Electronic Supplementary Material (ESI) for RSC Advances.

N-Heterocyclic Carbene (NHC)-Catalyzed Oxidation of Unactivated Aldimines to Amides via Imine Umpolung under Aerobic Conditions

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General information

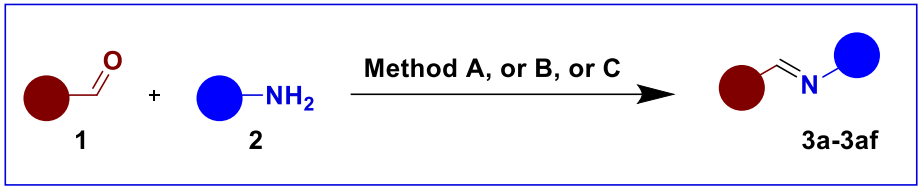
All the reactions were carried out with an oven dried round bottom flask/Schlenk tube. Reactions were magnetically stirred and monitored by analytical thin layer chromatography (TLC). TLC was performed on Merck silica gel 60 F_{254}; UV lamp was used as visualizing agent, I_2 or $KMnO_4$ and Anisaldehyde as developing agents. Purification of products was carried out by column chromatography by using 60-120/100-200 mesh silica and EtOAc/hexane were used as eluents and concentration under reduced pressure was performed by rotary evaporator at 40-45 ^oC, at appropriate pressure. The yields were given to the isolated products.

All the solvents, which were used in the reactions were dried and freshly distilled solvents according to their standard procedures, wherever required, and transferred under argon. Dry solvents like DMC, DMF, DMSO, CH_3CN, *t*-BuOH, DME, THF and 1,4-dioxane were purchased from Finar Scientifics, India. These were stored over activated 4 Å molecular sieves.

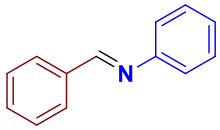
All the reagents, substrates, catalysts, deuterated solvents were purchased from commercial suppliers like as Alfa Aesar, Sigma Aldrich, TCI, S.D Fine chemicals, India. Those were used without further purification.

^{1}H-NMR spectra were recorded on 300, 400 and 500 MHz instruments. Chemical shifts are reported in ppm with the reference solvent as the internal standards (TMS = 0; $CDCl_3$ = 7.26; DMSO-d_6 = 2.50). The following abbreviations were used to explain the multiplicity of the spectra (s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, m = multiplet, brs = broad singlet). ^{13}C-NMR spectra were recorded on 75, 100, and 125 MHz spectrometers. Peaks which appear at 1.26, 0.86 in ^{1}H-NMR and 29.7 in ^{13}C-NMR corresponds to the residual grease present in the solvent (Gottlieb, H. E.; Kotlyar, V.; Nudelman, A. NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities. *J. Org. Chem.* **1997**, *62*, 7512-7515). Mass spectra were analysed by Electrospray Ionization (ESI) method and were obtained on a Shimadzu LCMS-2020 mass spectrometer. High resolution mass spectra were recorded on a Thermo scientific Exactive^{TM}Orbitrap mass spectrometer or Q STAR XL Hybrid MS/M. Infrared spectroscopy (IR-neat) was performed on a BRUKER FT-IR spectrophotometer in chloroform, and IR [KBr] spectra were recorded on a THERMO NICOLET NEXUS 670 FT-IR instrument.

General procedure for the synthesis of imines 3a-3af



Aldehyde Derivatives imines



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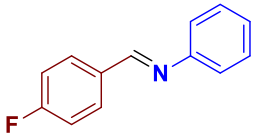

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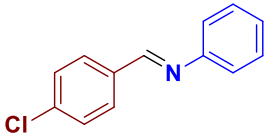

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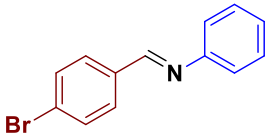

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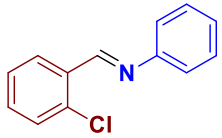

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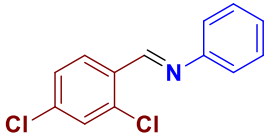

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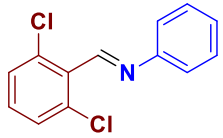

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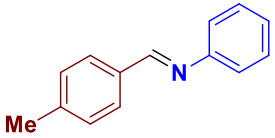

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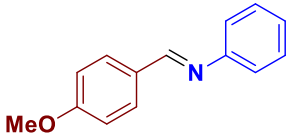

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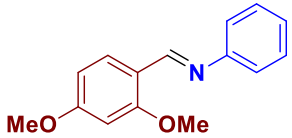

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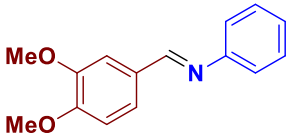

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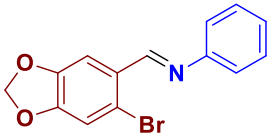

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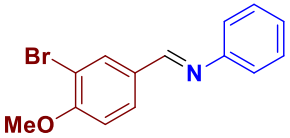

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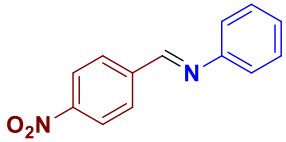

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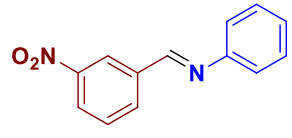

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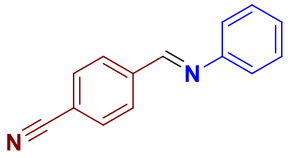

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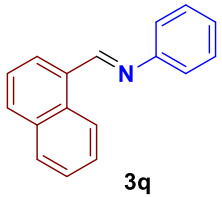

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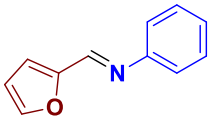

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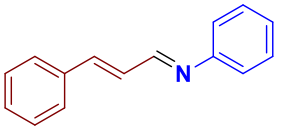

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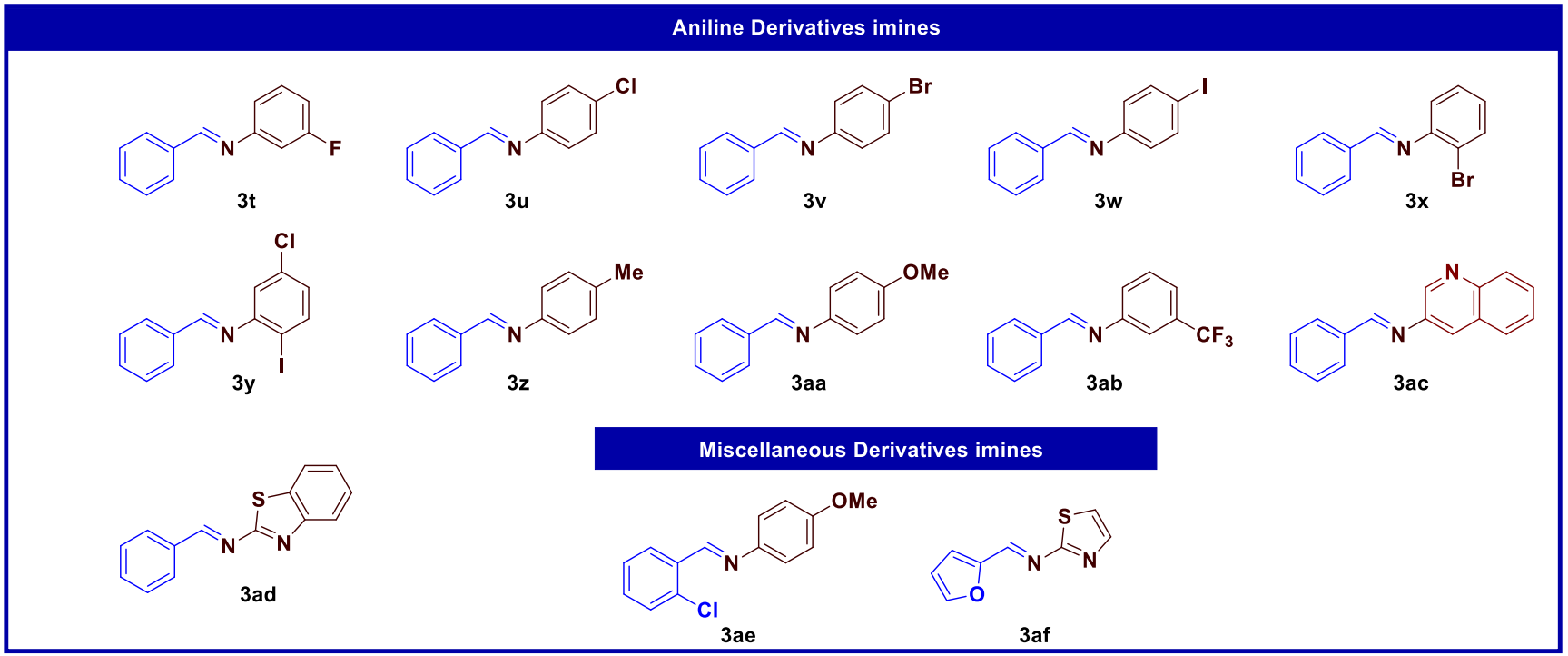


Procedure: A

To a flame dried flask was added 20 mL CH_2Cl_2, $MgSO_4$ (1.5 equiv, 7.5 mmol) followed by aniline **2** (1.0 equiv, 5 mmol). After stirring for 5 min, benzaldehyde **1** (1.0 equiv, 5 mmol) was added. The reaction mixture was stirred at room temperature for overnight. The reaction mixture was filtered through the pad of celite. The solvent of filtrate was removed under reduced pressure to afford the imines.

All the compounds **3c**, **3d**, **3e**, **3j**, **3k**, **3l**, **3m**, **3p**, **3q**, **3r**, **3s**, **3v**, **3w**, **3x**, **3y**, **3z**, **3aa**, **3ab**, **3ad**, **3ae** were prepared by using the above general **procedures A**. Spectral data were in good agreement with the reported data for the compounds as follows: **3c,**[1] **3d,**[3]**,3e,**[30] **3j,**[16] **3k,**[16] **3l,**[5] **3m**, **3p,**[16] **3q,**[19] **3r,**[18] **3s,**[18] **3v,**[1] **3w,**[15] **3x,**[12] **3y,**[13] **3z,**[11] **3aa,**[11] **3ab,**[2] **3ad,**[9] **3ae.**[8]

Procedure: B

To a flame dried flask was added benzaldehyde **1** (1.0 equiv, 5 mmol), aniline **2** (1.0 equiv, 5 mmol), and ethanol (10 mL). The reaction mixture was stirred at room temperature for overnight in the absence of light. The solvent was removed under reduced pressure to afford the imines.

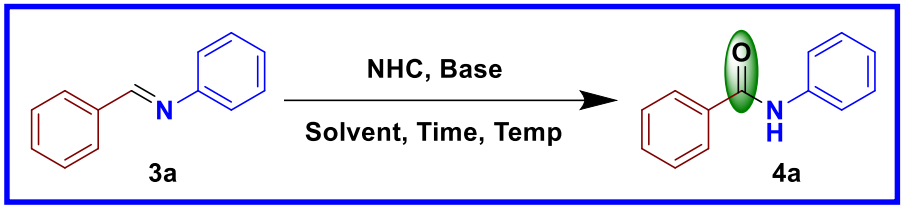
All the compounds **3b**, **3h**, **3i**, **3n**, **3t**, **3u** were prepared by using the above general **procedures B**. Spectral data were in good agreement with the reported data for the compounds as follows: **3b**, [7] **3h**,[1] **3i**,[6] **3n**,[6] **3t**,[2] **3u.**[11]

Procedure: C

To a flame dried flask was added benzaldehyde **1** (1.0 equiv, 5 mmol), aniline **2** (1.0 equiv, 5 mmol), and ethanol (10 mL). The reaction mixture was stirred at reflux temperature until both the starting materials were consumed. Then, the solvent was removed under reduced pressure and the product was recrystallization from cold ethanol to afford pure imines.

All the compounds **3a**, **3f**, **3g**, **3o**, **3ac**, **3af** were prepared by using the above general **procedures C**. Spectral data were in good agreement with the reported data for the compounds as follows: **3a**,[13] **3f**,[10] **3g**,[10] **3o**,[10] **3ac**,[4] **3af.**[14]

General procedure for the optimization study

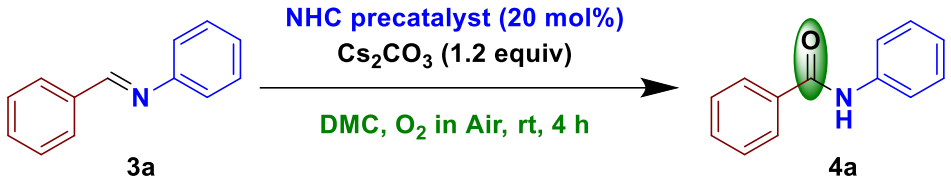


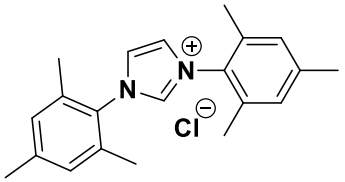
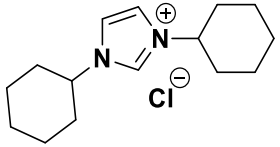
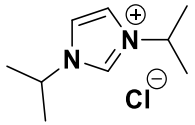
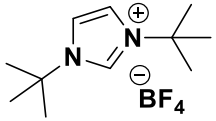
Imine **3a** (1 equiv, 0.5 mmol, 90 mg), NHC precatalyst (20 mol%, 0.1 mmol), and base (1.2 equiv, 0.6 mmol) were taken in a clean and dried two necked round bottom flask and it was evacuated and back filled with argon gas (2-3 cycles). Then solvent (4.0 mL) was added by syringe under argon atmosphere. Subsequently, the reaction mixture was stirred at the room temperature for 10 min under argon atmosphere. Later, the reaction mixture was stirred under open-air atmosphere at room temperature and time as mentioned in optimization Tables S1-S5. After completion of reaction, water (10 mL) was added to the reaction mixture and extracted with EtOAc (2 x 15 mL). The combined organic layer was washed with brine (20 mL), the organic phase was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to obtain a crude residue. The crude was kept for high vacuum for few minutes. Purification using recrystallization by using cold *n*-pentane and dichloromethane (few drops) to get amide **4a** as a pure product.

Note: **please see tables S1-S5, for screening of various NHCs, bases, solvents and their ratios/quantities**

Optimization survey

Table S1: Screening of various NHC precatalysts



Entry	NHC precatalyst (20 mol %)	Structure of NHC precatalyst	% of Yield 4a
1	1,3-Bis(2,4,6-trimethylphenyl) imidazolium chloride **A1**		53
2	1,3-Dicyclohexylimidazolium chloride **A2**		-
3	1,3-diisopropyl imidazolium chloride **A3**		-
4	1,3-Di-*tert*-butylimidazolium tetrafluoroborate **A4**		-

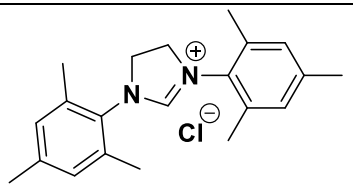
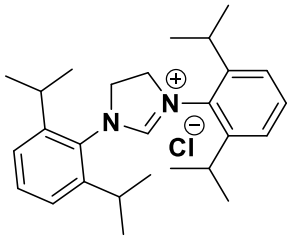
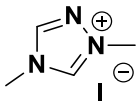
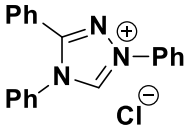
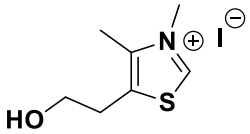
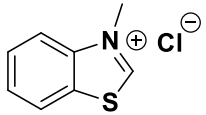
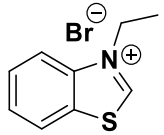
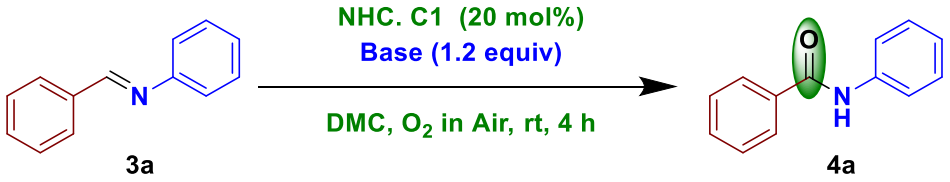
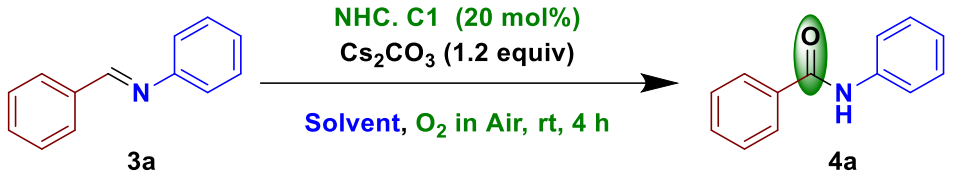
5	1,3-Bis(2,4,6-trimethylphenyl) imidazolinium chloride B**1**		-
6	1,3-Bis(2,6-diisopropylphenyl) imidazolinium chloride **B2**		-
7	1,4-Dimethyl-1,2,4-triazolium iodide C**1**		87
8	1,3,4-triphenyl-1*H*-1,2,4-triazol-4-ium chloride C**2**		-
9	5-(2-Hydroxyethyl)-3,4-dimethylthiazolium iodide **D1**		-
10	3-Methylbenzothiazolium iodide **D2**		-
11	3-Ethylbenzothiazolium bromide **D3**		-

Table S2: Screening of Bases



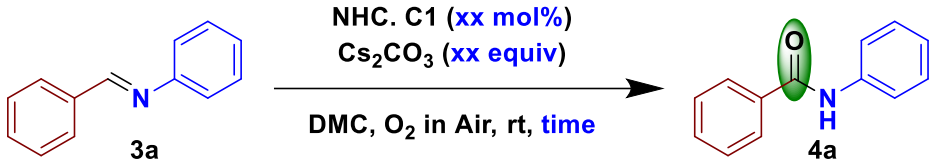
Entry	Base (1.2 equiv)	% Yield of 4a
1	K_2CO_3	55
2	K_3PO_4	41
3	Et_3N	29
4	1,4-Diazabicyclo[2.2.2]octane (DABCO)	65
5	NaH	72
6	**Cs_2CO_3**	**87**
7	1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU)	71

Table S3: Screening of Solvents



Entry	Solvent	% Yield of 4a
1	THF	75
2	**Dimethyl carbonate**	**87**
3	CH_3CN	52
4	1,4-Dioxane	65
5	Dimethyl sulfoxide (DMSO)	63
6	1,2-Dimethoxyethane (DME)	61
7	*t*-BuOH	traces
8	EtOAc	65
9	Toluene	–
10	DMF	49
11	EtOH	-
12	H_2O	-

Table S4: Screening of amounts of NHC, Base and time



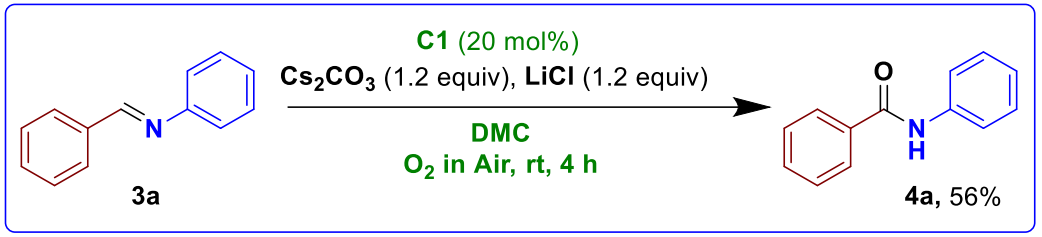
Entry	NHC. C1 (xx mol%)	Cs_2CO_3 (xx mol%)	Temp. (°C)	Time (h)	% Yield of 4a
1	10	120	rt	4	40
2	15	120	rt	4	70
3	**20**	**120**	rt	**4**	**87**
4	20	100	rt	4	72
5	20	50	rt	4	45
9	20	120	rt	12	85
10	20	120	rt	24	87

Table S5: Reaction without using NHC precatalyst (or) base

(Optimized conditions mentioned entry 1, Table S4 were used)

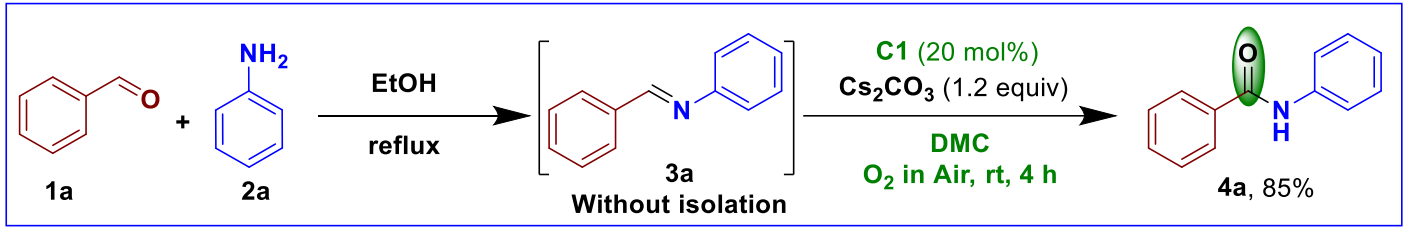
Entry	NHC precatalyst	Base	Solvent	% Yield of 4a
1	1,4-Dimethyl-1,2,4-triazolium iodide **C1**	**No base**	DMC	–
2	**No catalyst**	Cs_2CO_3	DMC	–

Experimental Procedure to know the effect of LiCl on optimized reaction conditions



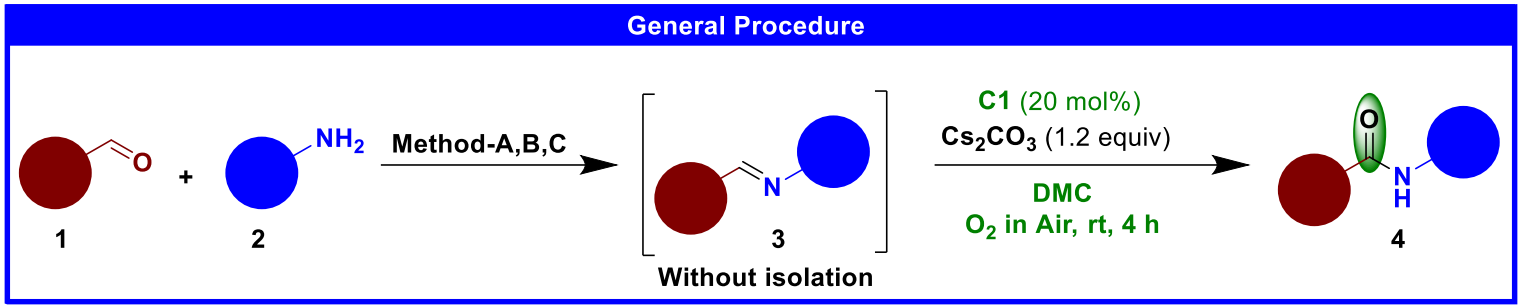
Imine 3a (1 equiv, 0.5 mmol, 90 mg), NHC precatalyst (20 mol%, 0.1 mmol, 22.5 mg), Cs_2CO_3 (1.2 equiv, 0.6 mmol, 196 mg) and anhydrous LiCl (1.5 equiv, 0.6 mmol, 25 mg) were taken in a clean and dried two necked round bottom flask and it was evacuated and back filled with argon gas (2-3 cycles). Then solvent DMC (4.0 mL) was added by syringe under argon atmosphere. Subsequently, the reaction mixture was stirred at the room temperature for 10 min under argon atmosphere. Later, the reaction was stirred under open-air for 4 h. After completion of reaction, water was added to the reaction mixture (10 mL) and extracted with EtOAc (2 x 15 mL). The combined organic extract was washed with brine (15 mL), the organic phase was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure on a rotavapor to obtain a crude residue. The crude was kept for high vacuum. Then recrystallization with cold n-pentane and DCM (few drops) afford the pure products. **4a** off-white solid with 56% yield

Sequential imine formation, NHC-catalyzed construction of benzanilide 4a.



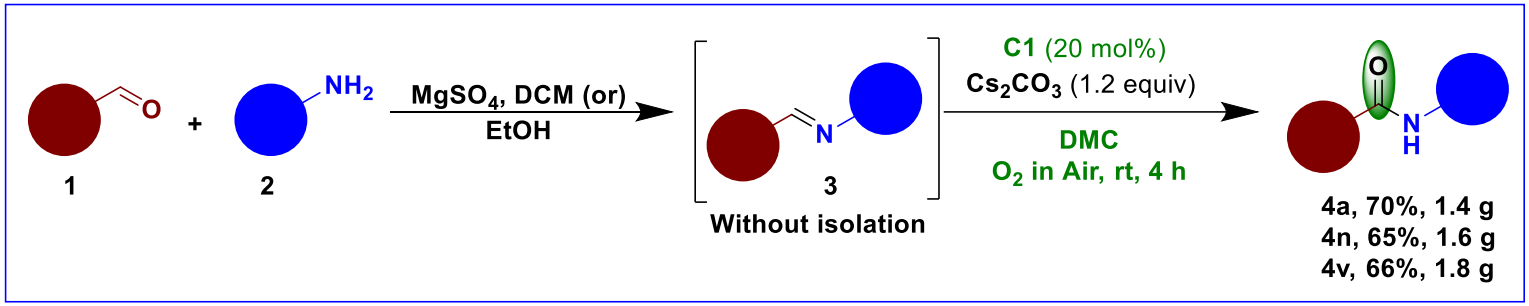
The imine **3a** was prepared by **procedure C**, which was used in the NHC catalyzed transformation. The crude imine **3a** (1.0 equiv, 1.0 mmol), 1,4-dimethyl-1,2,4-triazolium iodide **C1** (20 mol%, 0.2 mmol, 45 mg), and Cs_2CO_3 (1.2 equiv, 1.2 mmol, 390 mg) were taken in a clean and dried two necked round bottom flask and it was evacuated and back filled with argon gas (2-3 cycles). Then solvent dimethyl carbonate (DMC) (8.0 mL) was added by syringe under argon atmosphere. Subsequently, the reaction mixture was stirred at the room temperature for 10 min under argon atmosphere. Later, the reaction was stirred under open-air for 4 h. After completion of reaction, water was added to the reaction mixture (15 mL) and extracted with EtOAc (2 x 20 mL). The combined organic extract was washed with brine (20 mL), the organic phase was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure on a rotavapor to obtain a crude residue. The crude was kept for high vacuum. Then recrystallization with cold *n*-pentane and DCM (few drops) afford the pure products. **4a** off-white solid with 85% yield.

General procedure for the synthesis of 4a-4af



The crude imine **3a-af** (1.0 equiv, 1.0 mmol), 1,4-dimethyl-1,2,4-triazolium iodide **C1** (20 mol%, 0.2 mmol, 45 mg), and Cs_2CO_3 (1.2 equiv, 1.2 mmol, 390 mg) were taken in a clean and dried two necked round bottom flask and it was evacuated and back filled with argon gas (2-3 cycles). Then solvent dimethyl carbonate (DMC) (8.0 mL) was added by syringe under argon atmosphere. Subsequently, the reaction mixture was stirred at the room temperature for 10 min under argon atmosphere. Later, the reaction was stirred under open-air for 4 h. After completion of reaction, water was added to the reaction mixture (15 mL) and extracted with EtOAc (2 x 20 mL). The combined organic extract was washed with brine (20 mL), the organic phase was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure on a rotavapor to obtain a crude residue. The crude was kept for high vacuum. Then recrystallization with cold *n*-pentane and DCM (few drops) afford the pure products **4a, 4b, 4c, 4d, 4e, 4f, 4g, 4i, 4m, 4n, 4o, 4p, 4t, 4u, 4v, 4w, 4x, 4aa, 4ab.** and the products **4h, 4j, 4k, 4l, 4q, 4r, 4s, 4y, 4z, 4ac, 4ad, 4ae, 4af** were purified by using column chromatography.

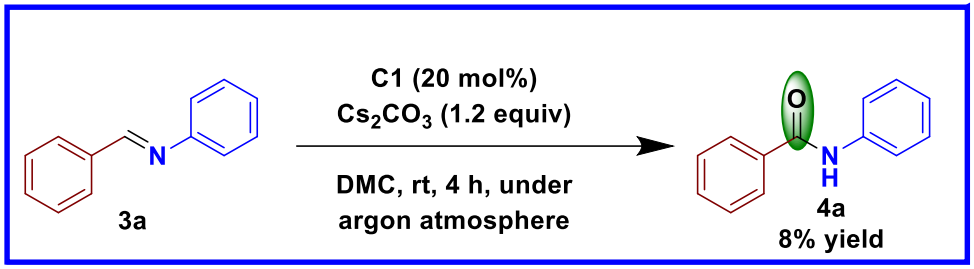
Experimental procedure for the NHC catalyzed gram-scale syntheses of 4a, 4n, and 4v



The imine **3a**, **3n**, and, **3v** were prepared by following method **A**, **B**, or **C**. Then the crude imine **3a**, **3n**, and **3v** (1.0 equiv, 10 mmol), 1,4-dimethyl-1,2,4-triazolium iodide **C1** (20 mol%, 2.0 mmol, 450 mg), and Cs_2CO_3 (1.2 equiv, 12 mmol, 3.9 g) were taken in a clean and dried two necked round bottom flask and it was evacuated and back filled with argon gas (2-3 cycles). Then solvent DMC (50 mL) was added by syringe under argon atmosphere. Subsequently, the reaction mixture was stirred at the room temperature for 10 min under argon atmosphere. Later, the reaction was stirred under open-air for 4 h. After completion of reaction, water was added to the reaction mixture (80 mL) and extracted with EtOAc (2 x 50 mL). The combined organic extract was washed with brine (100 mL), the organic phase was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure on a rotavapor to obtain a crude residue. The crude was kept for high vacuum. Then recrystallization with cold *n*-pentane and DCM (few drops) afford the pure product. **4a**, **4n**, and **4v** with 70%, 65%, and 66% yield respectively.

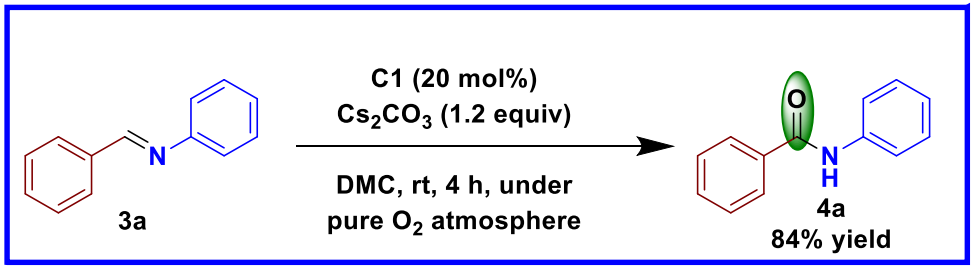
Control Experiments

➢ Under Argon Atmosphere



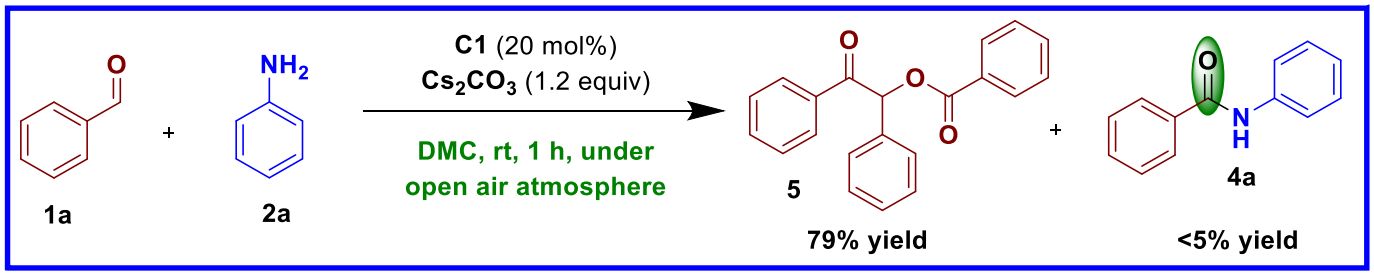
The imine **3a** (1 equiv, 0.5 mmol, 91 mg), NHC precatalyst **C1** (20 mol%, 0.1mmol, 22.5 mg), and Cs_2CO_3 (1.2 equiv, 0.6 mmol, 197 mg) were taken in a clean and dried two necked round bottom flask and it was evacuated and back filled with argon gas (2-3 cycles). Then DMC (4 mL) solvent was added by syringe under argon atmosphere. Later, the reaction mixture was continued at room temperature for 4 h under argon atmosphere. After completion of reaction, water was added to the reaction mixture (10 mL) and extracted with EtOAc (2 x 15 mL). The combined organic extract was washed with brine (20 mL), the organic phase was dried over anhydrous Na_2SO_4 and filtered. After solvent evaporation, the residue was purified by silica gel chromatography to afford the desired product **4a** with 8% yield.

➢ Under Pure Oxygen Atmosphere



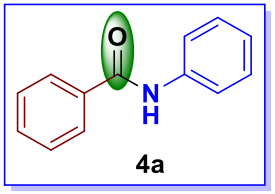
The imine **3a** (1 equiv, 0.5 mmol, 91 mg), NHC precatalyst **C1** (20 mol%, 0.1mmol, 22.5 mg), and Cs_2CO_3 (1.2 equiv, 0.6 mmol, 197 mg) were taken in a clean and dried two necked round bottom flask. It was evacuated and back filled with argon gas (2-3 cycles). Then were added DMC (4 mL) solvent by syringe under argon atmosphere. Later, the reaction mixture was continued at room temperature for 4 h under pure oxygen atmosphere. After completion of reaction, water was added to the reaction mixture (20 mL) and extracted with EtOAc (2 x 10 mL). The combined organic extract was washed with brine (10 mL), the organic phase was dried over anhydrous Na_2SO_4 and filtered. Then recrystallization with cold *n*-pentane and DCM (few drops) afford the pure products. **4a** off-white solid in 84% yield.

➢ Direct Reaction of 1a and 2a



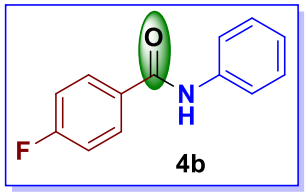
The aniline **2a** (1.0 equiv, 1 mmol, 0.091 mL), benzaldehyde **1a** (1.0 equiv, 1 mmol, 0.1 mL) and NHC precatalyst **C1** (20 mol%, 0.2 mmol, 45 mg) were added in a clean round bottom flask. Then dry DMC (8 mL) was added by syringe followed by addition of Cs_2CO_3 (1.2 equiv, 1.2 mmol, 391 mg). Then the reaction mixture was stirred at the room temperature for 1 h under open air. After completion of reaction, water was added to the reaction mixture (20 mL) and extracted with EtOAc (2 x 20 mL). The combined organic extract was washed with brine (15 mL), the organic phase was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure on a rotavapor to obtain a crude residue. The crude product was purified EtOAc/Hex by using column chromatography to give 5 in 79% yield. The spectroscopic data were in good agreement with the reported data reported by Cheon *et al.* (ref: *Org. Lett.*, 2014, **16,** 2514.)

Spectroscopic data



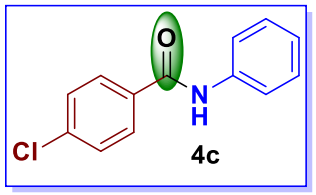
4a

***N*-phenyl benzamide (4a):**- Off-white solid, 167 mg (0.85 mmol), 85% yield, R_f = 0.5 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 755, 1076, 1221, 1588, 1686, 3034 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.16 (d, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 2H), 7.44-7.58 (m, 3H), 7.64 (d, *J* = 7.7 Hz, 2H), 7.84-7.90 (m, 2H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 120.8, 124.1, 128.1, 128.8, 129.1, 132.0, 135.5, 139.6, 166.0; **MS** (ESI, *m/z*): $[M+H]^+$ 198; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{12}NO$ $[M+H]^+$ 198.0914, found 198.0913. The spectroscopic data were in good agreement with the reported data.[22]

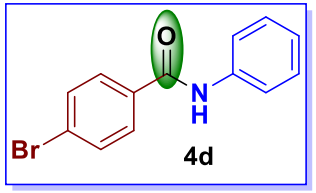


4b

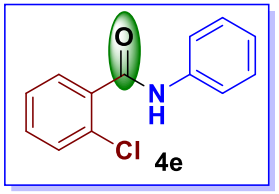
4-Fluoro-*N*-phenylbenzamide (4b):- White solid, 159 mg (0.74 mmol), 74% yield, R_f = 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 763, 1171, 1226, 1599, 1689, 3079 cm^{-1}; **^{1}H-NMR** (400 MHz, DMSO-d_6) δ = 7.12 (s, 1H), 7.36 (d, *J* = 6.2 Hz, 4H), 7.76 (d, *J* = 7.5 Hz, 2H), 8.04 (s, 2H), 10.25 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 115.7, 115.9, 120.9, 124.2, 129.1, 130.8, 130.9, 131.8, 139.5, 164.5 (*J* = 250 Hz), 164.9; **^{19}F-NMR** (376 MHz, $CDCl_3$) δ = -107.4; **MS** (ESI, *m/z*): $[M+H]^+$ 216; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}NOF$ $[M+H]^+$ 216.0823 found. 216.0817. The spectroscopic data were in good agreement with the reported data.[34]



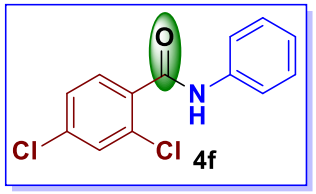
4-Chloro-*N*-phenylbenzamide(4c):- White solid, 173 mg (0.75 mmol), 75% yield, R_f = 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 755, 1324, 1532, 1653, 3345 cm^{-1}; **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 7.17 (t, *J* = 7.4 Hz, 1H), 7.38 (*J* = 7.9 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 7.8 Hz, 2H), 7.77 (s, 1H), 7.82 (d, *J* = 8.4 Hz, 2H); **^{13}C{^{1}H}NMR** (126 MHz, DMSO-d_6 & $CDCl_3$) δ = 121.0, 124.1, 128.5, 128.7, 129.6, 133.8, 137.2, 139.1, 165.0; **MS** (ESI, *m/z*): $[M+H]^+$ 232; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}NOCl$ $[M+H]^+$ 232.0529 found. 232.0524. The spectroscopic data were in good agreement with the reported data.[22]



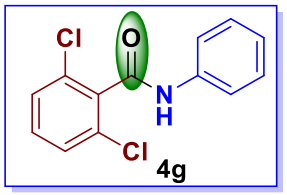
4-Bromo-*N*-phenylbenzamide (4d):- White solid, 222 mg (0.81 mmol), 81% yield, R_f = 0.5 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$), 753, 1286, 1442, 1533, 1653, 3341 cm^{-1}; **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 7.17 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 2H), 7.57-7.68 (m, 4H), 7.75 (d, *J* = 8.5 Hz, 3H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 120.9, 124.3, 125.9, 129.1, 130.3, 131.9, 134.5, 139.4, 165.0; **MS** (ESI, *m/z*): $[M+H]^+$ 276; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}BrNO$ $[M+H]^+$ 276.0023 found 276.0020.The spectroscopic data were in good agreement with the reported data.[22]



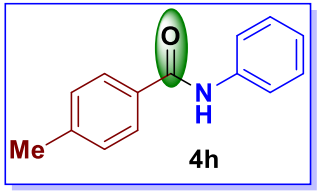
2-Chloro-*N*-phenylbenzamide (4e):- Black solid, 168 mg (0.73 mmol), 73% yield, R_f = 0.45 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 759, 1329, 1443, 1541, 1603, 1665, 3072 cm^{-1}**; ^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.17 (m, 1H), 7.30-7.34 (m, 1H), 7.36 (d, *J* = 2.9 Hz, 1H), 7.38-7.39 (m, 1H), 7.41-7.42 (d, *J* = 1.0 Hz, 1H), 7.61-7.67 (m, 4H), 7.72 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 119.3, 120.1, 125.1, 127.8, 129.0, 129.8, 131.5, 133.5, 137.5, 137.8, 165.6; **MS** (ESI, *m/z*): $[M+H]^+$ 232; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}ONCl$ $[M+H]^+$ 232.0519 found 232.0523. The spectroscopic data were in good agreement with the reported data.[22]



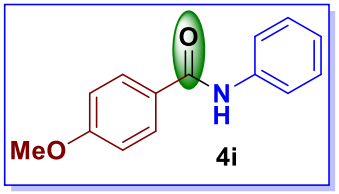
2,4-Dichloro-*N*-phenylbenzamide (4f): -White solid, 209 mg (0.79 mmol), 79% yield, R_f = 0.5 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 751, 1156, 1222, 1599, 1688, 3079 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.18 (d, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 3H), 7.47 (s, 1H), 7.64 (s, 2H), 7.72 (d, *J* = 8.3 Hz, 1H) 7.93 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 120.3, 125.1, 127.7, 129.2, 130.1, 131.4, 131.5, 133.6, 137.2, 137.4, 163.6; **MS** (ESI, *m/z*): $[M+H]^+$ 266; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{10}ONCl_2$ $[M+H]^+$ 266.0135 found 266.0134.



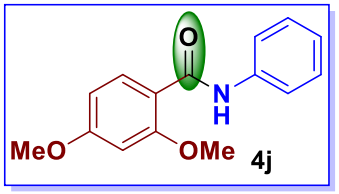
2,6-Dichloro-*N*-phenylbenzamide (4g):- White solid, 185 mg (0.70 mmol), 70% yield, R_f = 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 763, 1171, 1226, 1561, 1689, 3076 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.20 (t, *J* = 7.4 Hz, 1H), 7.31 (dd, *J* = 9.2, 6.7 Hz, 1H), 7.35-7.44 (m, 4H), 7.64 (d, *J* = 7.8 Hz, 2H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 120.4, 125.3, 128.3, 129.2, 131.0, 132.5, 135.9, 137.1, 162.4; **MS** (ESI, *m/z*): $[M+H]^+$ 266; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{10}NOCl_2$ $[M+H]^+$ 266.0144 found. 266.0141.The spectroscopic data were in good agreement with the reported data.[25]



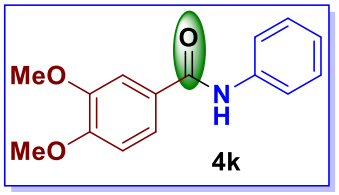
4-Methyl-*N*-phenylbenzamide (4h):- White solid, 158 mg (0.75 mmol), 75% yield, R_f = 0.45 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$), 753, 1467, 1533, 1656, 3348 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 2.42 (s, 3H), 7.12-7.18 (m, 1H), 7.28 (d, *J* = 7.9 Hz, 2H), 7.34-7.39 (m, 2H), 7.62-7.66 (m, 2H), 7.76-7.79 (m, 2H), 7.80 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 21.5, 120.2, 124.5, 127.0, 129.1, 129.5, 132.1, 138.1, 142.4, 165.6; **MS** (ESI, *m/z*): $[M+H]^+$ 212; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{14}ON$ $[M+H]^+$ 212.1065 found 212.1070.The spectroscopic data were in good agreement with the reported data.[22]



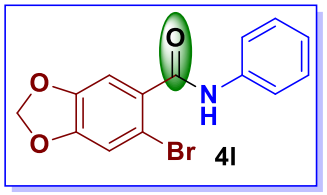
4-Methoxy-*N*-phenylbenzamide (4i):-White solid, 172 mg (0.76 mmol), 76% yield, R_f = 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 762, 1217, 1442, 1599, 1654, 2965, 3256; cm^{-1}; **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 3.88 (s, 3H), 6.98 (d, *J* = 8.2 Hz, 2H), 7.14 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.77 (s, 1H), 7.85 (d, *J* = 8.6 Hz, 2H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 55.5, 114.0, 120.2, 124.4, 127.2, 128.9, 129.1, 138.1, 162.5, 165.2; **MS** (ESI, *m/z*): $[M+H]^+$ 228; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{14}N_2O$ $[M+H]^+$ 228.1019 found 228.1018.The spectroscopic data were in good agreement with the reported data.[22]



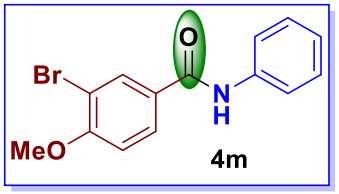
***N*-(2,4-Dimethoxyphenyl) benzamide (4j)**:- White solid, 182 mg (0.71 mmol), 71% yield, R_f = 0.40 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 757, 836, 1036, 1075, 1256, 1603, 1666, 2958, 3363 cm^{-1}; **^{1}H-NMR** (400 MHz, DMSO-d_6) δ = 3.84 (s, 3H), 3.93 (s, 3H), 6.61-6.79 (m, 2H), 7.08 (d, *J* = 6.7 Hz, 1H), 7.33 (t, *J* = 7.0 Hz, 2H), 7.65-7.83 (m, 3H), 9.92 (s, 1H) **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$ & DMSO-d_6) δ = 56.0, 56.6, 99.0, 106.2, 113.1, 116.4, 120.3, 124.1, 130.0, 132.6, 139.4, 158.8, 163.5, 163.9 ; **MS** (ESI, *m/z*): $[M+H]^+$ 258; **HRMS** (ESI, *m/z*): calcd for $C_{15}H_{16}O_3N$ $[M+H]^+$ 258.1125, found 258.1123.



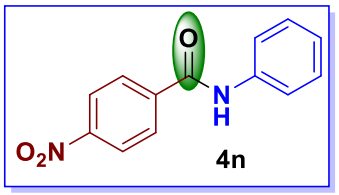
3,4-Dimethoxy-*N*-phenylbenzamide (4k):- White solid,187 mg (0.73 mmol), 73% yield, R_f = 0.45 (EtOAc/Hex, 20:80); **IR** ($CHCl_3$) 758, 1171, 1226, 1599, 1689, 3079 cm^{-1}; **^{1}H-NMR** (400 MHz, DMSO-d_6) δ =3.92 (s, 3H), 3.93 (s, 3H), 6.87-6.95 (m, 1H), 7.02 (d, *J* = 7.3 Hz, 1H), 7.24 (t, *J* = 7.8 Hz, 2H), 7.51 (s, 1H), 7.58 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 2H), 9.88 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 56.1, 56.2, 111.4, 111.5, 120.8, 120.9, 121.5, 123.9, 127.5, 129.03, 139.7, 148.8, 152.1, 165.4; **MS** (ESI, *m/z*): $[M-H]^+$ 258; **HRMS** (ESI, *m/z*): calcd for $C_{15}H_{16}O_3N$ $[M+H]^+$ 258.1125 found 258.1125. The spectroscopic data were in good agreement with the reported data.[23]



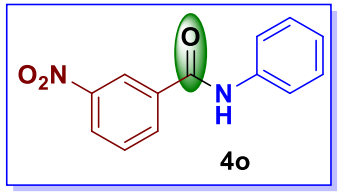
6-Bromo-*N*-phenylbenzo[*d*][1,3]dioxole-5-carboxamide (4l):- White solid, 229 mg (0.72 mmol), 72% yield, R_f= 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 760, 1040, 1249, 1484, 1545, 1662, 2925, 3281 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 6.04 (s, 2H), 7.03 (s, 1H), 7.09-7.21 (m, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.62 (d, *J* = 7.8 Hz, 2H), 7.76 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 102.4, 109.9, 110.8, 113.3, 120.1, 124.8, 129.1, 131.0, 137.6, 147.7, 150.0, 165.0; **MS** (ESI, *m/z*): $[M+H]^+$ 320; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{11}NO_3Br$ $[M+H]^+$ 319.991 found 319.990. The spectroscopic data were in good agreement with the reported data.[36]



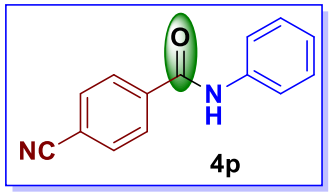
3-Bromo-4-methoxy-*N*-phenylbenzamide (4m):- Light yellow solid, 225 mg (0.74 mmol), 74% yield, R_f = 0.45; (EtOAc/Hex, 10:90) **IR** ($CHCl_3$) 594, 762, 1059, 1266, 1502, 1658, 2926, 3362 cm^{-1}; **^{1}H-NMR** (400 MHz, DMSO-d_6) δ = 3.95 (s, 3H), 7.10 (t, *J* = 7.3 Hz, 1H), 7.26 (d, *J* = 8.7 Hz, 1H), 7.35 (t, *J* = 7.7 Hz, 2H), 7.76 (d, *J* = 7.9 Hz, 2H), 8.02 (d, *J* = 7.1 Hz, 1H), 8.24 (s, 1H), 10.18 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 57.1, 110.8, 112.6, 120.8, 124.1, 128.6, 128.9, 129.6, 132.7, 139.6, 158.4, 164.0; **MS** (ESI, *m/z*): $[M+H]^+$ 306; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{13}O_2NBr$ $[M+H]^+$ 306.0124 found 306.0117.



