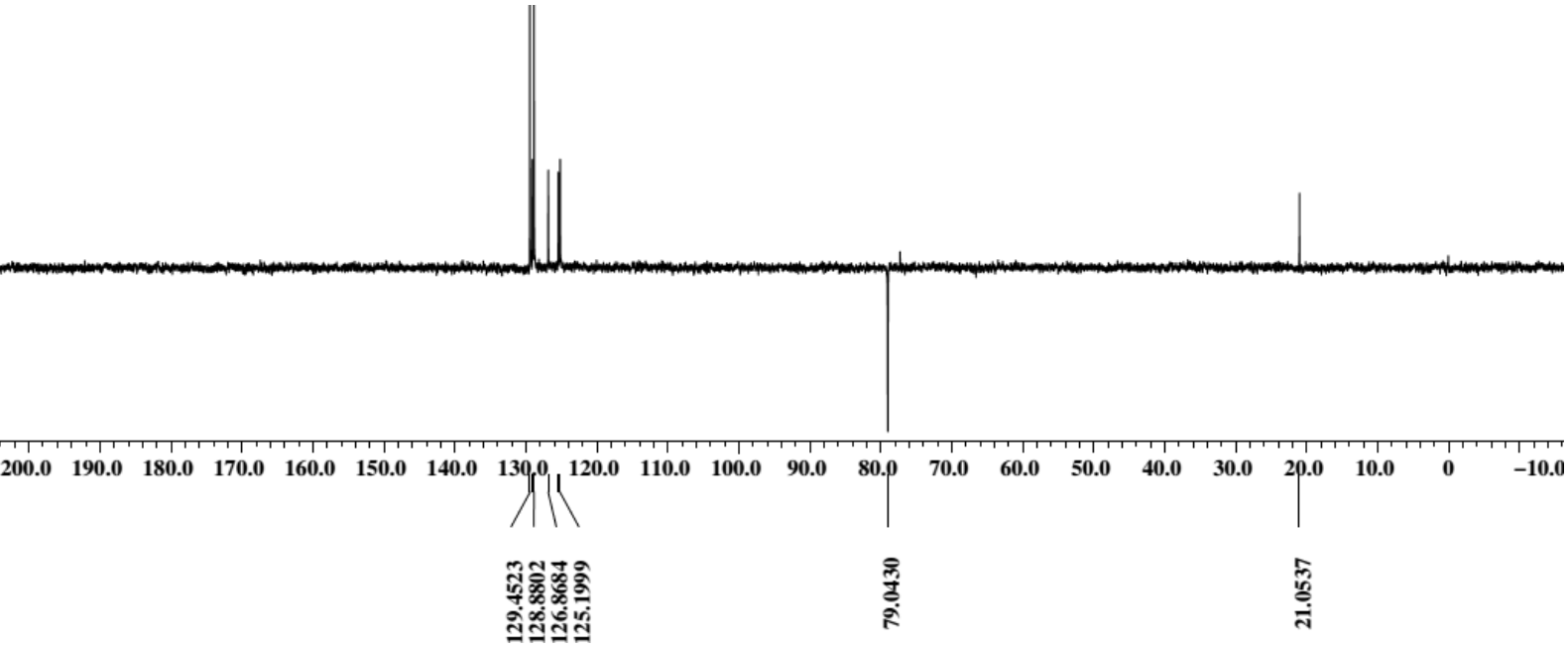
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1d



^{13}C-NMR ($CDCl_3$, 100 MHz) of 1d



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1d



HRMS of 1d

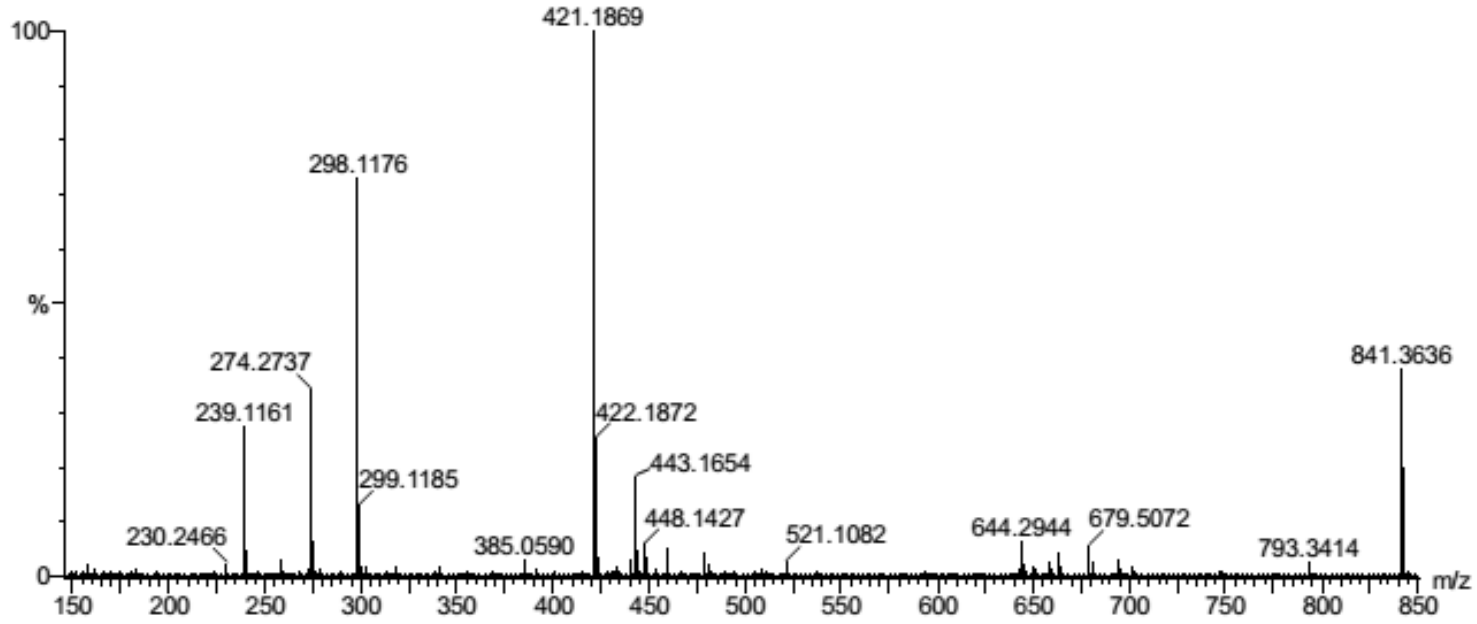
Elemental Composition Report

Single Mass Analysis

Tolerance = 25.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

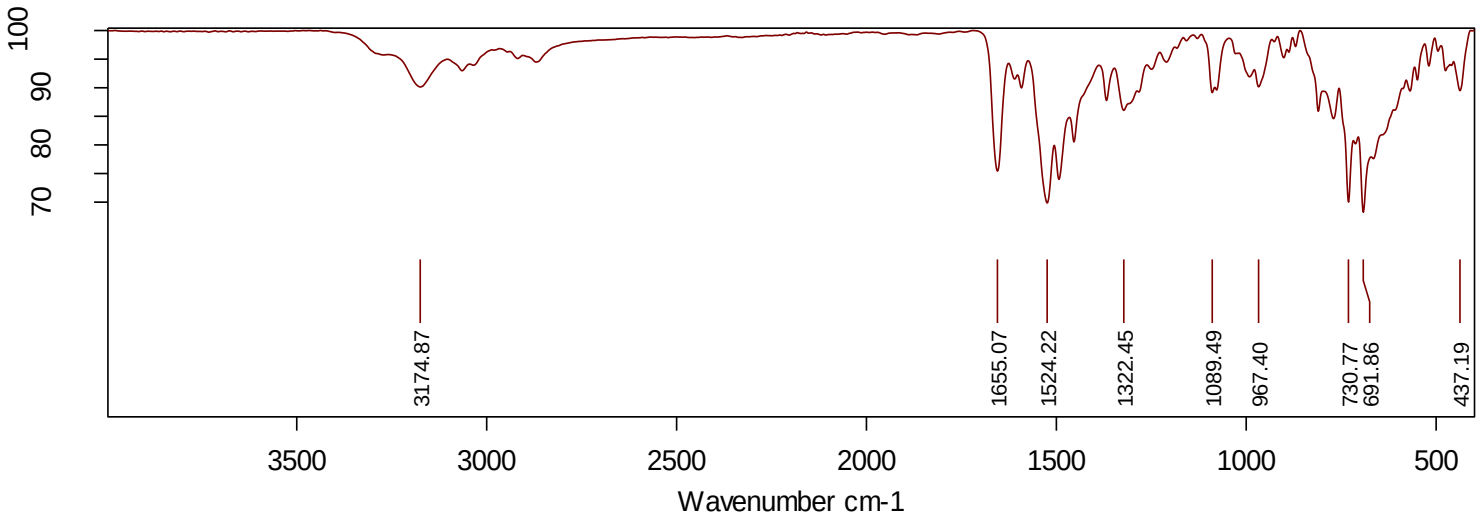
Monoisotopic Mass, Even Electron Ions
15 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-25 H: 11-25 N: 0-4 O: 1-5

Sample Name : 18-01-321 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
231019-18-01-321 18 (0.183) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (18:20) 1: TOF MS ES+
1.04e+007



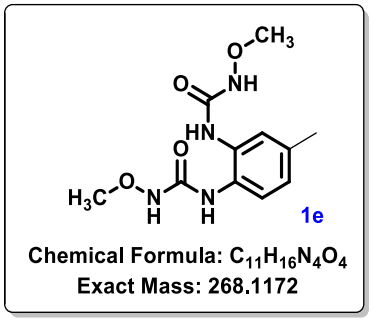
Minimum:				-1.5				
Maximum:		5.0	25.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
421.1869	421.1876	-0.7	-1.7	13.5	716.3	n/a	n/a	C23 H25 N4 O4

FTIR of 1d



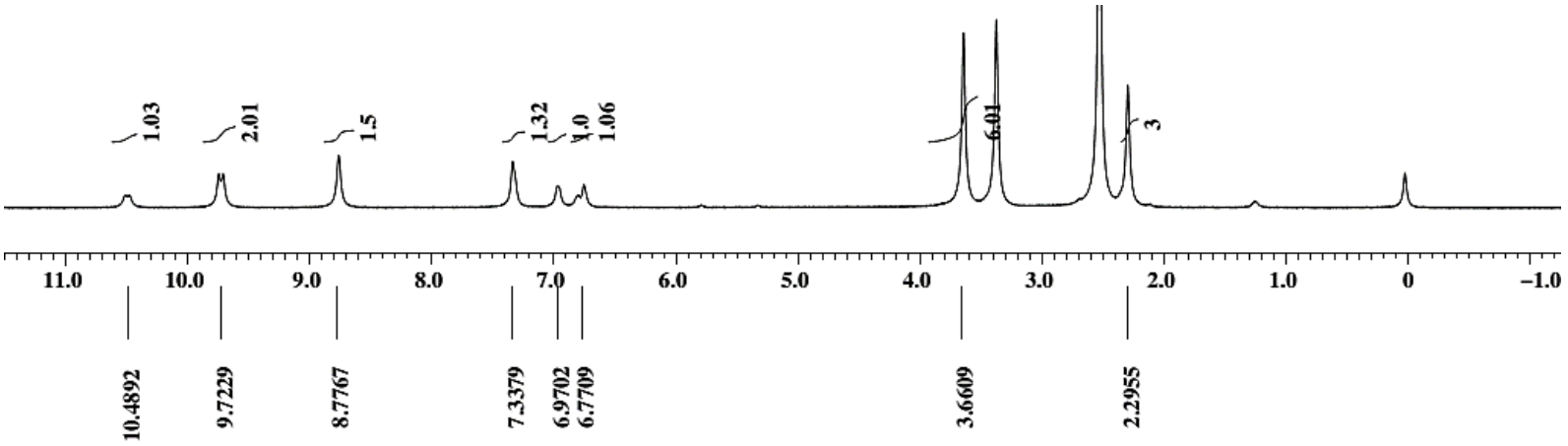
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-321.0	18-01-321	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	0.999538
3996.073013	0.999531
3994.643803	0.999525
3993.214592	0.999522
3991.785381	0.999522
3990.356171	0.999524
3988.926960	0.999533
3987.497749	0.999556
3986.068539	0.999601
3984.639328	0.999665
3983.210117	0.999742
3981.780907	0.999822
3980.351696	0.999900
3978.922485	0.999966
3977.493275	1.000000
3976.064064	0.999976
3974.634853	0.999875
3973.205643	0.999706
3971.776432	0.999506
3970.347221	0.999330
3968.918011	0.999219

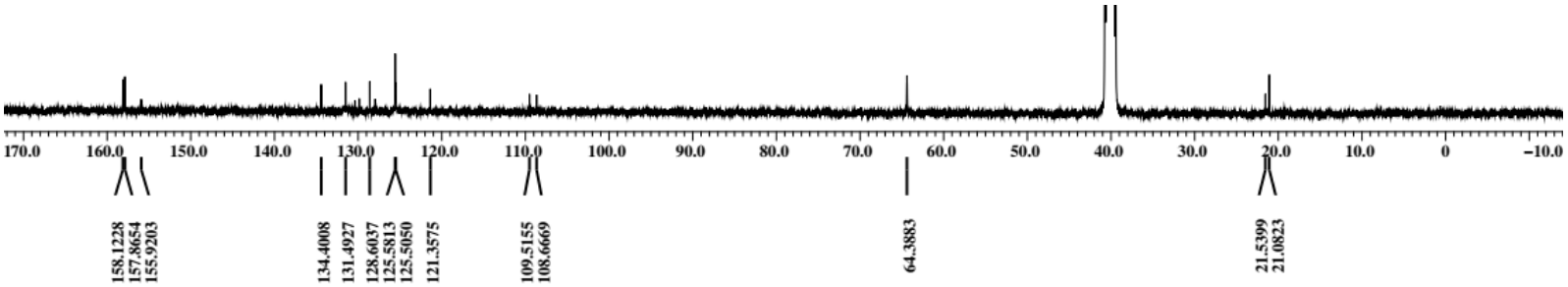


Chemical Formula: $C_{11}H_{16}N_4O_4$
Exact Mass: 268.1172

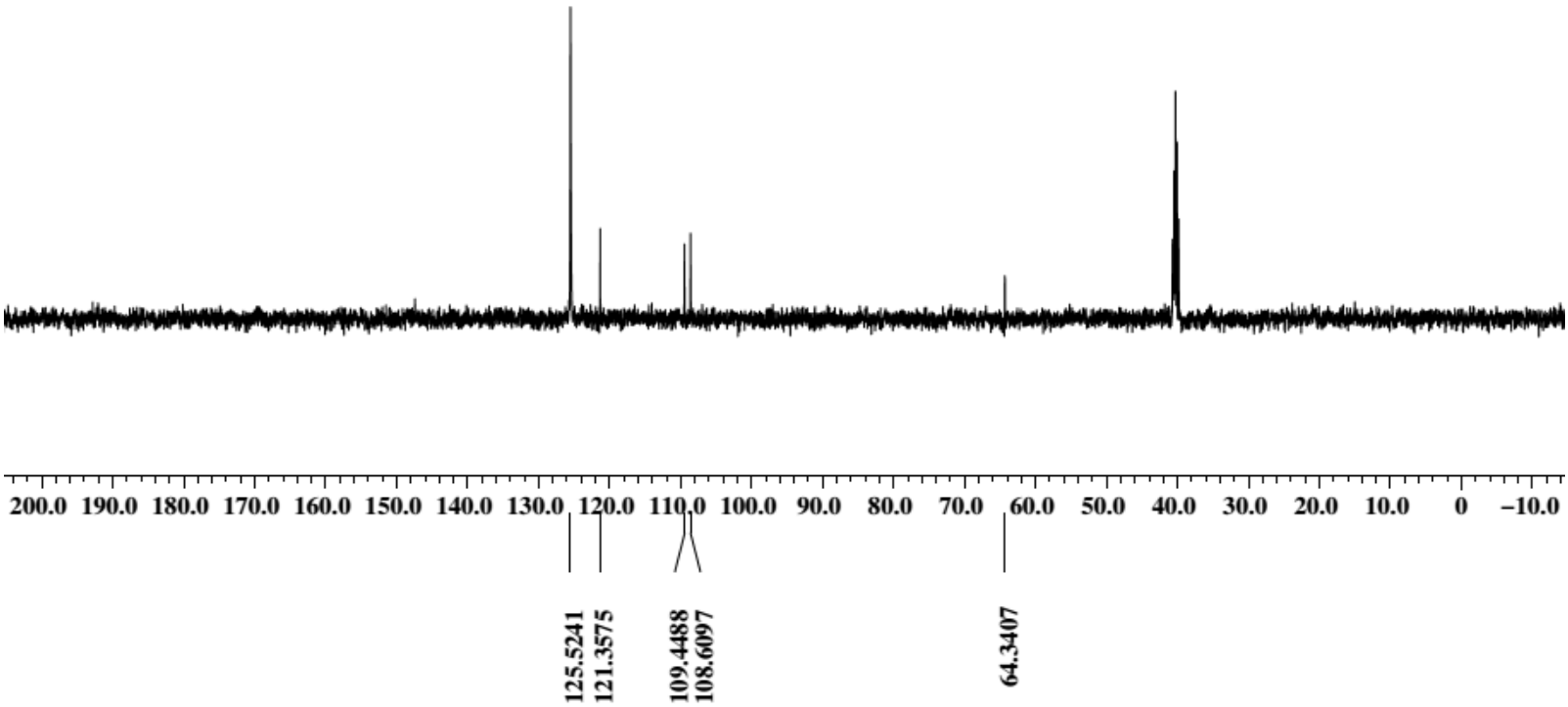
^{1}H-NMR (DMSO-d6, 400 MHz) of 1e



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



^{13}C-DEPT (DMSO-d6, 100 MHz) of 1e



HRMS of 1e

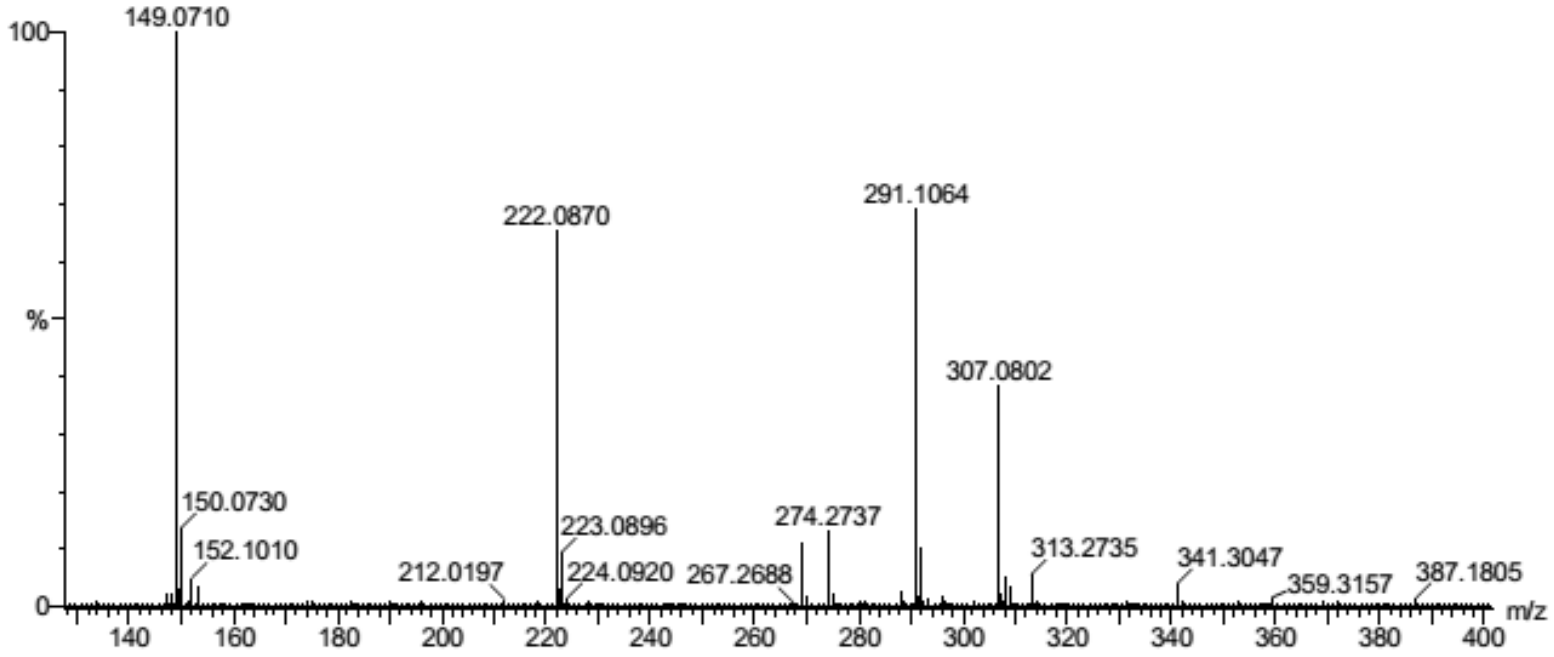
Elemental Composition Report

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 = 3

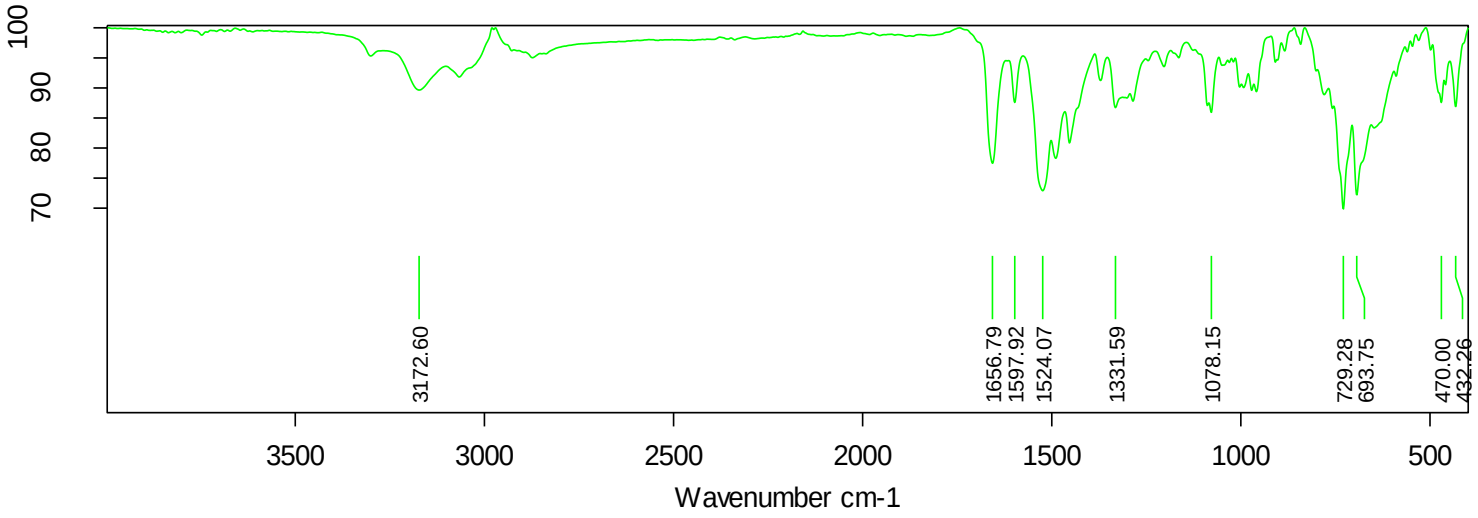
Monoisotopic Mass, Even Electron Ions
69 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-30 H: 7-25 N: 0-5 O: 0-6

Sample Name : 18-01-386 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
231219-18-01-386 12 (0.131) 1: TOF MS ES+
1.20e+008



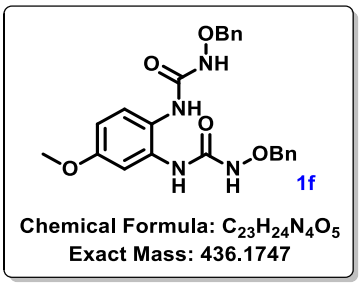
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
269.1242	269.1250	-0.8	-3.0	5.5	921.9	n/a	n/a	C11 H17 N4 O4

FTIR of 1e



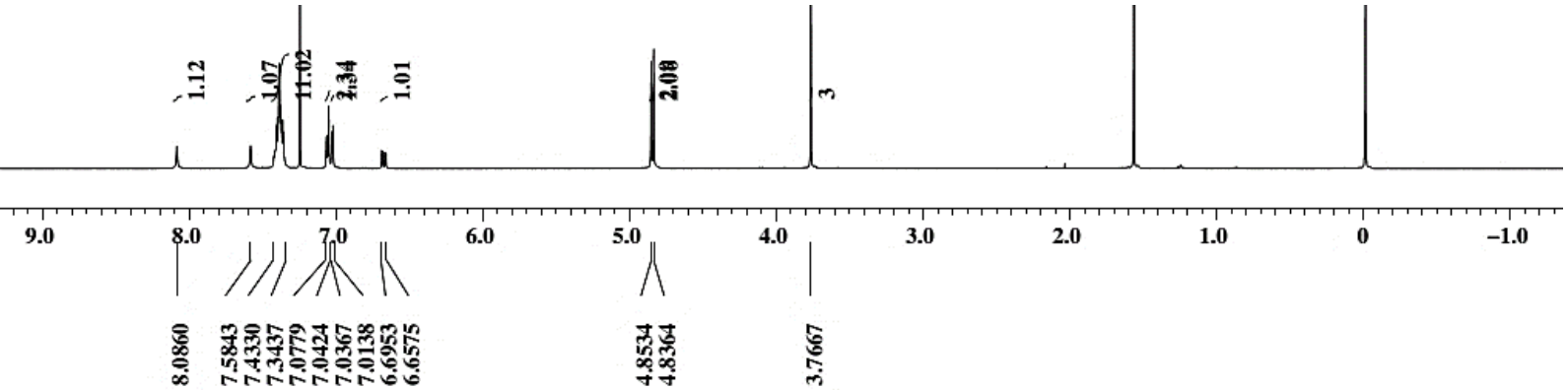
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-387.0	18-01-387	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	1.000010
3996.073013	1.000016
3994.643803	1.000000
3993.214592	0.999946
3991.785381	0.999848
3990.356171	0.999710
3988.926960	0.999549
3987.497749	0.999393
3986.068539	0.999264
3984.639328	0.999176
3983.210117	0.999139
3981.780907	0.999163
3980.351696	0.999243
3978.922485	0.999347
3977.493275	0.999417
3976.064064	0.999400
3974.634853	0.999294
3973.205643	0.999150
3971.776432	0.999036
3970.347221	0.998987
3968.918011	0.998999

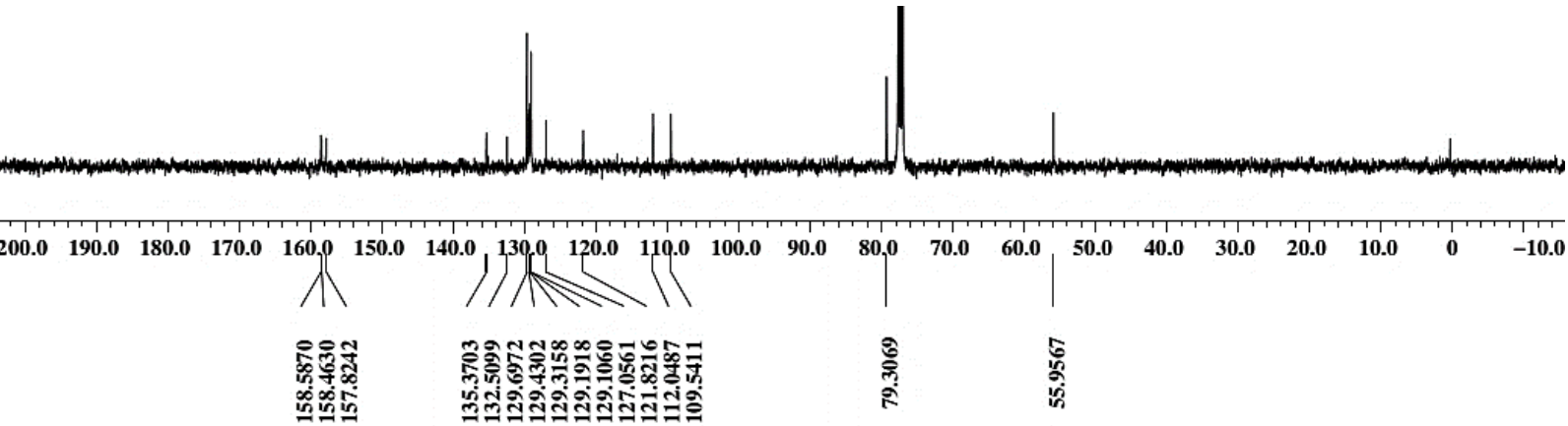


Chemical Formula: $C_{23}H_{24}N_4O_5$
Exact Mass: 436.1747

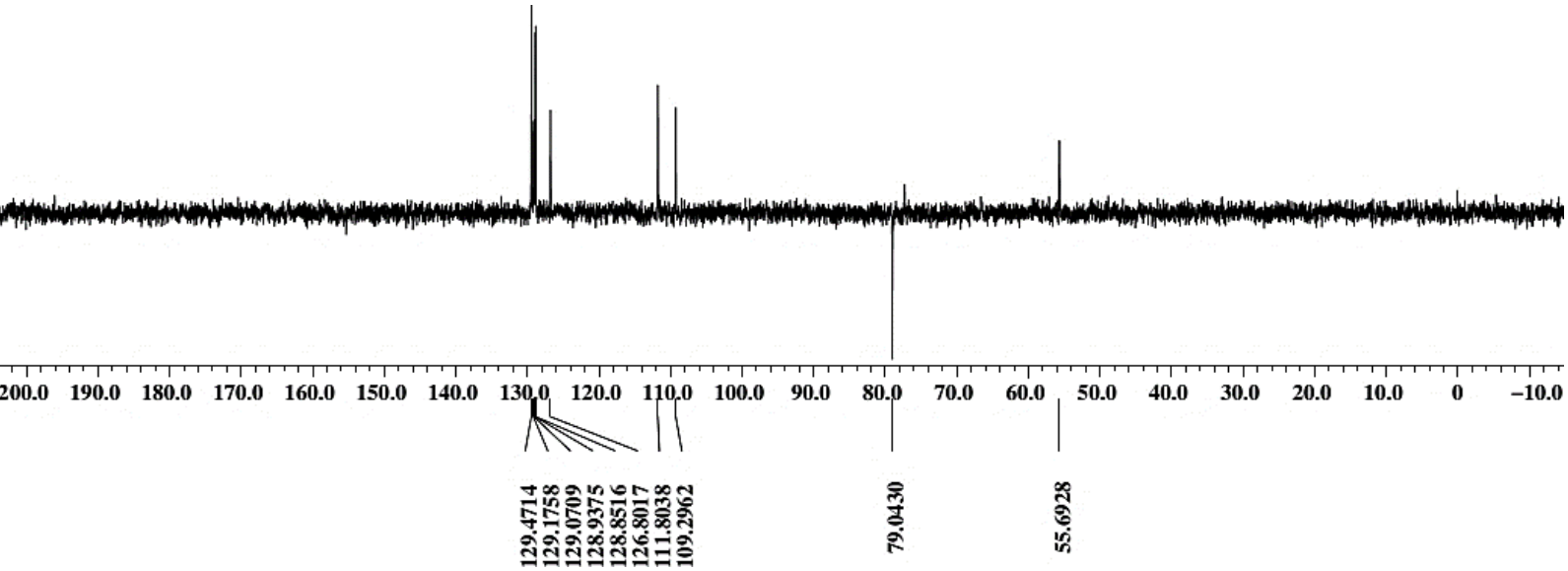
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1f



^{13}C-NMR ($CDCl_3$, 100 MHz) of 1f



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1f



HRMS of 1f

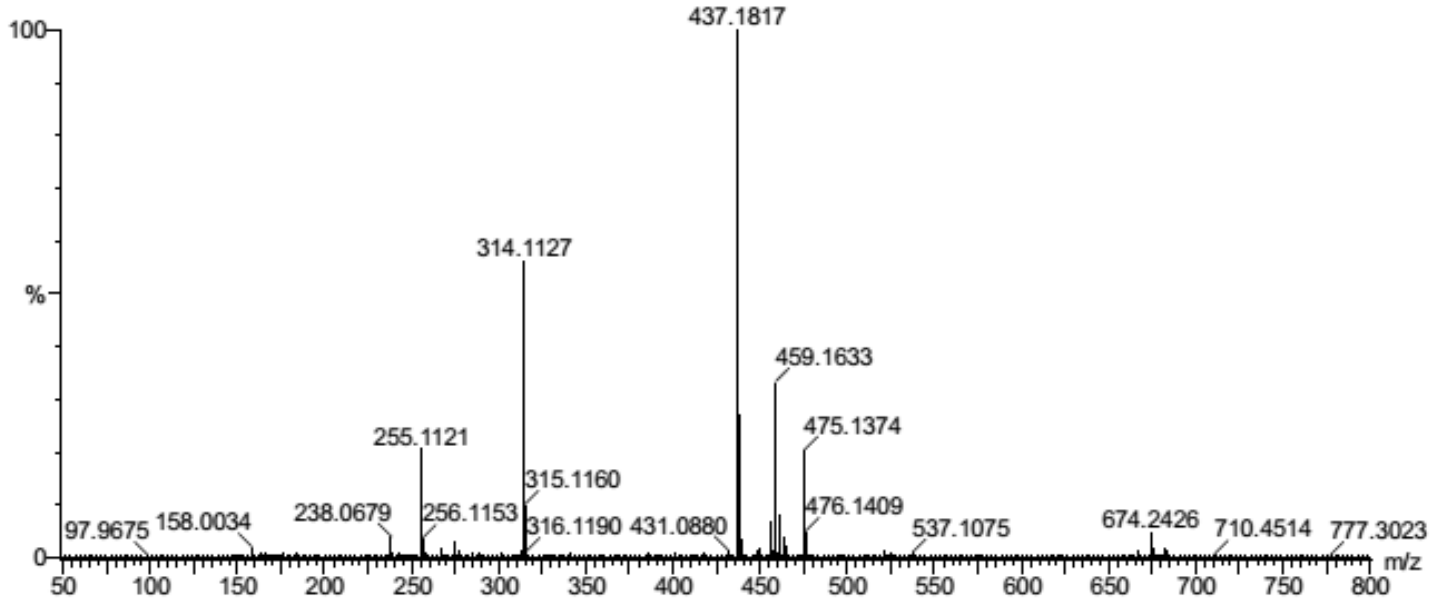
Elemental Composition Report

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 = 3

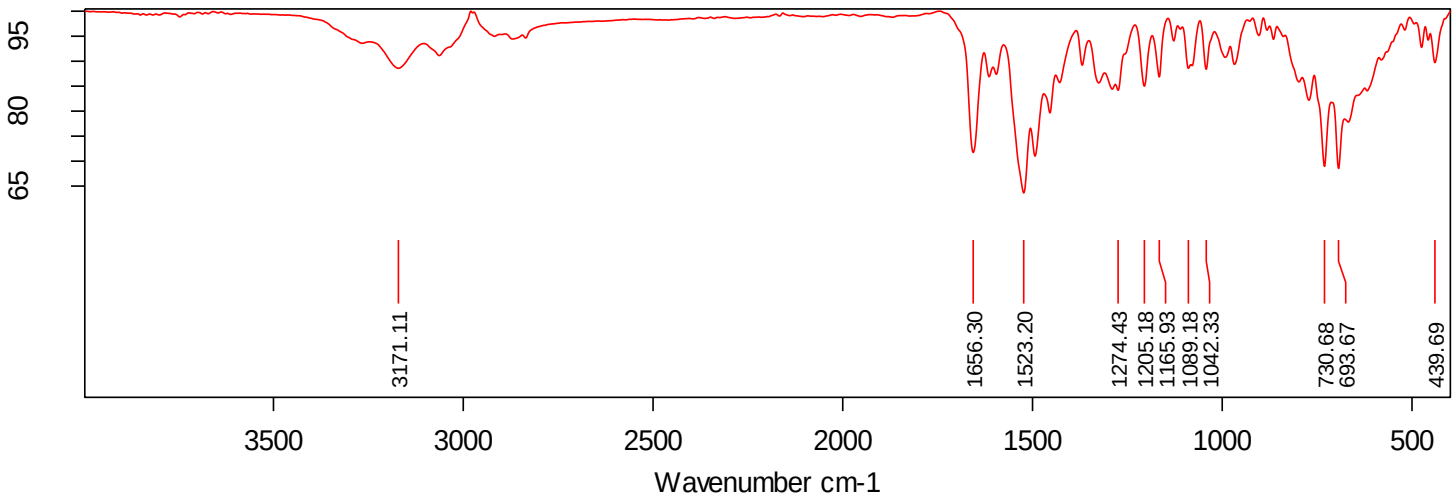
Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-25 H: 11-30 N: 0-4 O: 1-5

Sample Name : 18-01-342 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
081119-18-01-342 16 (0.165) AM2 (Ar,22000.0,0.00,0.00); Cm (16:22) 1: TOF MS ES+
2.66e+007



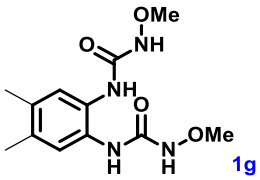
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
437.1817	437.1825	-0.8	-1.8	13.5	759.4	n/a	n/a	C23 H25 N4 O5

FTIR of 1f



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-342.0	18-01-342	Instrument type and / or accessory	1/6/2020

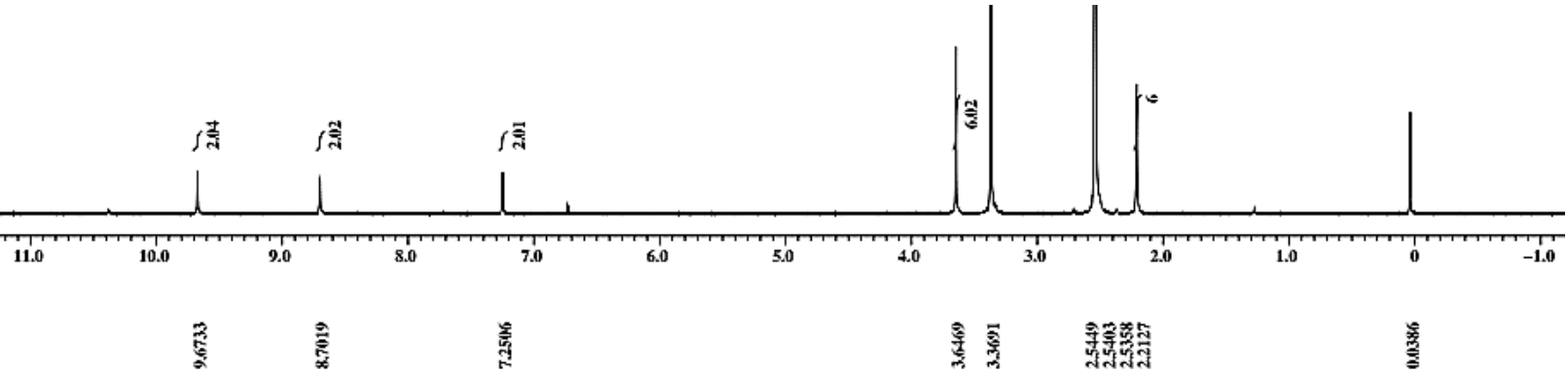
Wavenumber cm-1	Transmittance [%]
3997.502224	0.999801
3996.073013	0.999908
3994.643803	0.999984
3993.214592	1.000000
3991.785381	0.999937
3990.356171	0.999789
3988.926960	0.999577
3987.497749	0.999343
3986.068539	0.999141
3984.639328	0.999017
3983.210117	0.998992
3981.780907	0.999069
3980.351696	0.999222
3978.922485	0.999404
3977.493275	0.999550
3976.064064	0.999604
3974.634853	0.999553
3973.205643	0.999429
3971.776432	0.999284
3970.347221	0.999154
3968.918011	0.999053



1g

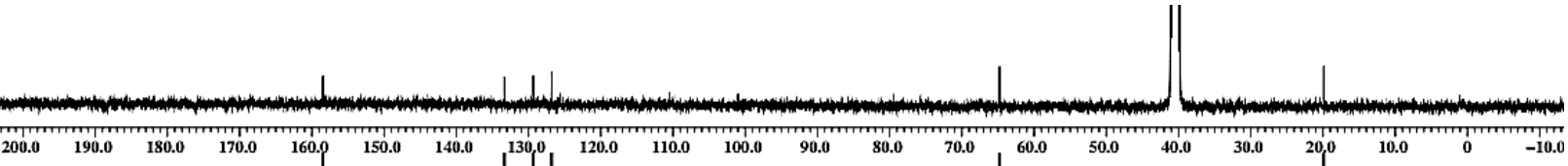
Chemical Formula: $C_{12}H_{18}N_4O_4$
Exact Mass: 282.1328

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



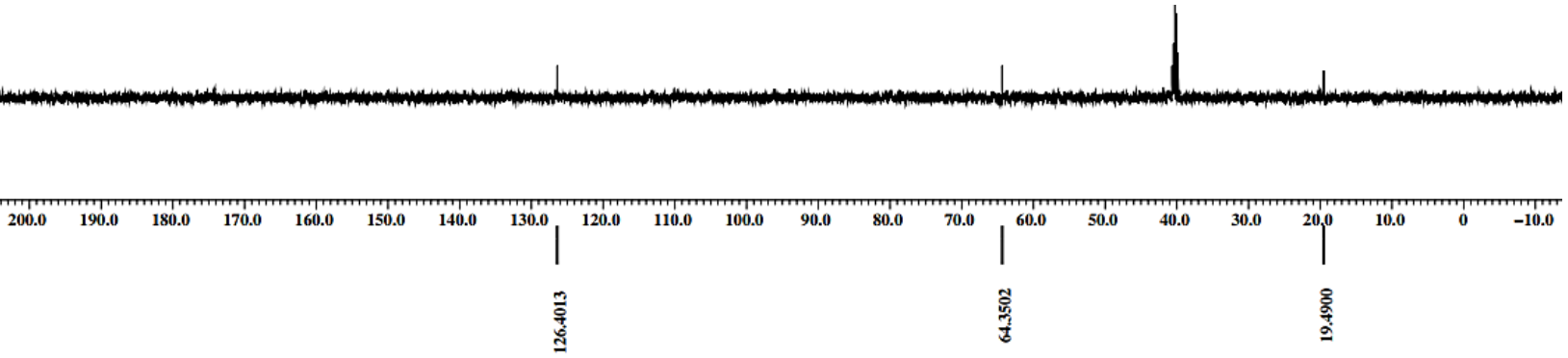
9.6733 8.7019 7.2506 3.6469 3.3691 2.5449 2.5403 2.5358 2.2127 0.0386

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



158.4700 133.3177 129.3227 126.7960 64.7831 19.8847

^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1g



HRMS of 1g

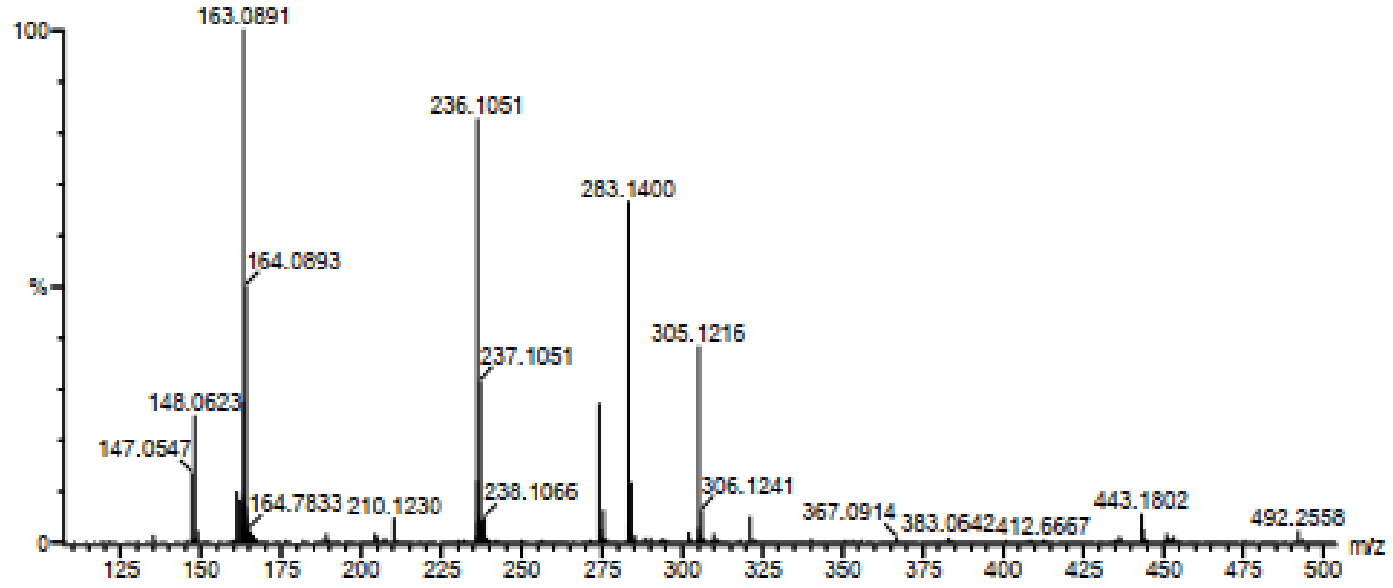
Elemental Composition Report

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 = 6

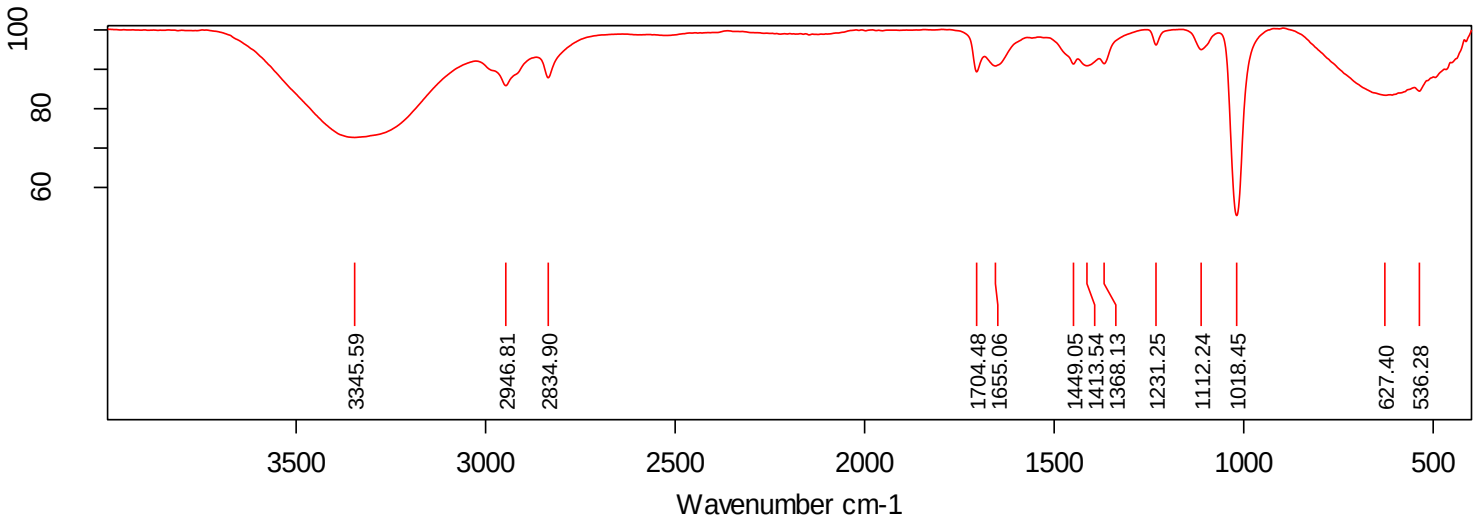
Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 11-20 H: 11-25 N: 0-4 O: 0-5

Sample Name : 18-01-411 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
170920-18-01-411- 15 (0.157) 1: TOF MS ES+
6.66e+007



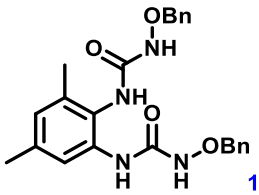
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
283.1400	283.1406	-0.6	-2.1	5.5	1161.1	n/a	n/a	C12 H19 N4 O4

FTIR of 1g



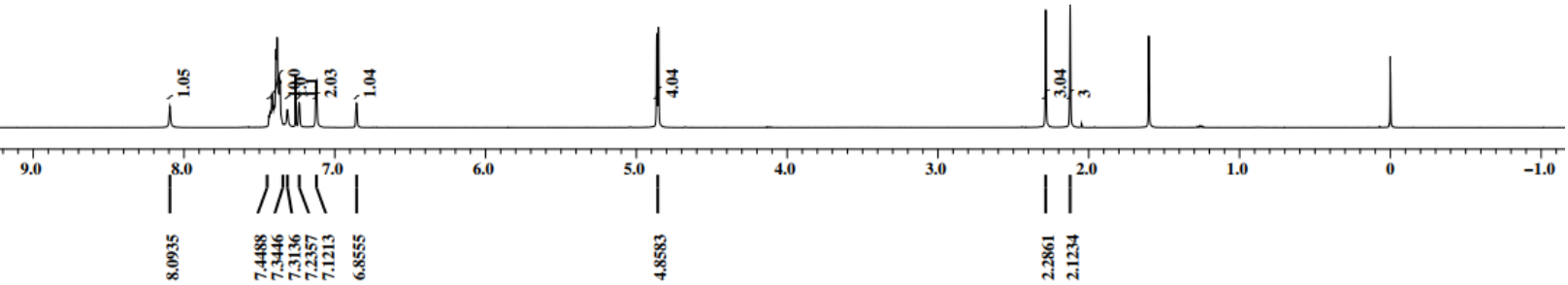
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-411.0	18-01-411	Instrument type and / or accessory	10/21/2020

Wavenumber cm-1	Transmittance [%]
3997.658602	1.001773
3996.229335	1.001633
3994.800069	1.001500
3993.370802	1.001387
3991.941536	1.001301
3990.512269	1.001230
3989.083002	1.001158
3987.653736	1.001073
3986.224469	1.000987
3984.795203	1.000921
3983.365936	1.000887
3981.936670	1.000875
3980.507403	1.000870
3979.078136	1.000862
3977.648870	1.000847
3976.219603	1.000818
3974.790337	1.000769
3973.361070	1.000689
3971.931804	1.000576
3970.502537	1.000439
3969.073270	1.000294

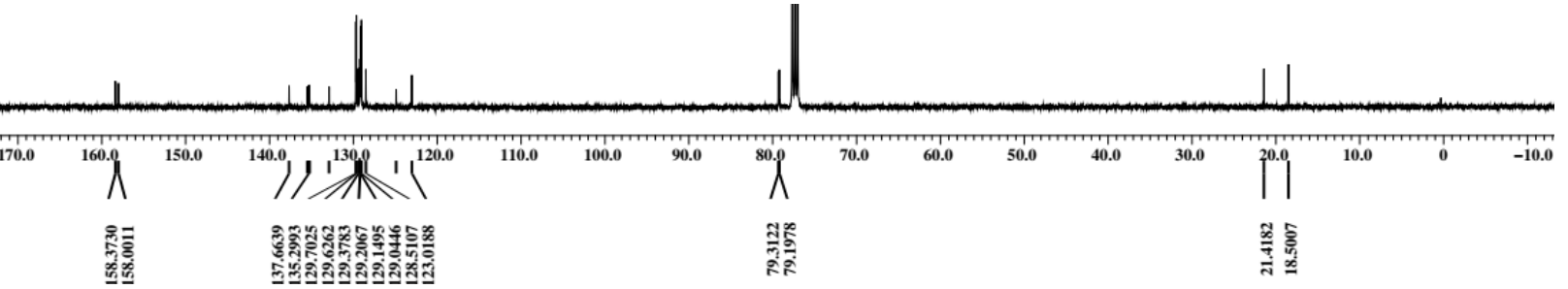


Chemical Formula: $C_{24}H_{26}N_4O_4$
Exact Mass: 434.1954

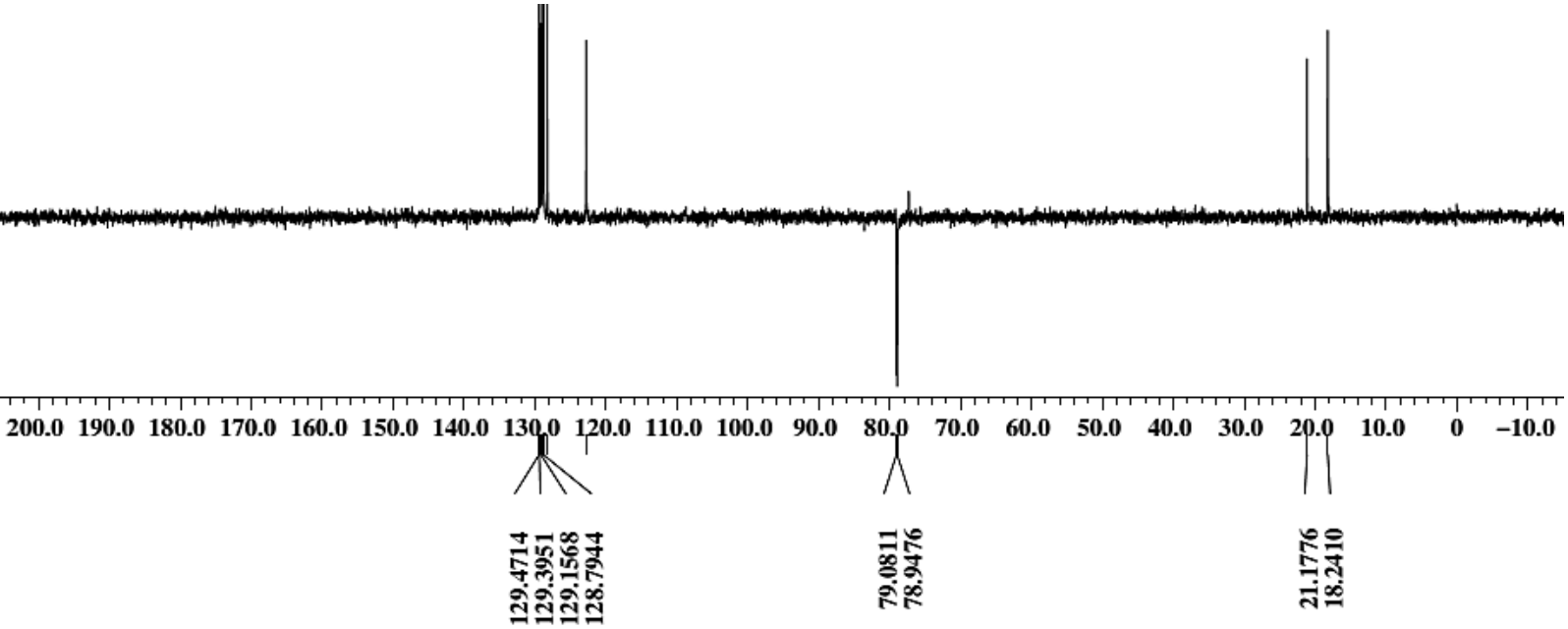
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1h