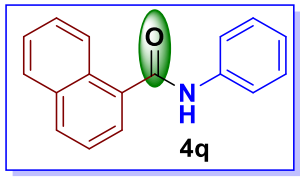
4-Nitro-*N*-phenylbenzamide (4n):- White solid, 191 mg (0.79 mmol), 79% yield, R_f = 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 758, 1327, 1544, 1669, 2233, 3353 cm^{-1}; **^{1}H-NMR** (400 MHz, DMSO-d_6) δ = 7.15 (s, 1H), 7.38 (s, 2H), 7.78 (d, *J* = 7.3 Hz, 2H), 8.19 (d, *J* = 7.8 Hz, 2H), 8.38 (d, *J* = 7.7 Hz, 2H), 10.57 (s, 1H); **^{13}C{^{1}H}NMR** (126 MHz, $CDCl_3$) δ = 120.5, 123.5, 124.2, 128.7, 129.2, 138.6, 140.6, 149.1, 163.9; **MS** (ESI, *m/z*): $[M+H]^+$ 243; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}N_2O_3$ $[M+H]^+$ 243.0761 found 243.0764. The spectroscopic data were in good agreement with the reported data.[29]



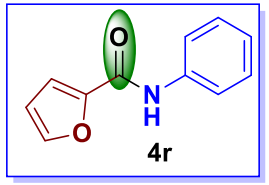
3-Nitro-*N*-phenylbenzamide (4o):- White solid, 176 mg (0.73 mmol), 73% yield, R_f = 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 768, 1081, 1262, 1452, 1607, 1669, 2245, 3080 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.21 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.66 (d, *J* = 7.8 Hz, 2H), 7.71 (t, *J* = 8.0 Hz, 1H), 7.98 (s, 1H), 8.26 (d, *J* = 7.6 Hz, 1H), 8.41 (d, *J* = 8.1 Hz, 1H), 8.70 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 120.5, 121.8, 125.3, 126.4, 129.3, 130.1, 133.4, 136.6, 137.3, 148.3, 163.3; **MS** (ESI, *m/z*): $[M+H]^+$ 243; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}N_2O_3$ $[M+H]^+$ 243.0764, found 243.0765.The spectroscopic data were in good agreement with the reported data.[31]



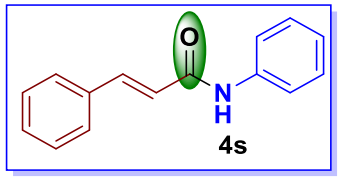
4-Cyano-*N*-phenylbenzamide (4p):- White solid, 171 mg (0.77 mmol), 77% yield, R_f = 0.50 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 760, 1077, 1288, 1454, 1541, 1670, 2232, 3178, 3353 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.20 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.63 (d, *J* = 7.7 Hz, 2H), 7.80 (d, *J* = 8.2 Hz, 2H), 7.86 (s, 1H), 7.98 (d, *J* = 8.1 Hz, 2H); **^{13}C{^{1}H}NMR** (126 MHz, $CDCl_3$) δ = 115.5, 117.9, 120.4, 125.3, 127.8, 129.3, 132.7, 137.3, 138.9, 163.9; **MS** (ESI, *m/z*): $[M-H]^+$ 223; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{11}ON_2$ $[M+H]^+$ 223.0866 found 223.0863.The spectroscopic data were in good agreement with the reported data.[22]



***N*-phenyl-1-naphthamide (4q)**:- White solid, 192 mg (0.78 mmol), 78% yield, R_f = 0.45 (EtOAc/Hex, 8:92); **IR** ($CHCl_3$) 756, 1215, 1535, 1600, 1657, 3019 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.18 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.50 (dd, *J* = 15.0, 7.4 Hz, 1H), 7.56 (dt, *J* = 5.8, 3.5 Hz, 2H), 7.71 (dd, *J* = 15.7, 7.2 Hz, 4H), 7.90 (dd, *J* = 6.1, 3.2 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 8.30-8.42 (m, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 120.0, 124.7, 124.8, 125.1, 125.3, 126.6, 127.4, 128.5, 129.2, 130.1, 131.1, 133.8, 134.5, 138.1, 167.6; MS (ESI, *m/z*): $[M+H]^+$ 248; **HRMS** (ESI, *m/z*): calcd for C_{17} $H_{14}ON$ $[M+H]^+$ 248.1070, found 248.1066.The spectroscopic data were in good agreement with the reported data.[33]

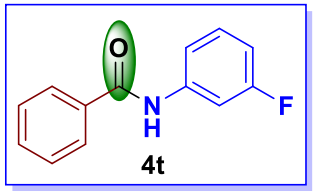


***N*-phenylfuran-2-carboxamide (4r)**:- White solid, 120 mg (0.64 mmol), 64% yield, R_f= 0.45 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 756, 1155, 1216, 1443, 1604, 1668, 2922, 3021, cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 6.57 (dd, *J* = 3.5, 1.8 Hz, 1H), 7.13-7.20 (m, 1H), 7.25 (dd, *J* = 3.5, 0.7 Hz, 1H), 7.30-7.43 (m, 2H), 7.52 (dd, *J* = 1.7, 0.8 Hz, 1H), 7.65 (dd, *J* = 8.6, 1.0 Hz, 2H), 8.06 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 112.7, 115.3, 119.9, 124.6, 129.1, 137.4, 144.2, 148.1, 156.0; **MS** (ESI, *m/z*): $[M+H]^+$ 188; **HRMS** (ESI, *m/z*): calcd for $C_{11}H_{10}O_2N$ $[M+H]^+$ 188.0706 found 188.0705. The spectroscopic data were in good agreement with the reported data.[22]



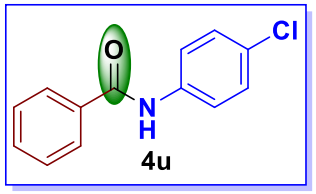
4s

***N*-phenylcinnamamide (4s)**:-White solid, 122 mg (0.55 mmol), 55% yield, R_f = 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 761, 1184, 1249, 1348, 1449,1547, 1626 1667, 3283 cm^{-1}; **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 6.55 (d, *J* = 15.5 Hz, 1H), 7.14 (t, *J* = 7.0 Hz, 1H), 7.37 (dt, *J* = 15.7, 6.8 Hz, 6H), 7.55 (d, *J* = 5.3 Hz, 2H), 7.61 (s, 2H), 7.77 (d, *J* = 15.5 Hz, 1H); **^{13}C{^{1}H}NMR** (126 MHz, $CDCl_3$) δ = 119.0, 120.8, 124.5, 128.0, 129.0, 129.1, 130.0, 134.6, 138.0, 142.5, 164.1; **MS** (ESI, *m/z*): $[M+H]^+$ 224; **HRMS** (ESI, *m/z*): calcd for $C_{15}H_{14}ON$ $[M+H]^+$ 224.1070, found 224.1071.The spectroscopic data were in good agreement with the reported data.[35]

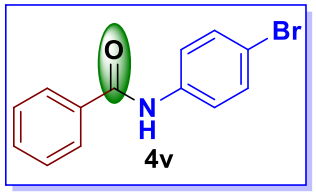


4t

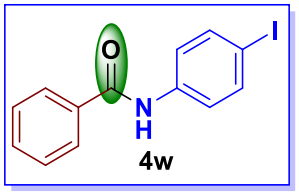
***N*-(3-fluorophenyl) benzamide (4t)**:- White solid, 165 mg (0.77 mmol), 77% yield, R_f = 0.45 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 705, 1493, 1541, 1609, 1667, 2925, 2960, 3343 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 6.86 (m, 1H), 7.25-7.34 (m, 2H), 7.47-7.56 (m, 2H), 7.56-7.66 (m, 1H), 7.86 (dd, *J* = 5.3, 3.3 Hz, 2H); **^{13}C{^{1}H}NMR** (126 MHz, $CDCl_3$) δ = 107.6, 107.8, 111.2, 111.4, 115.4, 127.0, 129.0, 130.1, 130.2, 132.1, 134.6, 139.4, 139.5, 163.1 (*J* = 258 Hz), 165.7; **^{19}F-NMR** (376 MHz, $CDCl_3$) δ = 111.28; **MS** (ESI, *m/z*): $[M+H]^+$ 216; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}OFN$ $[M+H]^+$ 216.0825 found 216.0824. The spectroscopic data were in good agreement with the reported data.[32]



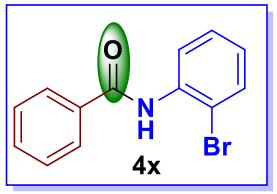
***N*-(4-chlorophenyl) benzamide (4u):-** White solid, 182 mg (0.79 mmol), 79% yield, R_f = 0.45 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 830, 1127, 1401, 1524, 1660, 2923, 2964, 3352 cm^{-1}; **^{1}H-NMR** (400 MHz, DMSO-d_6) δ = 7.39-7.46 (m, 2H), 7.50-7.58 (m, 2H) ,7.61 (m, 1H), 7.78-7.89 (m, 2H) , 7.95 (dd, *J* = 5.3, 3.3 Hz, 2H), 10.38 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 122.3, 127.7, 128.2, 128.9, 129.0, 132.2, 135.2, 138.6, 166.1; **MS** (ESI, *m/z*): $[M+H]^+$ 232; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}OClN$ $[M+H]^+$ 232.05237 found 232.05214.The spectroscopic data were in good agreement with the reported data.[33]



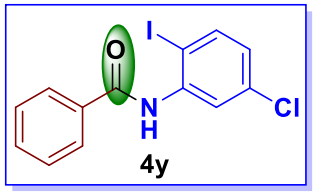
***N*-(4-bromophenyl) benzamide (4v):-** White solid, 217 mg (0.79 mmol), 79% yield, R_f = 0.50 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 1000, 1217, 1590, 1689, 2922, 3076 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.48 (d, *J* = 2.2 Hz, 1H), 7.51 (d, *J* = 8.2 Hz, 3H), 7.56 (dd, *J* = 11.9, 5.3 Hz, 3H), 7.80 (s, 1H), 7.83-7.90 (m, 2H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 115.8, 122.7, 128.1, 128.9, 131.9, 132.2, 135.1, 139.1, 166.1; **MS** (ESI, *m/z*): $[M+H]^+$ 276; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}NOBr$ $[M+H]^+$ 276.0027 found 276.0024. The spectroscopic data were in good agreement with the reported data.[27]



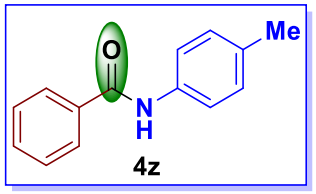
***N*-(4-iodophenyl) benzamide (4w):-** White solid, 245 mg (0.76 mmol), 76% yield, R_f = 0.50 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 799, 1073, 1155, 1277, 1464, 1590, 3071 cm^{-1}; **^{1}H-NMR** (400 MHz, DMSO-d_6) δ = 7.52 (t, *J* = 7.4 Hz, 2H), 7.55 (s, 1H), 7.64 (d, *J* = 8.8 Hz, 2H), 7.70 (d, *J* = 8.8 Hz, 2H), 7.94 (d, *J* = 7.2 Hz, 2H), 10.34 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 87.8, 122.9, 128.2, 128.9, 132.2, 135.2, 137.7, 139.5, 166.1; **MS** (ESI, *m/z*): $[M+H]^+$ 324; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}ONI$ $[M+H]^+$ 324.0905 found 324.0905. The spectroscopic data were in good agreement with the reported data.[27]



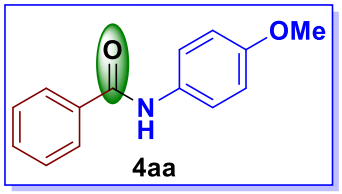
***N*-(2-bromophenyl) benzamide (4v):-** White solid, 198 mg (0.72 mmol), 72% yield, R_f = 0.40 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 757, 1034, 1216, 1444, 1603, 1669, 3020, 3305 cm^{-1}; **^{1}H-NMR** (400 MHz, DMSO-d_6) δ = 7.10 (d, *J* = 6.8 Hz, 1H), 7.22 (d, *J* = 6.7 Hz, 1H), 7.35 (t, *J* = 7.3 Hz, 2H), 7.43 (d, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.55 (d, *J* = 6.5 Hz, 1H), 7.73 (s, 2H), 10.47 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 119.5, 120.0, 124.3, 128.2, 129.2, 129.3, 131.6, 133.2, 139.4, 139.6, 166.3; **MS** (ESI, *m/z*): $[M+H]^+$ 276; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{11}NOBr$ $[M+H]^+$ 276.0025 found 276.0024. The spectroscopic data were in good agreement with the reported data.[24]



***N*-(5-chloro-2-iodophenyl)benzamide (4y):-** White solid, 278 mg (0.78 mmol), 78% yield, R_f = 0.45 (EtOAc/Hex, 5:95); **IR** ($CHCl_3$) 800, 1074, 1283, 1462, 1649, 2925, 3136 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 6.90 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.55 (t, *J* = 7.4 Hz, 2H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 7.5 Hz, 2H), 8.30 (s, 1H), 8.60 (d, *J* = 1.6 Hz, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 86.7, 121.2, 126.0, 127.2, 129.1, 132.5, 134.2, 135.6, 139.2, 165.3; **MS** (ESI, *m/z*): $[M+H]^+$ 358; **HRMS** (ESI, *m/z*): calcd for $C_{13}H_{10}IClO$ $[M+H]^+$ 358.0506 found 358.0506. The spectroscopic data were in good agreement with the reported data.[20]

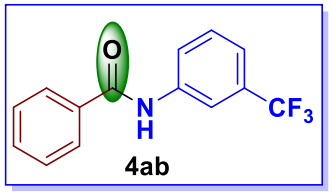


***N*-(*p*-tolyl) benzamide (4z):-** Yellow solid, 156 mg (0.74 mmol), 74% yield, R_f = 0.45 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 808, 1262, 1524, 1653, 1724, 2924, 3345 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 2.34 (s, 3H), 7.18 (d, *J* = 8.2 Hz, 2H), 7.45-7.58 (m, 5H), 7.78 (s, 1H), 7.83-7.90 (m, 2H); **^{13}C{^{1}H}NMR** (126 MHz, $CDCl_3$) δ = 21.0, 120.3, 127.0, 128.8, 129.6, 131.8, 134.3, 135.1, 135.3, 165.7; **MS** (ESI, *m/z*): $[M+H]^+$ 212; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{14}ON$ $[M+H]^+$ 212.1071 found 212.1070. The spectroscopic data were in good agreement with the reported data.[27]



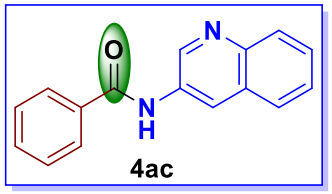
4aa

***N*-(4-methoxyphenyl) benzamide (4aa):-** Brown solid, 158 mg (0.75 mmol), 75% yield, R_f = 0.5 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 760, 1036, 1259, 1525, 1650, 2923, 2961, 3325 cm^{-1}; **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 3.82 (s, 3H), 6.91 (d, *J* = 8.7 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.52-7.57 (m, 3H), 7.76 (s, 1H), 7.86 (d, *J* = 7.4 Hz, 2H); **^{13}C{^{1}H}NMR** (126 MHz, $CDCl_3$) δ = 55.7, 114.3, 122.1, 128.8, 129.0, 131.7, 135.0, 156.7, 165.6, **MS** (ESI, *m/z*): $[M+H]^+$ 228; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{14}O_2N$ $[M+H]^+$ 228.1020 found 228.1020. The spectroscopic data were in good agreement with the reported data.[27]



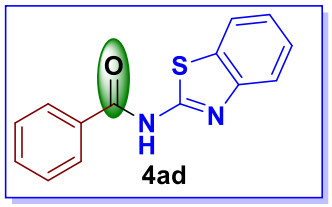
4ab

***N*-(3-(trifluoromethyl)phenyl)benzamide (4ab):-** Light yellow solid, 207 mg (0.78 mmol), 78% yield, R_f = 0.40 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 705, 1037, 1124, 1329, 1442, 1550, 1607,1668, 2923, 3076, 3278 cm^{-1}; **^{1}H-NMR** (500 MHz, DMSO-d_6) δ = 7.45 (d, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.4 Hz, 2H), 7.60 (dd, *J* = 16.3, 8.0 Hz, 2H), 7.97 (d, *J* = 7.4 Hz, 2H), 8.03 (d, *J* = 8.0 Hz, 1H), 8.25 (s, 1H), 10.56 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 116.8, 116.9, 120.5, 123.3, 124.3, 126.1, 128.2, 128.9, 129.3,129.7, 130.0, 130.4, 132.4, 134.8, 140.4, 166.5; **^{19}F-NMR** (376 MHz, $CDCl_3$) δ = -62.7; **MS** (ESI, *m/z*): $[M+H]^+$ 266; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{11}ONF_3$ $[M+H]^+$ 266.0787, found. 266.0782. The spectroscopic data were in good agreement with the reported data.[21]



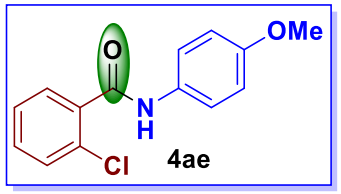
4ac

***N*-(quinolin-3-yl)benzamide (4ac):-** Light yellow solid, 190 mg (0.77 mmol), 77% yield, R_f = 0.45 (EtOAc/Hex, 20:80); **IR** ($CHCl_3$) 757, 1132, 1283, 1372, 1548, 1668, 2926, 3068 cm^{-1}; **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 7.58 (dd, *J* = 19.1, 7.1 Hz, 5H), 7.64 (s, 1H), 7.83 (s,1H), 7.96 (d, *J* = 7.5 Hz, 1H), 8.05 (s, 1H), 8.36 (s, 1H), 8.90 (d, *J* = 9.7 Hz, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 124.6, 127.2, 127.4, 127.9, 128.2, 128.5, 128.8, 128.9, 131.6, 132.4, 134.2, 144.1, 145.1, 166.3; **MS** (ESI, *m/z*): $[M+H]^+$ 249; **HRMS** (ESI, *m/z*): calcd for $C_{16}H_{13}ON_2$ $[M+H]^+$ 249.1030 found 249.1028. The spectroscopic data were in good agreement with the reported data.[26]

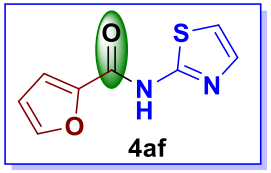


4ad

***N*-(benzo[*d*]thiazol-2-yl) benzamide (4ad):-** White solid, 203 mg (0.80 mmol), 80% yield, R_f = 0.45 (EtOAc/Hex, 10:90); **IR** ($CHCl_3$) 759, 1283, 1302, 1548, 1679, 3070, 3176 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.33 (d, *J* = 5.1 Hz, 3H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.84-7.92 (m, 1H), 8.04 (d, *J* = 7.6 Hz, 2H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 120.7, 121.5, 124.2, 126.3, 128.0, 129.0, 132.0, 133.2, 147.4, 165.6; **MS** (ESI, *m/z*): $[M+H]^+$ 255; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{10}ON_2S$ [M+H] 255.0587 found 255.0584 The spectroscopic data were in good agreement with the reported data.[28]



2-chloro-*N*-(4-methoxyphenyl) benzamide (4ae):- White solid, 188 mg (0.72 mmol), 72% yield, R_f = 0.45 (EtOAc/Hex, 15:85); **IR** ($CHCl_3$) 752, 1076, 1130, 1285, 1603, 1678, 2855, 2925, 3071 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 3.82 (s, 3H), 6.92 (d, *J* = 9.0 Hz, 2H), 7.41 (m, 3H), 7.55 (d, *J* = 8.9 Hz, 2H), 7.77 (dt, *J* = 11.9, 5.7 Hz, 2H); **^{13}C{^{1}H}NMR** (101 MHz, DMSO-d_6) δ = 55.7, 114.4, 121.5, 127.7, 129.4, 130.1, 131.4, 132.6, 137.6, 156.0, 164.9; **MS** (ESI, *m/z*): $[M+H]^+$ 262; **HRMS** (ESI, *m/z*): calcd for $C_{14}H_{13}O_2NCl$ $[M+H]^+$ 262.0636 found 262.0634.



***N*-(thiazol-2-yl) furan-2-carboxamide (4af):-** Light brown solid, 135 mg (0.70 mmol), 70% yield, R_f = 0.45 (EtOAc/Hex, 20:80); **IR** ($CHCl_3$) 763, 1168, 1314, 1546, 1671, 2922, 2962, 3080 cm^{-1}; **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 6.61 (d, *J* = 1.7 Hz, 1H),7.03 (d, *J* = 3.4 Hz, 1H), 7.36 (d, *J* = 3.3 Hz, 1H), 7.51 (d, *J* = 3.4 Hz, 1H), 7.58 (s, 1H), 10.24 (s, 1H); **^{13}C{^{1}H}NMR** (101 MHz, $CDCl_3$) δ = 113.0, 114.0, 117.2, 137.6, 145.4, 146.2, 155.3, 158.1; **MS** (ESI, *m/z*): $[M+H]^+$ 195; **HRMS** (ESI, *m/z*): calcd for $C_8H_7O_2N_2S$ $[M+H]^+$ 195.0223, found 195.0218. The spectroscopic data were in good agreement with the reported data.[30]

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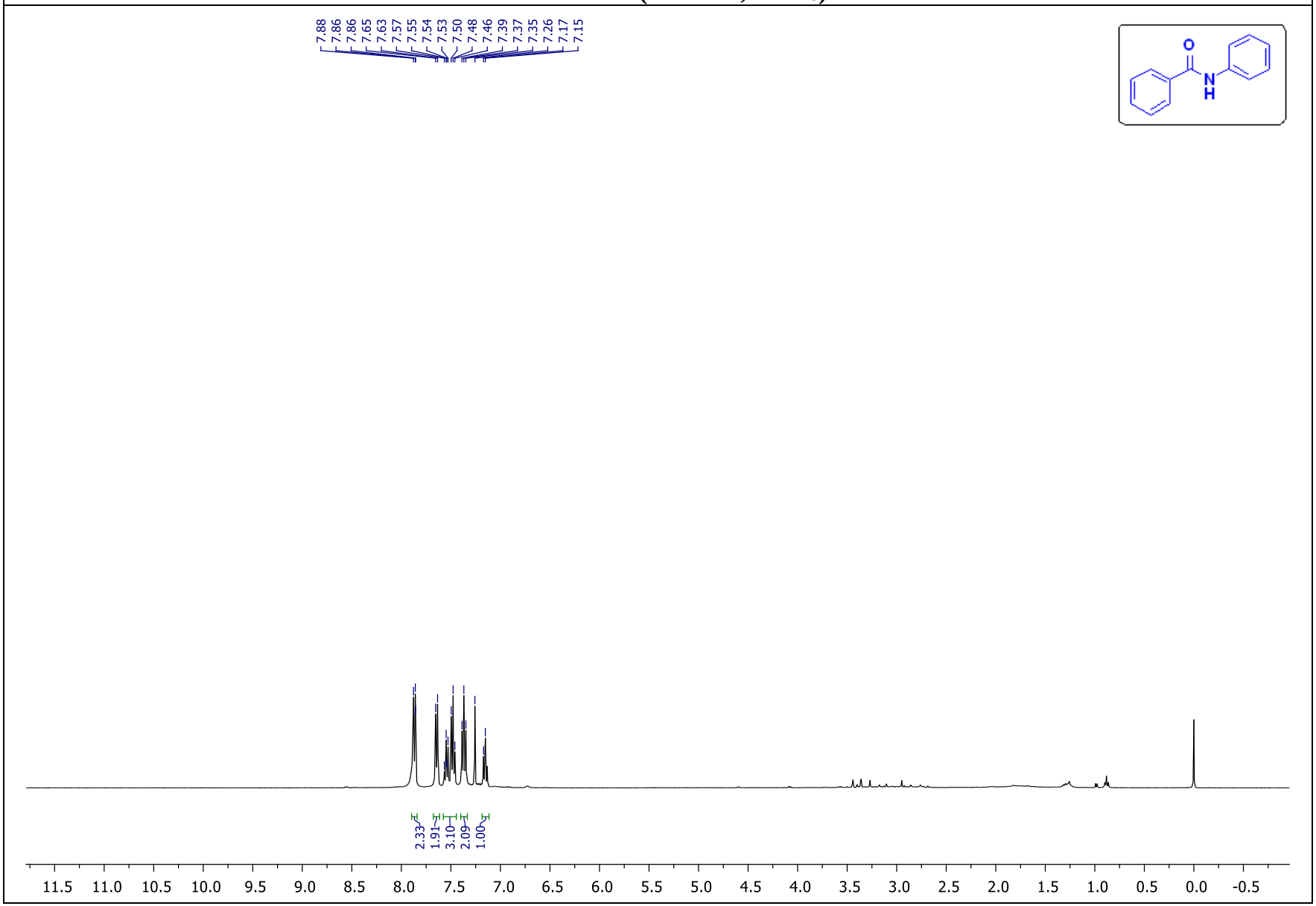
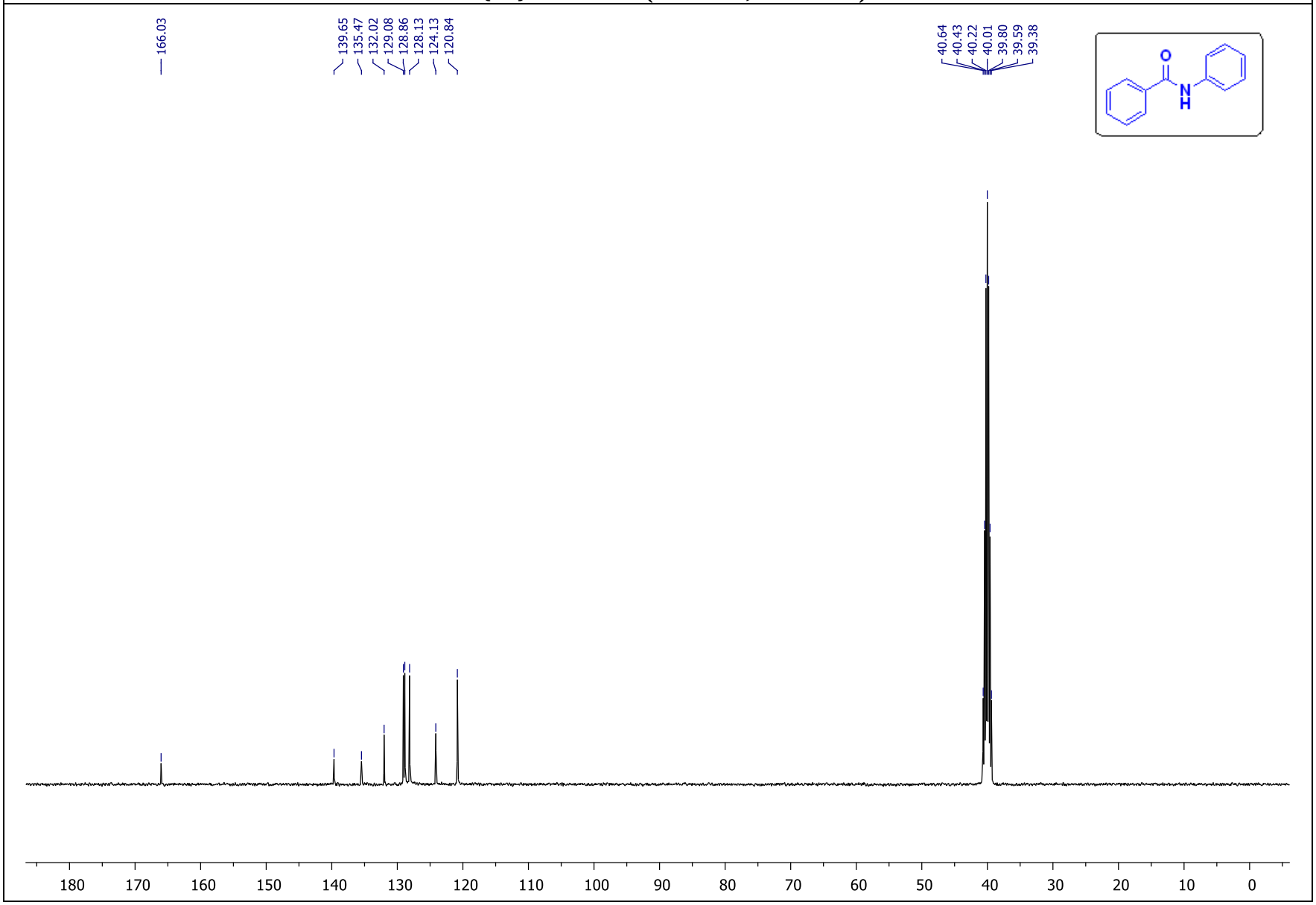
^{1}H NMR of 4a (400 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$NMR of 4a (101 MHz, DMSO-d_6)



HRMS of 4a

D:\Sai krishna Important\...\SUR-RR-BA

CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
DEPARTMENT OF ANALYTICAL& STRUCTURAL CHEMISTRY

4/22/2021 1:27:05 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

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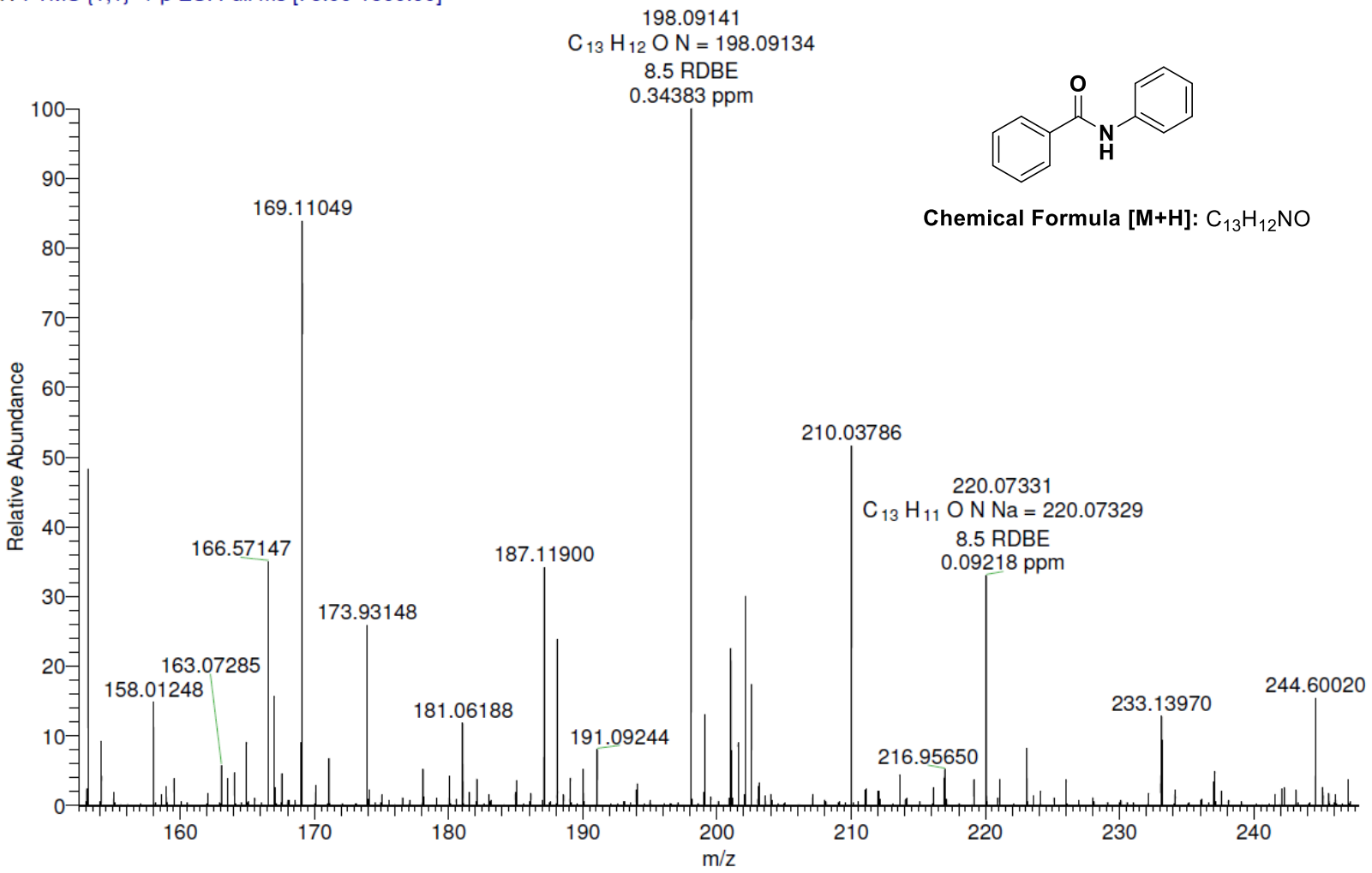
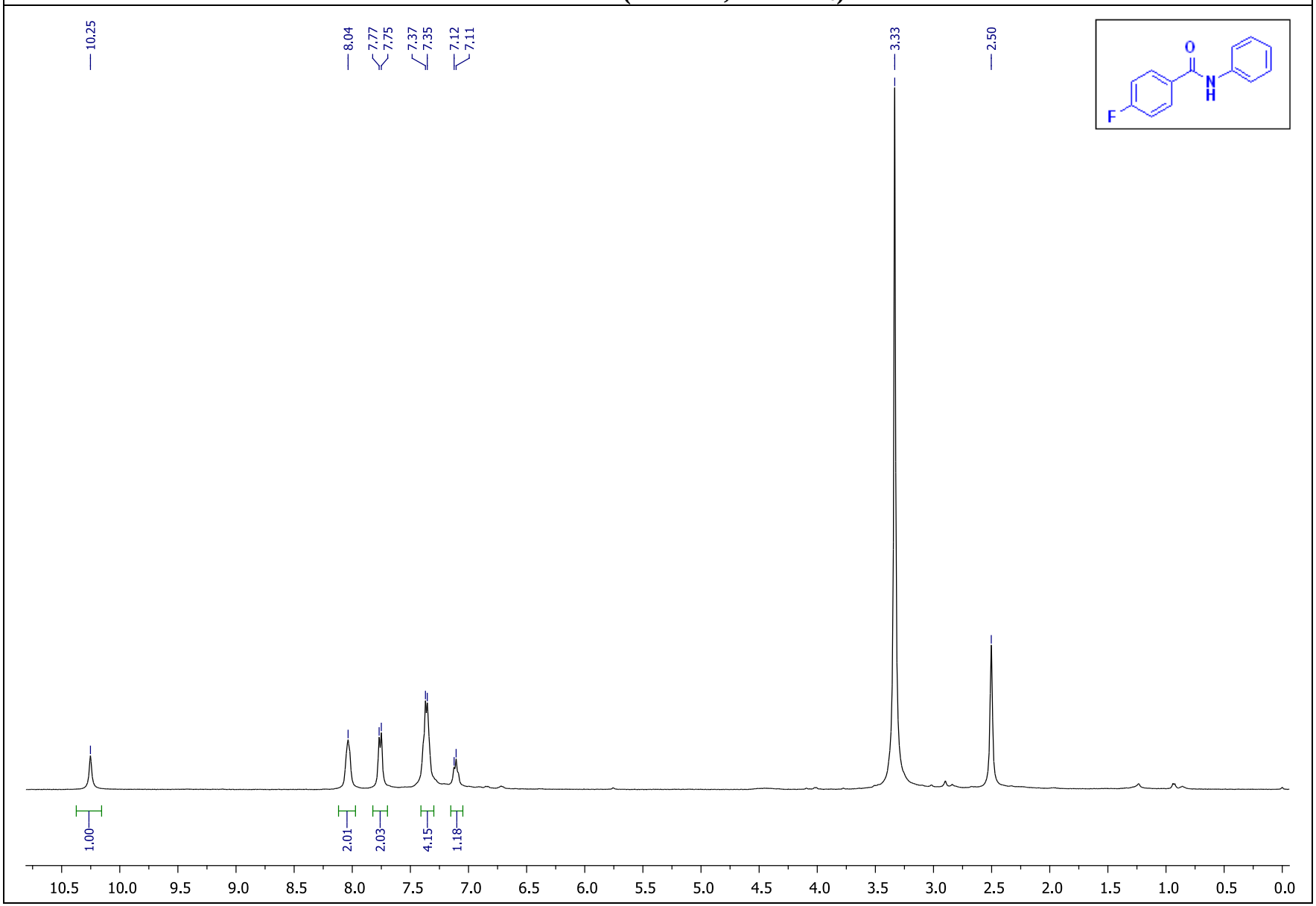
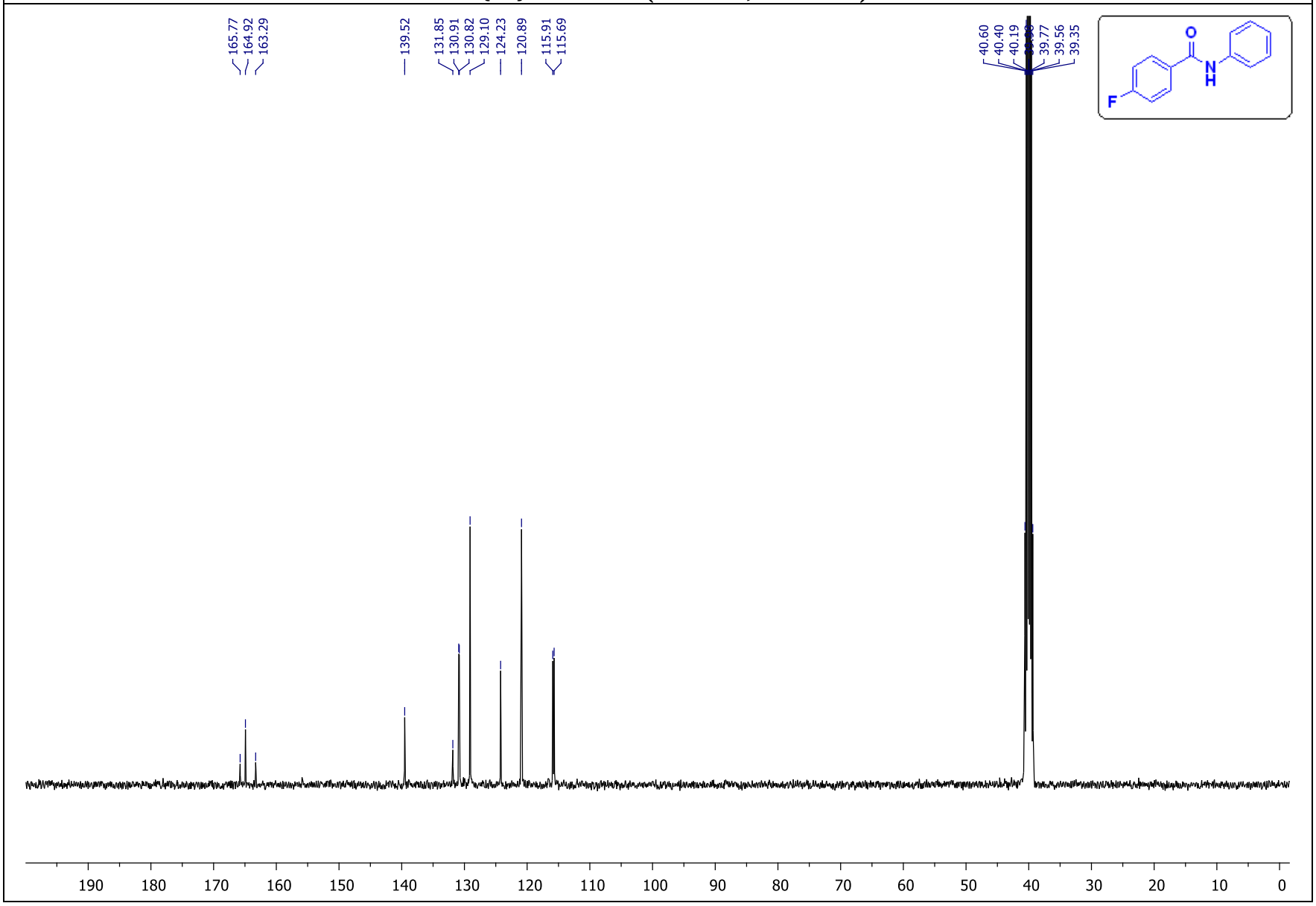


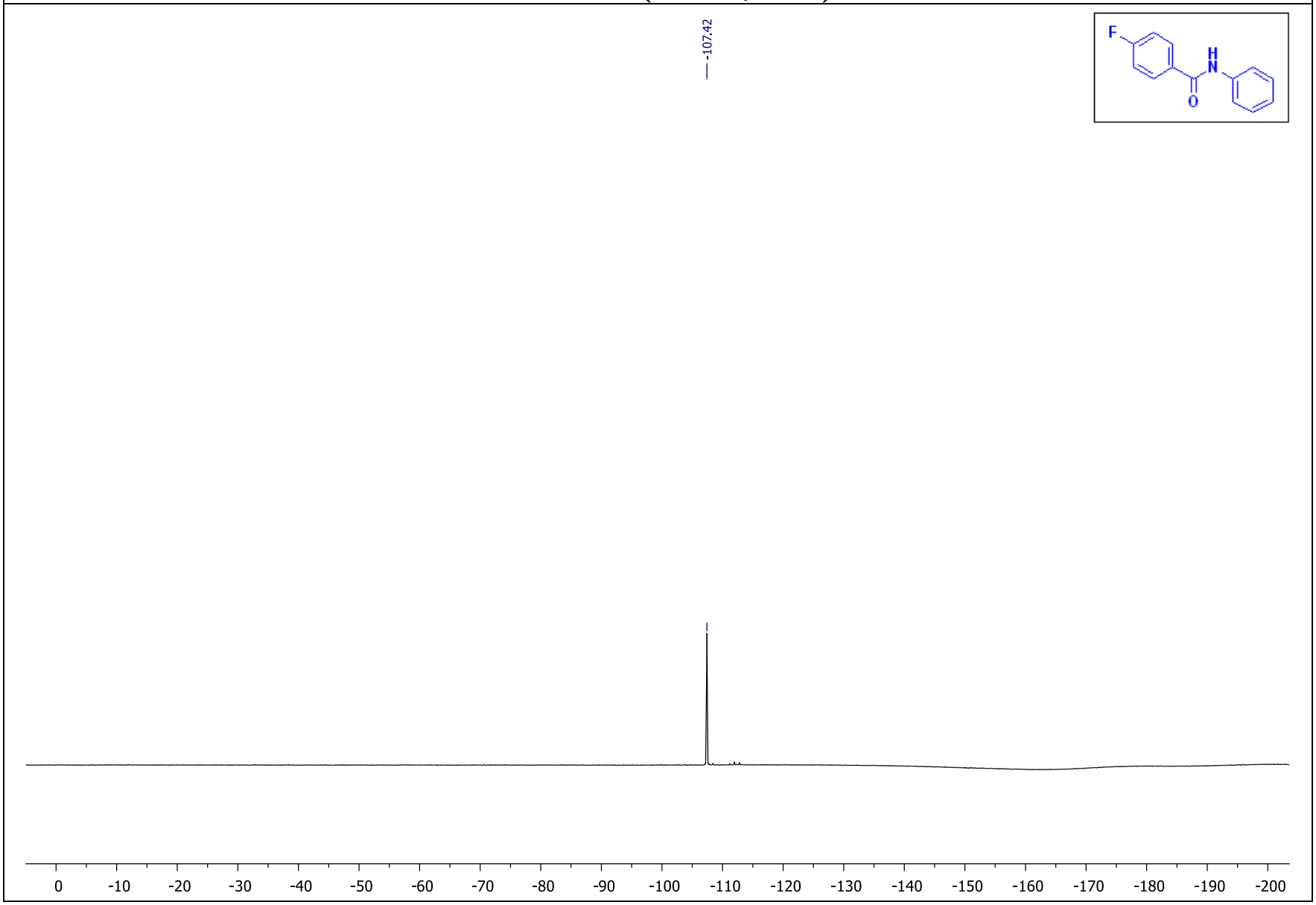
^{1}H NMR of 4b (400 MHz, DMSO-d$_6$)



$^{13}C\{^{1}H\}$NMR of 4b (101 MHz, DMSO-d_6)



^{19}F-NMR of 4b (376 MHz, $CDCl_3$)



HRMS of 4b

Qualitative Analysis Report

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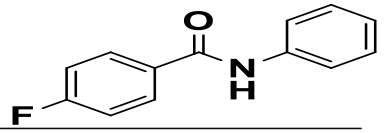
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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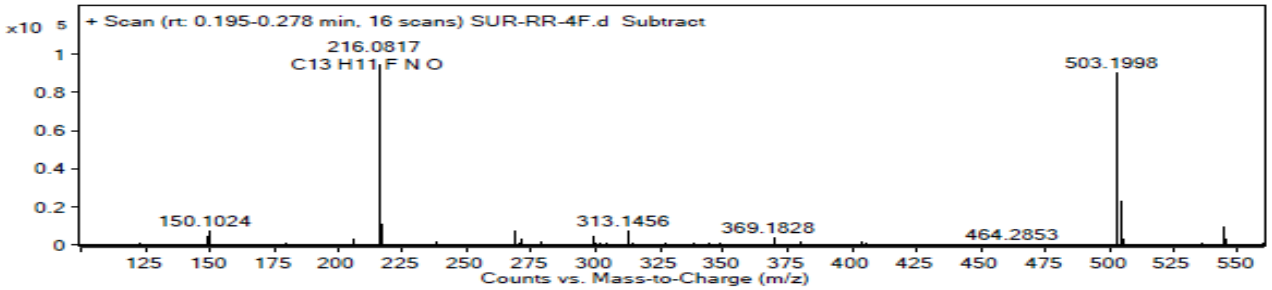
Chemical Formula [M+H]: $C_{13}H_{11}FNO$



Peak List

m/z	z	Abund	Formula	Ion
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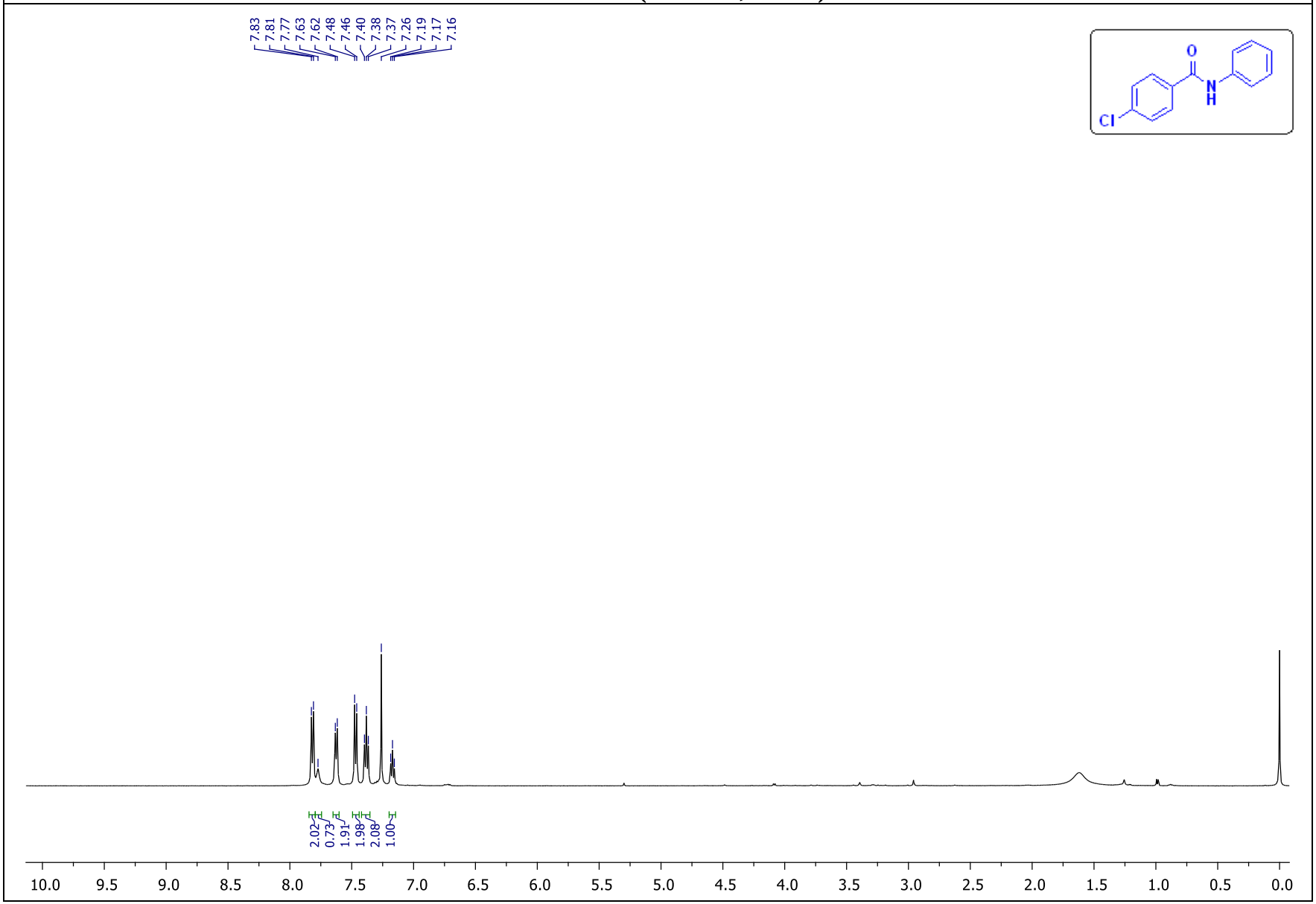
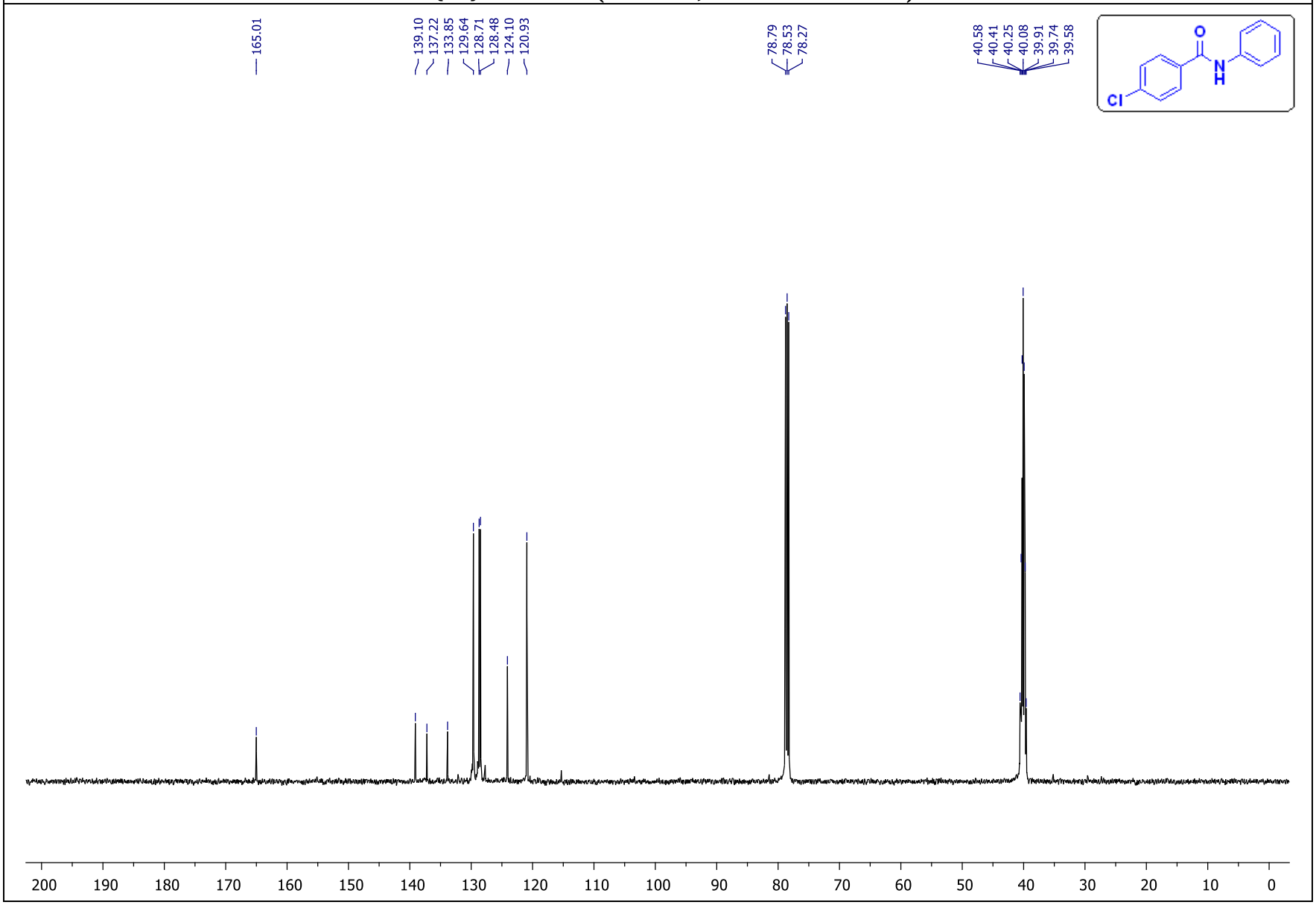
^{1}H NMR of 4c (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$NMR of 4c (101 MHz, $CDCl_3$ & DMSO-d_6)



HRMS of 4C

Qualitative Analysis Report

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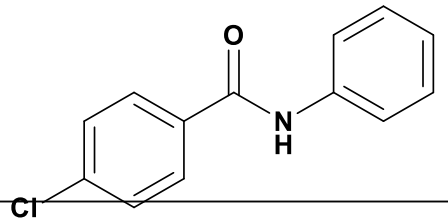
User Spectra



Fragmentor Voltage	Collision Energy	Ionization Mode
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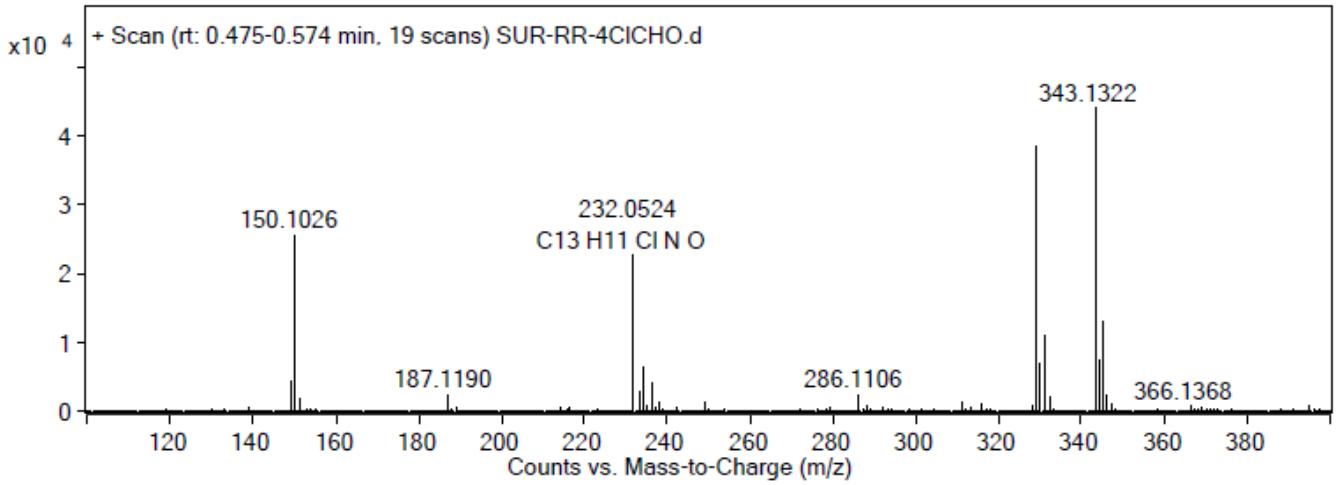
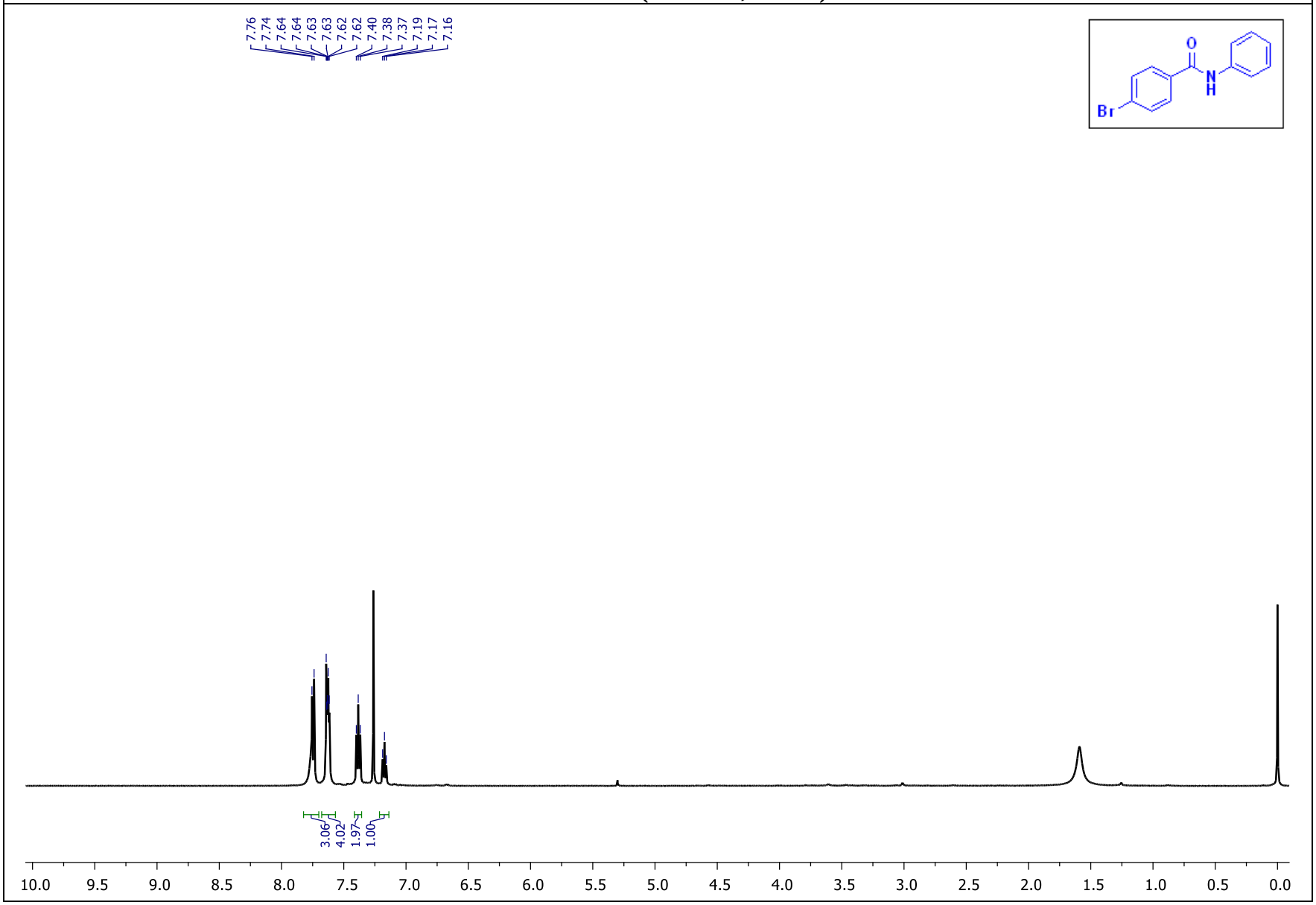
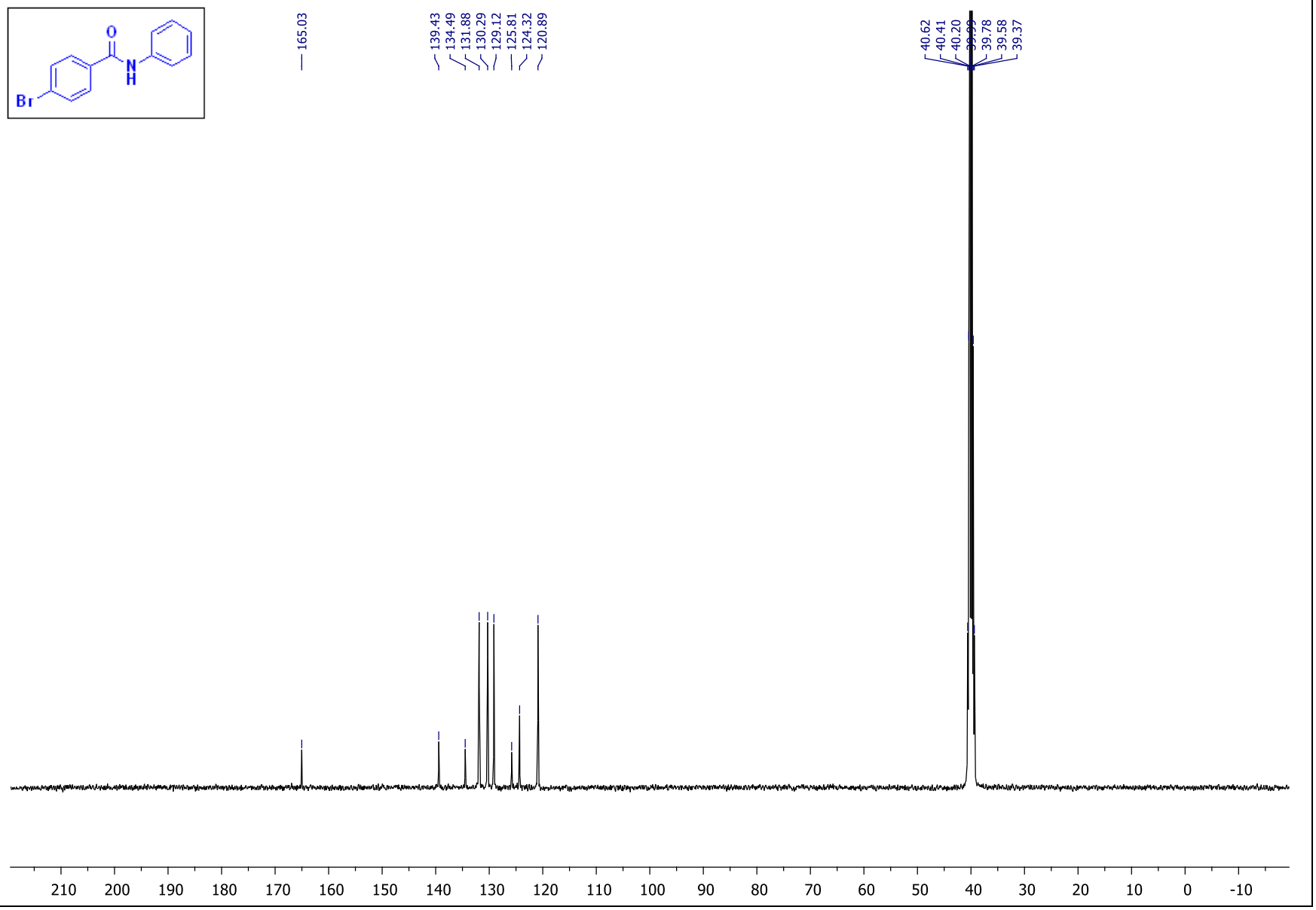


^{1}H NMR of 4d (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$NMR of 4d (101 MHz, DMSO-d_6))



HRMS of 4d

Qualitative Analysis Report

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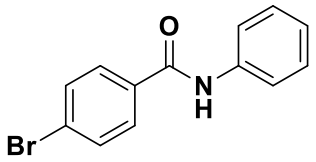
User Spectra



Fragmentor Voltage	Collision Energy	Ionization Mode
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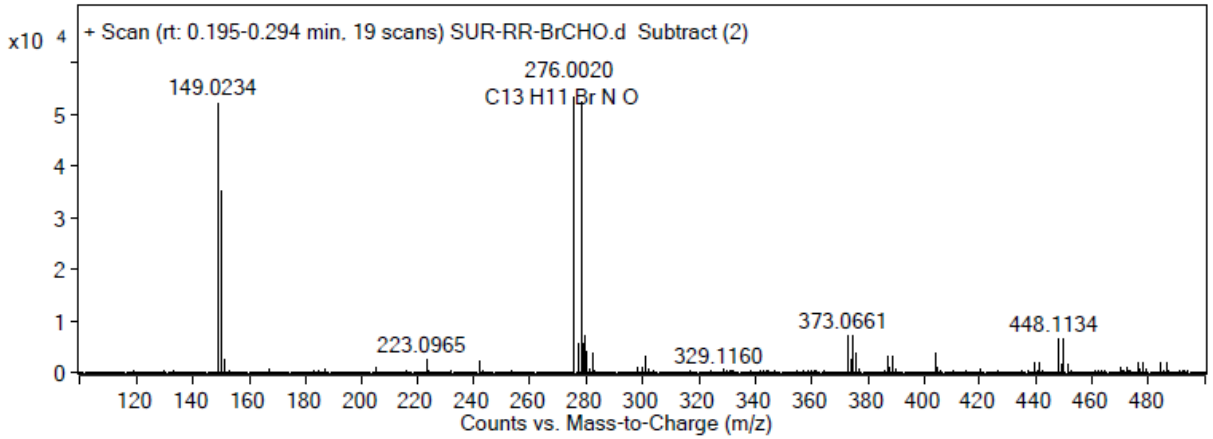
Chemical Formula [M+H]: $C_{13}H_{11}BrNO$



Peak List

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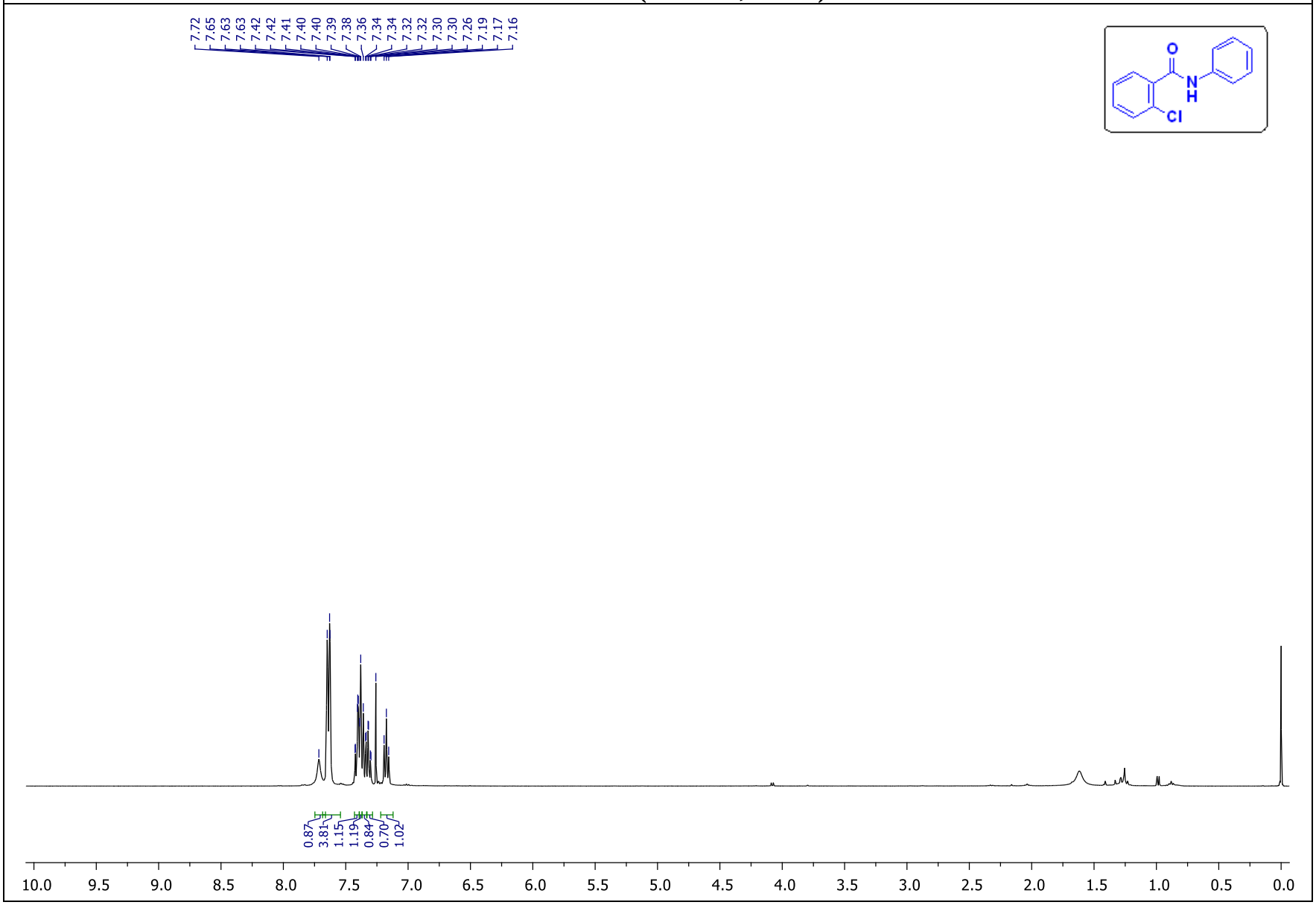
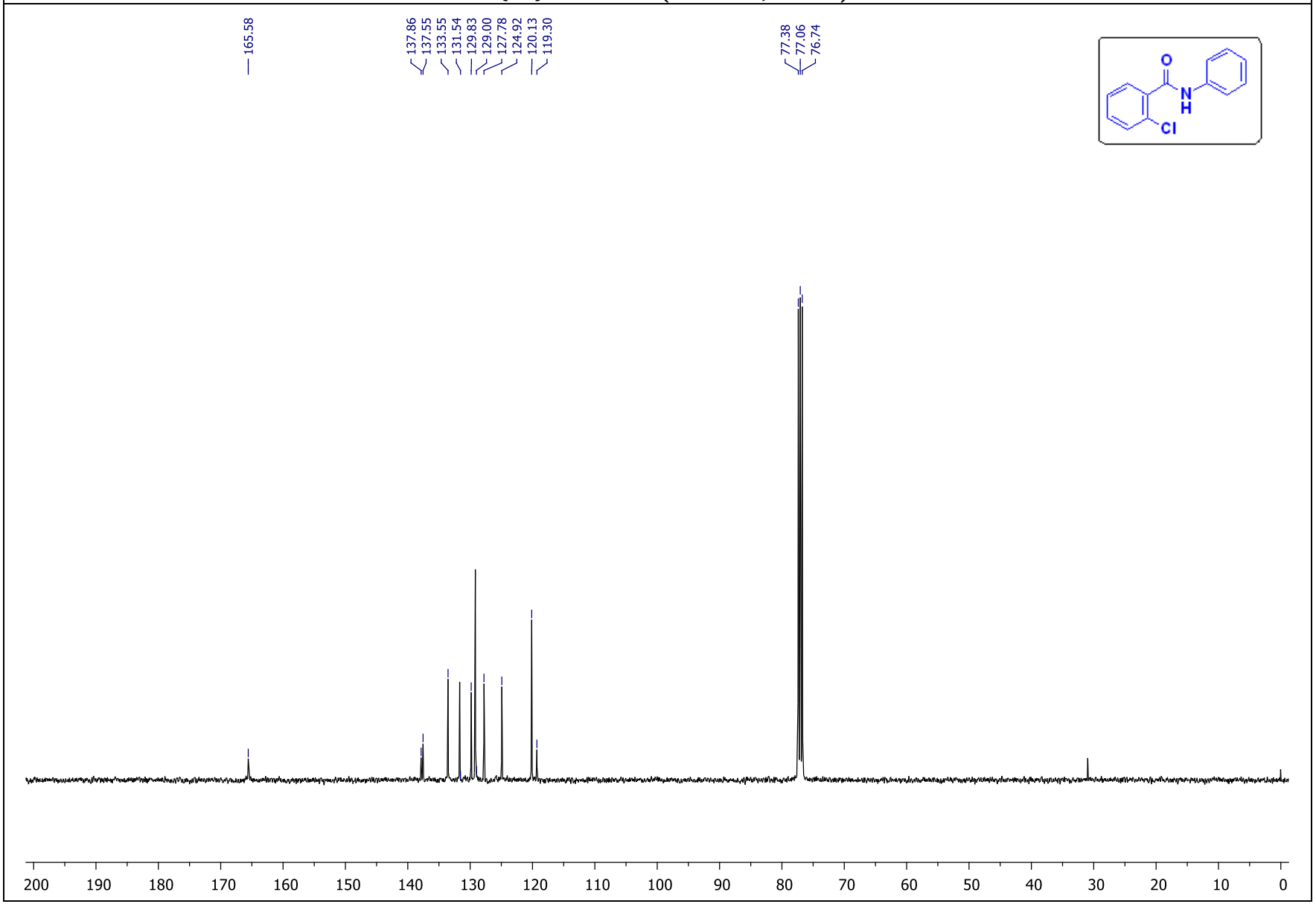
--- End Of Report ---

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



$^{13}C\{^{1}H\}$NMR of 4e (101 MHz, $CDCl_3$)



HRMS of 4e

D:\HRMS\...\14-12-2021\SUR-RR-2-CL

CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
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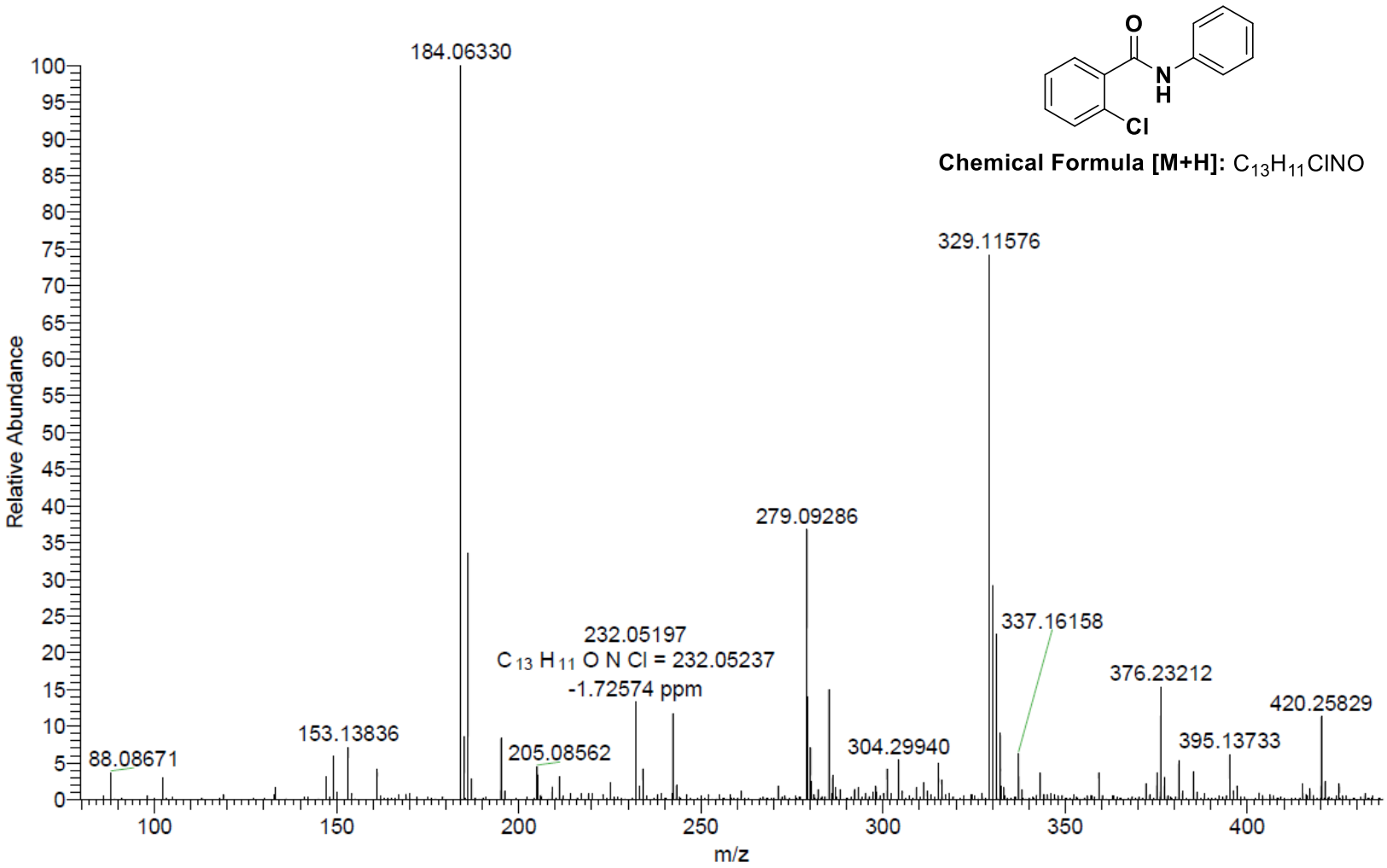
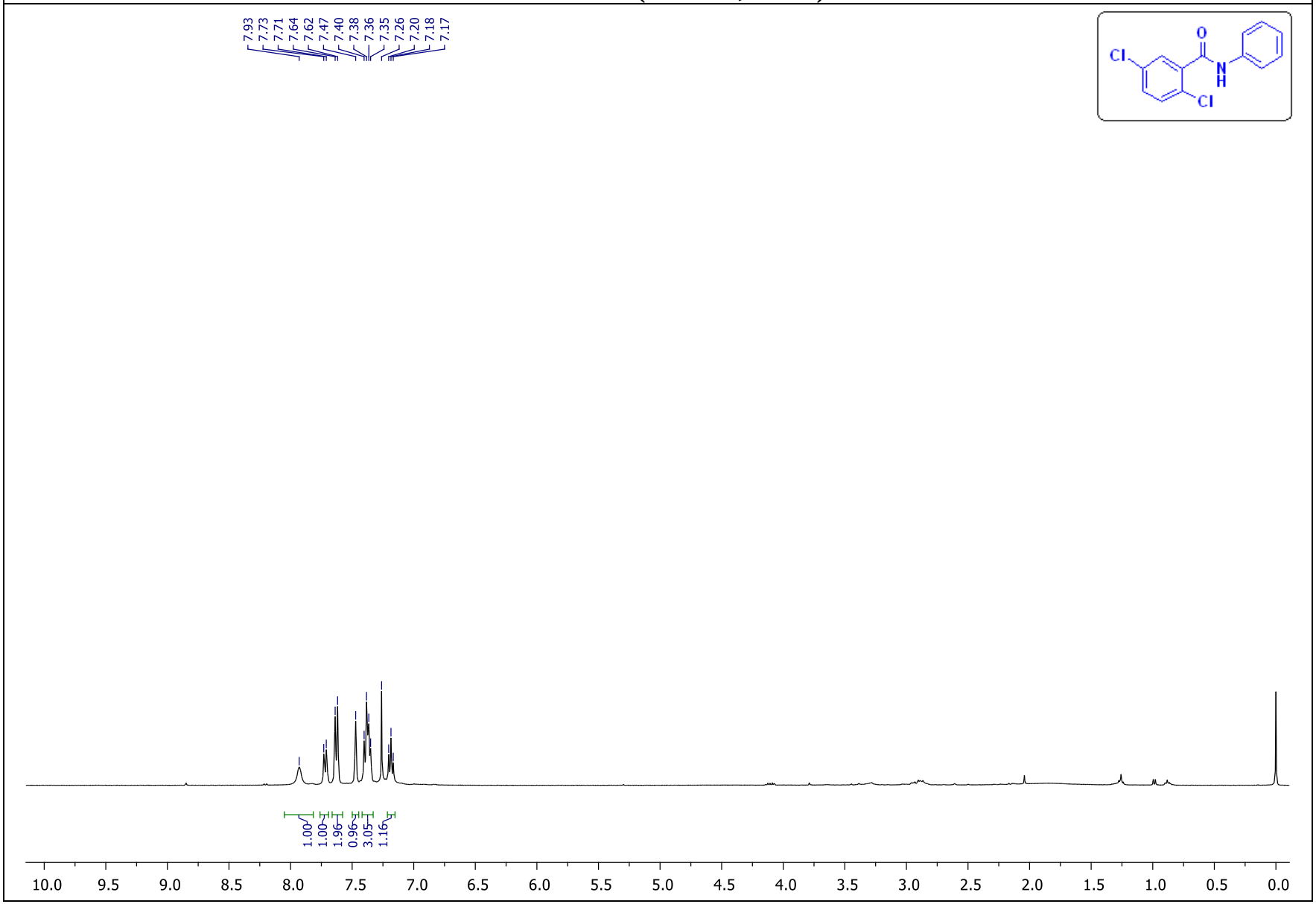
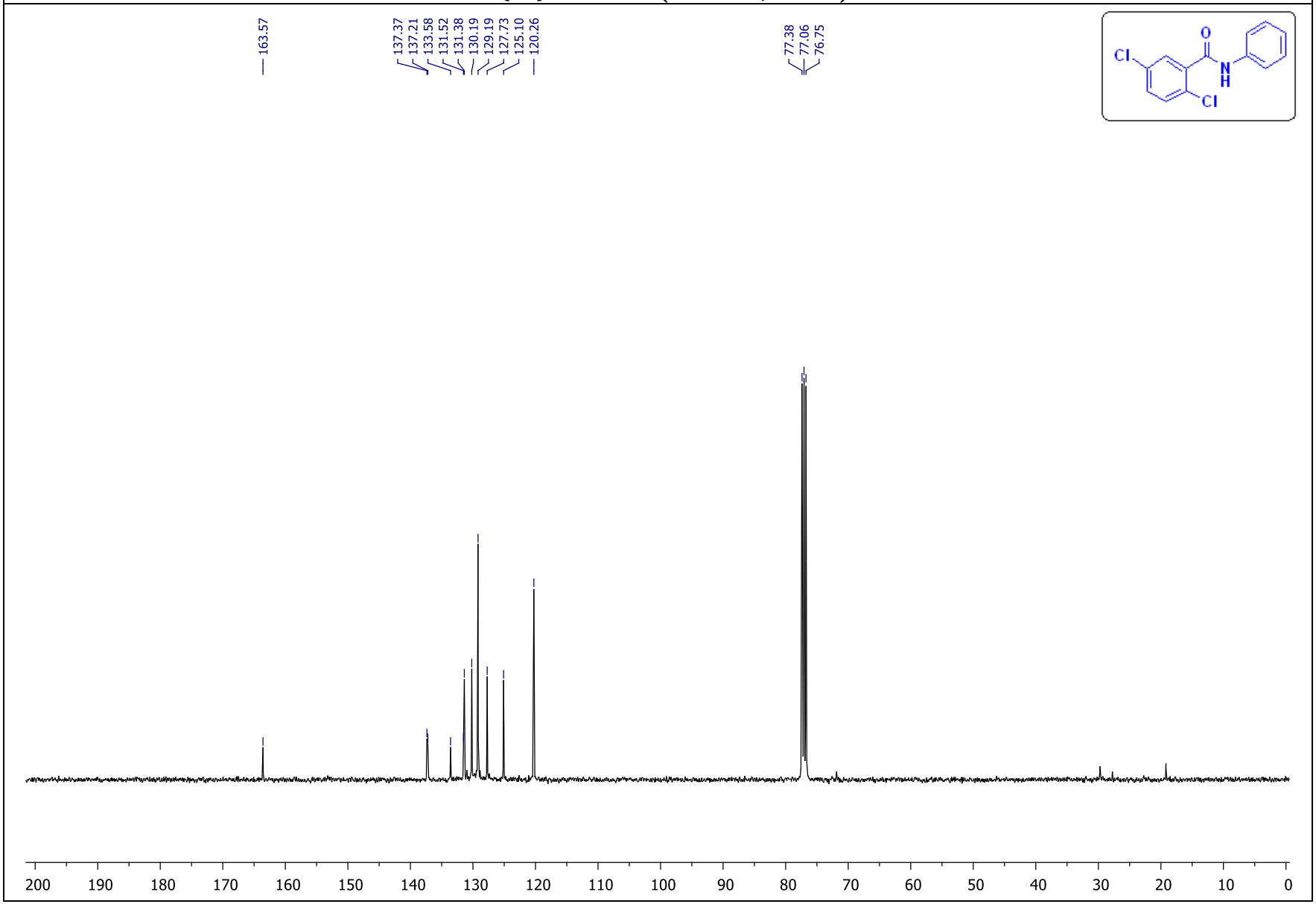
12/14/21 13:13:38
1180111042
Thermo Scientific Orbitrap Exploris 120
Analysed by G SAIKRISHNA
SUR-RR-2-CL #8-24 RT: 0.02-0.06 AV: 17 SB: 251 0.56-1.14 NL: 6.42E7
T: FTMS + p ESI Full ms [50.0000-3000.0000]



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



$^{13}C\{^{1}H\}$NMR of 4f (101 MHz, $CDCl_3$)



HRMS of 4f

SUR-RR-2-4-CLAM

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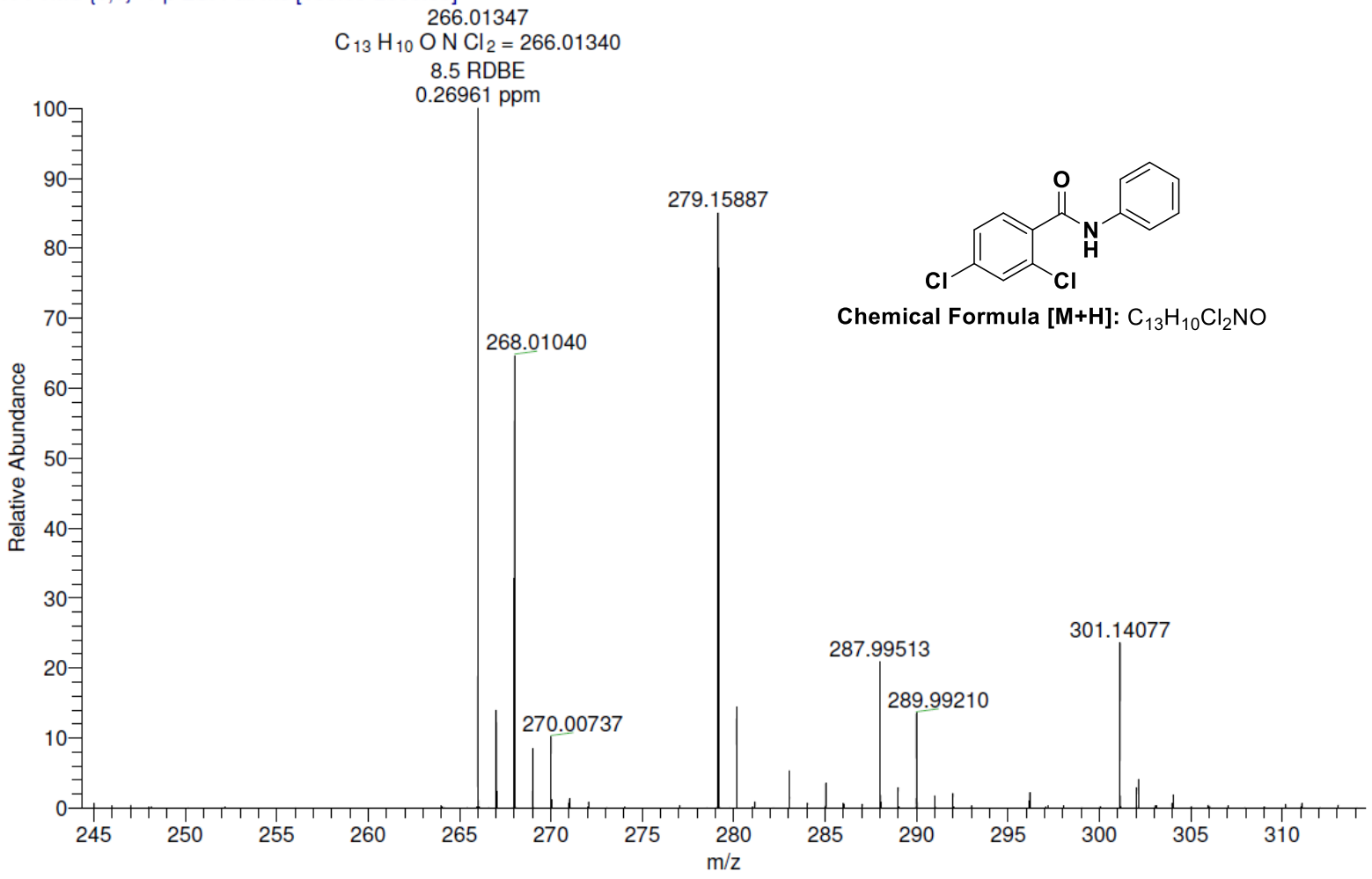
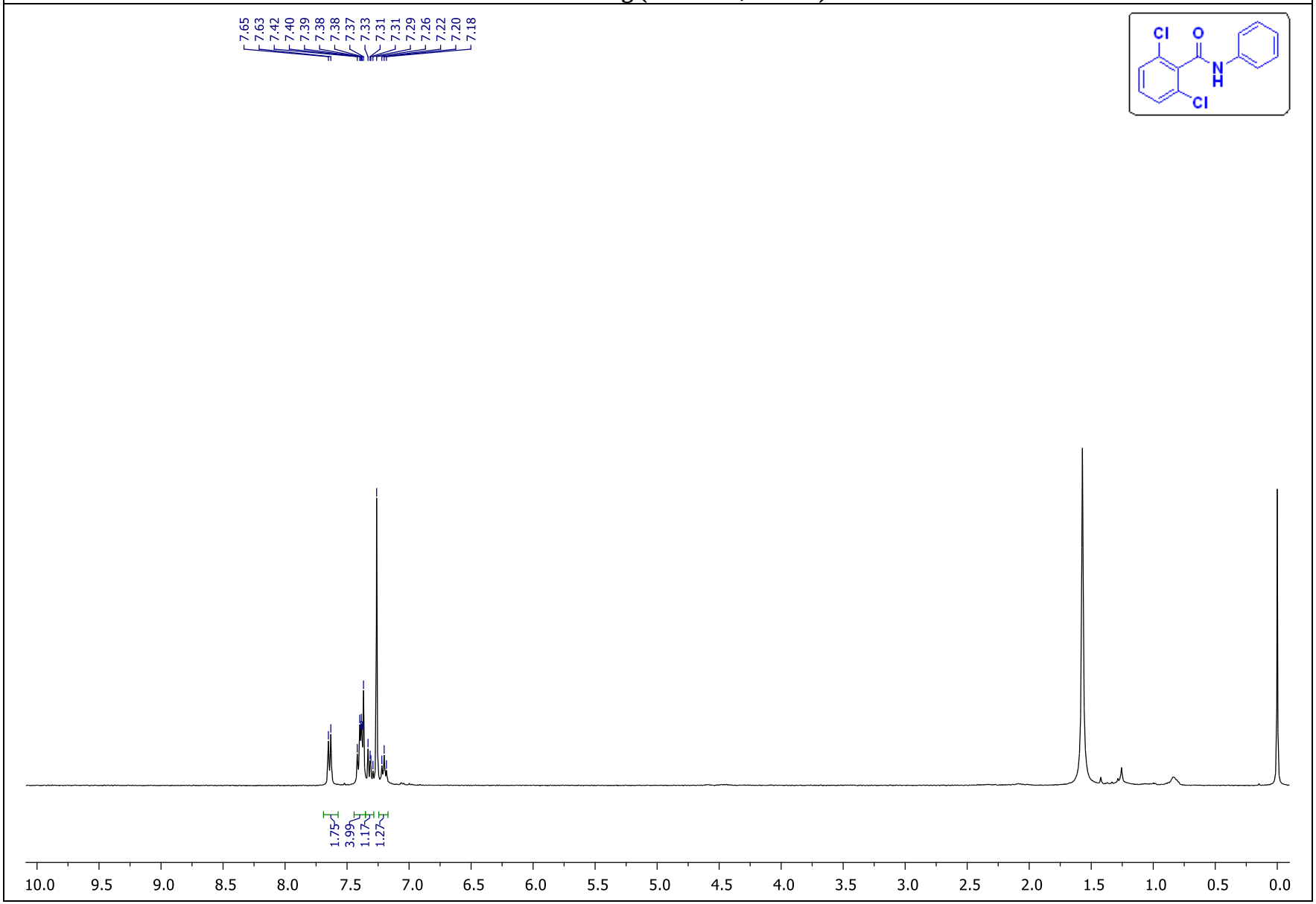
3/16/2021 5:19:16 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR-2-4-CLAM #8-25 RT: 0.06-0.18 AV: 18 SB: 40 0.38-0.67 NL: 2.41E7
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

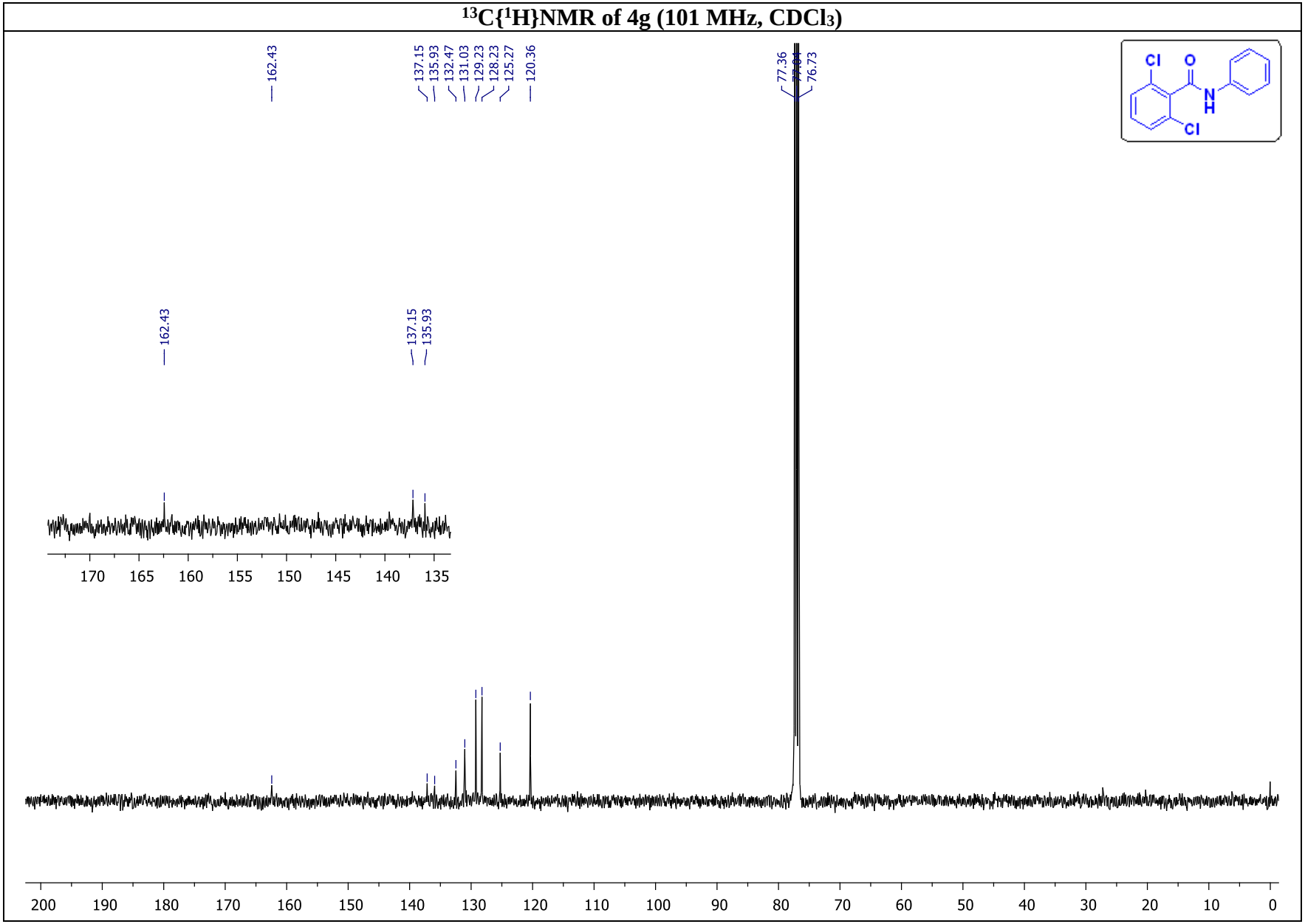


Chemical Formula [M+H]: $C_{13}H_{10}Cl_2NO$

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



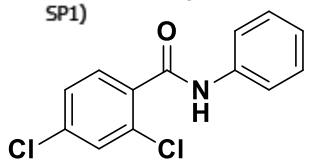
$^{13}C\{^{1}H\}$NMR of 4g (101 MHz, $CDCl_3$)



HRMS of 4g

Qualitative Analysis Report

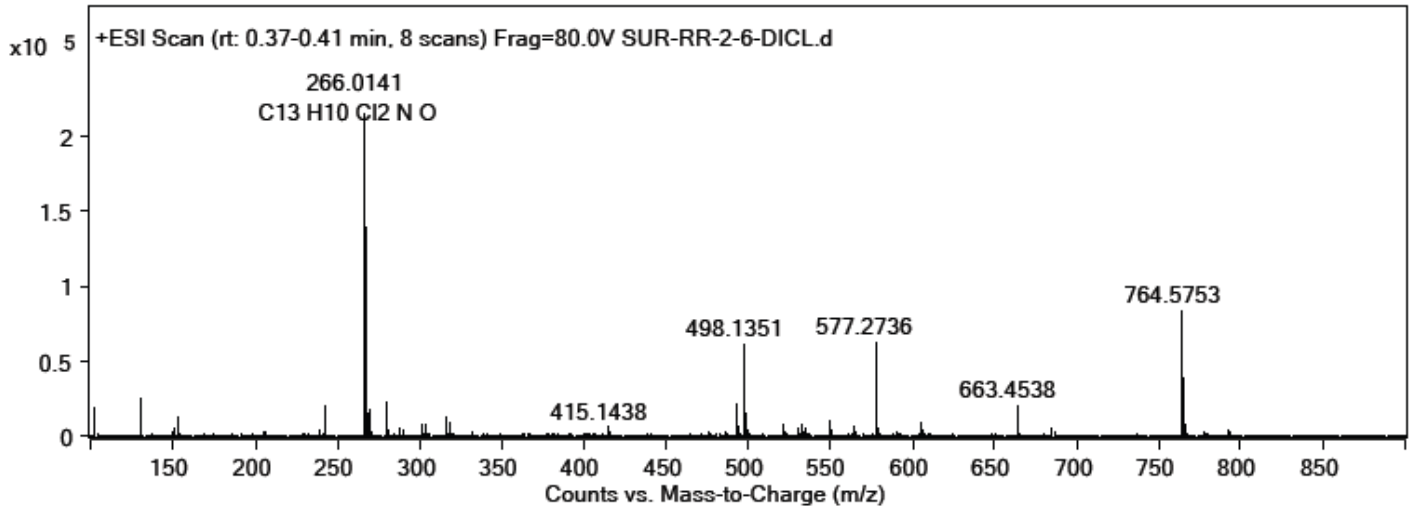
Data File	SUR-RR-2-6-DICL.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	07-07-2021 12:29:43
IRM Calibration Status	Success	**DA Method**	11.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



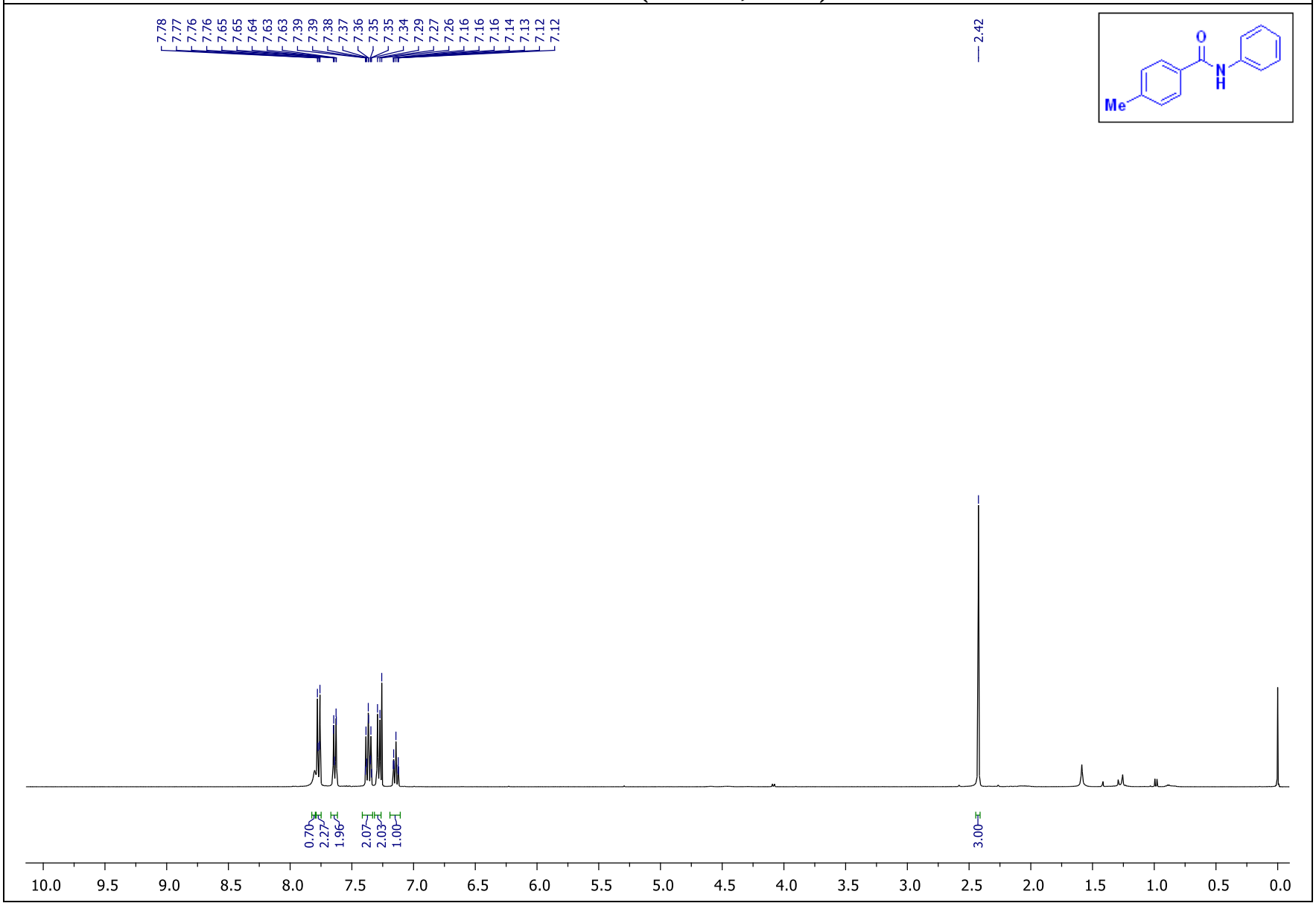
Chemical Formula [M+H]: $C_{13}H_{10}Cl_2NO$

User Spectra

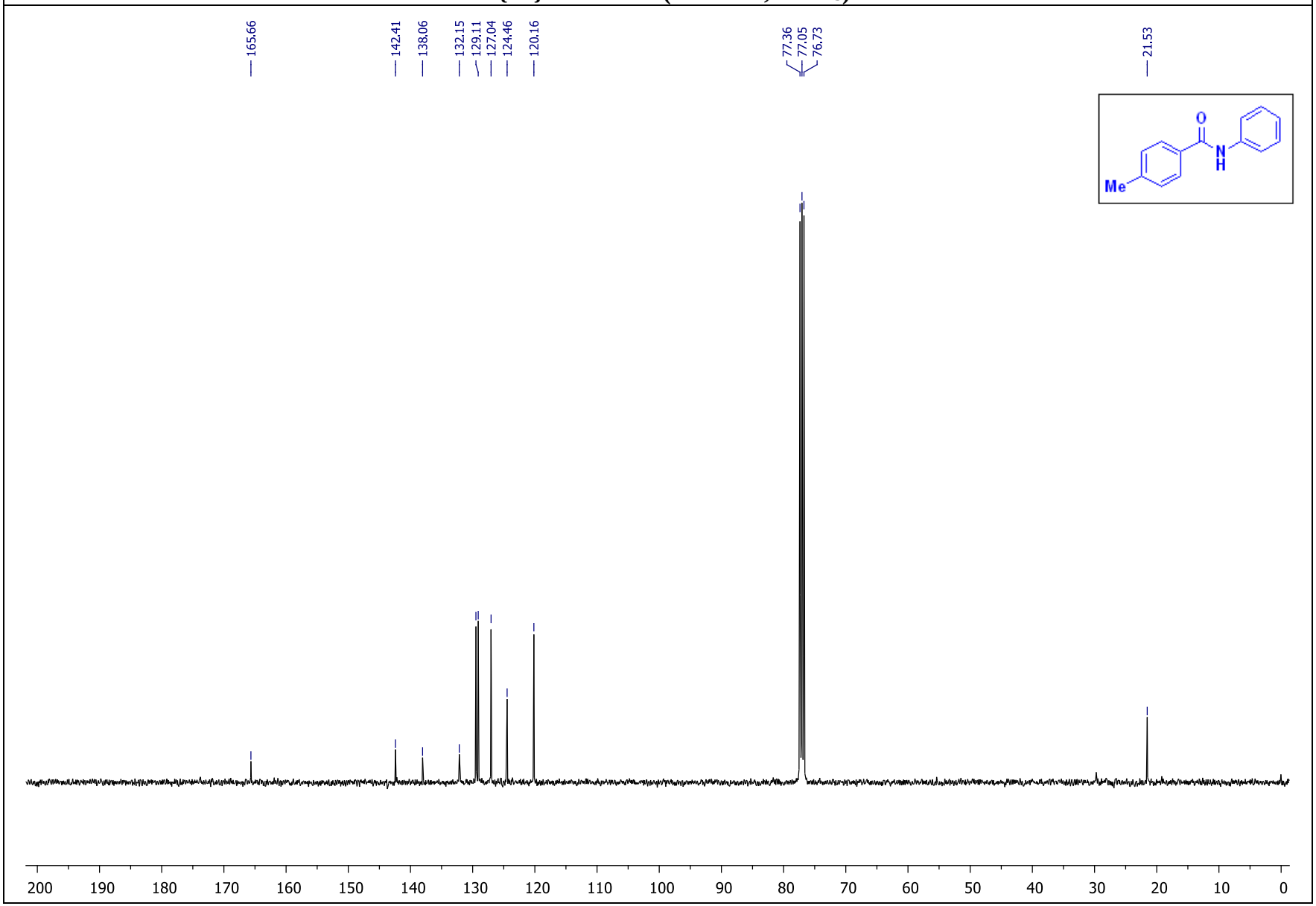
Fragmentor Voltage	Collision Energy	Ionization Mode
80	0	ESI