^{13}C-NMR ($CDCl_3$, 100 MHz) of 1h



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1h



HRMS of 1h

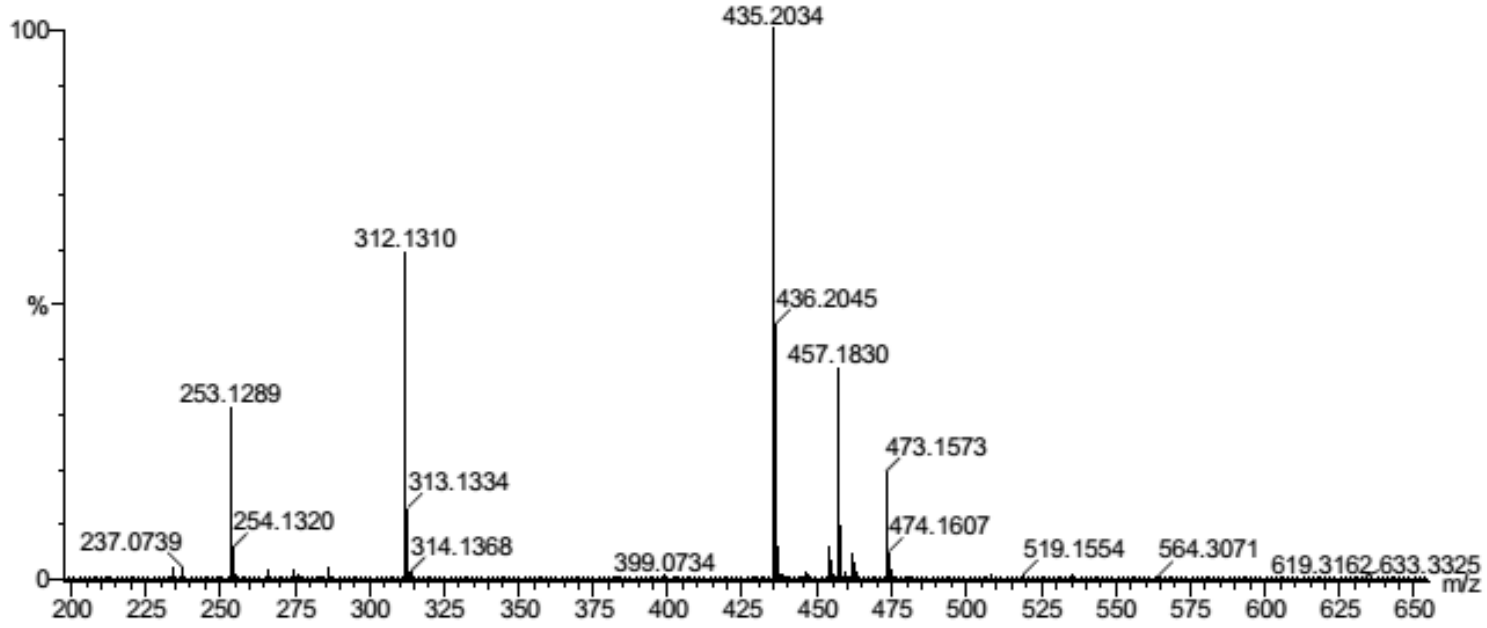
Elemental Composition Report

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 = 3

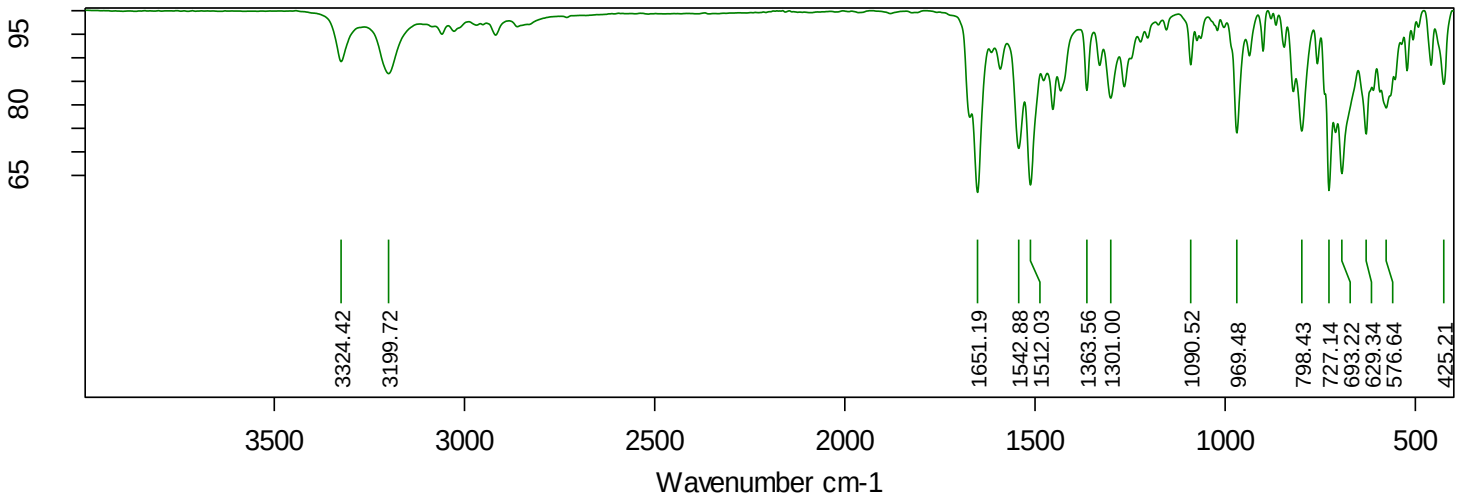
Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-25 H: 11-30 N: 0-5 O: 1-5

Sample Name : 18/01/316 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
051119-18-01-316 17 (0.174) AM2 (Ar,22000.0,0.00,0.00); Cm (17:20) 1: TOF MS ES+
4.64e+007



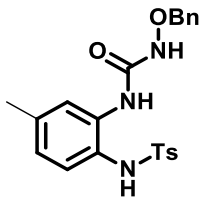
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
435.2034	435.2032	0.2	0.5	13.5	903.7	n/a	n/a	C24 H27 N4 O4

FTIR of 1h



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-316.0	18-01-316	Instrument type and / or accessory	1/6/2020

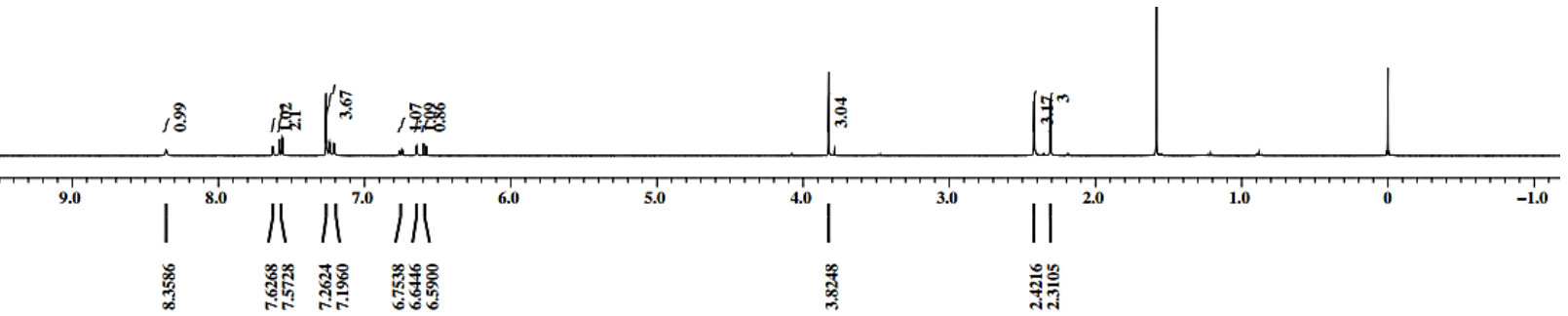
Wavenumber cm-1	Transmittance [%]
3997.502224	1.000853
3996.073013	1.000867
3994.643803	1.000878
3993.214592	1.000880
3991.785381	1.000872
3990.356171	1.000850
3988.926960	1.000811
3987.497749	1.000754
3986.068539	1.000686
3984.639328	1.000611
3983.210117	1.000540
3981.780907	1.000482
3980.351696	1.000448
3978.922485	1.000442
3977.493275	1.000457
3976.064064	1.000475
3974.634853	1.000478
3973.205643	1.000456
3971.776432	1.000418
3970.347221	1.000386
3968.918011	1.000378



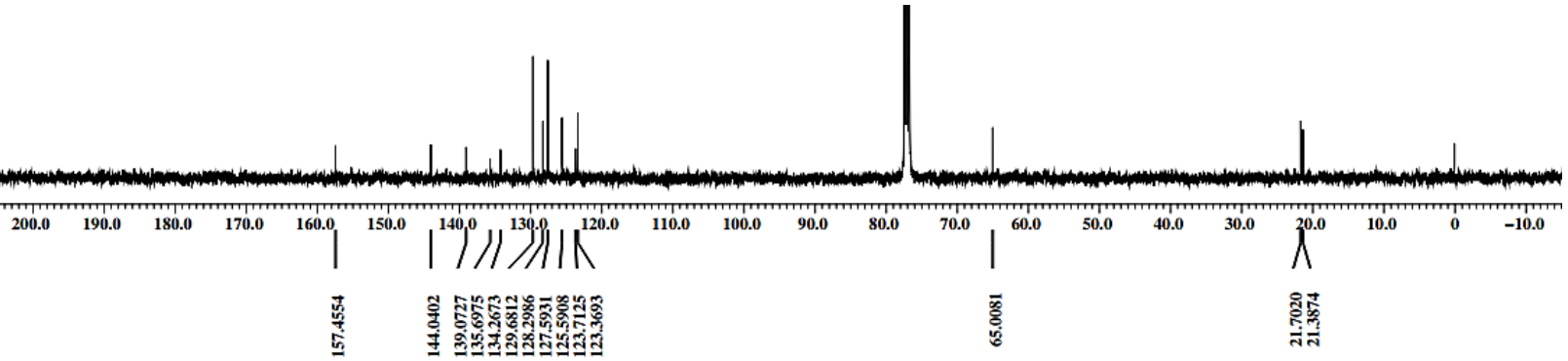
1i

Chemical Formula: $C_{22}H_{23}N_{3O4S}$
Exact Mass: 425.1409

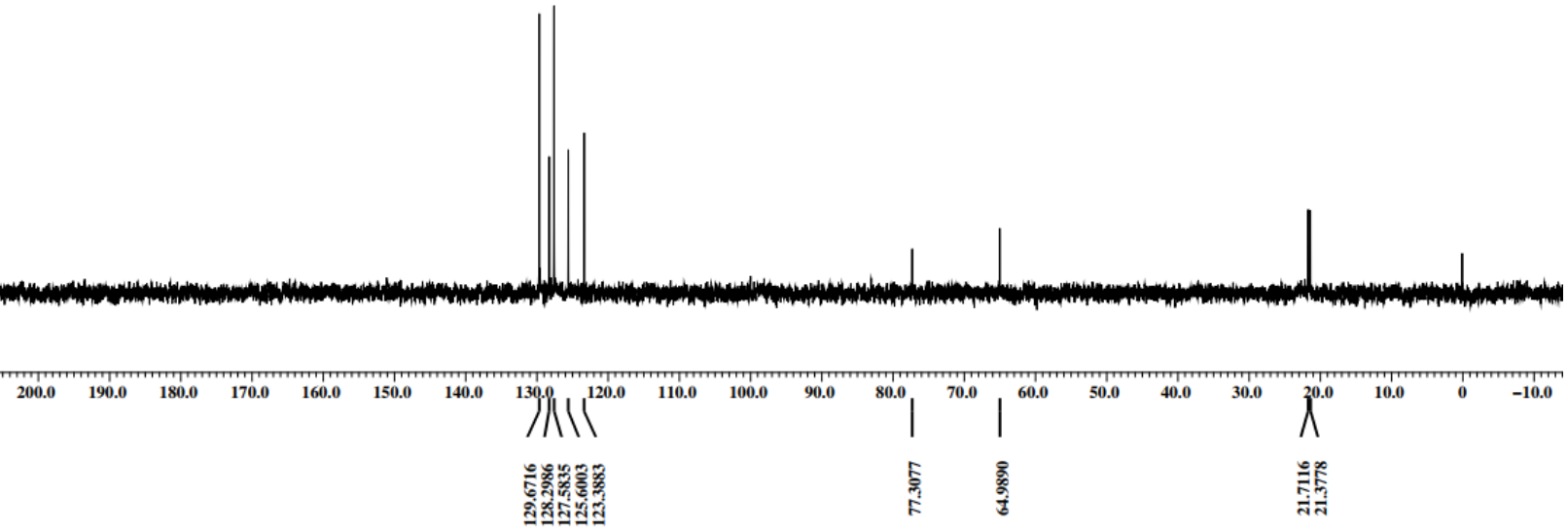
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1i



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1i



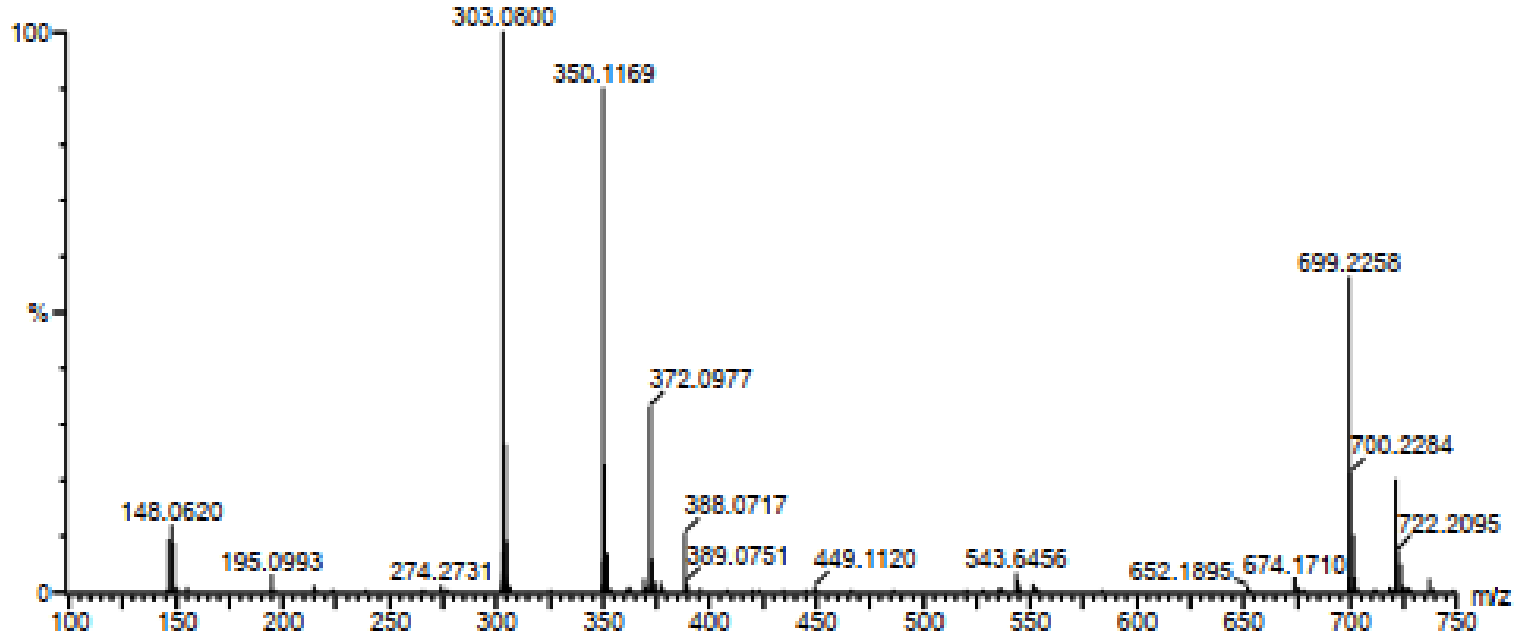
Elemental Composition Report

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 = 6

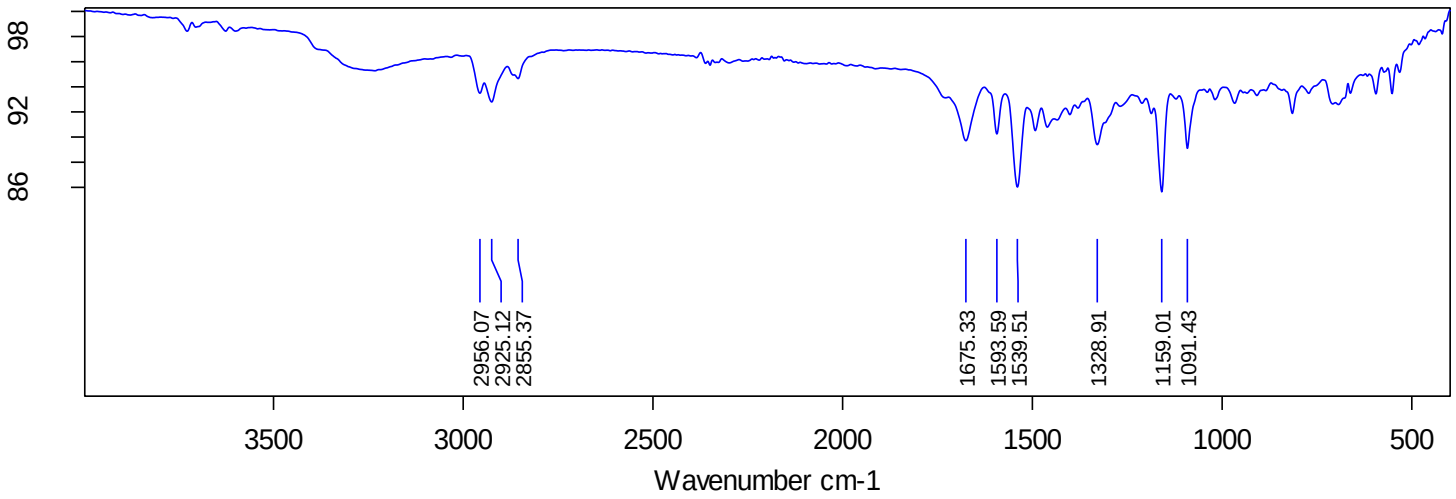
Monoisotopic Mass, Even Electron Ions
100 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 11-25 H: 10-25 N: 1-3 O: 0-6 S: 1-4

Sample Name : 18-01-444-2 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
221020-18-01-444-2- 12 (0.131) 1: TOF MS ES+
1.16e+008



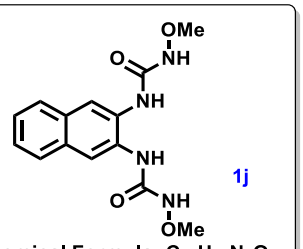
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
350.1169	350.1175	-0.6	-1.7	8.5	1815.8	n/a	n/a	C16 H20 N3 O4 S

FTIR of 1i



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-444.0	18-01-444	Instrument type and / or accessory	10/23/2020

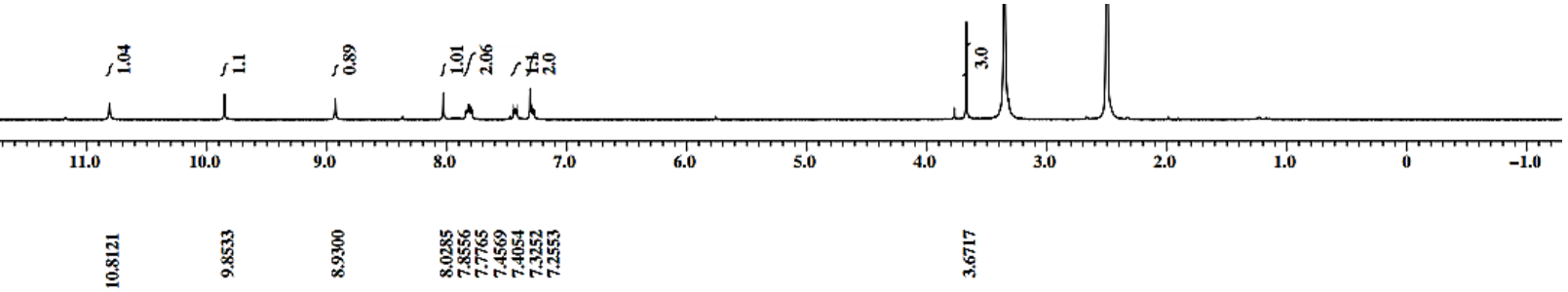
Wavenumber cm-1	Transmittance [%]
3997.658602	1.000565
3996.229335	1.000590
3994.800069	1.000599
3993.370802	1.000577
3991.941536	1.000523
3990.512269	1.000453
3989.083002	1.000396
3987.653736	1.000370
3986.224469	1.000373
3984.795203	1.000383
3983.365936	1.000372
3981.936670	1.000320
3980.507403	1.000226
3979.078136	1.000108
3977.648870	0.999991
3976.219603	0.999895
3974.790337	0.999826
3973.361070	0.999781
3971.931804	0.999757
3970.502537	0.999763
3969.073270	0.999806



1j

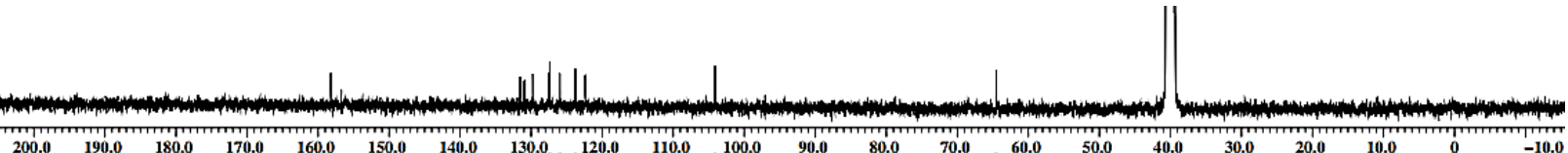
Chemical Formula: $C_{14}H_{16}N_4O_4$
Exact Mass: 304.1172

^{1}H-NMR (DMSO-d6, 400 MHz) of 1j



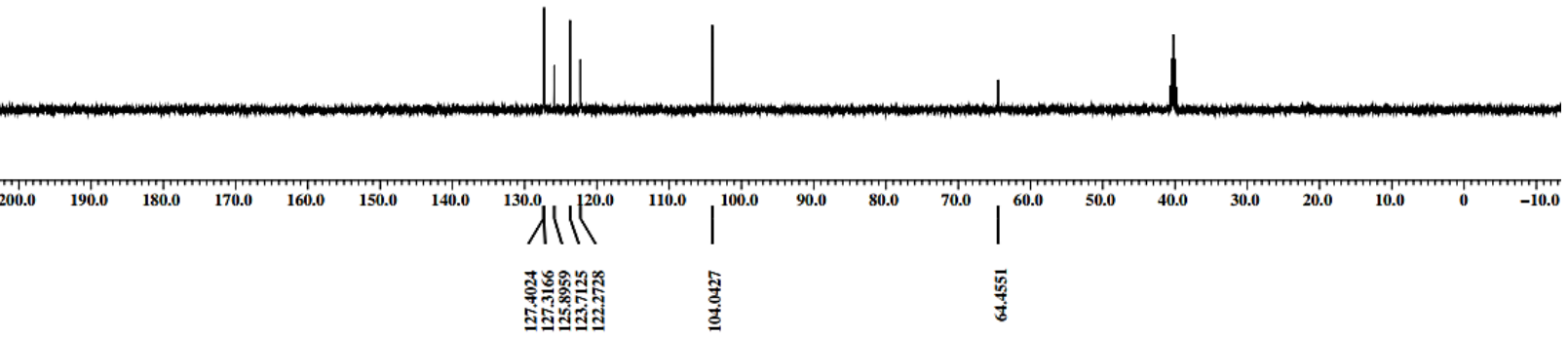
10.8121, 9.8533, 8.9300, 8.0285, 7.8556, 7.7765, 7.4569, 7.4054, 7.3252, 7.2553, 3.6717

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



158.1705, 131.5881, 129.7479, 127.3738, 125.9817, 123.8078, 122.3681, 104.1189, 64.5314

^{13}C-DEPT (DMSO-d6, 100 MHz) of 1j



127.4024
127.3166
125.8959
123.7125
122.2728
104.0427
64.4551

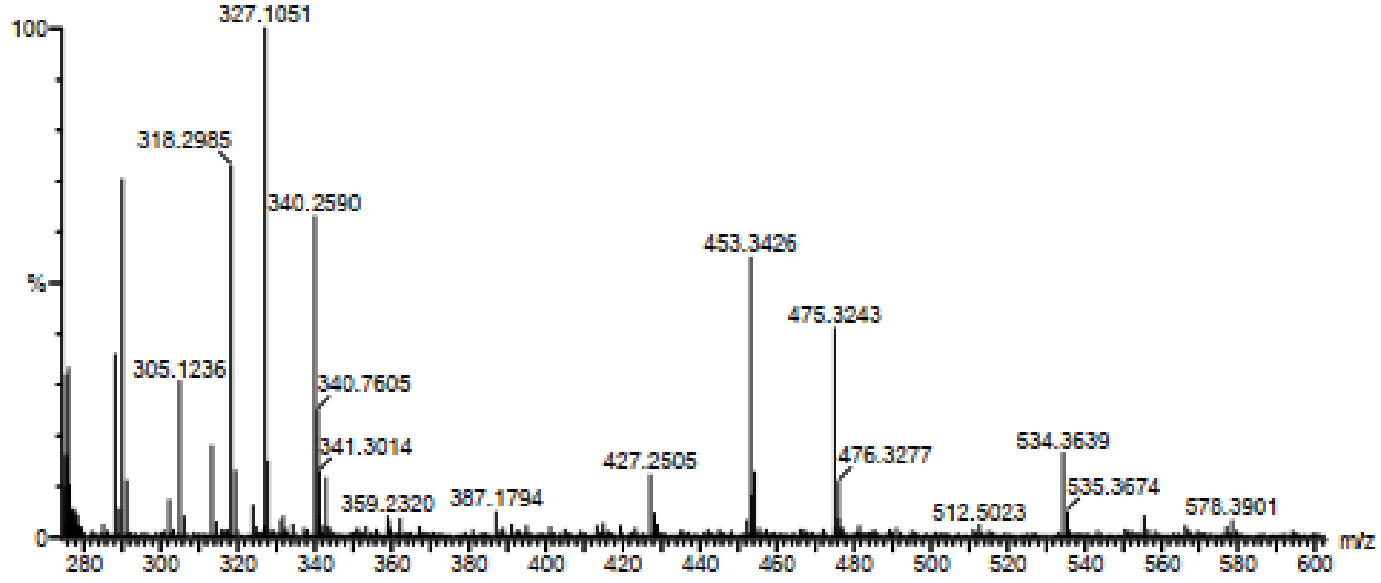
Elemental Composition Report

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 = 6

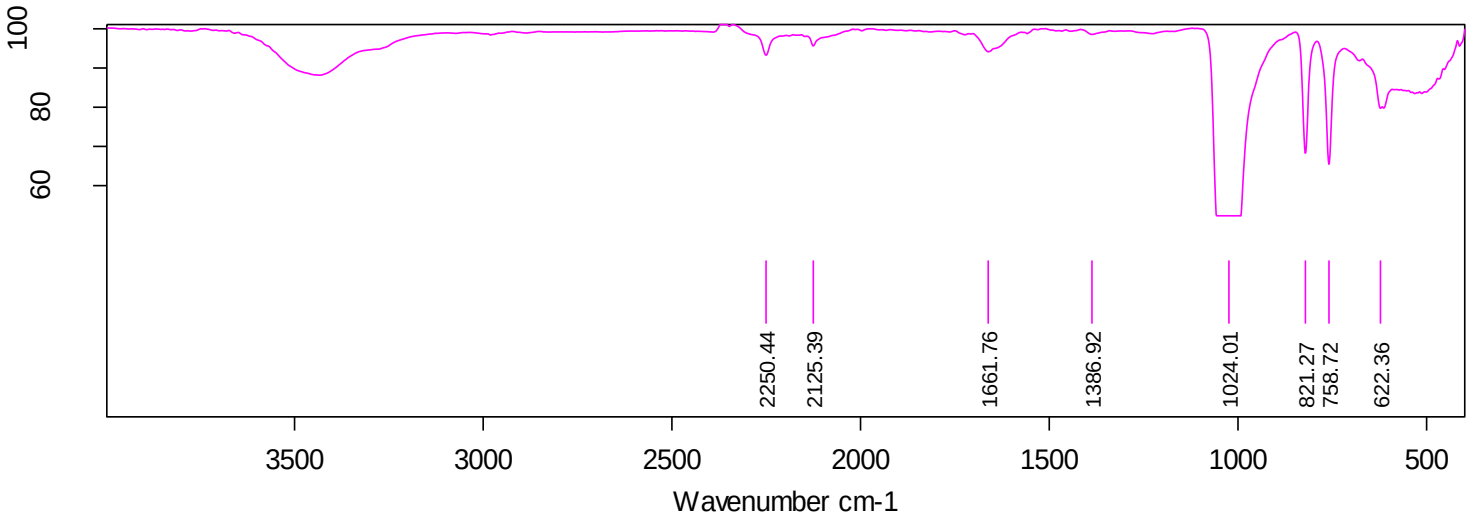
Monoisotopic Mass, Even Electron Ions
42 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-20 H: 11-25 N: 0-4 O: 0-4 Na: 0-1

Sample Name : 18-01-413-02 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
220920-18-01-413-02_ 12 (0.131) 1: TOF MS ES+
2.05e+007



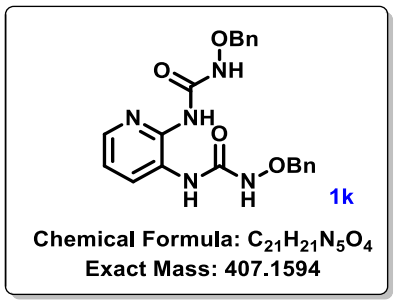
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
327.1051	327.1069	-1.8	-5.5	8.5	1634.6	n/a	n/a	C14 H16 N4 O4 Na

FTIR of 1j



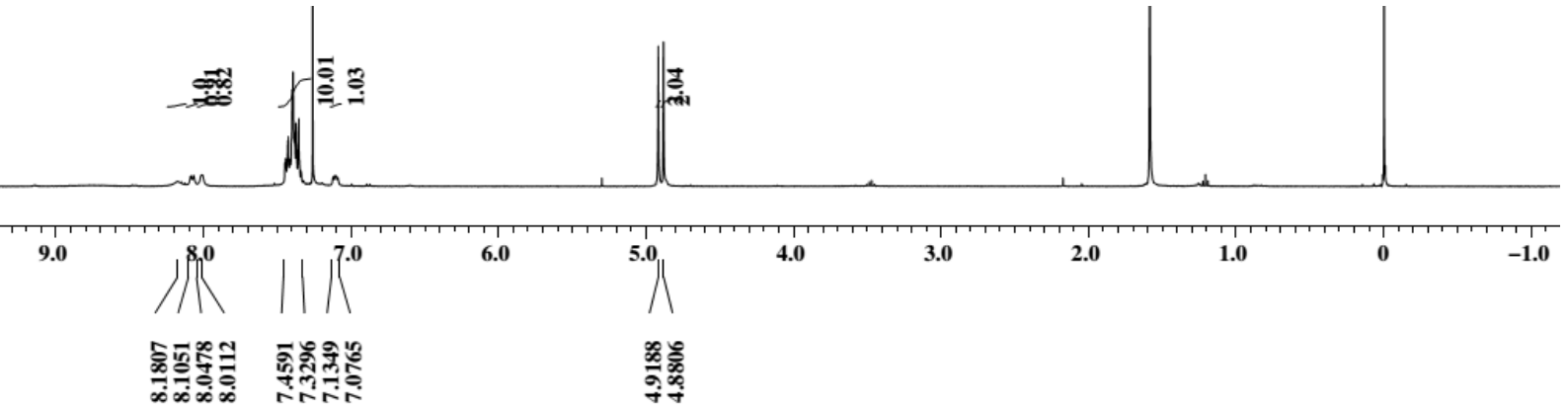
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-413.0	18-01-413	Instrument type and / or accessory	10/21/2020

Wavenumber cm-1	Transmittance [%]
3997.658602	1.002613
3996.229335	1.002399
3994.800069	1.002204
3993.370802	1.002045
3991.941536	1.001925
3990.512269	1.001831
3989.083002	1.001750
3987.653736	1.001673
3986.224469	1.001605
3984.795203	1.001553
3983.365936	1.001515
3981.936670	1.001483
3980.507403	1.001446
3979.078136	1.001393
3977.648870	1.001320
3976.219603	1.001230
3974.790337	1.001129
3973.361070	1.001010
3971.931804	1.000861
3970.502537	1.000685
3969.073270	1.000499

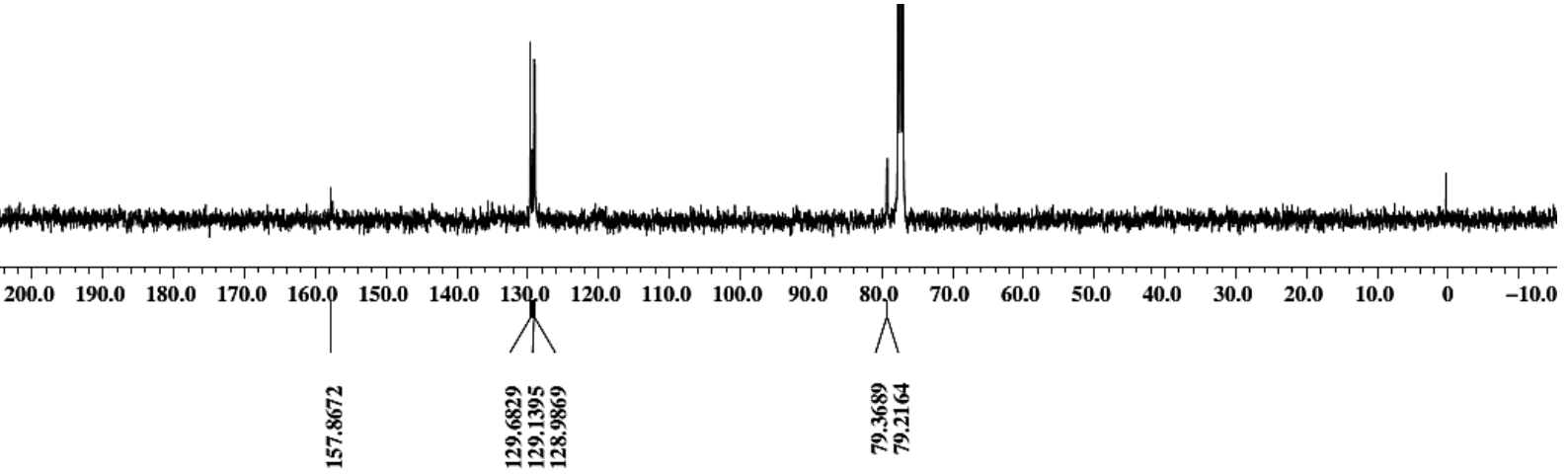


Chemical Formula: $C_{21}H_{21}N_5O_4$
Exact Mass: 407.1594

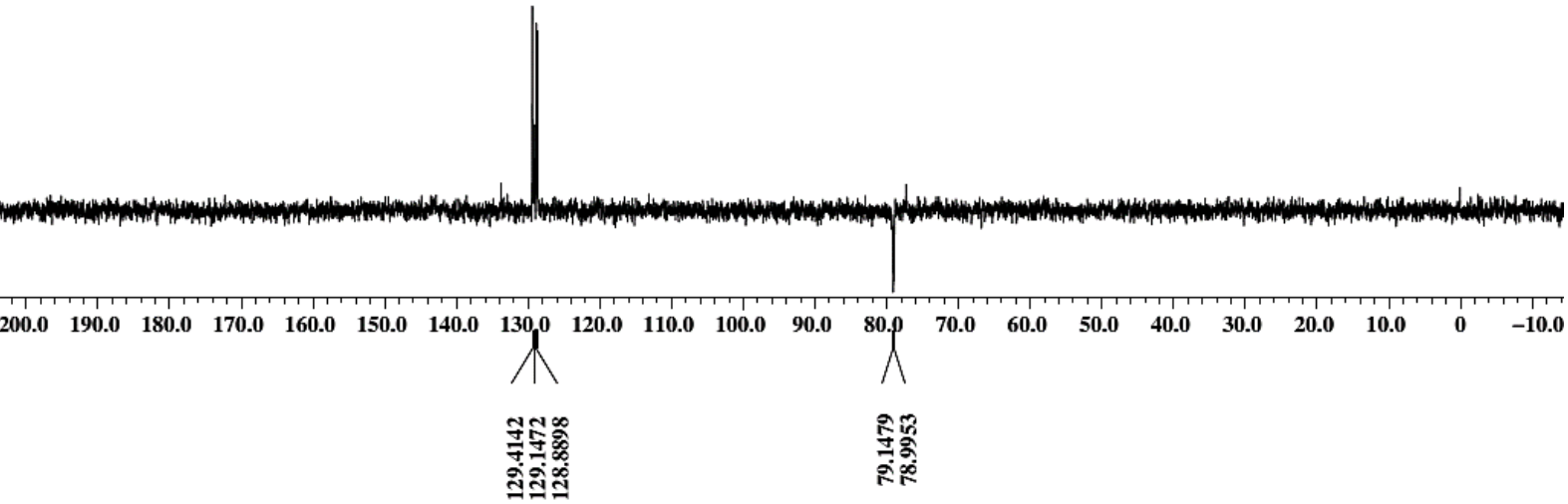
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1k



^{13}C-NMR ($CDCl_3$, 100 MHz) of 1k



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1k



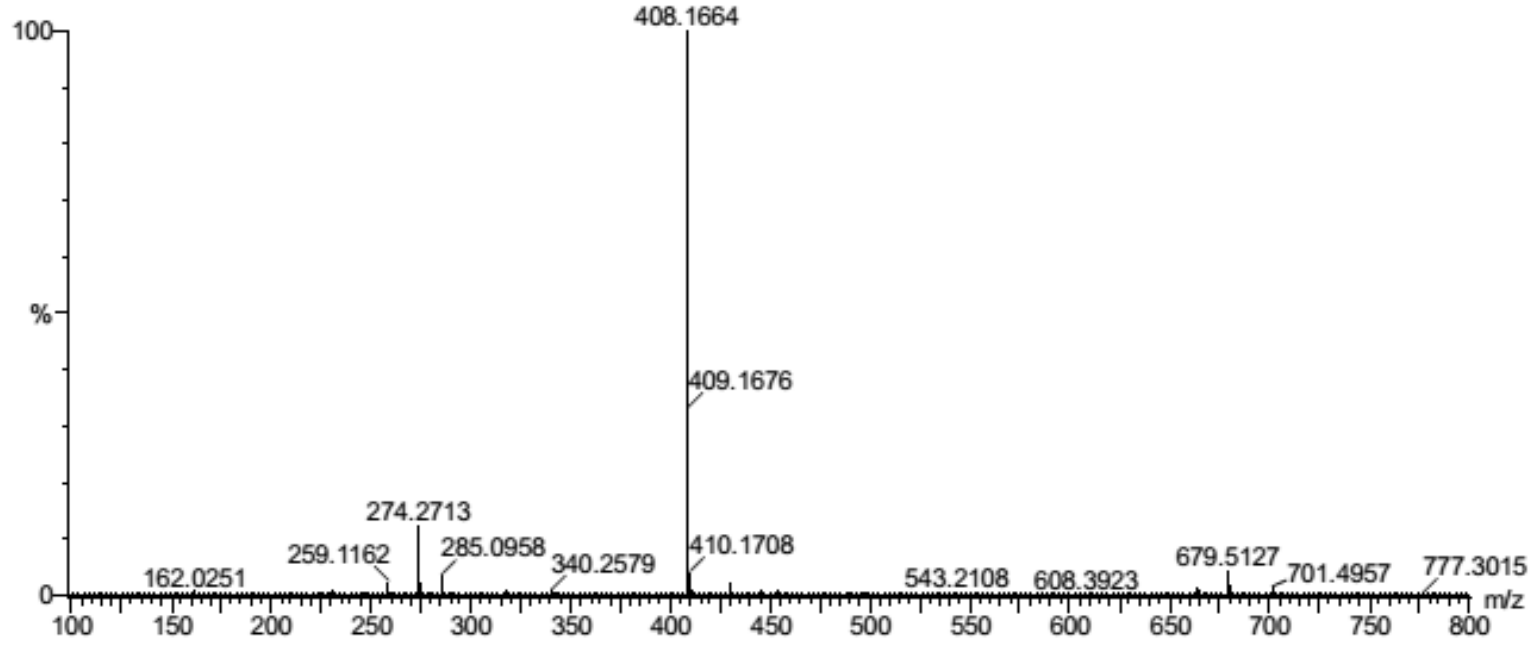
Elemental Composition Report

Single Mass Analysis

Tolerance = 8.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

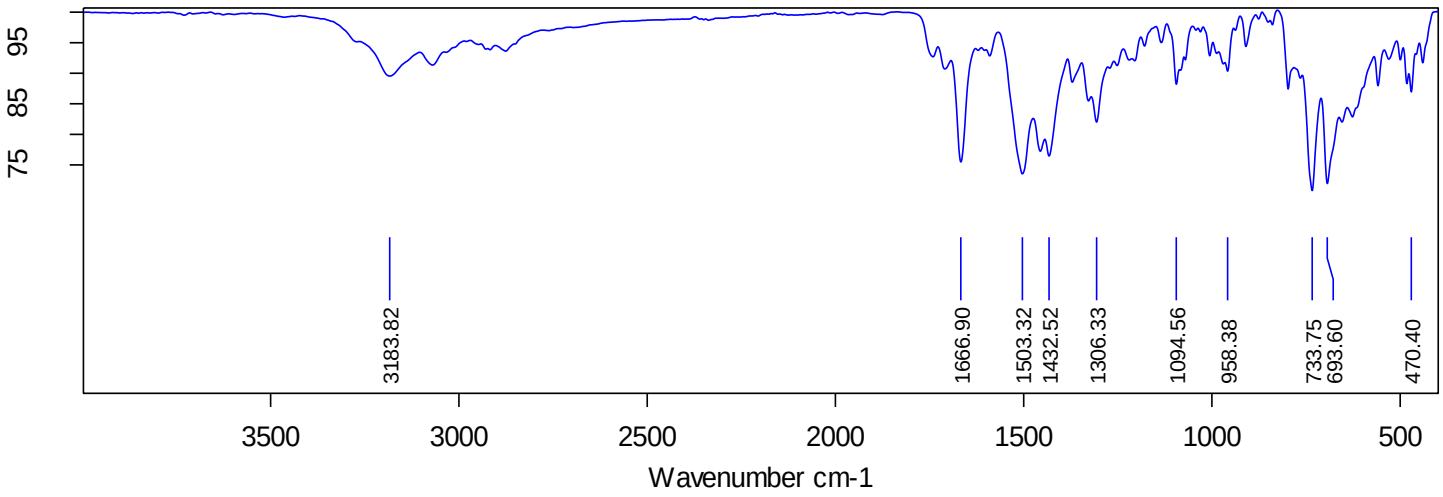
Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-21 H: 9-30 N: 0-5 O: 1-5

Sample Name : 18-01-355 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
181119-18-01-355- 18 (0.183) AM2 (Ar,22000.0,0.00,0.00); Cm (18:19) 1: TOF MS ES+
1.82e+007



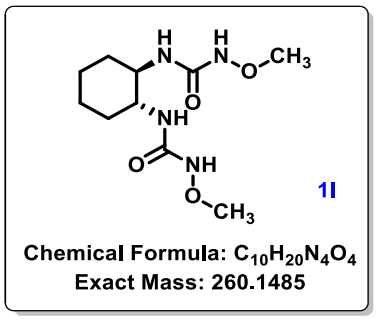
Minimum:				-1.5				
Maximum:		5.0	8.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
408.1664	408.1672	-0.8	-2.0	13.5	811.9	n/a	n/a	C21 H22 N5 O4

FTIR of 1k

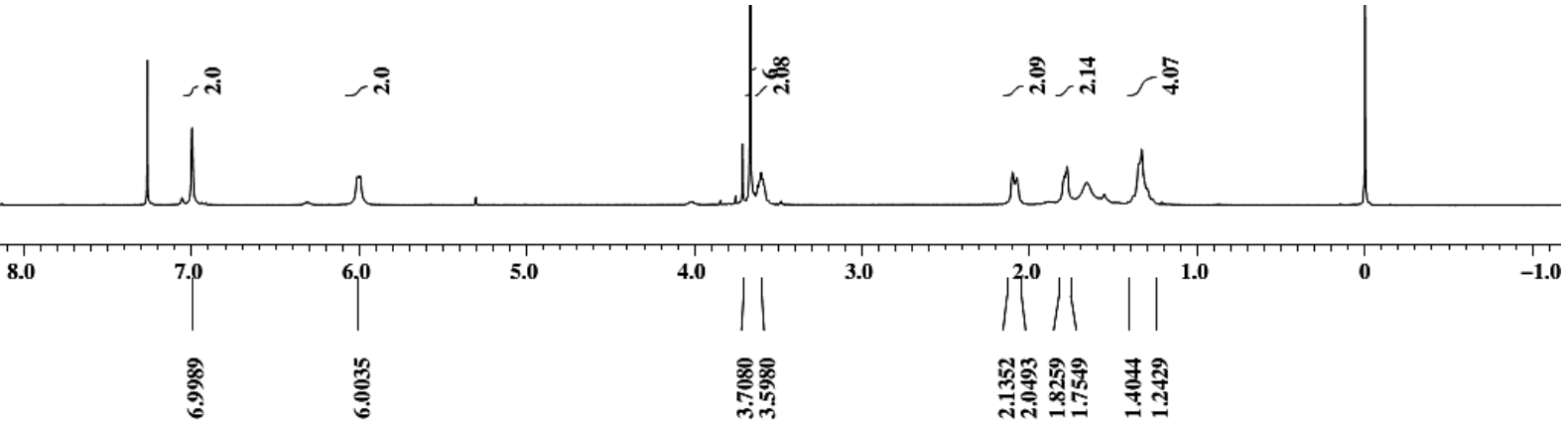


D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-355.0	18-01-355	Instrument type and / or accessory	1/6/2020

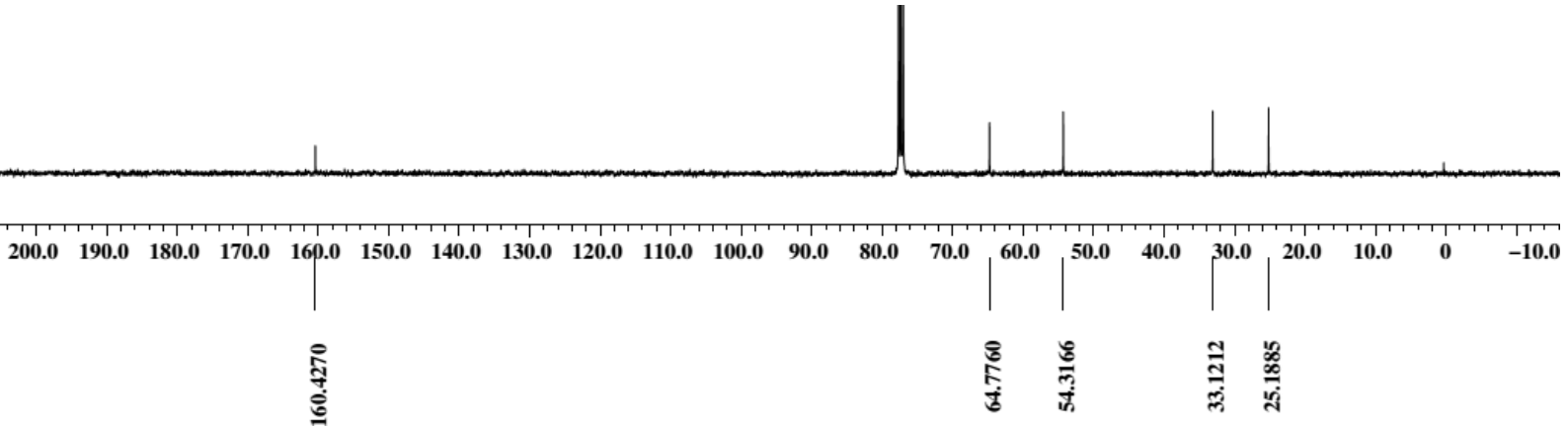
Wavenumber cm-1	Transmittance [%]
3997.502224	0.999754
3996.073013	0.999796
3994.643803	0.999831
3993.214592	0.999856
3991.785381	0.999871
3990.356171	0.999886
3988.926960	0.999912
3987.497749	0.999950
3986.068539	0.999988
3984.639328	1.000000
3983.210117	0.999964
3981.780907	0.999874
3980.351696	0.999743
3978.922485	0.999602
3977.493275	0.999483
3976.064064	0.999408
3974.634853	0.999379
3973.205643	0.999382
3971.776432	0.999402
3970.347221	0.999439
3968.918011	0.999497



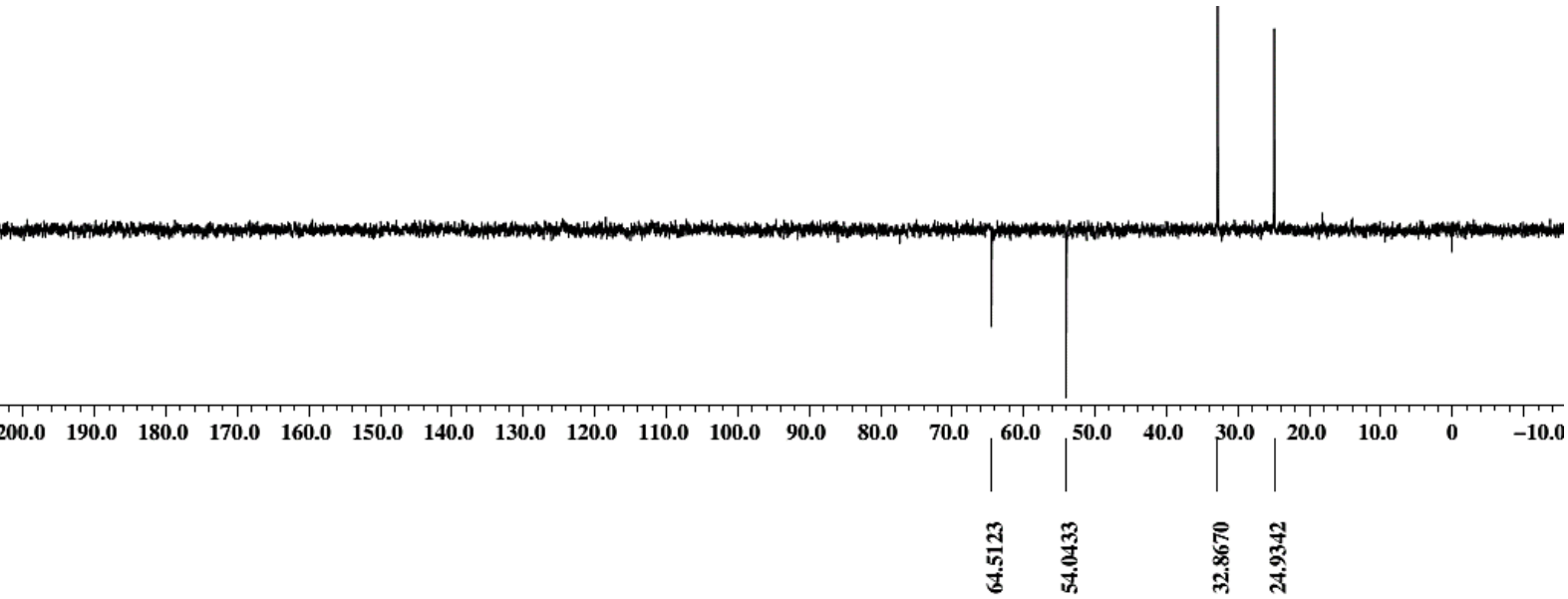
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1l



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



^{13}C-DEPT ($CDCl_3$, 100MHz) of 1l



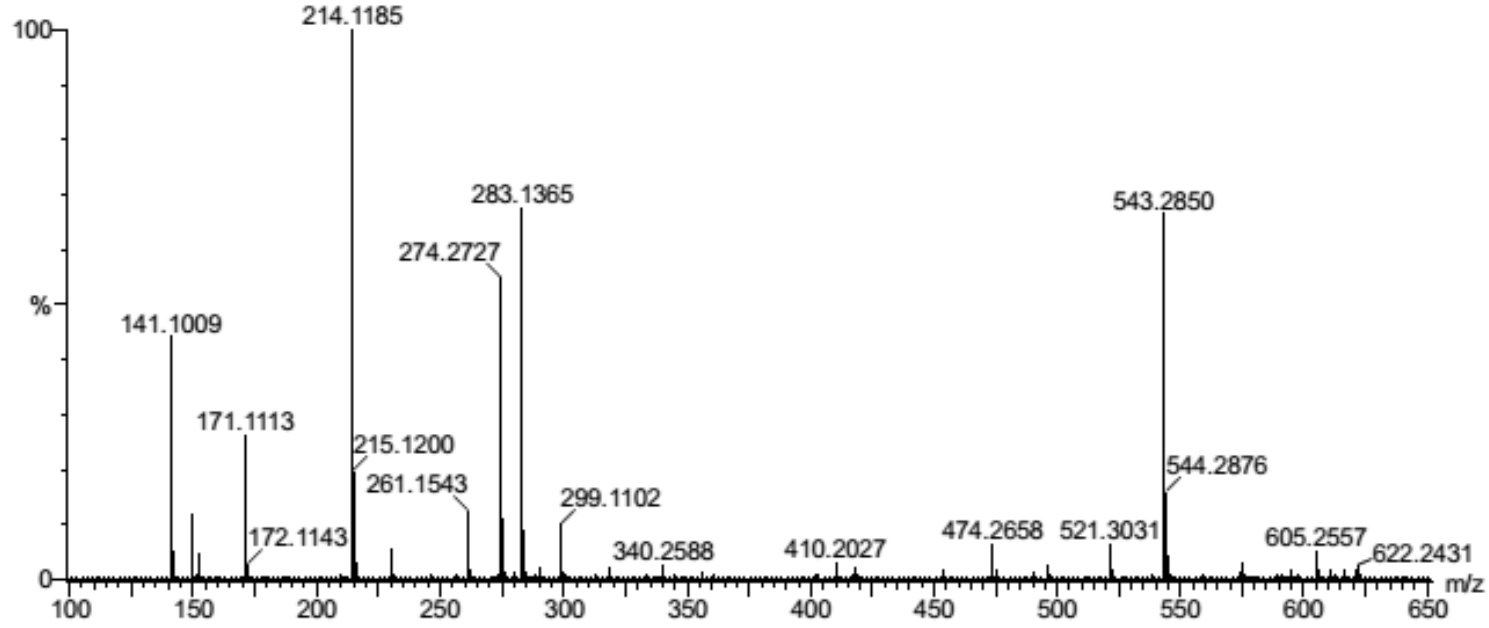
Elemental Composition Report

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 = 3

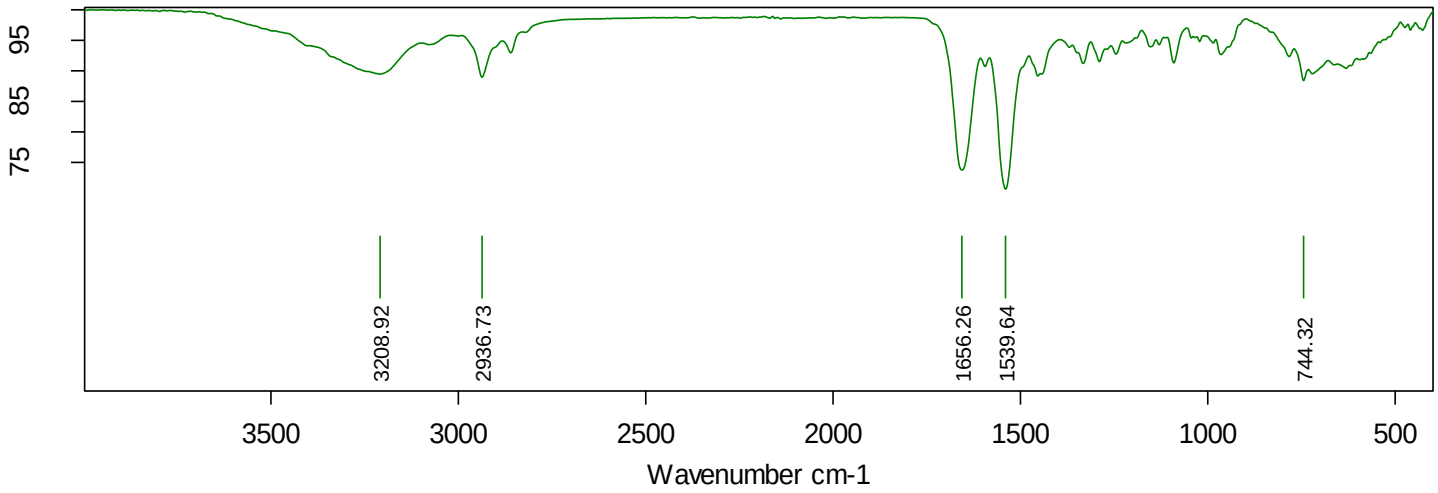
Monoisotopic Mass, Even Electron Ions
62 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-35 H: 7-40 N: 0-4 O: 1-5

Sample Name : 18-01-370 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
031219-18-01-370 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (7:21) 1: TOF MS ES+
1.53e+008



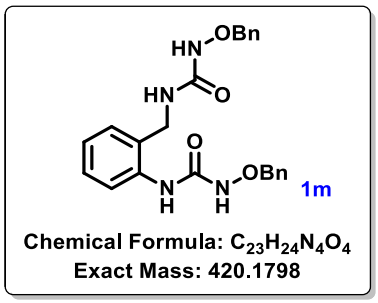
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
261.1543	261.1563	-2.0	-7.7	2.5	884.3	n/a	n/a	C10 H21 N4 O4

FTIR of 1l



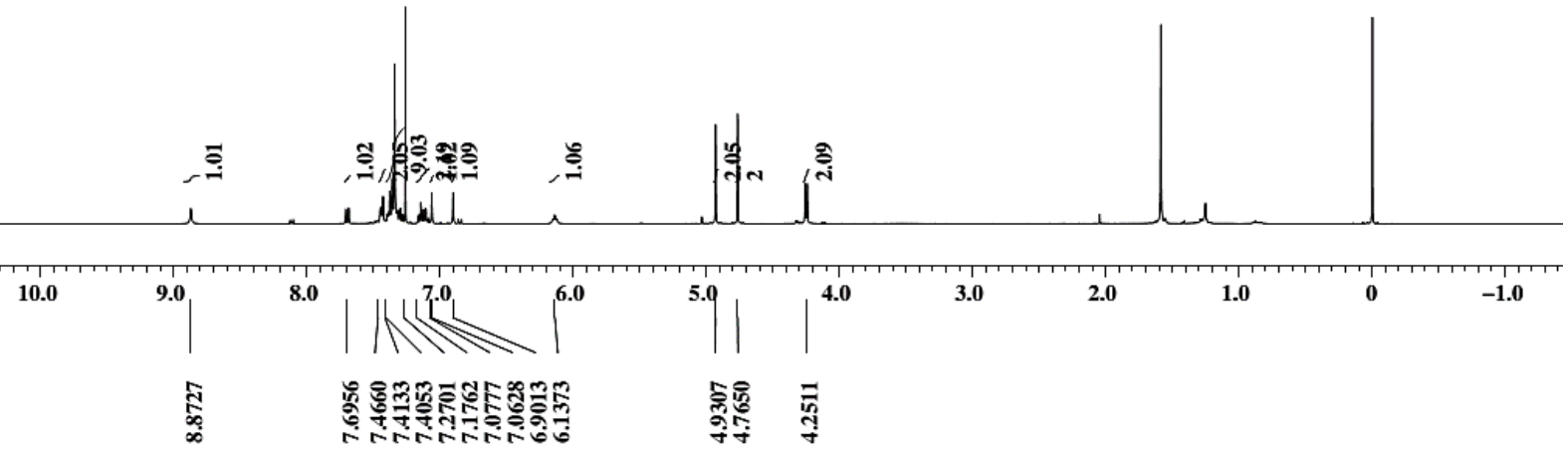
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-370.0	18-01-370	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	1.000203
3996.073013	0.999932
3994.643803	0.999686
3993.214592	0.999500
3991.785381	0.999403
3990.356171	0.999406
3988.926960	0.999490
3987.497749	0.999621
3986.068539	0.999763
3984.639328	0.999889
3983.210117	0.999989
3981.780907	1.000063
3980.351696	1.000113
3978.922485	1.000136
3977.493275	1.000125
3976.064064	1.000075
3974.634853	0.999993
3973.205643	0.999898
3971.776432	0.999809
3970.347221	0.999736
3968.918011	0.999678

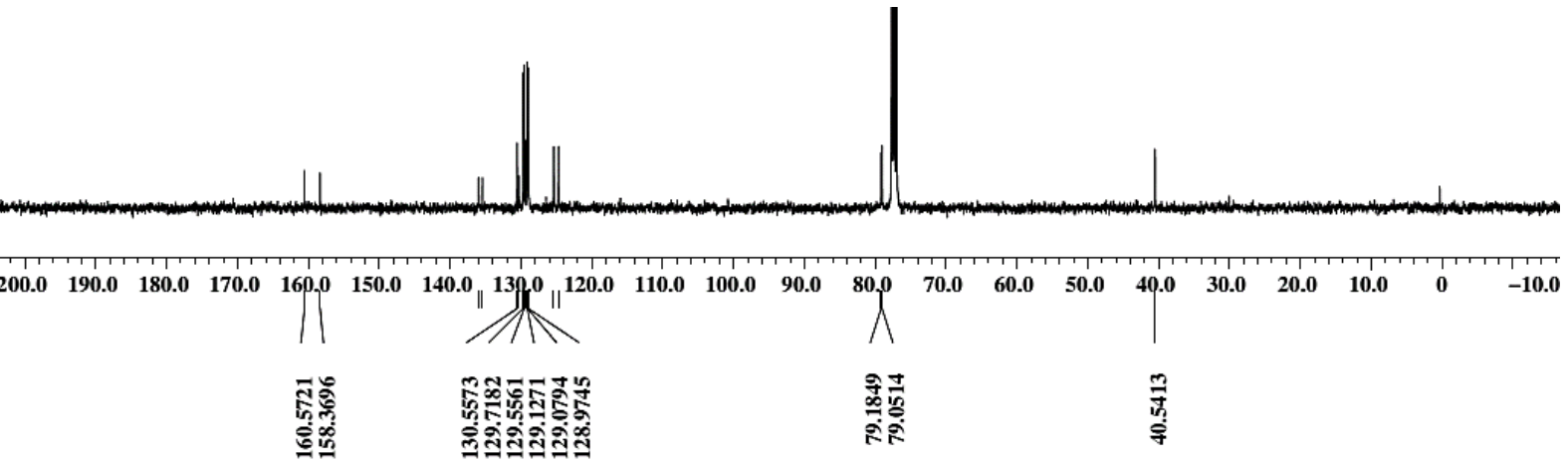


Chemical Formula: $C_{23}H_{24}N_4O_4$
Exact Mass: 420.1798

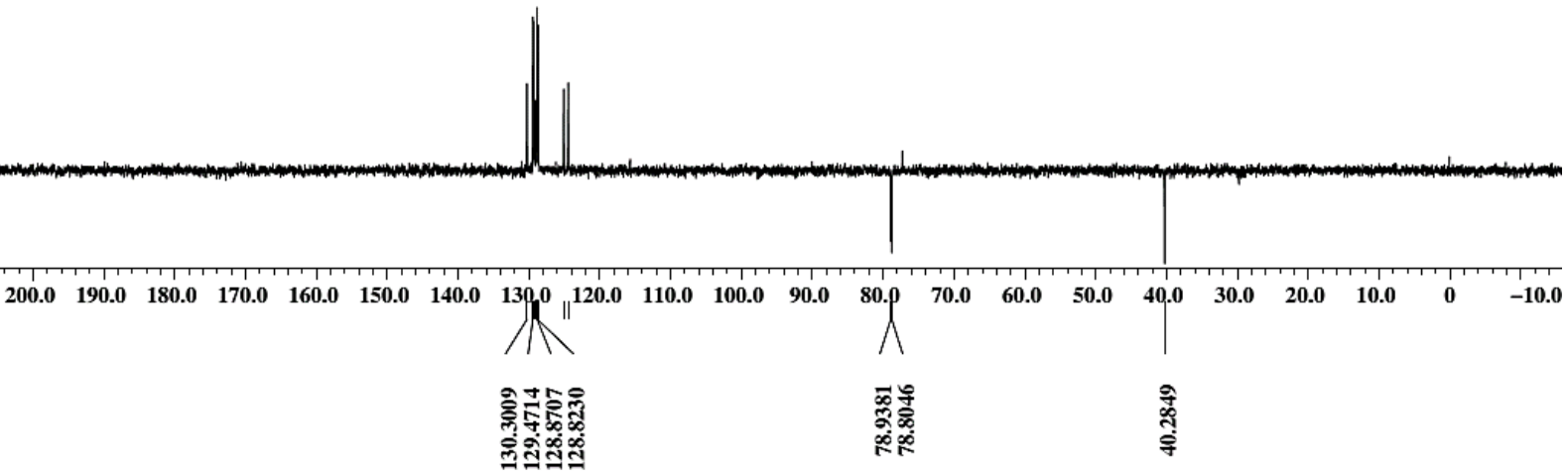
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1m



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1m



HRMS of 1m

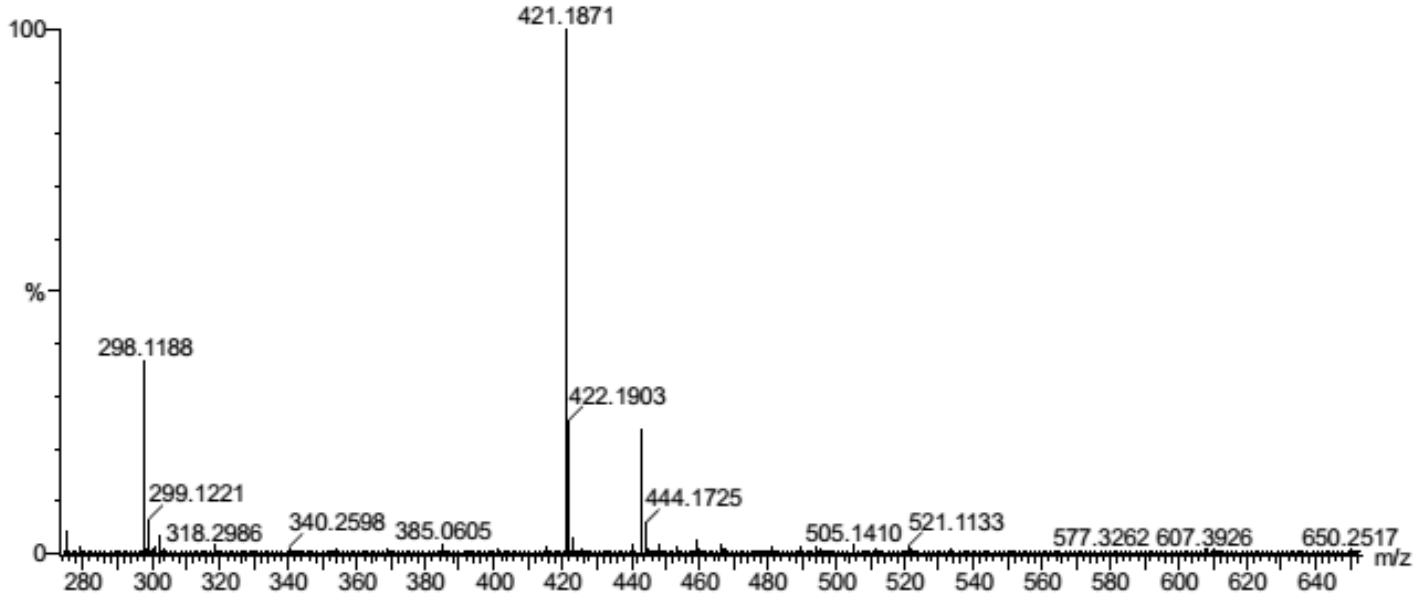
Elemental Composition Report

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 = 3

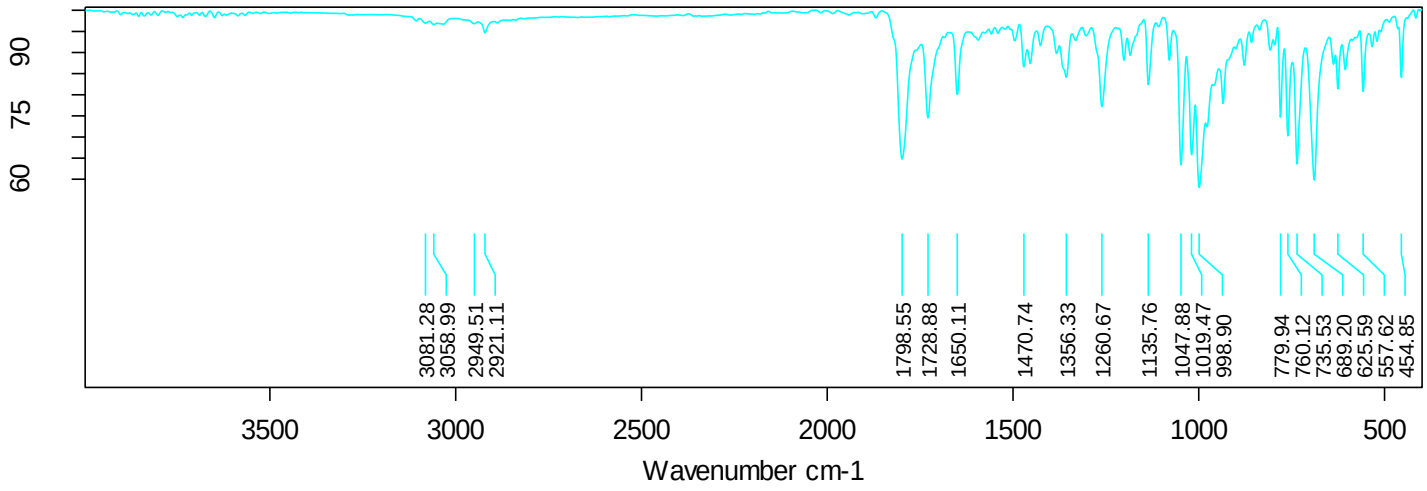
Monoisotopic Mass, Even Electron Ions
79 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-25 H: 11-30 N: 0-6 O: 1-5 S: 0-1

Sample Name : 18-01-300-2 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
300919-18-01-300-2 19 (0.203) AM2 (Ar,22000.0,0.00,0.00); Cm (19:23) 1: TOF MS ES+
1.62e+007



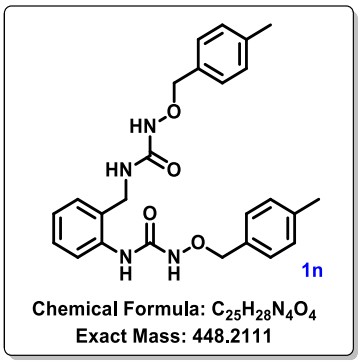
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
421.1871	421.1876	-0.5	-1.2	13.5	734.6	n/a	n/a	C23 H25 N4 O4

FTIR of 1m



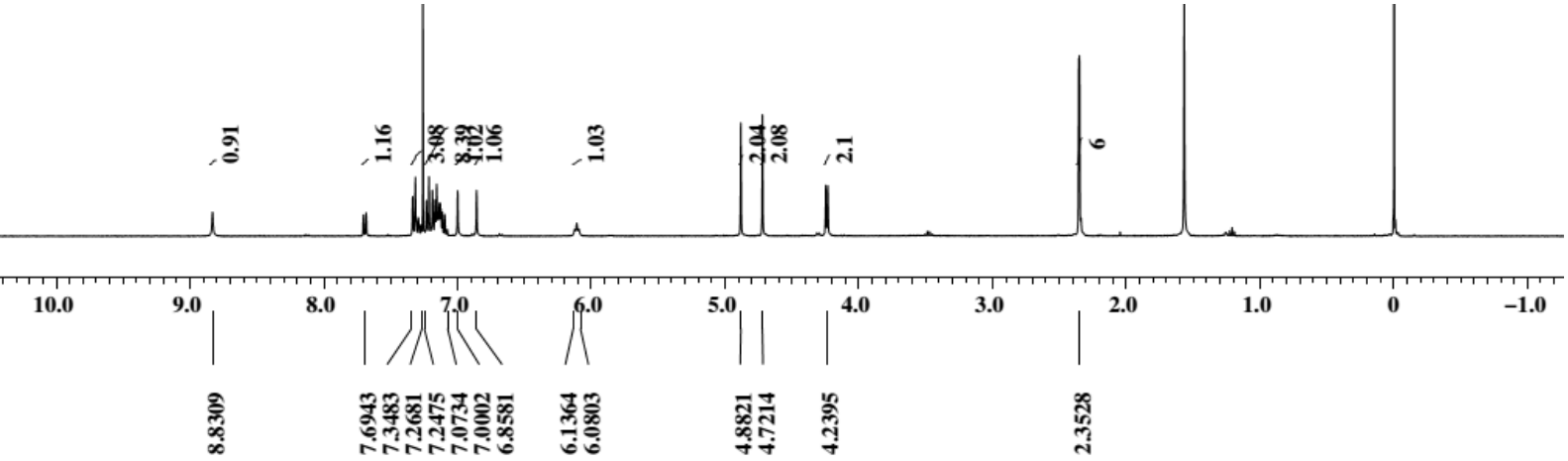
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-300-02.0	18-01-300-02	Instrument type and / or access	2/4/2020

Wavenumber cm-1	Transmittance [%]
3997.524564	0.999572
3996.095345	0.999554
3994.666126	0.999535
3993.236908	0.999517
3991.807689	0.999515
3990.378470	0.999560
3988.949252	0.999673
3987.520033	0.999828
3986.090814	0.999958
3984.661596	1.000000
3983.232377	0.999928
3981.803159	0.999753
3980.373940	0.999496
3978.944721	0.999170
3977.515503	0.998809
3976.086284	0.998486
3974.657065	0.998278
3973.227847	0.998218
3971.798628	0.998281
3970.369409	0.998409
3968.940191	0.998544

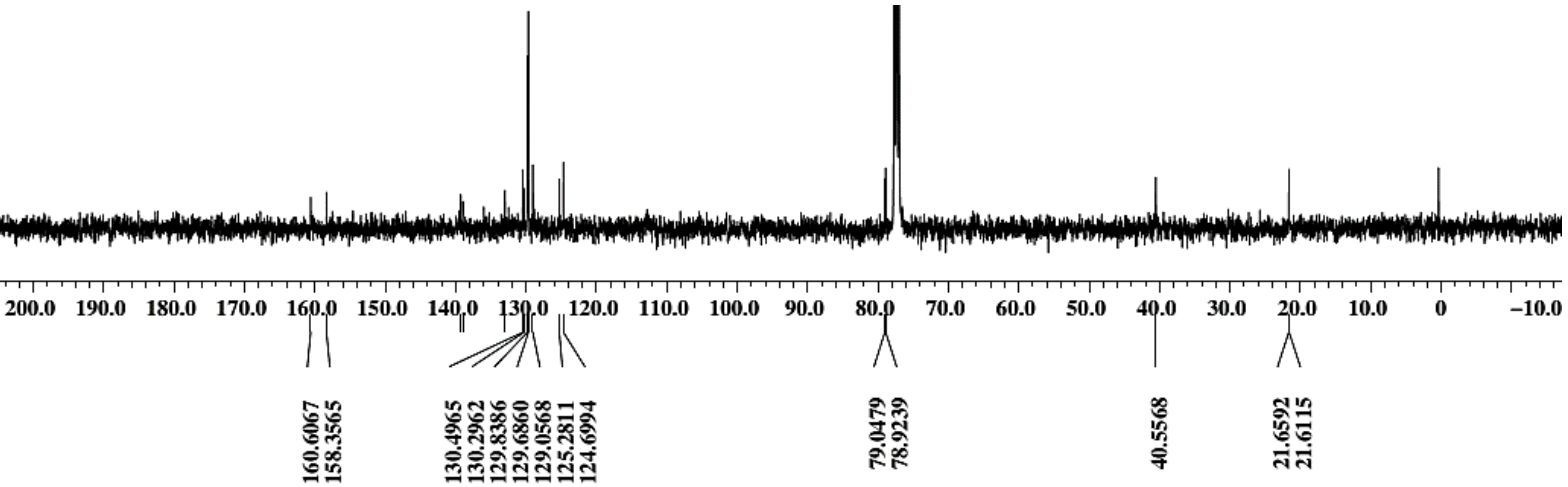


Chemical Formula: $C_{25}H_{28}N_4O_4$
Exact Mass: 448.2111

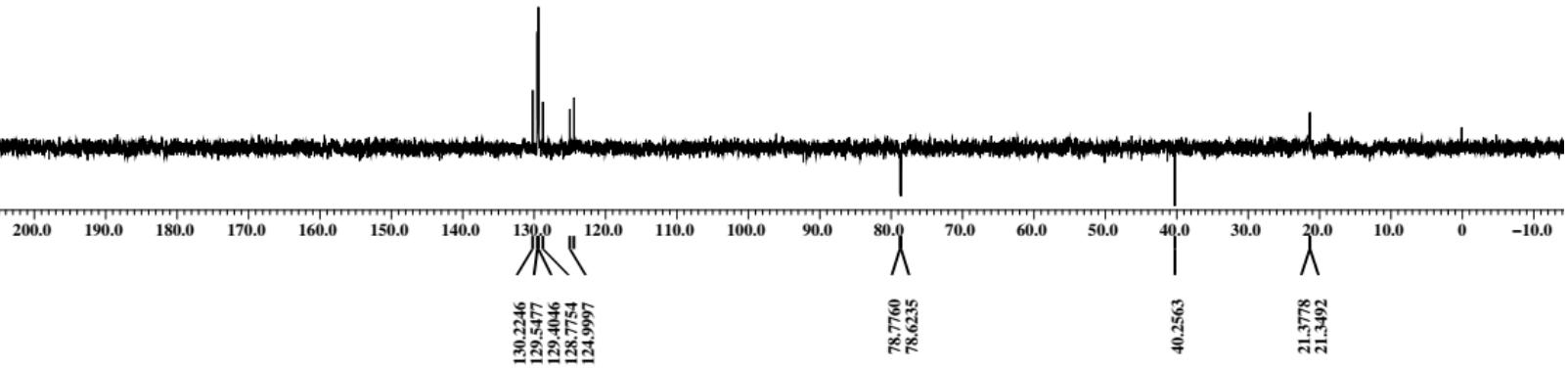
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1n



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1n



130.2246
129.5477
129.4046
128.7754
124.9997

78.7760
78.6235

40.2563

21.3778
21.3492

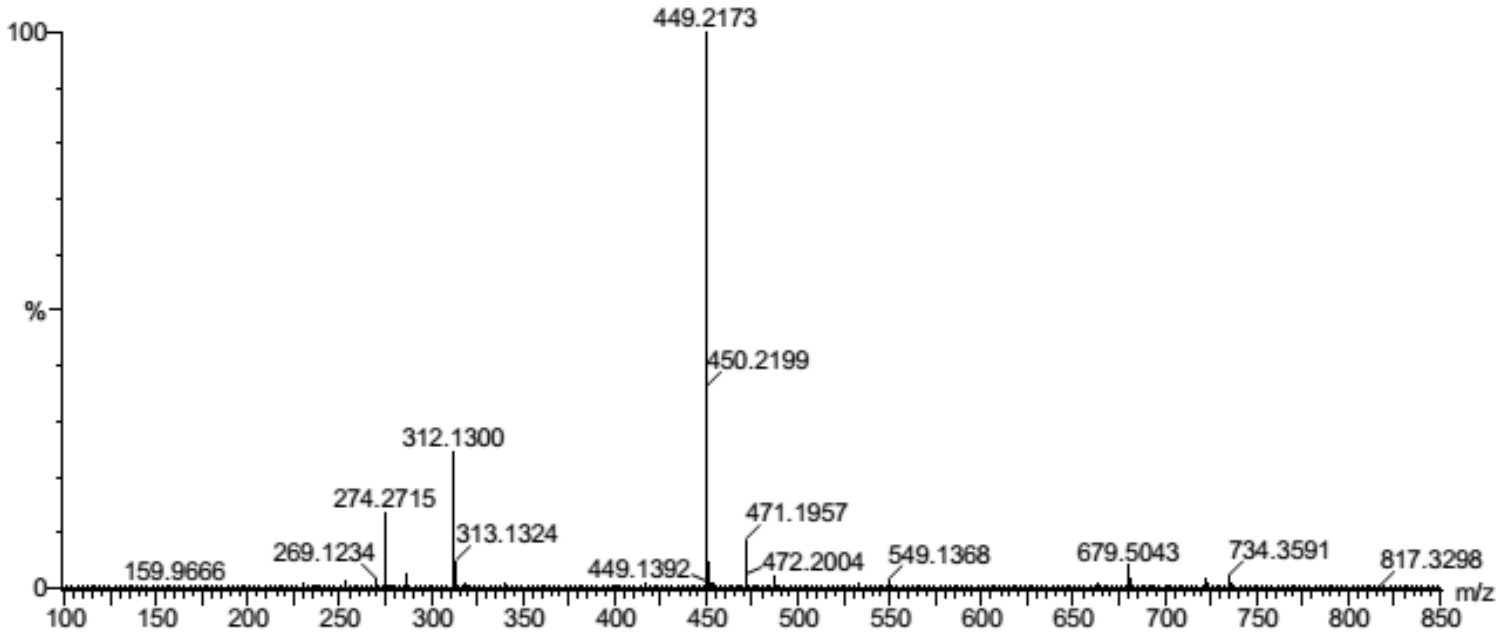
Elemental Composition Report

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 = 3

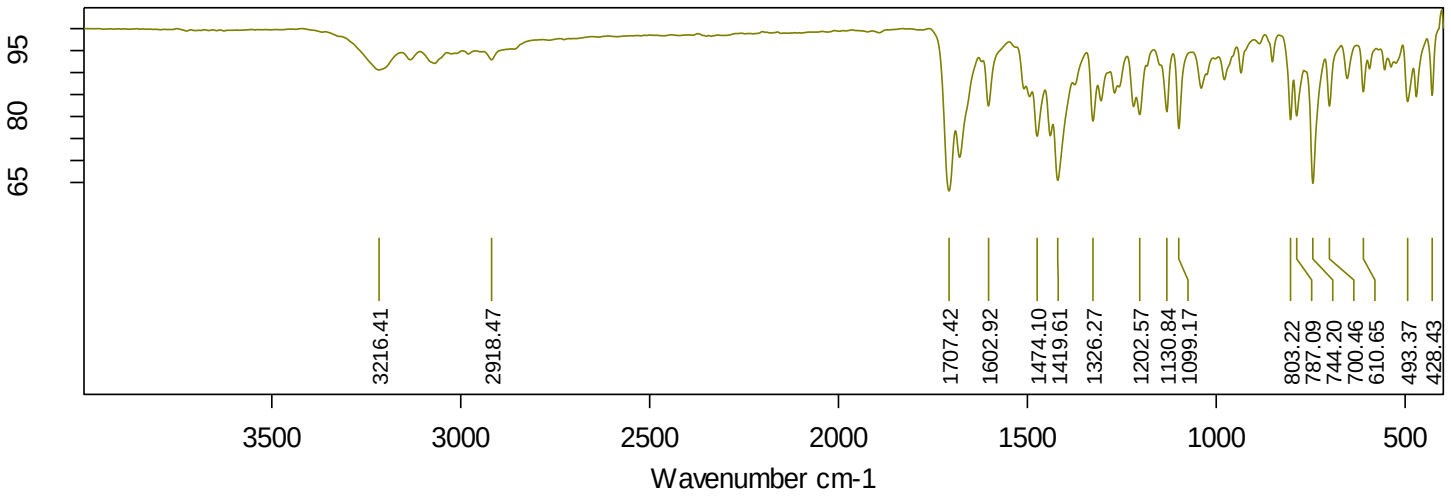
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 7-30 N: 0-4 O: 1-5

Sample Name : 18-01-362 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
271119-18-01-362 17 (0.174) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (17:18) 1: TOF MS ES+
2.45e+007



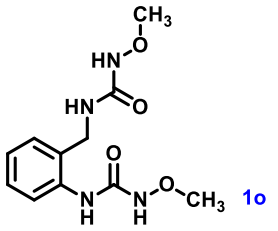
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
449.2173	449.2189	-1.6	-3.6	13.5	963.4	n/a	n/a	C25 H29 N4 O4

FTIR of 1n



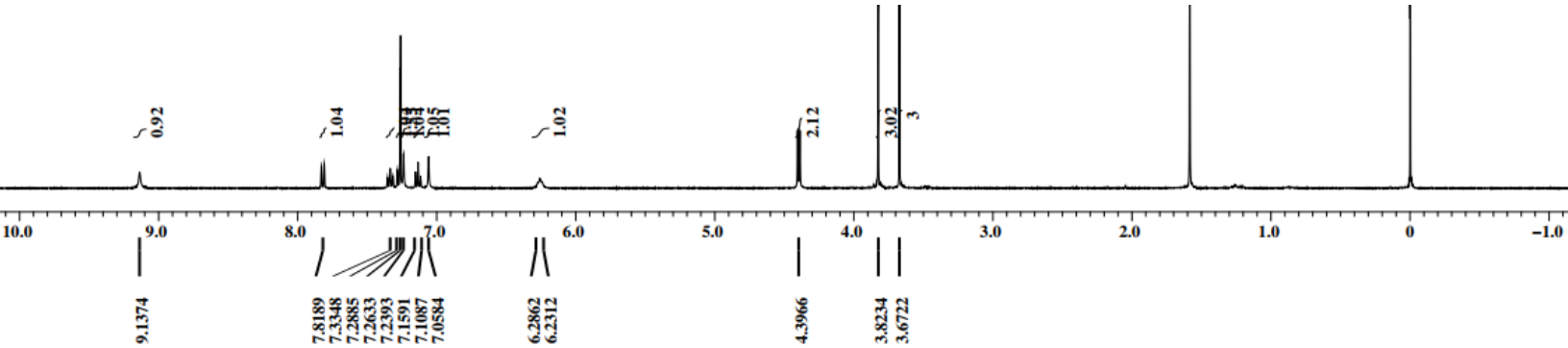
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-362.0	18-01-362	Instrument type and / or accessory	2/4/2020

Wavenumber cm-1	Transmittance [%]
3997.524564	1.000507
3996.095345	1.000379
3994.666126	1.000256
3993.236908	1.000145
3991.807689	1.000058
3990.378470	1.000005
3988.949252	0.999995
3987.520033	1.000017
3986.090814	1.000047
3984.661596	1.000057
3983.232377	1.000031
3981.803159	0.999975
3980.373940	0.999904
3978.944721	0.999832
3977.515503	0.999773
3976.086284	0.999738
3974.657065	0.999734
3973.227847	0.999752
3971.798628	0.999776
3970.369409	0.999796
3968.940191	0.999815

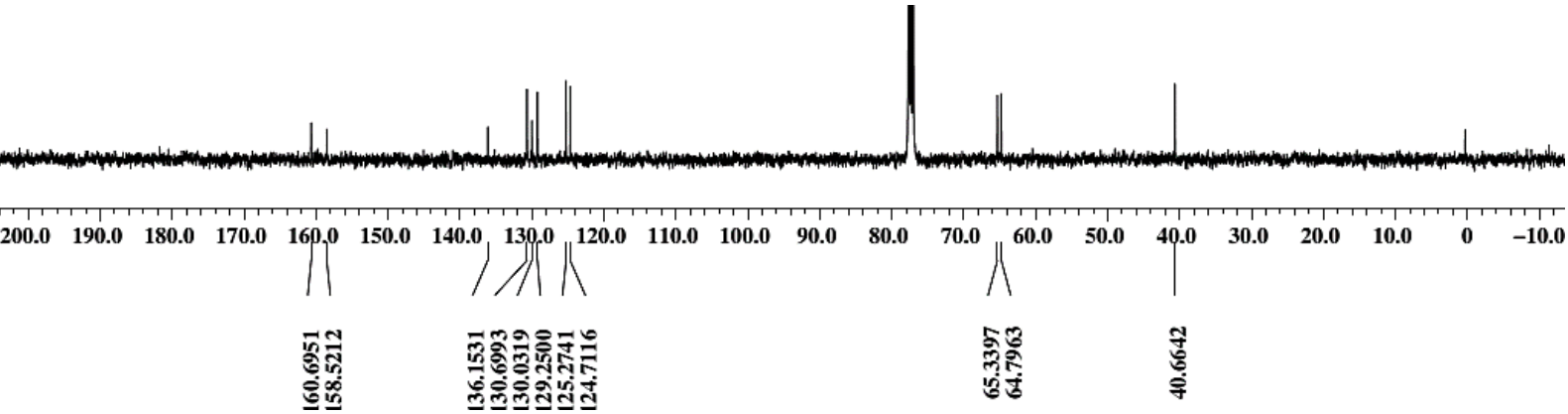


Chemical Formula: $C_{11}H_{16}N_4O_4$
Exact Mass: 268.1172

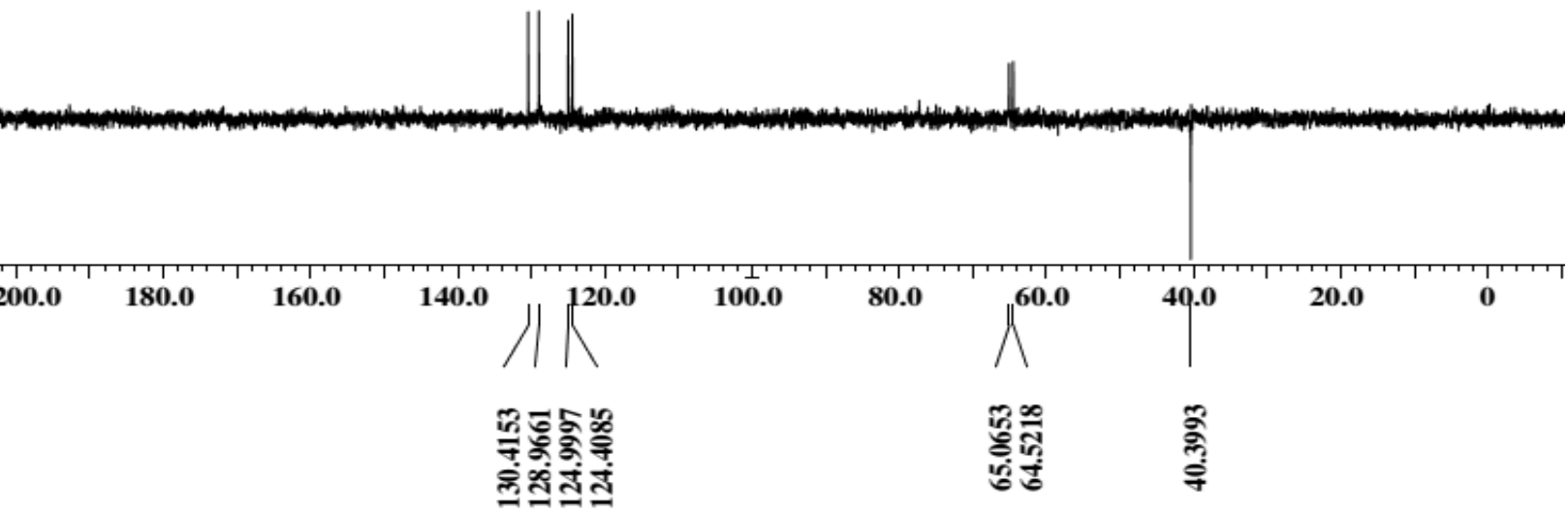
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1o



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1o



130.4153
128.9661
124.9997
124.4085
65.0653
64.5218
40.3993

HRMS of 1o

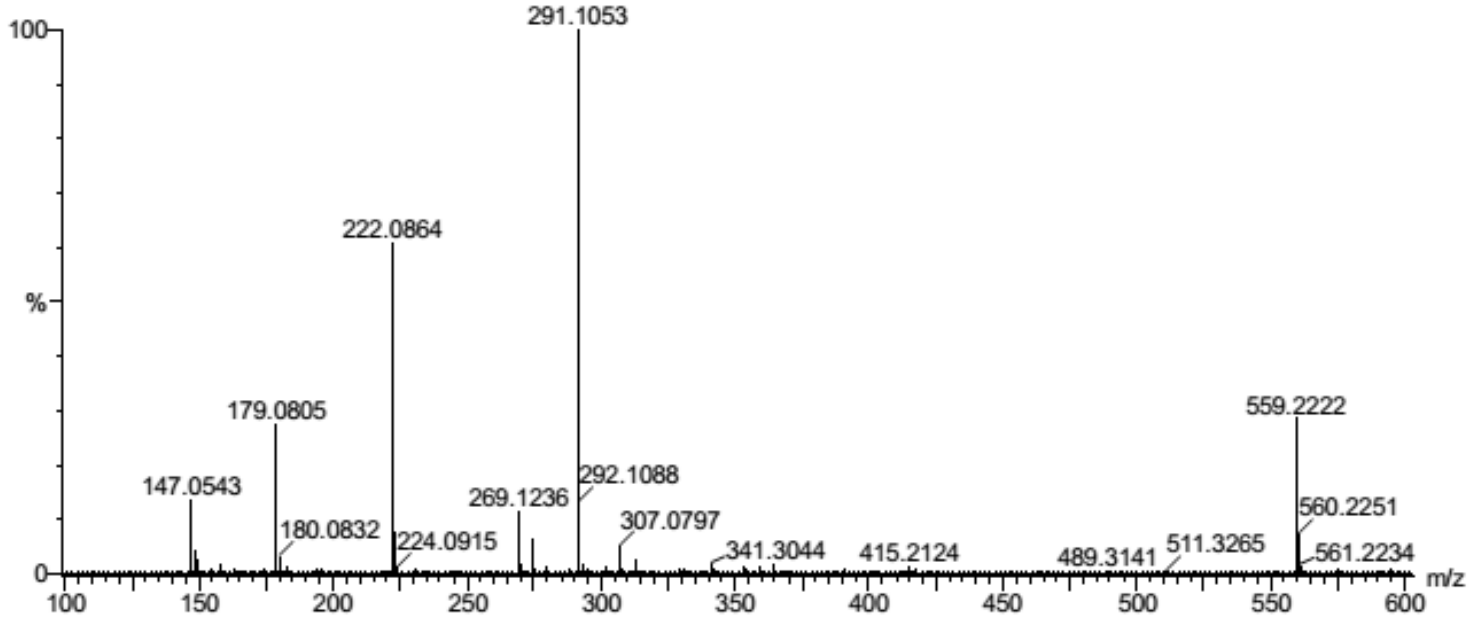
Elemental Composition Report

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 = 3

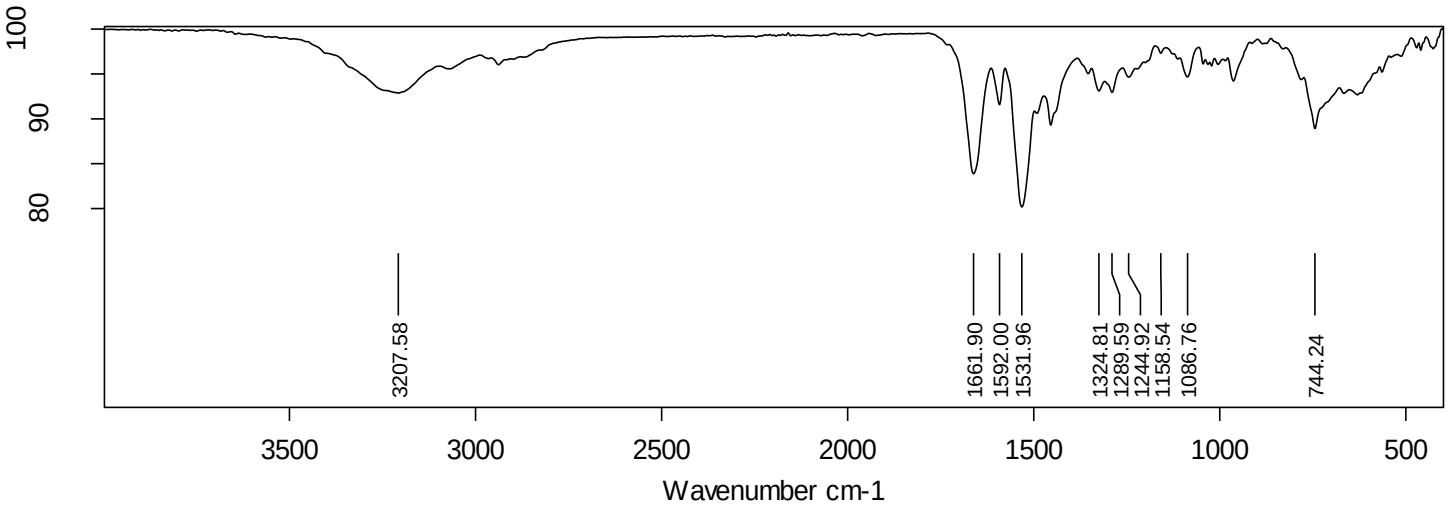
Monoisotopic Mass, Even Electron Ions
110 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-19 H: 10-35 N: 0-4 O: 0-5 Na: 0-1

Sample Name : 18-01-366 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
201219-18-01-366 17 (0.174) 1: TOF MS ES+
1.15e+007



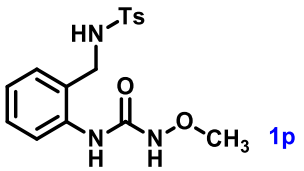
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
269.1236	269.1250	-1.4	-5.2	5.5	830.5	n/a	n/a	C11 H17 N4 O4

FTIR of 1o



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-366.0	18-01-366	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	1.000000
3996.073013	0.999883
3994.643803	0.999773
3993.214592	0.999685
3991.785381	0.999634
3990.356171	0.999624
3988.926960	0.999643
3987.497749	0.999677
3986.068539	0.999716
3984.639328	0.999756
3983.210117	0.999798
3981.780907	0.999832
3980.351696	0.999849
3978.922485	0.999842
3977.493275	0.999817
3976.064064	0.999783
3974.634853	0.999752
3973.205643	0.999729
3971.776432	0.999715
3970.347221	0.999697
3968.918011	0.999662

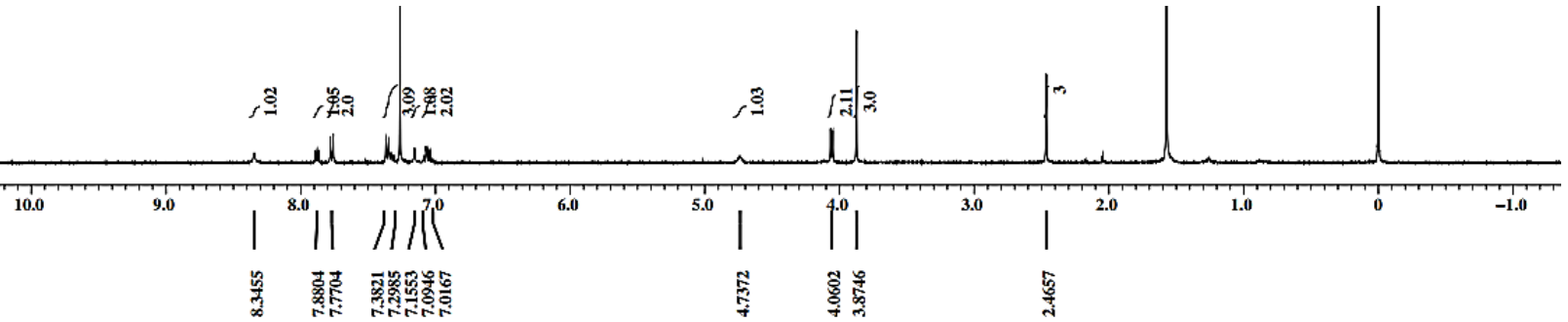


1p

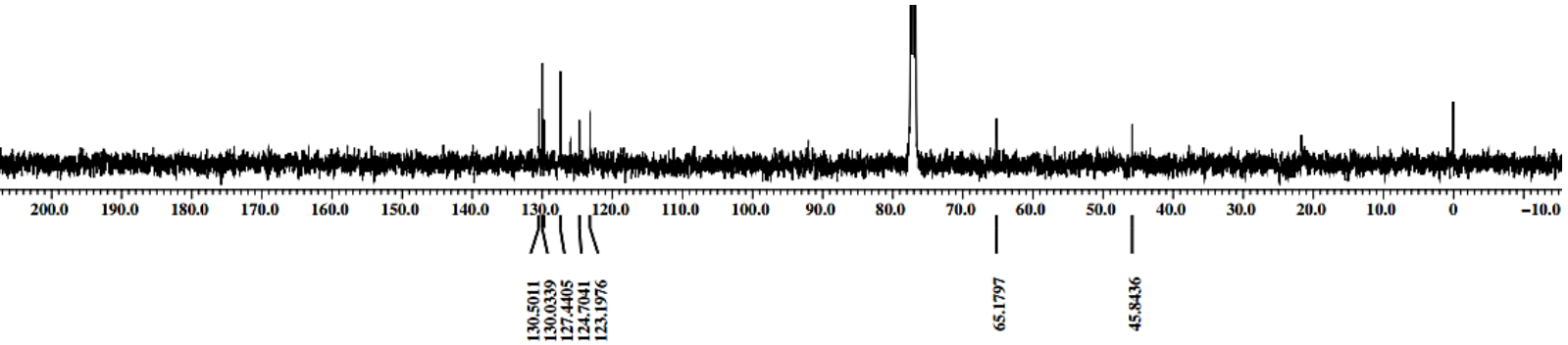
Chemical Formula: $C_{16}H_{19}N_3O_4S$

Exact Mass: 349.1096

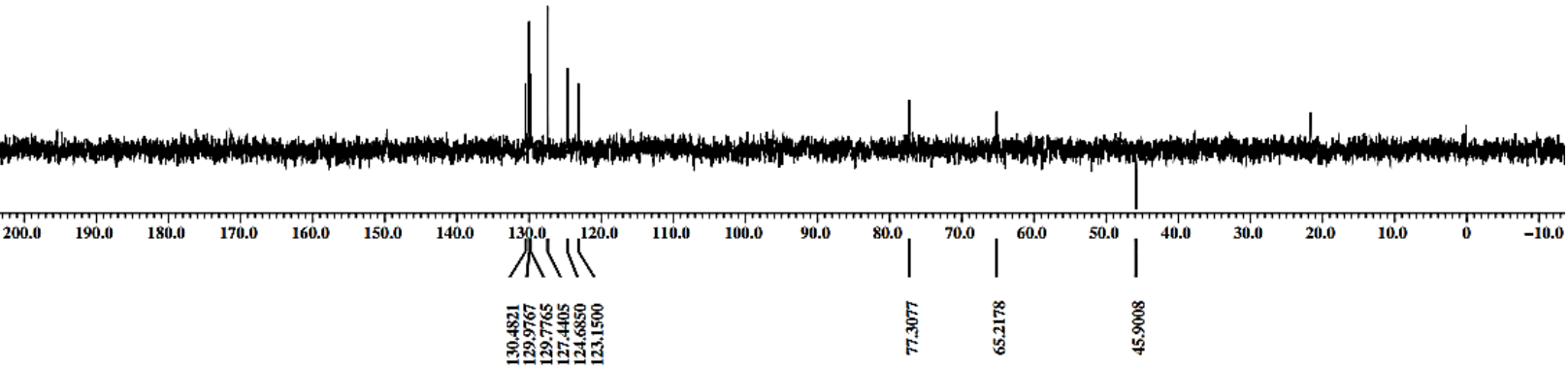
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1p



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1p



HRMS of 1p

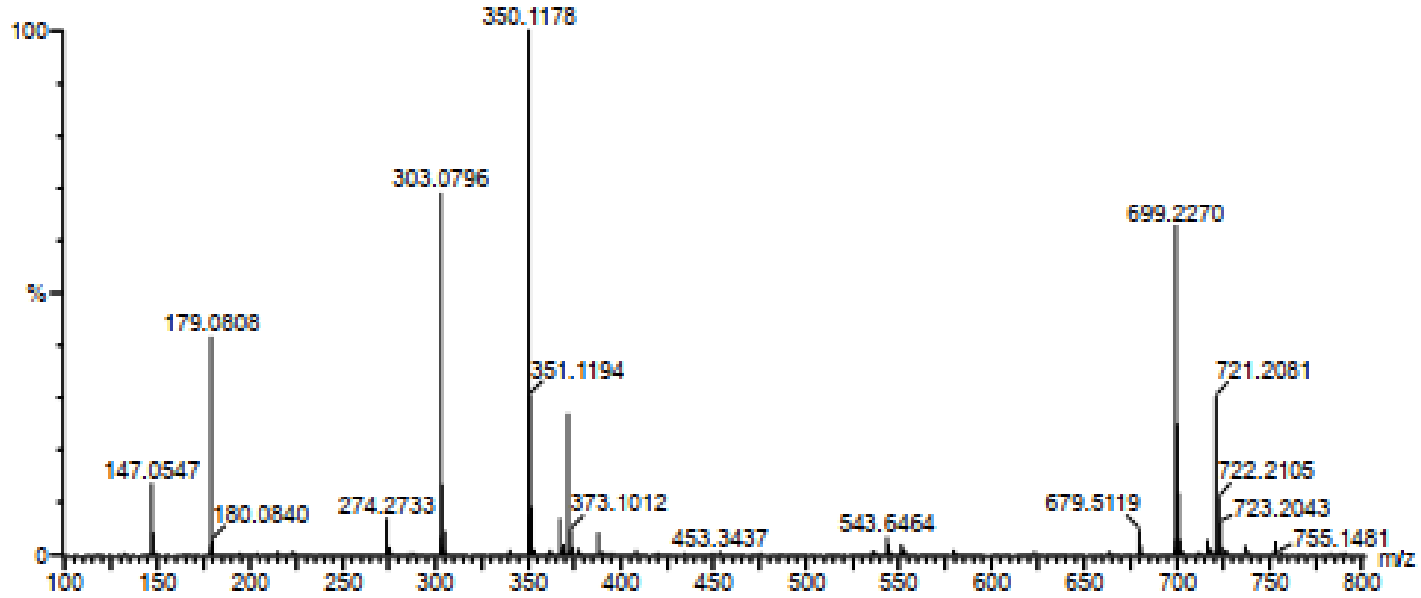
Elemental Composition Report

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 = 6

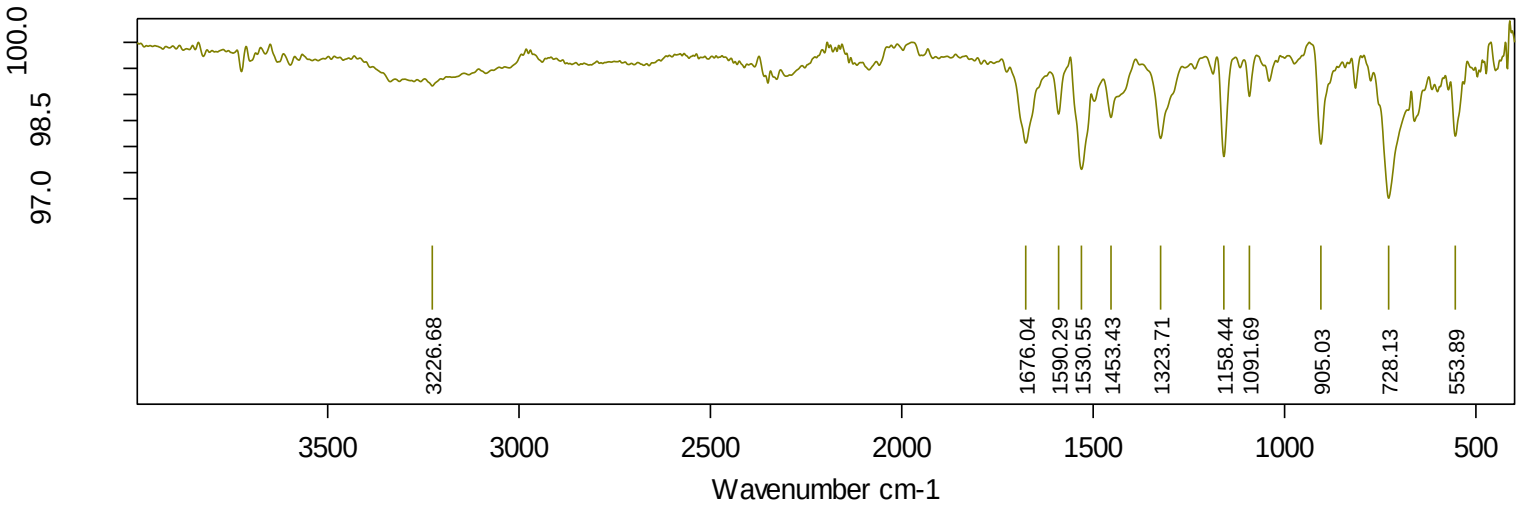
Monoisotopic Mass, Even Electron Ions
47 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-20 H: 11-20 N: 1-3 O: 0-4 S: 1-4

Sample Name : 18-01-429-2 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
081020-18-01-429-2- 17 (0.174) 1: TOF MS ES+
3.57e+007



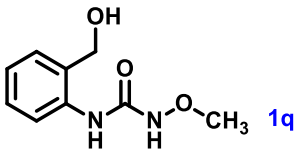
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
350.1178	350.1175	0.3	0.9	8.5	1215.7	n/a	n/a	C16 H20 N3 O4 S

FTIR of 1p



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-429.2	18-01-429	Instrument type and / or accessory	10/21/2020

Wavenumber cm-1	Transmittance [%]
3997.658602	1.000000
3996.229335	0.999860
3994.800069	0.999750
3993.370802	0.999696
3991.941536	0.999704
3990.512269	0.999752
3989.083002	0.999797
3987.653736	0.999798
3986.224469	0.999730
3984.795203	0.999594
3983.365936	0.999420
3981.936670	0.999258
3980.507403	0.999153
3979.078136	0.999131
3977.648870	0.999182
3976.219603	0.999267
3974.790337	0.999336
3973.361070	0.999355
3971.931804	0.999328
3970.502537	0.999283
3969.073270	0.999260