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



$^{13}C\{^{1}H\}$NMR of 4h (101 MHz, $CDCl_3$)



HRMS of 4h

D:\Sai krishna Important\...\SUR-RR-4ME

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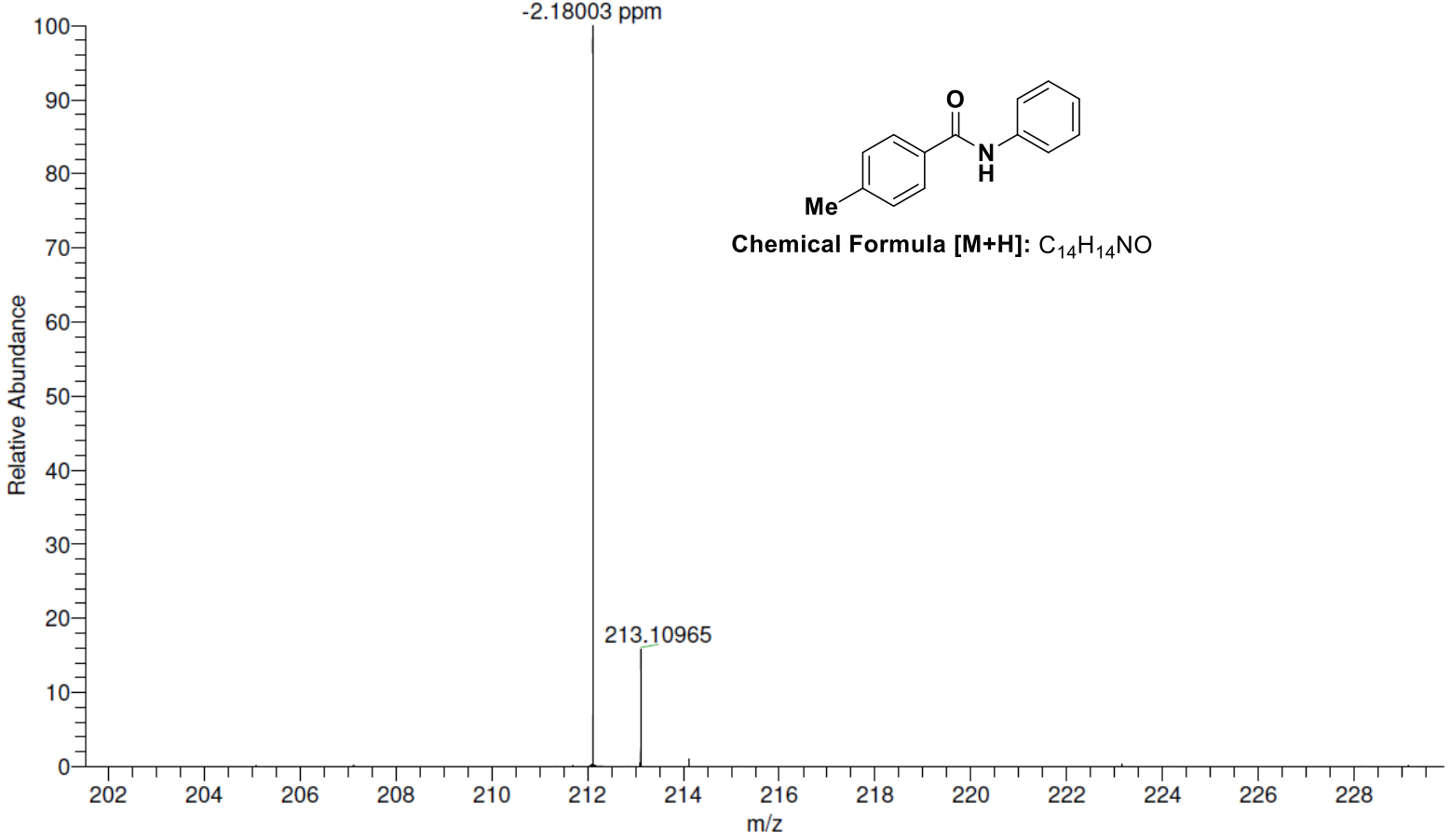
3/23/2021 7:59:04 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

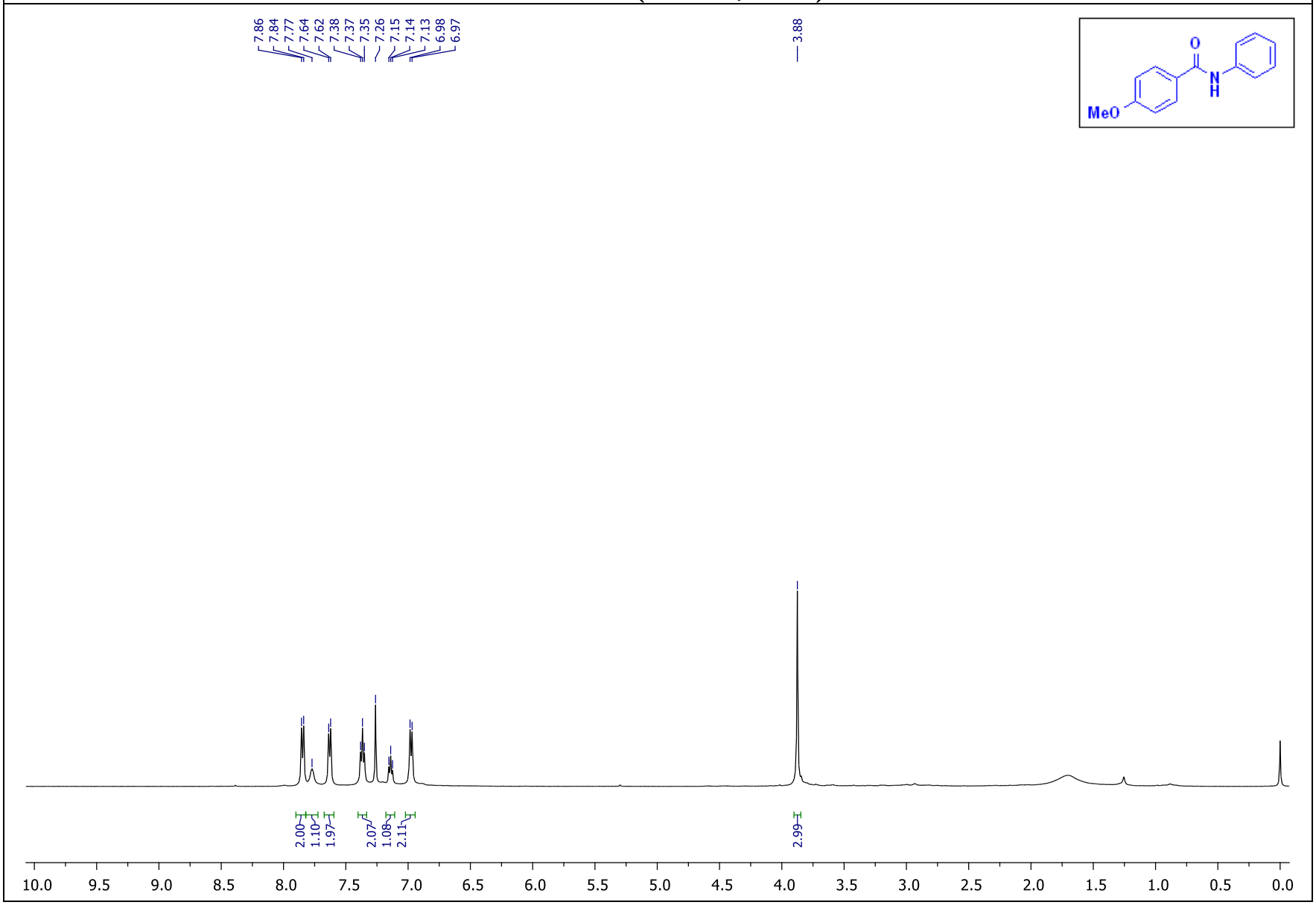
SUR-RR-4ME #8-25 RT: 0.06-0.18 AV: 18 NL: 2.21E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

212.10653
$C_{14}H_{14}ON$ = 212.10699
8.5 RDBE
-2.18003 ppm

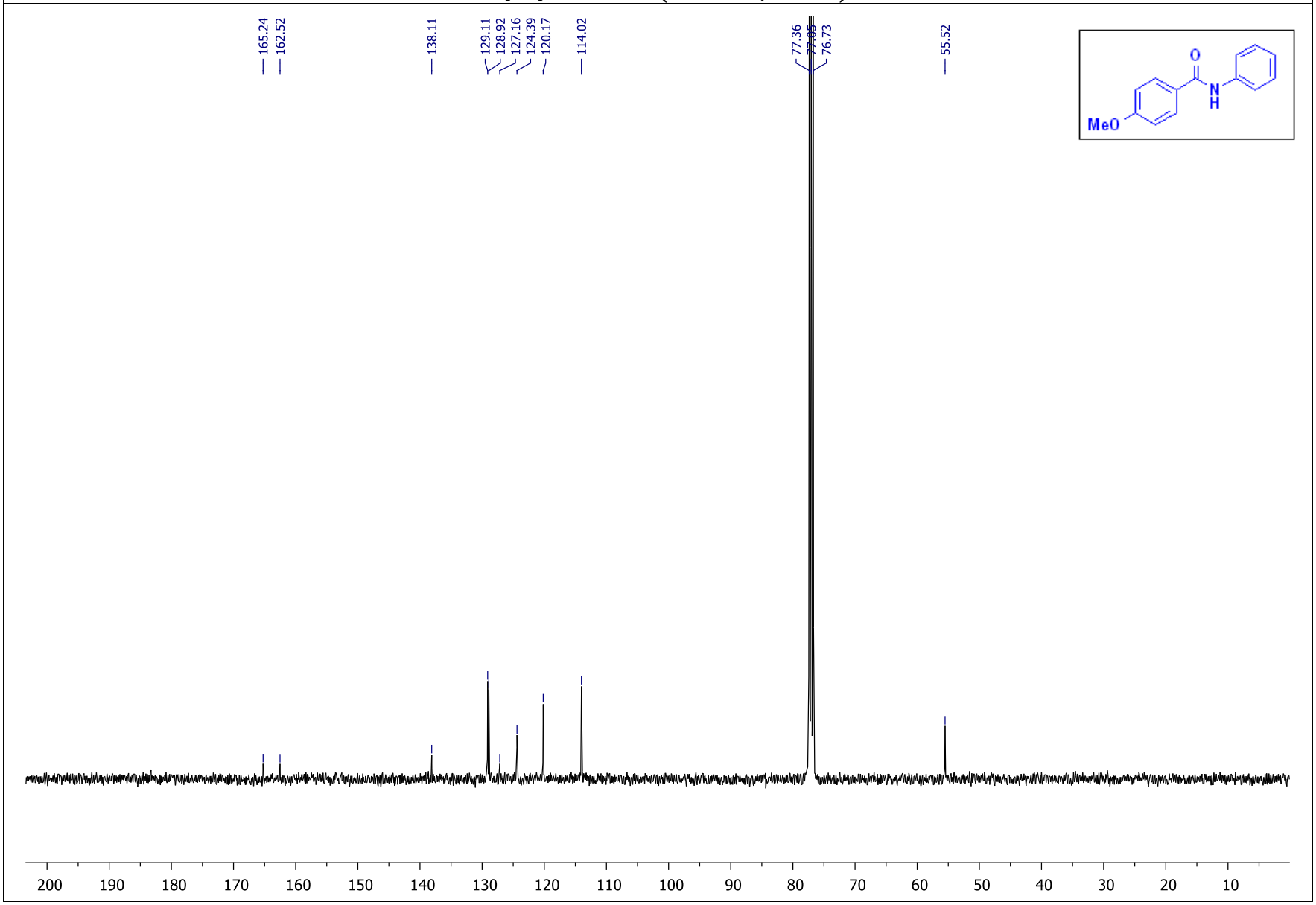


Chemical Formula [M+H]: $C_{14}H_{14}NO$

^{1}H NMR of 4i (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$NMR of 4i (101 MHz, $CDCl_3$)



HRMS of 4i

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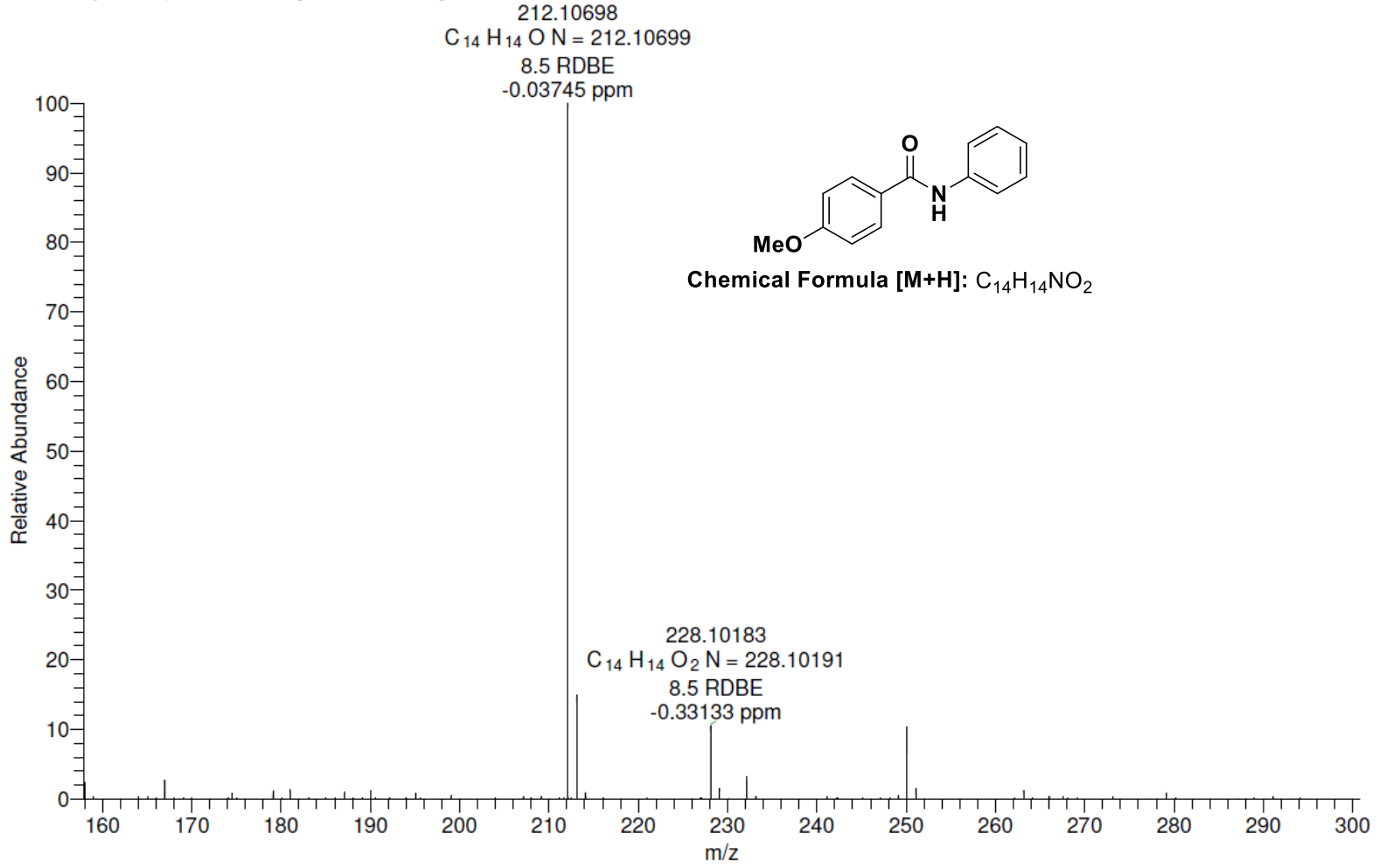
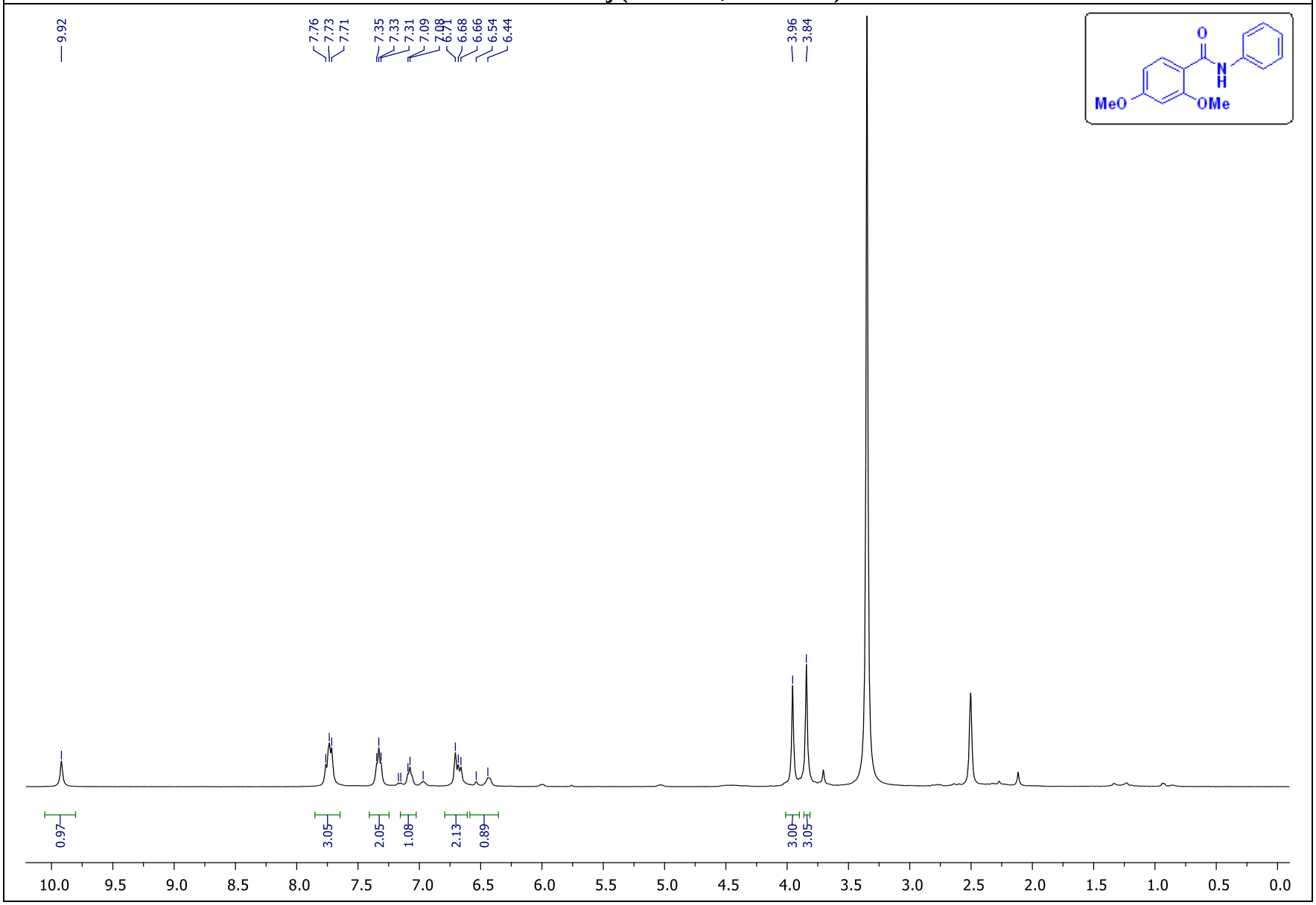
4/22/2021 1:19:26 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR-4OME #19-40 RT: 0.14-0.30 AV: 22 NL: 5.73E7
T: FTMS {1,1} + p ESI Full ms [75.00-1500.00]

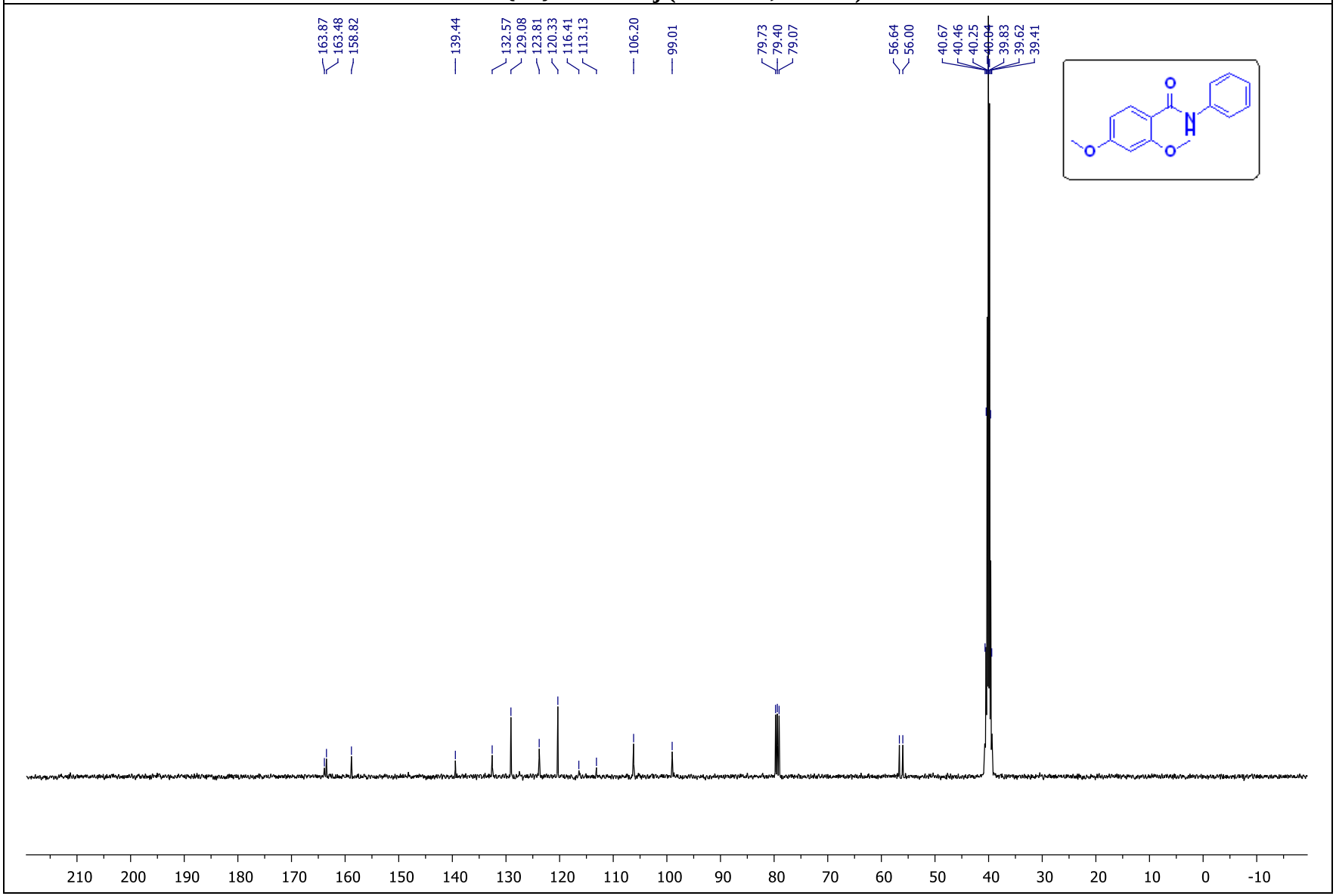


Chemical Formula [M+H]: $C_{14}H_{14}NO_2$

^{1}H NMR of 4j (400 MHz, DMSO-d_6)



$^{13}C\{^{1}H\}$NMR of 4j (101 MHz, DMSO)



HRMS of 4j

SUR-R-R-2-4-DIOME

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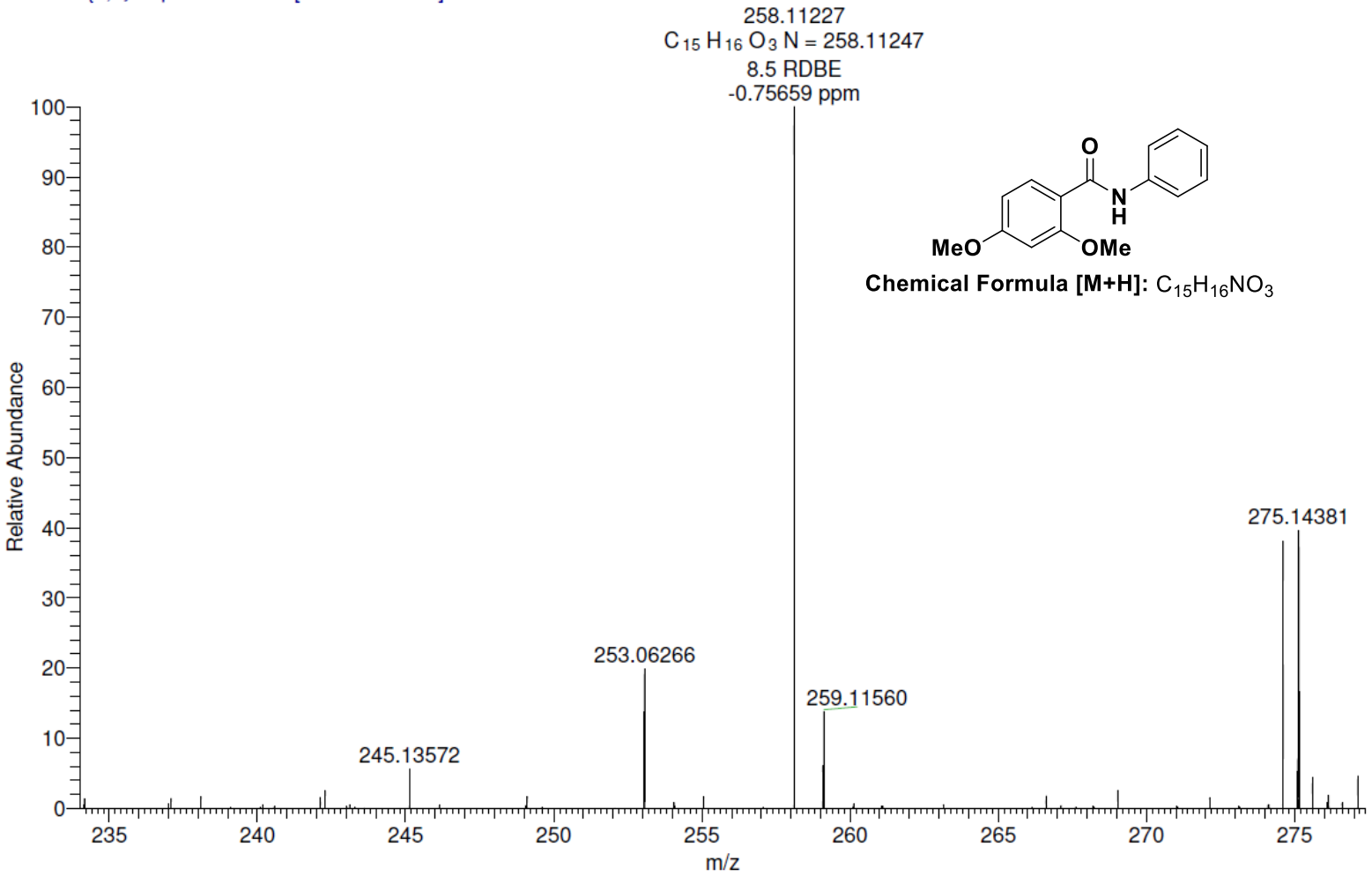
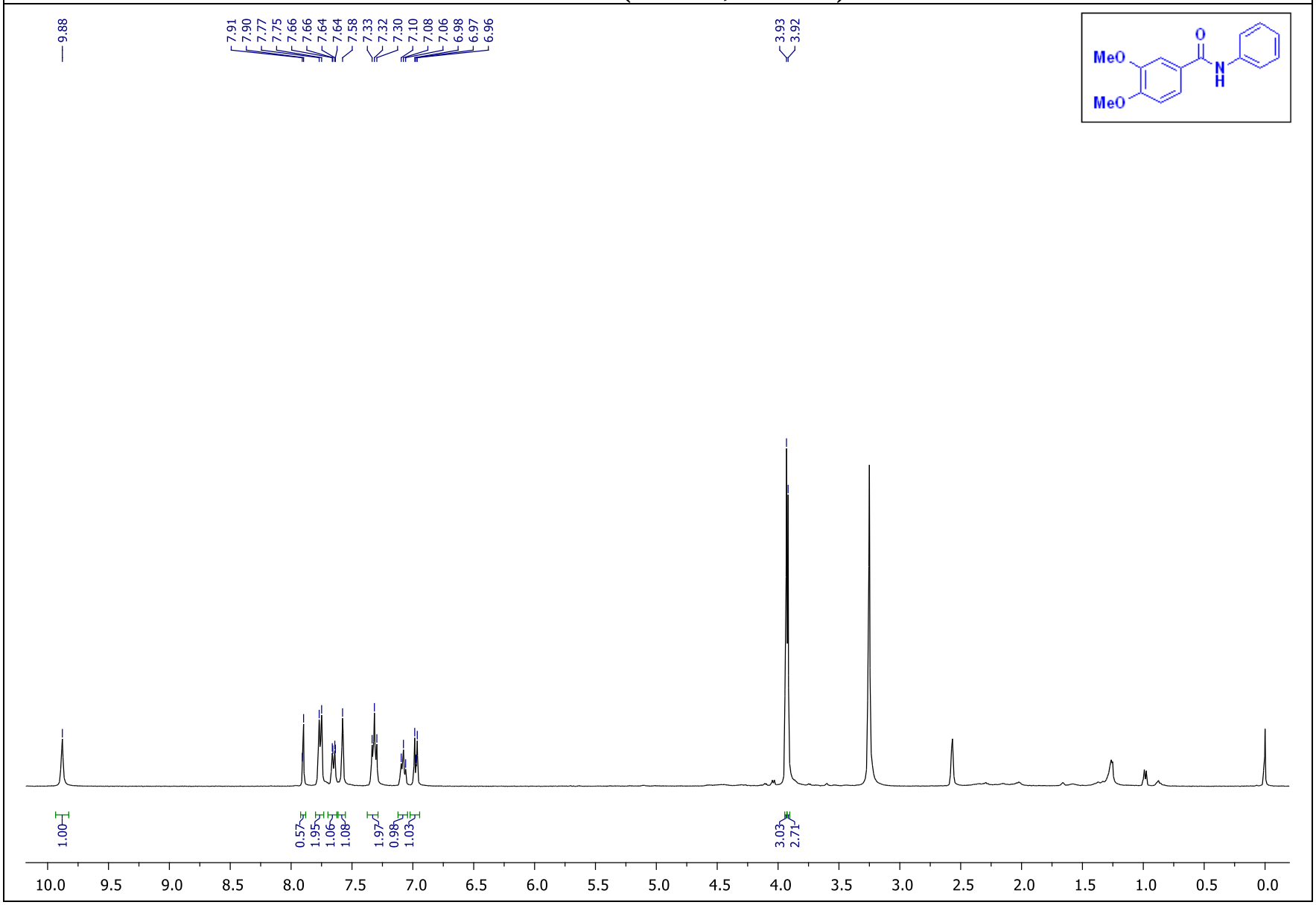
4/22/2021 1:28:37 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

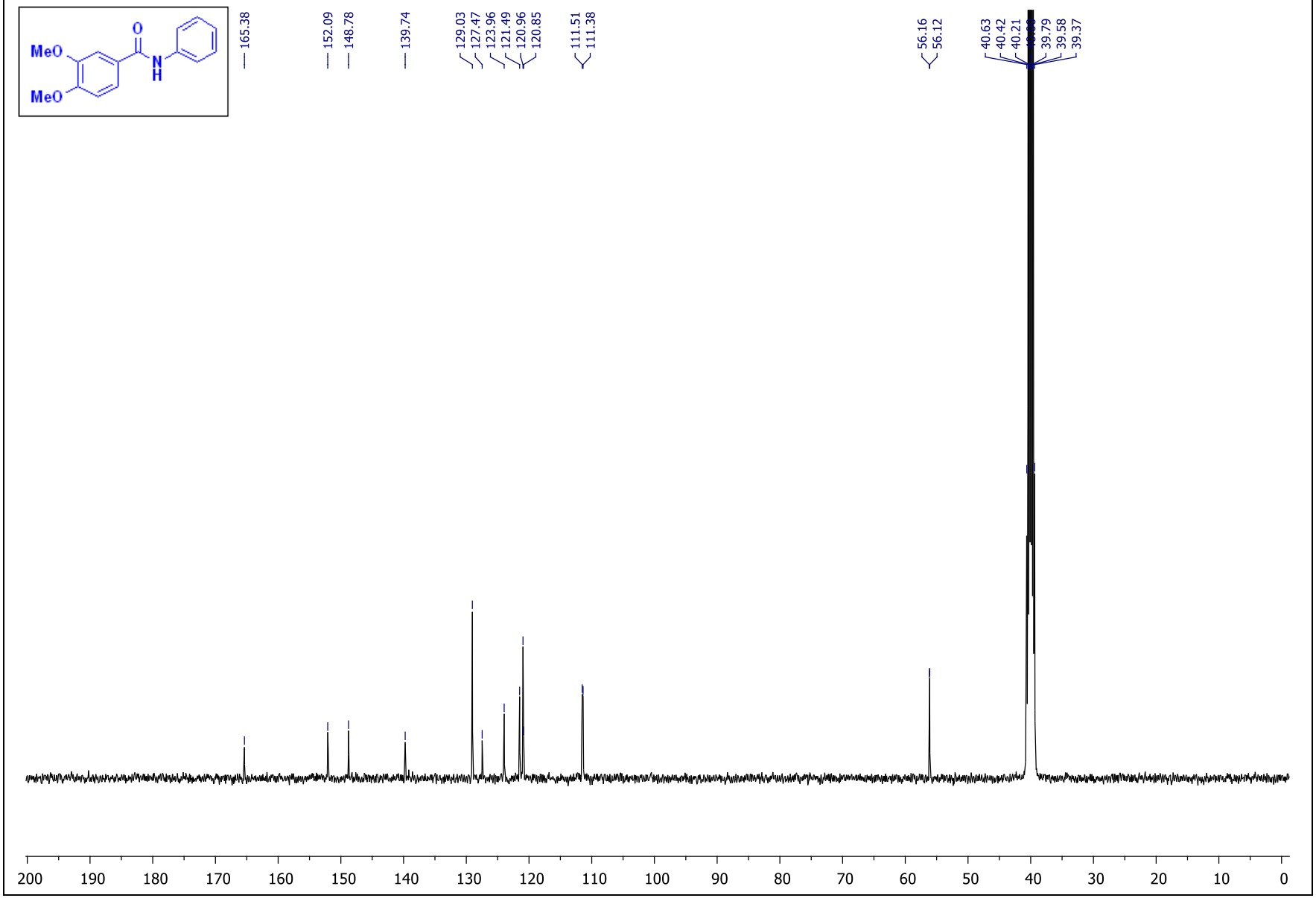
SUR-R-R-2-4-DIOME #23-44 RT: 0.17-0.32 AV: 22 NL: 4.73E6
T: FTMS {1,1} + p ESI Full ms [75.00-1500.00]



^{1}H NMR of 4k (400 MHz, DMSO-d$_6$)



$^{13}C\{^{1}H\}$NMR of 4k (101 MHz, DMSO-d_6)



HRMS of 4k

SUR-RR--3-4-DIOME

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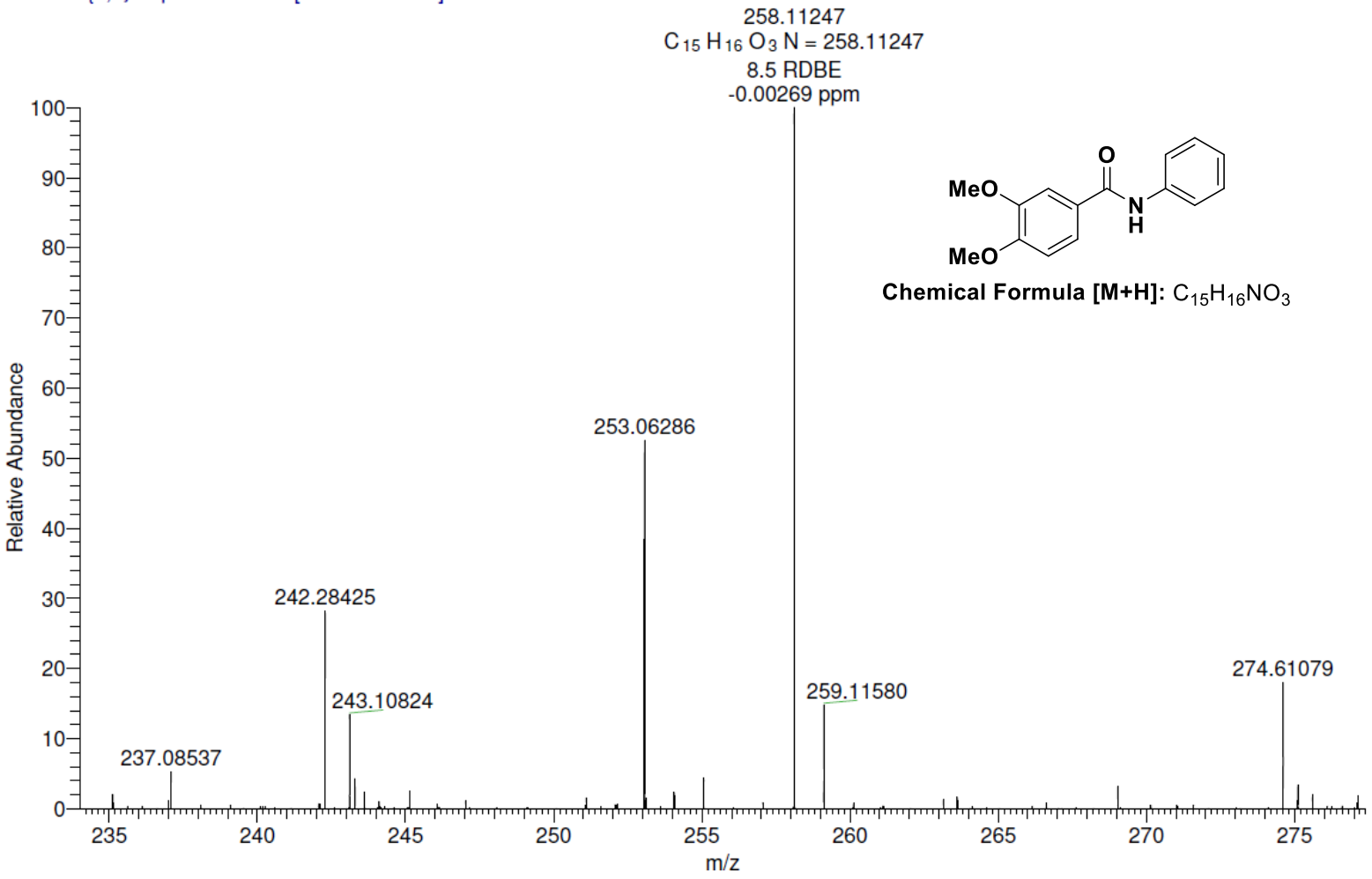
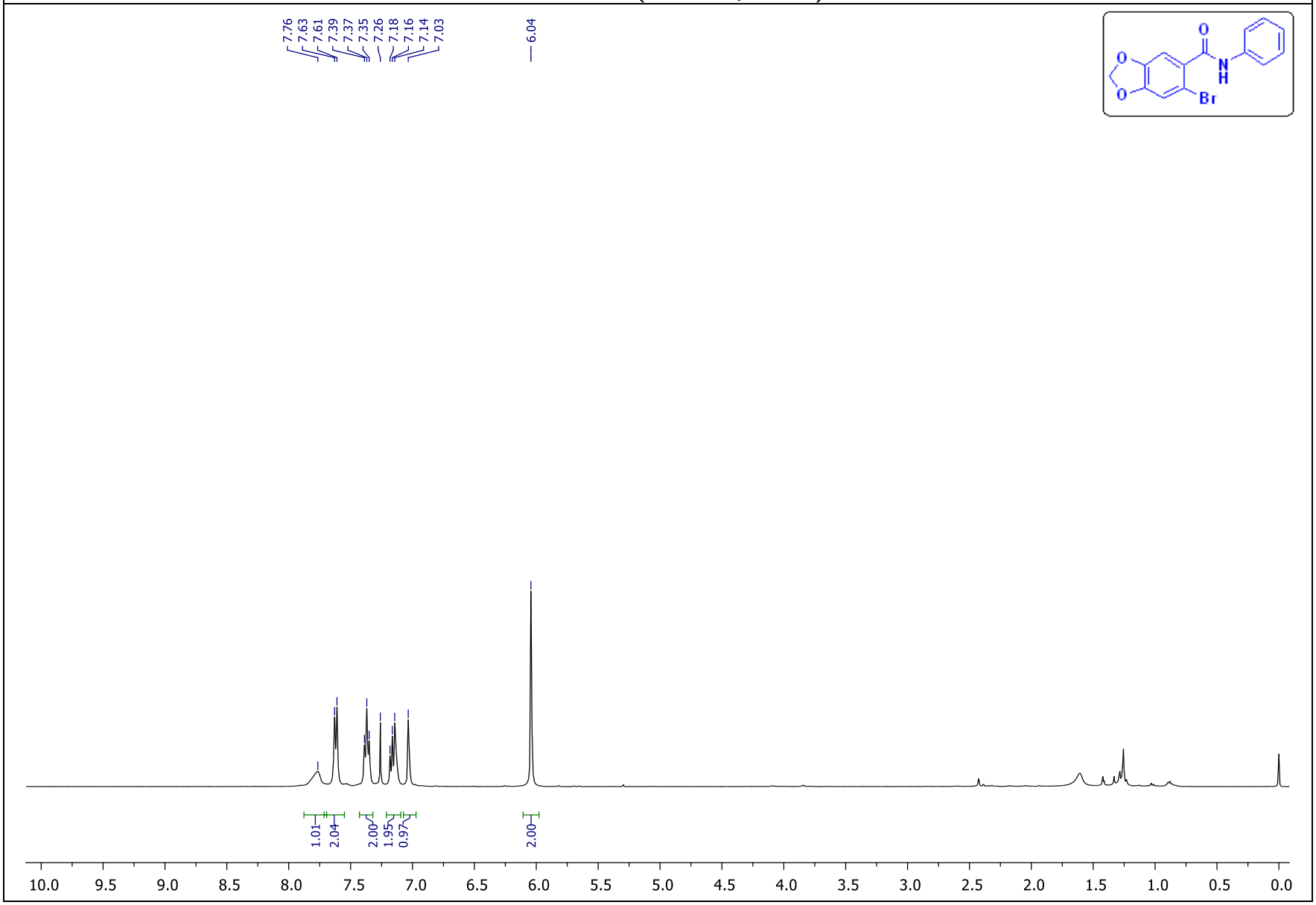
4/22/2021 1:30:10 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR--3-4-DIOME #23-45 RT: 0.17-0.33 AV: 23 NL: 4.12E6
T: FTMS {1,1} + p ESI Full ms [75.00-1500.00]

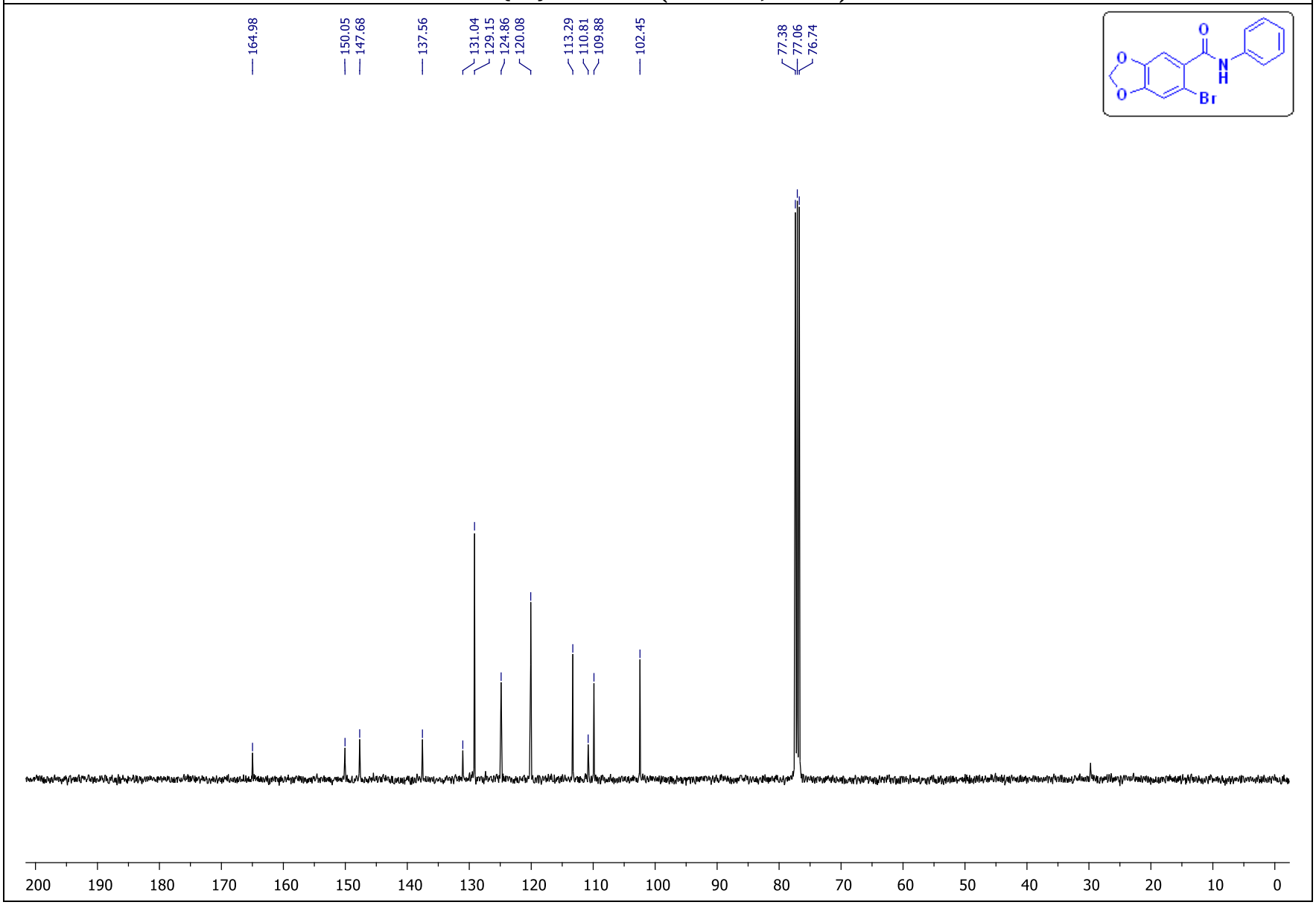


Chemical Formula [M+H]: $C_{15}H_{16}NO_3$

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



$^{13}C\{^{1}H\}$NMR of 4l (101 MHz, $CDCl_3$)

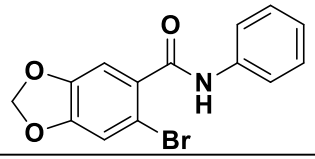


HRMS of 4l

Qualitative Analysis Report

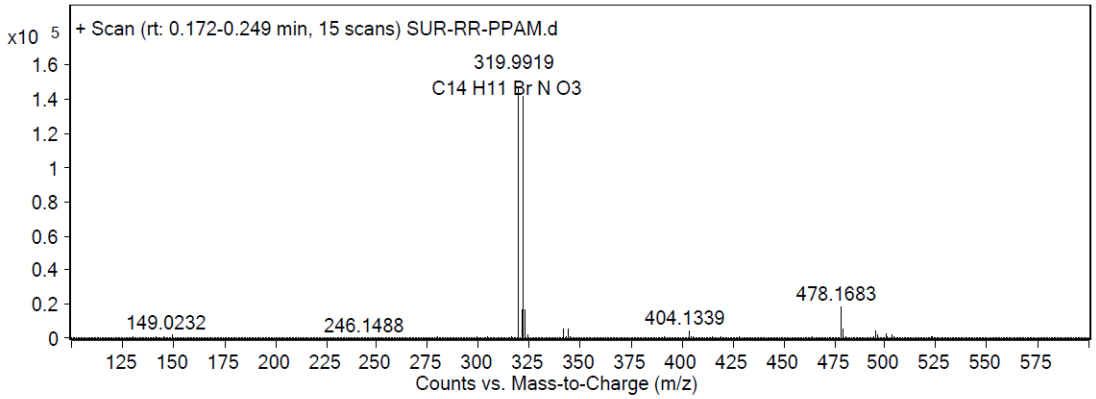
Data File	SUR-RR-PPAM.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	26-08-2021 12:42:58
IRM Calibration Status	Success	**DA Method**	11.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra



Fragmentor Voltage	Collision Energy	Ionization Mode
60	0	ESI

Chemical Formula [M+H]: $C_{14}H_{11}BrNO_3$

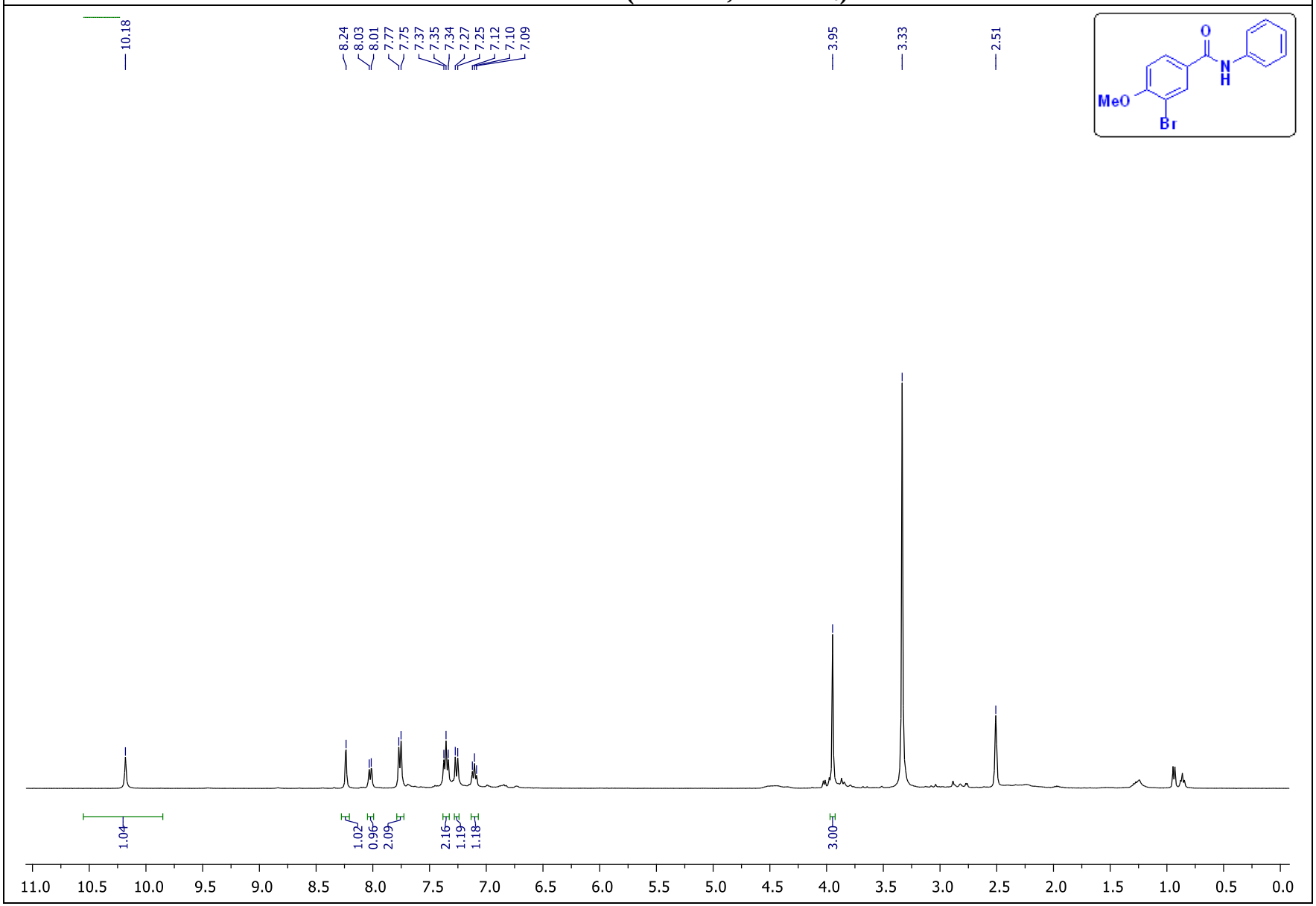


Peak List

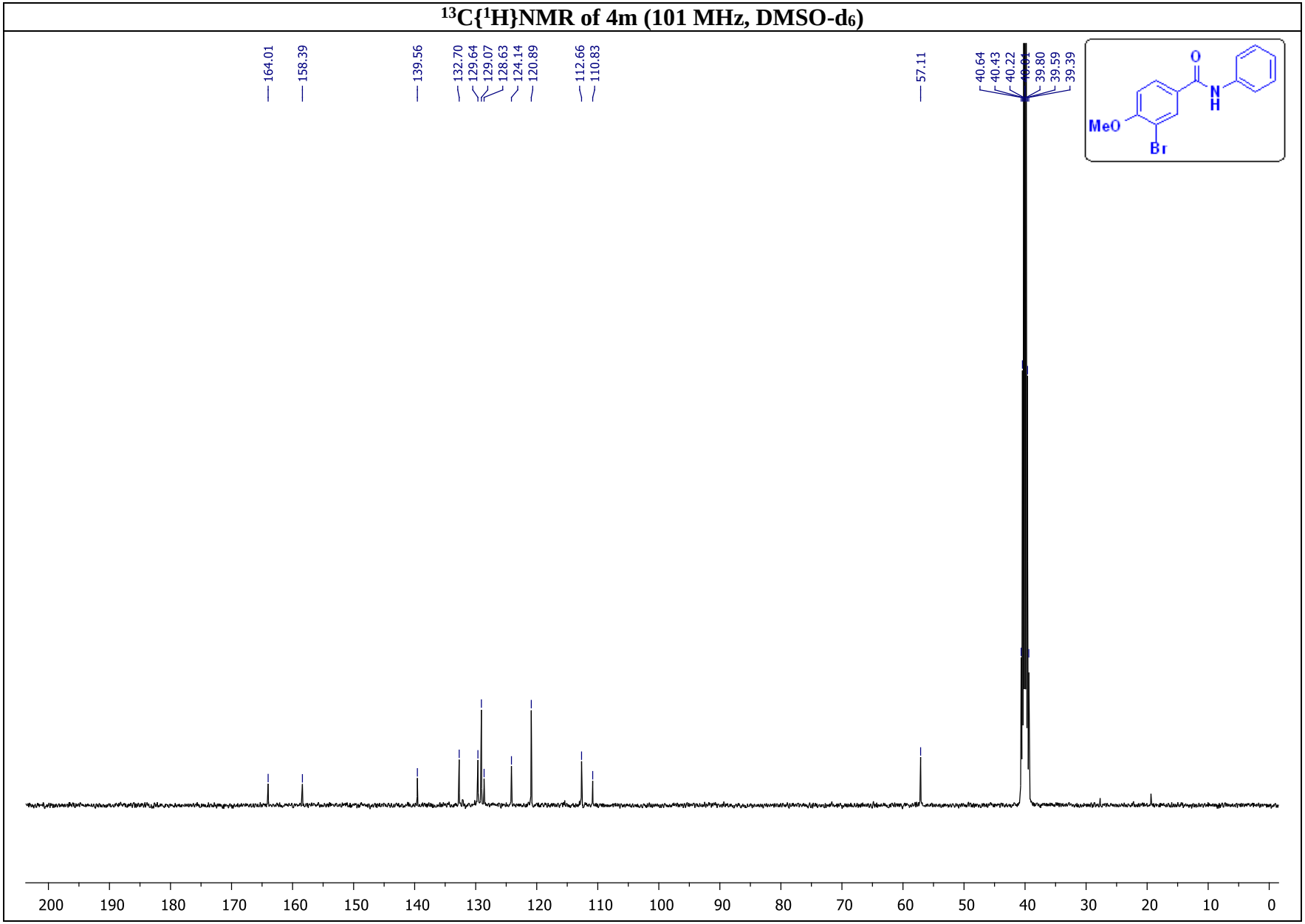
m/z	z	Abund	Formula	Ion
319.9919	1	146442.94	C14 H11 Br N O3	M+

--- End Of Report ---

^{1}H NMR of 4m (400 MHz, DMSO-d$_6$)



$^{13}C\{^{1}H\}$NMR of 4m (101 MHz, DMSO-d_6)



HRMS of 4m

SUR-RR-3-BR4OME

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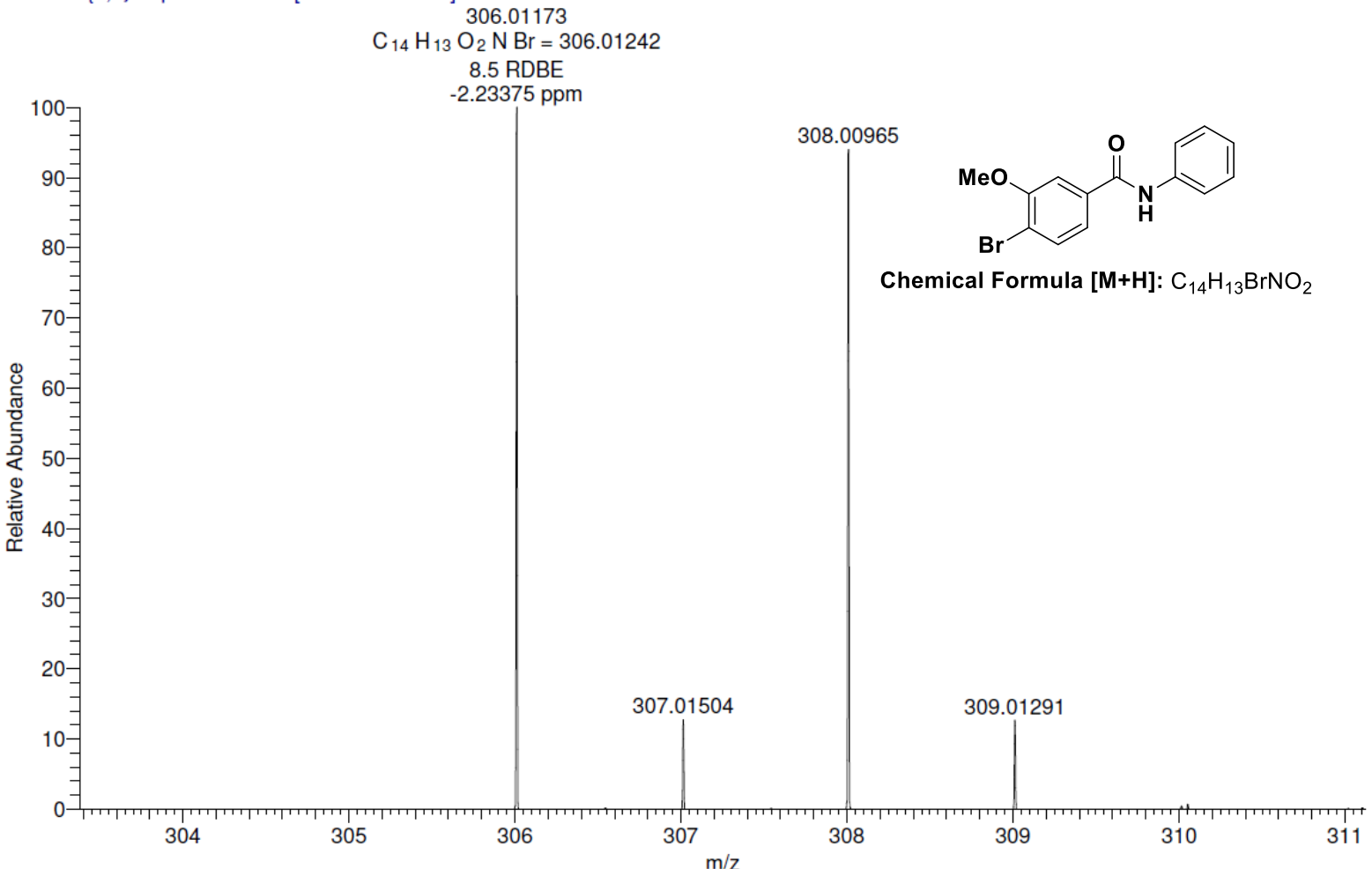
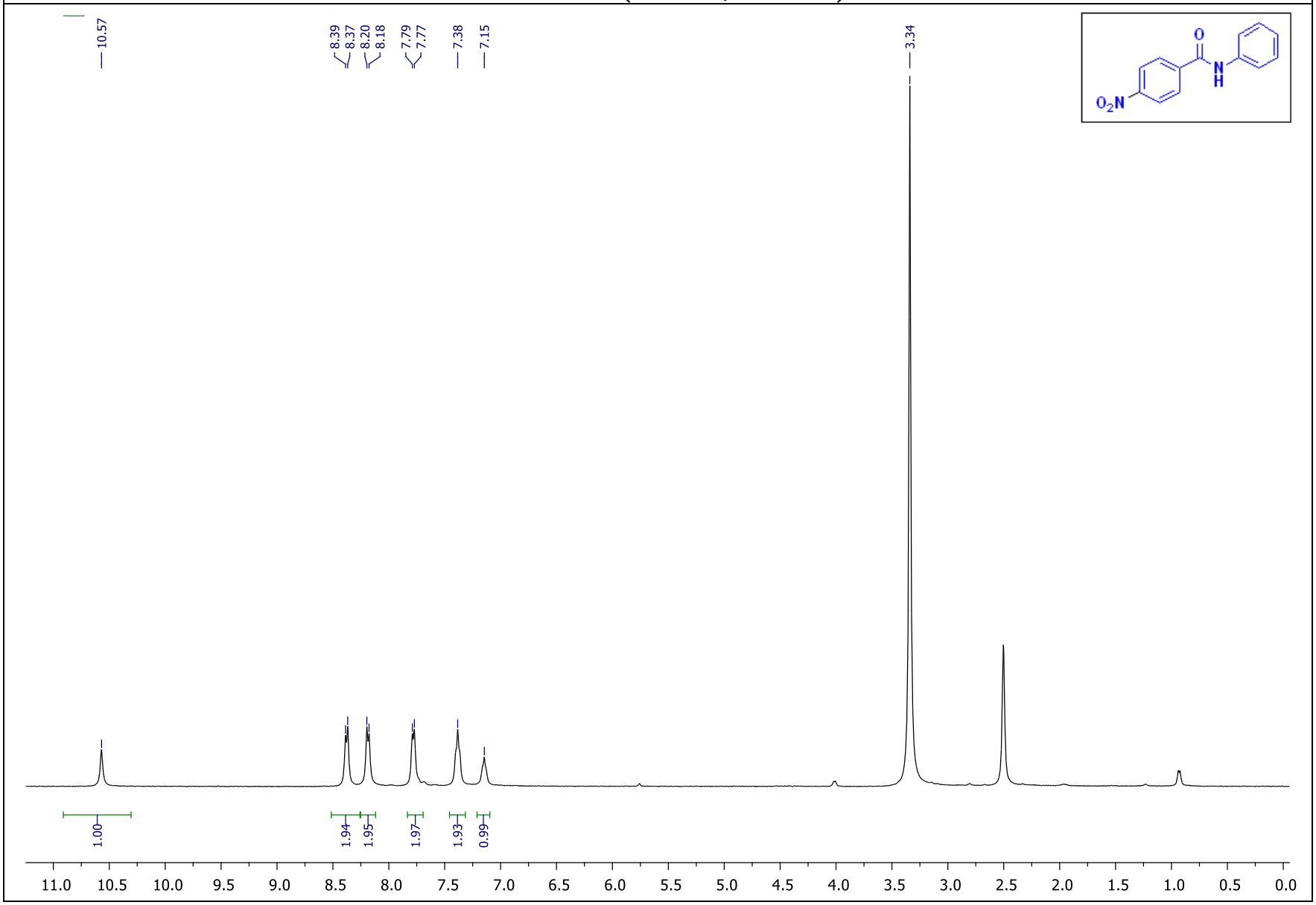
3/16/2021 5:29:20 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

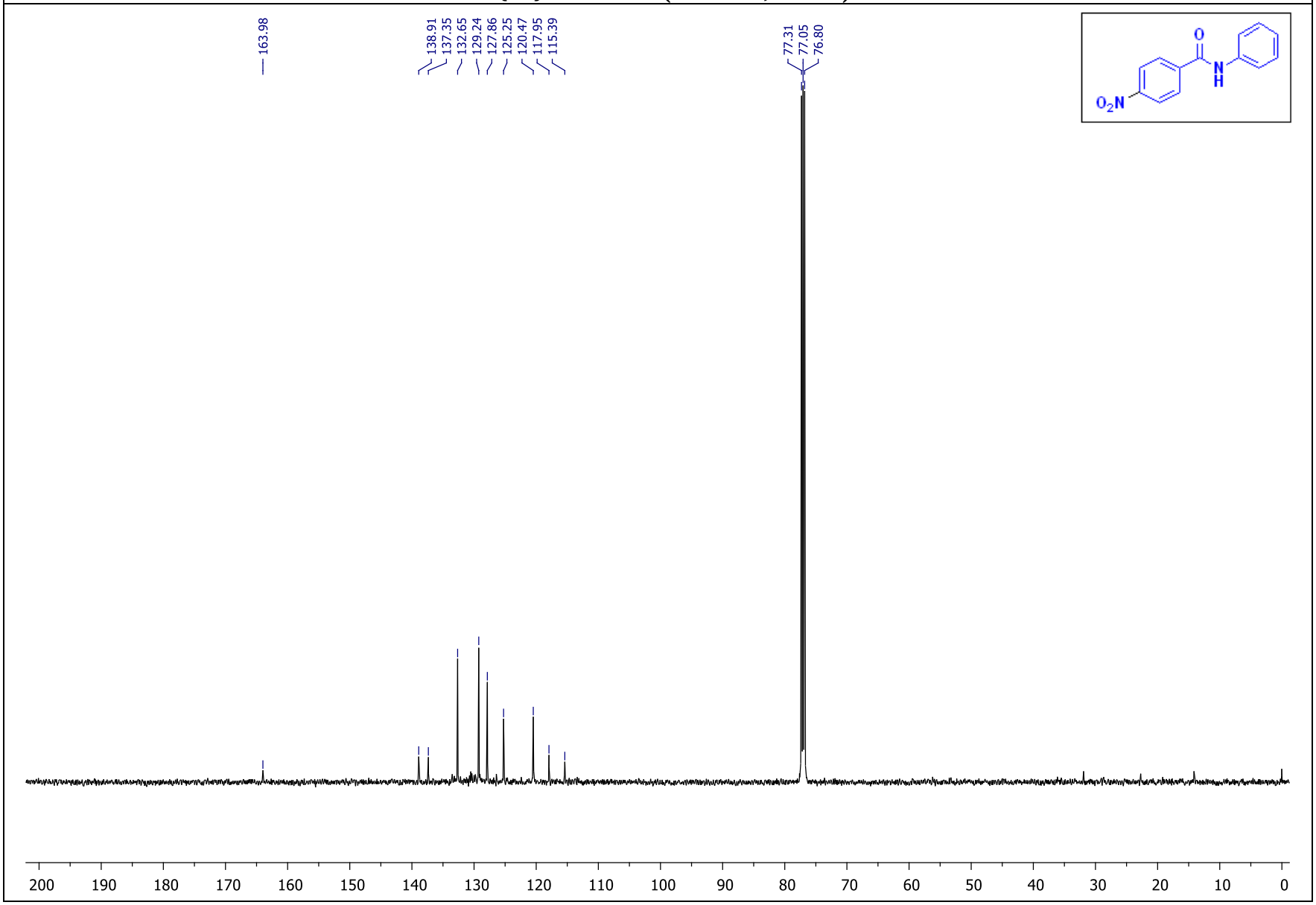
SUR-RR-3-BR4OME #10-22 RT: 0.07-0.16 AV: 13 SB: 42 0.37-0.68 NL: 2.86E6
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



^{1}H NMR of 4n (400 MHz, DMSO-d$_6$)



$^{13}C\{^{1}H\}$NMR of 4n (126 MHz, $CDCl_3$)



HRMS of 4n

D:\HRMS\...\14-12-2021\SUR-RR-4NO2

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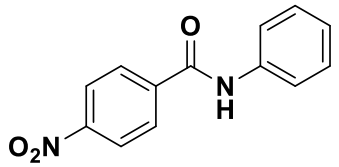
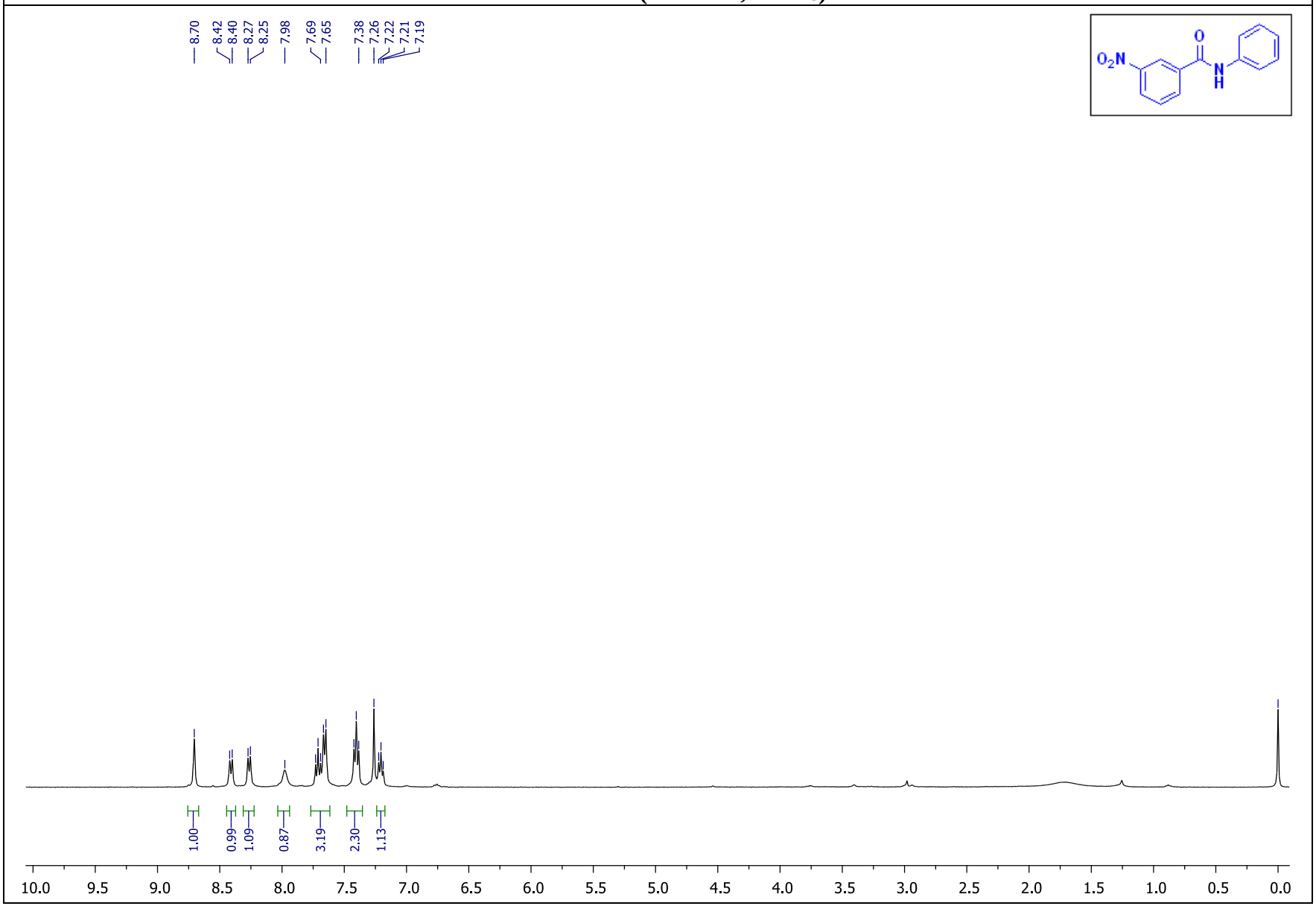
12/14/21 13:10:44
1180111041
Thermo Scientific Orbitrap Exploris 120
Analysed by G SAIKRISHNA
SUR-RR-4NO2 #11-31 RT: 0.03-0.07 AV: 21 SB: 252 0.56-1.14 NL: 1.44E7
T: FTMS + p ESI Full ms [50.0000-3000.0000]

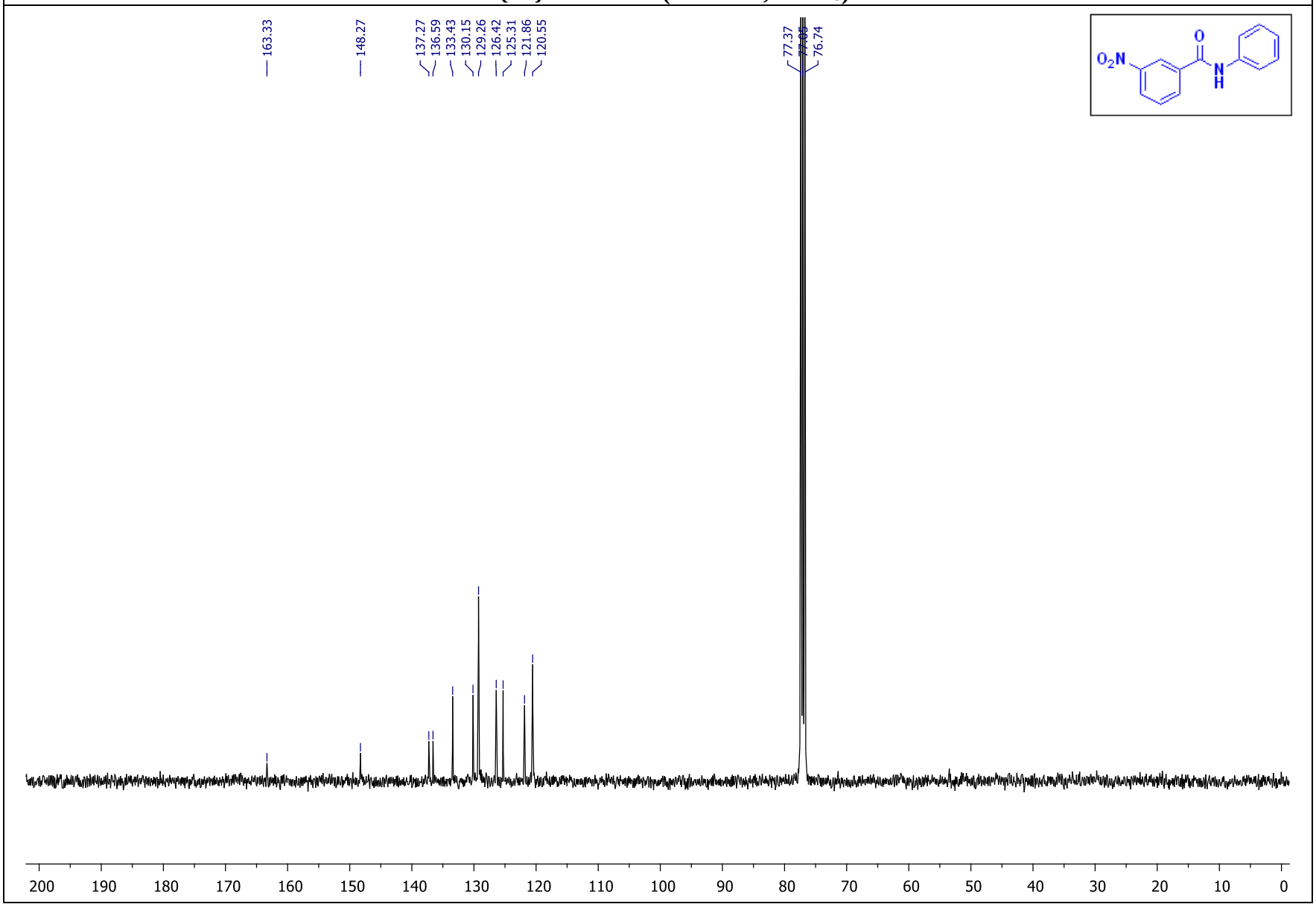


Chemical Formula [M+H]: $C_{13}H_{11}N_2O_3$

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



$^{13}C\{^{1}H\}$NMR of 4o (101 MHz, $CDCl_3$)



HRMS of 4o

D:\Sai krishna Important\...\SUR-RR-3NO2

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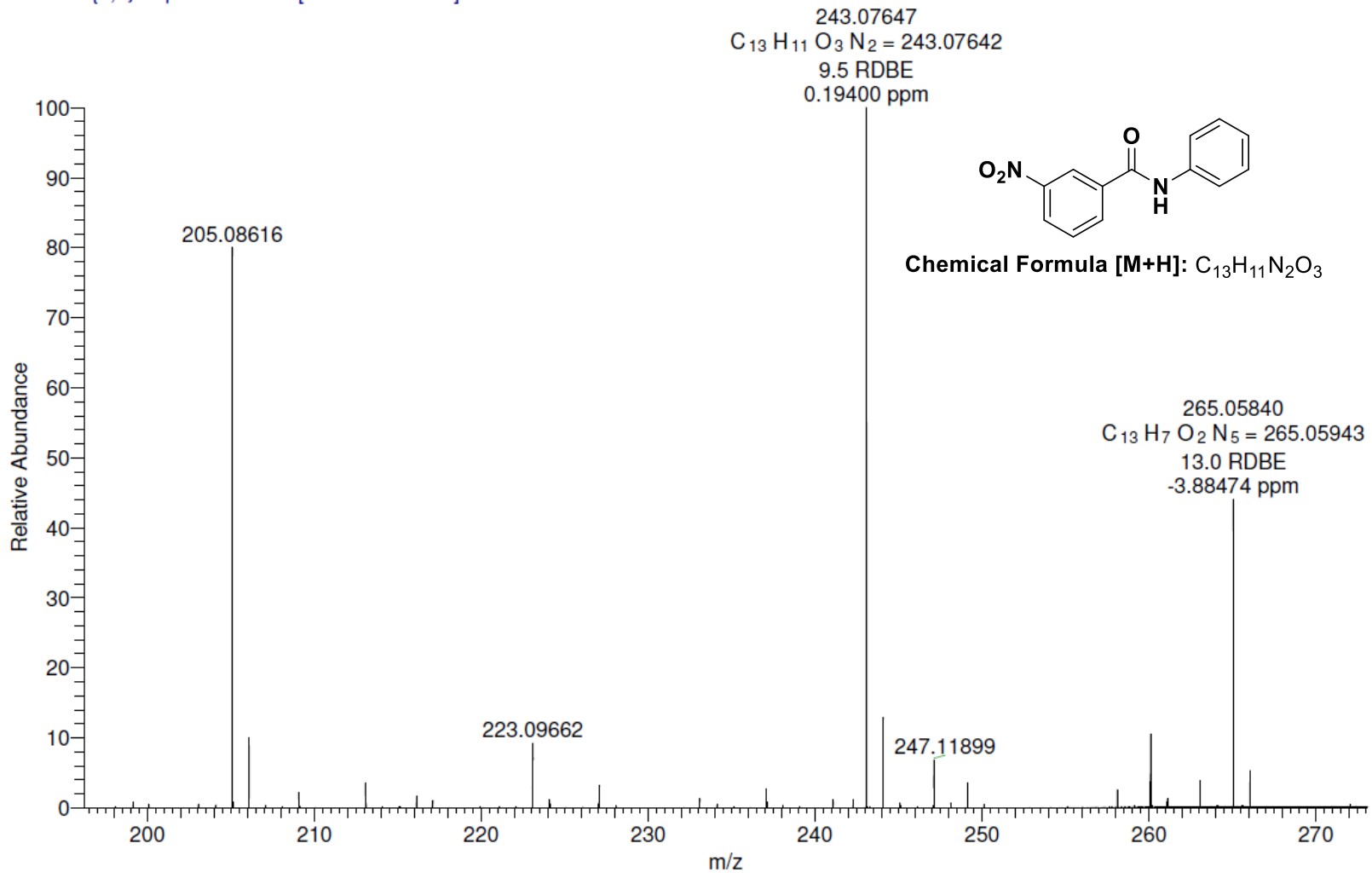
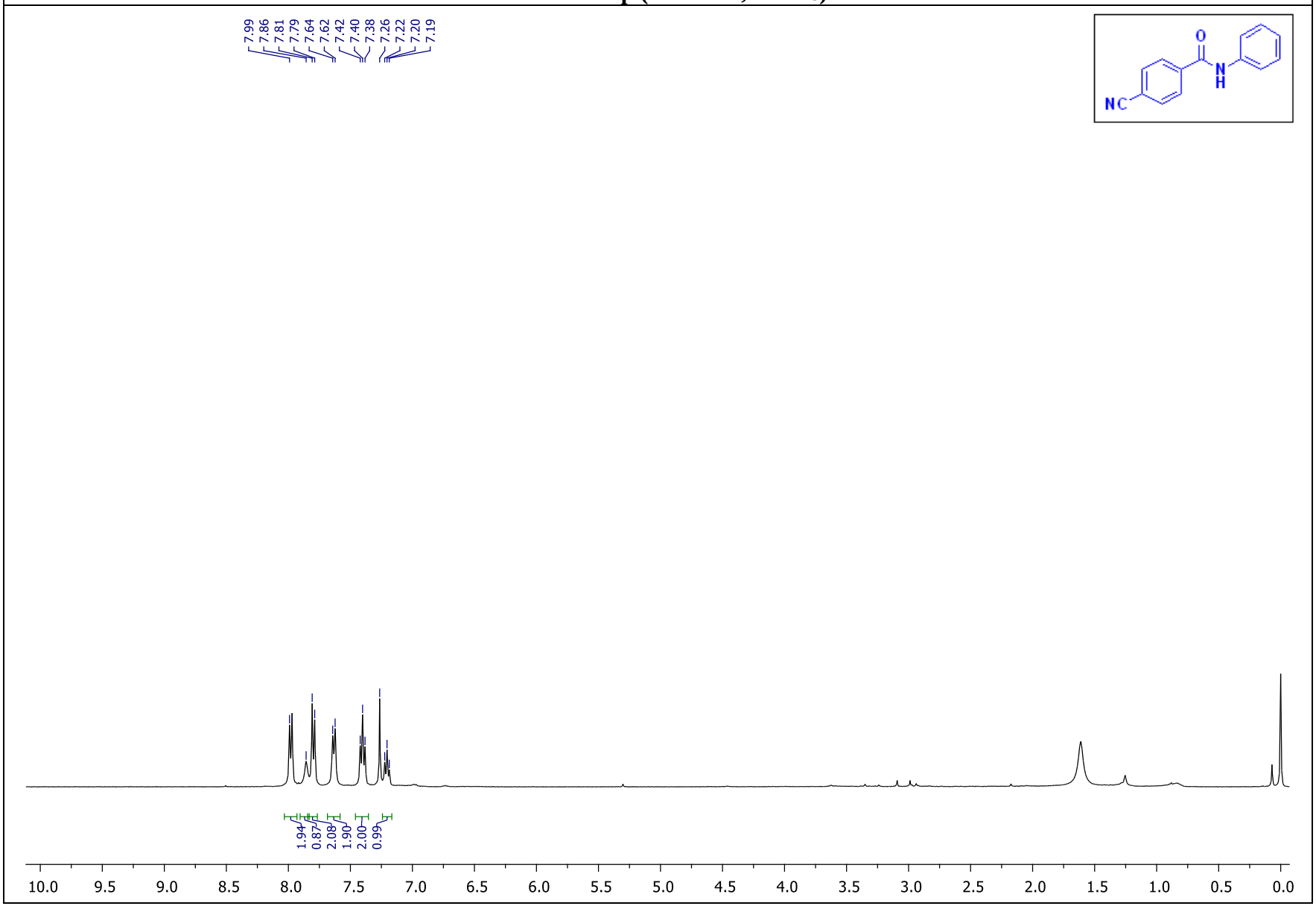
3/16/2021 5:16:47 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR-3NO2 #10-22 RT: 0.07-0.16 AV: 13 SB: 41 0.37-0.68 NL: 4.63E6
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

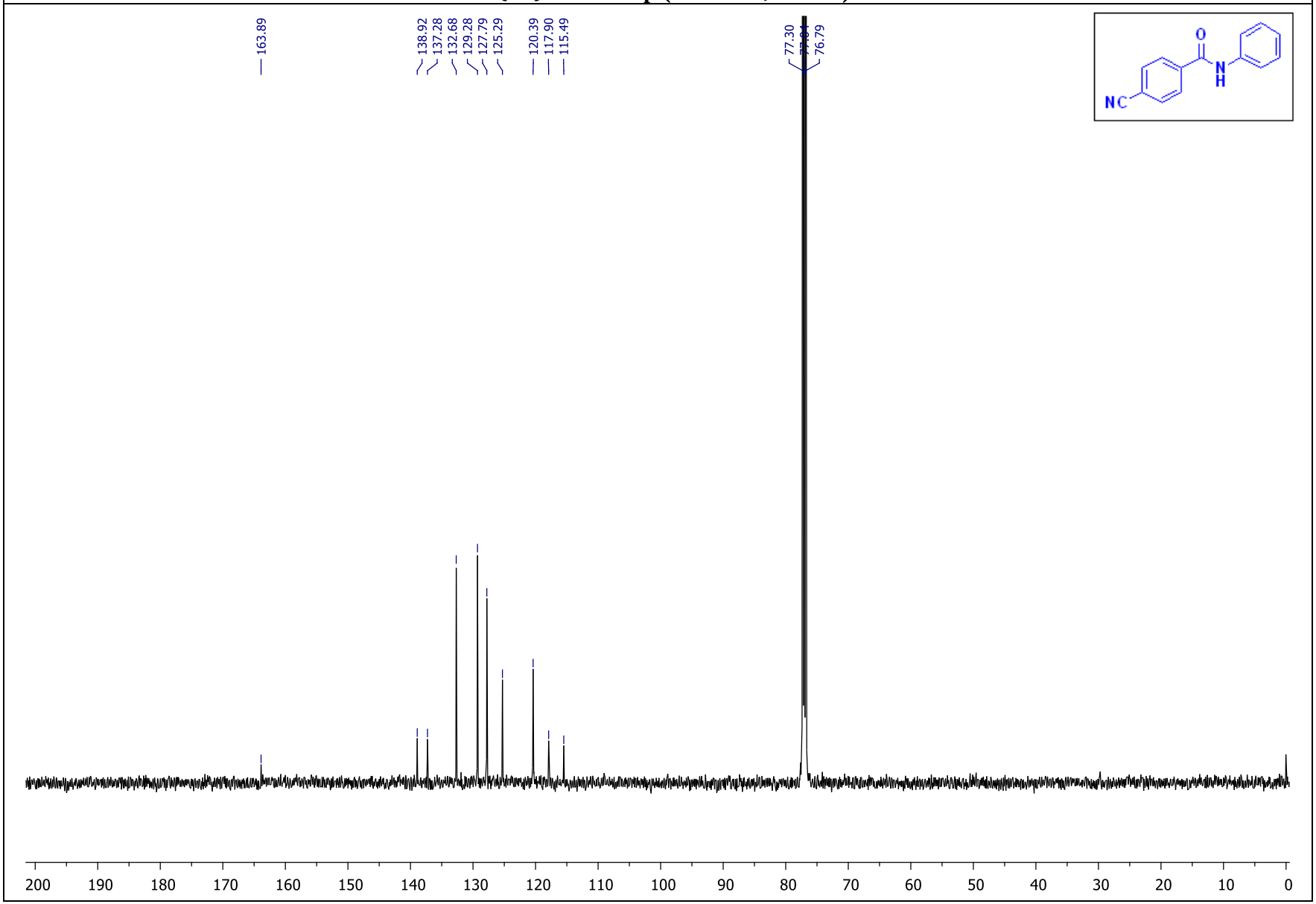


Chemical Formula [M+H]: $C_{13}H_{11}N_2O_3$

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



$^{13}C\{^{1}H\}$NMR of 4p (126 MHz, $CDCl_3$)



HRMS of 4p

D:\Sai krishna Important\...\SUR-RR-4CN

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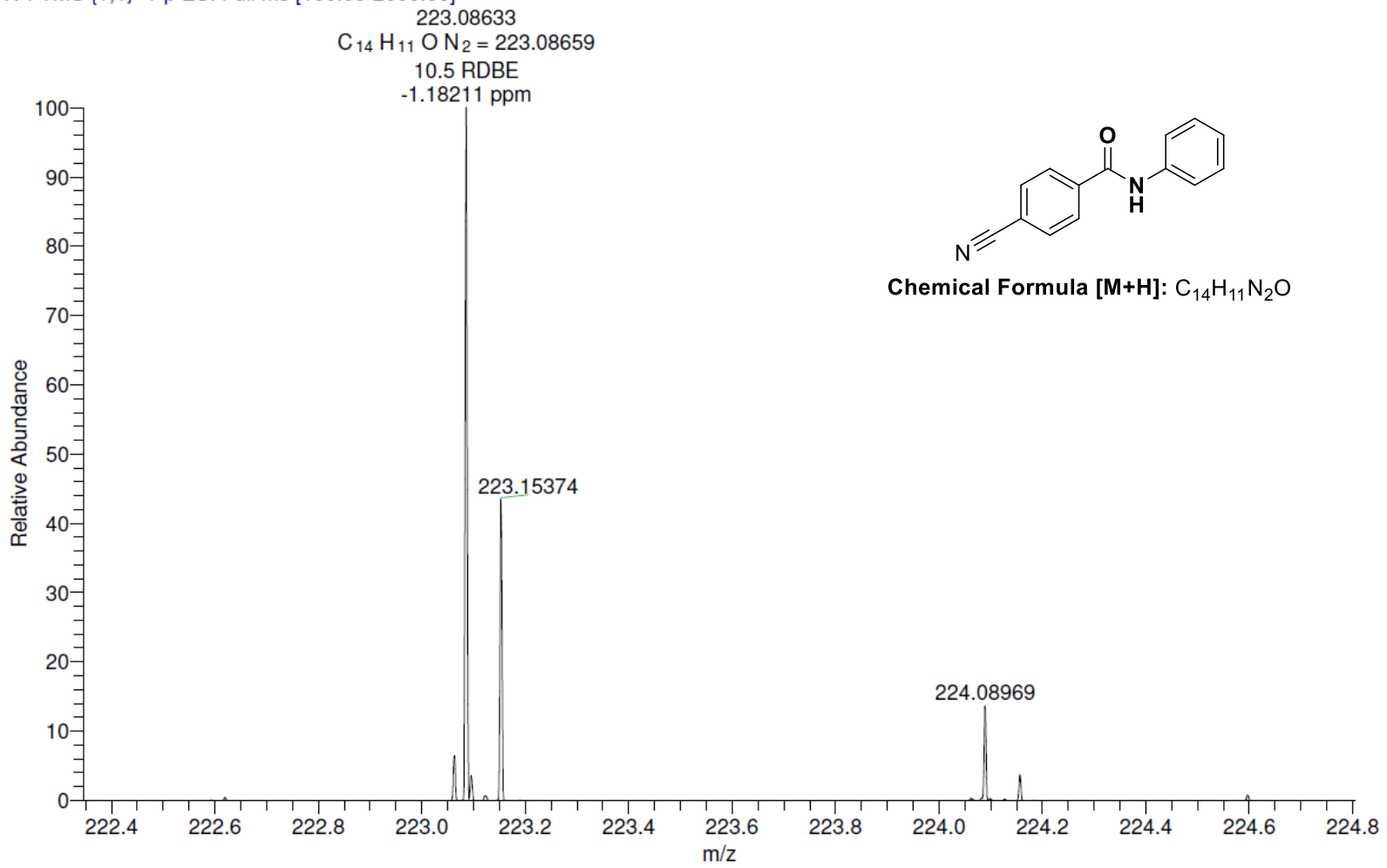
DEPARTMENT OF ANALYTICAL& STRUCTURAL CHEMISTRY

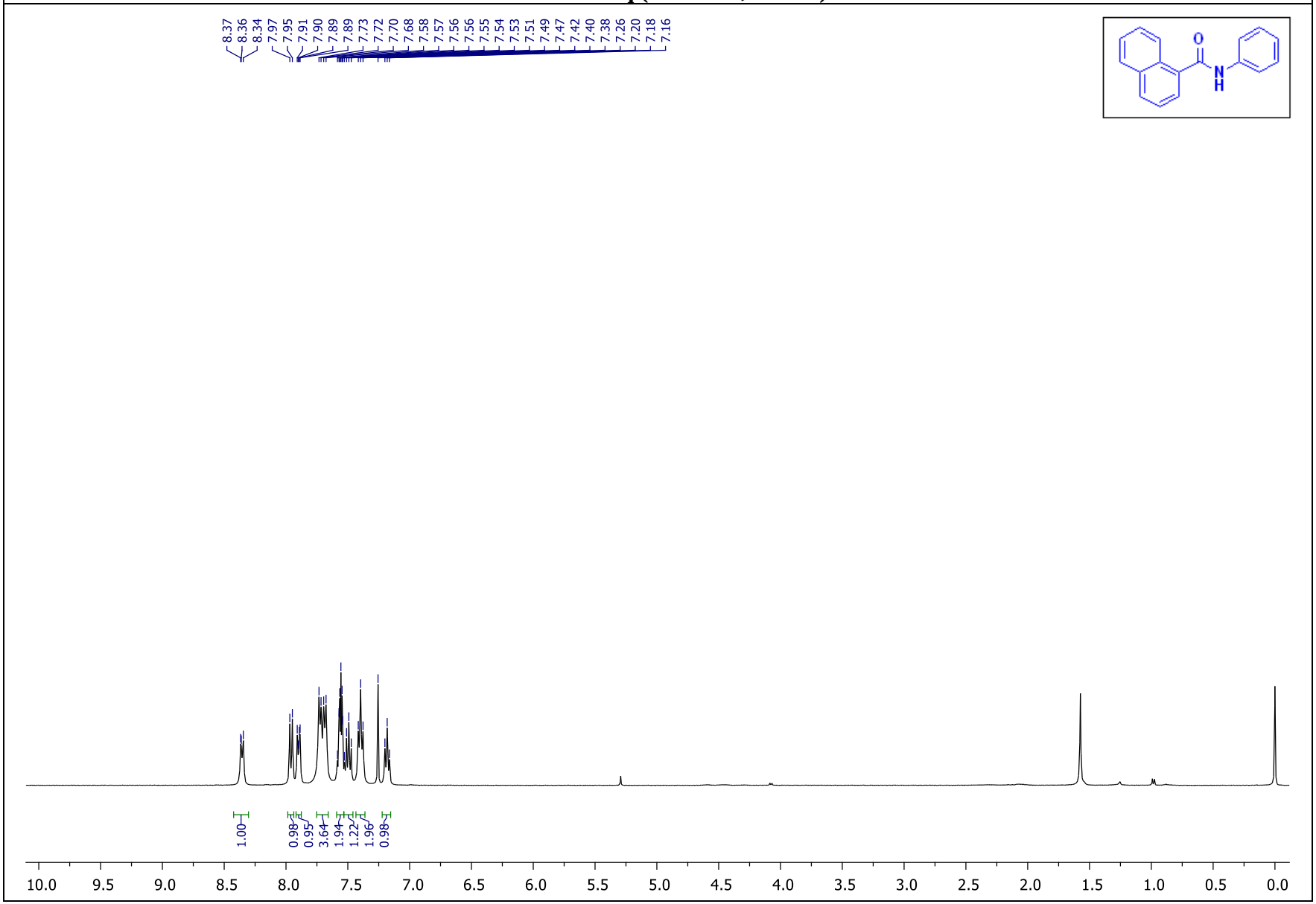
3/23/2021 8:01:35 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR-4CN #8-25 RT: 0.06-0.18 AV: 18 NL: 7.80E5
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

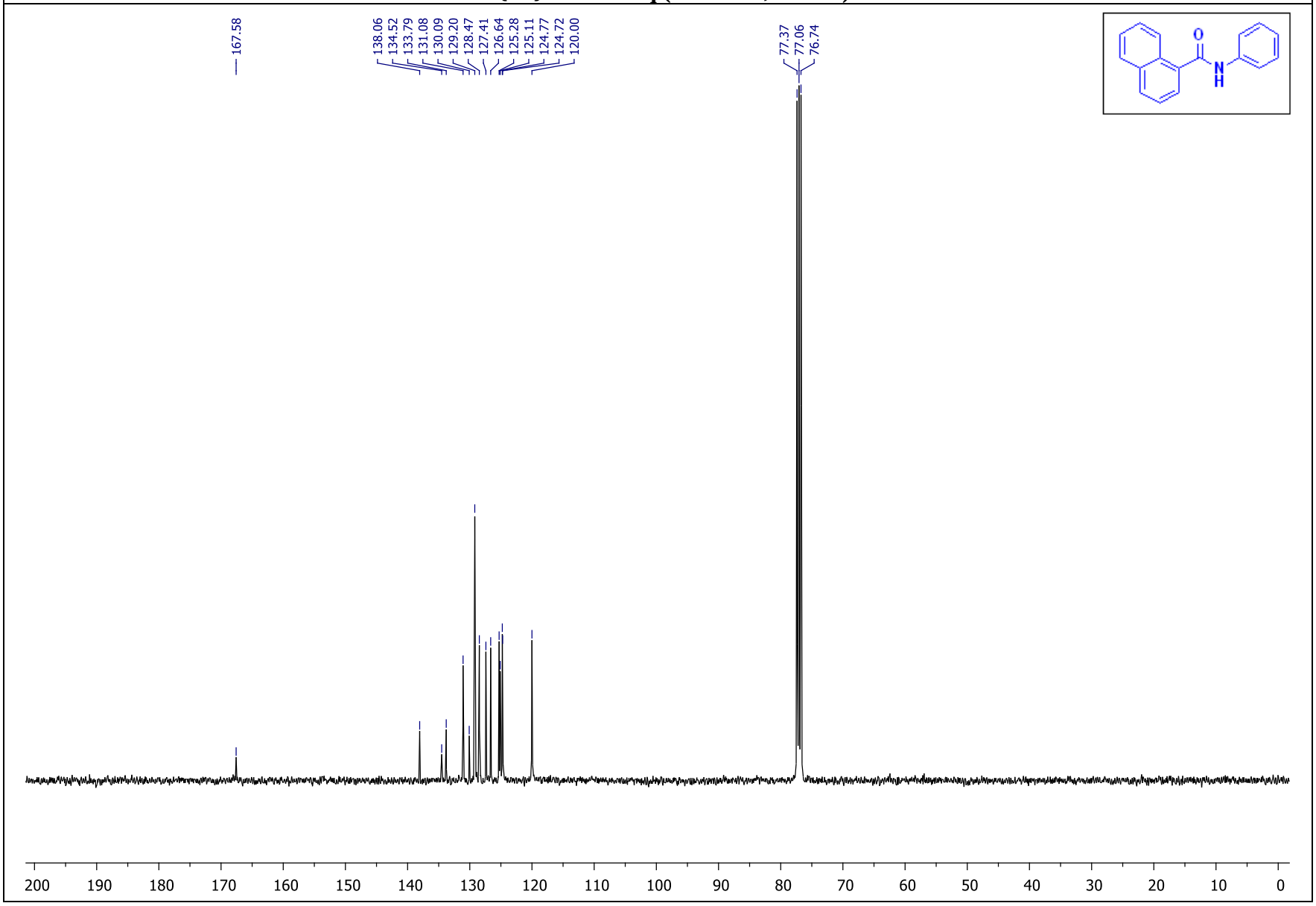


Chemical Formula [M+H]: $C_{14}H_{11}N_2O$

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



$^{13}C\{^{1}H\}$NMR of 4q (101 MHz, $CDCl_3$)