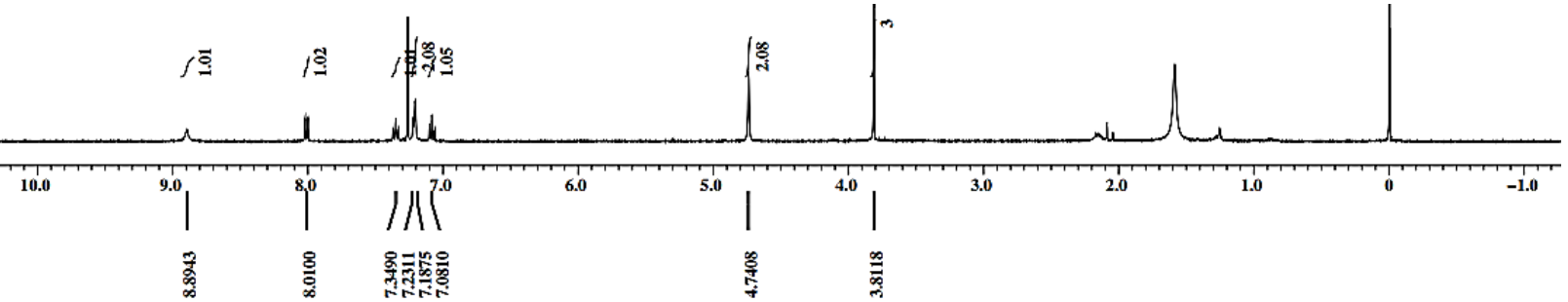


1q

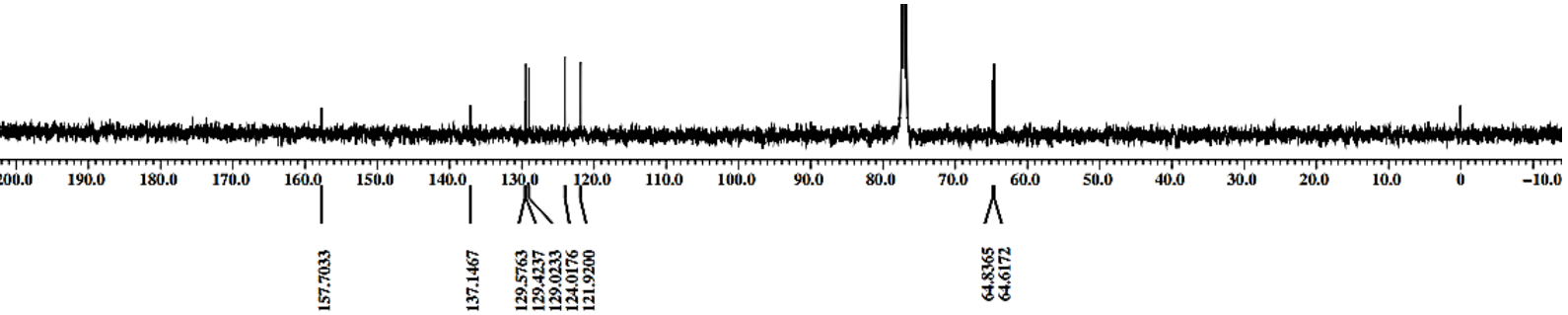
Chemical Formula: $C_9H_{12}N_2O_3$

Exact Mass: 196.0848

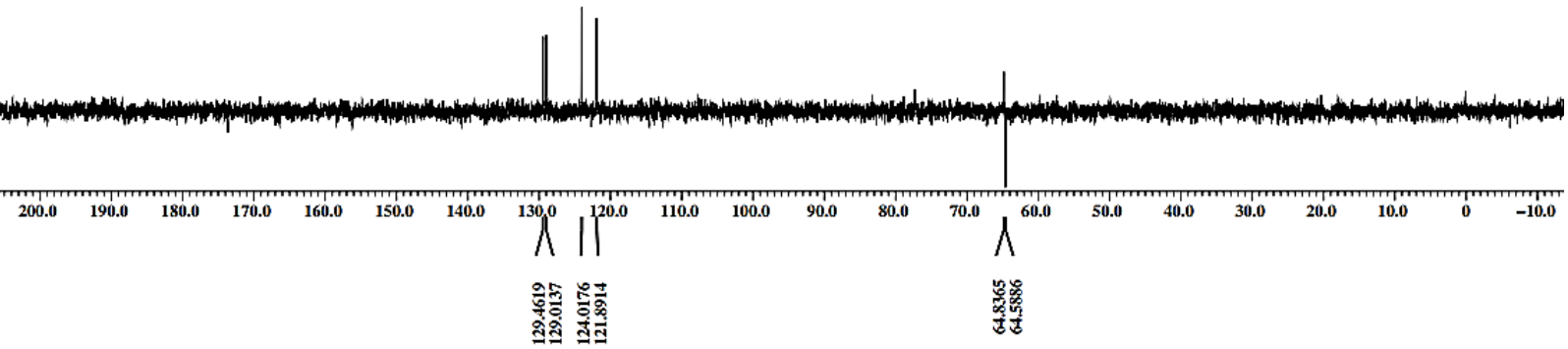
^{1}H-NMR ($CDCl_3$, 400 MHz) of 1q



^{13}C-NMR ($CDCl_3$, 100 MHz) of 1q



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 1q



HRMS of 1q

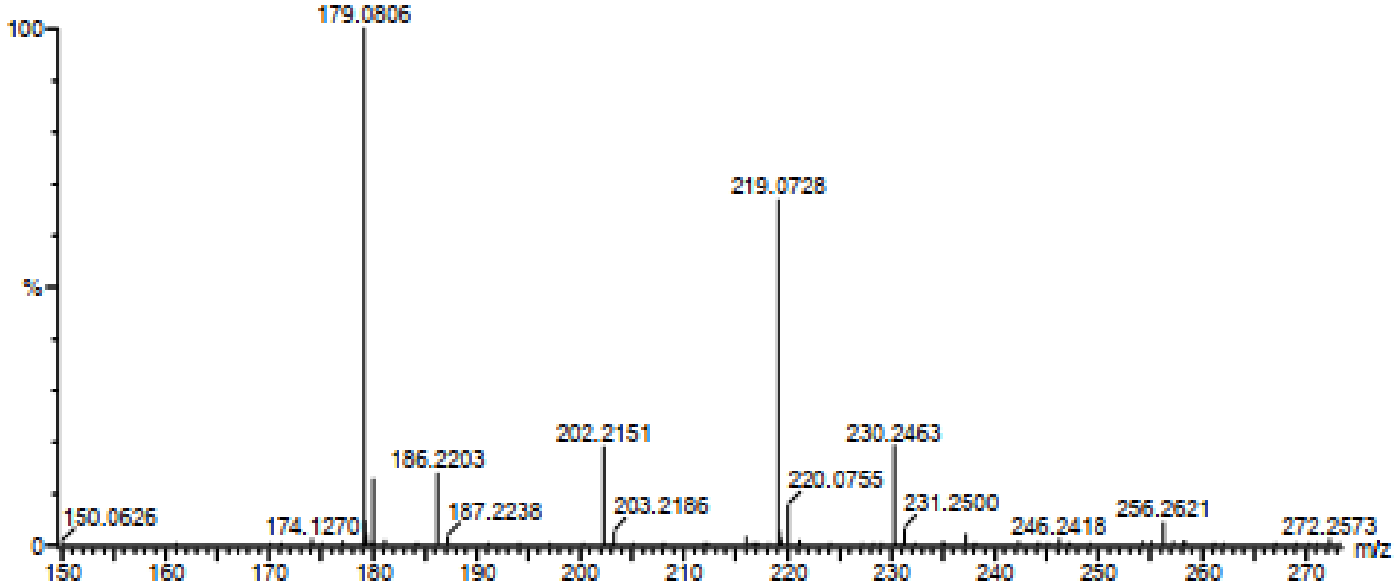
Elemental Composition Report

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 = 6

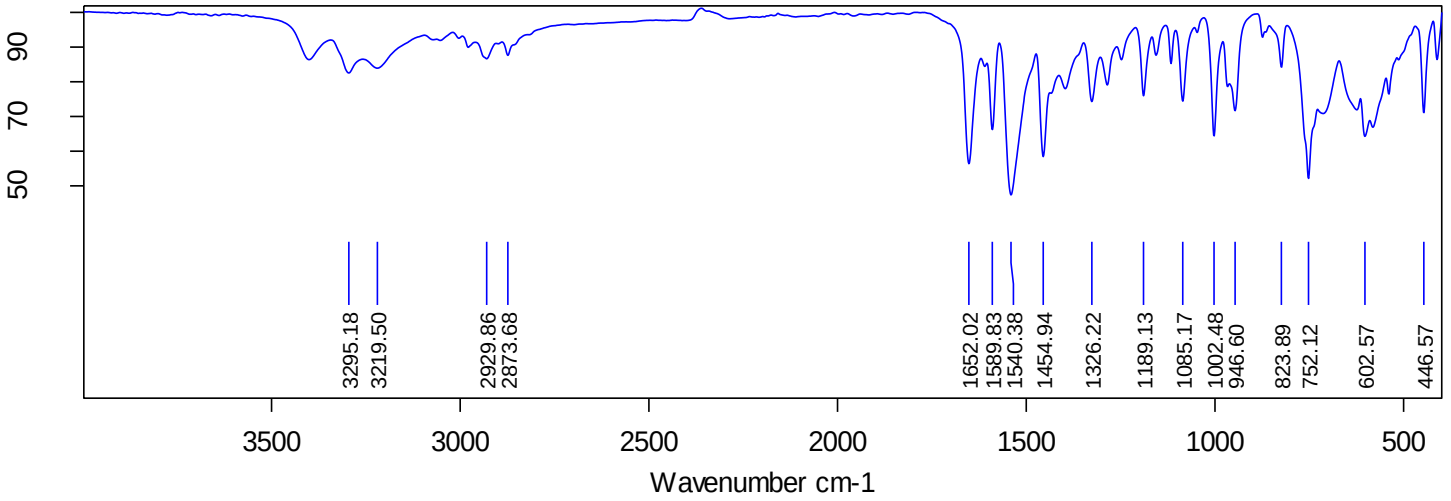
Monoisotopic Mass, Even Electron Ions
97 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 8-40 H: 11-45 N: 0-4 O: 0-4 Na: 0-1

Sample Name : 18-01-423 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
011020-18-01-423 12 (0.131) 1: TOF MS ES+
9.65e+007



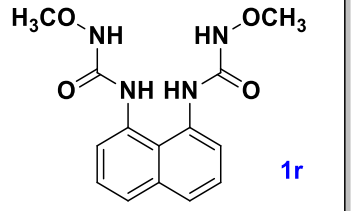
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
219.0728	219.0746	-1.8	-8.2	4.5	2266.1	n/a	n/a	C9 H12 N2 O3 Na

FTIR of 1q



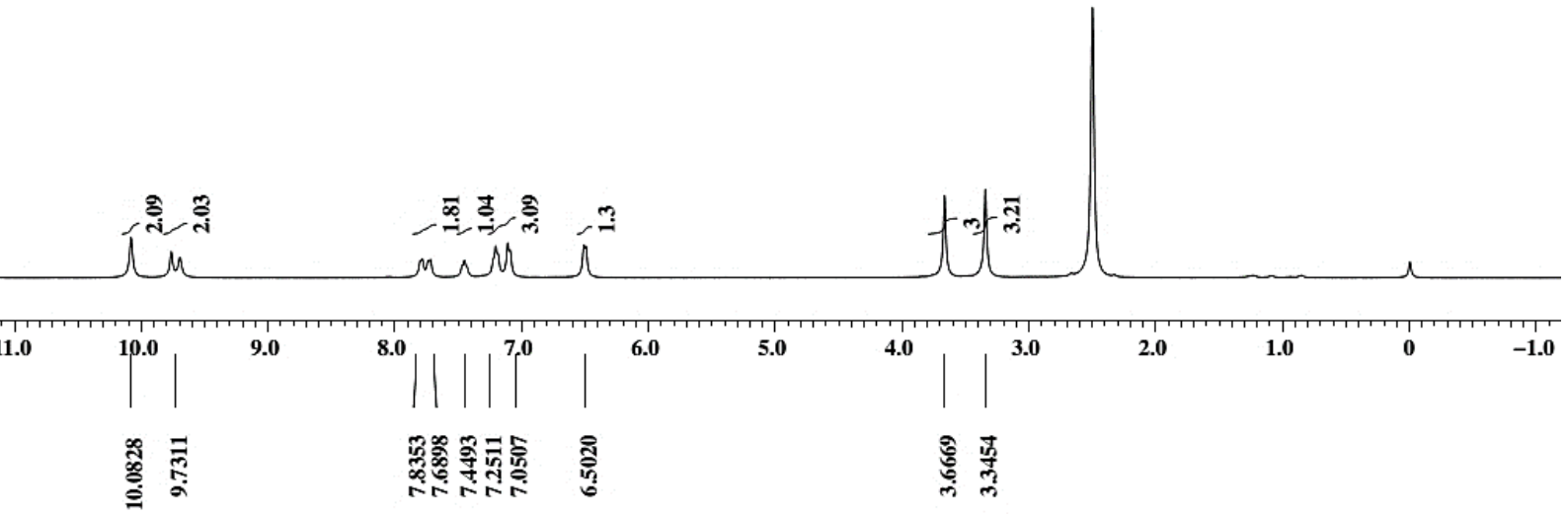
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-423.0	18-01-423	Instrument type and / or accessory	10/21/2020

Wavenumber cm-1	Transmittance [%]
3997.658602	1.002046
3996.229335	1.001923
3994.800069	1.001814
3993.370802	1.001730
3991.941536	1.001680
3990.512269	1.001669
3989.083002	1.001696
3987.653736	1.001741
3986.224469	1.001785
3984.795203	1.001817
3983.365936	1.001825
3981.936670	1.001793
3980.507403	1.001706
3979.078136	1.001560
3977.648870	1.001378
3976.219603	1.001204
3974.790337	1.001070
3973.361070	1.000978
3971.931804	1.000907
3970.502537	1.000832
3969.073270	1.000748

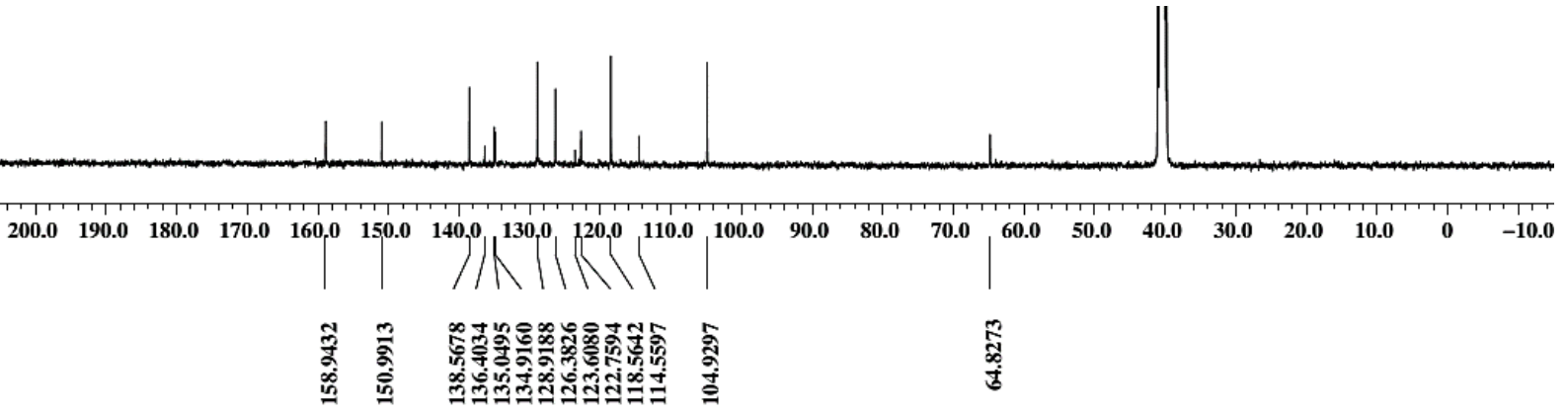


Chemical Formula: $C_{14}H_{16}N_4O_4$
Exact Mass: 304.1172

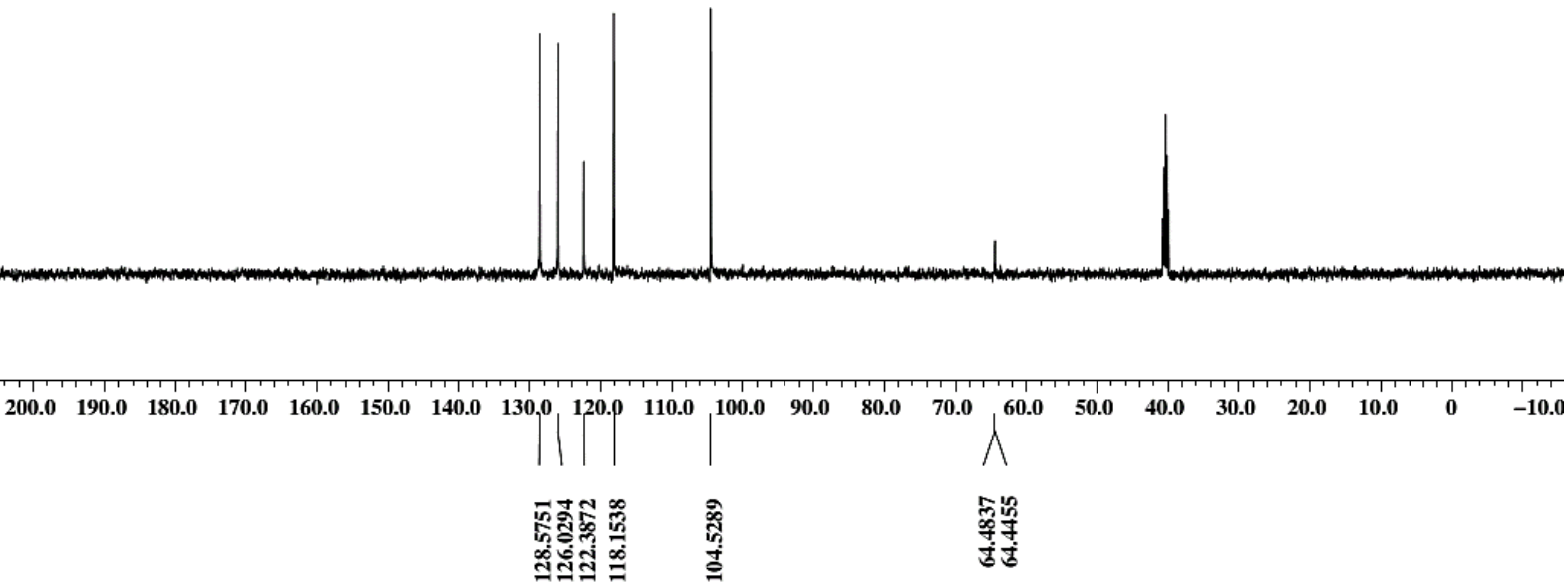
^{1}H-NMR (DMSO-d6, 400 MHz) of 1r



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



^{13}C-DEPT (DMSO-d6, 100 MHz) of 1r



HRMS of 1r

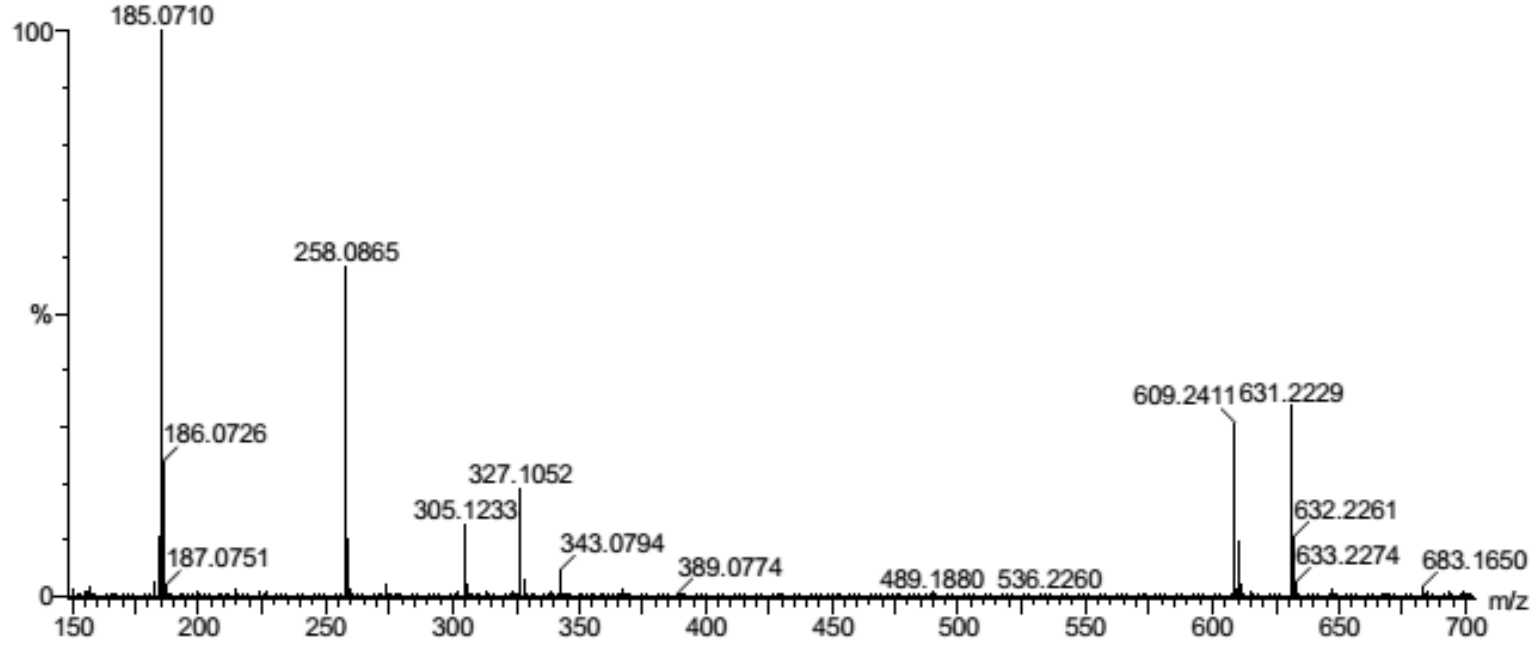
Elemental Composition Report

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 = 3

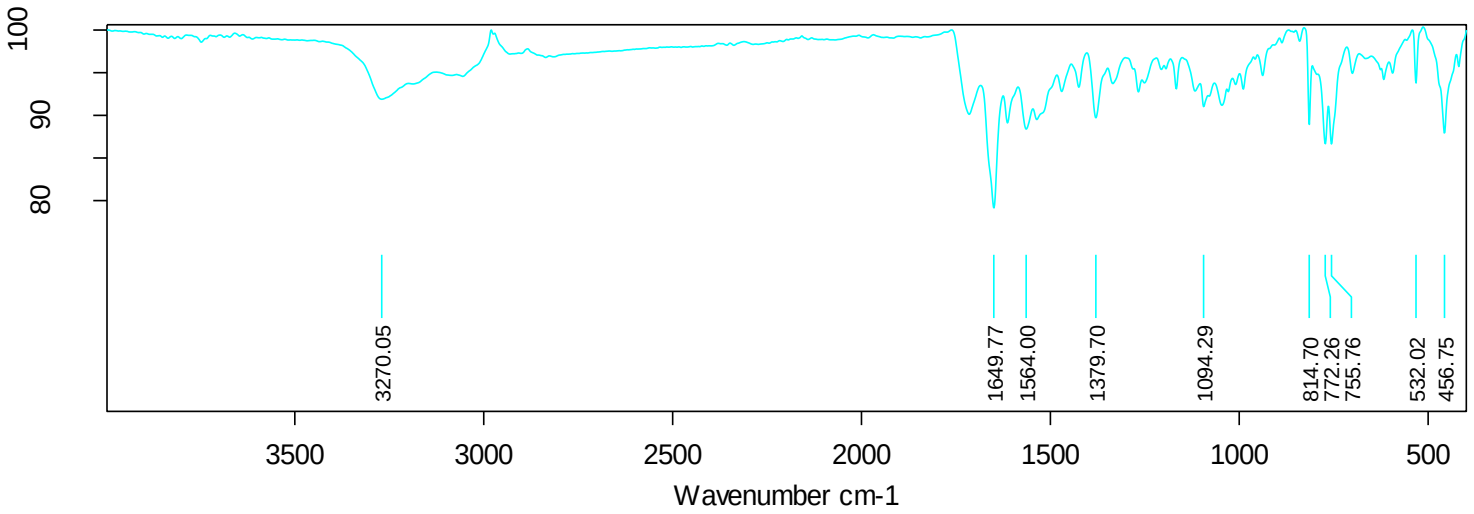
Monoisotopic Mass, Odd and Even Electron Ions
67 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-35 H: 11-35 N: 0-4 O: 1-4 I: 0-4

Sample Name : 18-01-372 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
051219-18-01-372- 16 (0.165) AM2 (Ar,22000.0,0.00,0.00); Cm (16:21) 1: TOF MS ES+
5.23e+007



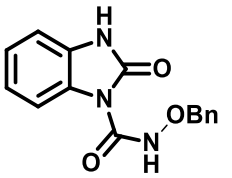
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
305.1233	305.1250	-1.7	-5.6	8.5	769.5	n/a	n/a	C14 H17 N4 O4

FTIR of 1r



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-372.0	18-01-372	Instrument type and / or accessory	1/6/2020

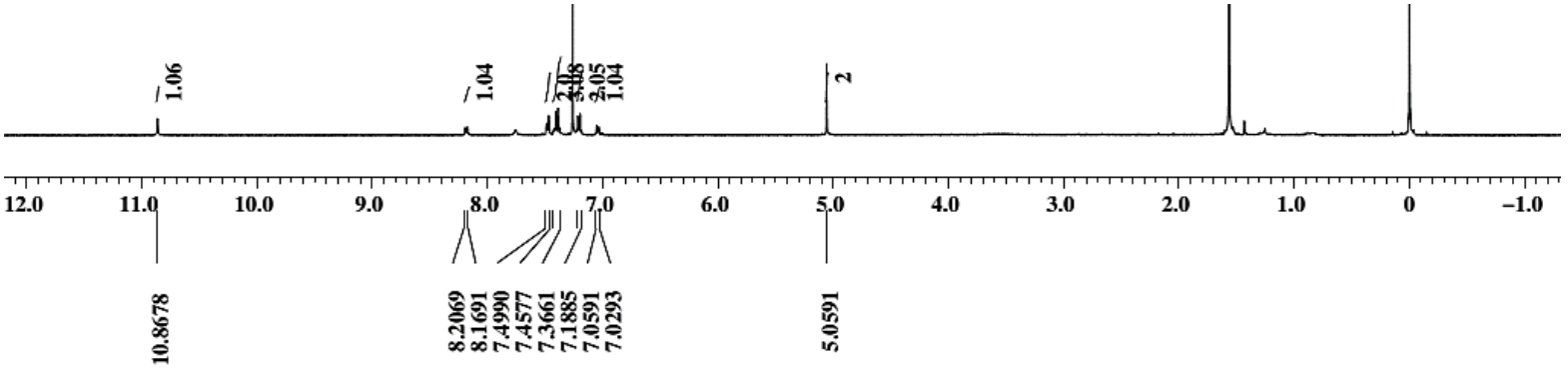
Wavenumber cm-1	Transmittance [%]
3997.502224	0.999866
3996.073013	0.999950
3994.643803	1.000004
3993.214592	1.000000
3991.785381	0.999916
3990.356171	0.999746
3988.926960	0.999507
3987.497749	0.999242
3986.068539	0.999005
3984.639328	0.998839
3983.210117	0.998772
3981.780907	0.998811
3980.351696	0.998939
3978.922485	0.999118
3977.493275	0.999281
3976.064064	0.999366
3974.634853	0.999348
3973.205643	0.999254
3971.776432	0.999134
3970.347221	0.999021
3968.918011	0.998929



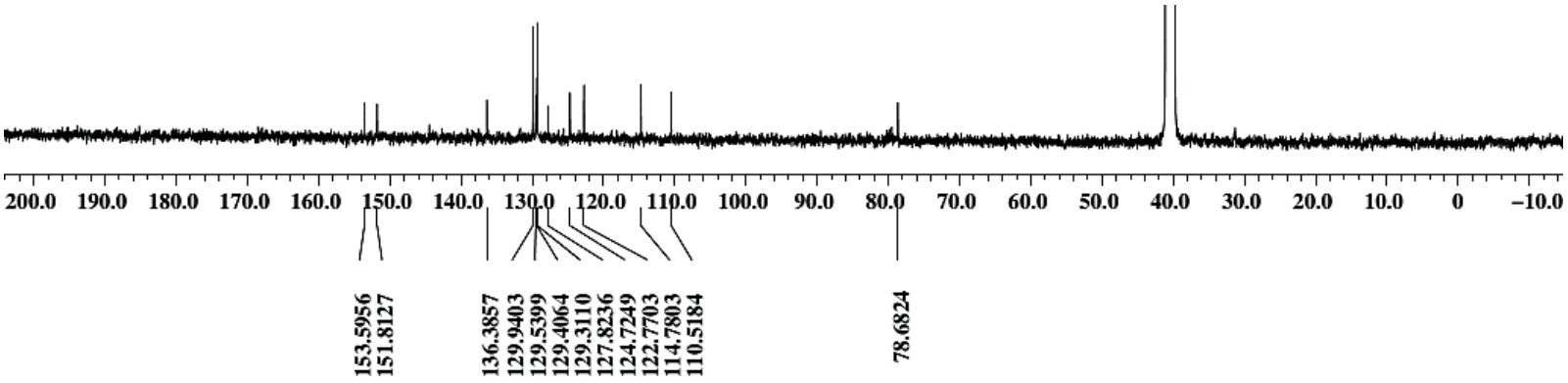
2a

Chemical Formula: $C_{15}H_{13}N_3O_3$
Exact Mass: 283.0957

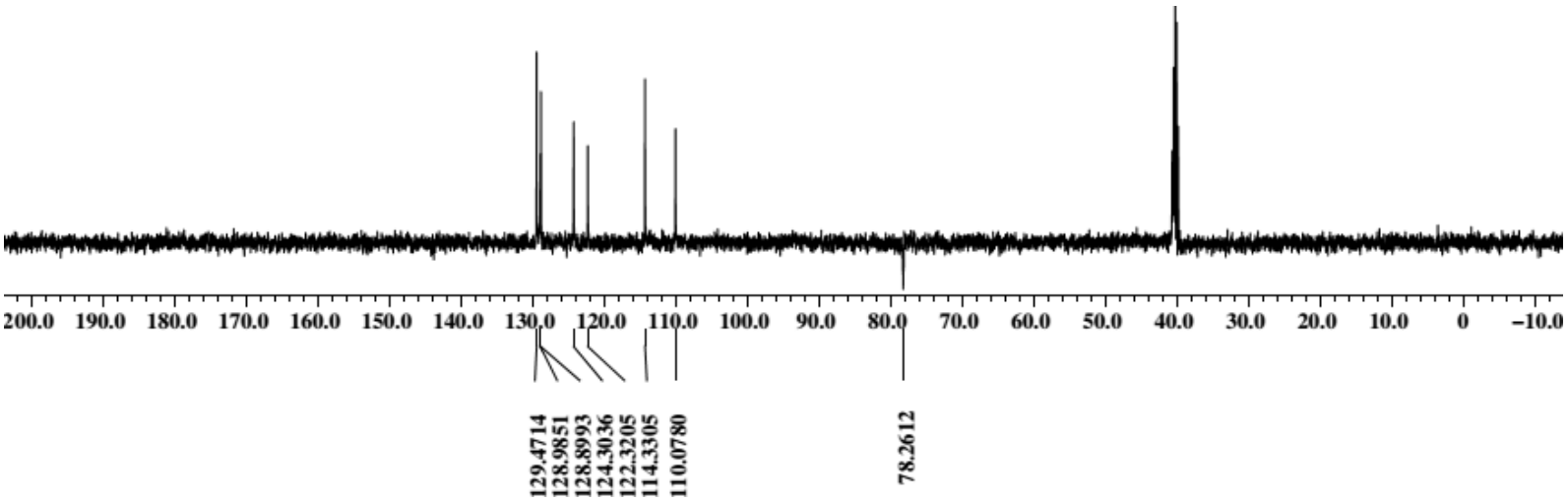
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2a



^{13}C-NMR (DMSO-d_6, 100 MHz) of 2a



^{13}C-DEPT (DMSO-d6, 100 MHz) of 2a



HRMS of 2a

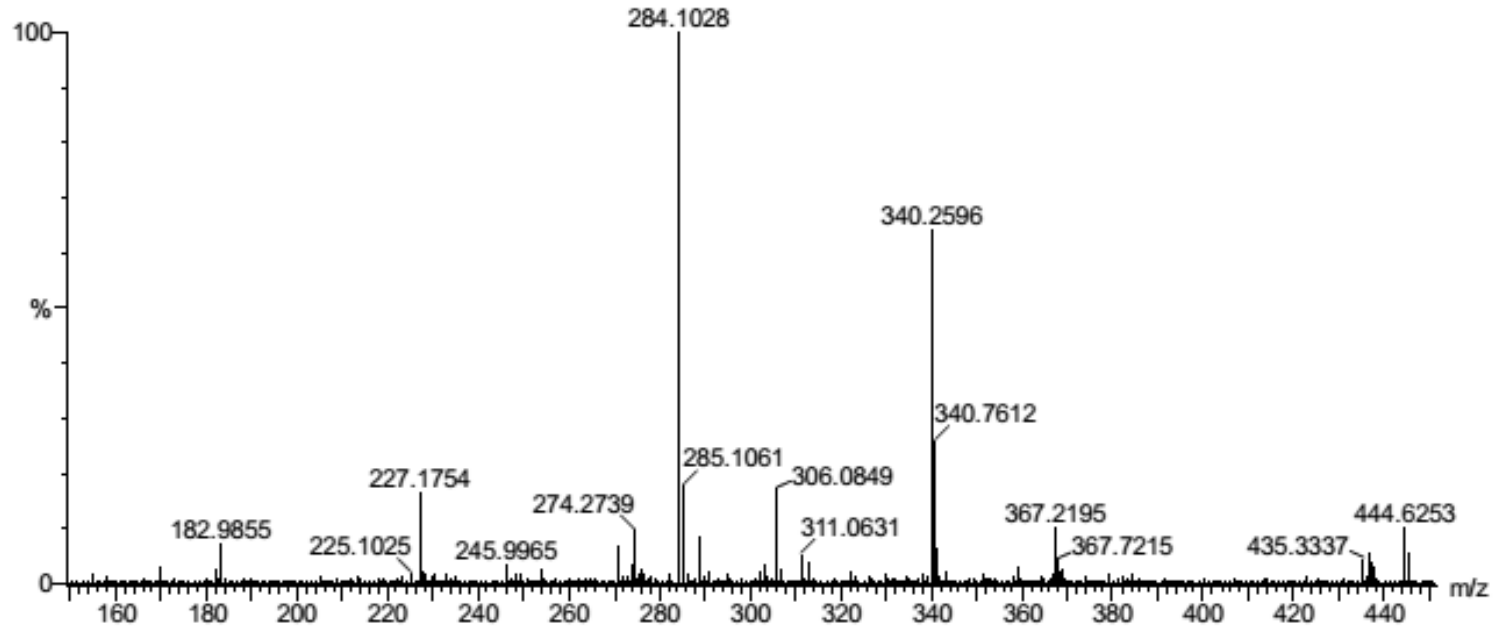
Elemental Composition Report

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 = 3

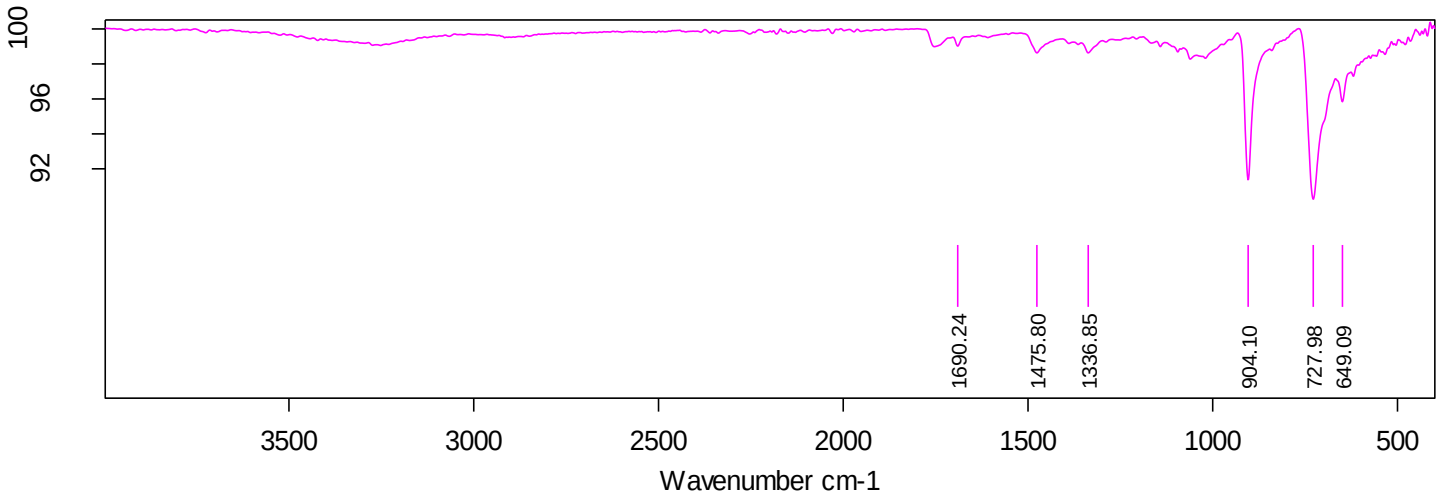
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-25 H: 5-25 N: 0-5 O: 1-4

Sample Name : 18-01-282 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
300819-18-01-282- 15 (0.157) AM2 (Ar,22000.0,0.00,0.00); Cm (15:18) 1: TOF MS ES+
1.86e+007



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
284.1028	284.1035	-0.7	-2.5	10.5	886.0	n/a	n/a	C15 H14 N3 O3

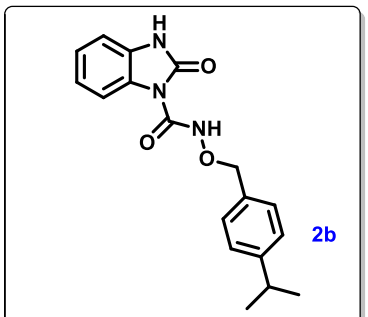
FTIR of 2a



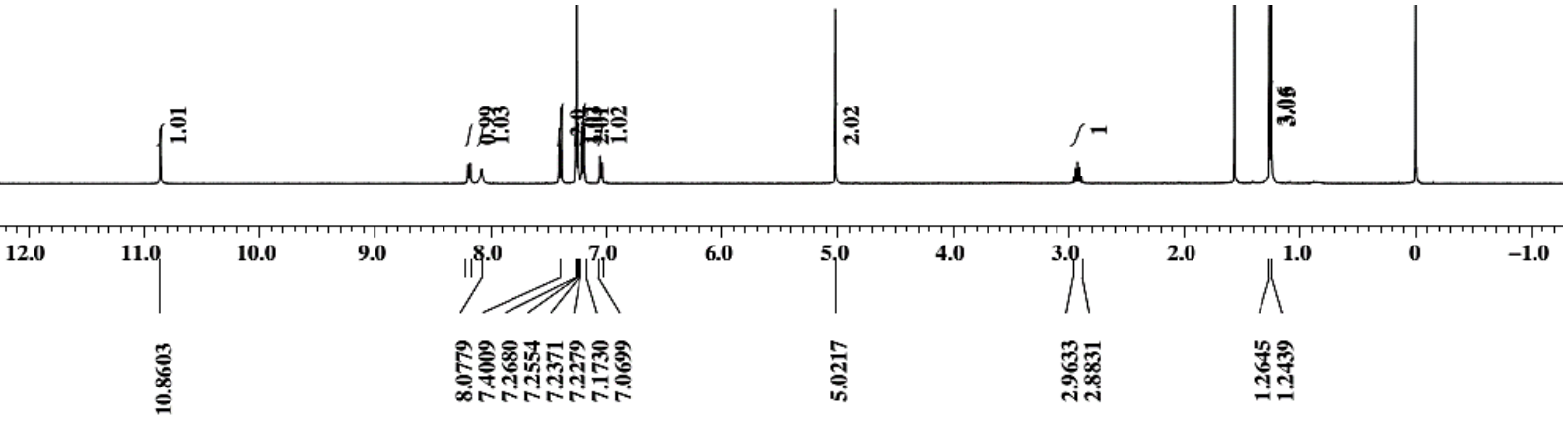
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-397.0	18-01-397	Instrument type and / or accessory	2/4/2020

Wavenumber cm-1	Transmittance [%]
3997.524564	1.000340
3996.095345	1.000353
3994.666126	1.000359
3993.236908	1.000347
3991.807689	1.000322
3990.378470	1.000295
3988.949252	1.000278
3987.520033	1.000269
3986.090814	1.000252
3984.661596	1.000214
3983.232377	1.000163
3981.803159	1.000119
3980.373940	1.000098
3978.944721	1.000101
3977.515503	1.000117
3976.086284	1.000137
3974.657065	1.000155
3973.227847	1.000163
3971.798628	1.000150
3970.369409	1.000108
3968.940191	1.000043

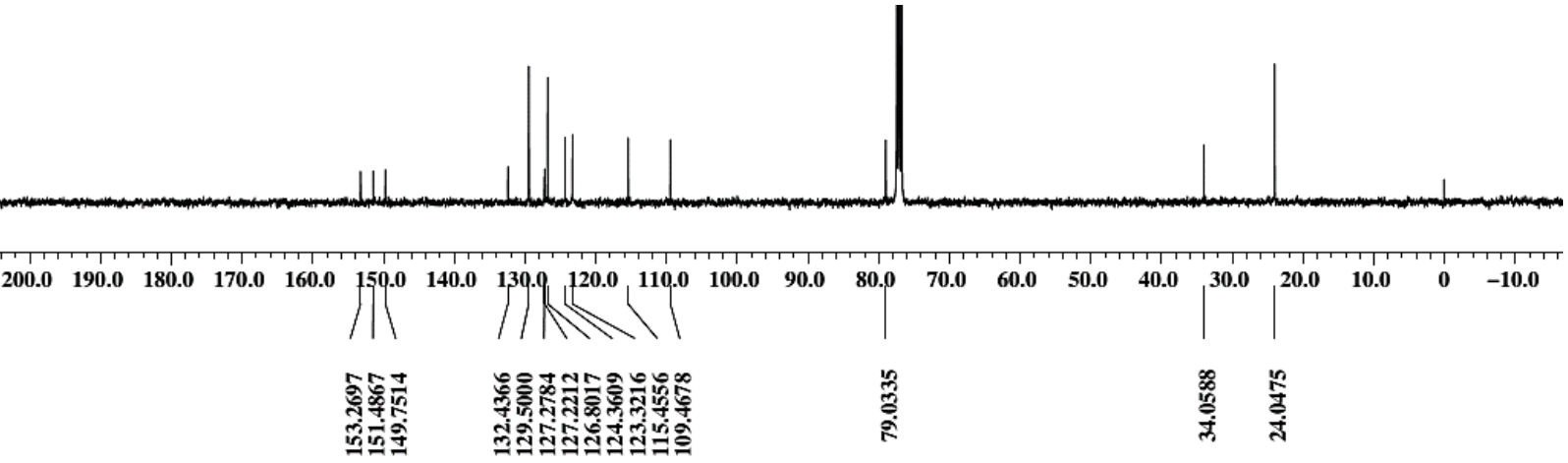
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2b



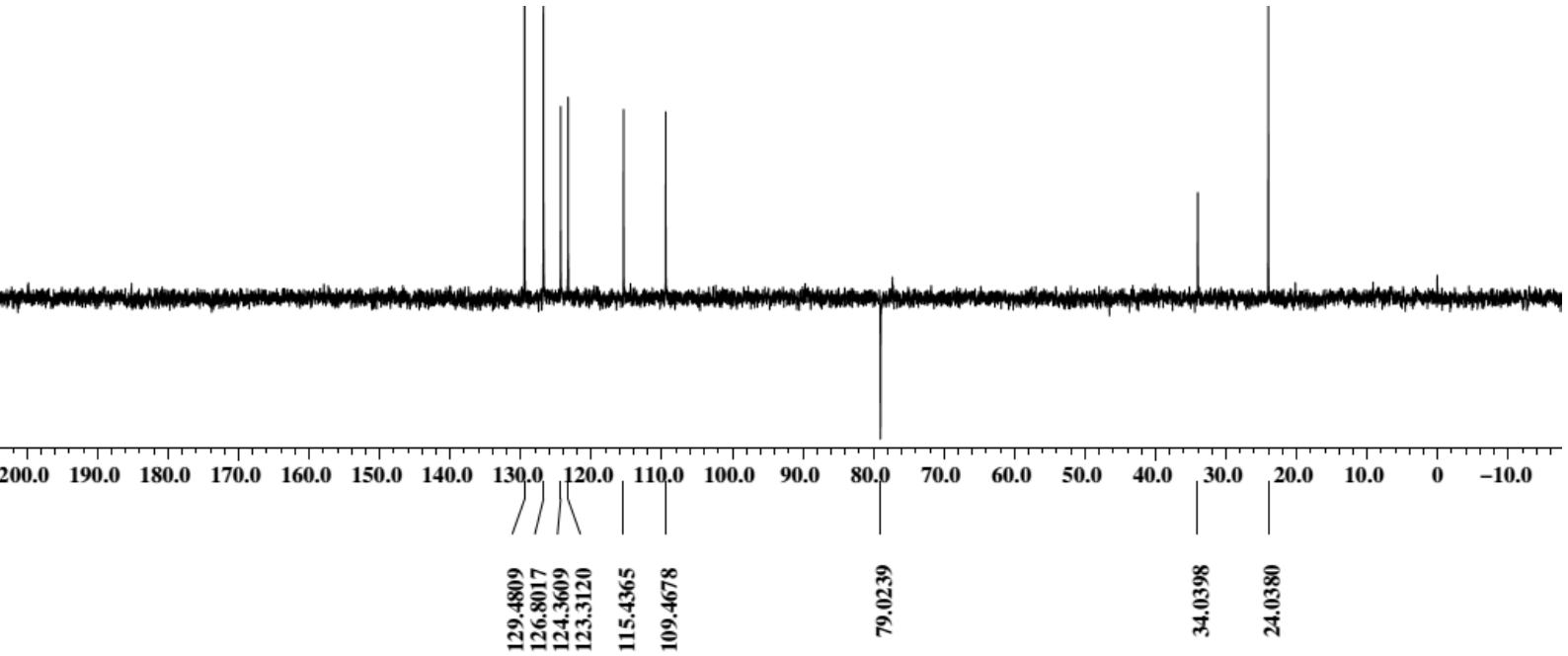
Chemical Formula: $C_{18}H_{19}N_3O_3$
Exact Mass: 325.1426



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2b



129.4809
126.8017
124.3609
123.3120
115.4365
109.4678
79.0239
34.0398
24.0380

HRMS of 2b

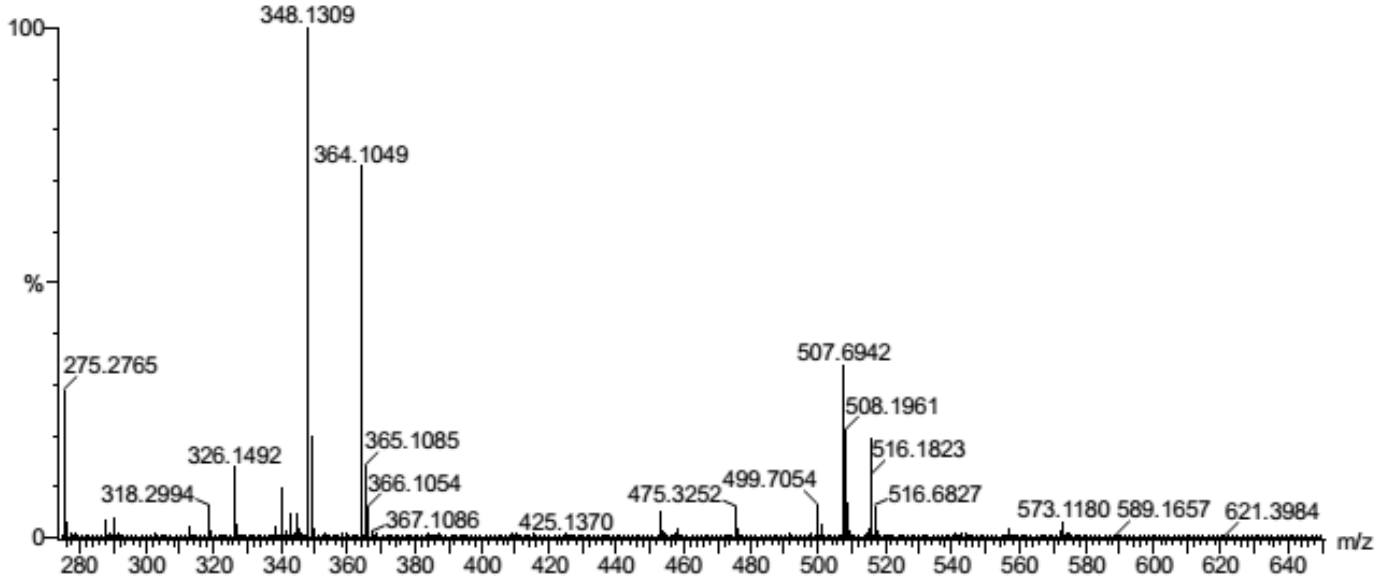
Elemental Composition Report

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 = 3

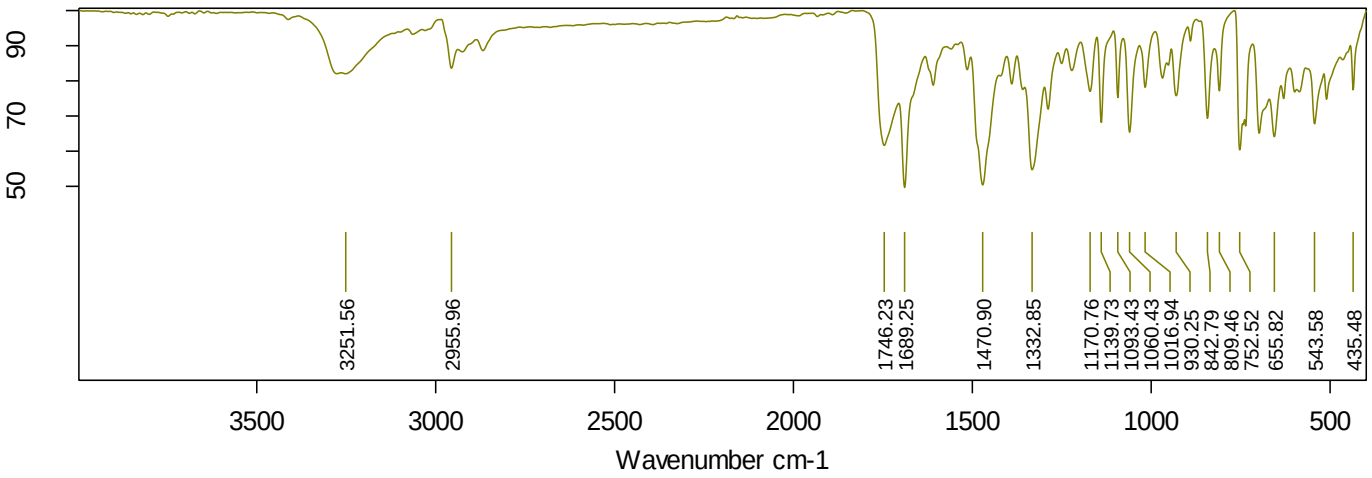
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-35 H: 11-35 N: 0-3 O: 1-5

Sample Name : 18/01/340 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
061119-18-01-340 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (8:18) 1: TOF MS ES+
4.47e+007



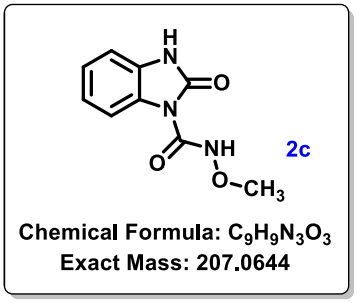
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
326.1492	326.1505	-1.3	-4.0	10.5	768.7	n/a	n/a	C18 H20 N3 O3

FTIR of 2b



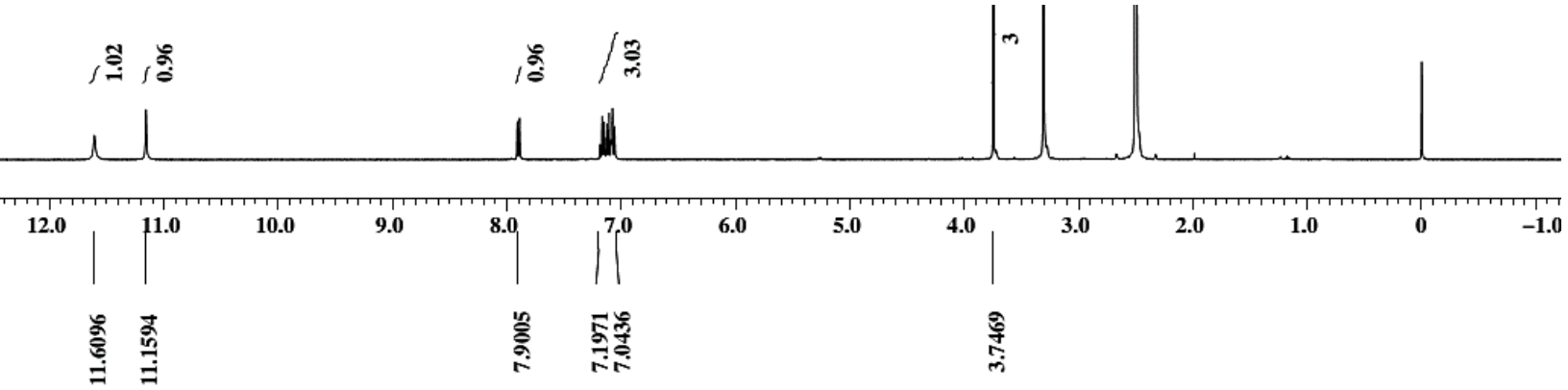
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-340.1	18-01-340	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	1.000000
3996.073013	0.999880
3994.643803	0.999746
3993.214592	0.999591
3991.785381	0.999413
3990.356171	0.999213
3988.926960	0.999000
3987.497749	0.998796
3986.068539	0.998631
3984.639328	0.998531
3983.210117	0.998512
3981.780907	0.998571
3980.351696	0.998687
3978.922485	0.998820
3977.493275	0.998919
3976.064064	0.998942
3974.634853	0.998891
3973.205643	0.998808
3971.776432	0.998741
3970.347221	0.998712
3968.918011	0.998717

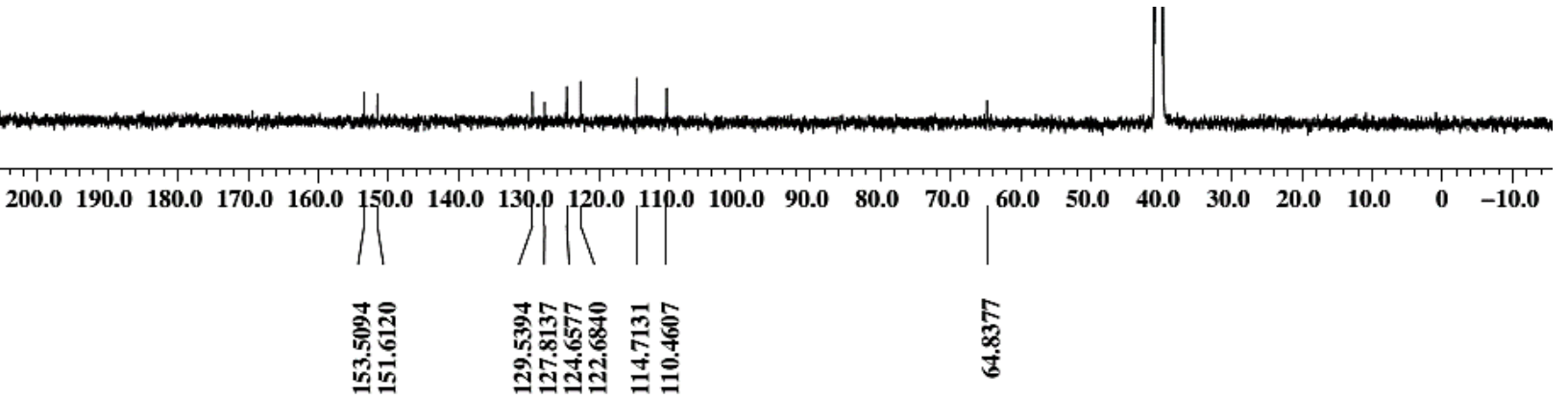


Chemical Formula: $C_9H_9N_3O_3$
Exact Mass: 207.0644

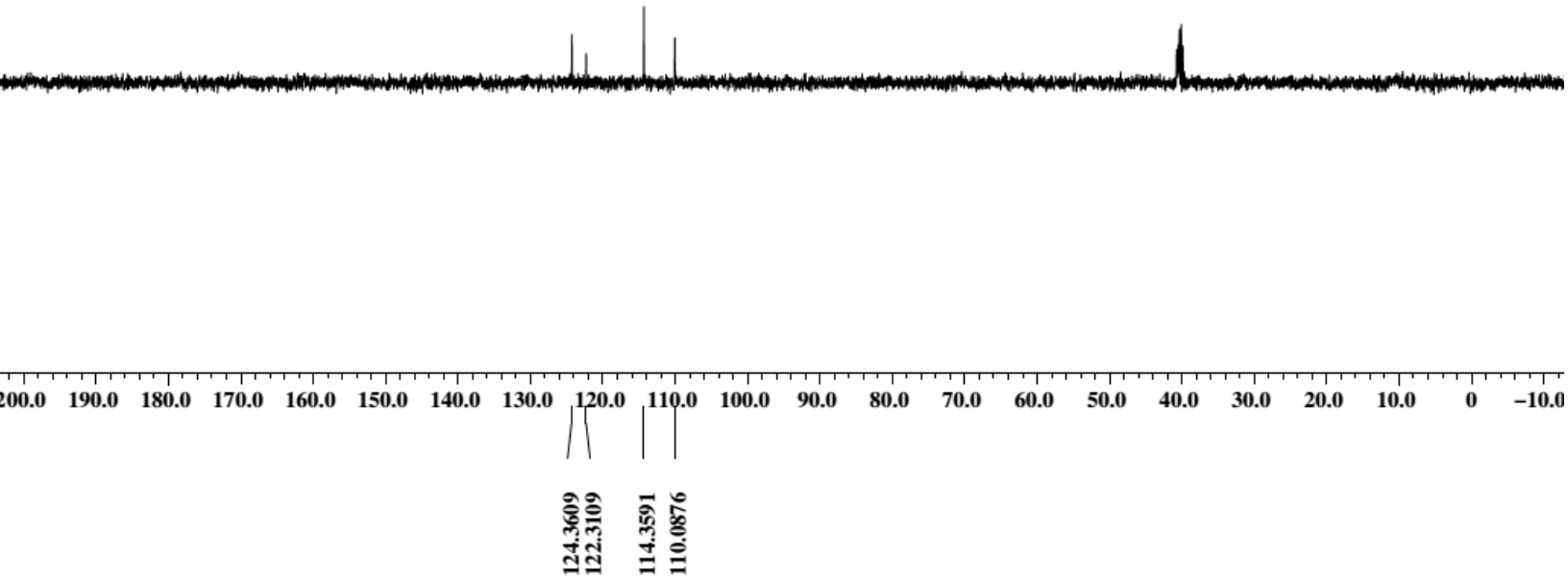
^{1}H-NMR (DMSO-d6, 400 MHz) of 2c



^{13}C-NMR (DMSO-d_6, 100 MHz) of 2c



^{13}C-DEPT (DMSO-d6, 100 MHz) of 2c



HRMS of 2c

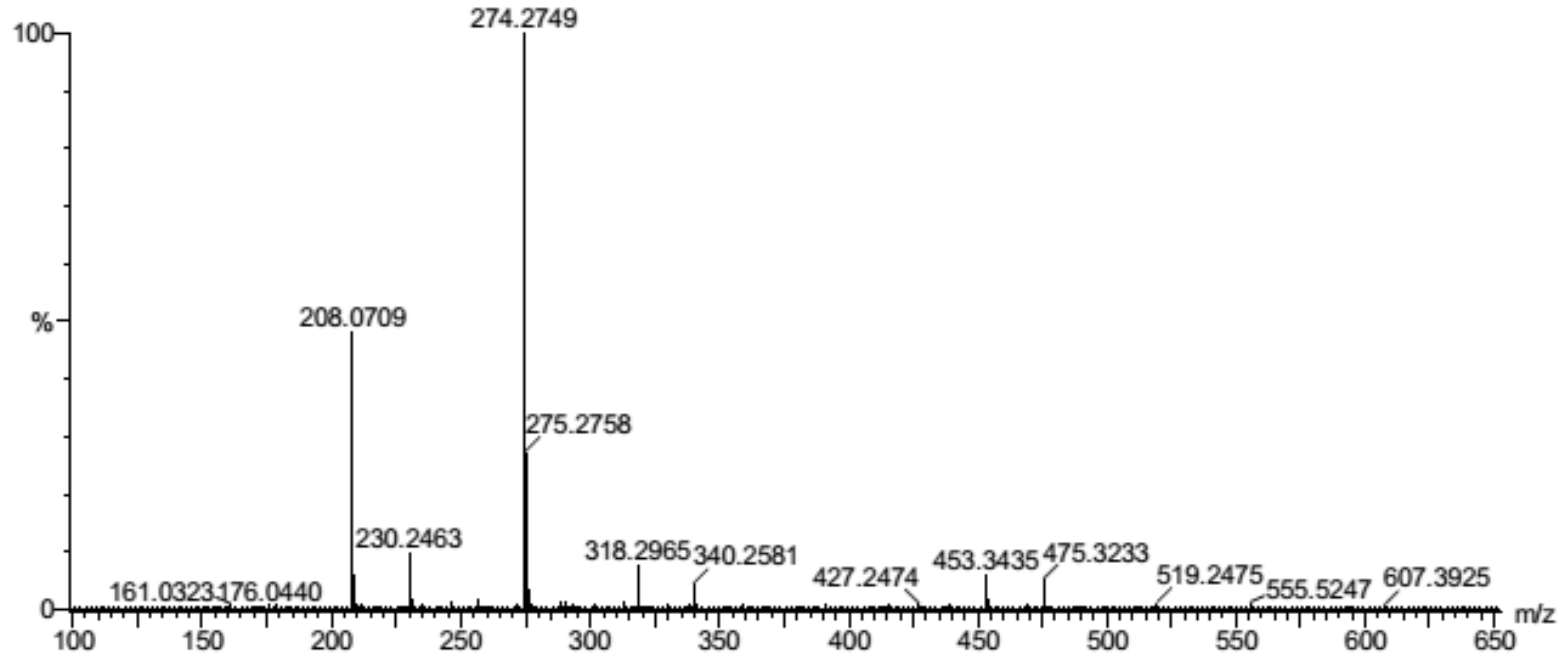
Elemental Composition Report

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 = 3

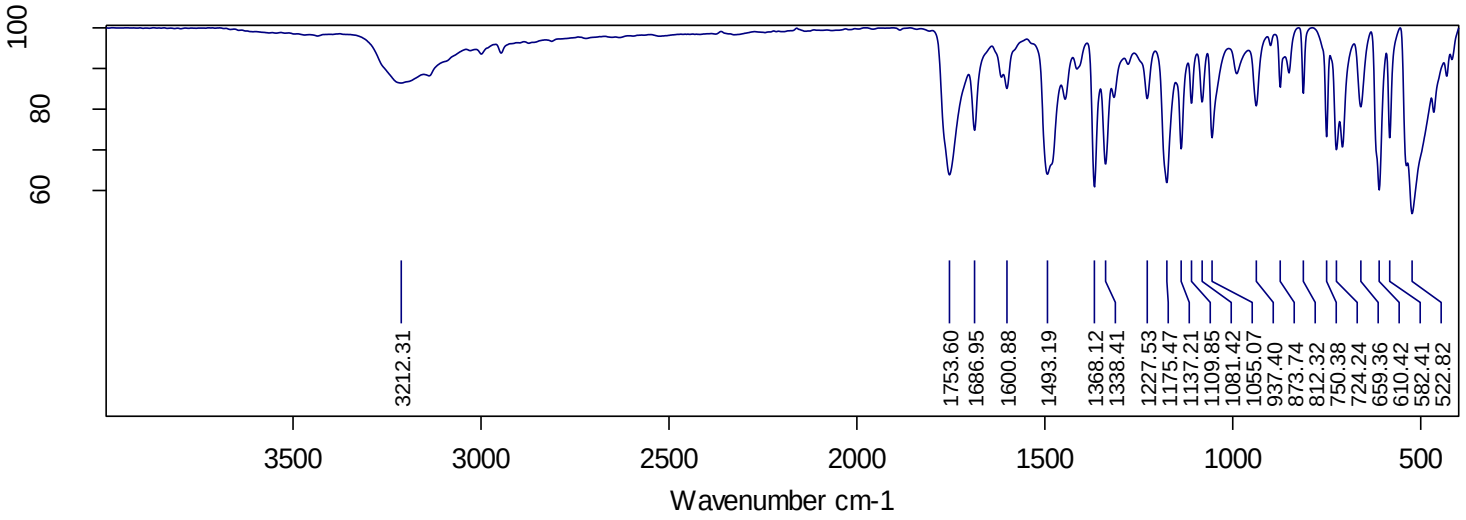
Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 7-30 N: 0-4 O: 1-5

Sample Name : 18-01-368 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
291119-18-01-368 12 (0.131) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (8:18) 1: TOF MS ES+
1.22e+008



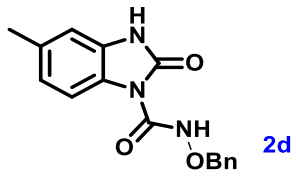
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
208.0709	208.0722	-1.3	-6.2	6.5	1461.5	n/a	n/a	C9 H10 N3 O3

FTIR of 2c



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-379.0	18-01-379	Instrument type and / or accessory	1/6/2020

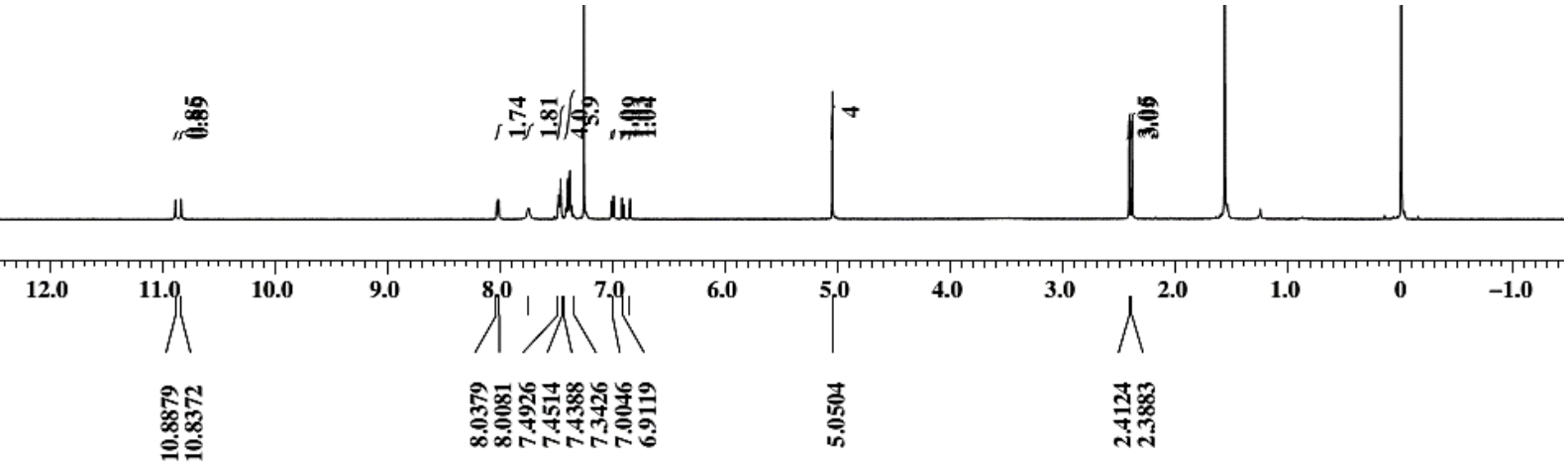
Wavenumber cm-1	Transmittance [%]
3997.502224	1.000169
3996.073013	0.999956
3994.643803	0.999745
3993.214592	0.999556
3991.785381	0.999424
3990.356171	0.999378
3988.926960	0.999432
3987.497749	0.999569
3986.068539	0.999752
3984.639328	0.999942
3983.210117	1.000109
3981.780907	1.000232
3980.351696	1.000290
3978.922485	1.000271
3977.493275	1.000181
3976.064064	1.000049
3974.634853	0.999918
3973.205643	0.999822
3971.776432	0.999770
3970.347221	0.999751
3968.918011	0.999741



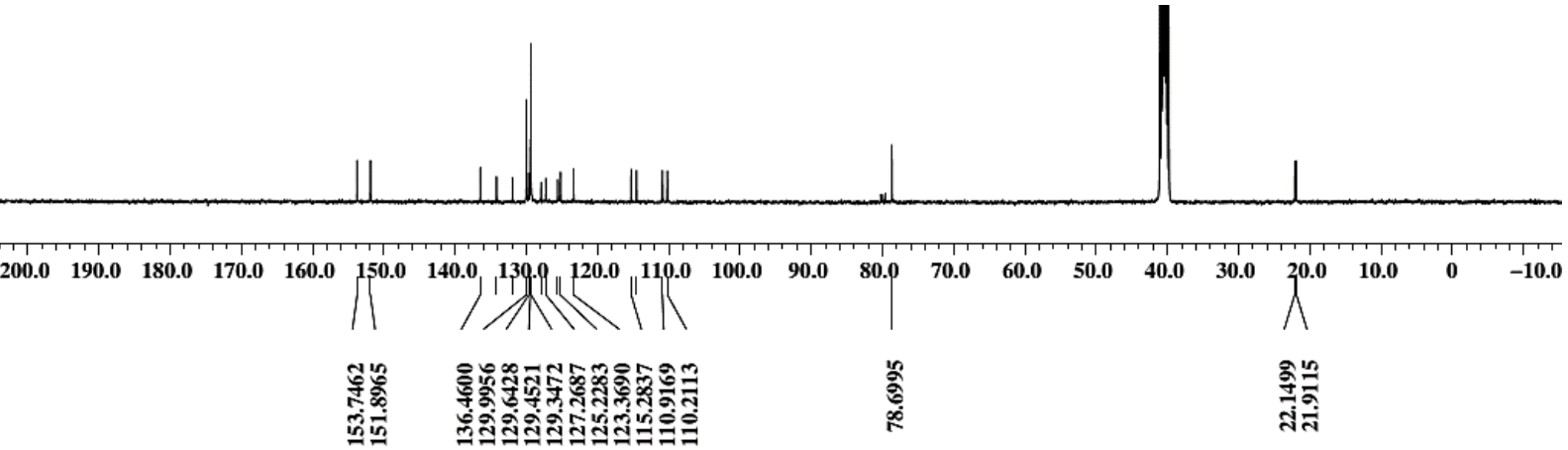
2d

Chemical Formula: $C_{16}H_{15}N_3O_3$
Exact Mass: 297.1113

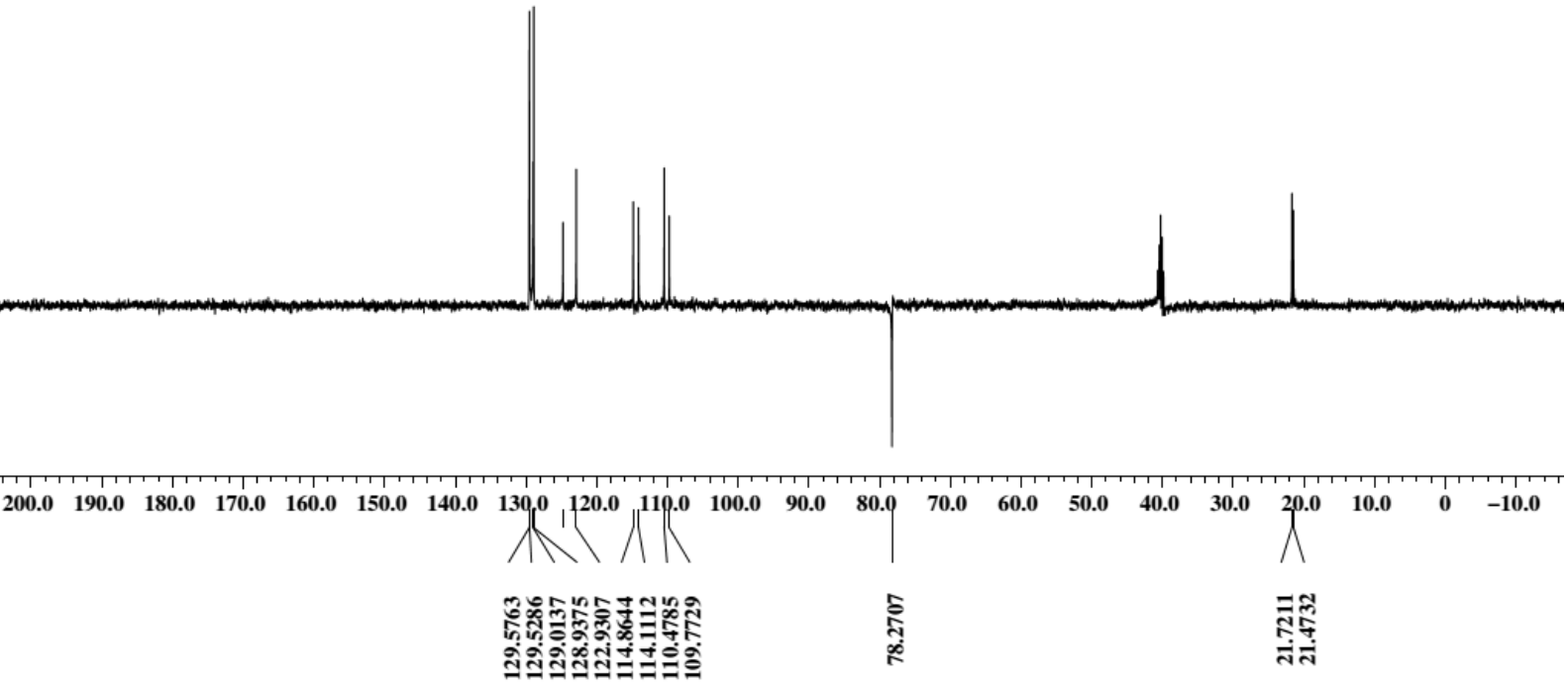
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2d



^{13}C-NMR ($DMSO\text{-}d_6$, 100 MHz) of 2d



^{13}C-DEPT (DMSO-d6, 100 MHz) of 2d



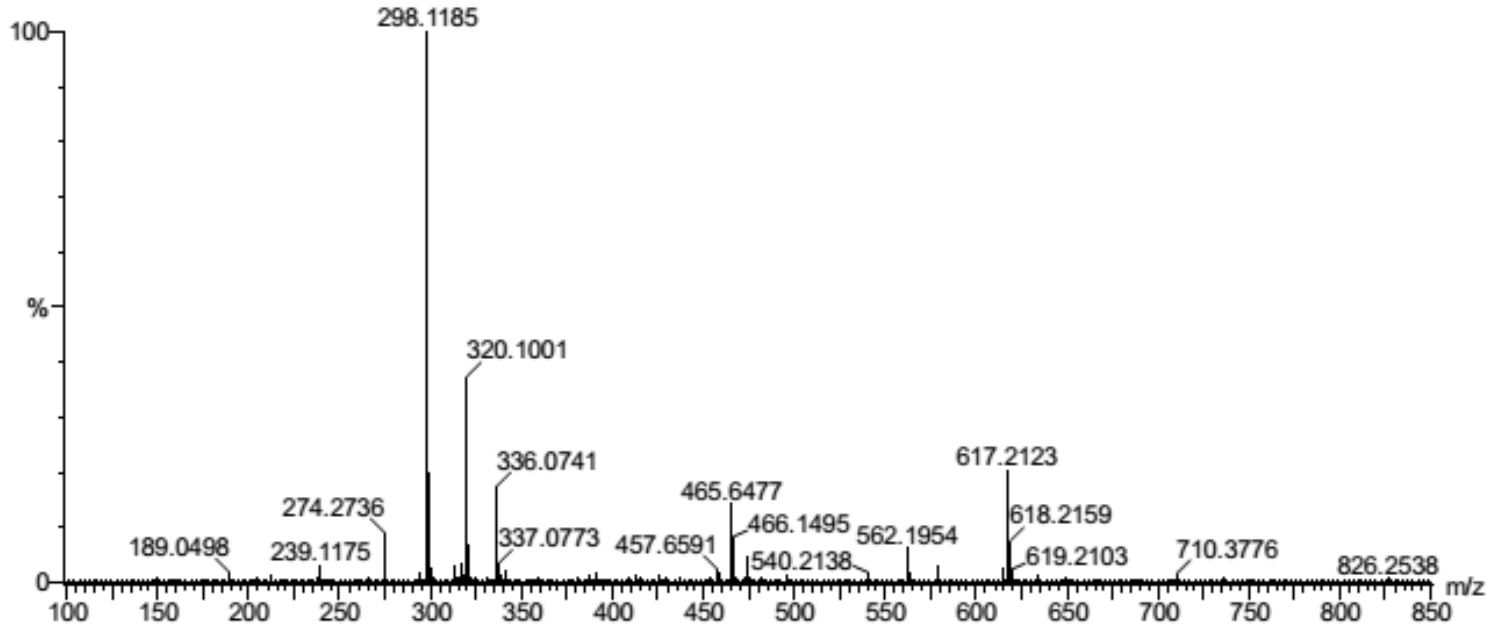
Elemental Composition Report

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 = 3

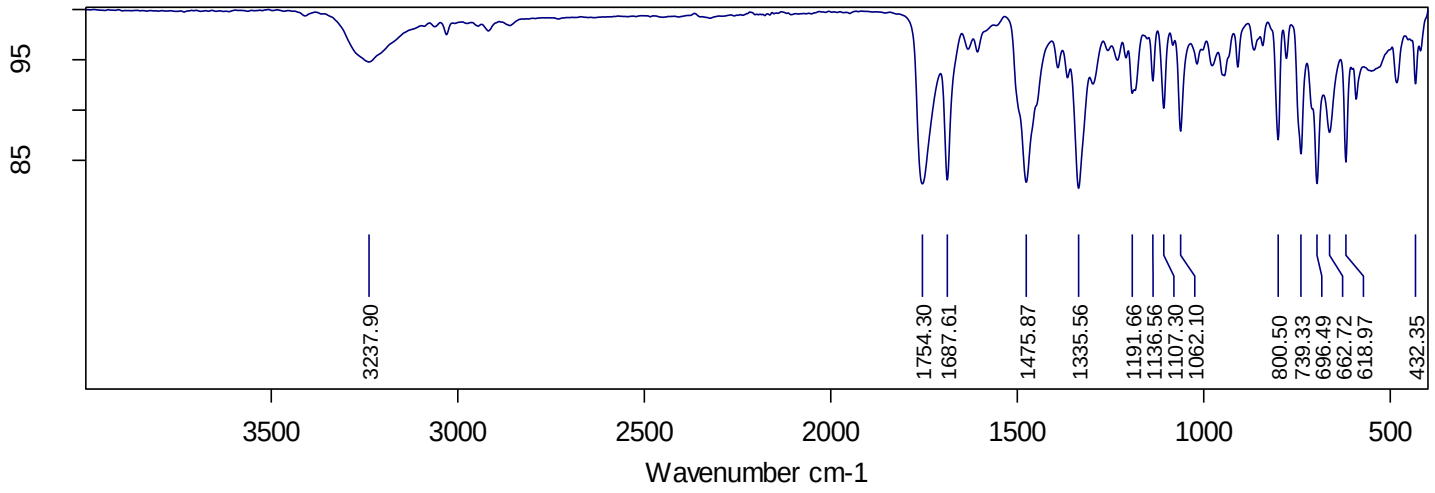
Monoisotopic Mass, Even Electron Ions
49 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-25 H: 11-30 N: 0-5 O: 1-5

Sample Name : 18/01/323 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
051119-18-01-323 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (12:15) 1: TOF MS ES+
3.83e+007



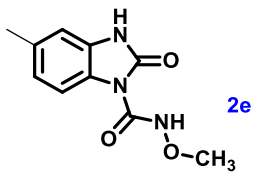
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
298.1185	298.1192	-0.7	-2.3	10.5	845.2	n/a	n/a	C16 H16 N3 O3

FTIR of 2d



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-323.0	18-01-323	Instrument type and / or accessory	1/6/2020

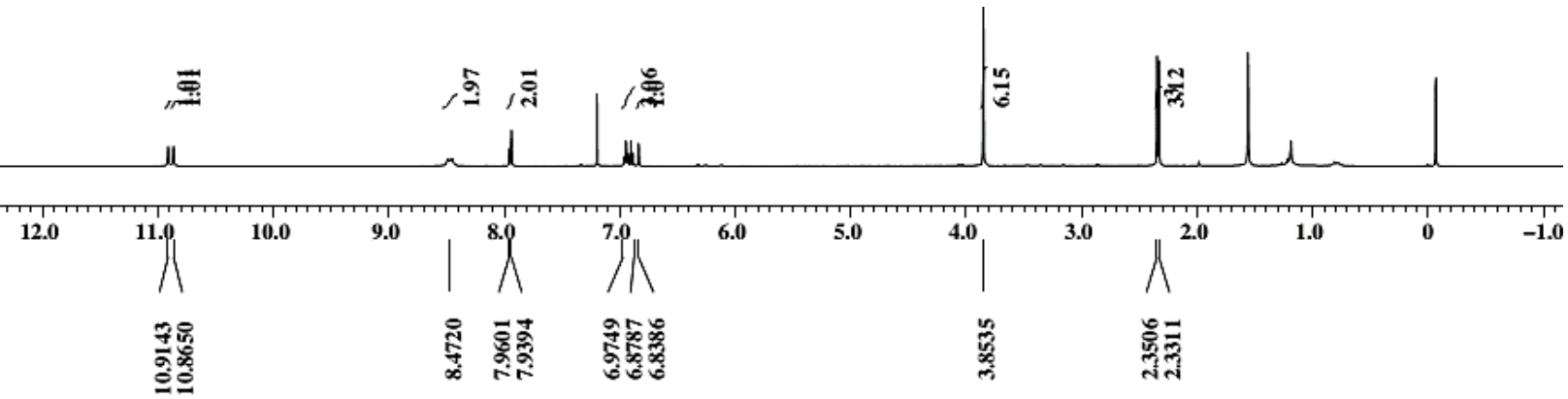
Wavenumber cm-1	Transmittance [%]
3997.502224	0.999687
3996.073013	0.999745
3994.643803	0.999799
3993.214592	0.999836
3991.785381	0.999839
3990.356171	0.999807
3988.926960	0.999754
3987.497749	0.999704
3986.068539	0.999674
3984.639328	0.999670
3983.210117	0.999695
3981.780907	0.999746
3980.351696	0.999817
3978.922485	0.999893
3977.493275	0.999960
3976.064064	1.000000
3974.634853	1.000000
3973.205643	0.999955
3971.776432	0.999877
3970.347221	0.999789
3968.918011	0.999715



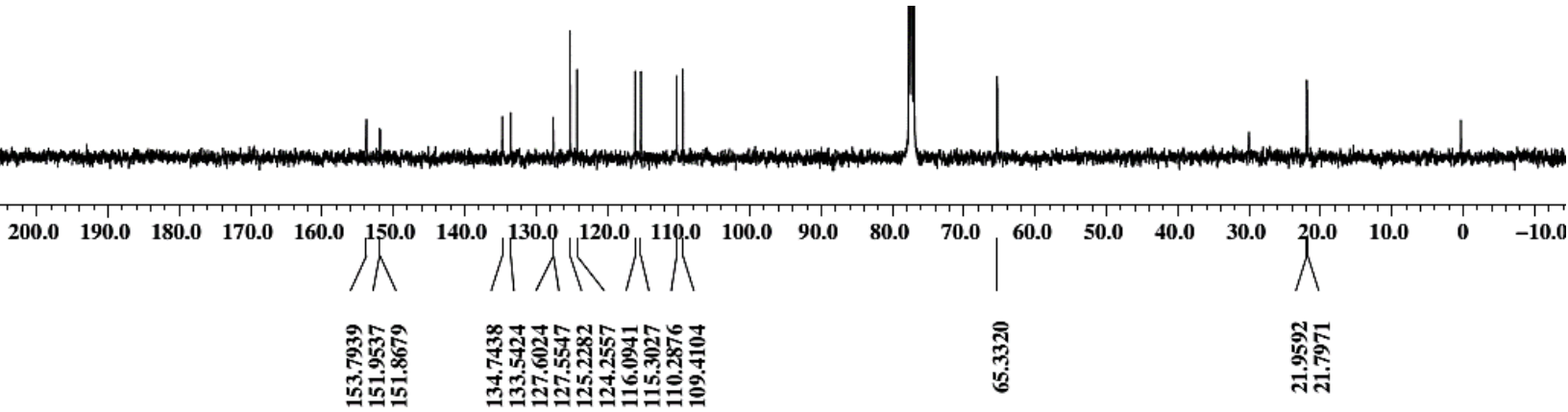
2e

Chemical Formula: $C_{10}H_{11}N_3O_3$
Exact Mass: 221.0800

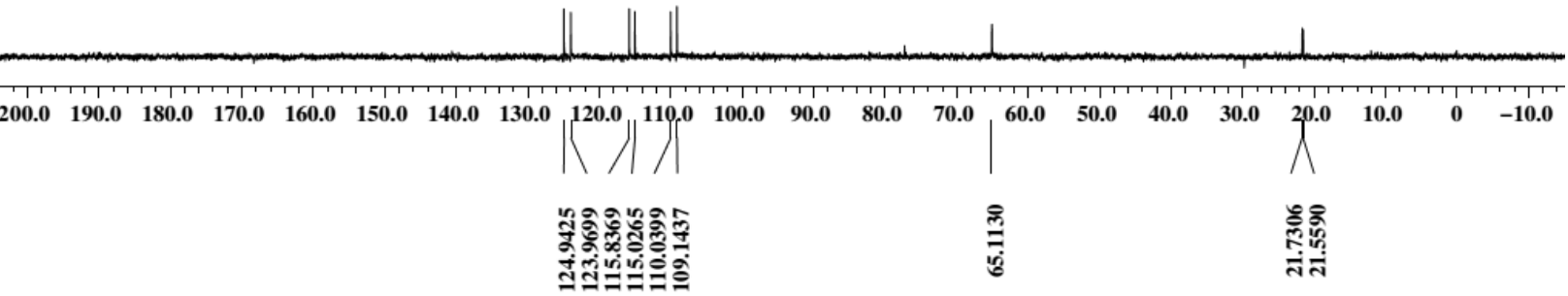
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2e



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2e



124.9425
123.9699
115.8369
115.0265
110.0399
109.1437

65.1130

21.7306
21.5590

HRMS of 2e

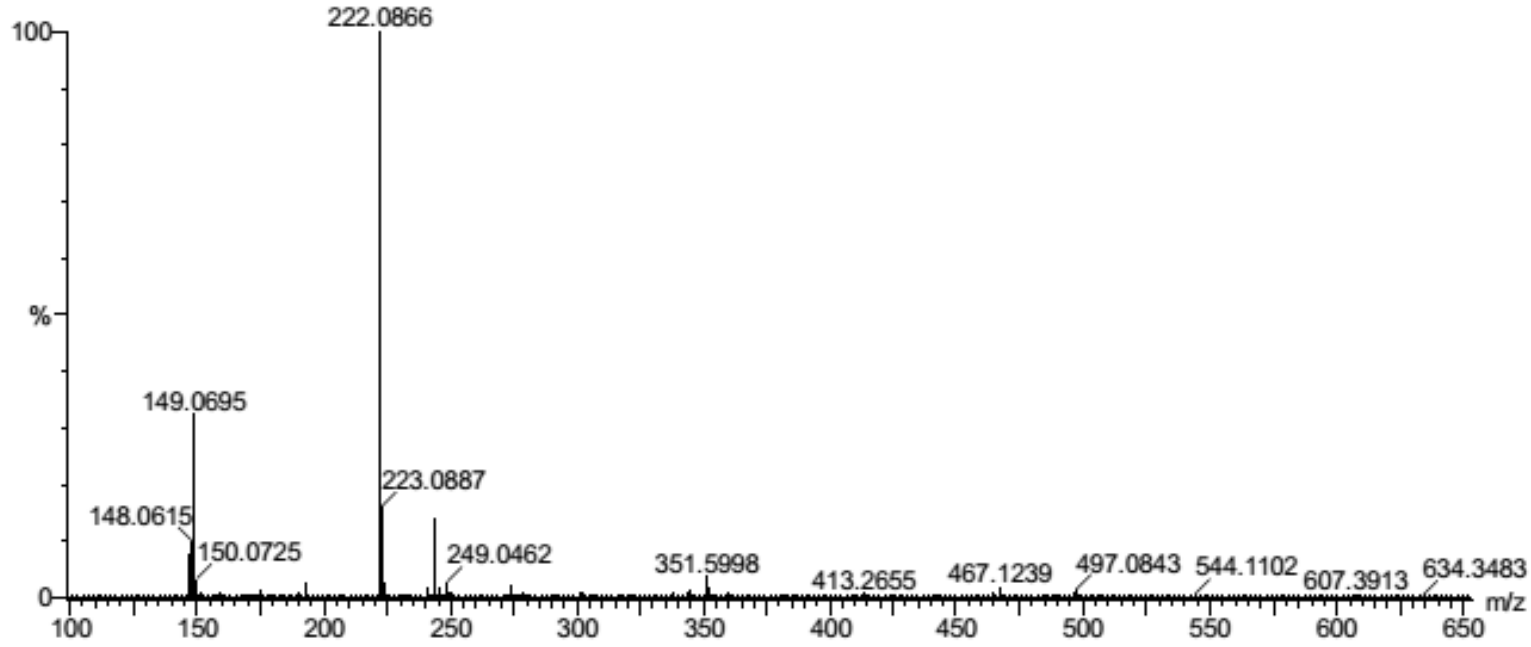
Elemental Composition Report

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 = 3

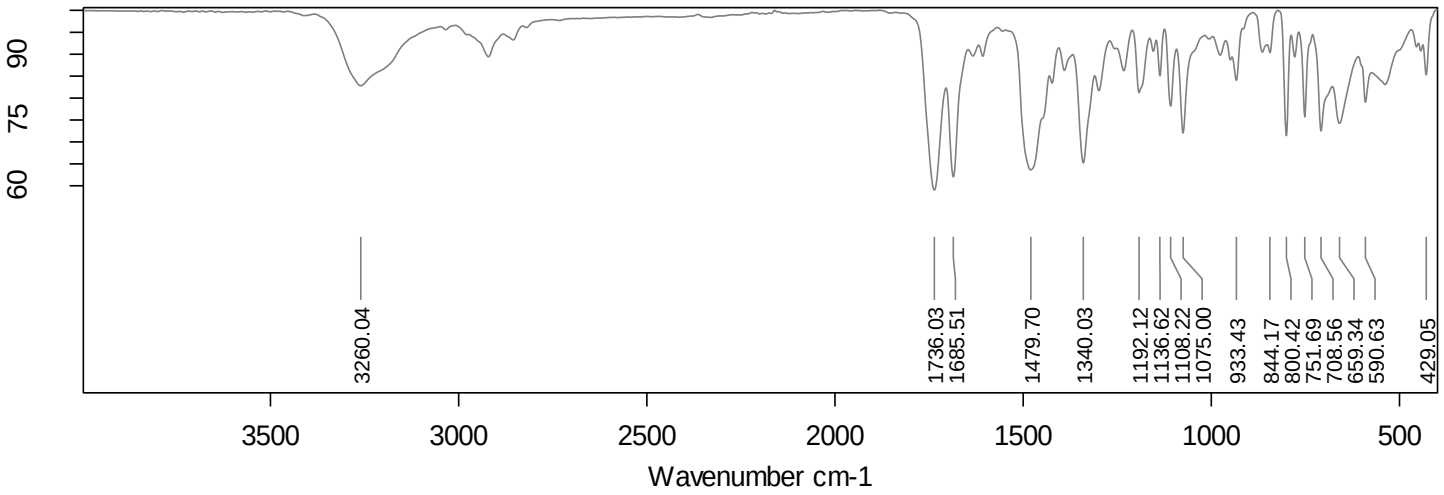
Monoisotopic Mass, Even Electron Ions
55 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-30 H: 7-25 N: 0-5 O: 0-6

Sample Name : 18-01-388 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
231219-18-01-388 12 (0.131) 1: TOF MS ES+
8.66e+007



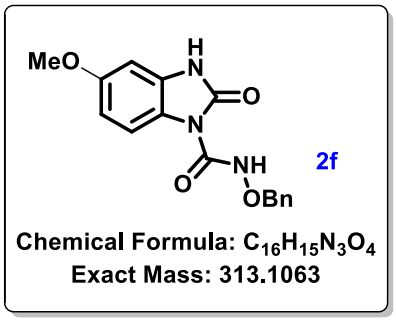
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
222.0866	222.0879	-1.3	-5.9	6.5	1259.1	n/a	n/a	C10 H12 N3 O3

FTIR of 2e



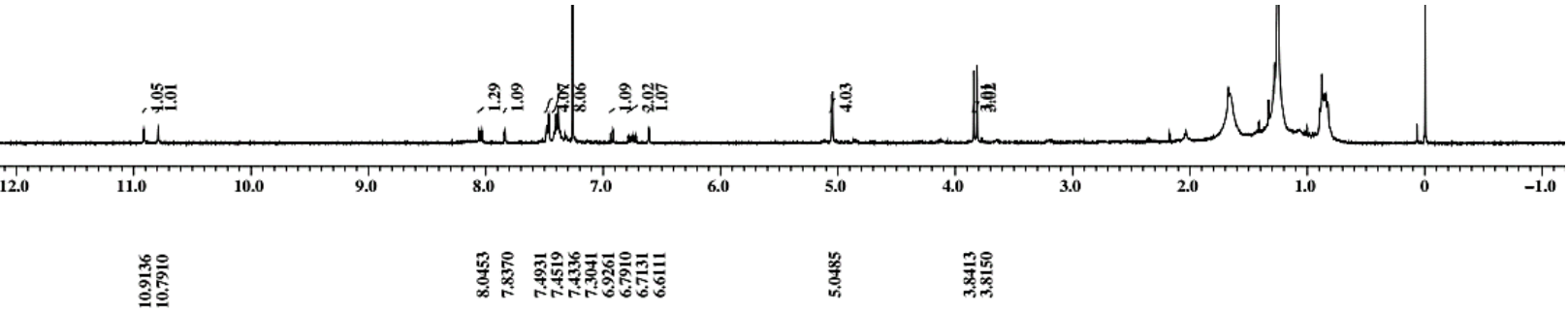
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-388.0	18-01-388	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	1.000000
3996.073013	0.999880
3994.643803	0.999754
3993.214592	0.999624
3991.785381	0.999501
3990.356171	0.999403
3988.926960	0.999340
3987.497749	0.999315
3986.068539	0.999325
3984.639328	0.999365
3983.210117	0.999426
3981.780907	0.999491
3980.351696	0.999536
3978.922485	0.999542
3977.493275	0.999508
3976.064064	0.999453
3974.634853	0.999406
3973.205643	0.999383
3971.776432	0.999384
3970.347221	0.999391
3968.918011	0.999379

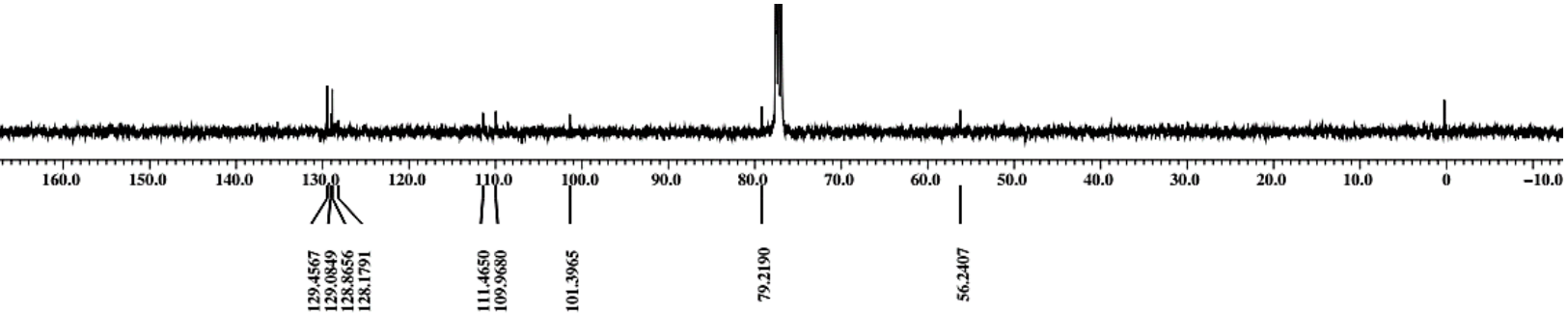


Chemical Formula: $C_{16}H_{15}N_3O_4$
Exact Mass: 313.1063

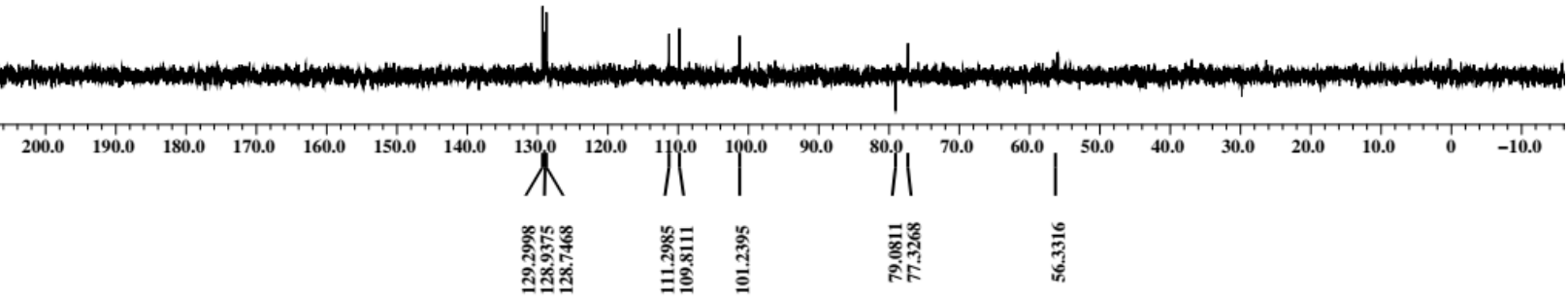
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2f



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2f



HRMS of 2f

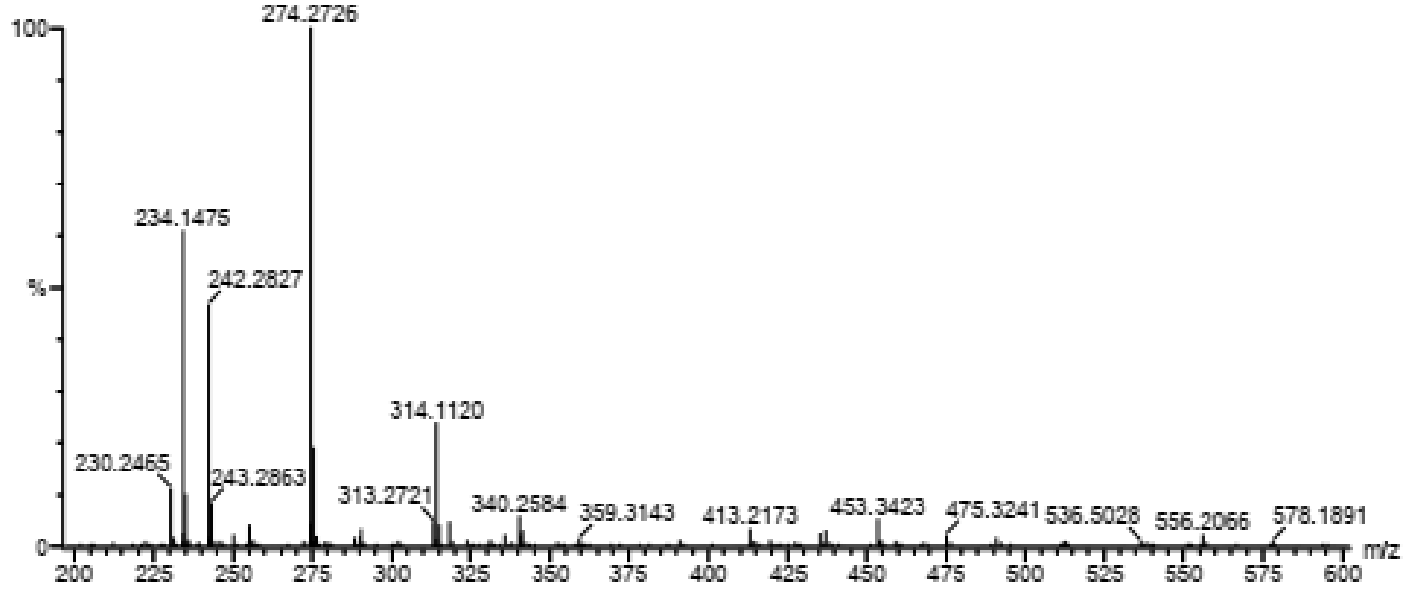
Elemental Composition Report

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 = 3

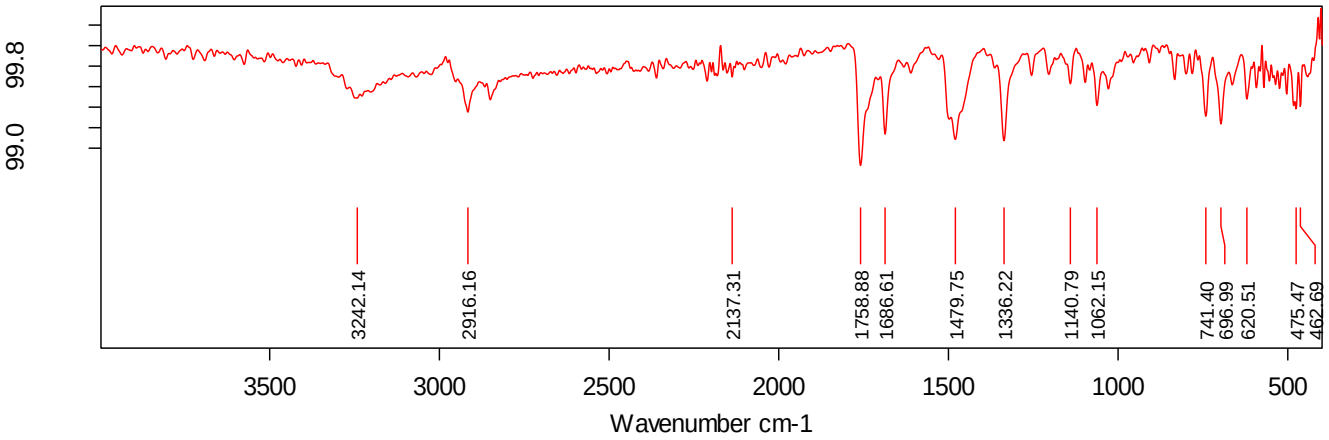
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-40 H: 15-45 N: 0-3 O: 1-4

Sample Name : 18-01-344 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
141119-18-01-344 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (7:18) 1: TOF MS ES+
7.63e+007



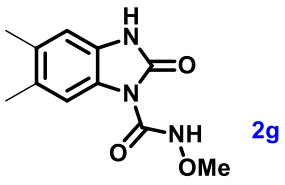
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
314.1120	314.1141	-2.1	-6.7	10.5	815.0	n/a	n/a	C16 H16 N3 O4

FTIR of 2f



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-344.1	18-01-344	Instrument type and / or accessory	2/4/2020

Wavenumber cm-1	Transmittance [%]
3997.524564	0.999643
3996.095345	0.999622
3994.666126	0.999600
3993.236908	0.999579
3991.807689	0.999572
3990.378470	0.999595
3988.949252	0.999653
3987.520033	0.999732
3986.090814	0.999804
3984.661596	0.999840
3983.232377	0.999834
3981.803159	0.999798
3980.373940	0.999750
3978.944721	0.999700
3977.515503	0.999649
3976.086284	0.999601
3974.657065	0.999563
3973.227847	0.999530
3971.798628	0.999490
3970.369409	0.999431
3968.940191	0.999352

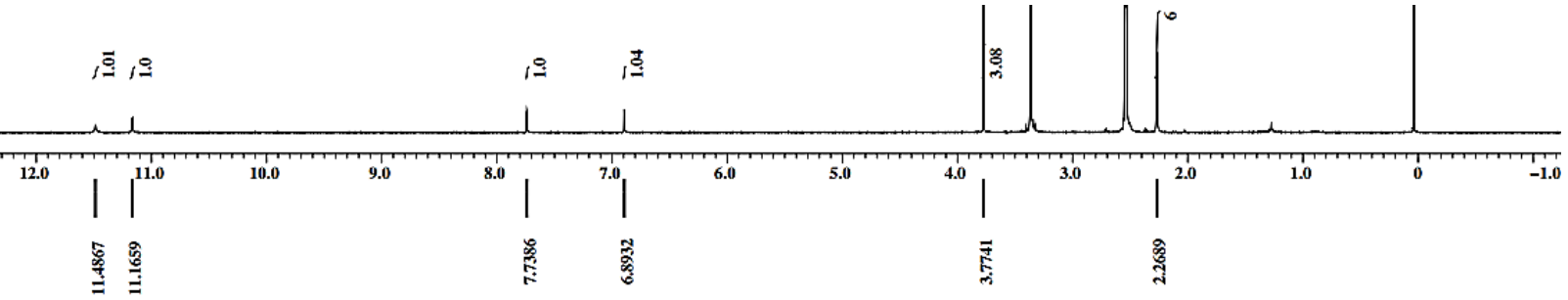


2g

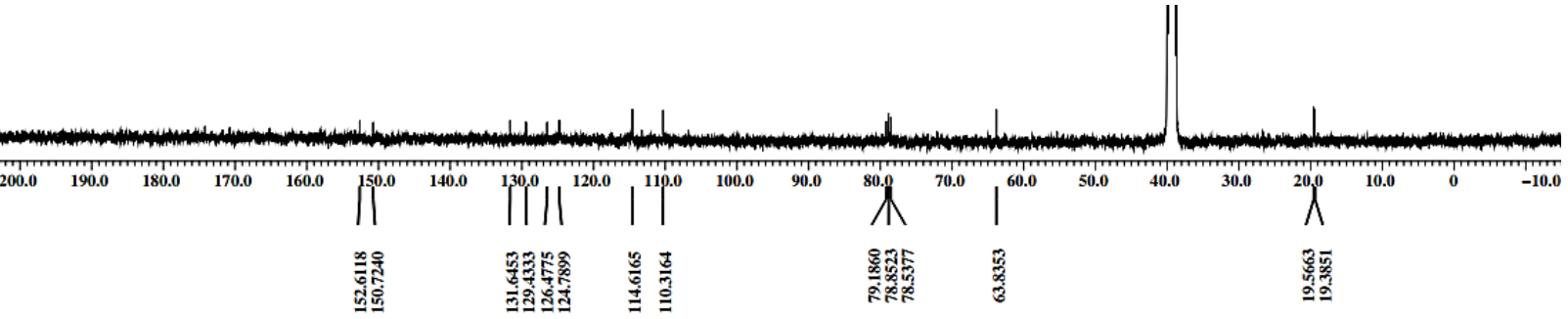
Chemical Formula: $C_{11}H_{13}N_3O_3$

Exact Mass: 235.0957

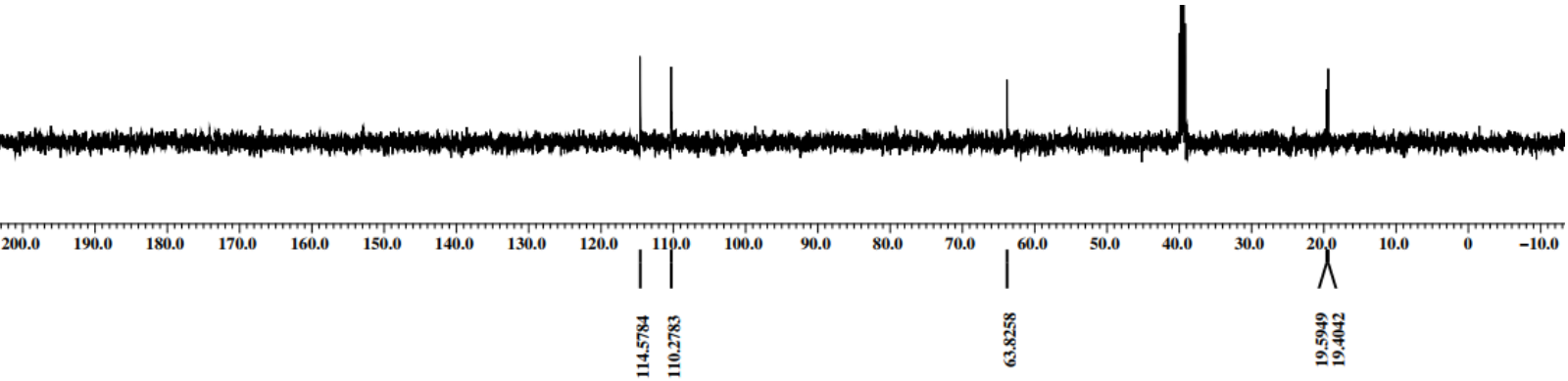
^{1}H-NMR (DMSO-d6, 400 MHz) of 2g



^{13}C-NMR (DMSO-d6, 100 MHz) of 2g



^{13}C-DEPT (DMSO-d6, 100 MHz) of 2g


200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
114.5784
110.2783
63.8258
19.5949
19.4042

HRMS of 2g

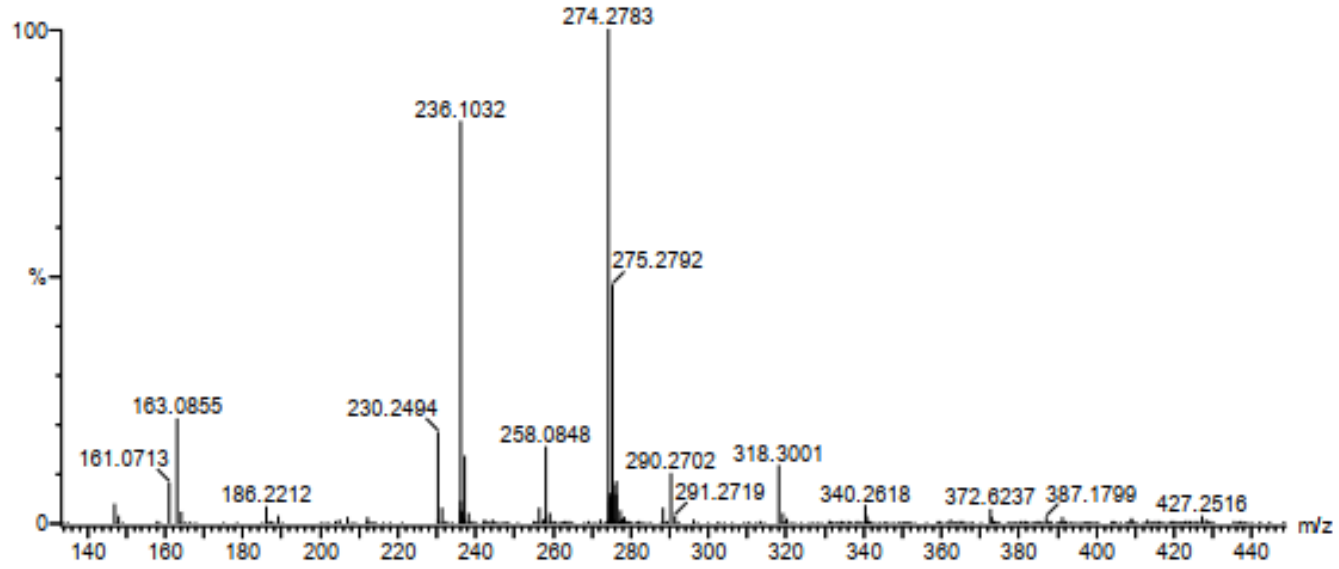
Elemental Composition Report

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 = 6

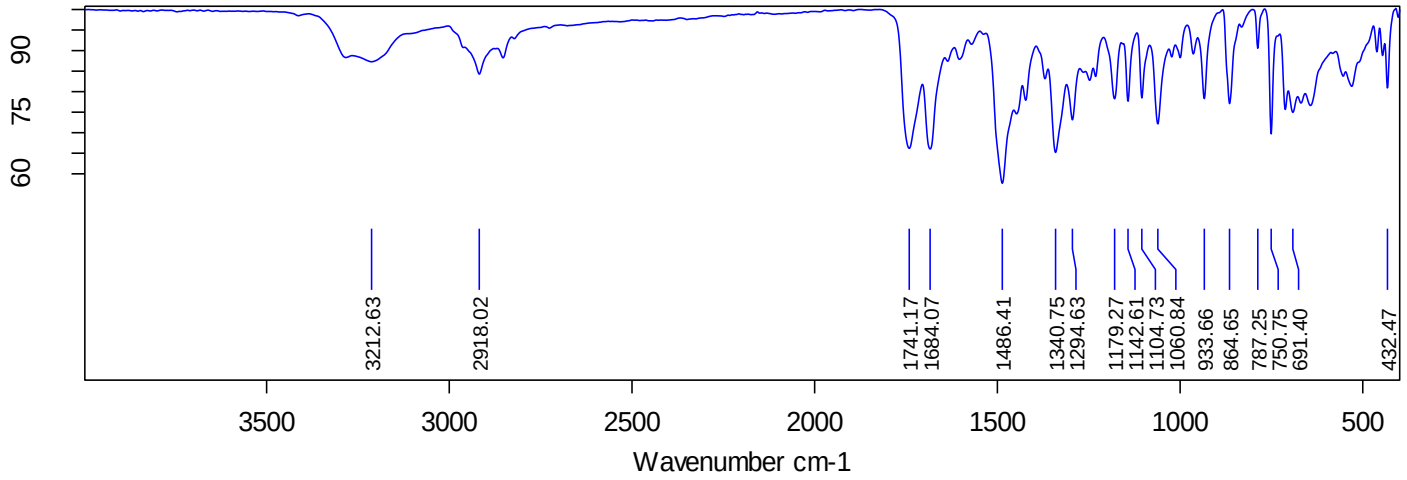
Monoisotopic Mass, Even Electron Ions
39 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 11-20 H: 11-30 N: 0-3 O: 0-3 Se: 0-1