HRMS of 4q

SUR-RR-NAPAM

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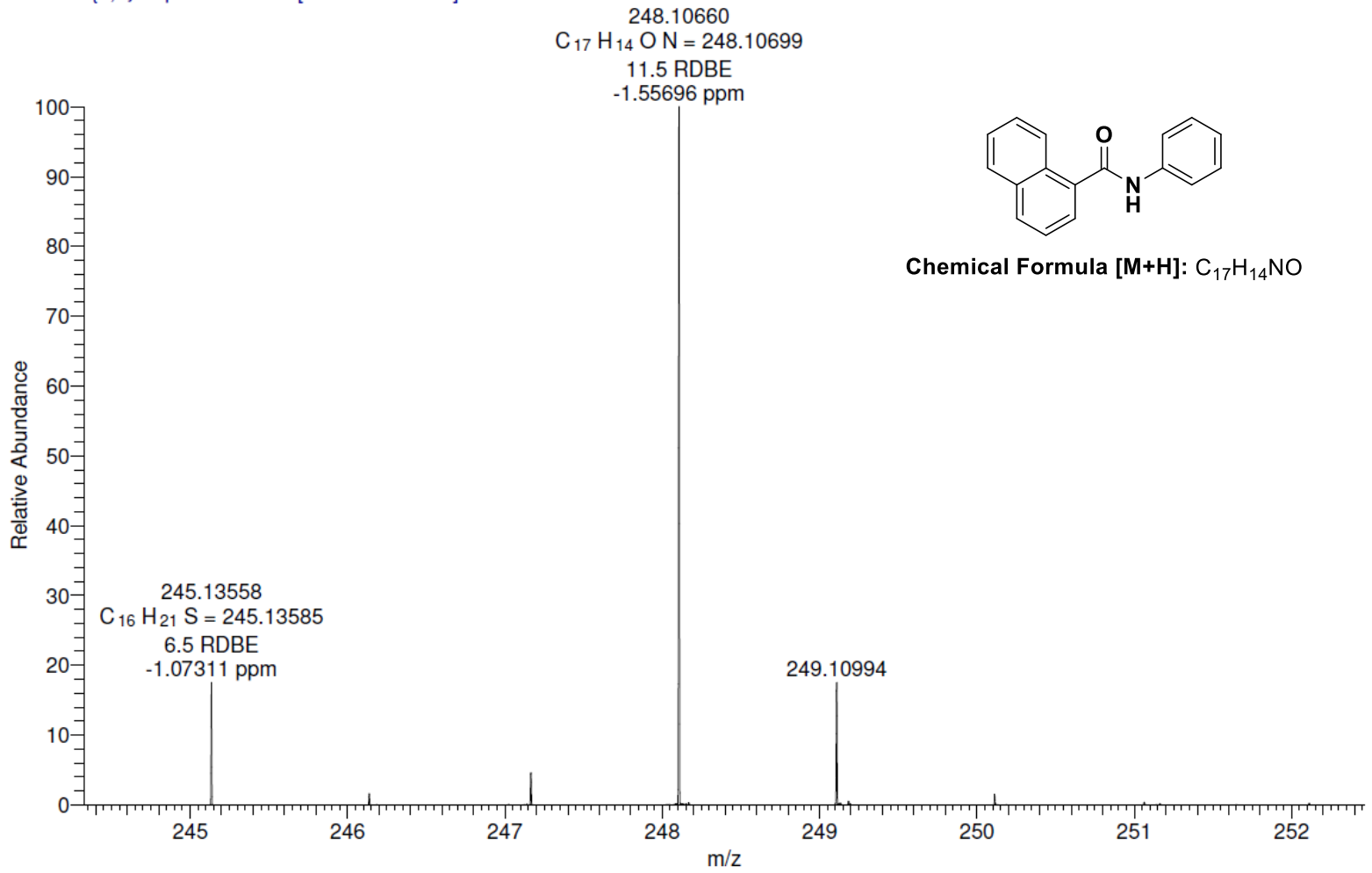
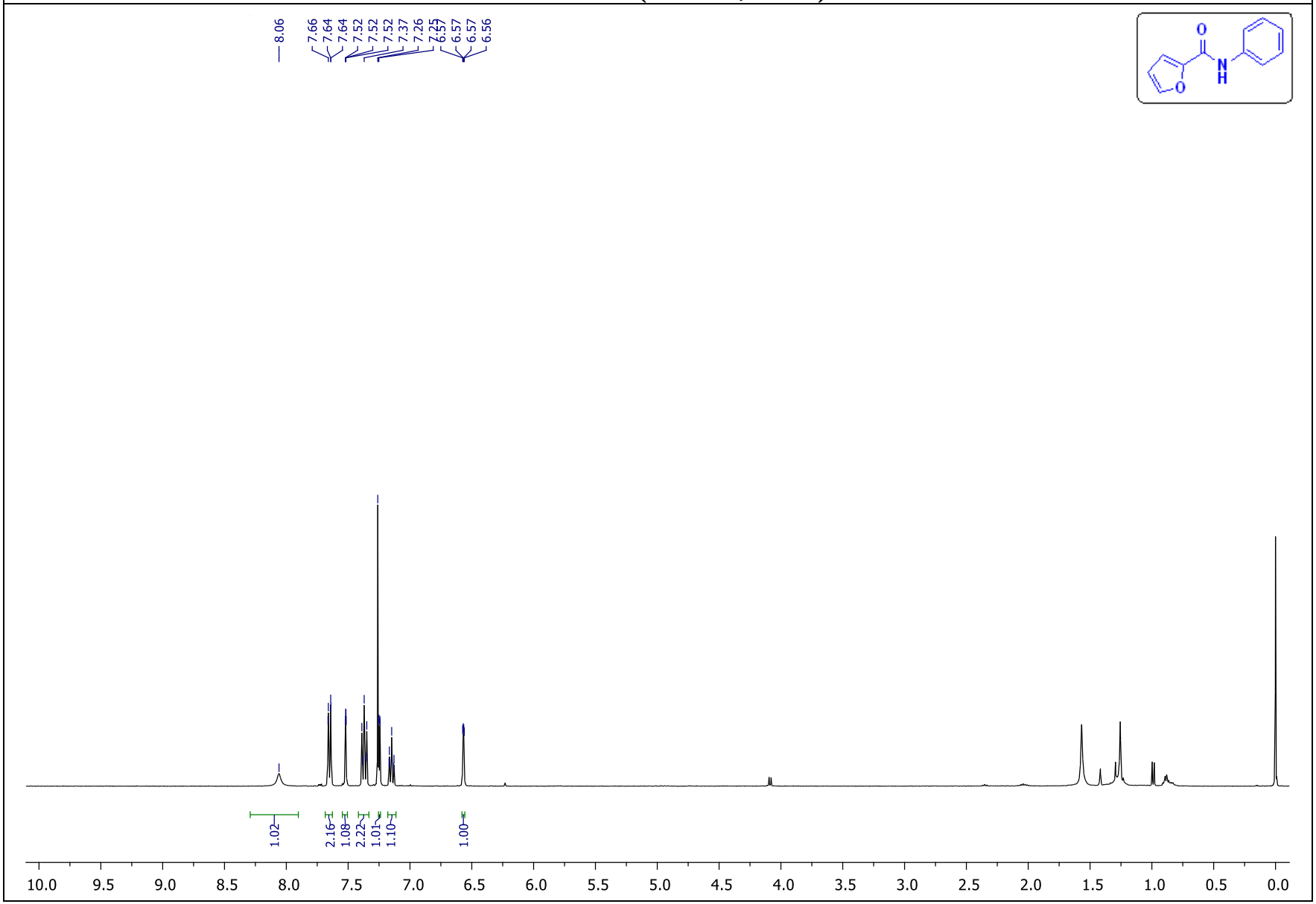
3/23/2021 8:06:33 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR-NAPAM #8-24 RT: 0.06-0.18 AV: 17 NL: 2.68E6
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

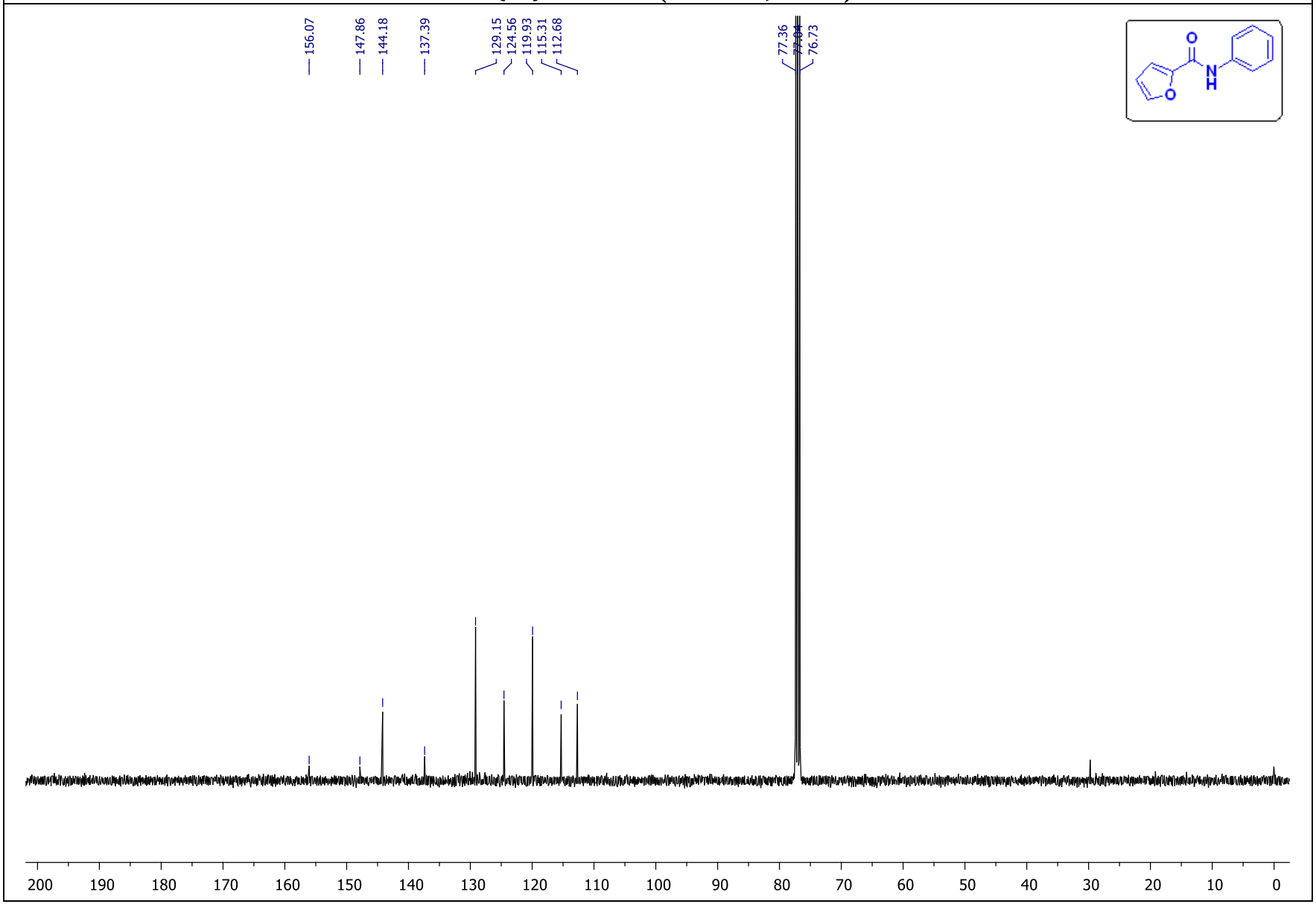


Chemical Formula [M+H]: $C_{17}H_{14}NO$

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



$^{13}C\{^{1}H\}$NMR of 4r (101 MHz, $CDCl_3$)



HRMS of 4r

D:\Sai krishna Important\...\SUR-RR-FA

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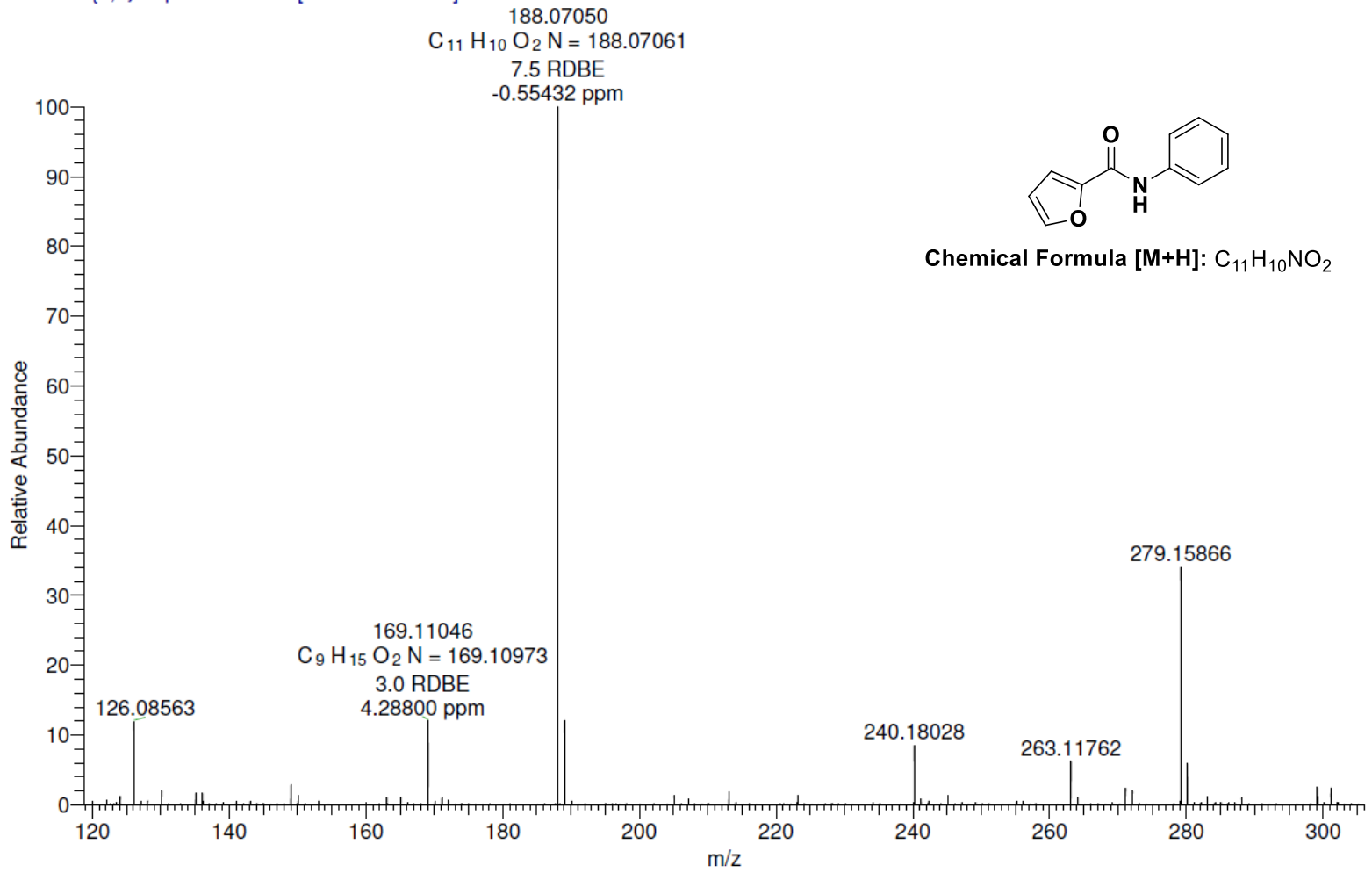
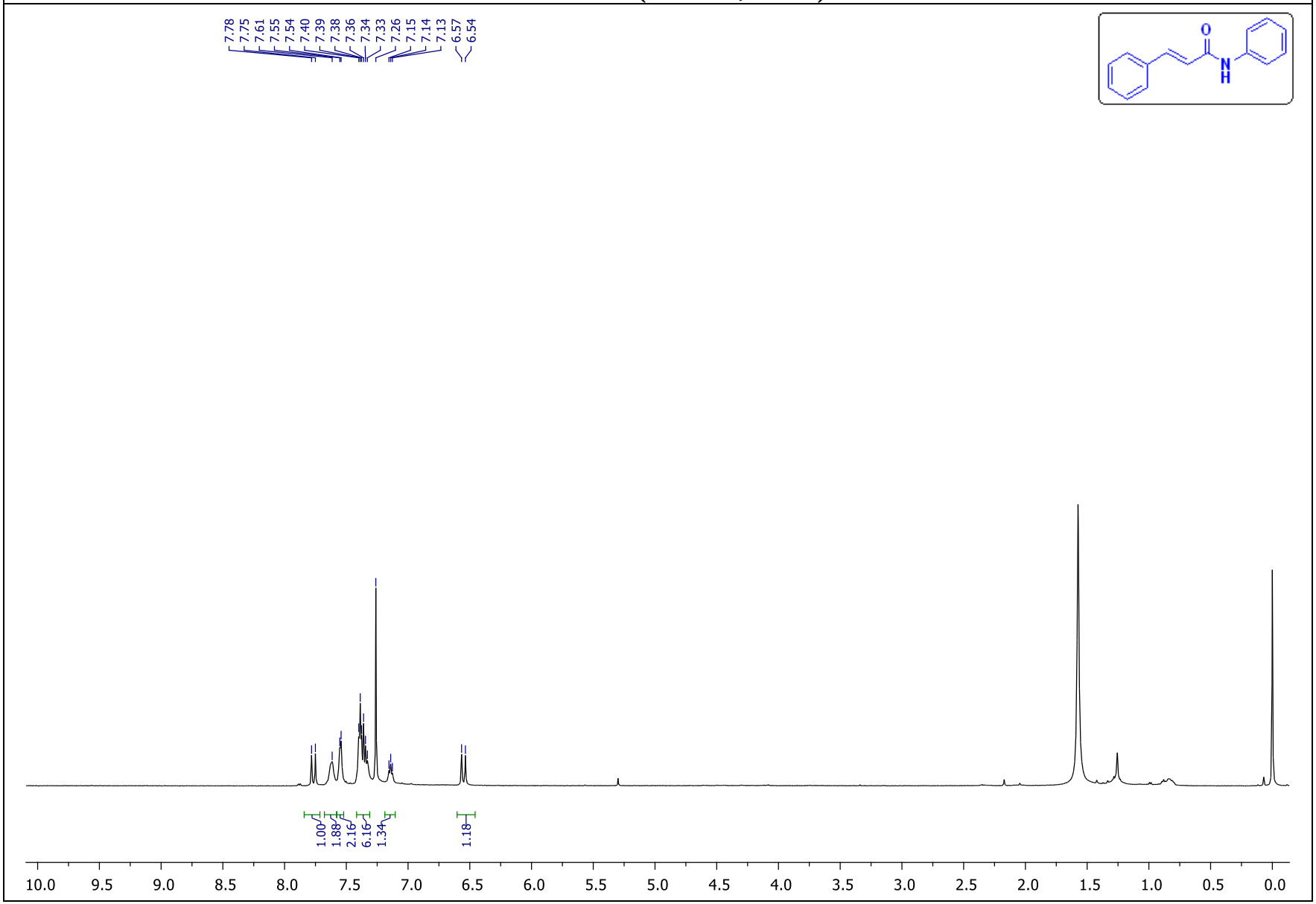
3/23/2021 7:54:04 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR-FA #8-24 RT: 0.06-0.18 AV: 17 NL: 3.71E7
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

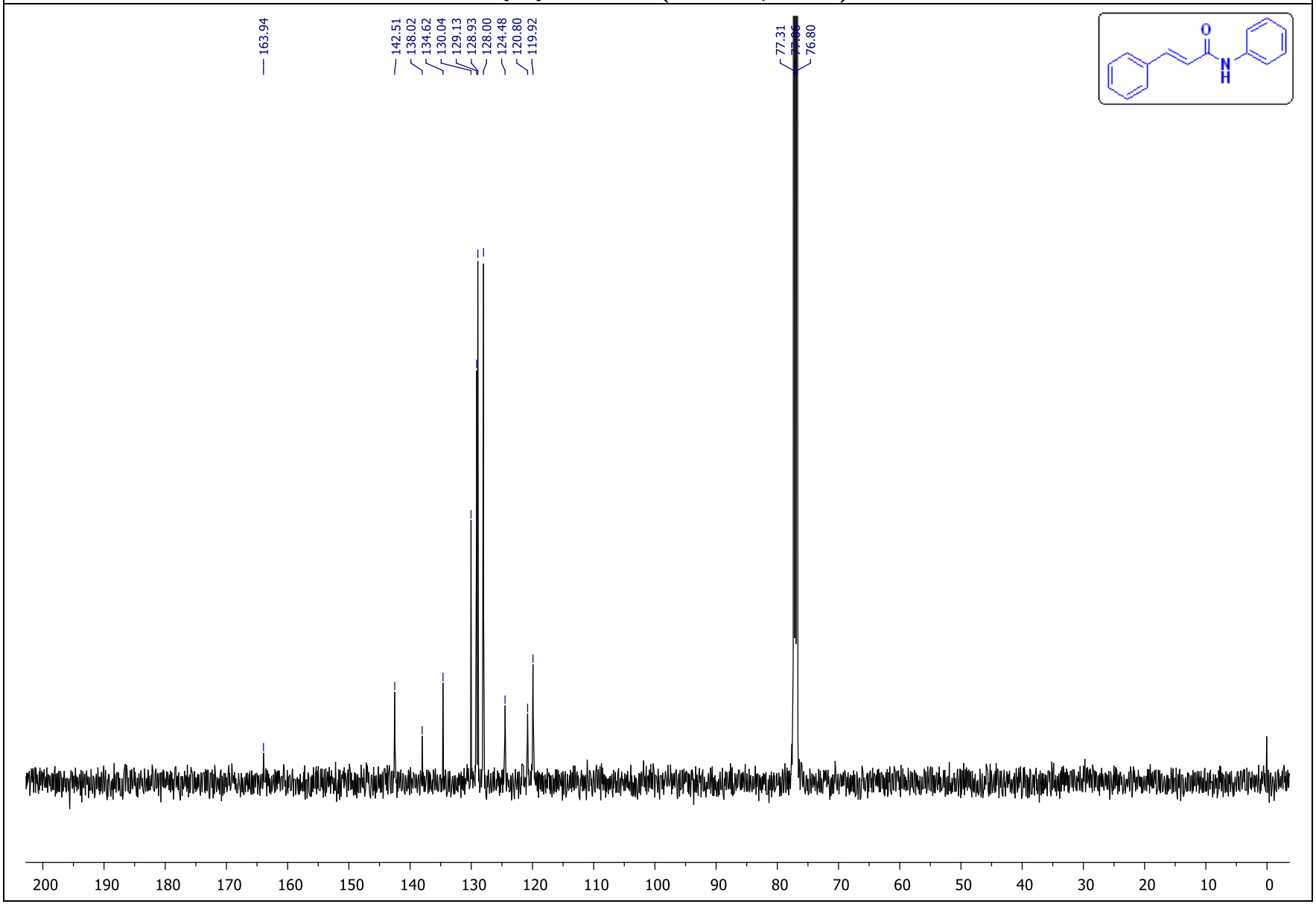


Chemical Formula [M+H]: $C_{11}H_{10}NO_2$

^{1}H NMR of 4s (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$NMR of 4s (126 MHz, $CDCl_3$)



HRMS of 4s

SUR-RR-CINAM

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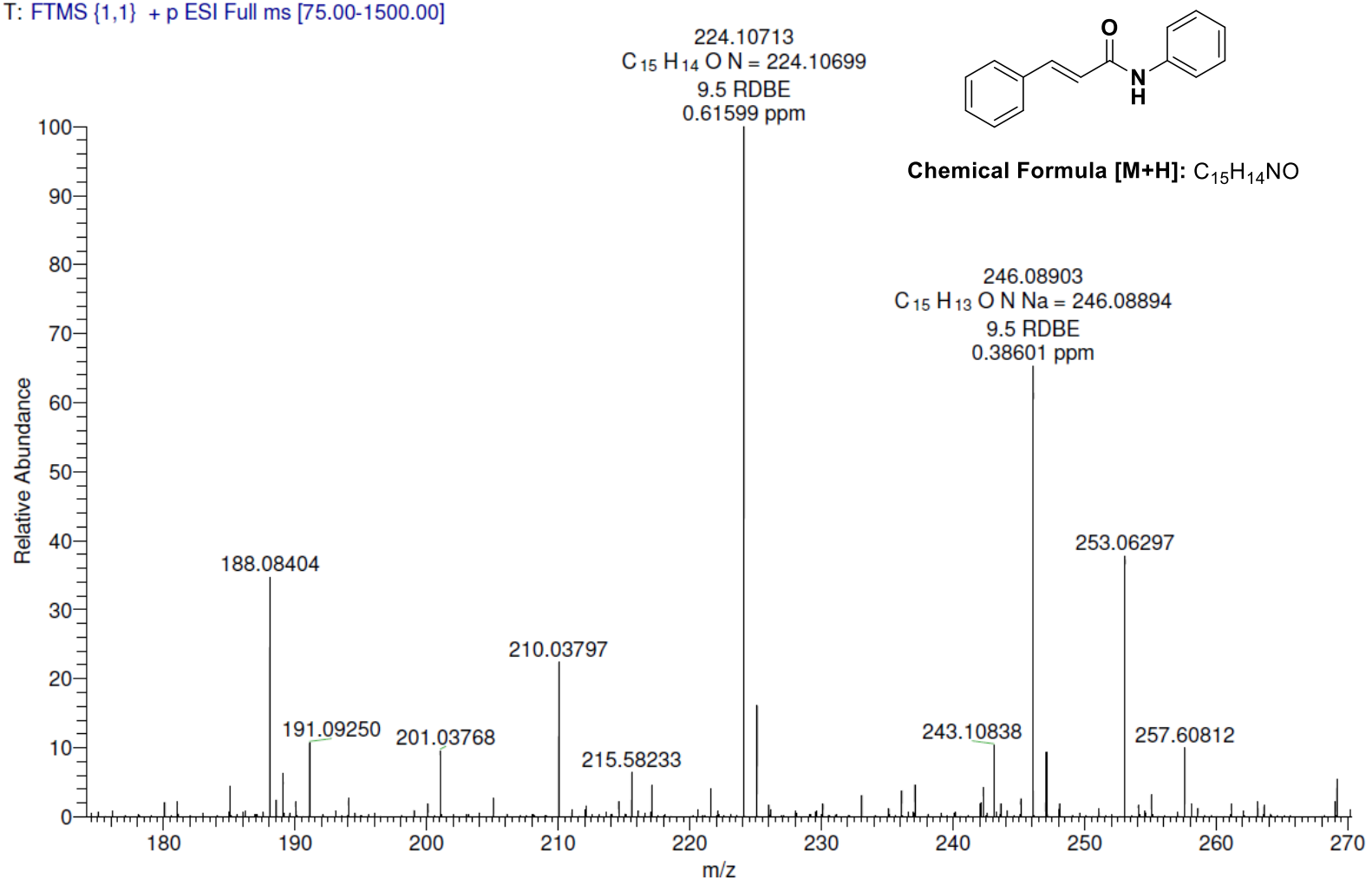
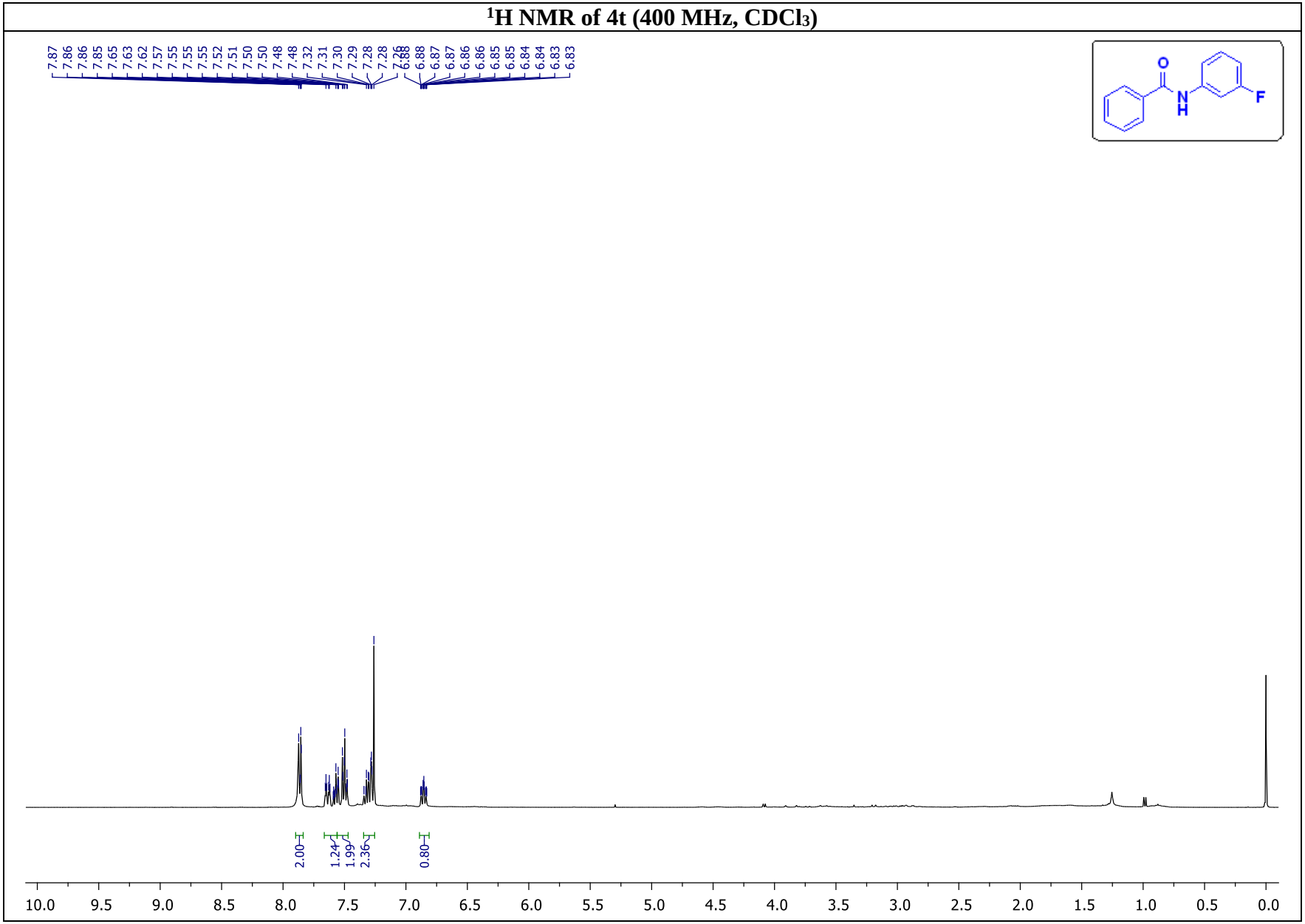
4/22/2021 1:25:32 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR-CINAM #21-42 RT: 0.15-0.31 AV: 22 NL: 3.68E6
T: FTMS {1,1} + p ESI Full ms [75.00-1500.00]

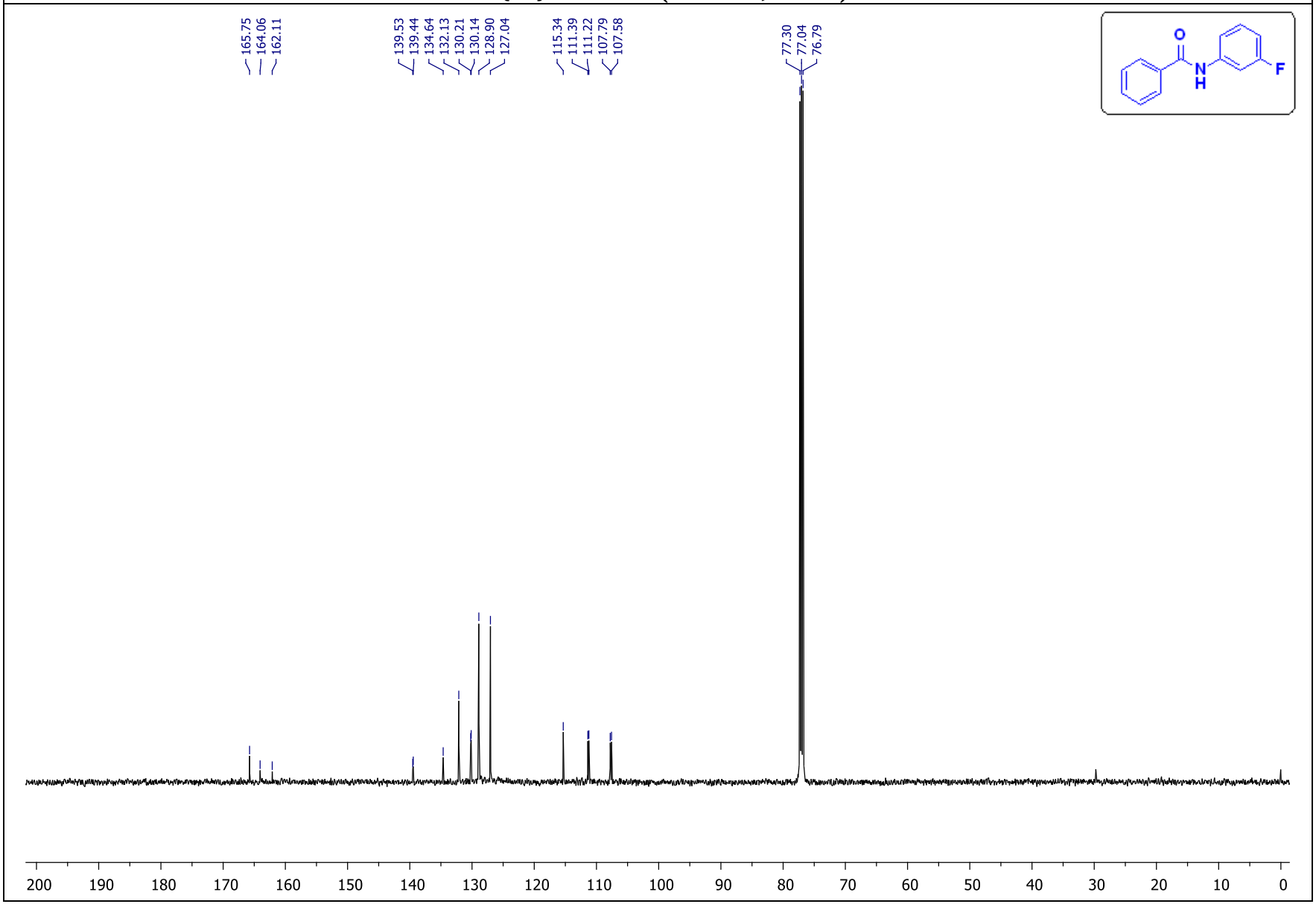


Chemical Formula [M+H]: $C_{15}H_{14}NO$

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



$^{13}C\{^{1}H\}$NMR of 4t (126 MHz, $CDCl_3$)

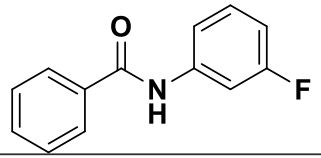


HRMS of 4t

Qualitative Analysis Report

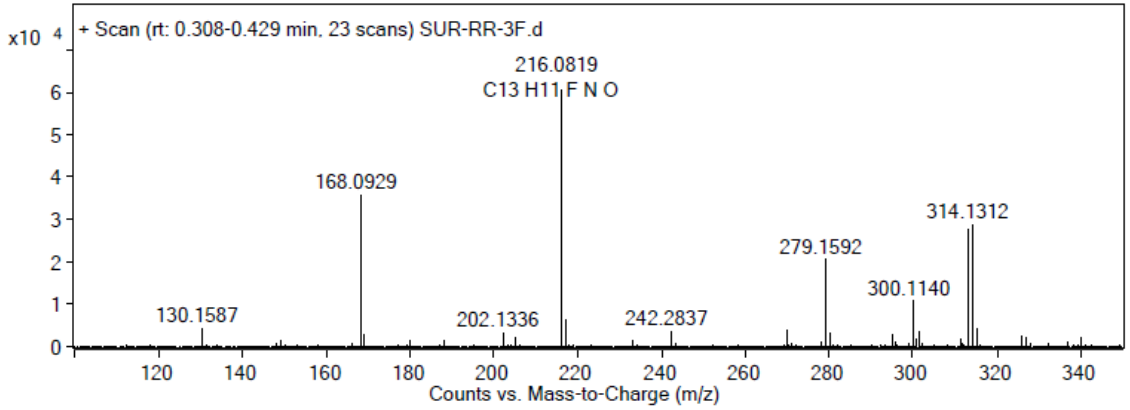
Data File	SUR-RR-3F.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	03-09-2021 12:06:55
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra



Fragmentor Voltage	Collision Energy	Ionization Mode
60	0	ESI

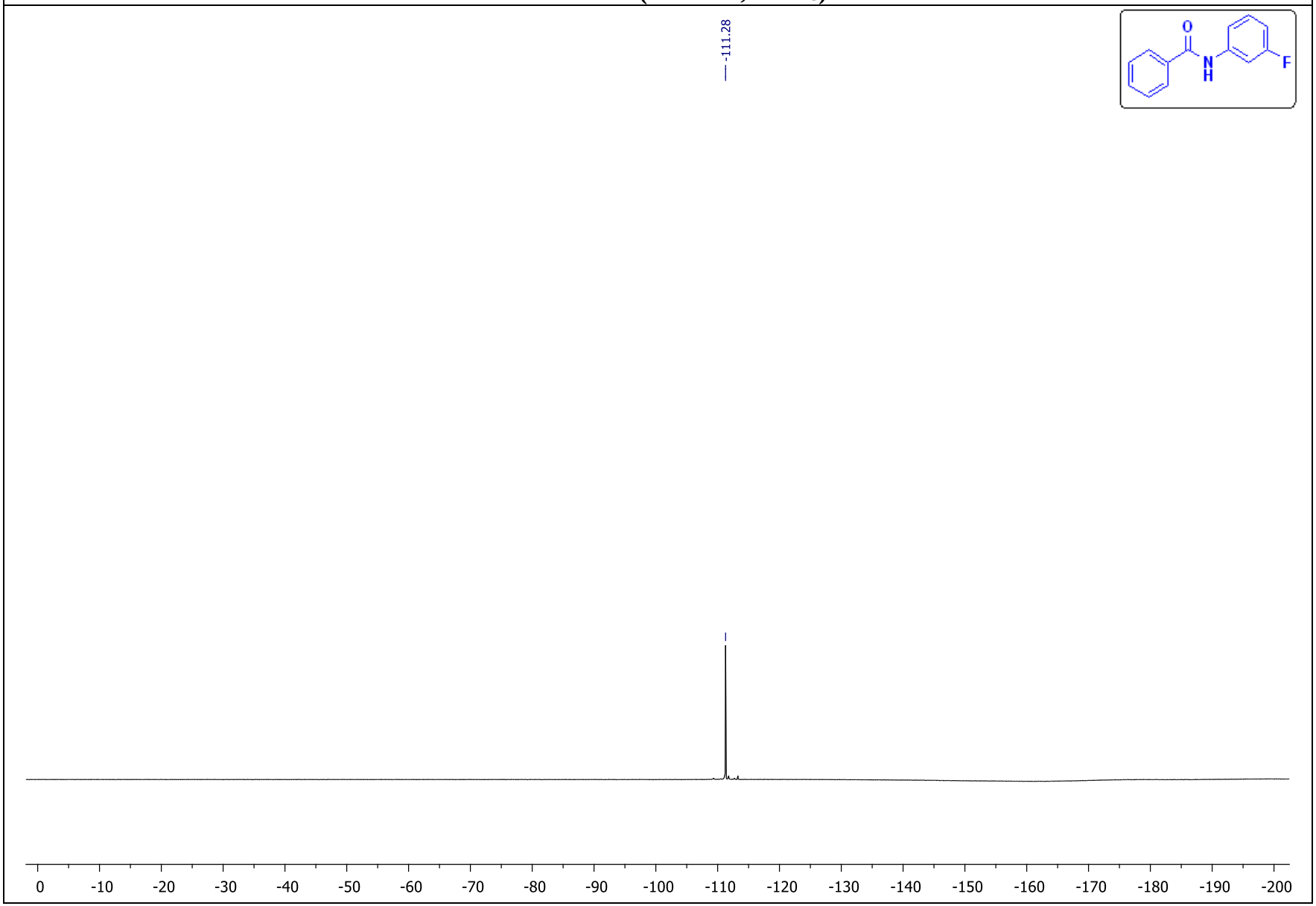
Chemical Formula [M+H]: $C_{13}H_{11}FNO$



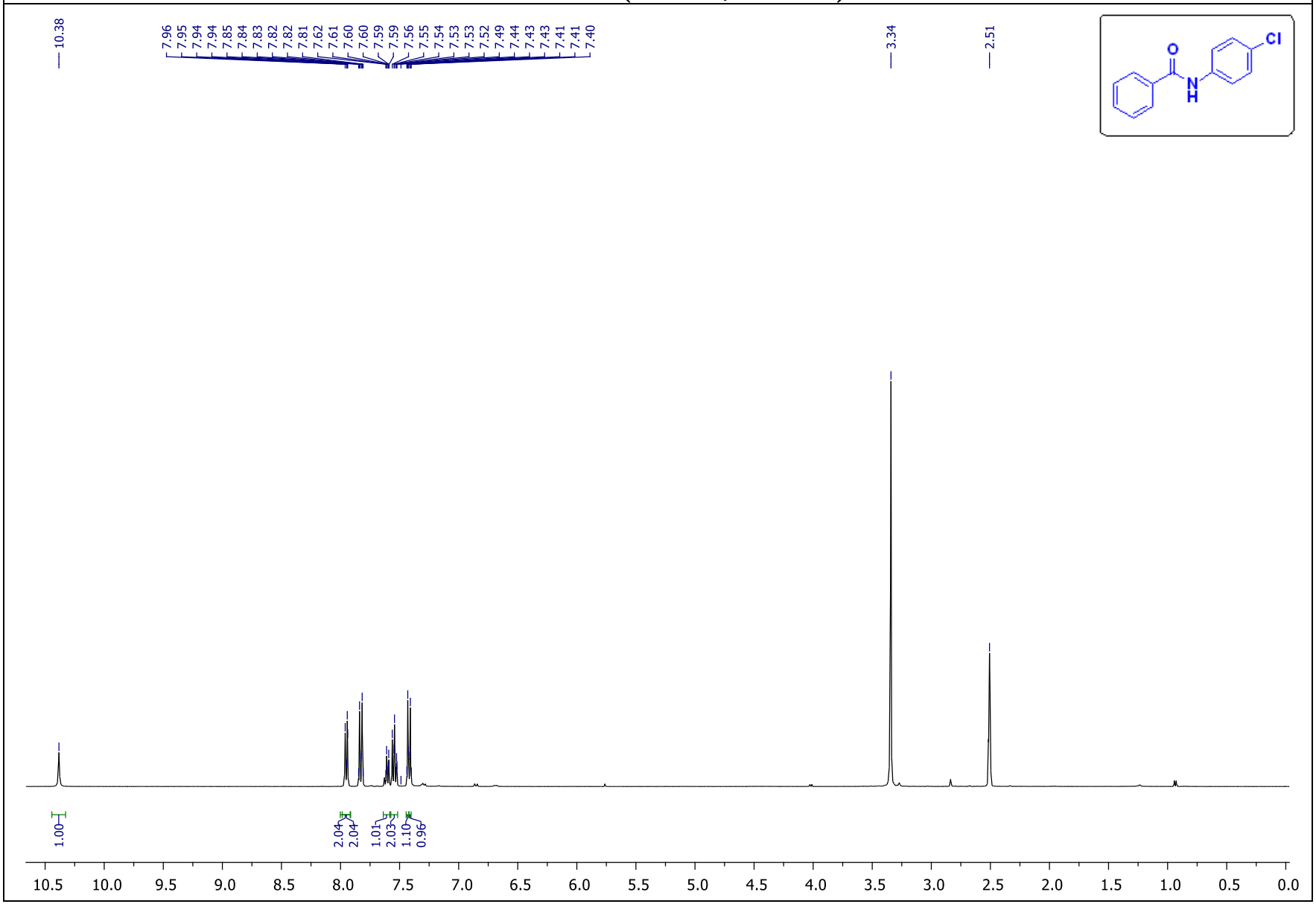
Peak List

m/z	z	Abund	Formula	Ion
216.0819	1	60376	C13 H11 F N O	M+

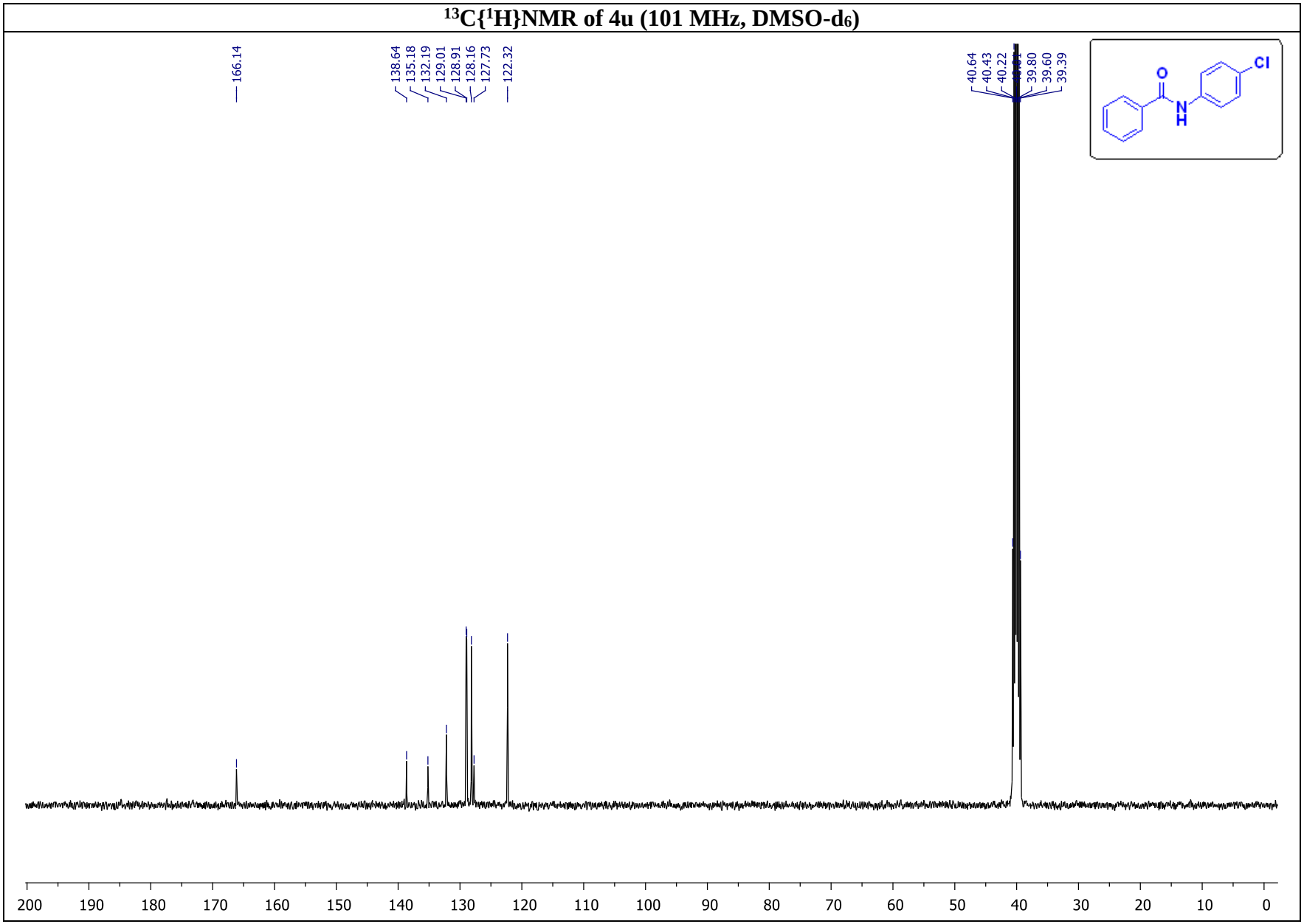
^{19}F NMR of 4t (376 MHz, $CDCl_3$)



^{1}H NMR of 4u (400 MHz, DMSO-d$_6$)



$^{13}C\{^{1}H\}$NMR of 4u (101 MHz, DMSO-d_6)



HRMS of 4u

D:\HRMS\...\20-10-2021\SUR-RR-4CIN

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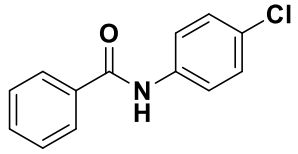
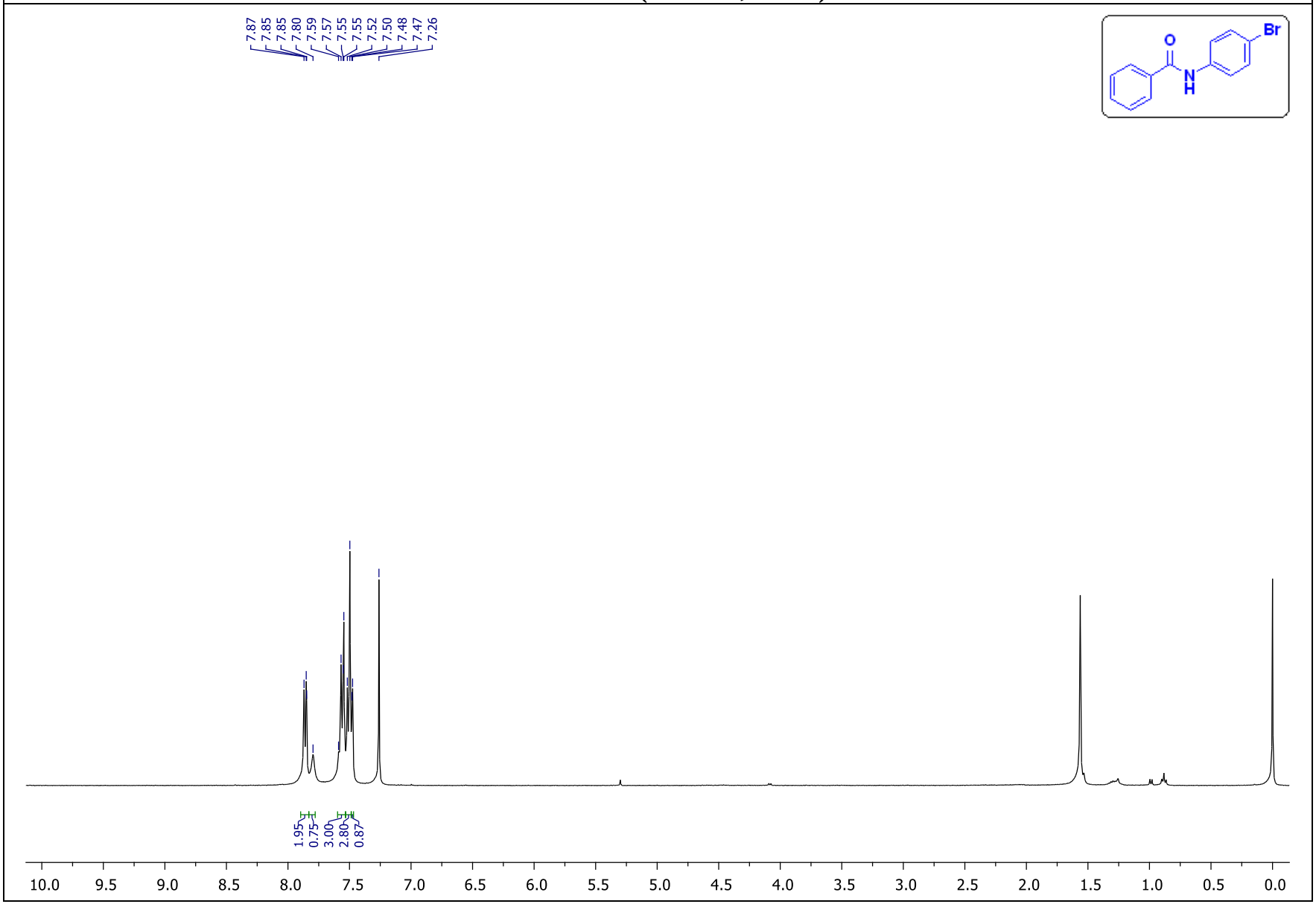
10/20/21 14:06:25
1180101083
SUR-RR-4CIN #116-144 RT: 0.27-0.33 AV: 29 SB: 184 1.16-1.58 NL: 1.31E6
T: FTMS + p ESI Full ms [50.0000-1600.0000]