Sample Name : 18-01-414 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
220920-18-01-414 12 (0.131) 1: TOF MS ES+
6.88e+007



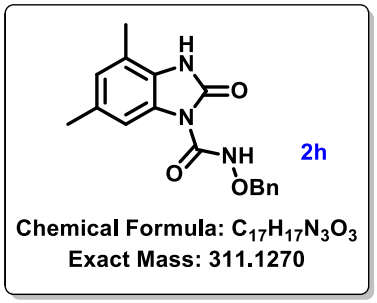
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
236.1032	236.1035	-0.3	-1.3	6.5	446.5	n/a	n/a	C11 H14 N3 O3

FTIR of 2g



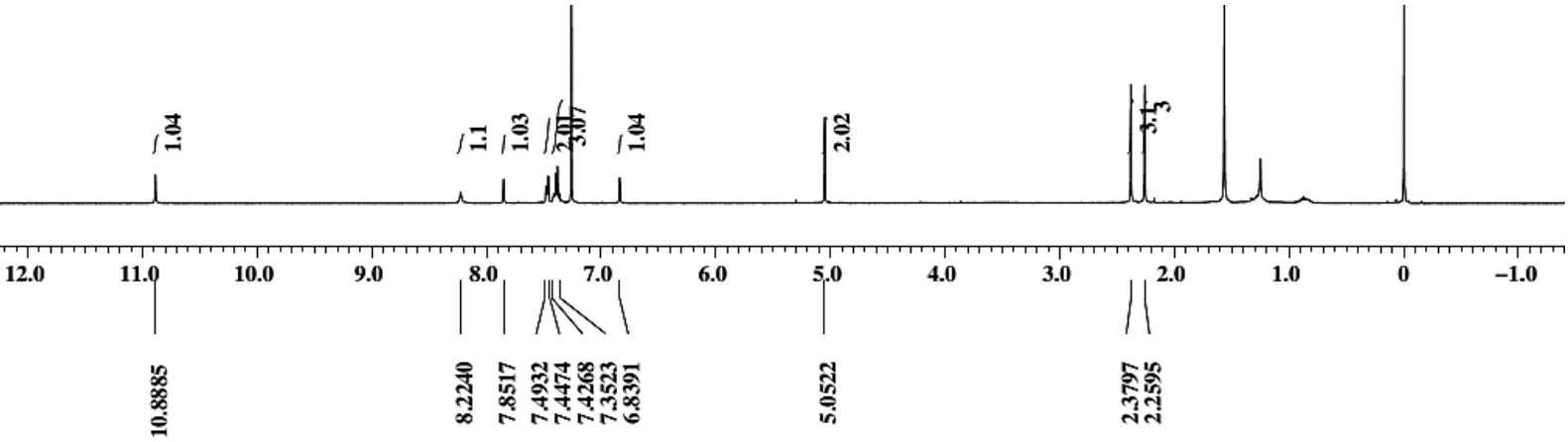
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-414.0	18-01-414	Instrument type and / or accessory	10/21/2020

Wavenumber cm-1	Transmittance [%]
3997.658602	1.000113
3996.229335	1.000018
3994.800069	0.999934
3993.370802	0.999876
3991.941536	0.999861
3990.512269	0.999891
3989.083002	0.999950
3987.653736	0.999999
3986.224469	1.000000
3984.795203	0.999933
3983.365936	0.999812
3981.936670	0.999680
3980.507403	0.999575
3979.078136	0.999512
3977.648870	0.999477
3976.219603	0.999442
3974.790337	0.999388
3973.361070	0.999300
3971.931804	0.999176
3970.502537	0.999019
3969.073270	0.998849

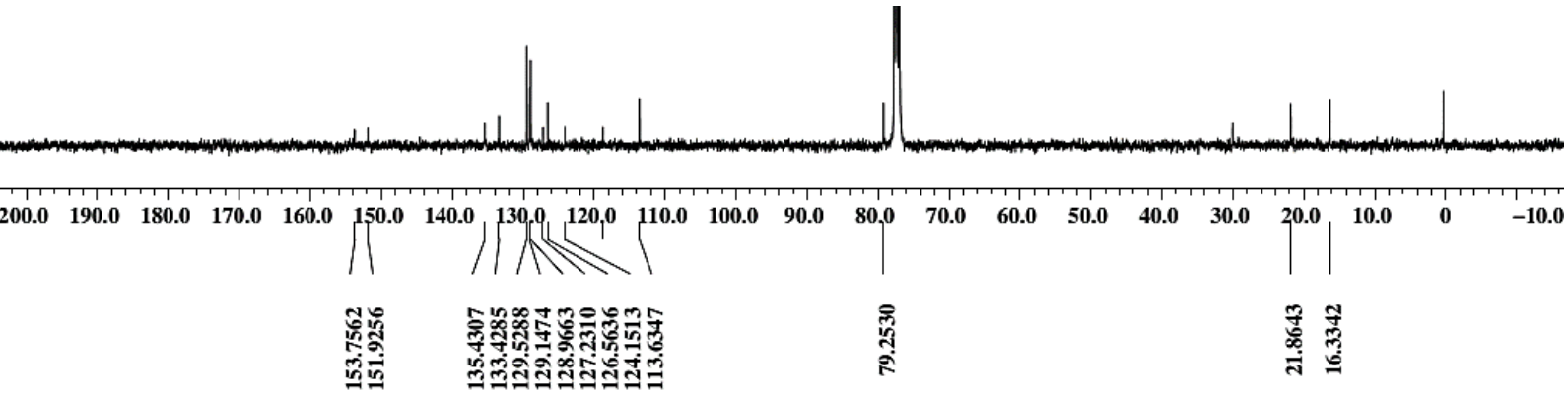


Chemical Formula: $C_{17}H_{17}N_3O_3$
Exact Mass: 311.1270

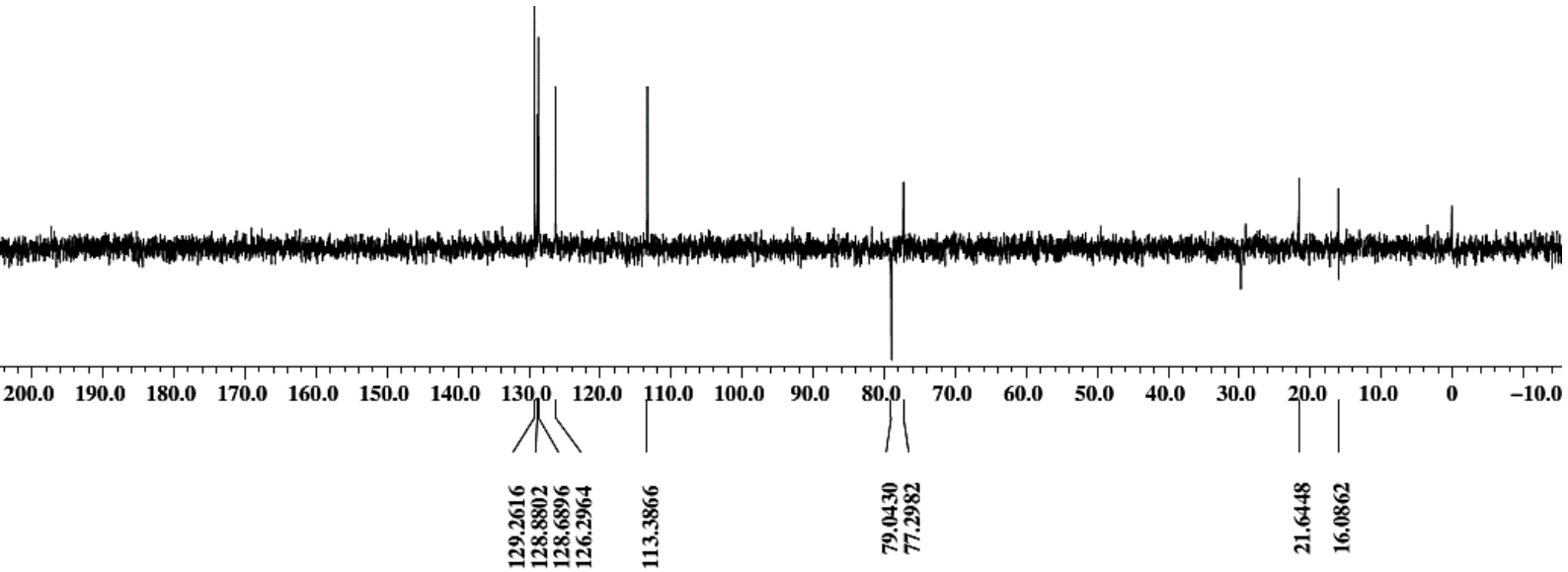
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2h



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2h



HRMS of 2h

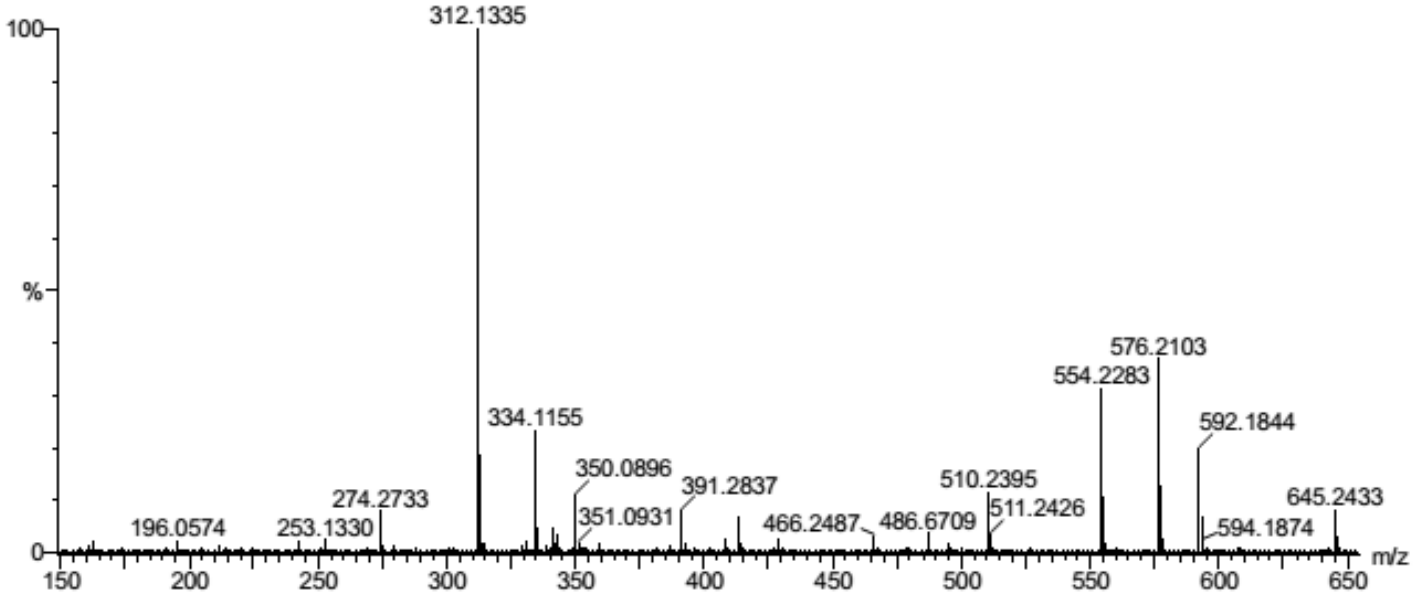
Elemental Composition Report

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 = 3

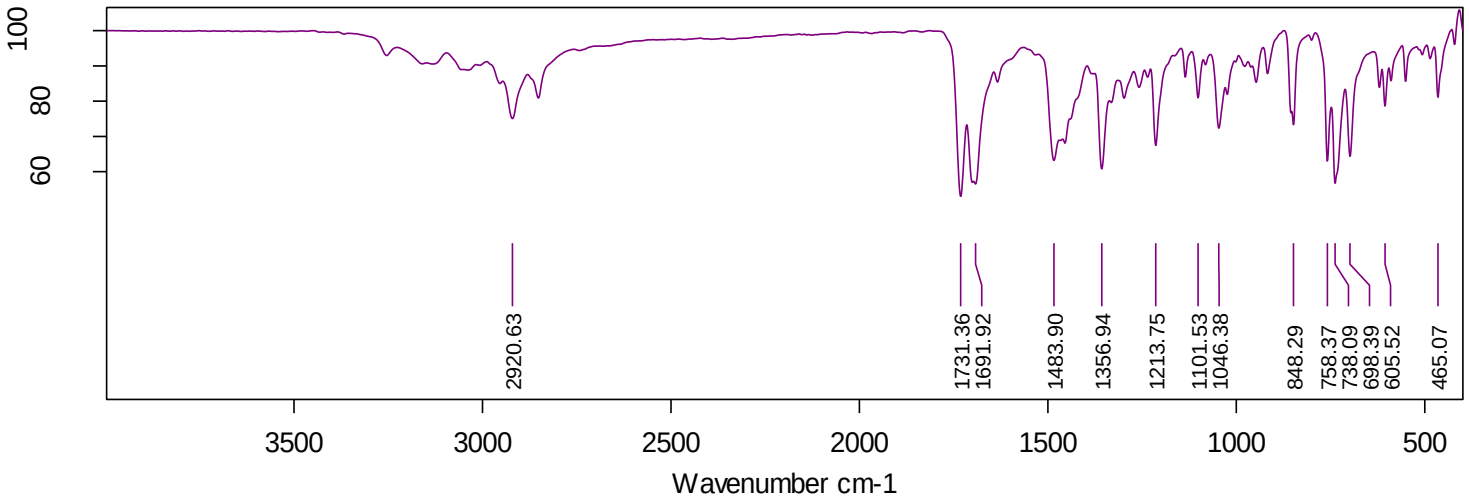
Monoisotopic Mass, Even Electron Ions
50 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-25 H: 11-30 N: 0-5 O: 1-5

Sample Name : 18/01/328 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
051119-18-01-328- 13 (0.140) AM2 (Ar,22000.0,0.00,0.00); Cm (13:18) 1: TOF MS ES+
2.68e+007



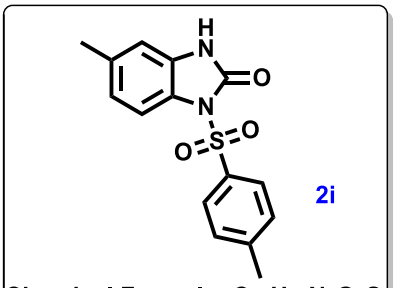
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.1335	312.1348	-1.3	-4.2	10.5	905.1	n/a	n/a	C17 H18 N3 O3

FTIR of 2h



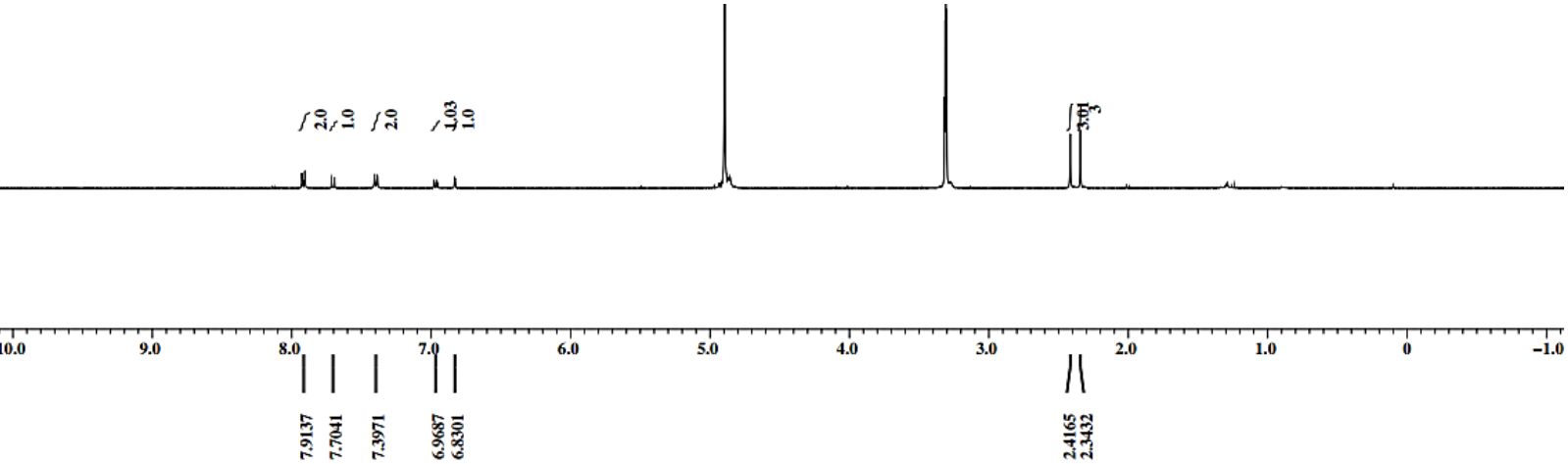
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-328.0	18-01-328	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	1.000146
3996.073013	1.000136
3994.643803	1.000129
3993.214592	1.000128
3991.785381	1.000127
3990.356171	1.000121
3988.926960	1.000110
3987.497749	1.000097
3986.068539	1.000084
3984.639328	1.000074
3983.210117	1.000067
3981.780907	1.000064
3980.351696	1.000064
3978.922485	1.000063
3977.493275	1.000053
3976.064064	1.000027
3974.634853	0.999978
3973.205643	0.999907
3971.776432	0.999831
3970.347221	0.999780
3968.918011	0.999782

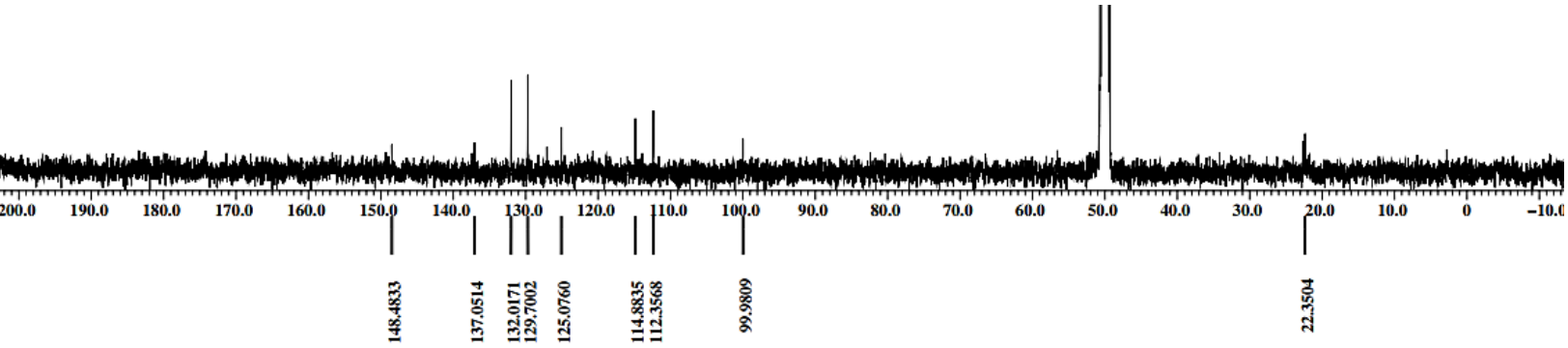


Chemical Formula: $C_{15}H_{14}N_2O_3S$
Exact Mass: 302.0725

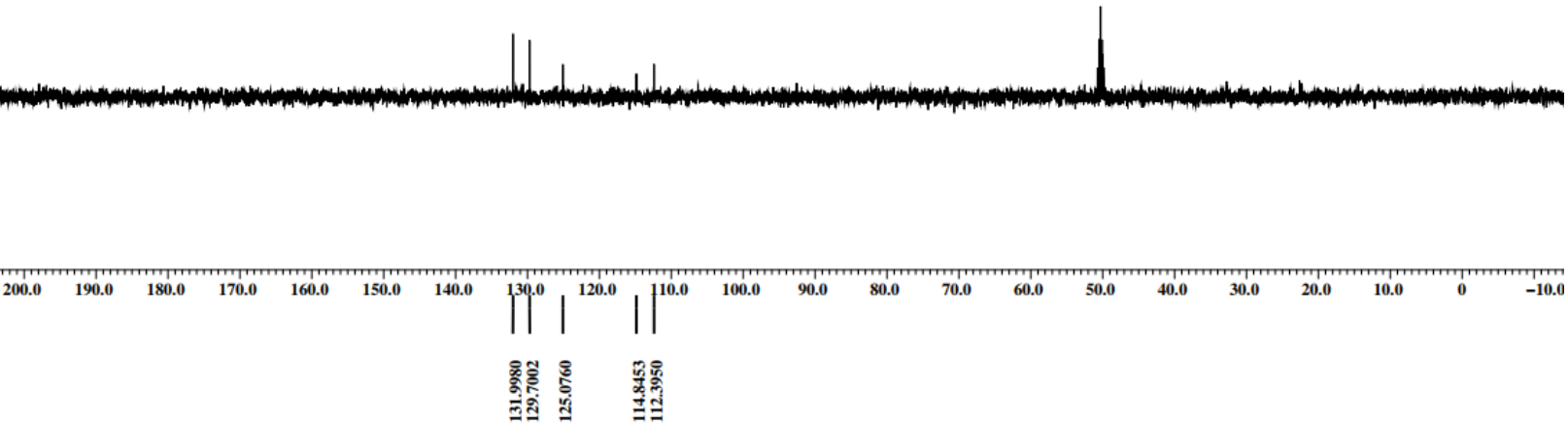
^{1}H-NMR (CD_3OD, 400 MHz) of 2i



^{13}C-NMR (CD_3OD, 100 MHz) of 2i



^{13}C-DEPT (CD_3OD, 100 MHz) of 2i



HRMS of 2i

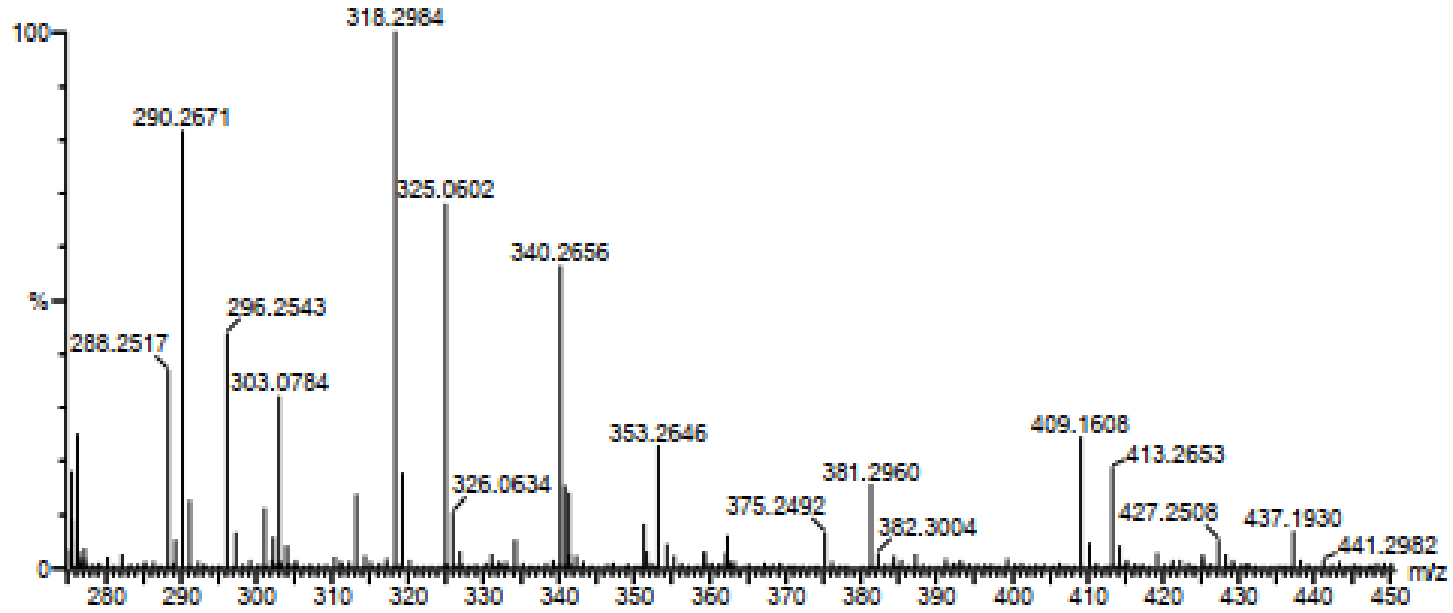
Elemental Composition Report

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 = 6

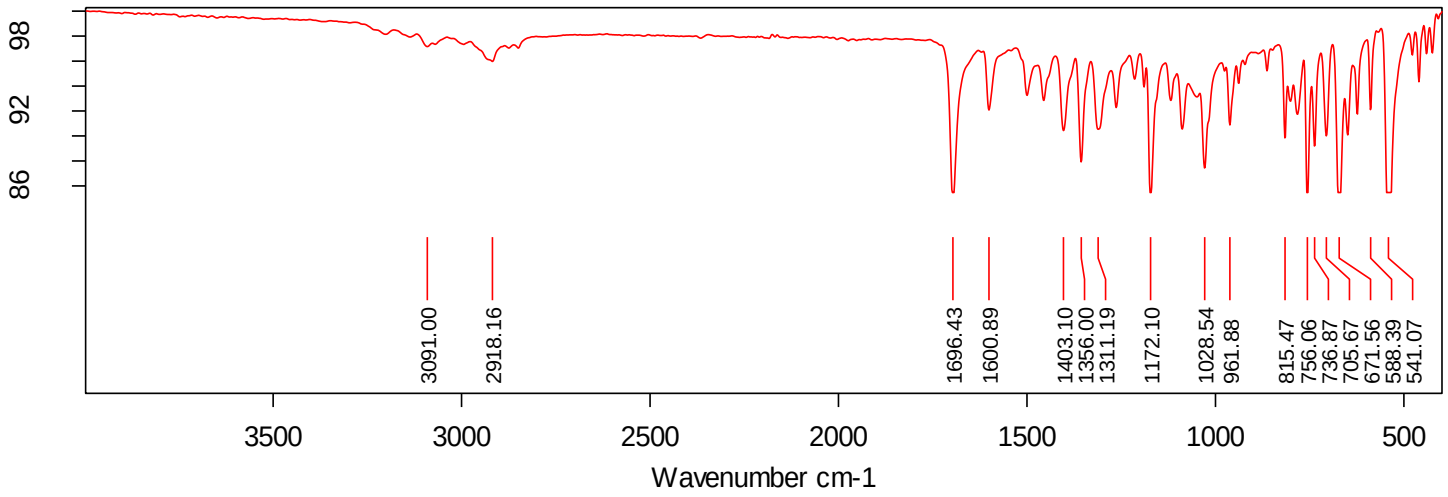
Monoisotopic Mass, Even Electron Ions
59 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 15-25 H: 12-25 N: 1-3 O: 0-4 Na: 0-1 S: 0-1

Sample Name : 18-01-445 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
221020-18-01-445 12 (0.131) 1: TOF MS ES+
1.16e+007



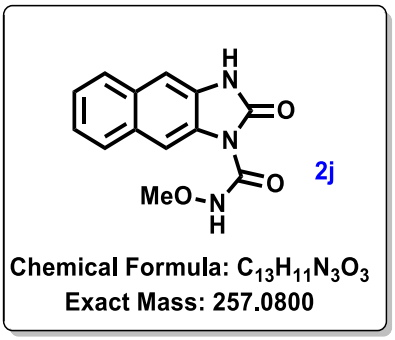
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
303.0784	303.0803	-1.9	-6.3	9.5	1514.2	n/a	n/a	C15 H15 N2 O3 S

FTIR of 2i



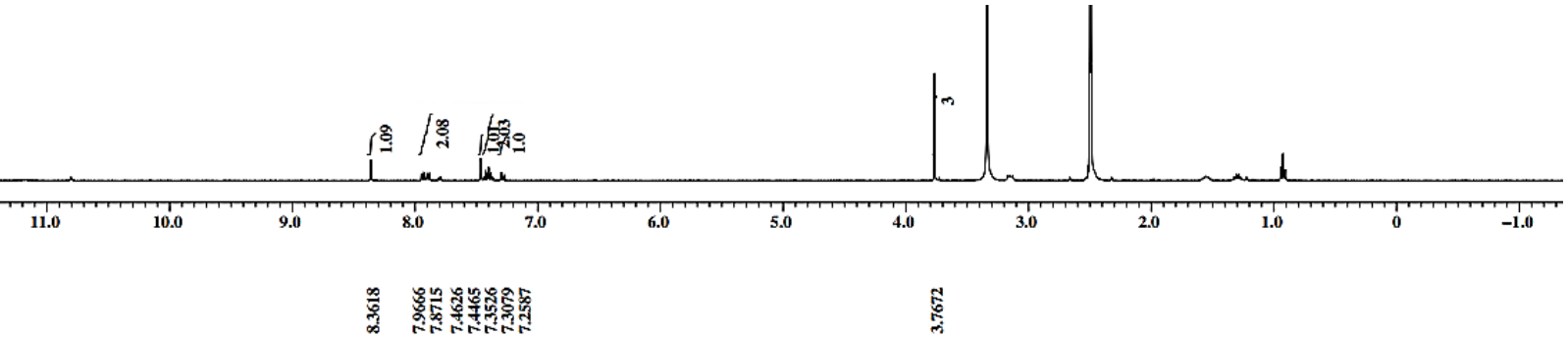
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-445.0	18-01-445	Instrument type and / or accessory	10/23/2020

Wavenumber cm-1	Transmittance [%]
3997.658602	0.999975
3996.229335	1.000031
3994.800069	1.000077
3993.370802	1.000097
3991.941536	1.000078
3990.512269	1.000018
3989.083002	0.999929
3987.653736	0.999839
3986.224469	0.999776
3984.795203	0.999754
3983.365936	0.999772
3981.936670	0.999815
3980.507403	0.999864
3979.078136	0.999906
3977.648870	0.999933
3976.219603	0.999946
3974.790337	0.999942
3973.361070	0.999914
3971.931804	0.999857
3970.502537	0.999782
3969.073270	0.999718



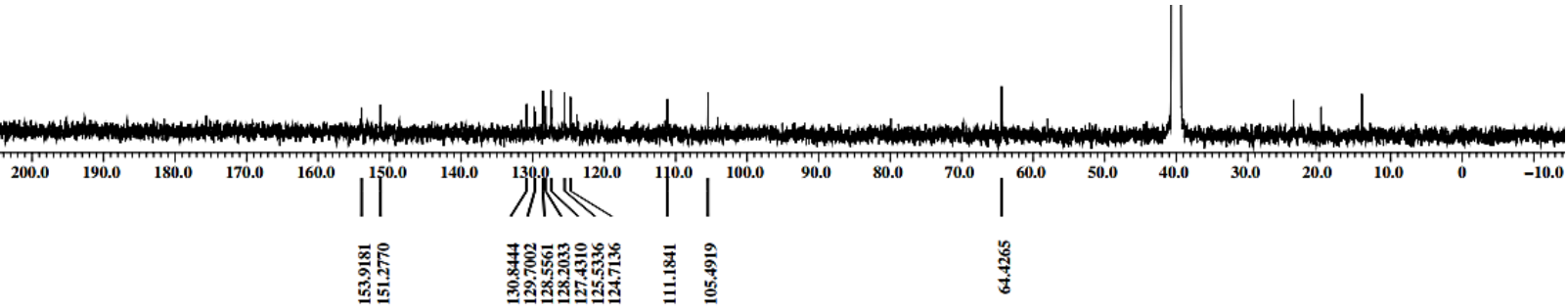
Chemical Formula: $C_{13}H_{11}N_3O_3$
Exact Mass: 257.0800

^{1}H-NMR (DMSO-d6, 400 MHz) of 2j



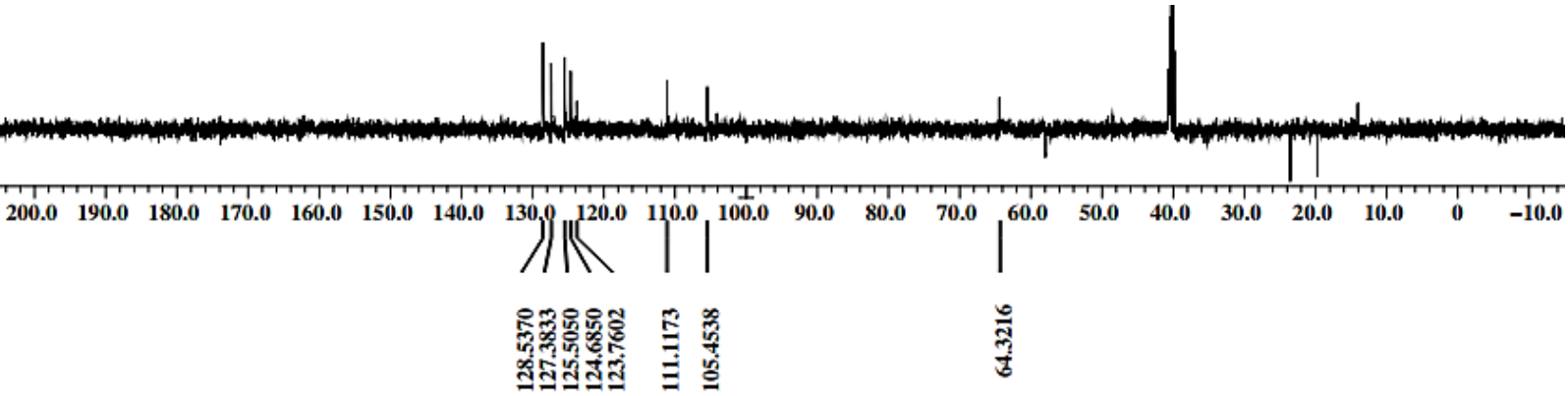
8.3618
7.9666
7.8715
7.4626
7.4465
7.3526
7.3079
7.2587
3.7672

^{13}C-NMR (DMSO-d6, 100 MHz) of 2j



153.9181
151.2770
130.8444
129.7002
128.5561
128.2033
127.4310
125.5336
124.7136
111.1841
105.4919
64.4265

^{13}C-DEPT (DMSO-d6, 100 MHz) of 2j



128.5370
127.3833
125.5050
124.6850
123.7602
111.1173
105.4538
64.3216

HRMS of 2j

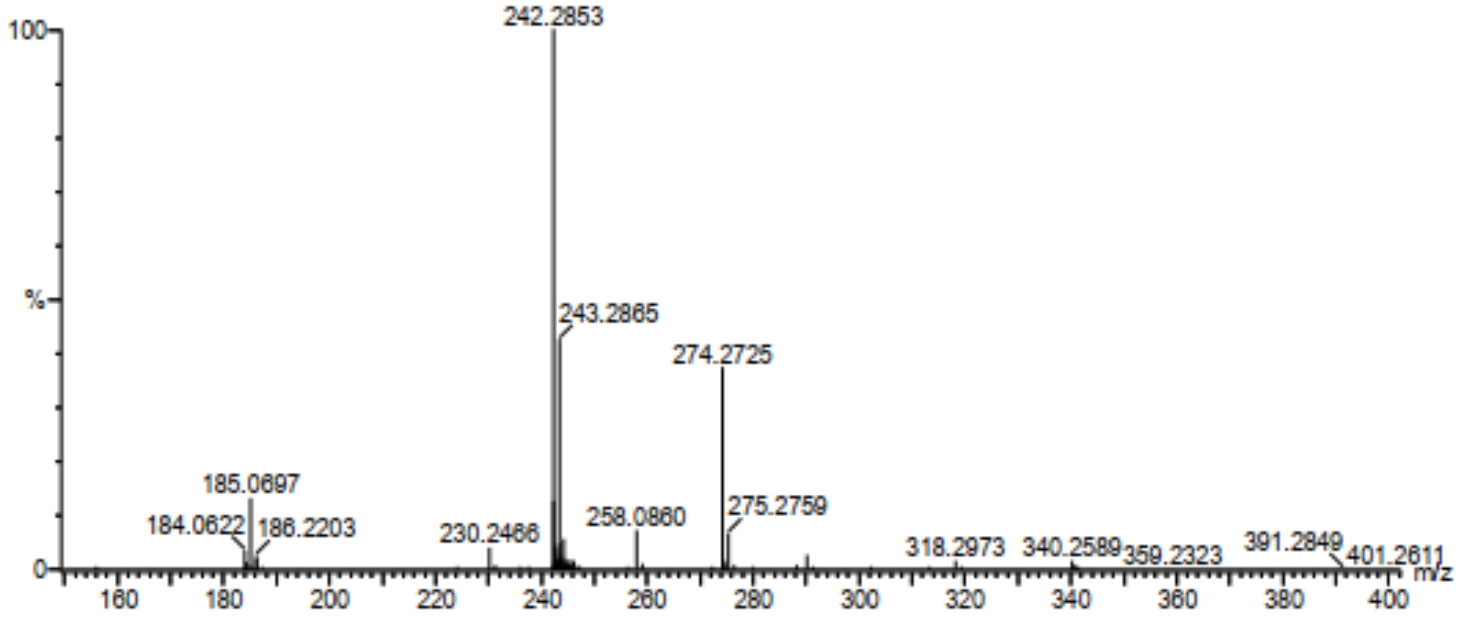
Elemental Composition Report

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 = 6

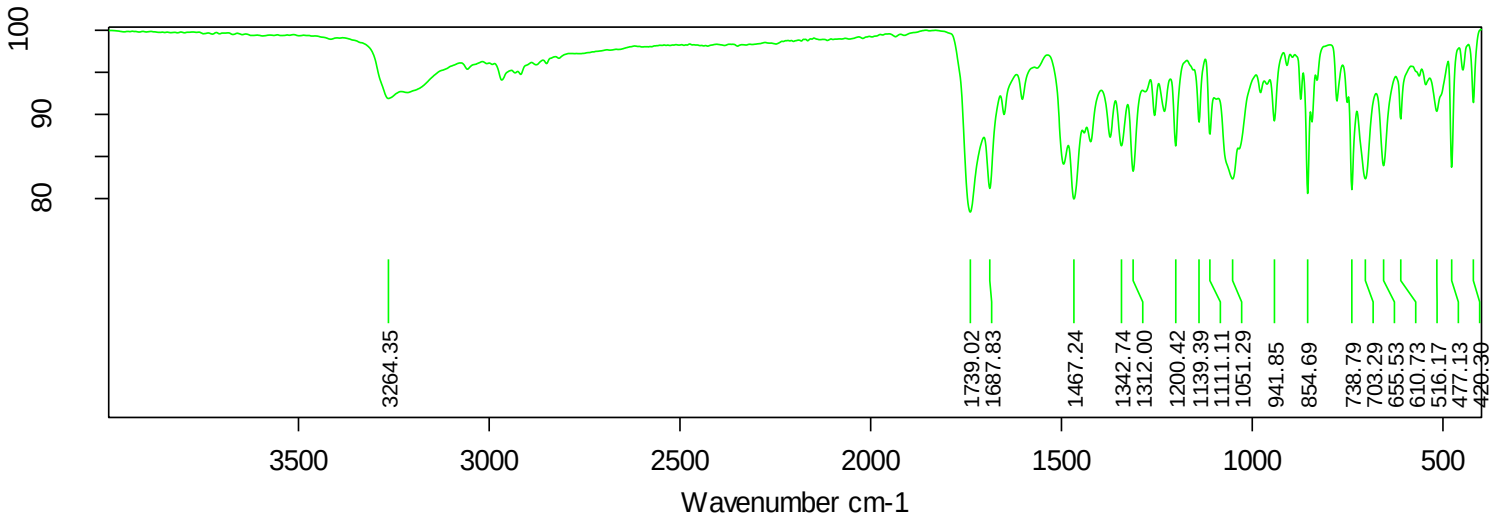
Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-25 H: 8-25 N: 0-4 O: 0-4

Sample Name : 18-01-419 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
240920-18-01-419 15 (0.157) 1: TOF MS ES+
2.19e+008



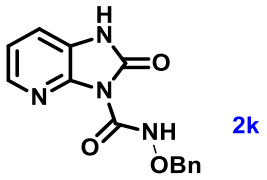
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
258.0860	258.0879	-1.9	-7.4	9.5	1854.5	n/a	n/a	C13 H12 N3 O3

FTIR of 2j



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-417.0	18-01-417	Instrument type and / or accessory	10/21/2020

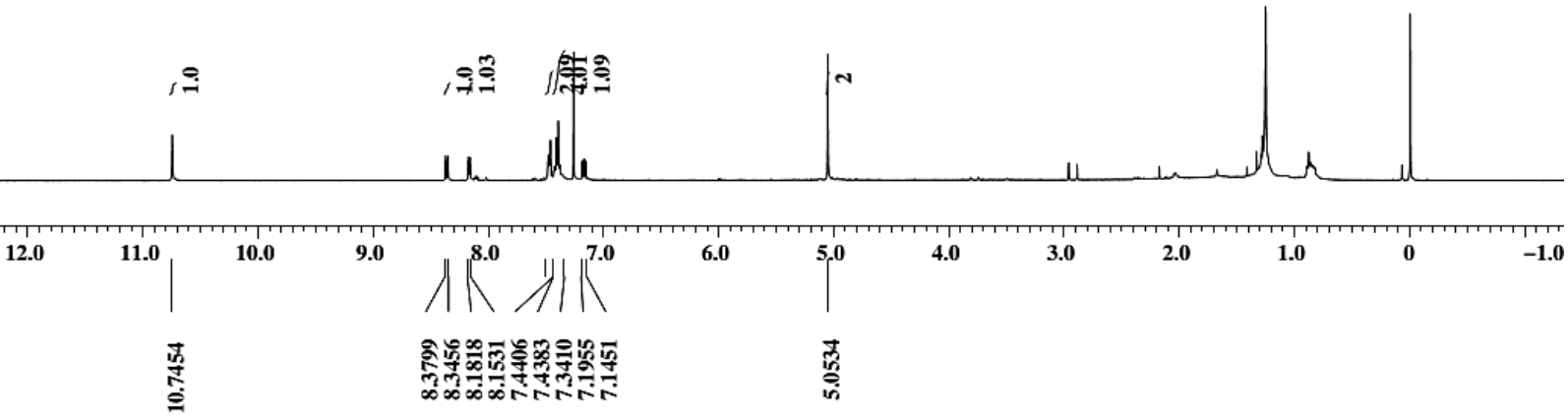
Wavenumber cm-1	Transmittance [%]
3997.658602	1.000000
3996.229335	0.999913
3994.800069	0.999841
3993.370802	0.999793
3991.941536	0.999767
3990.512269	0.999753
3989.083002	0.999739
3987.653736	0.999723
3986.224469	0.999704
3984.795203	0.999675
3983.365936	0.999634
3981.936670	0.999577
3980.507403	0.999506
3979.078136	0.999429
3977.648870	0.999355
3976.219603	0.999290
3974.790337	0.999231
3973.361070	0.999164
3971.931804	0.999078
3970.502537	0.998971
3969.073270	0.998853



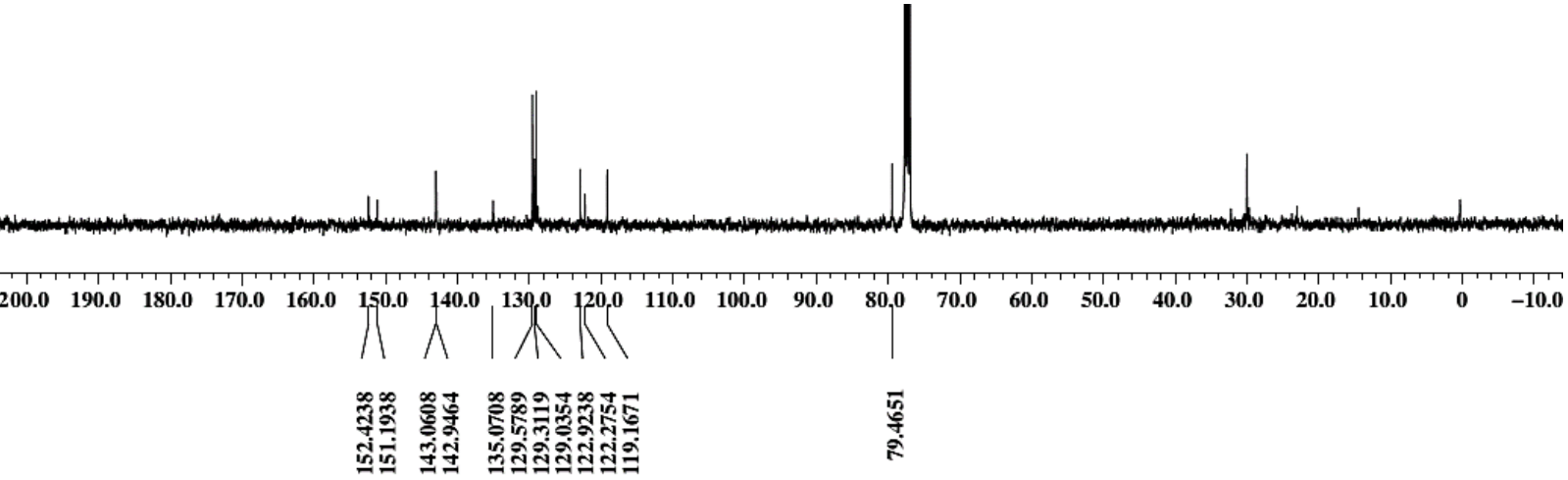
2k

Chemical Formula: $C_{14}H_{12}N_4O_3$
Exact Mass: 284.0909

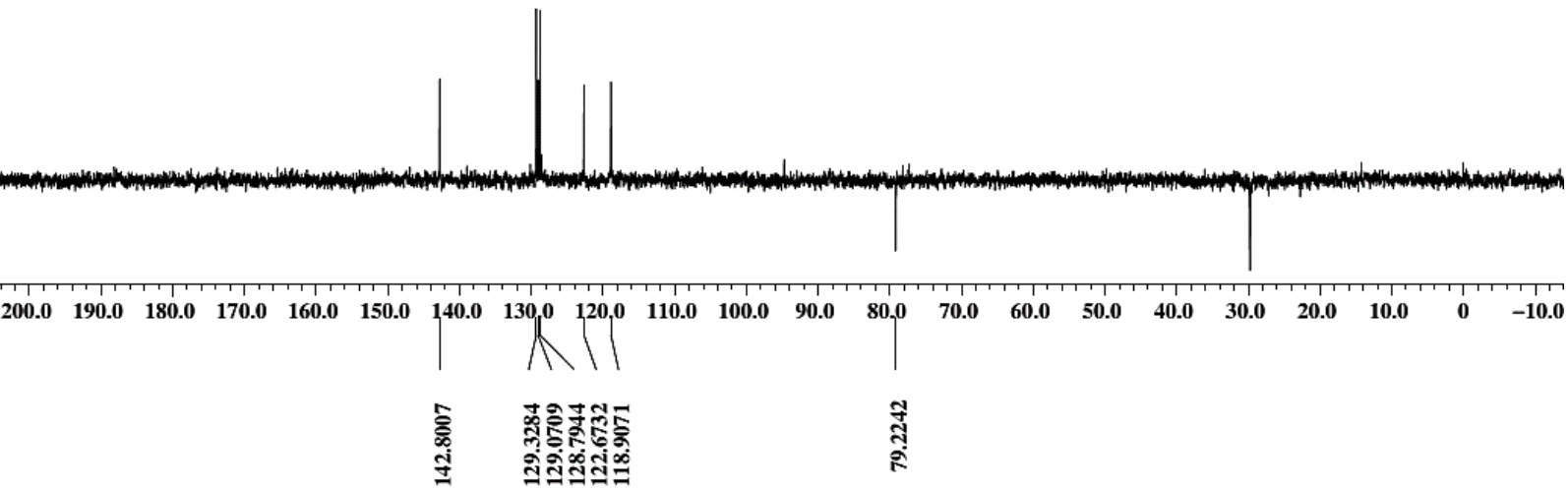
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2k



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2k



HRMS of 2k

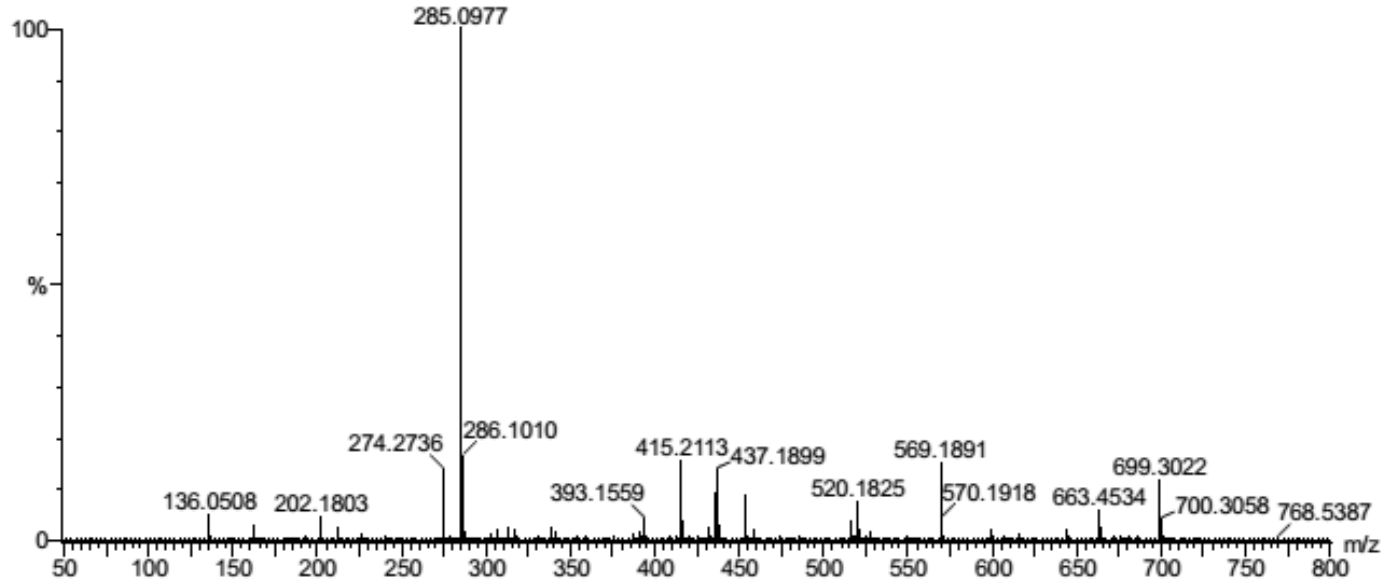
Elemental Composition Report

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 = 3

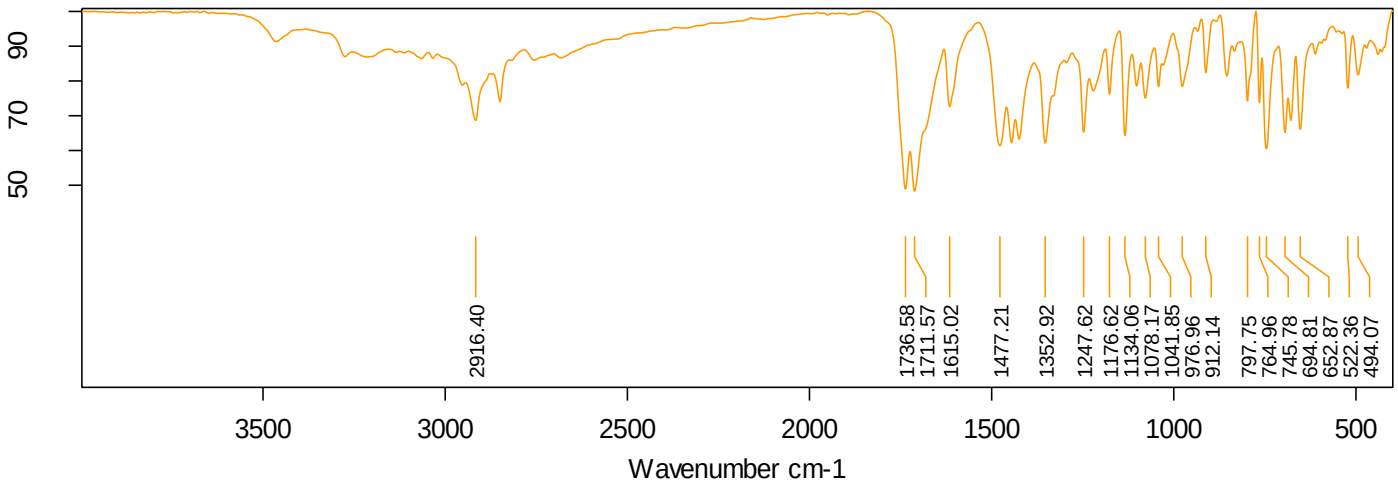
Monoisotopic Mass, Even Electron Ions
60 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-30 H: 7-35 N: 0-5 O: 1-4

Sample Name : 18-01-356 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
221119-18-01-356 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (8:18) 1: TOF MS ES+
3.72e+007



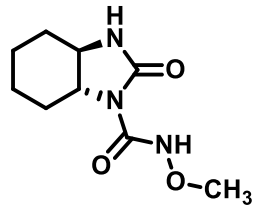
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
285.0977	285.0988	-1.1	-3.9	10.5	977.4	n/a	n/a	C14 H13 N4 O3

FTIR of 2k



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-356.0	18-01-356	Instrument type and / or accessory	1/6/2020

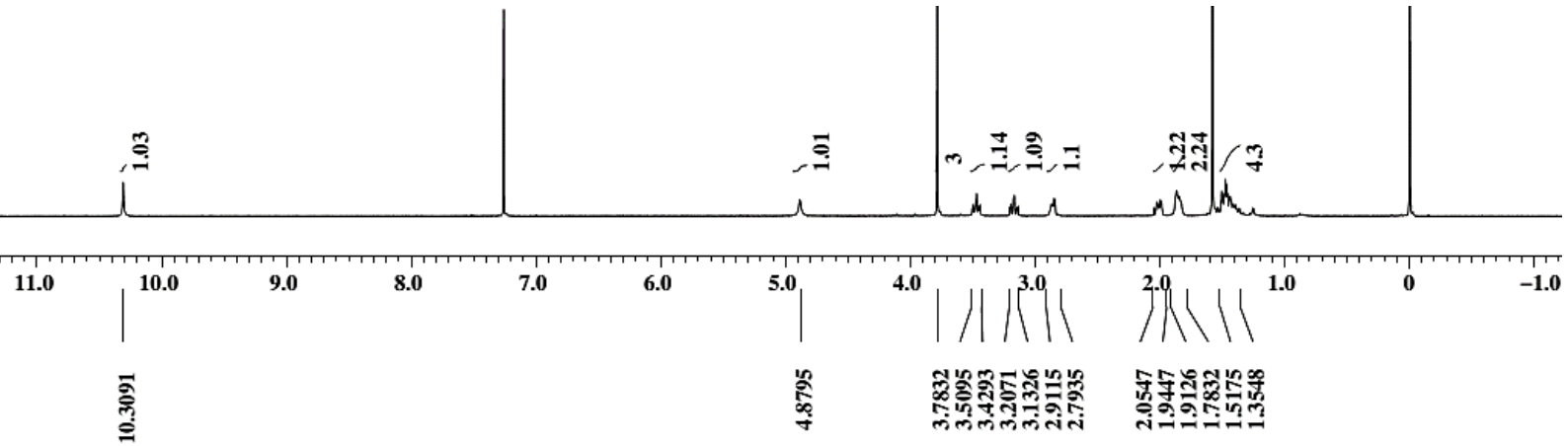
Wavenumber cm-1	Transmittance [%]
3997.502224	0.999644
3996.073013	0.999755
3994.643803	0.999865
3993.214592	0.999965
3991.785381	1.000038
3990.356171	1.000074
3988.926960	1.000071
3987.497749	1.000031
3986.068539	0.999963
3984.639328	0.999874
3983.210117	0.999781
3981.780907	0.999699
3980.351696	0.999636
3978.922485	0.999585
3977.493275	0.999546
3976.064064	0.999530
3974.634853	0.999550
3973.205643	0.999611
3971.776432	0.999701
3970.347221	0.999805
3968.918011	0.999907



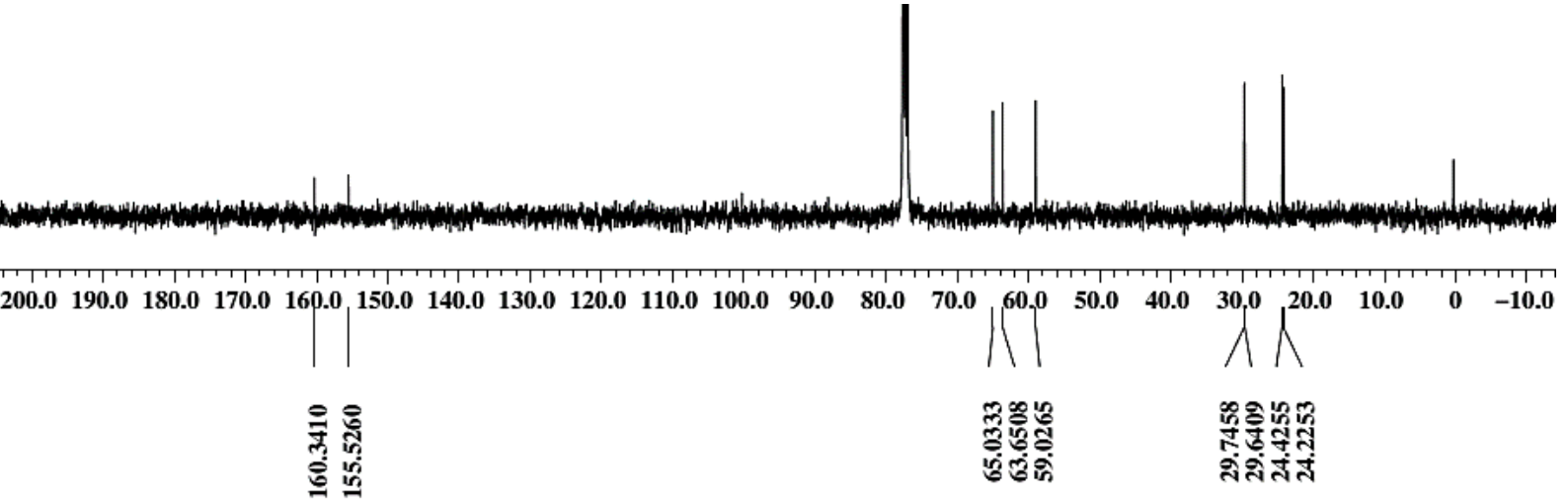
2l

Chemical Formula: $C_9H_{15}N_3O_3$
Exact Mass: 213.1113

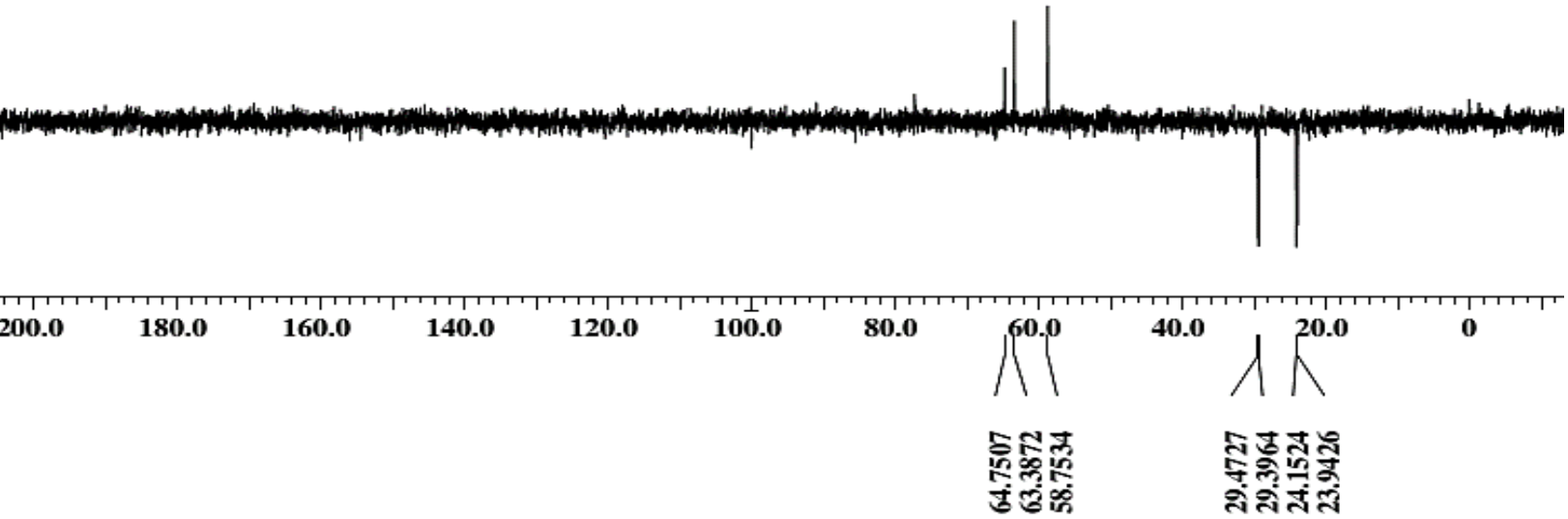
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2l



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2l



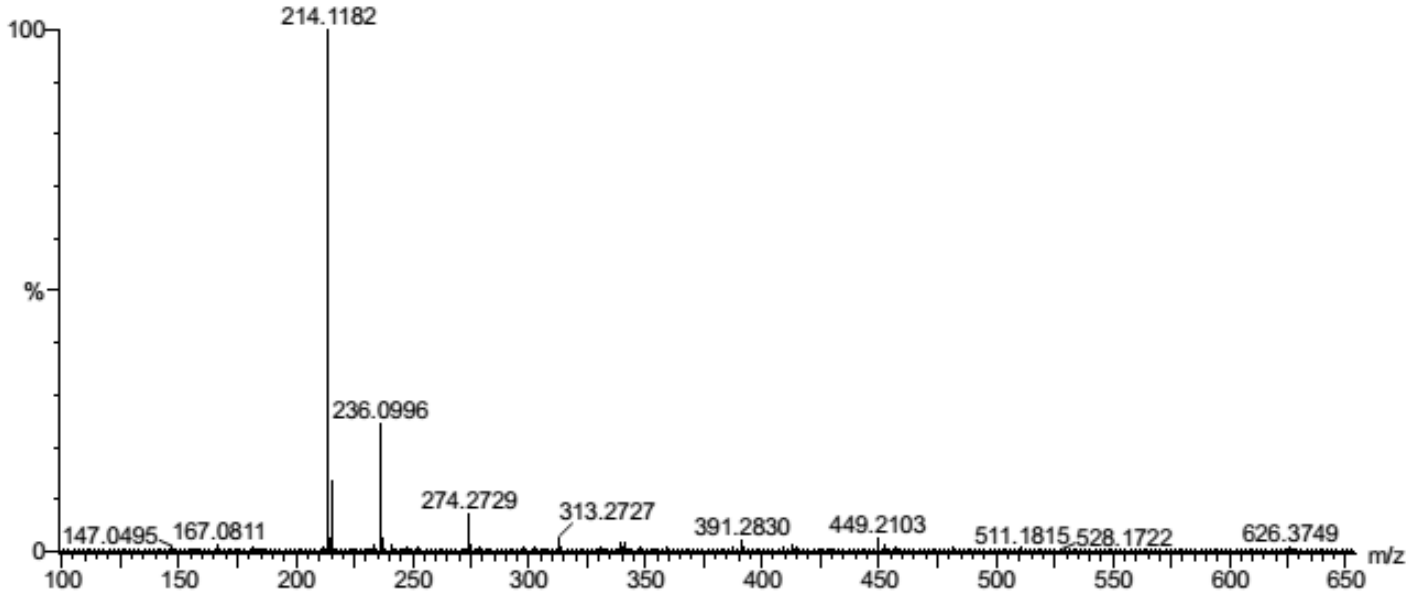
Elemental Composition Report

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 = 3

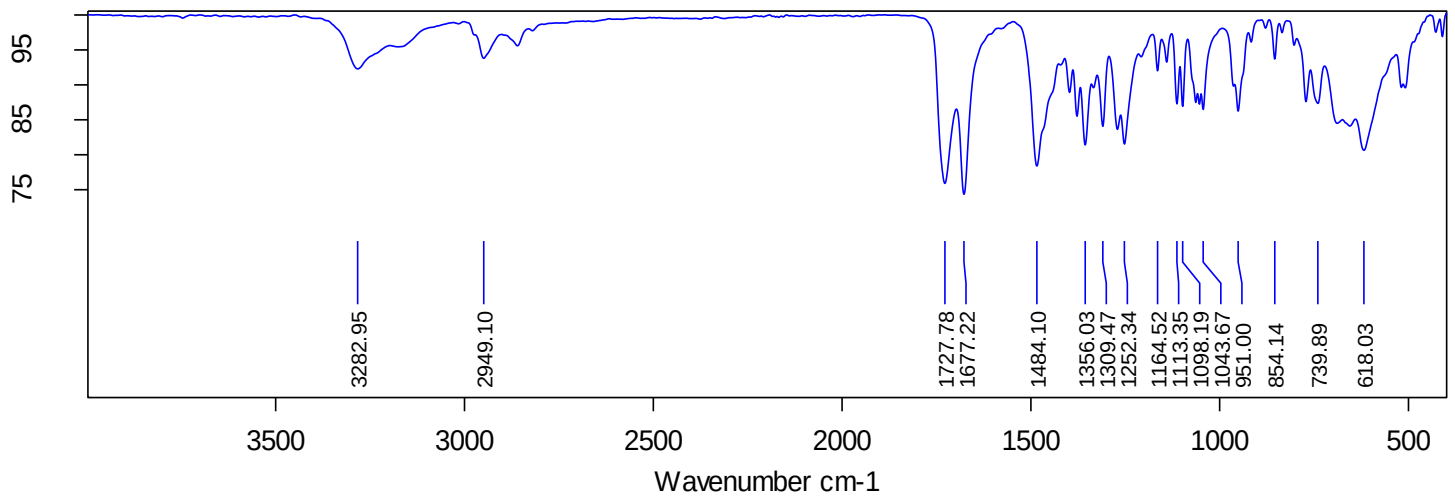
Monoisotopic Mass, Odd and Even Electron Ions
42 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-40 H: 11-45 N: 0-4 O: 1-4

Sample Name : 18-01-371 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
051219-18-01-371 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (7:18) 1: TOF MS ES+
7.04e+007



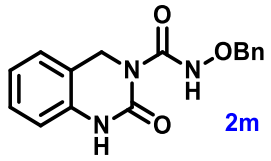
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
214.1182	214.1192	-1.0	-4.7	3.5	1205.4	n/a	n/a	C9 H16 N3 O3

FTIR of 2l



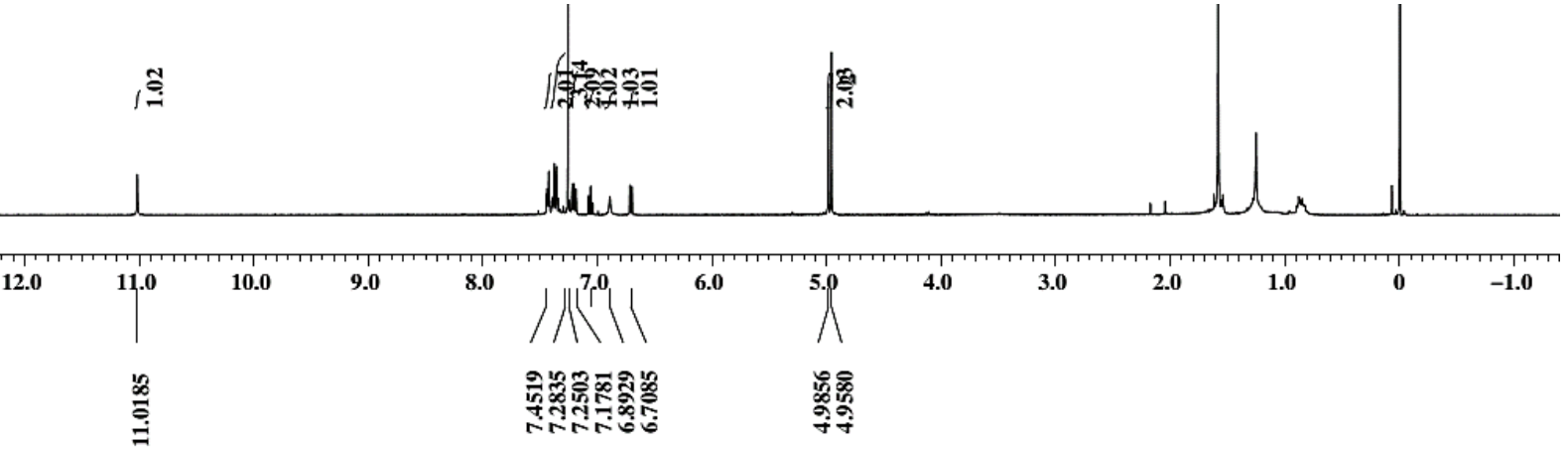
D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-371.0	18-01-371	Instrument type and / or accessory	1/6/2020

Wavenumber cm-1	Transmittance [%]
3997.502224	1.000014
3996.073013	1.000092
3994.643803	1.000158
3993.214592	1.000200
3991.785381	1.000207
3990.356171	1.000178
3988.926960	1.000124
3987.497749	1.000063
3986.068539	1.000012
3984.639328	0.999981
3983.210117	0.999978
3981.780907	1.000004
3980.351696	1.000051
3978.922485	1.000106
3977.493275	1.000158
3976.064064	1.000198
3974.634853	1.000221
3973.205643	1.000225
3971.776432	1.000216
3970.347221	1.000199
3968.918011	1.000181

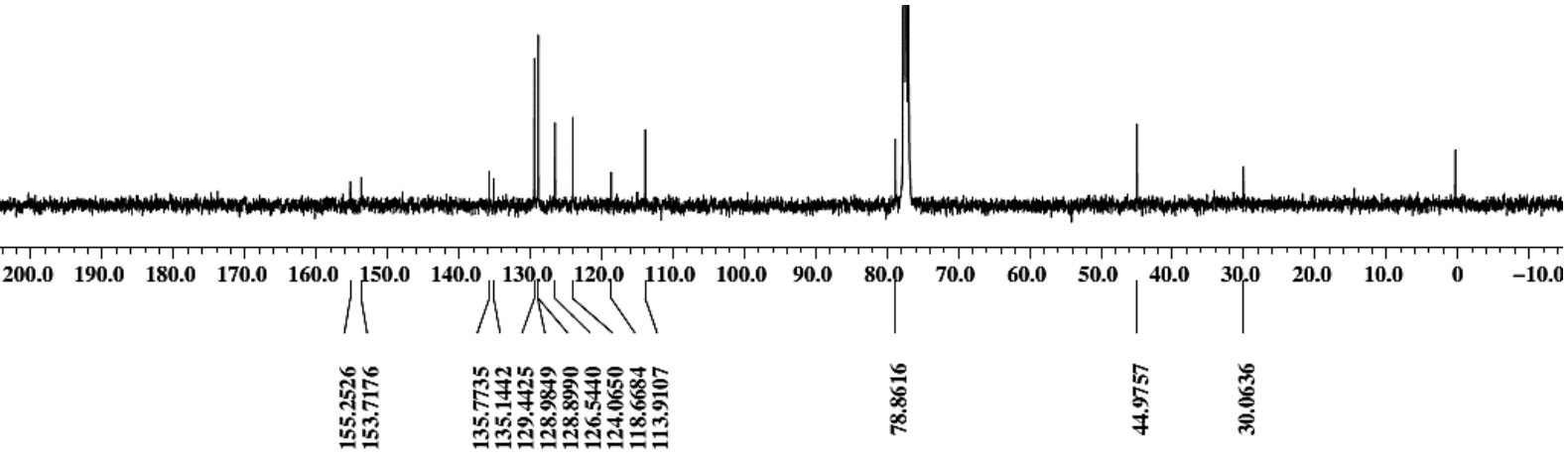


Chemical Formula: $C_{16}H_{15}N_3O_3$
Exact Mass: 297.1113

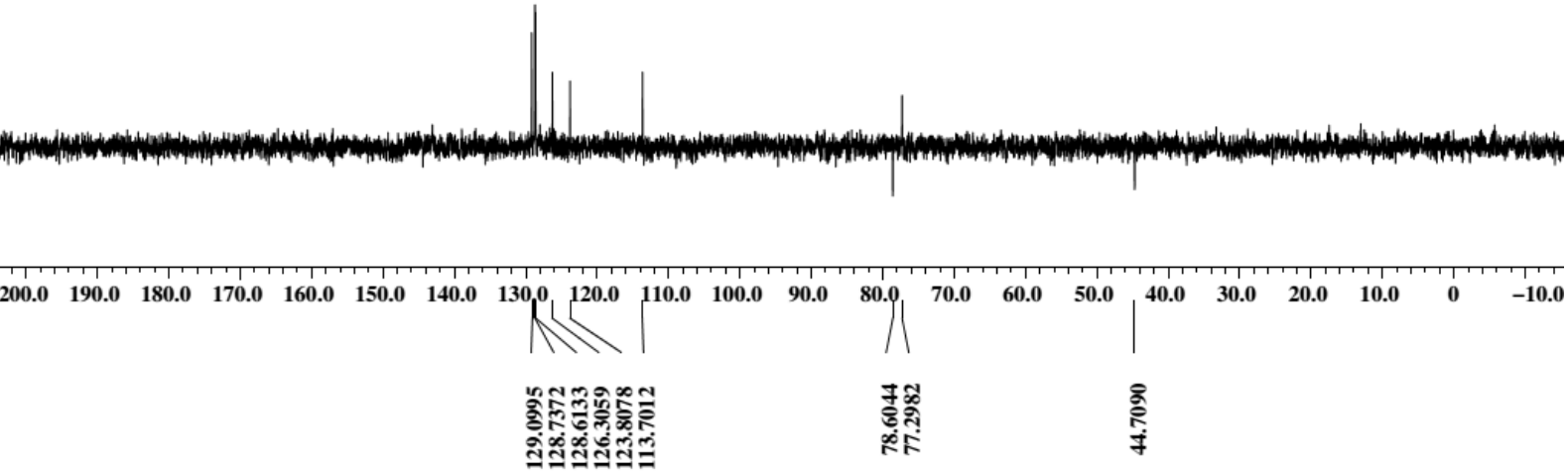
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2m



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2m



HRMS of 2m

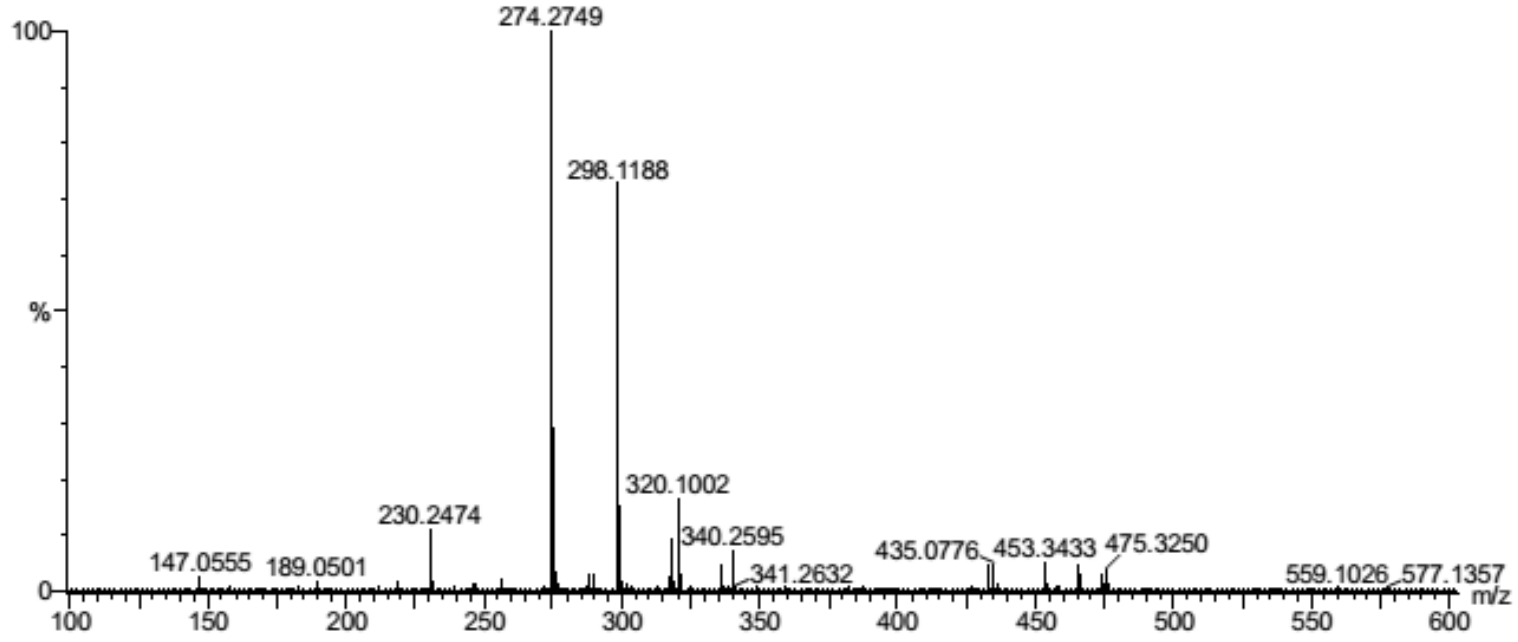
Elemental Composition Report

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 = 3

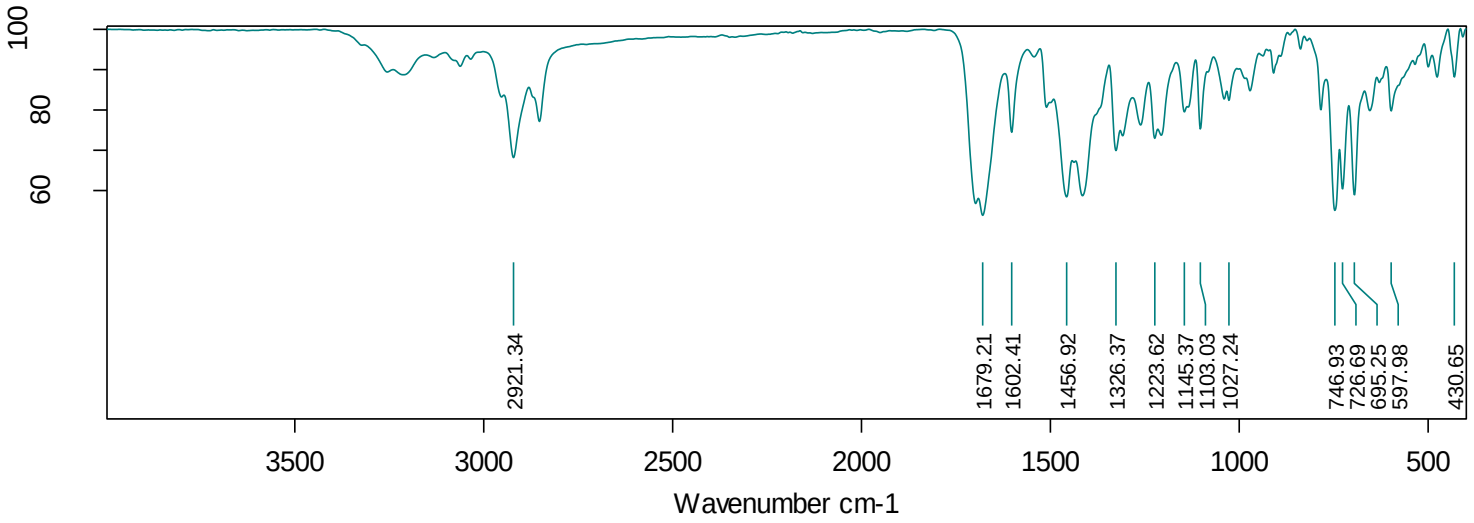
Monoisotopic Mass, Even Electron Ions
77 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-20 H: 10-25 N: 0-3 O: 1-5 F: 0-2

Sample Name : 18-01-302 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
011019-18-01-302 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (7:18) 1: TOF MS ES+
1.30e+008



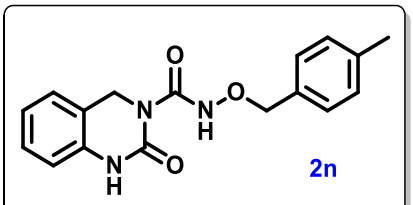
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
298.1188	298.1192	-0.4	-1.3	10.5	990.1	n/a	n/a	C16 H16 N3 O3

FTIR of 2m



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-302.0	18-01-302	Instrument type and / or accessory	1/6/2020

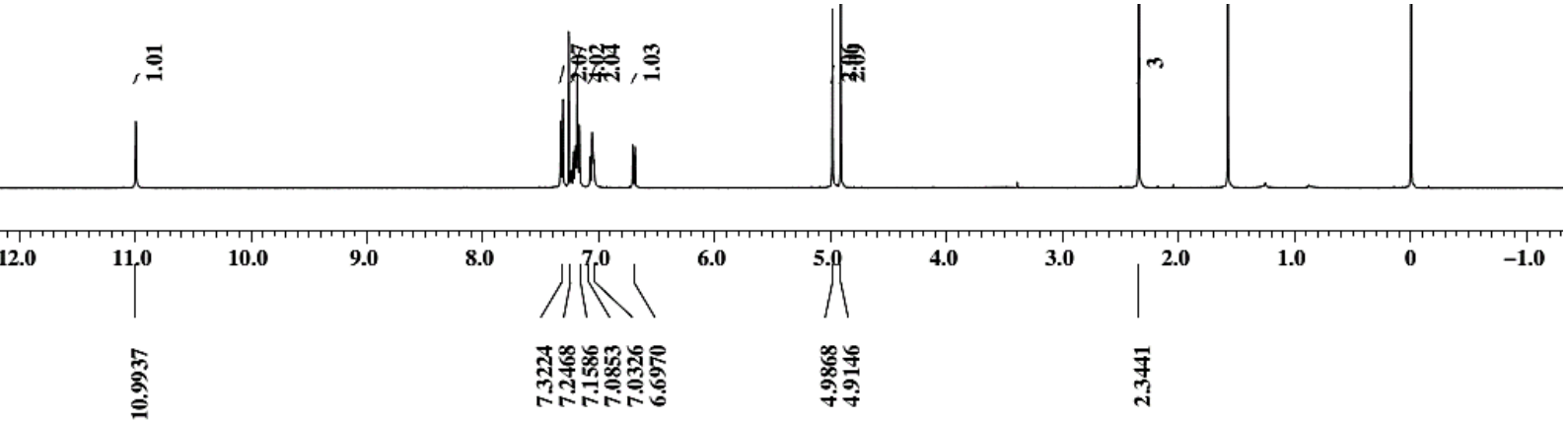
Wavenumber cm-1	Transmittance [%]
3997.502224	1.000031
3996.073013	0.999950
3994.643803	0.999886
3993.214592	0.999851
3991.785381	0.999846
3990.356171	0.999853
3988.926960	0.999849
3987.497749	0.999826
3986.068539	0.999787
3984.639328	0.999745
3983.210117	0.999720
3981.780907	0.999722
3980.351696	0.999746
3978.922485	0.999773
3977.493275	0.999786
3976.064064	0.999777
3974.634853	0.999753
3973.205643	0.999731
3971.776432	0.999724
3970.347221	0.999747
3968.918011	0.999801



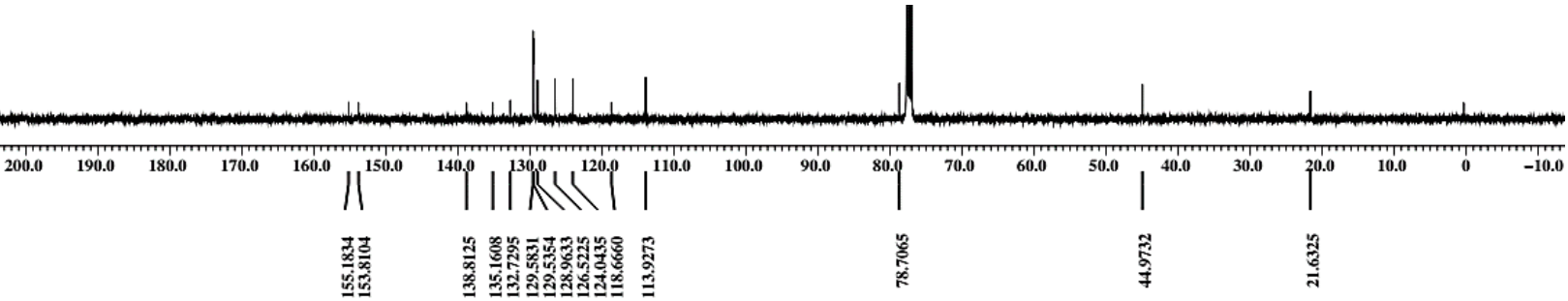
2n

Chemical Formula: $C_{17}H_{17}N_3O_3$
Exact Mass: 311.1270

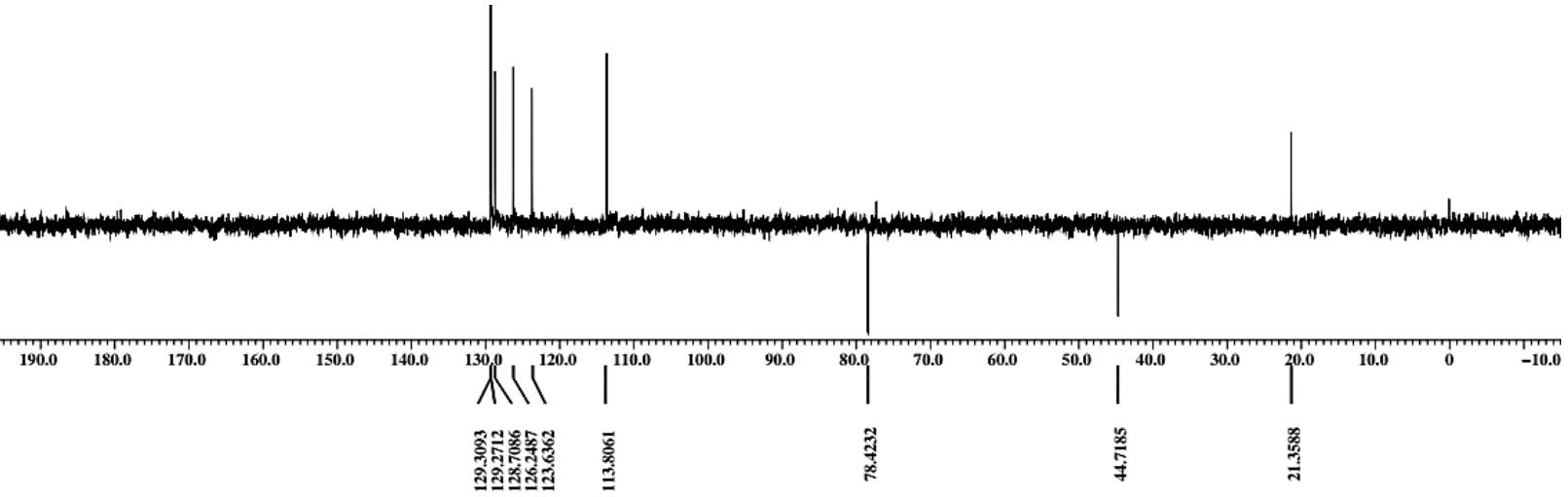
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2n



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2n



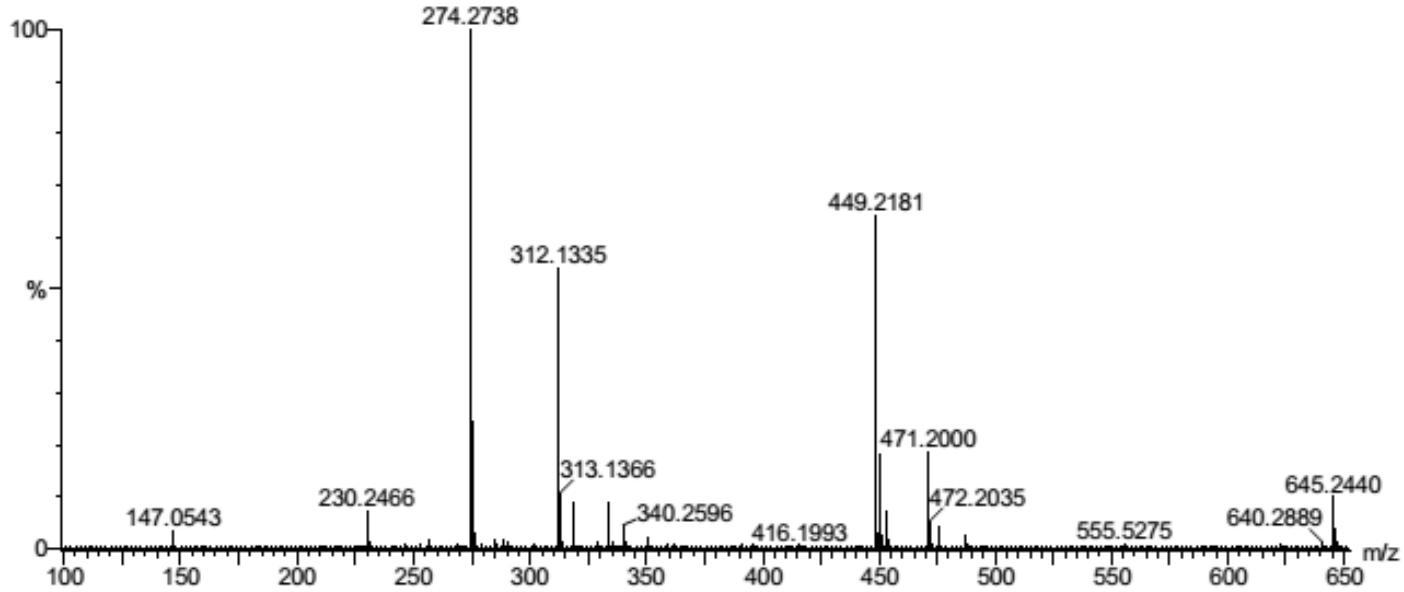
Elemental Composition Report

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 = 3

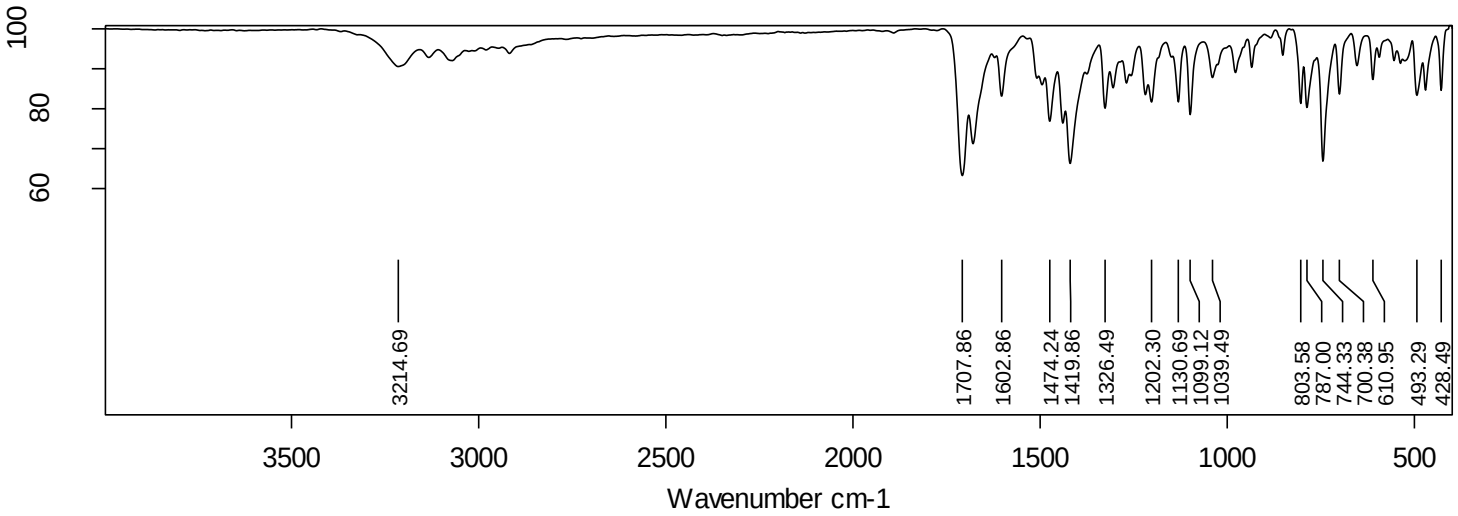
Monoisotopic Mass, Even Electron Ions
50 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 7-30 N: 0-4 O: 1-5

Sample Name : 18-01-364 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
281119-18-01-364 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (8:18) 1: TOF MS ES+
1.11e+008



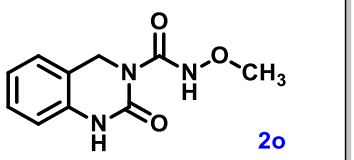
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.1335	312.1348	-1.3	-4.2	10.5	1000.5	n/a	n/a	C17 H18 N3 O3

FTIR of 2n



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-364.0	18-01-364	Instrument type and / or accessory	1/6/2020

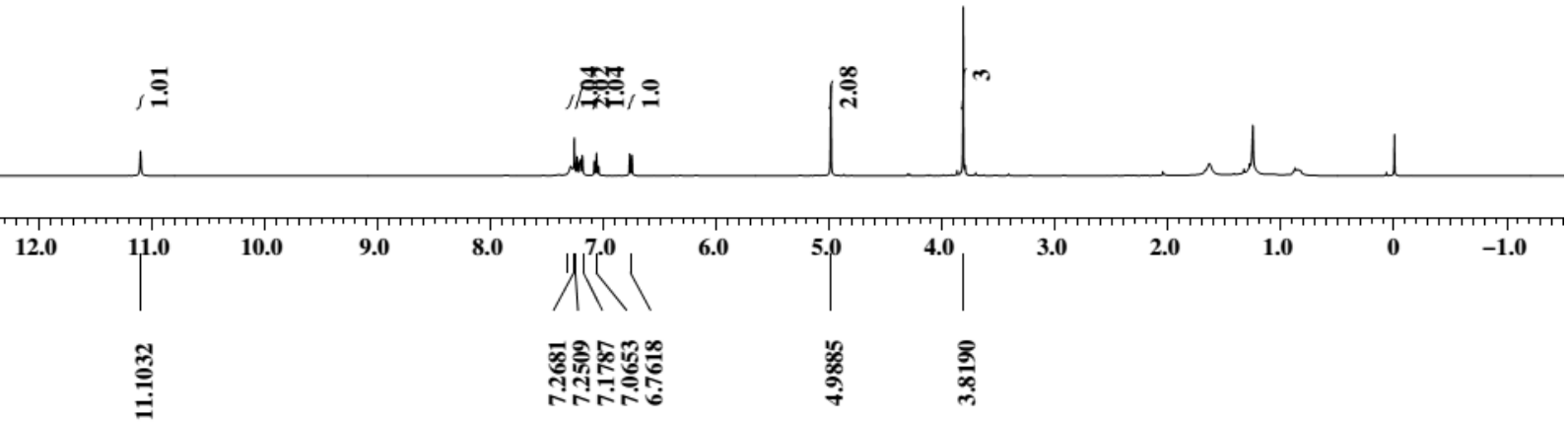
Wavenumber cm-1	Transmittance [%]
3997.502224	1.000471
3996.073013	1.000353
3994.643803	1.000236
3993.214592	1.000121
3991.785381	1.000012
3990.356171	0.999911
3988.926960	0.999821
3987.497749	0.999741
3986.068539	0.999674
3984.639328	0.999621
3983.210117	0.999593
3981.780907	0.999592
3980.351696	0.999618
3978.922485	0.999667
3977.493275	0.999736
3976.064064	0.999821
3974.634853	0.999911
3973.205643	0.999986
3971.776432	1.000031
3970.347221	1.000042
3968.918011	1.000028



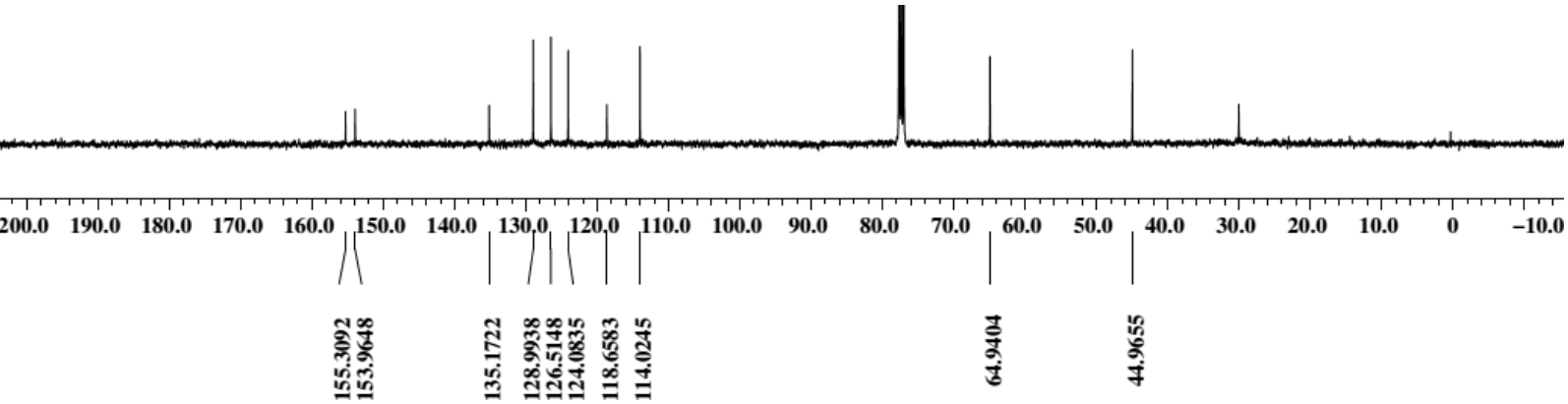
2o

Chemical Formula: $C_{10}H_{11}N_3O_3$
Exact Mass: 221.0800

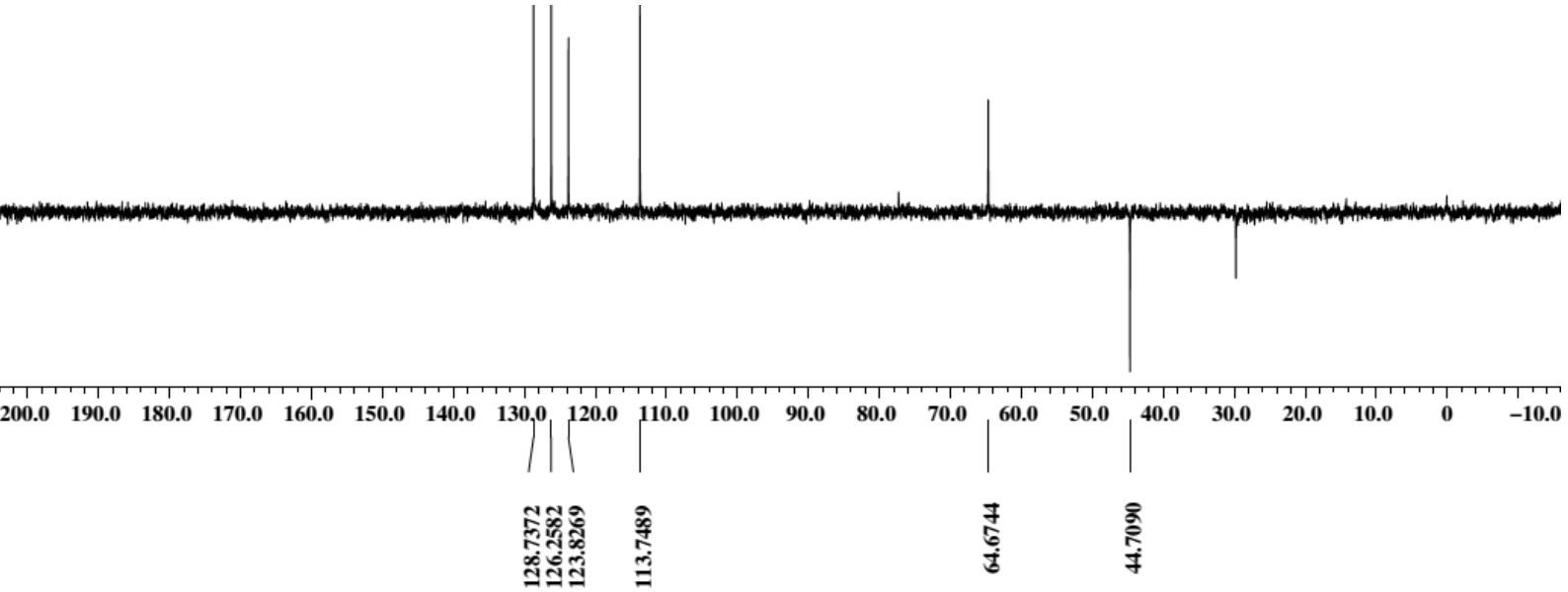
1H-NMR ($CDCl_3$, 400 MHz) of 2o



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2o



HRMS of 2o

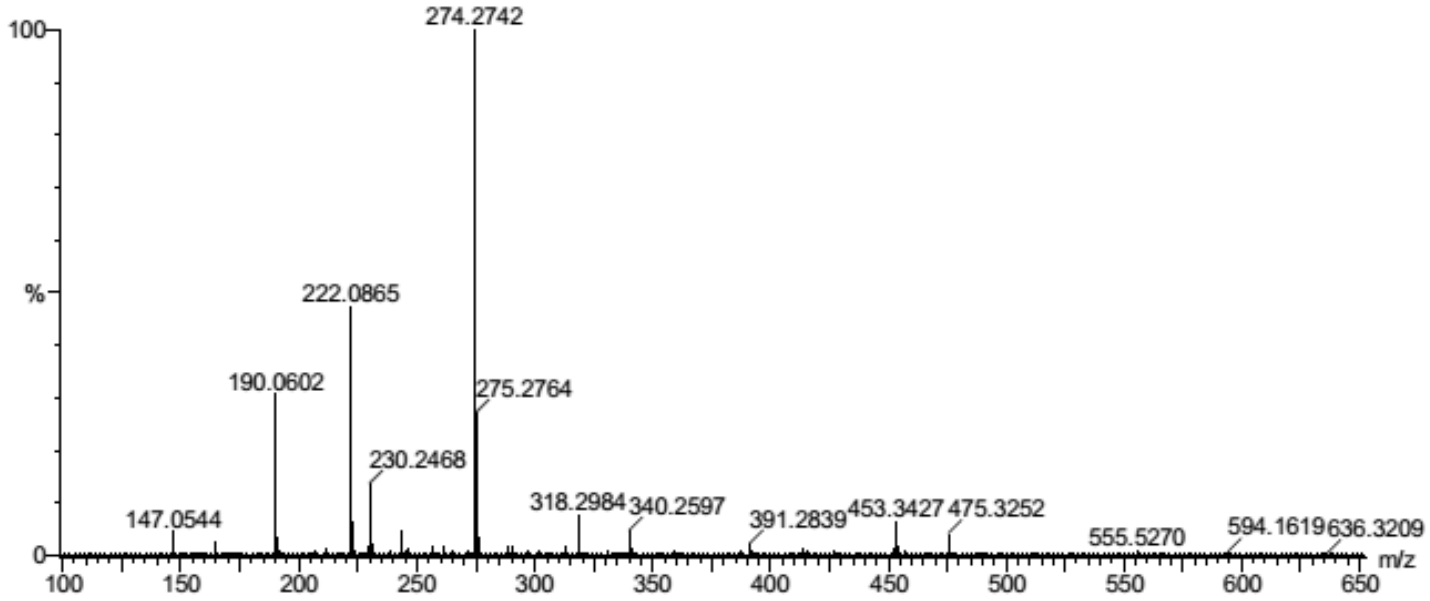
Elemental Composition Report

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 = 3

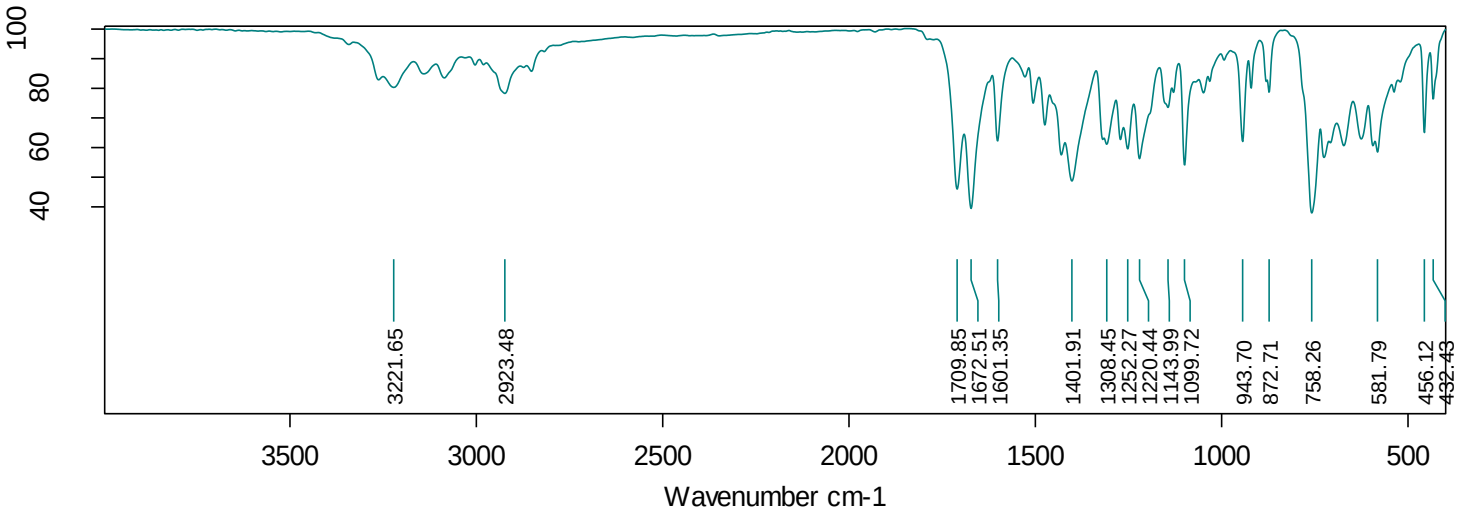
Monoisotopic Mass, Odd and Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-30 H: 7-35 N: 0-4 O: 1-6

Sample Name : 18-01-369 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
031219-18-01-369 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (8:18) 1: TOF MS ES+
1.22e+008



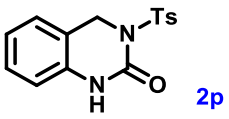
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
222.0865	222.0879	-1.4	-6.3	6.5	1237.5	n/a	n/a	C10 H12 N3 O3

FTIR of 2o



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-369.0	18-01-369	Instrument type and / or accessory	1/6/2020

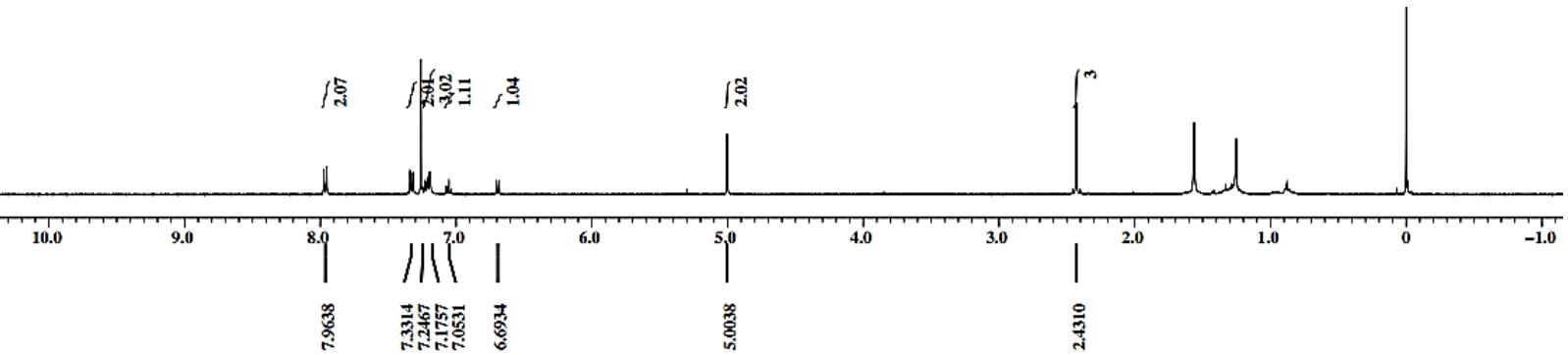
Wavenumber cm-1	Transmittance [%]
3997.502224	1.000146
3996.073013	0.999944
3994.643803	0.999747
3993.214592	0.999569
3991.785381	0.999431
3990.356171	0.999346
3988.926960	0.999318
3987.497749	0.999339
3986.068539	0.999402
3984.639328	0.999501
3983.210117	0.999629
3981.780907	0.999772
3980.351696	0.999902
3978.922485	0.999992
3977.493275	1.000024
3976.064064	1.000000
3974.634853	0.999938
3973.205643	0.999861
3971.776432	0.999789
3970.347221	0.999730
3968.918011	0.999679



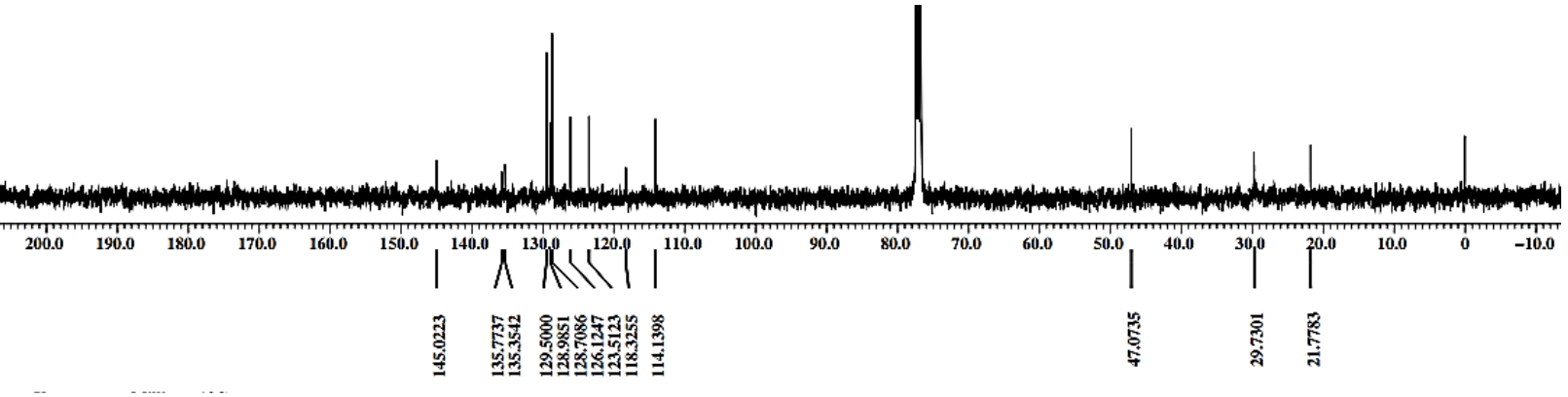
2p

Chemical Formula: $C_{15}H_{14}N_2O_3S$
Exact Mass: 302.0725

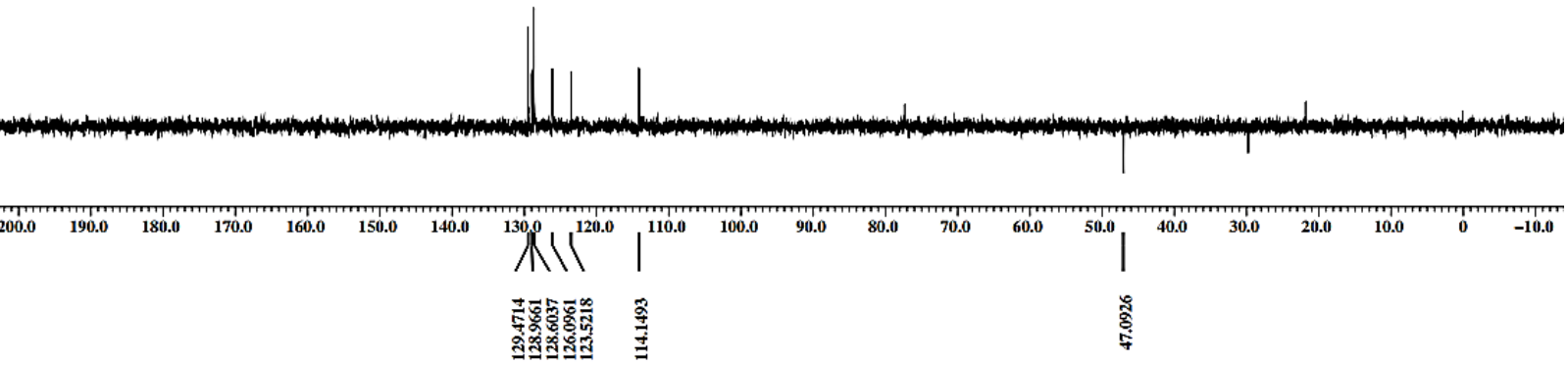
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2p