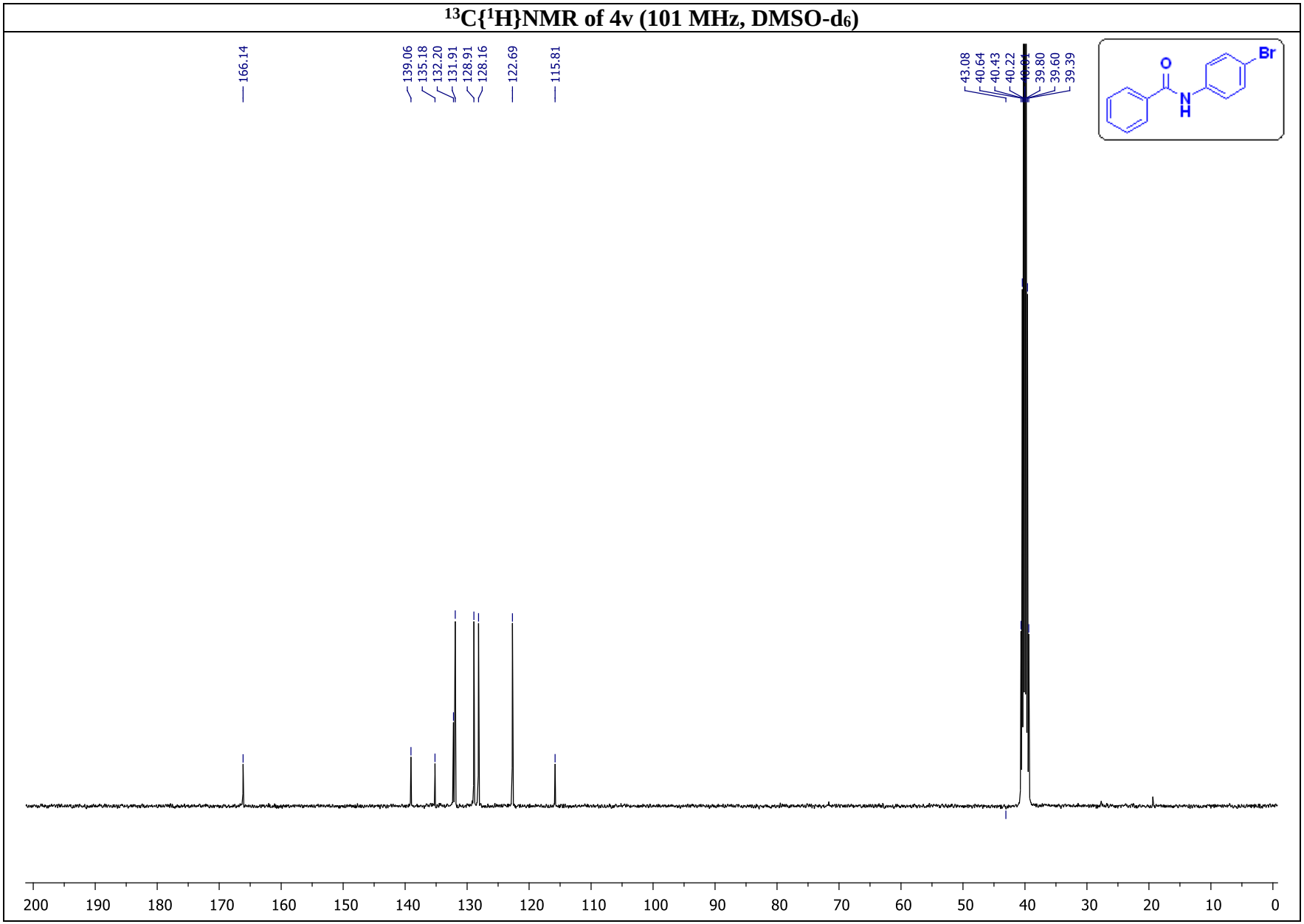


Chemical Formula [M+H]: $C_{13}H_{11}ClNO$

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



$^{13}C\{^{1}H\}$NMR of 4v (101 MHz, DMSO-d_6)



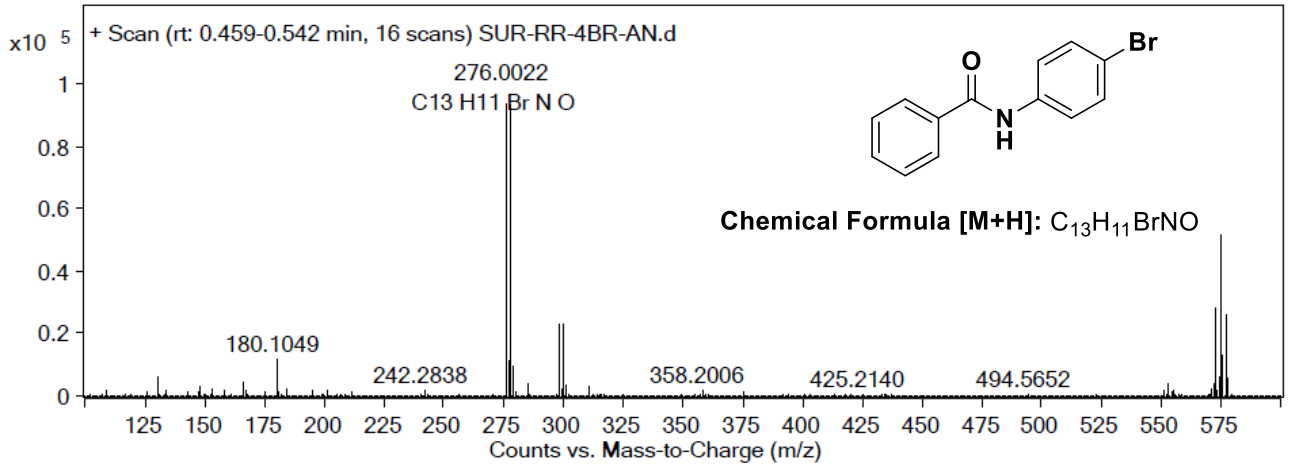
HRMS of 4v

Qualitative Analysis Report

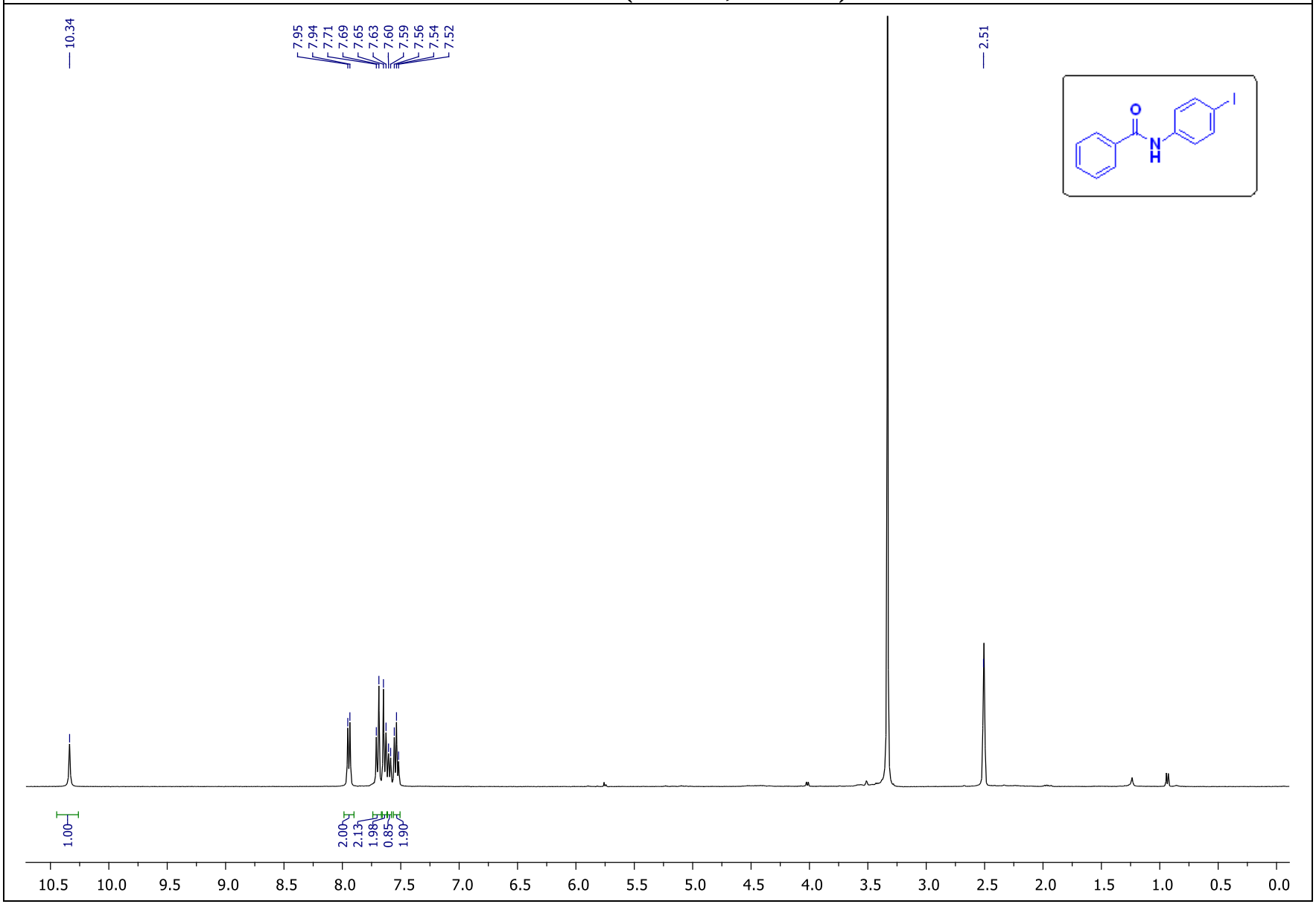
Data File	SUR-RR-4BR-AN.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	03-09-2021 15:40:31
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra

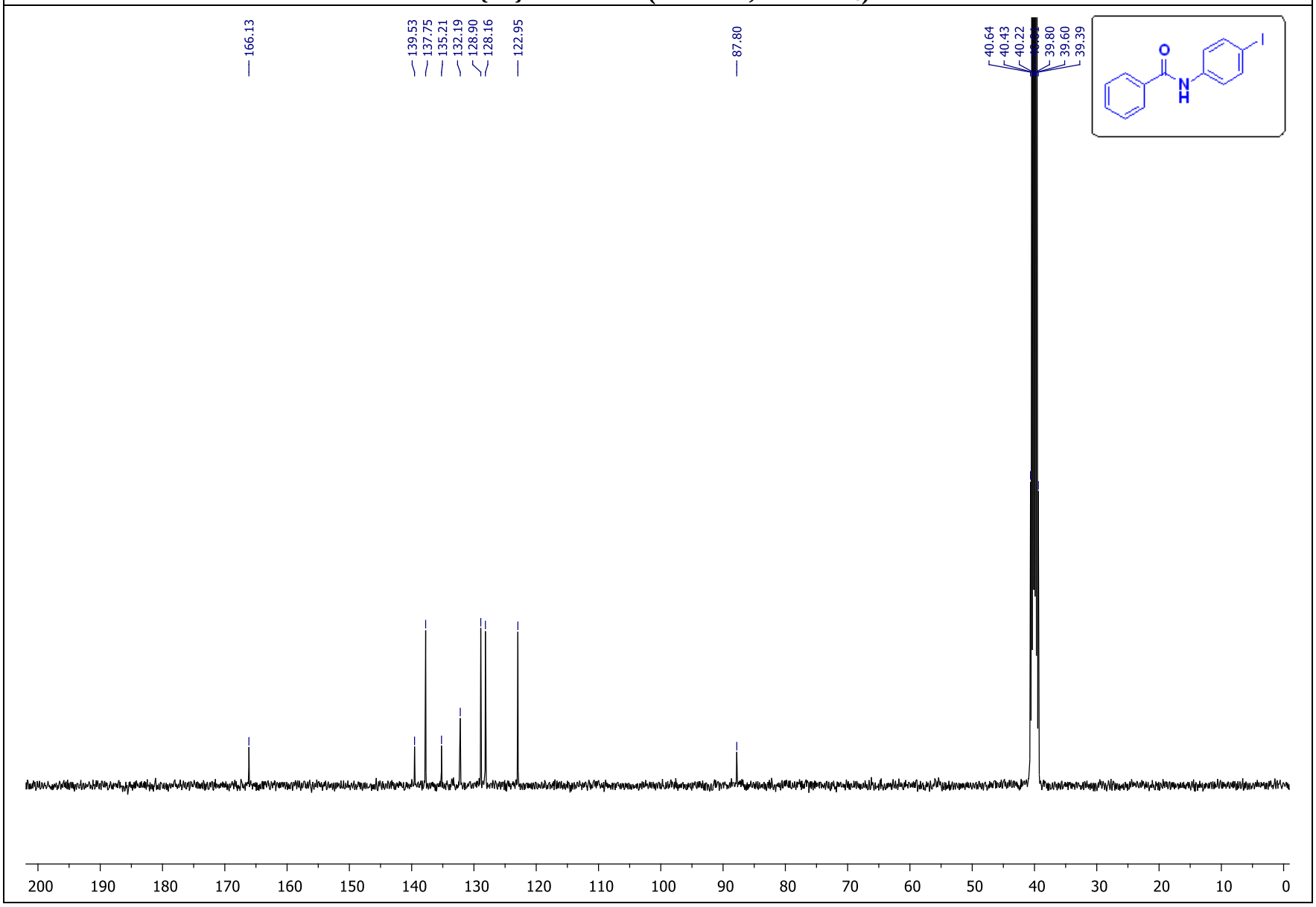
Fragmentor Voltage	Collision Energy	Ionization Mode
60	0	ESI



^{1}H NMR of 4w (400 MHz, DMSO-d$_6$)



$^{13}C\{^{1}H\}$NMR of 4w (101 MHz, DMSO-d_6)



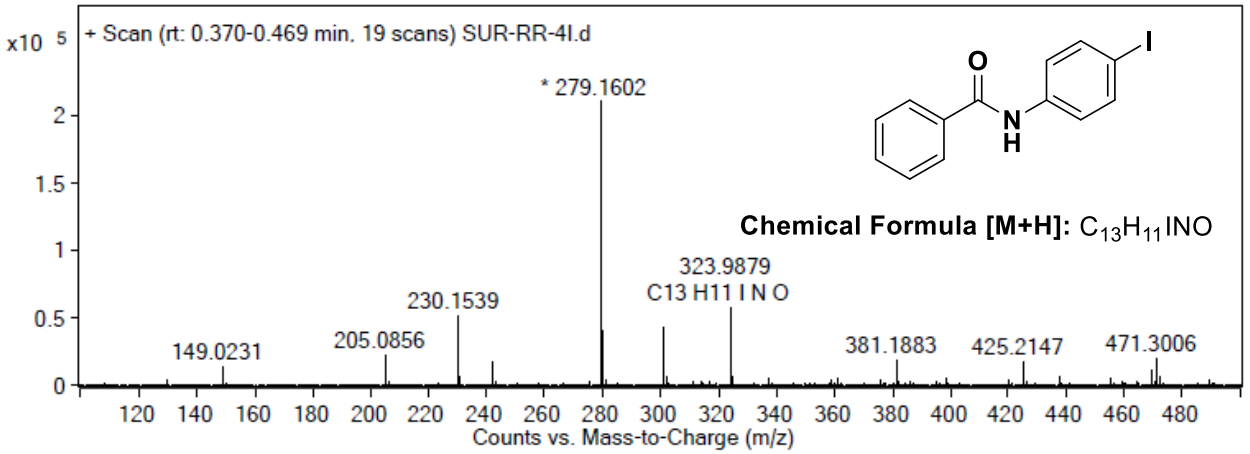
HRMS of 4w

Qualitative Analysis Report

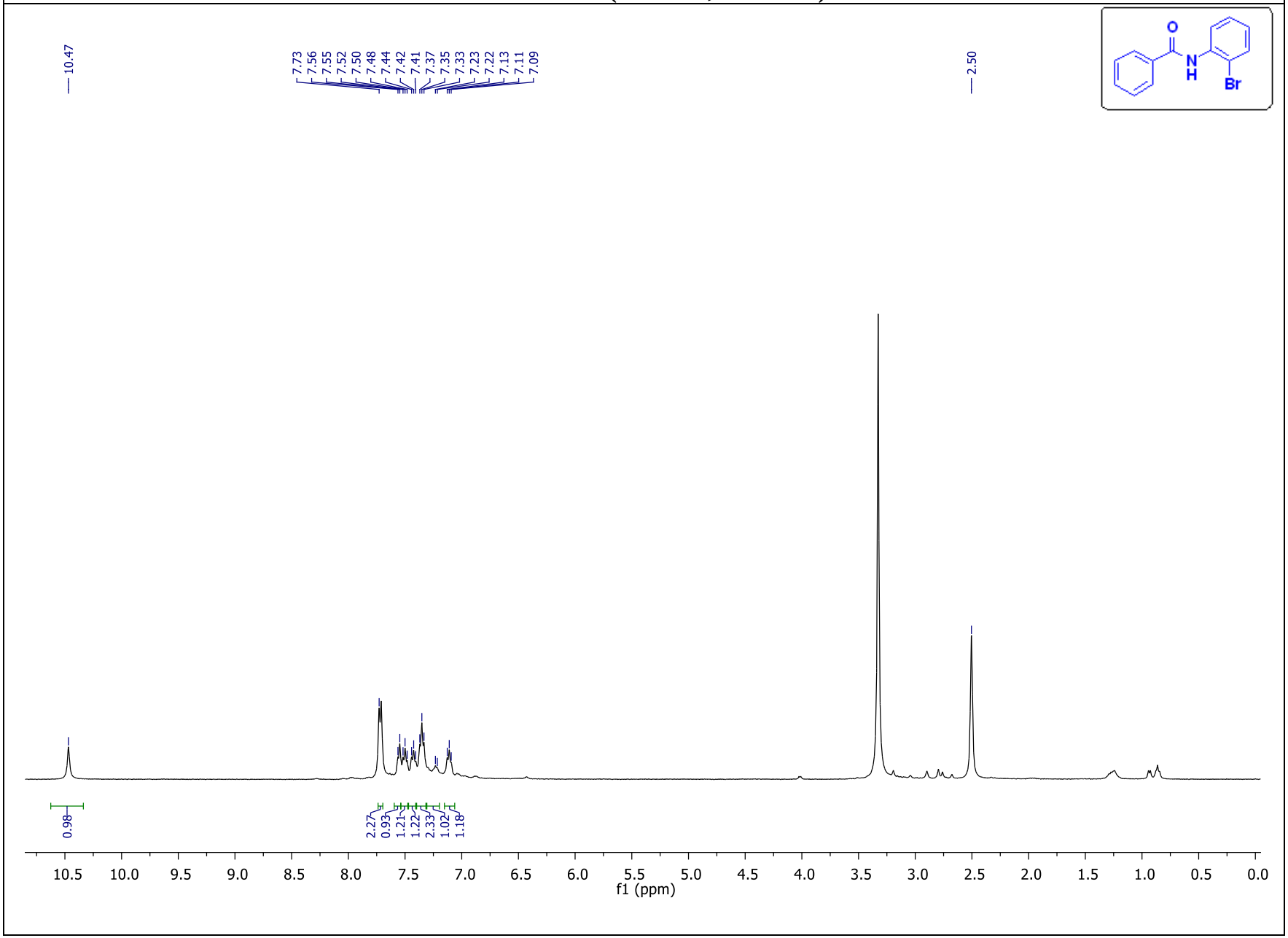
Data File	SUR-RR-4I.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	03-09-2021 15:42:36
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra

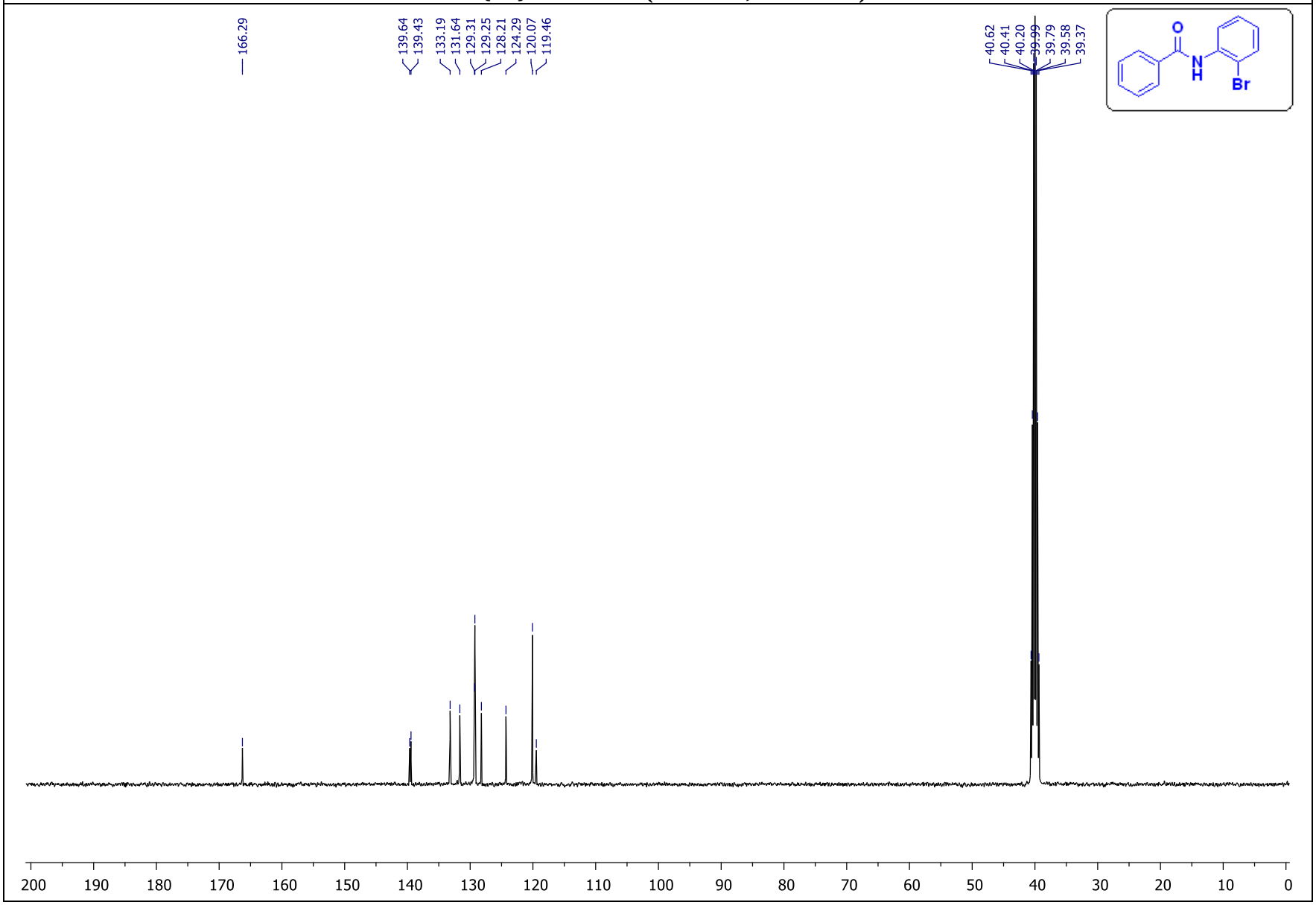
Fragmentor Voltage	Collision Energy	Ionization Mode
60	0	ESI



^{1}H NMR of 4x (400 MHz, DMSO-d_6)



$^{13}C\{^{1}H\}$NMR of 4x (101 MHz, DMSO-d_6)



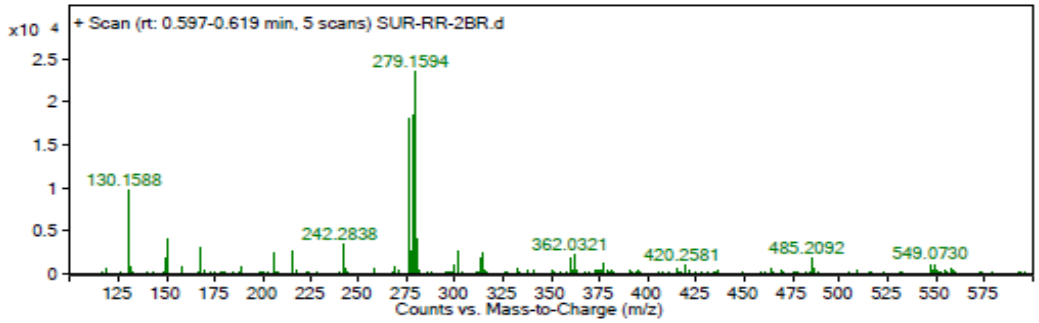
HRMS of 4x

Qualitative Analysis Report

Data File	SUR-RR-2BR.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	03-09-2021 12:08:40
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
60	0	ESI

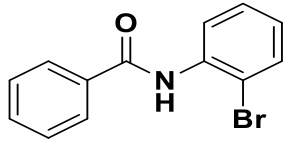


Peak List

m/z	z	Abund
279.1594	1	23432.78

Formula Calculator Element Limits

Element	Min	Max
C	10	15
H	0	60
O	0	2
N	0	2
S	0	0
Cl	0	0
Br	0	1

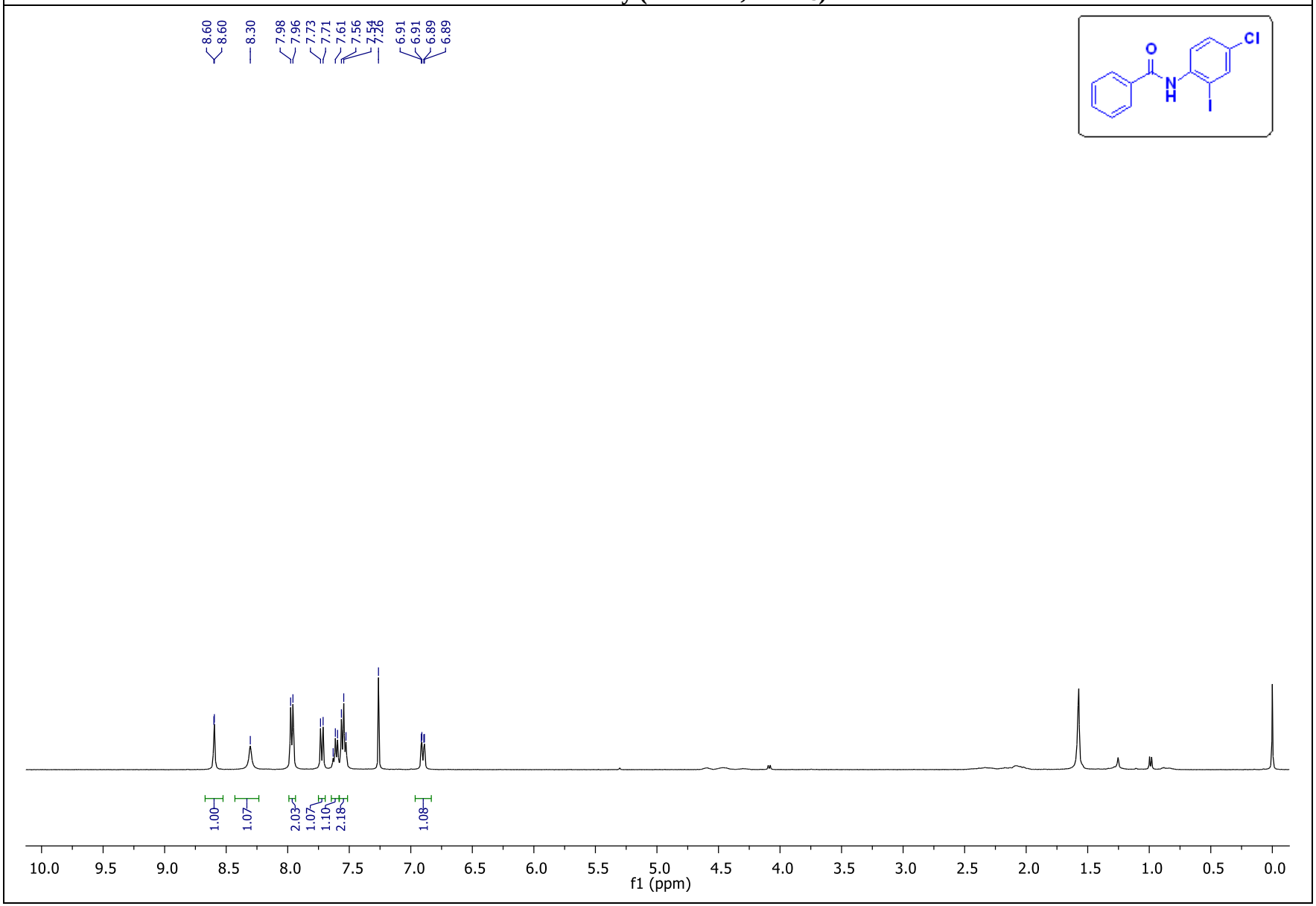


Chemical Formula [M+H]: $C_{13}H_{11}BrNO$

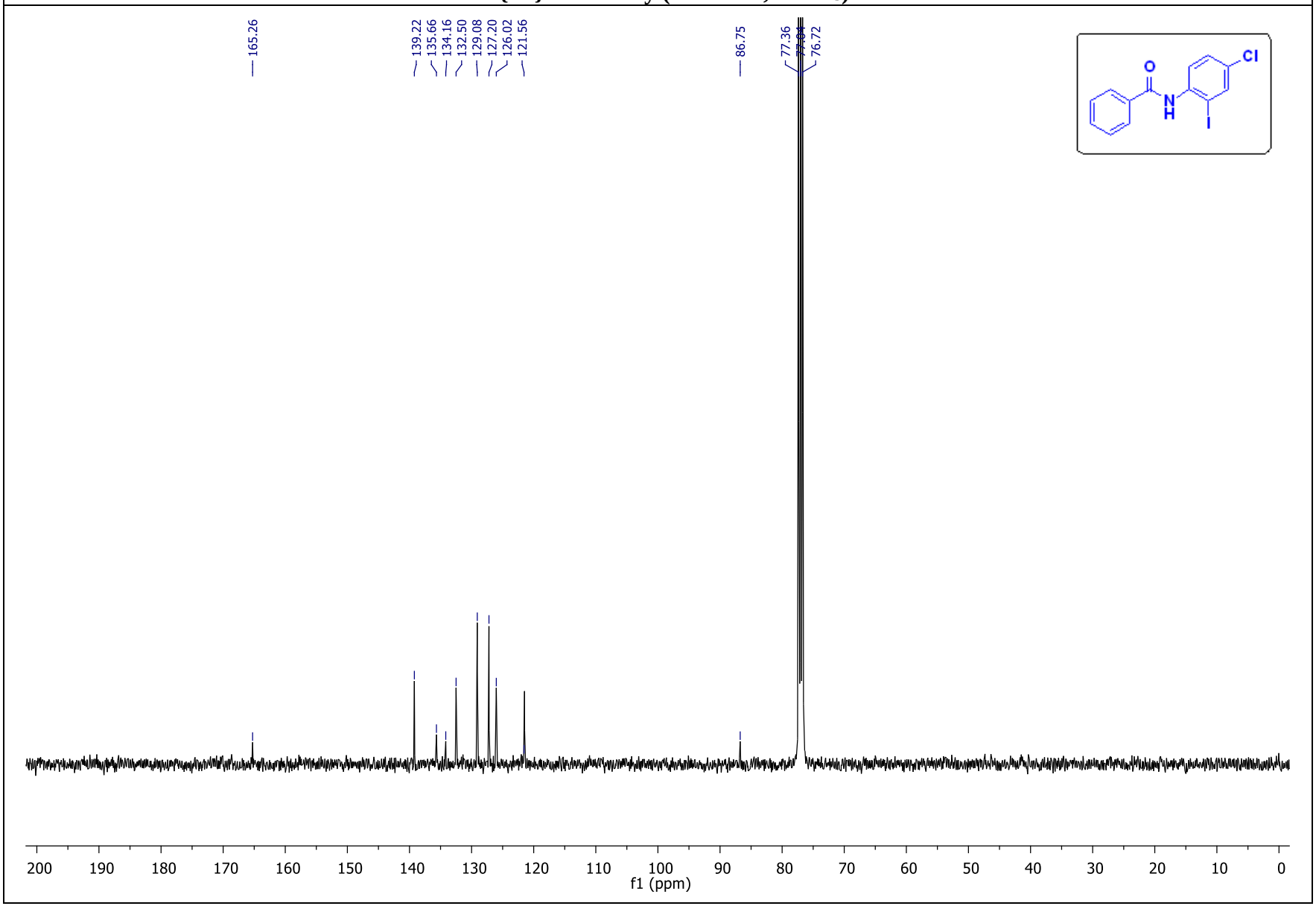
Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C13 H11 Br N O	True	276.00256	276.0024	-0.58	C13 H11 Br N O	98.35
C13 H10 Br N O	True	274.99474	274.99458	-0.58	C13 H11 Br N O	98.35

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



$^{13}C\{^{1}H\}$NMR of 4y (101 MHz, $CDCl_3$)



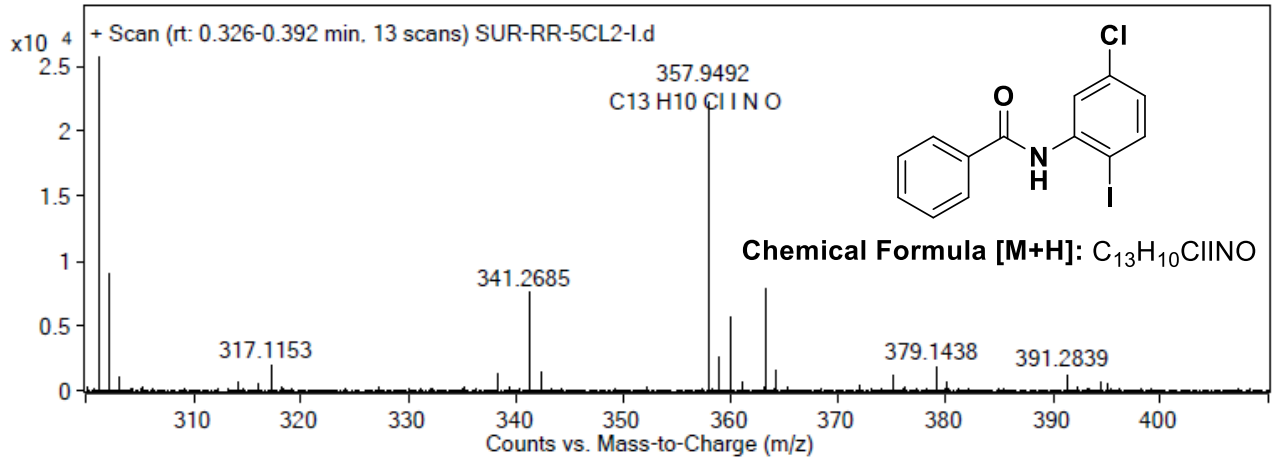
HRMS of 4y

Qualitative Analysis Report

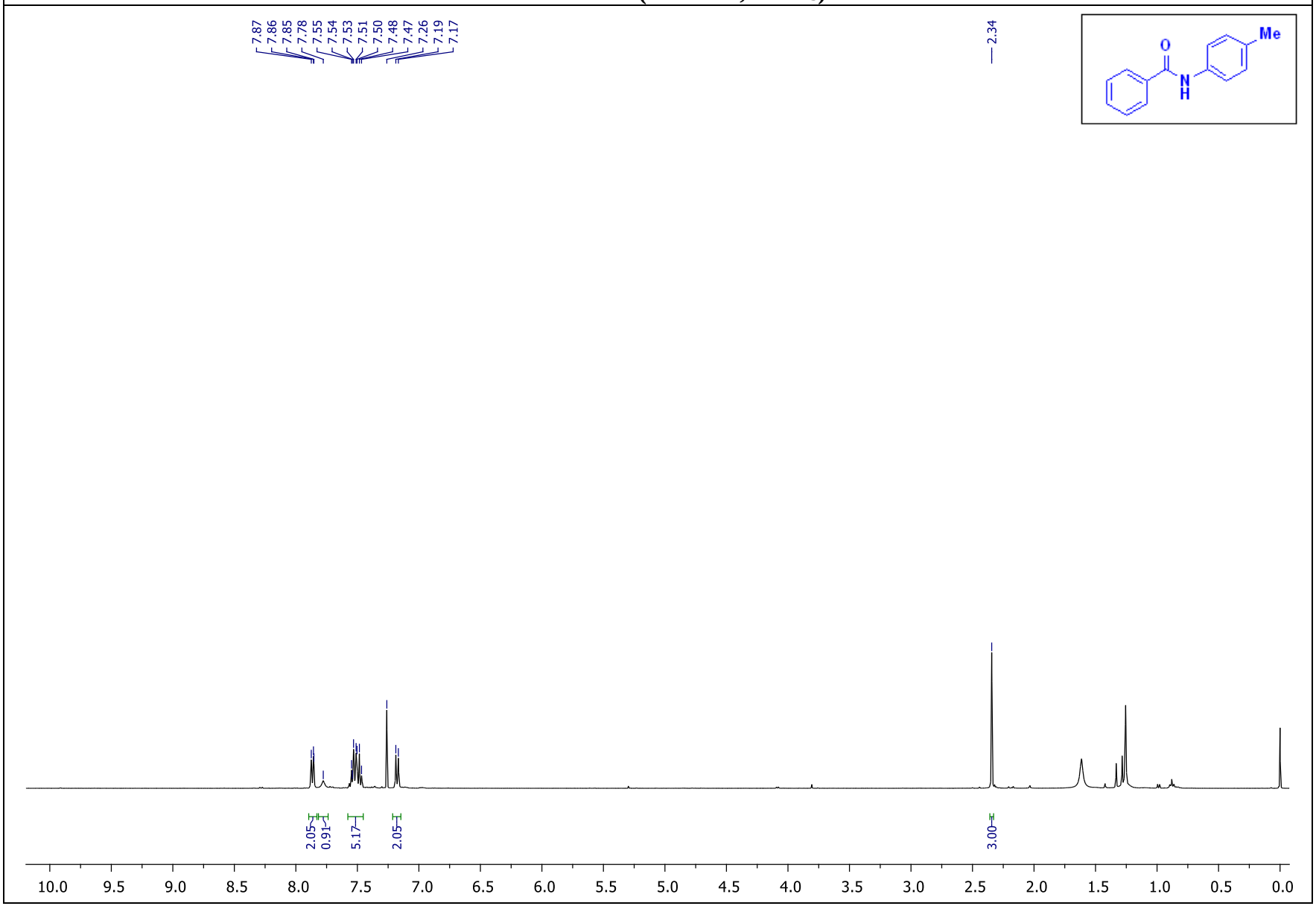
Data File	SUR-RR-5CL2-I.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	03-09-2021 12:05:26
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra

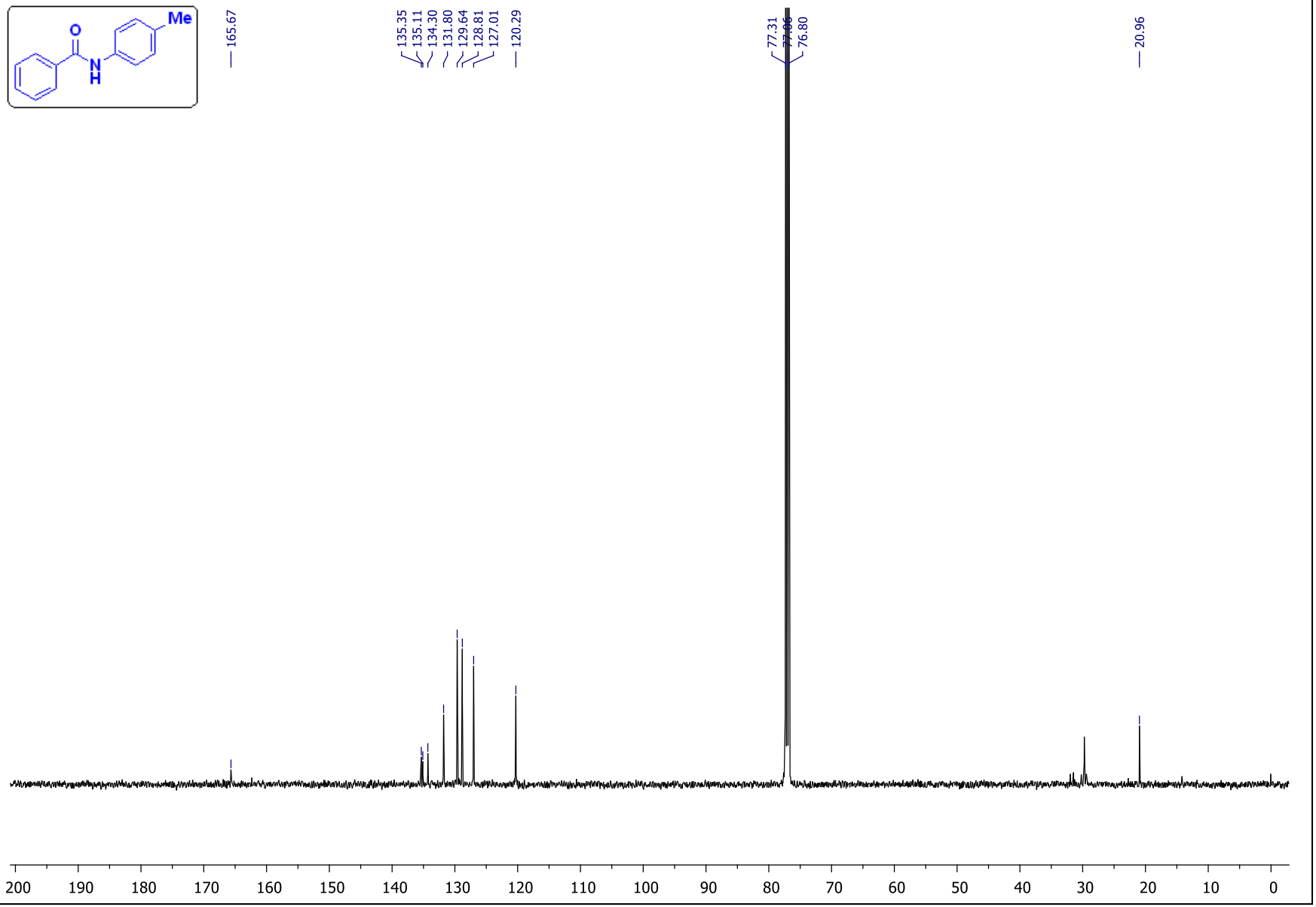
Fragmentor Voltage	Collision Energy	Ionization Mode
60	0	ESI



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



$^{13}C\{^{1}H\}$NMR of 4z (101 MHz, $CDCl_3$)



HRMS of 4z

D:\HRMS\...\20-10-2021\SUR-RR-4MEN

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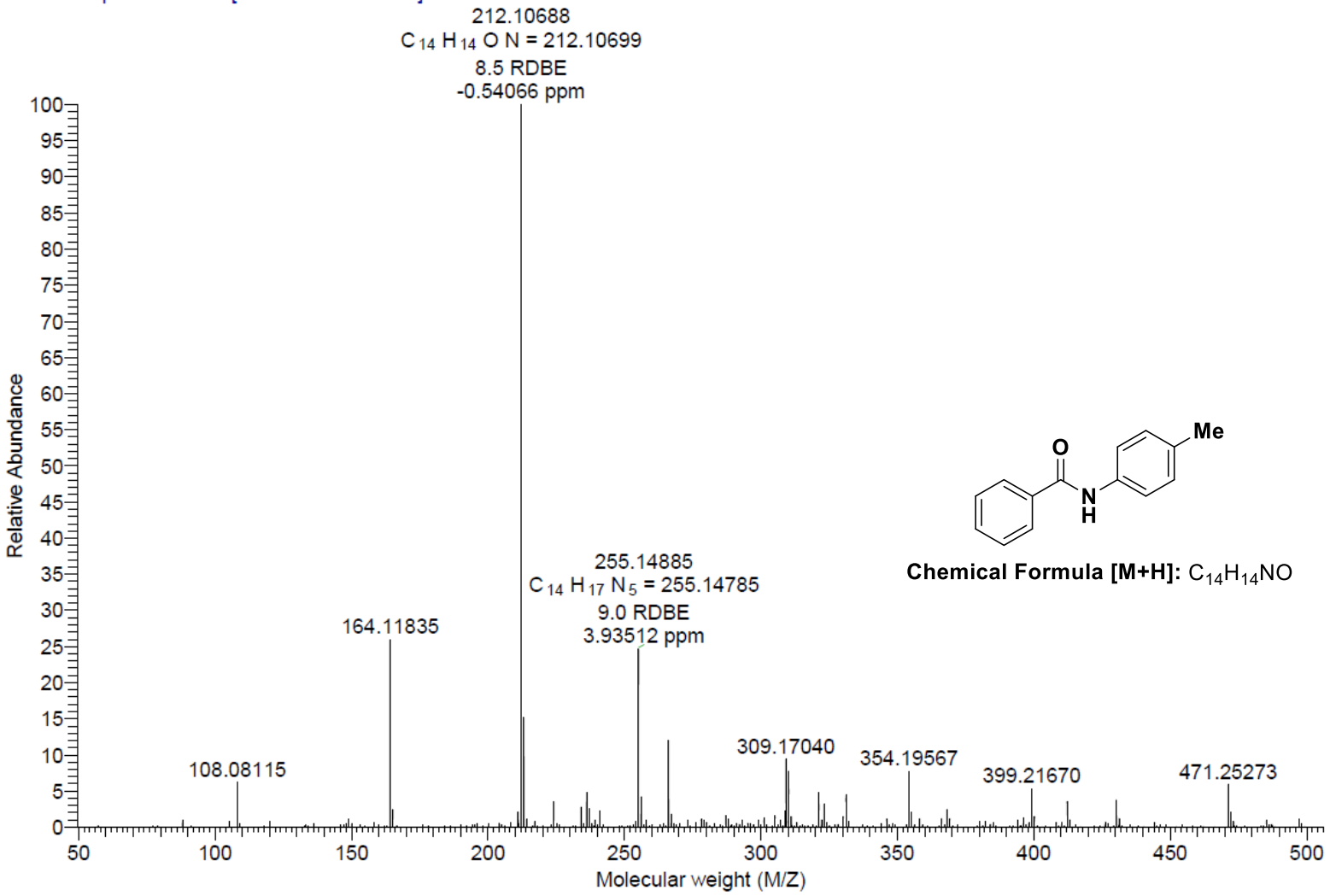
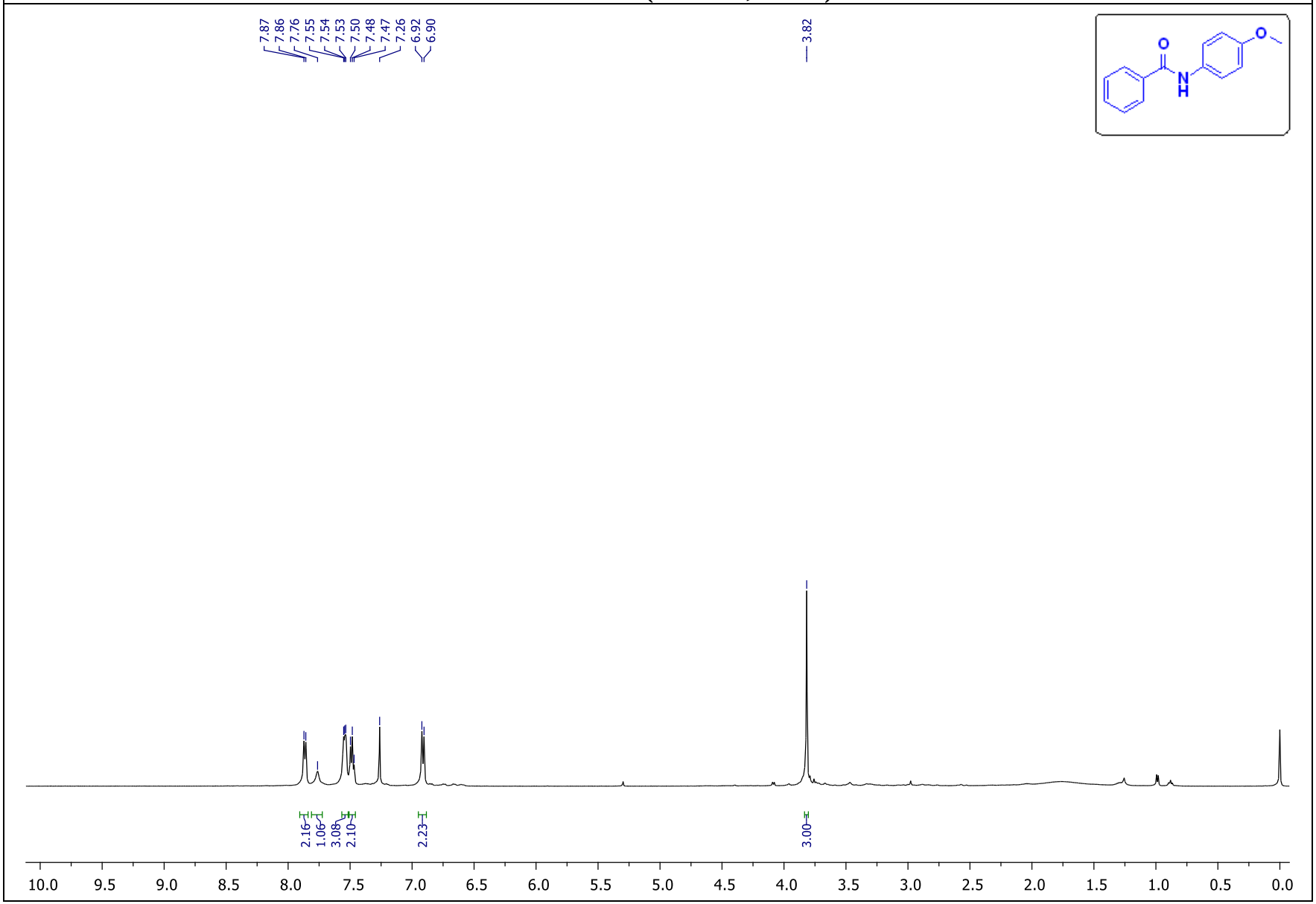
10/20/21 14:15:35
1180101101
SUR-RR-4MEN #80-111 RT: 0.18-0.25 AV: 32 SB: 184 1.16-1.58 NL: 1.31E8
T: FTMS + p ESI Full ms [50.0000-1600.0000]