^{13}C-NMR ($CDCl_3$, 100 MHz) of 2p



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2p



HRMS of 2p

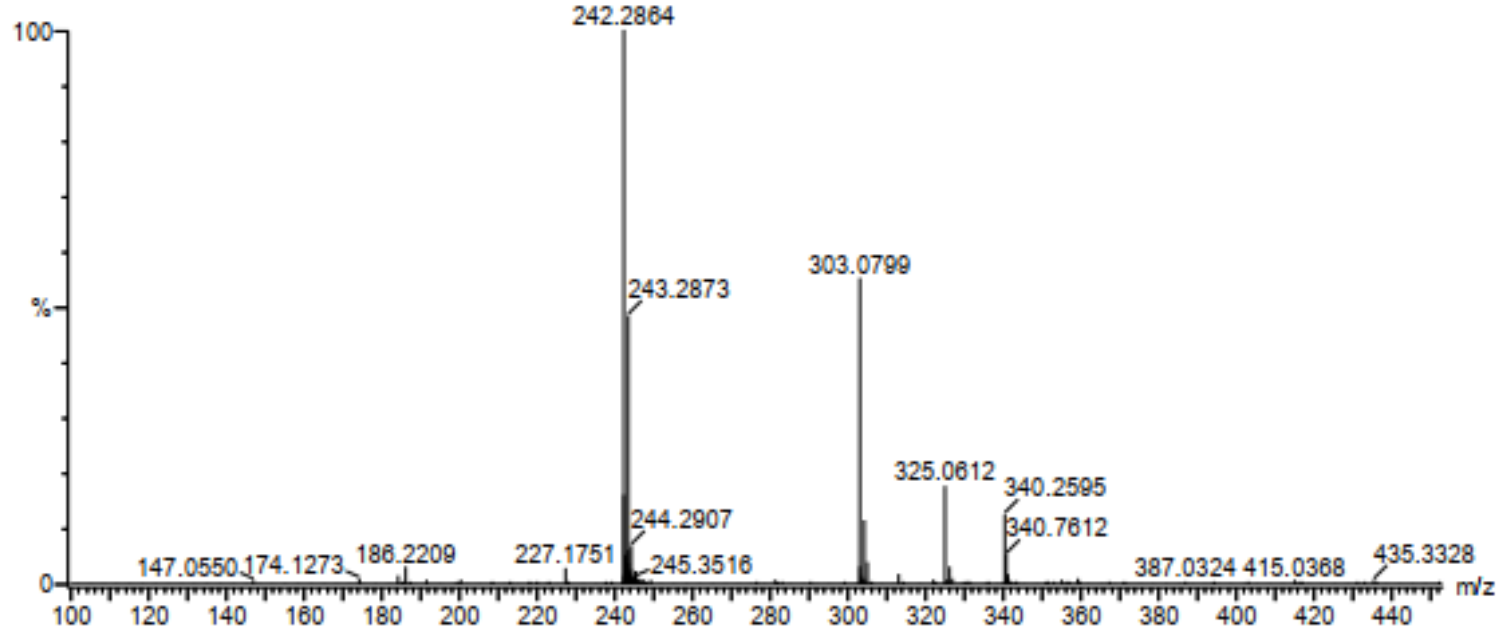
Elemental Composition Report

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 = 6

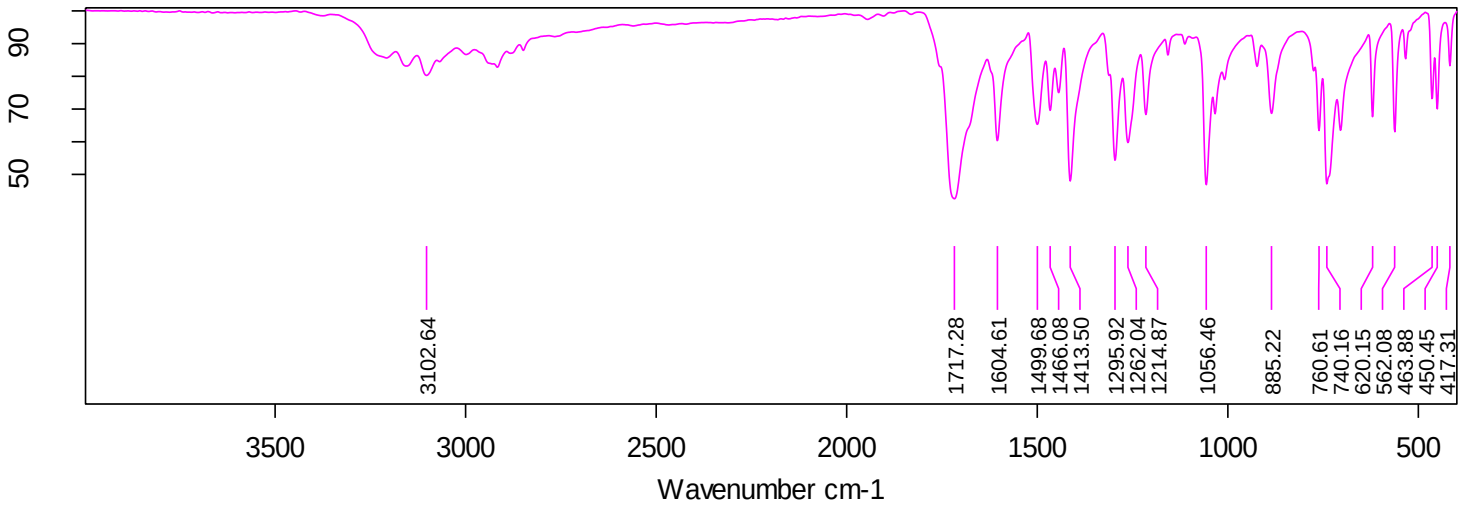
Monoisotopic Mass, Even Electron Ions
46 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-25 H: 11-25 N: 1-2 O: 0-4 S: 1-4

Sample Name : 18-01-431 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
091020-18-01-431 12 (0.131) 1: TOF MS ES+
1.75e+008



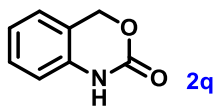
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
303.0799	303.0803	-0.4	-1.3	9.5	1671.7	n/a	n/a	C15 H15 N2 O3 S

FTIR of 2p



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-431.0	18-01-431	Instrument type and / or accessory	10/21/2020

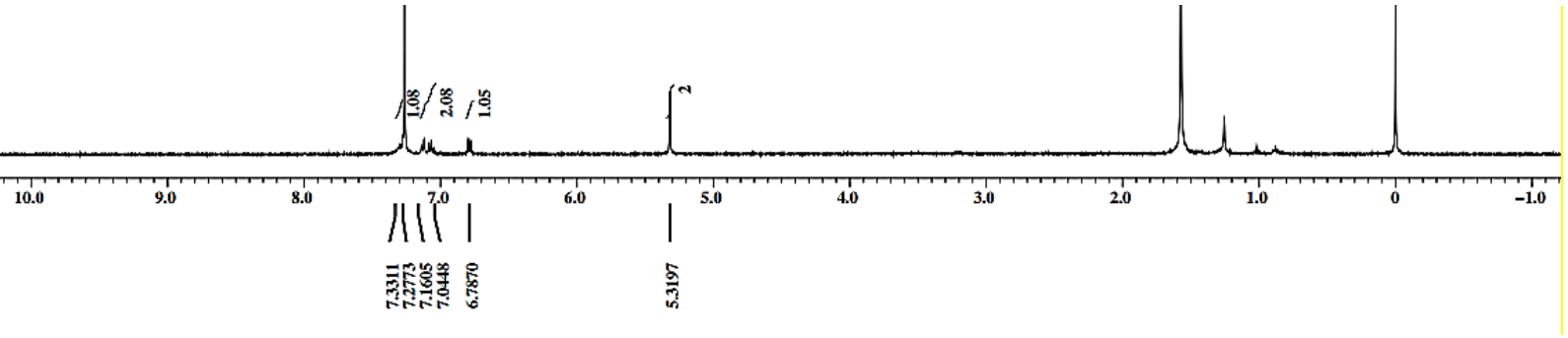
Wavenumber cm-1	Transmittance [%]
3997.658602	1.002051
3996.229335	1.001915
3994.800069	1.001769
3993.370802	1.001610
3991.941536	1.001449
3990.512269	1.001292
3989.083002	1.001138
3987.653736	1.000971
3986.224469	1.000774
3984.795203	1.000545
3983.365936	1.000310
3981.936670	1.000113
3980.507403	0.999998
3979.078136	0.999978
3977.648870	1.000029
3976.219603	1.000099
3974.790337	1.000145
3973.361070	1.000160
3971.931804	1.000166
3970.502537	1.000189
3969.073270	1.000229



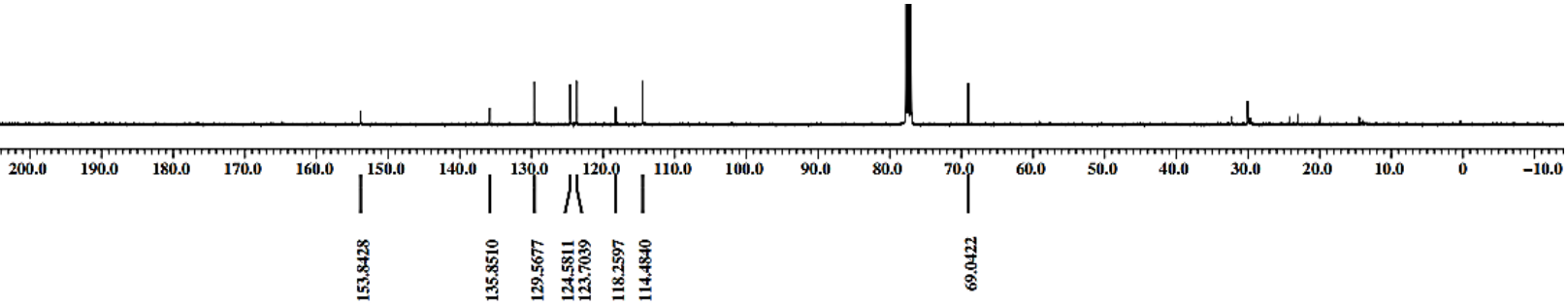
2q

Chemical Formula: $C_8H_7NO_2$
Exact Mass: 149.0477

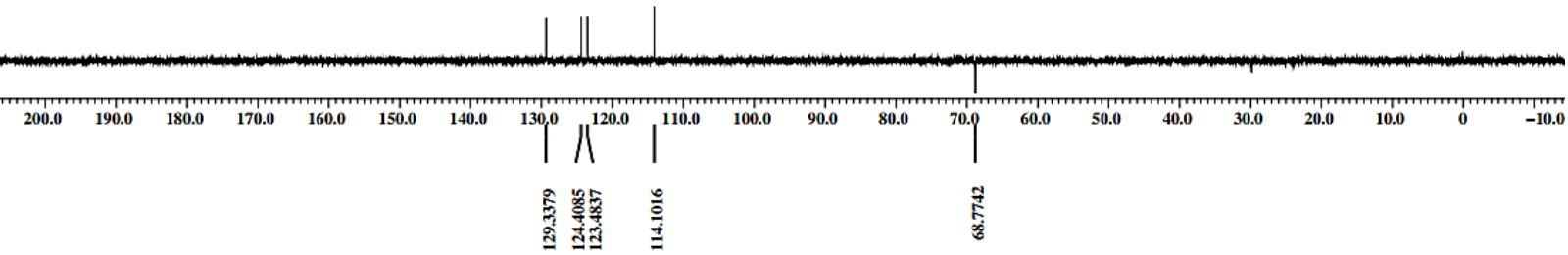
^{1}H-NMR ($CDCl_3$, 400 MHz) of 2q



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



^{13}C-DEPT ($CDCl_3$, 100 MHz) of 2q



129.3379
124.4085
123.4837
114.1016
68.7742

HRMS of 2q

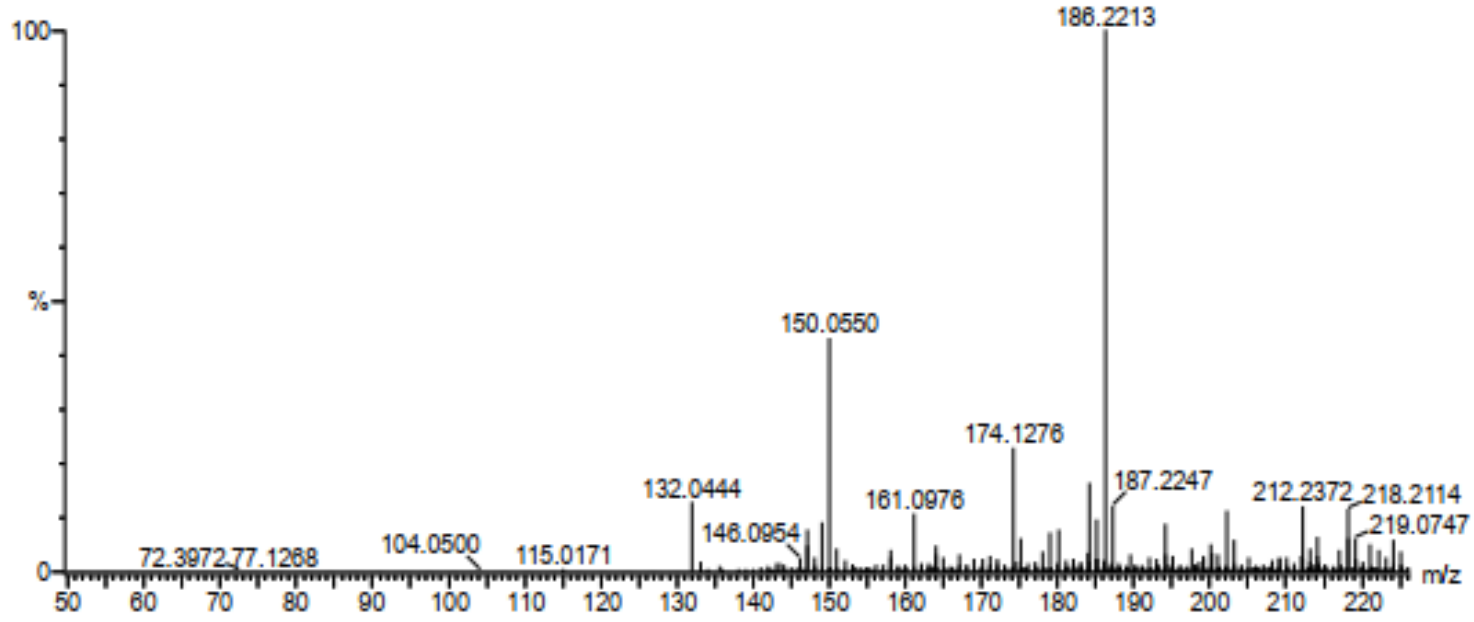
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 6

Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 8-25 H: 7-25 N: 0-4 O: 0-4

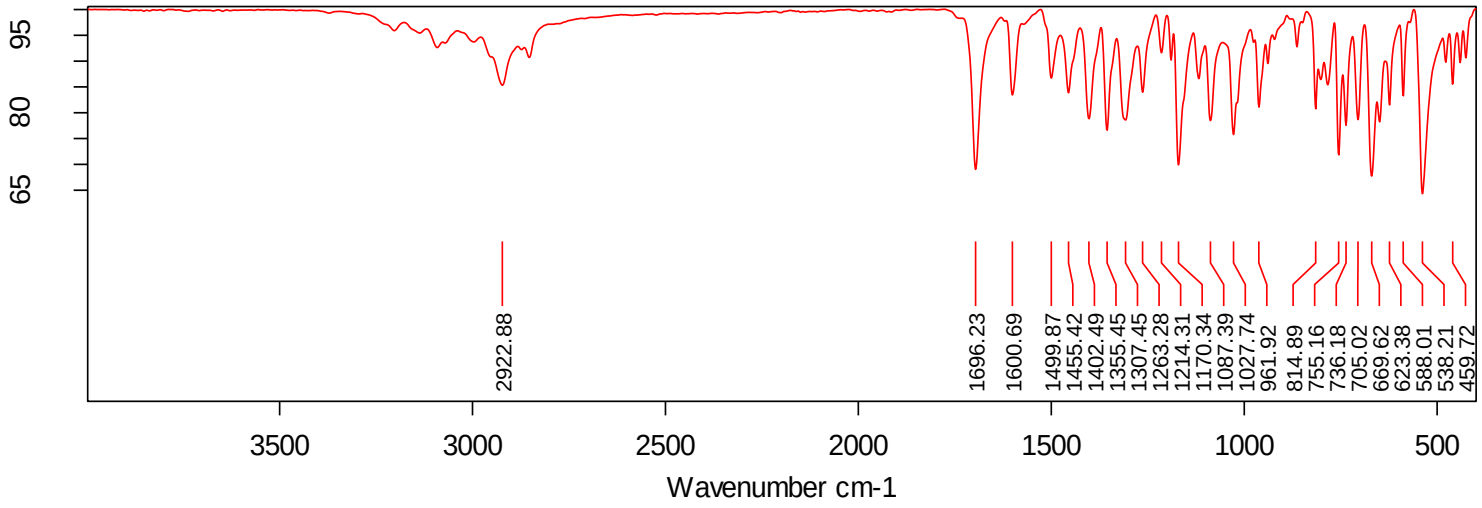
Sample Name : 18-01-425 IITRPR UPLC-XEVOG2XSQTOF
Test Name : HRMS-1
051020-18-01-425 12 (0.131)

1: TOF MS ES+
5.53e+006



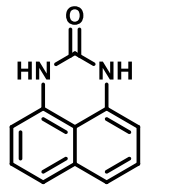
Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
150.0550	150.0555	-0.5	-3.3	5.5	2721.5	n/a	n/a	C8 H8 N O2

FTIR of 2q



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-425.0	18-01-425	Instrument type and / or accessory	10/21/2020

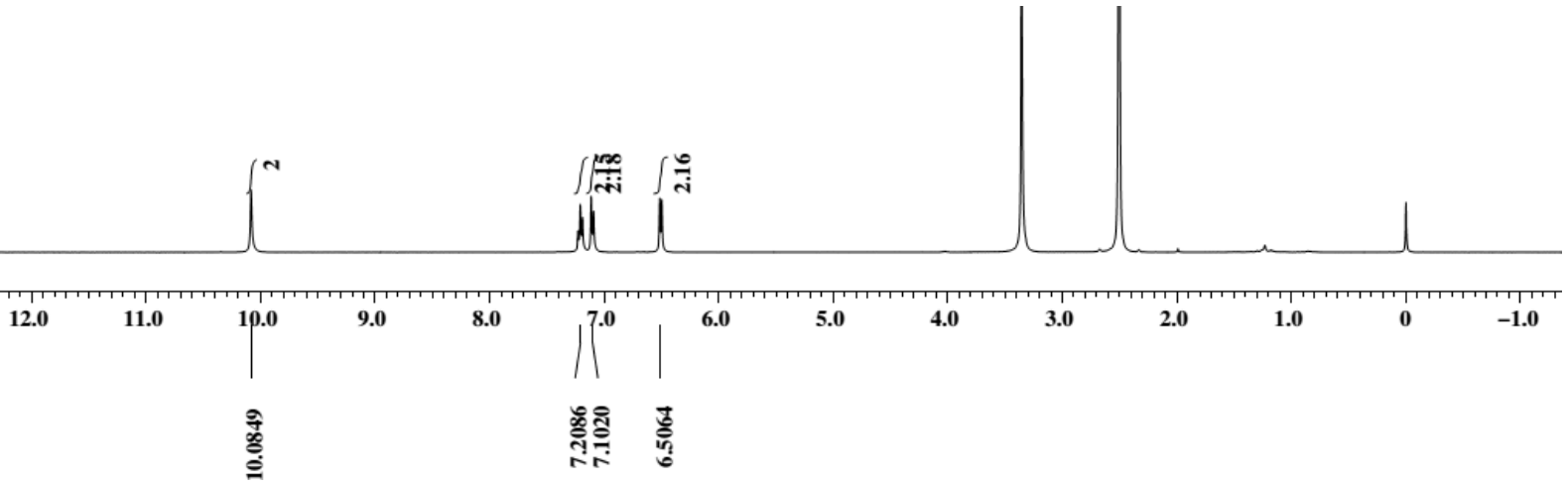
Wavenumber cm-1	Transmittance [%]
3997.658602	1.000390
3996.229335	1.000285
3994.800069	1.000180
3993.370802	1.000075
3991.941536	0.999977
3990.512269	0.999893
3989.083002	0.999831
3987.653736	0.999793
3986.224469	0.999782
3984.795203	0.999806
3983.365936	0.999875
3981.936670	0.999986
3980.507403	1.000103
3979.078136	1.000179
3977.648870	1.000181
3976.219603	1.000116
3974.790337	1.000022
3973.361070	0.999938
3971.931804	0.999885
3970.502537	0.999861
3969.073270	0.999861



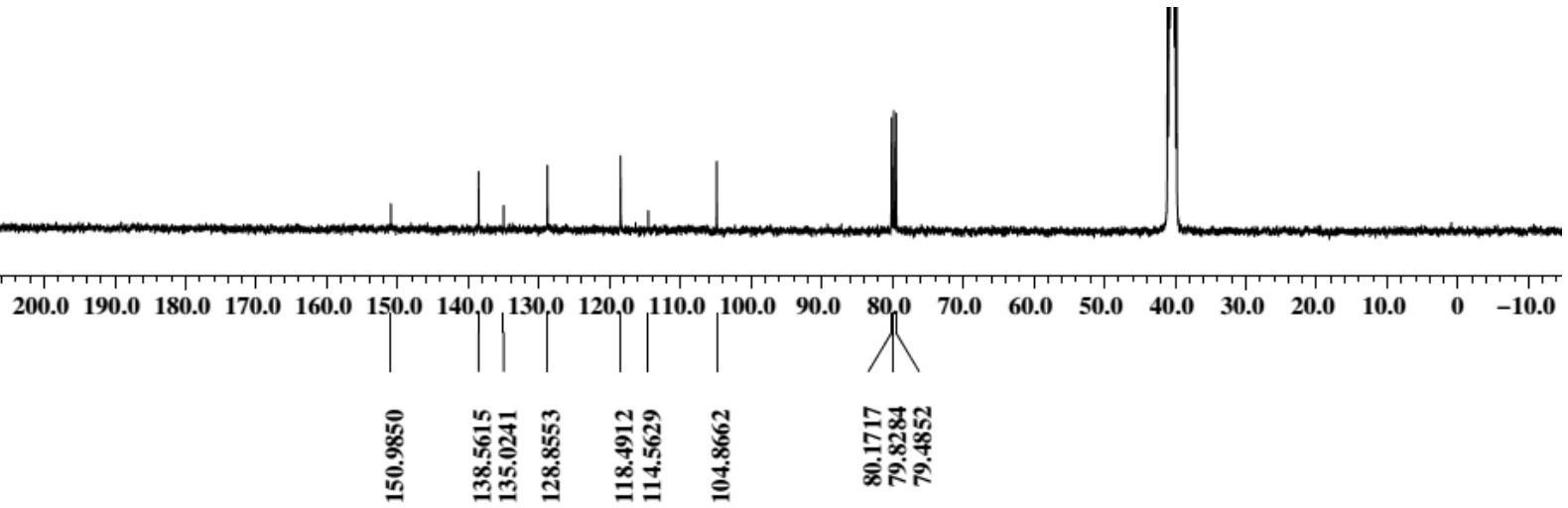
2r'

Chemical Formula: $C_{11}H_8N_2O$
Exact Mass: 184.0637

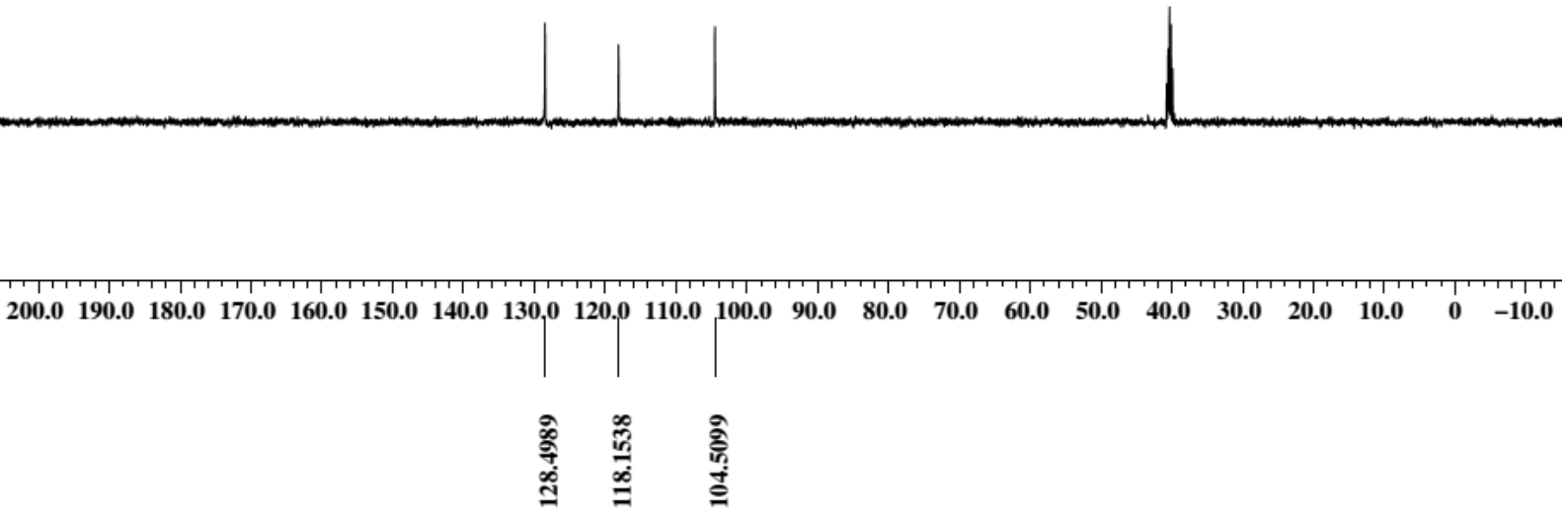
^{1}H-NMR (DMSO-d_6, 400 MHz) of 2r'



^{13}C-NMR (DMSO-d_6, 100 MHz) of 2r'



^{13}C-DEPT (DMSO-d_6, 100 MHz) of 2r'



HRMS of 2r'

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

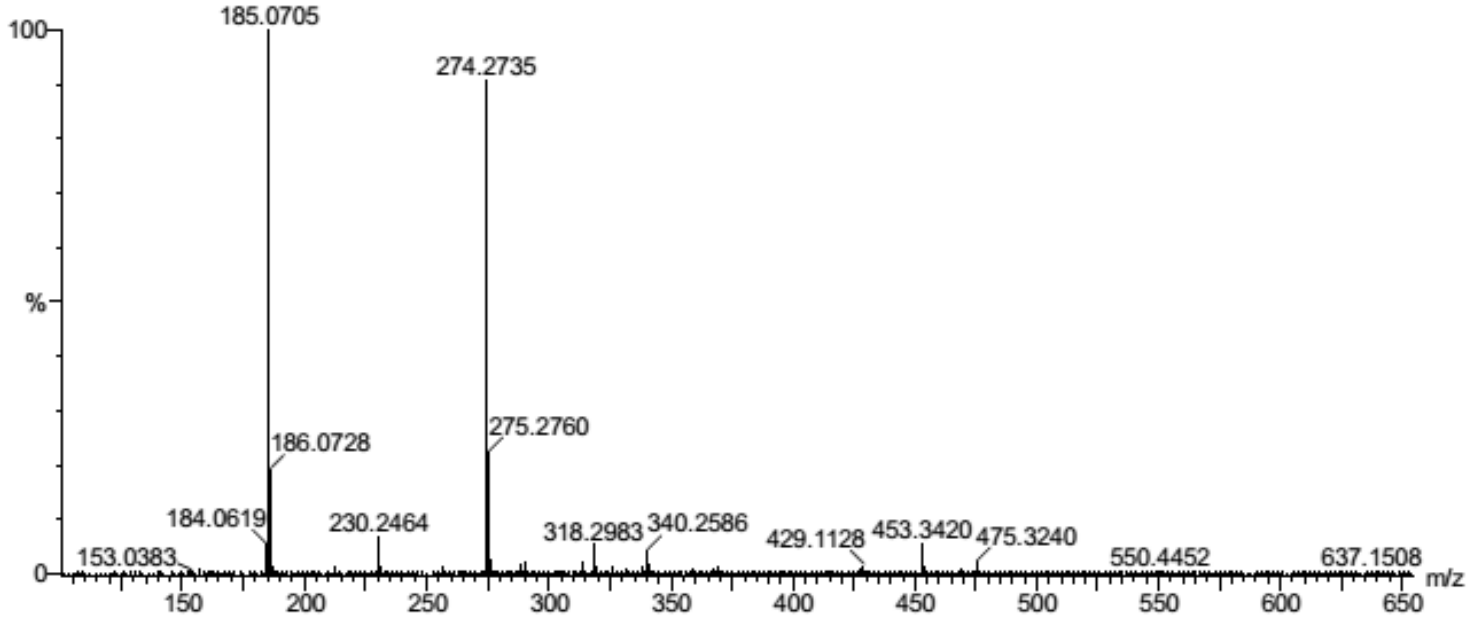
Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 8-35 N: 0-3 O: 0-5

Sample Name : 18-01-374
Test Name : HRMS-1
201219-18-01-374 15 (0.157)

IITRPR

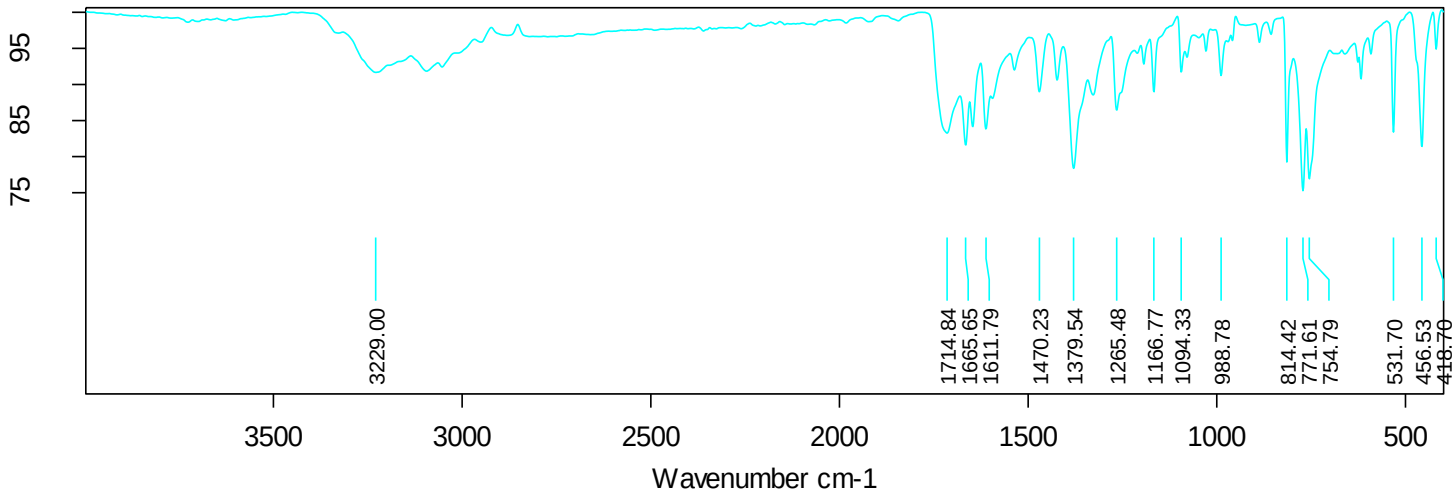
XEVO G2-XS QTOF

1: TOF MS ES+
3.66e+007



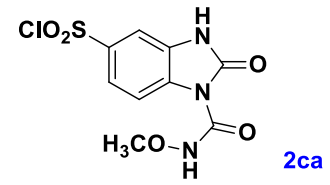
Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
185.0705	185.0715	-1.0	-5.4	8.5	877.9	n/a	n/a	C11 H9 N2 O

FTIR of 2r'



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-374.0	18-01-374	Instrument type and / or accessory	1/6/2020

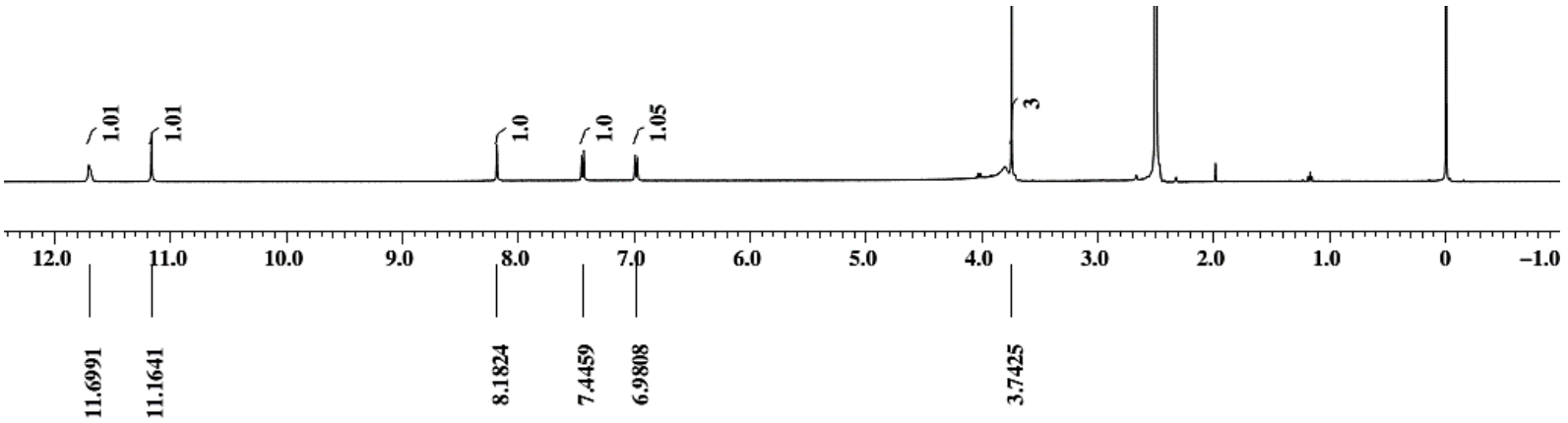
Wavenumber cm-1	Transmittance [%]
3997.502224	1.001109
3996.073013	1.000934
3994.643803	1.000756
3993.214592	1.000583
3991.785381	1.000430
3990.356171	1.000303
3988.926960	1.000202
3987.497749	1.000128
3986.068539	1.000089
3984.639328	1.000083
3983.210117	1.000099
3981.780907	1.000117
3980.351696	1.000122
3978.922485	1.000109
3977.493275	1.000072
3976.064064	1.000000
3974.634853	0.999882
3973.205643	0.999720
3971.776432	0.999534
3970.347221	0.999356
3968.918011	0.999213



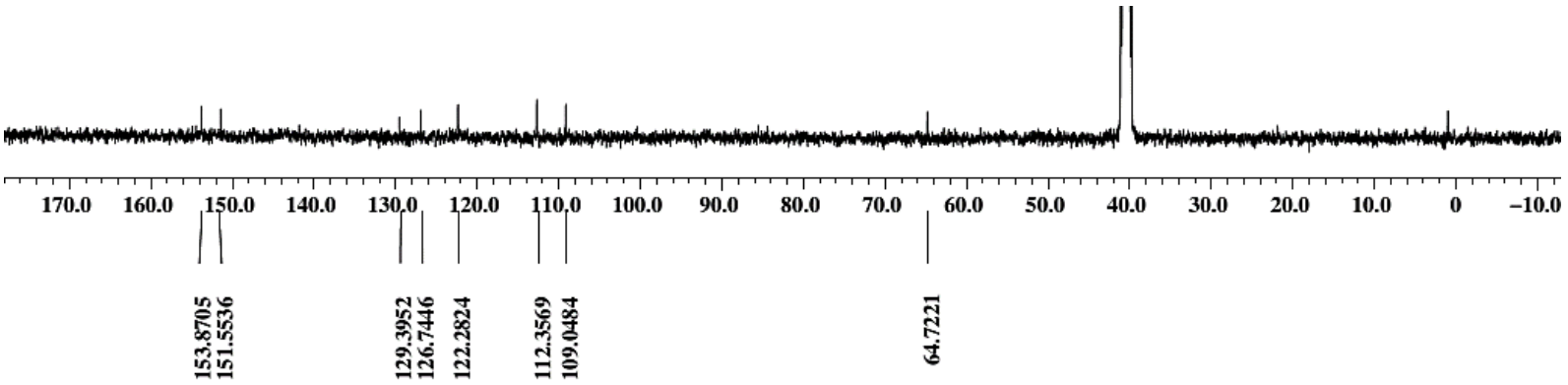
2ca

Chemical Formula: $C_9H_8ClN_3O_5S$
Exact Mass: 304.9873

^{1}H-NMR (DMSO-d6, 400 MHz) of 2ca



^{13}C-NMR (DMSO-d6, 100 MHz) of 2ca



HRMS of 2ca

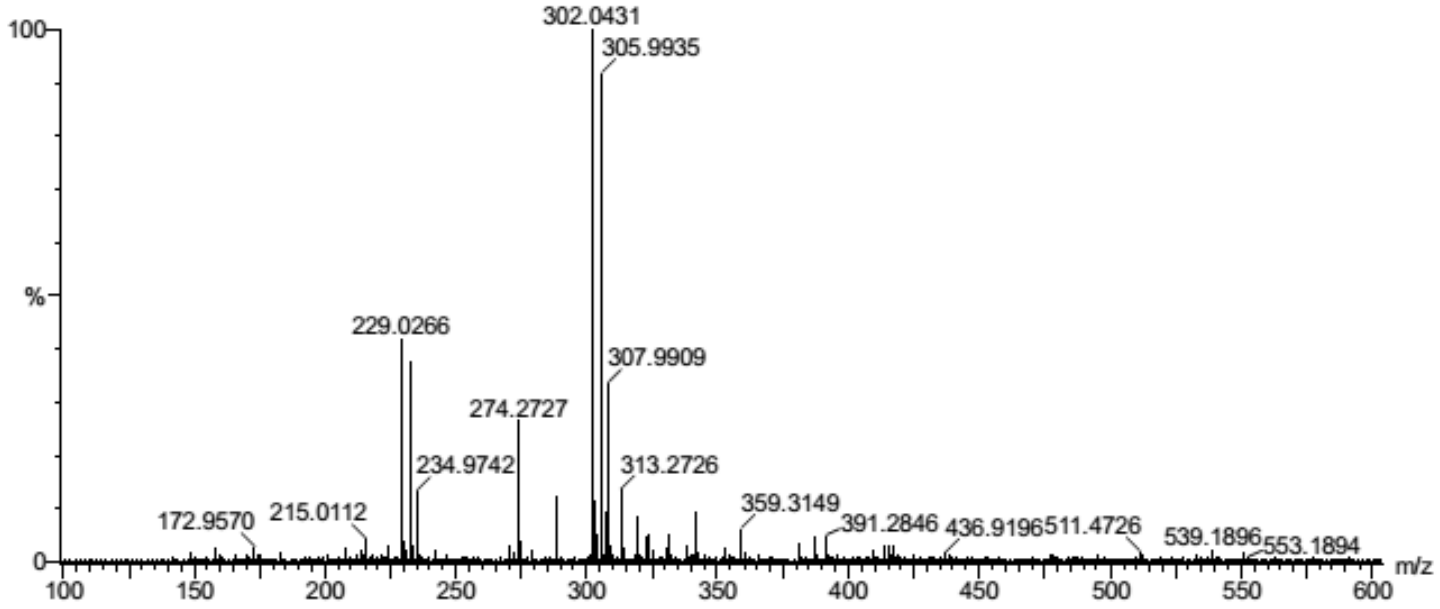
Elemental Composition Report

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 = 3

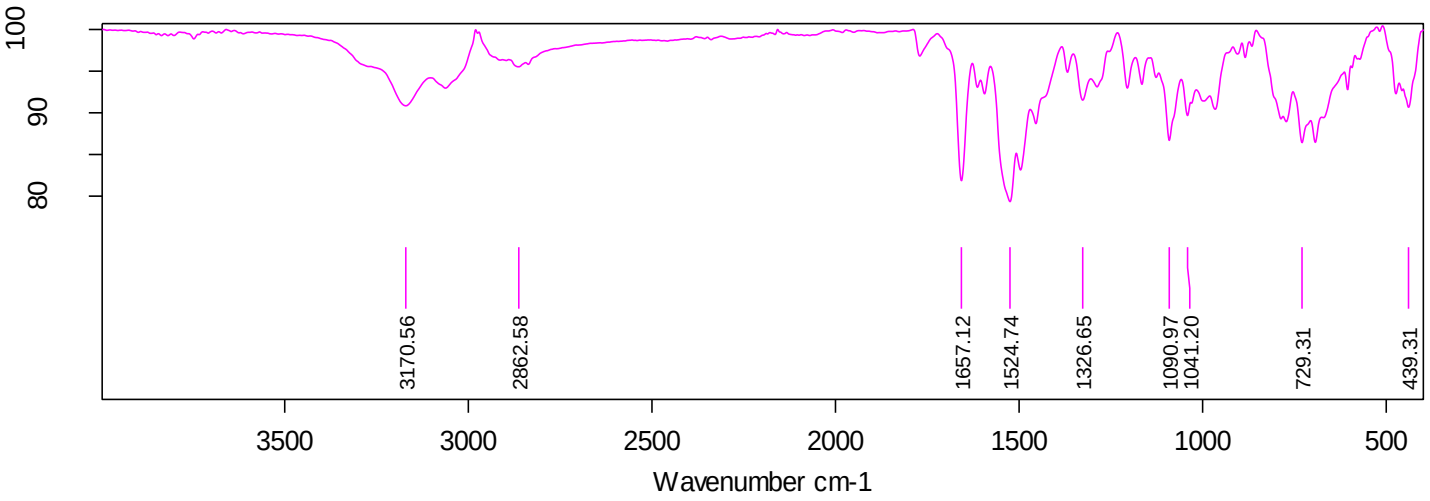
Monoisotopic Mass, Odd and Even Electron Ions
166 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 8-15 H: 7-45 N: 0-3 O: 0-5 S: 0-1 Cl: 0-1

Sample Name : 18-01-379 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
121219-18-01-379- 16 (0.165) AM2 (Ar,22000.0,0.00,0.00); Cm (16:18) 1: TOF MS ES+
3.53e+006



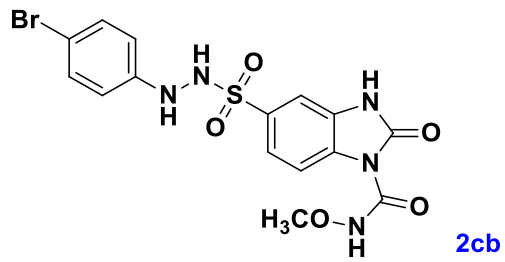
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
305.9935	305.9951	-1.6	-5.2	6.5	793.5	n/a	n/a	C9 H9 N3 O5 S Cl

FTIR of 2ca



D:\FTIR DATA\DR. PRABAL\Devarshi\18-01-376.0	18-01-376	Instrument type and / or accessory	1/6/2020

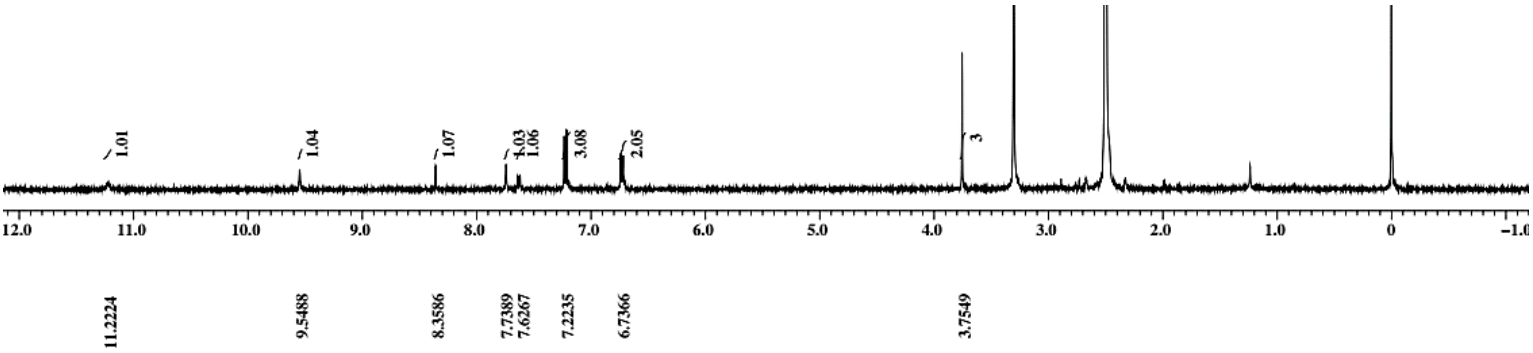
Wavenumber cm-1	Transmittance [%]
3997.502224	0.999734
3996.073013	0.999862
3994.643803	0.999960
3993.214592	1.000000
3991.785381	0.999958
3990.356171	0.999826
3988.926960	0.999621
3987.497749	0.999390
3986.068539	0.999191
3984.639328	0.999066
3983.210117	0.999037
3981.780907	0.999100
3980.351696	0.999228
3978.922485	0.999374
3977.493275	0.999483
3976.064064	0.999511
3974.634853	0.999453
3973.205643	0.999347
3971.776432	0.999242
3970.347221	0.999166
3968.918011	0.999129



2cb

Chemical Formula: $C_{15}H_{14}BrN_5O_5S$
Exact Mass: 454.9899

^{1}H-NMR (DMSO-d6, 400 MHz) of 2cb



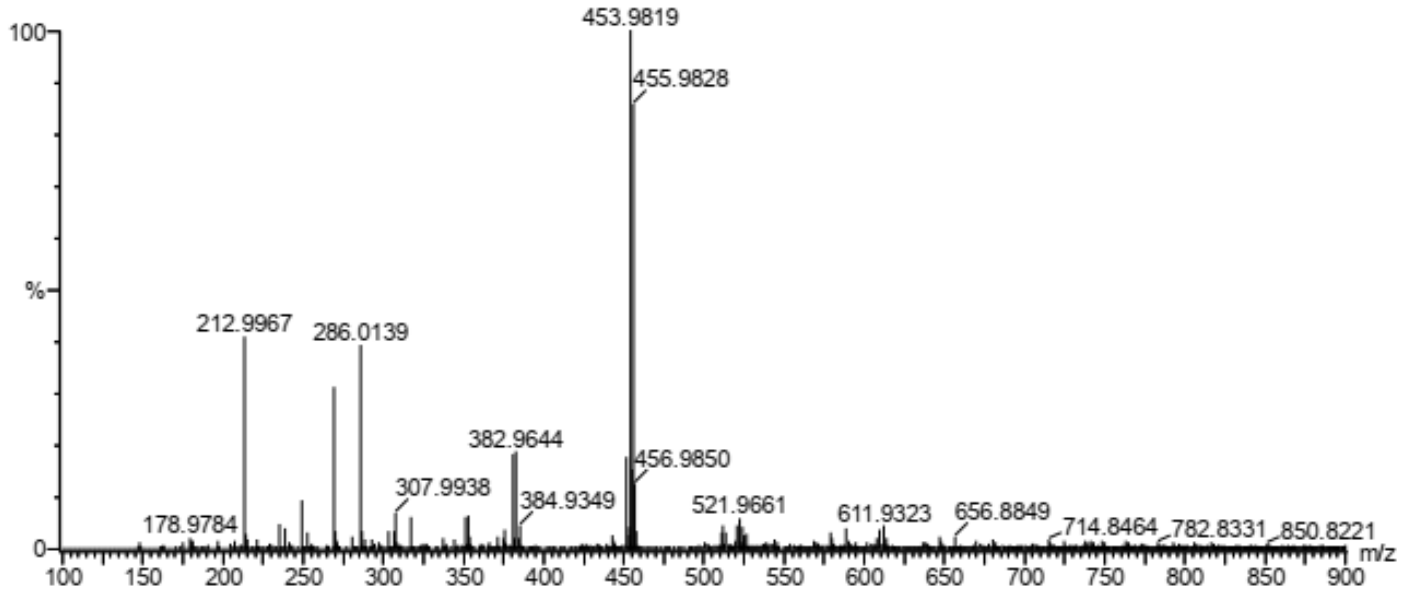
Elemental Composition Report

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 = 3

Monoisotopic Mass, Even Electron Ions
264 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-17 H: 7-20 N: 0-5 O: 0-7 S: 0-1 Br: 0-2

Sample Name : 18-01-380 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
131219-18-01-380-HRMS- 12 (0.131) AM (Top,4, Ar,10000.0,0.00,0.00); Sm (SG, 1x3.00); Cm (9:18) 1: TOF MS ES-
6.59e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
453.9819	453.9821	-0.2	-0.4	11.5	694.4	n/a	n/a	C15 H13 N5 O5 S Br

13) HRMS data for intermediate trap experiment

HRMS of adduct II

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

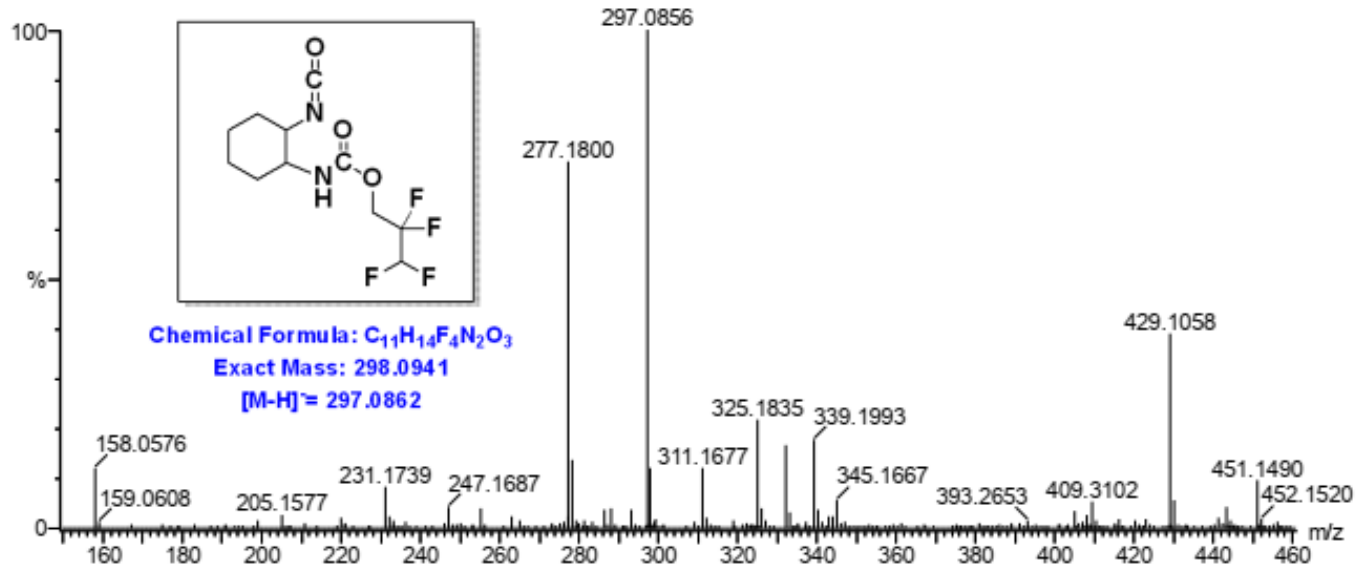
Monoisotopic Mass, Even Electron Ions
101 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-13 H: 6-25 N: 0-3 O: 0-4 F: 0-4

Sample Name : 18-01-398
Test Name : HRMS-1
130120-18-01-398_ 12 (0.131)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES-
3.16e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
297.0856	297.0862	-0.6	-2.0	4.5	1903.0	n/a	n/a	C11 H13 N2 O3 F4

HRMS of adduct I

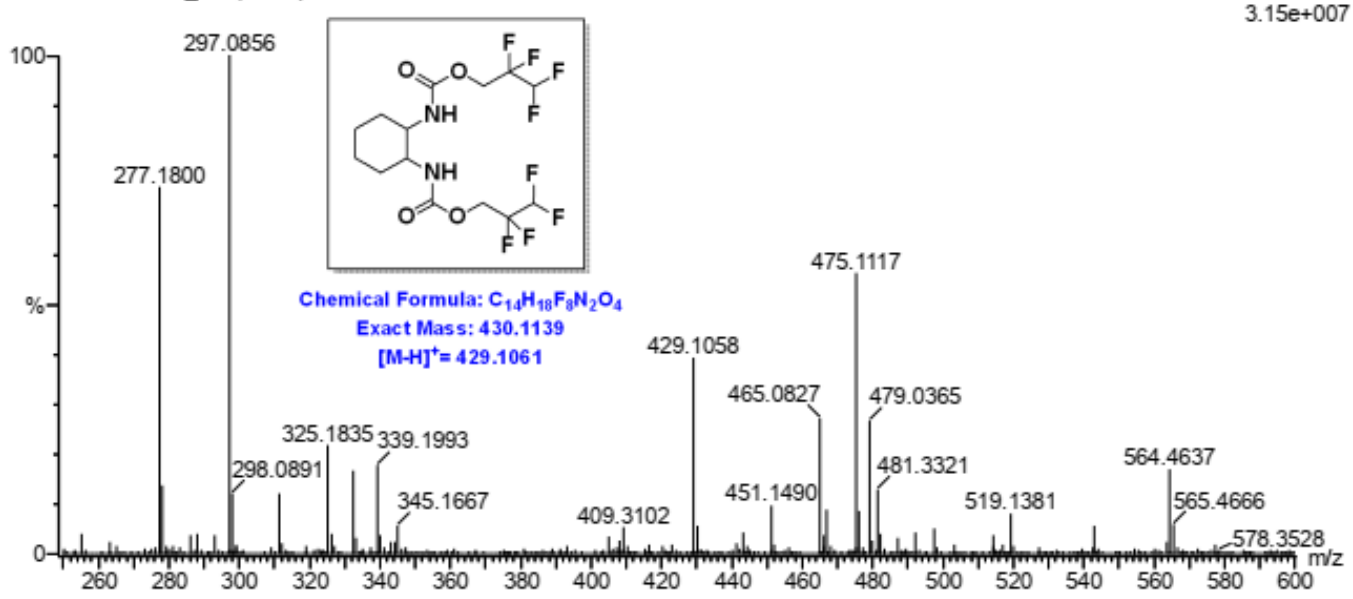
Elemental Composition Report

Single Mass Analysis

Tolerance = 2.0 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
179 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-20 H: 6-25 N: 0-3 O: 0-4 F: 0-8

Sample Name : 18-01-398 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
130120-18-01-398_ 12 (0.131) 1: TOF MS ES-
3.15e+007



Chemical Formula: $C_{14}H_{18}F_8N_2O_4$
Exact Mass: 430.1139
$[M-H]^+$= 429.1061

Minimum:				-1.5				
Maximum:		5.0	2.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
429.1058	429.1061	-0.3	-0.7	3.5	1609.4	n/a	n/a	C14 H17 N2 O4 F8

14) References

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