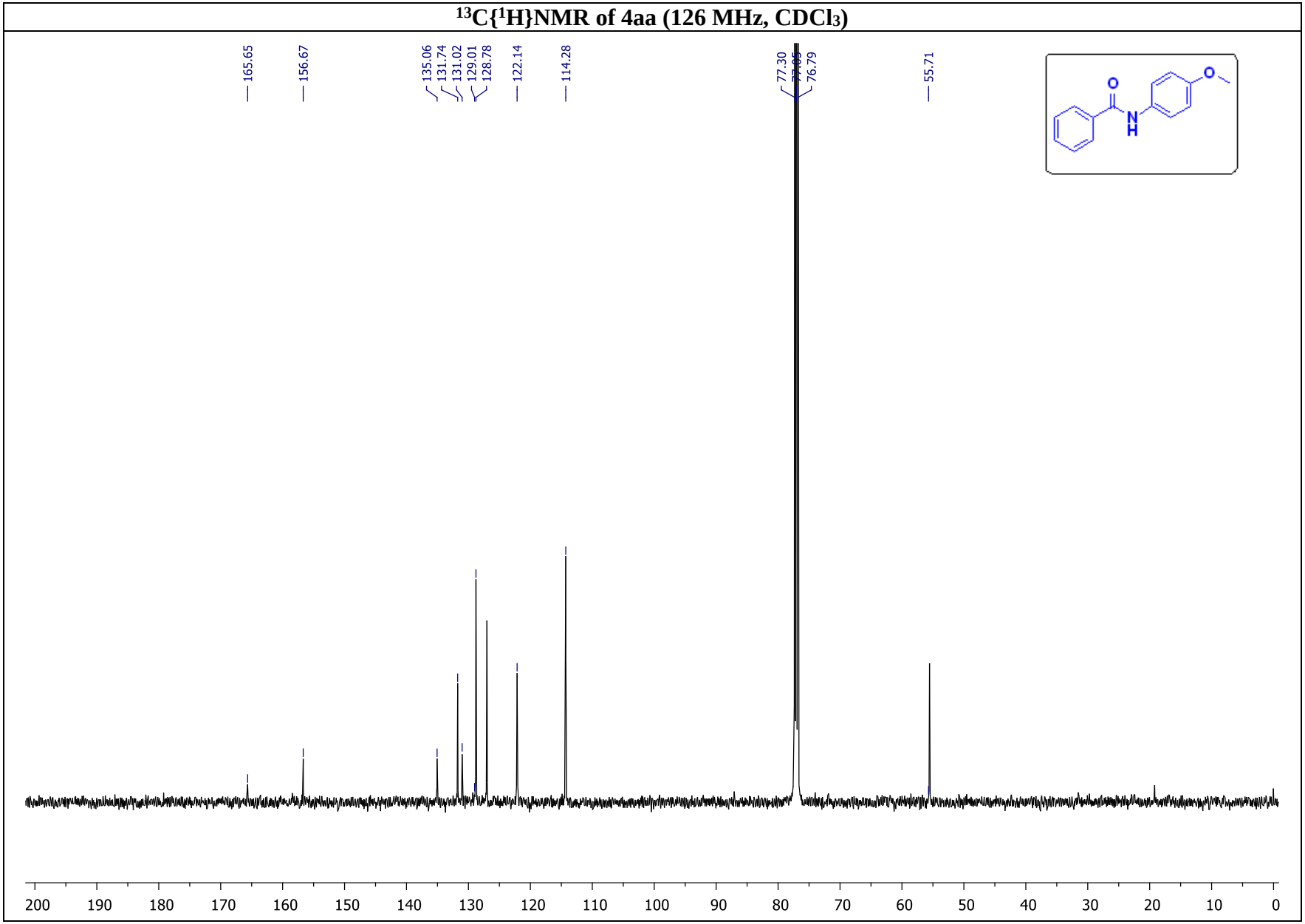


Chemical Formula [M+H]: $C_{14}H_{14}NO$

^{1}H NMR of 4aa (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$NMR of 4aa (126 MHz, $CDCl_3$)



HRMS of 4aa

BCSUR-RR-4OMEAN

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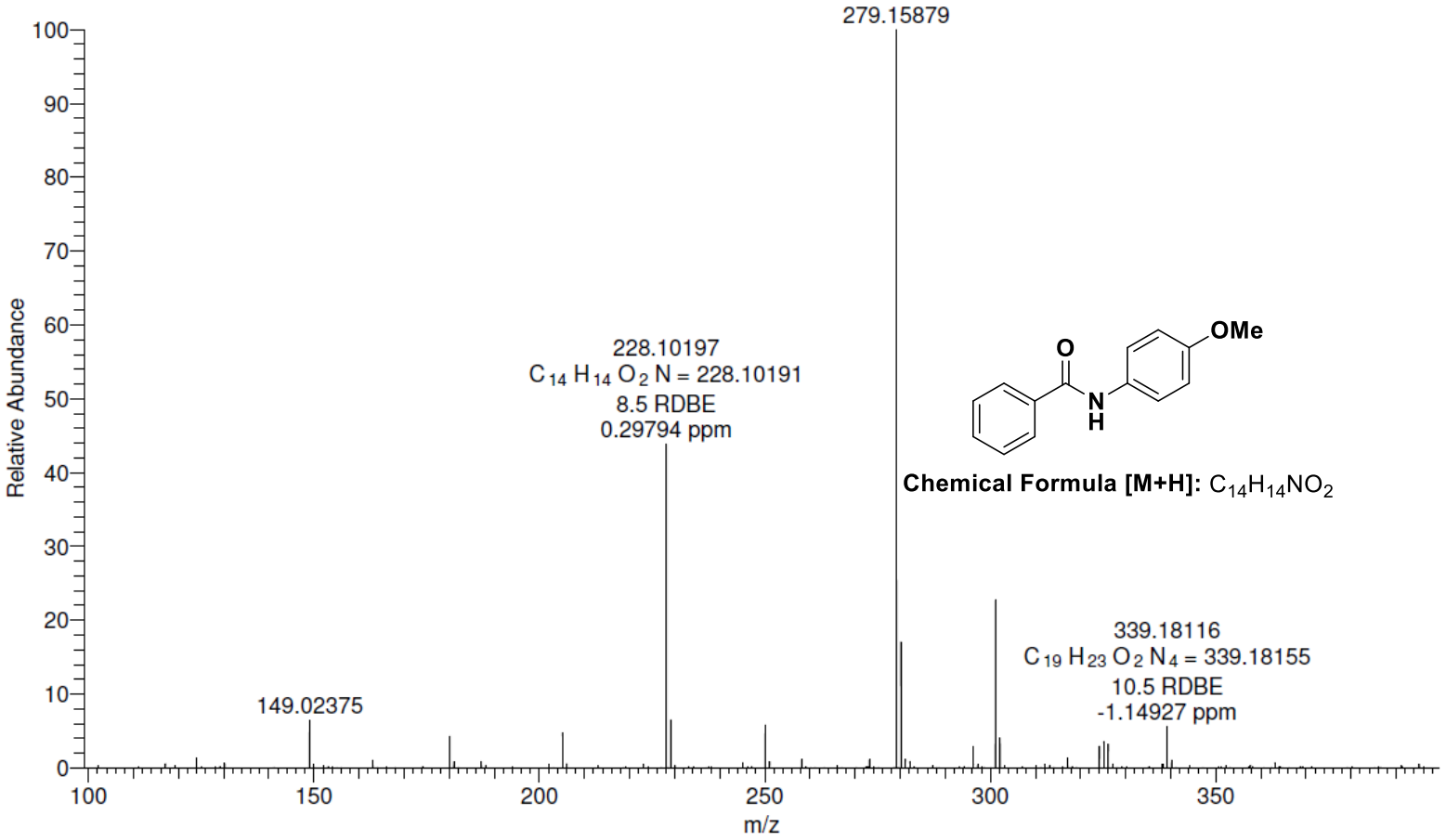
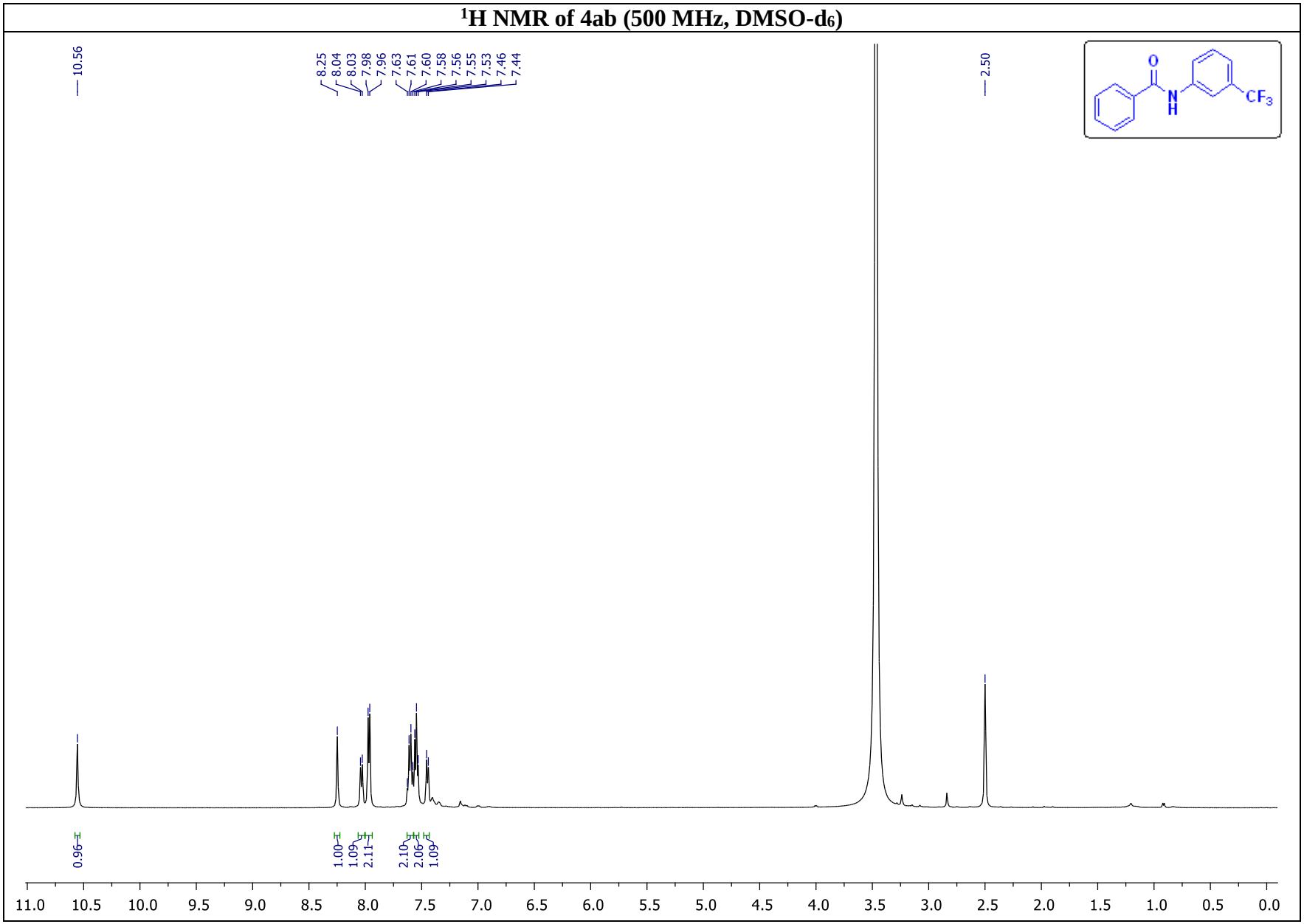
3/16/2021 5:14:17 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

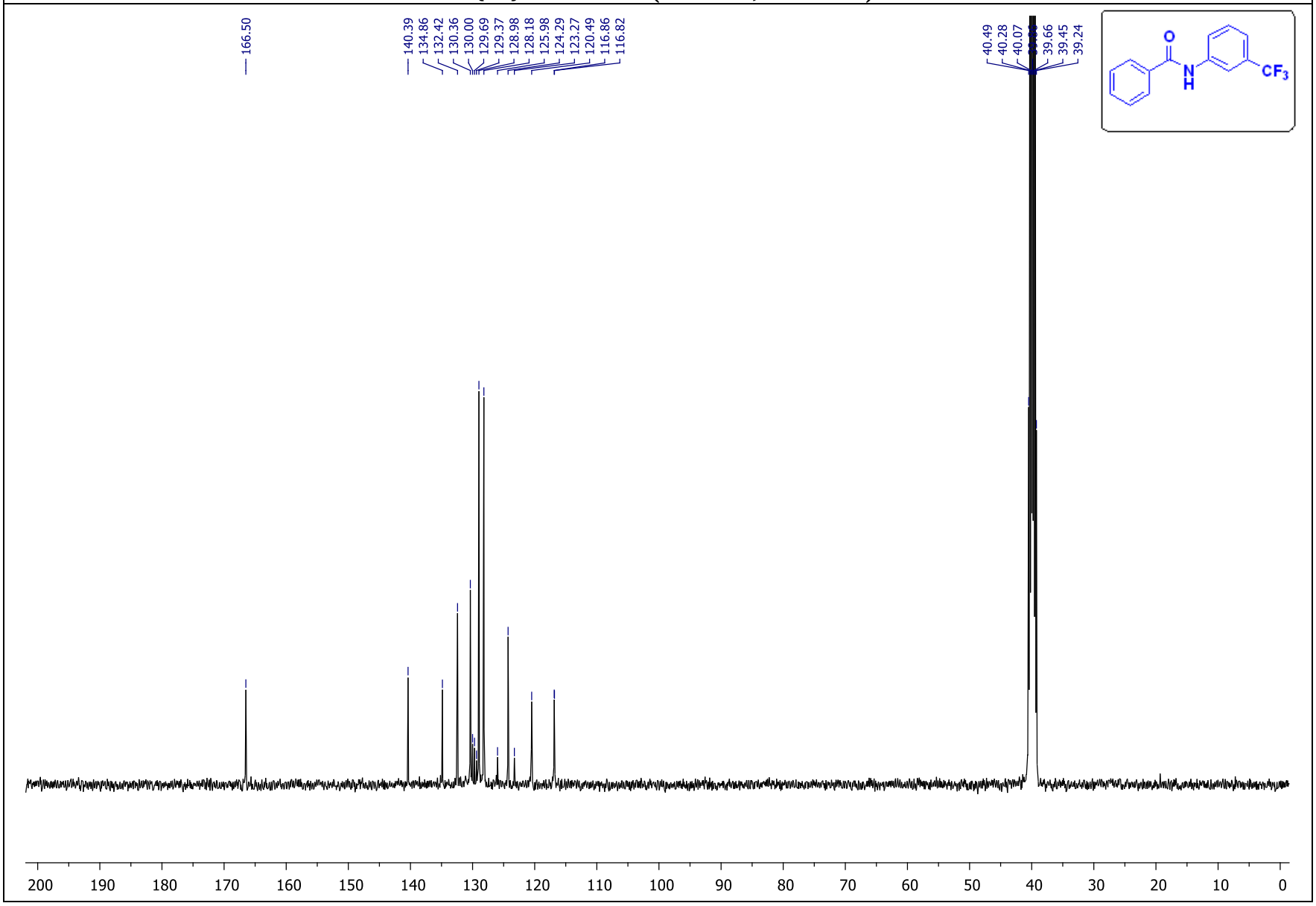
BCSUR-RR-4OMEAN #8-20 RT: 0.06-0.14 AV: 13 SB: 40 0.37-0.67 NL: 8.99E7
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



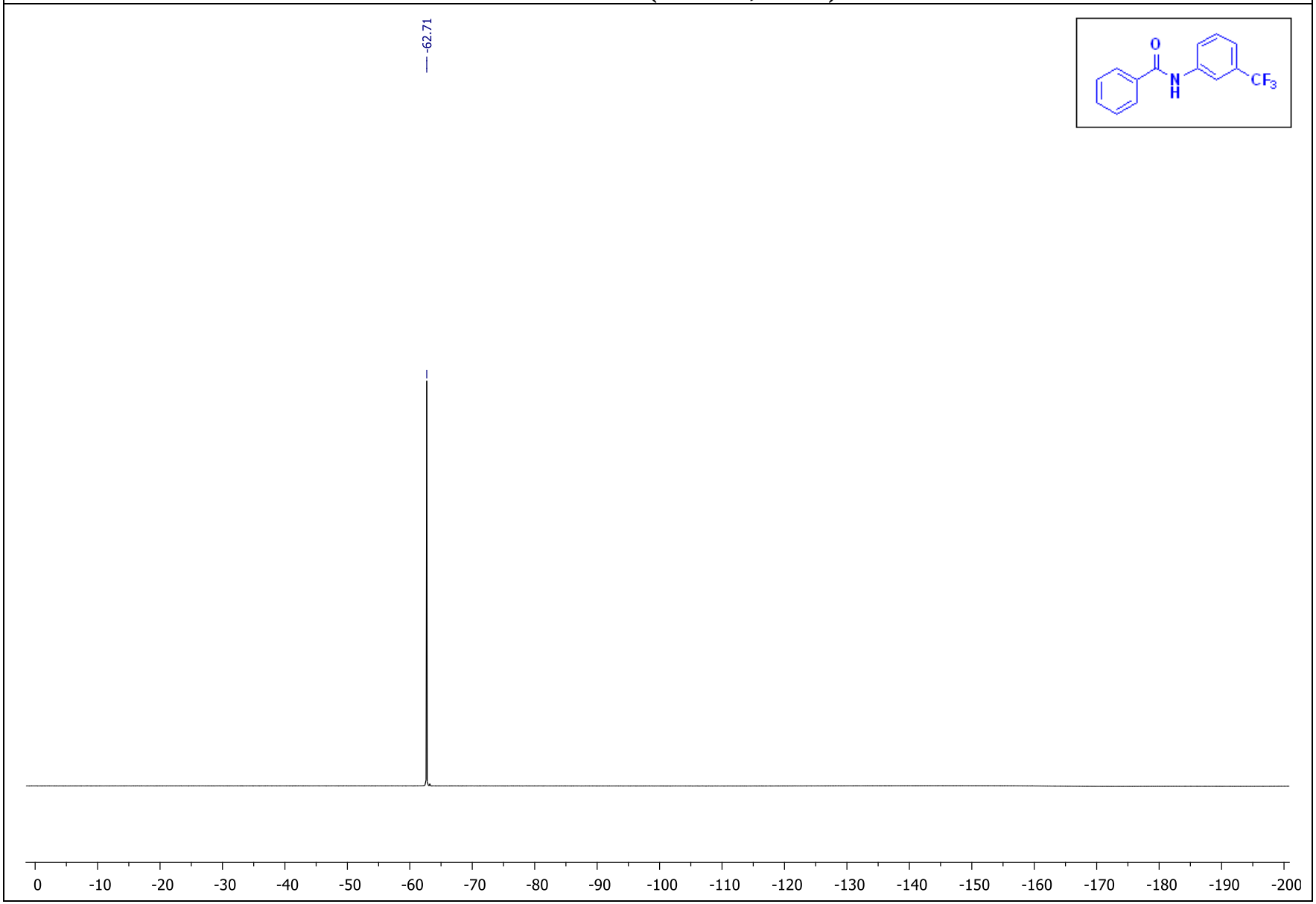
^{1}H NMR of 4ab (500 MHz, DMSO-d$_6$)



$^{13}C\{^{1}H\}$NMR of 4ab (101 MHz, DMSO-d_6)



^{19}F-NMR of 4ab (376 MHz, $CDCl_3$)



HRMS of 4ab

SUR--RR-3CF3

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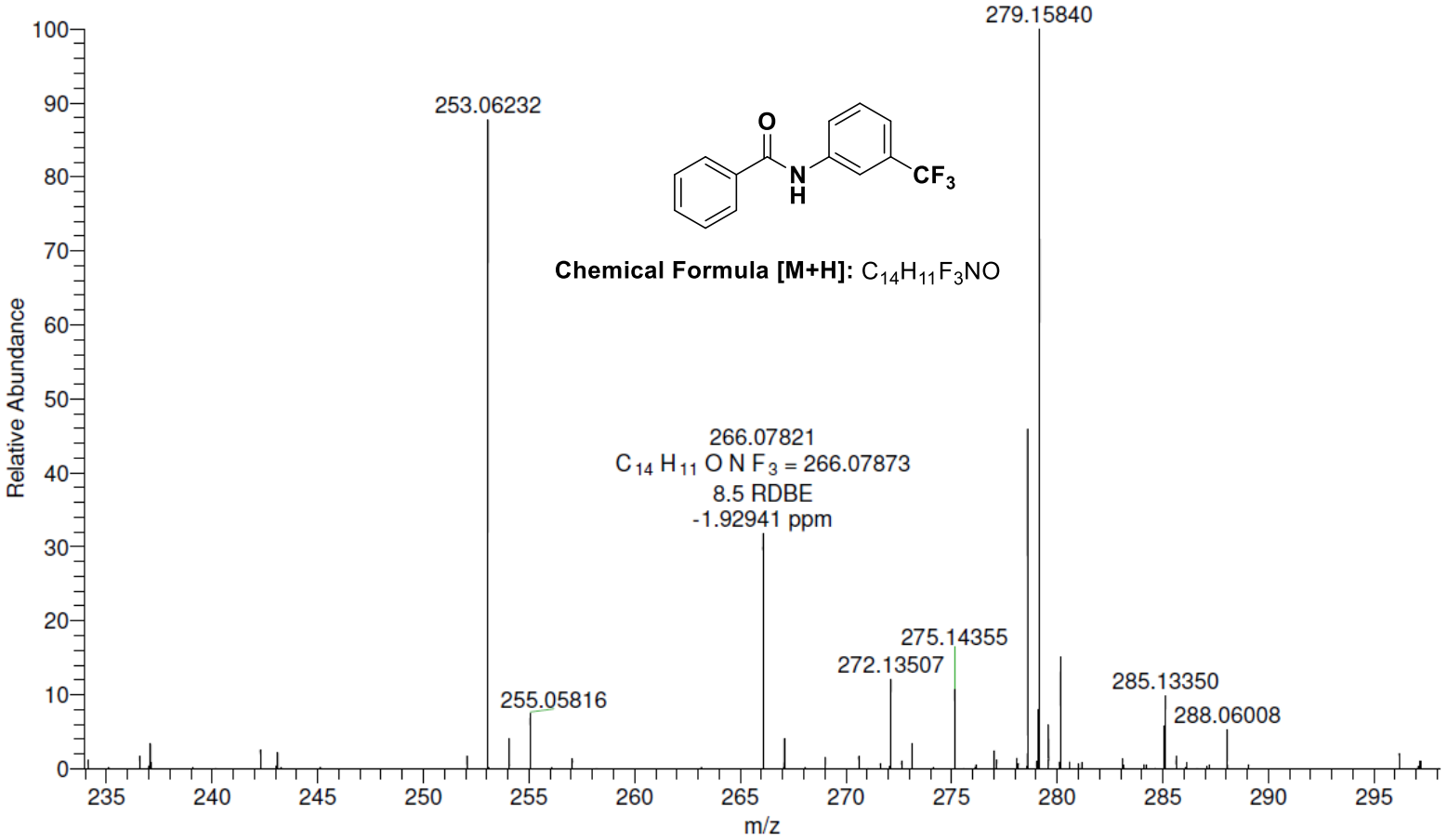
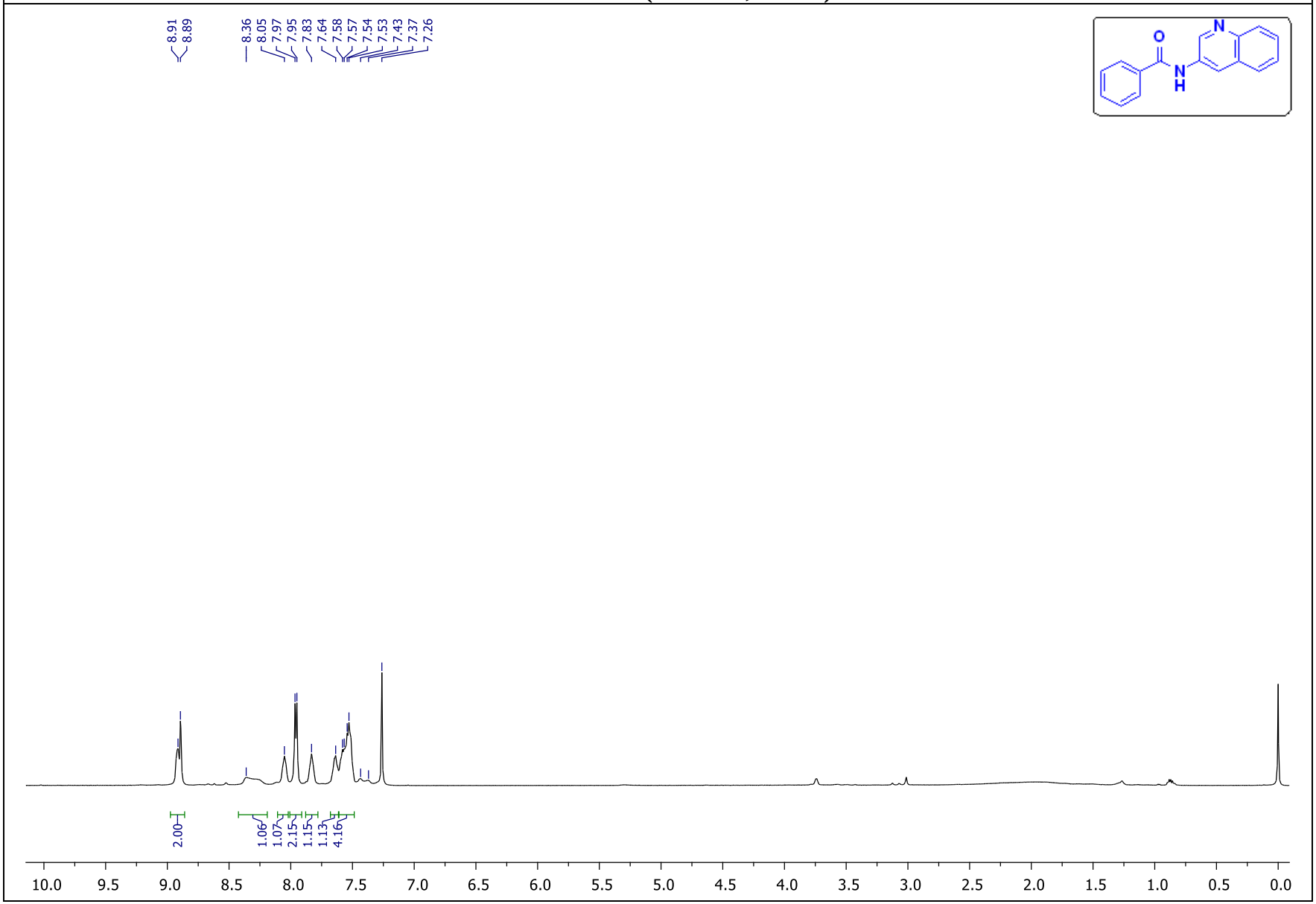
DEPARTMENT OF ANALYTICAL& STRUCTURAL CHEMISTRY

3/16/2021 5:21:49 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

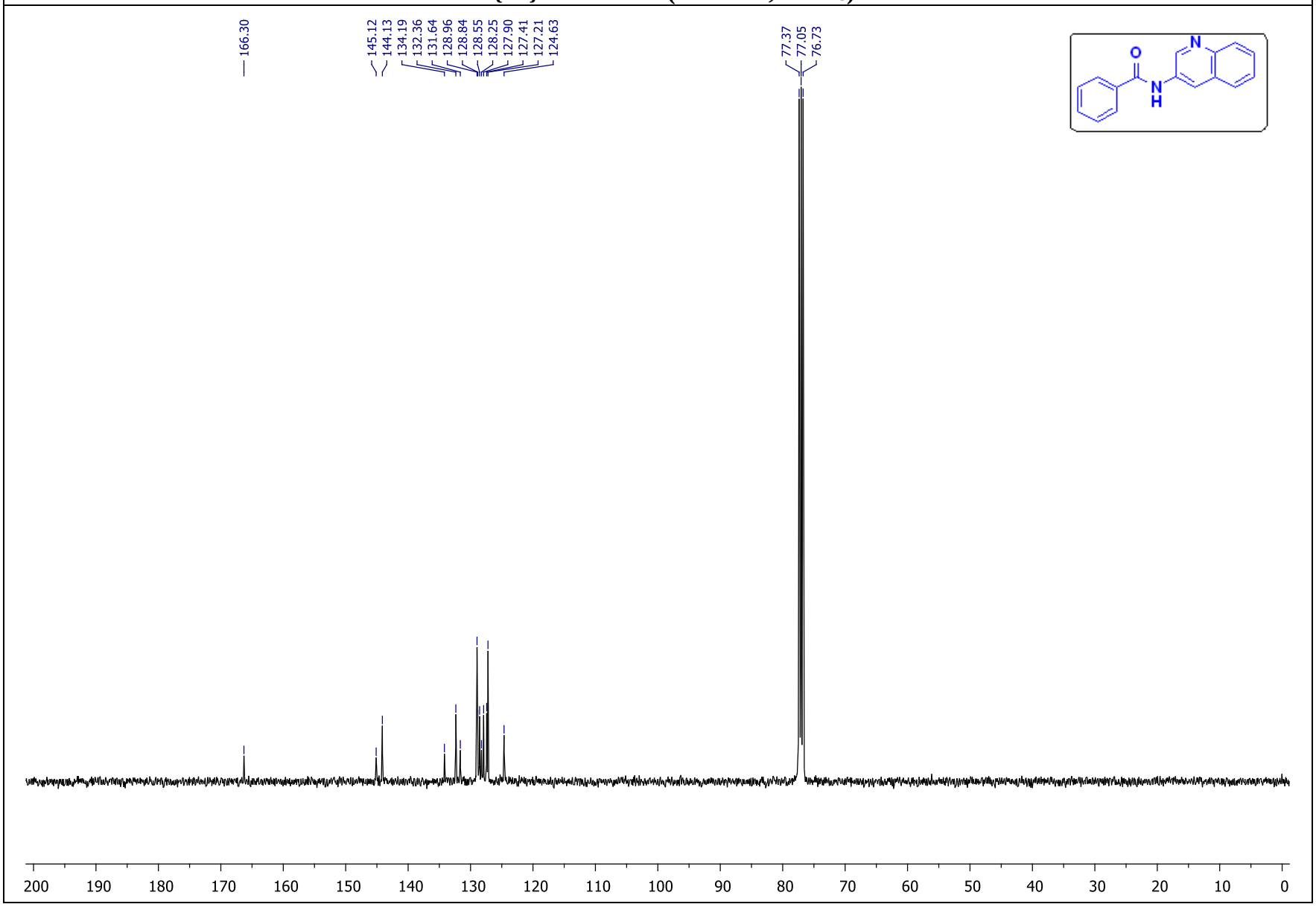
SUR--RR-3CF3 #11-25 RT: 0.08-0.18 AV: 15 SB: 41 0.37-0.67 NL: 4.10E6
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



^{1}H NMR of 4ac (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$NMR of 4ac (101 MHz, $CDCl_3$)

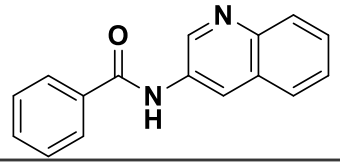


HRMS of 4ac

Qualitative Analysis Report

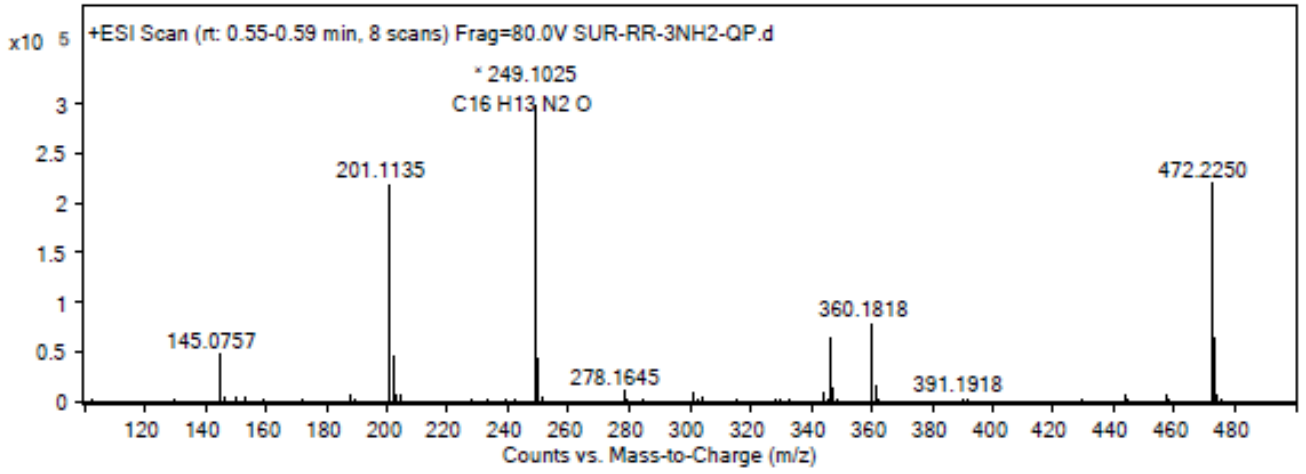
Data File	SUR-RR-3NH2-QP.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	07-07-2021 12:15:29
IRM Calibration Status	Success	**DA Method**	11.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra

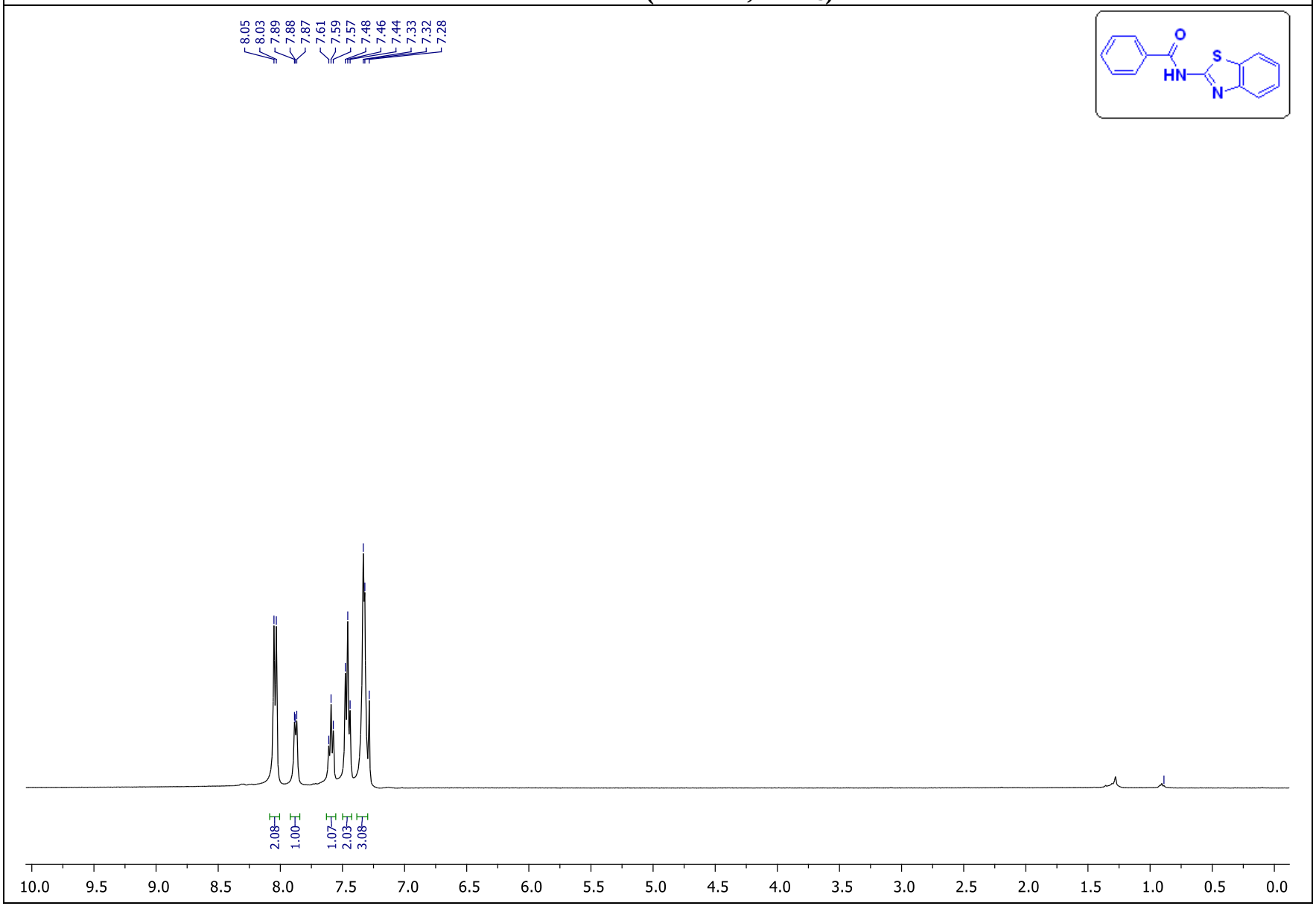


Fragmentor Voltage	Collision Energy	Ionization Mode
80	0	ESI

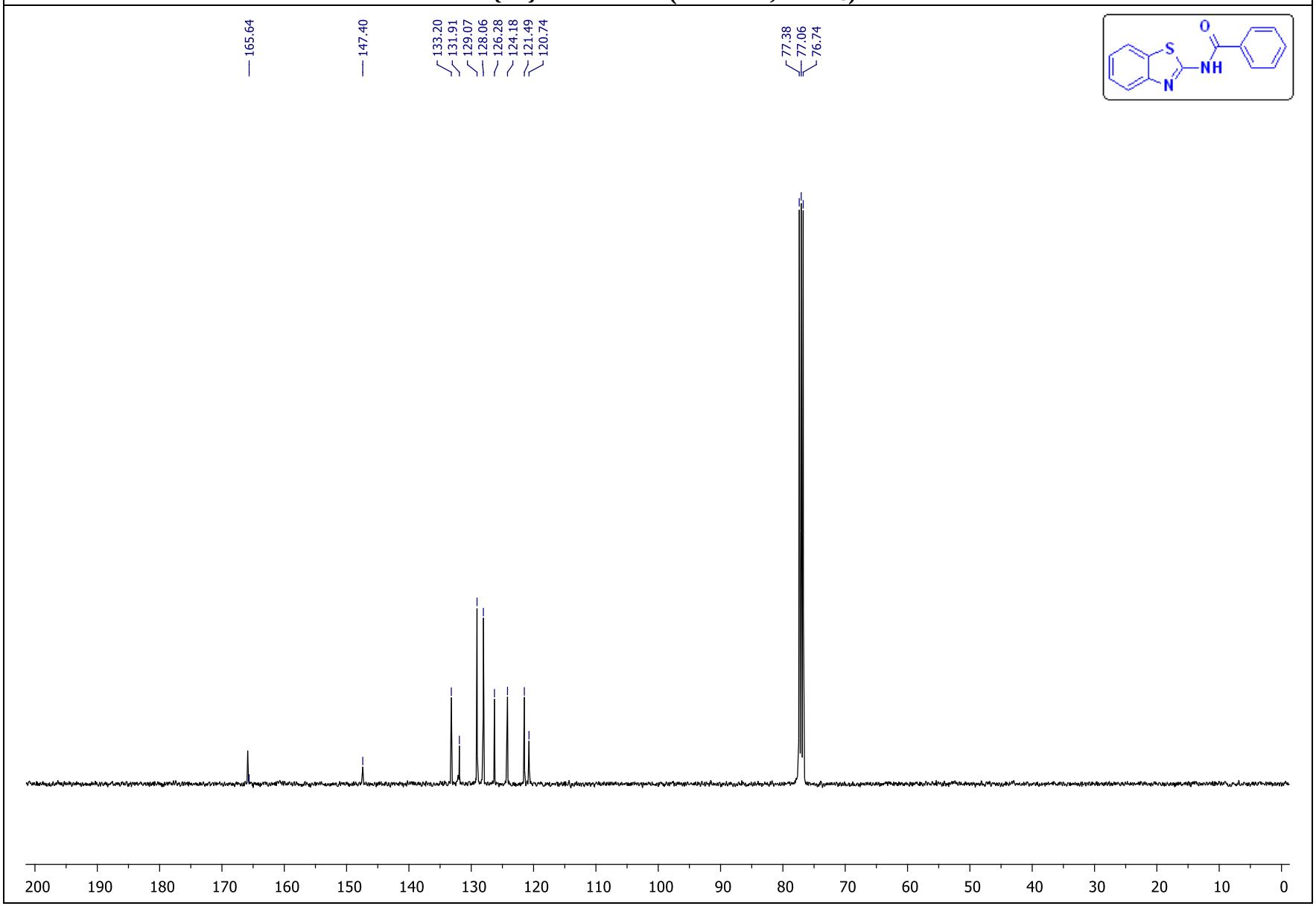
Chemical Formula [M+H]: $C_{16}H_{13}N_2O$



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



$^{13}C\{^{1}H\}$NMR of 4ad (101 MHz, $CDCl_3$)



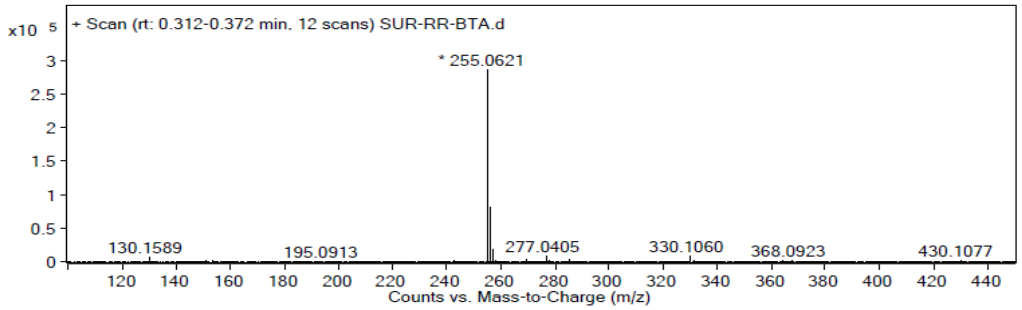
HRMS of 4ad

Qualitative Analysis Report

Data File	SUR-RR-BTA.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	03-09-2021 12:13:58
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

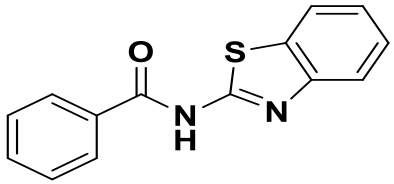
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
60	0	ESI



Peak List

m/z	z	Abund
255.0621	1	286324.84



Chemical Formula [M+H]: $C_{14}H_{11}N_2OS$

Formula Calculator Element Limits

Element	Min	Max
C	10	15
H	0	60
O	0	3
N	0	2
S	0	1
Cl	0	0
Br	0	1

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C14 H12 N O2 S	True	258.05829	258.05887	2.25	C14 H12 N O2 S	64.16
C14 H11 N O2 S	True	257.05047	257.05105	2.25	C14 H12 N O2 S	64.16
C11 H18 N2 O S	False	226.11252	226.11398	6.49	C11 H18 N2 Na O S	61.47

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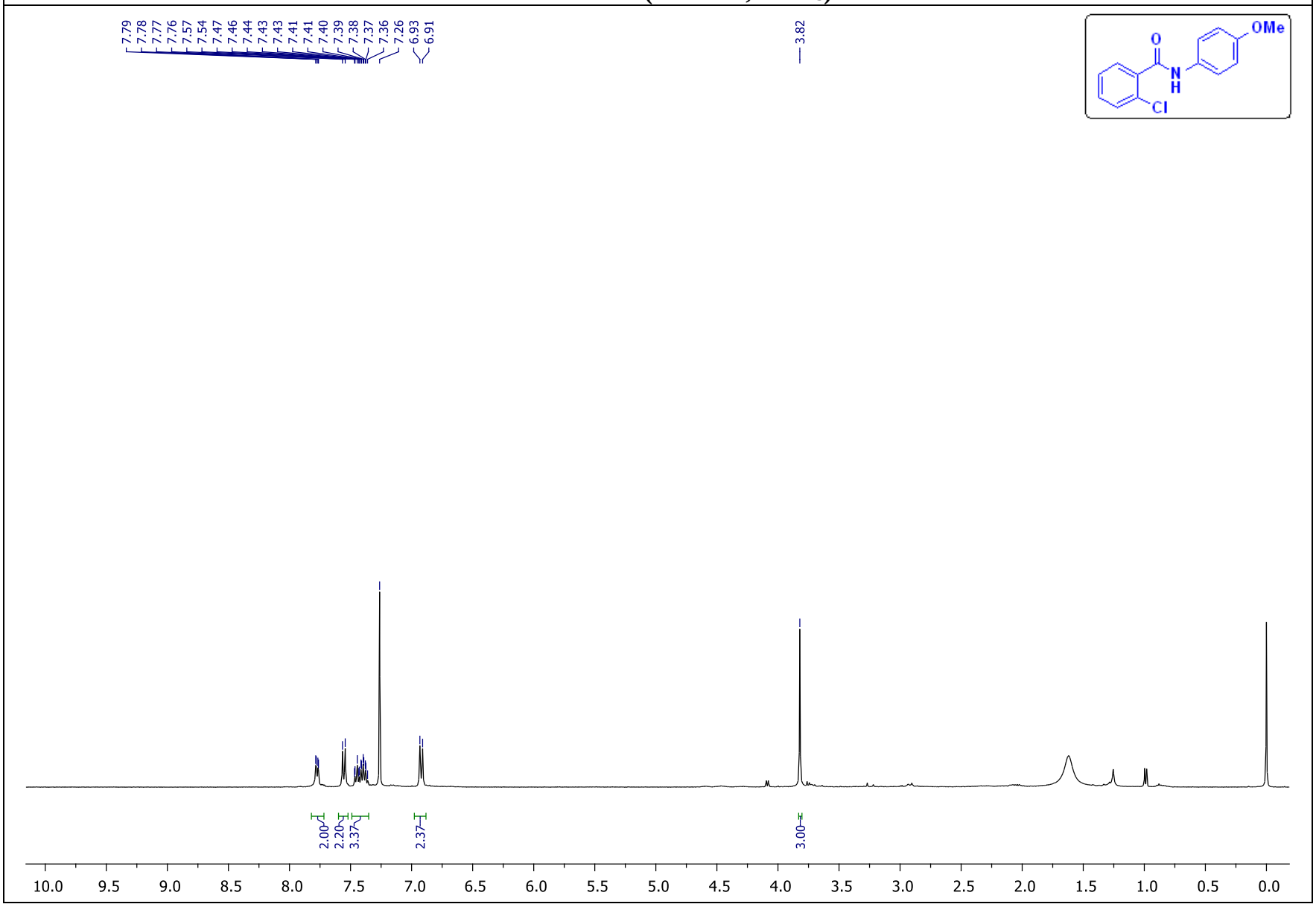
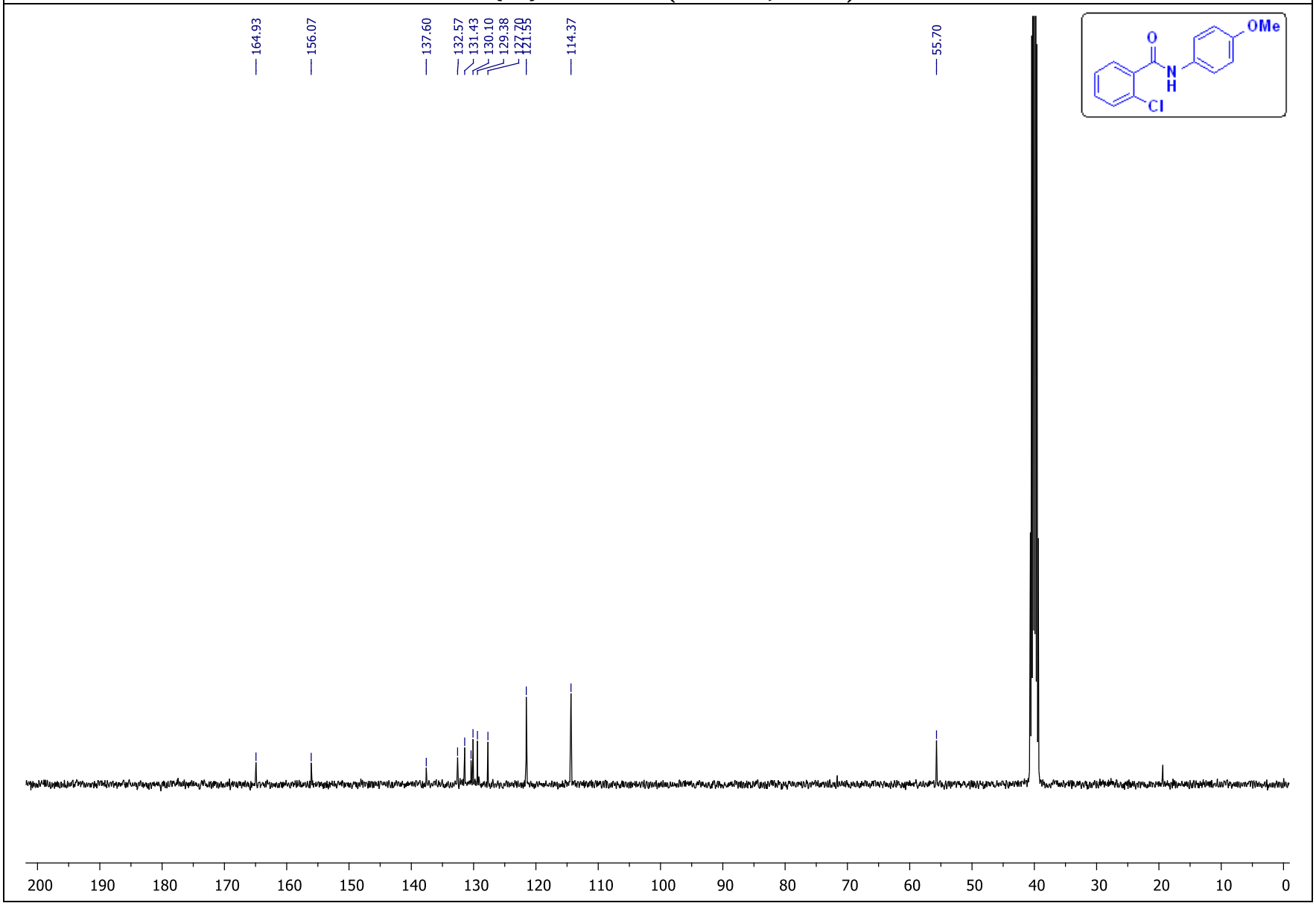
Agilent Technologies

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



$^{13}C\{^{1}H\}$NMR of 4ae (101 MHz, $CDCl_3$)



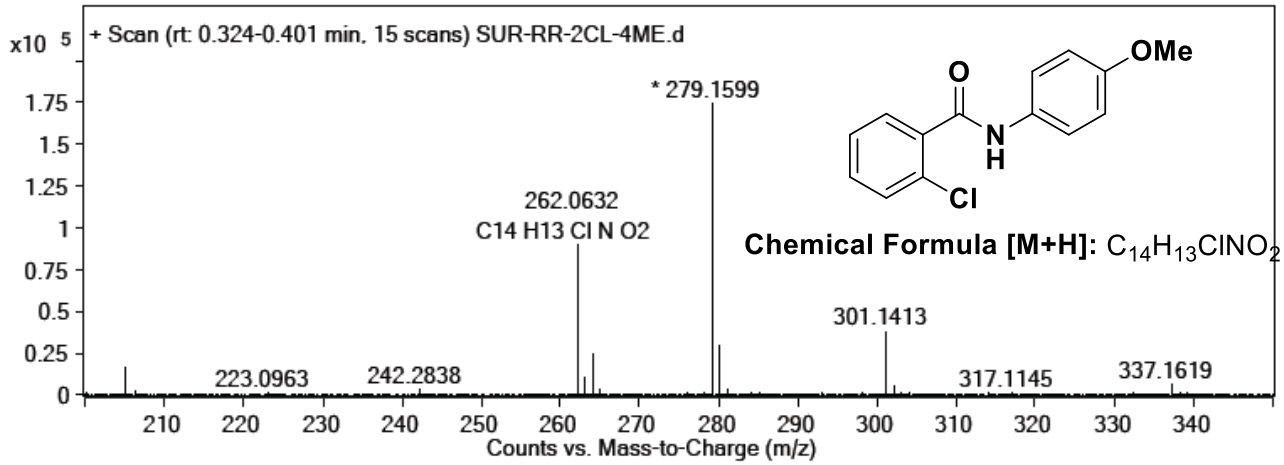
HRMS of 4ae

Qualitative Analysis Report

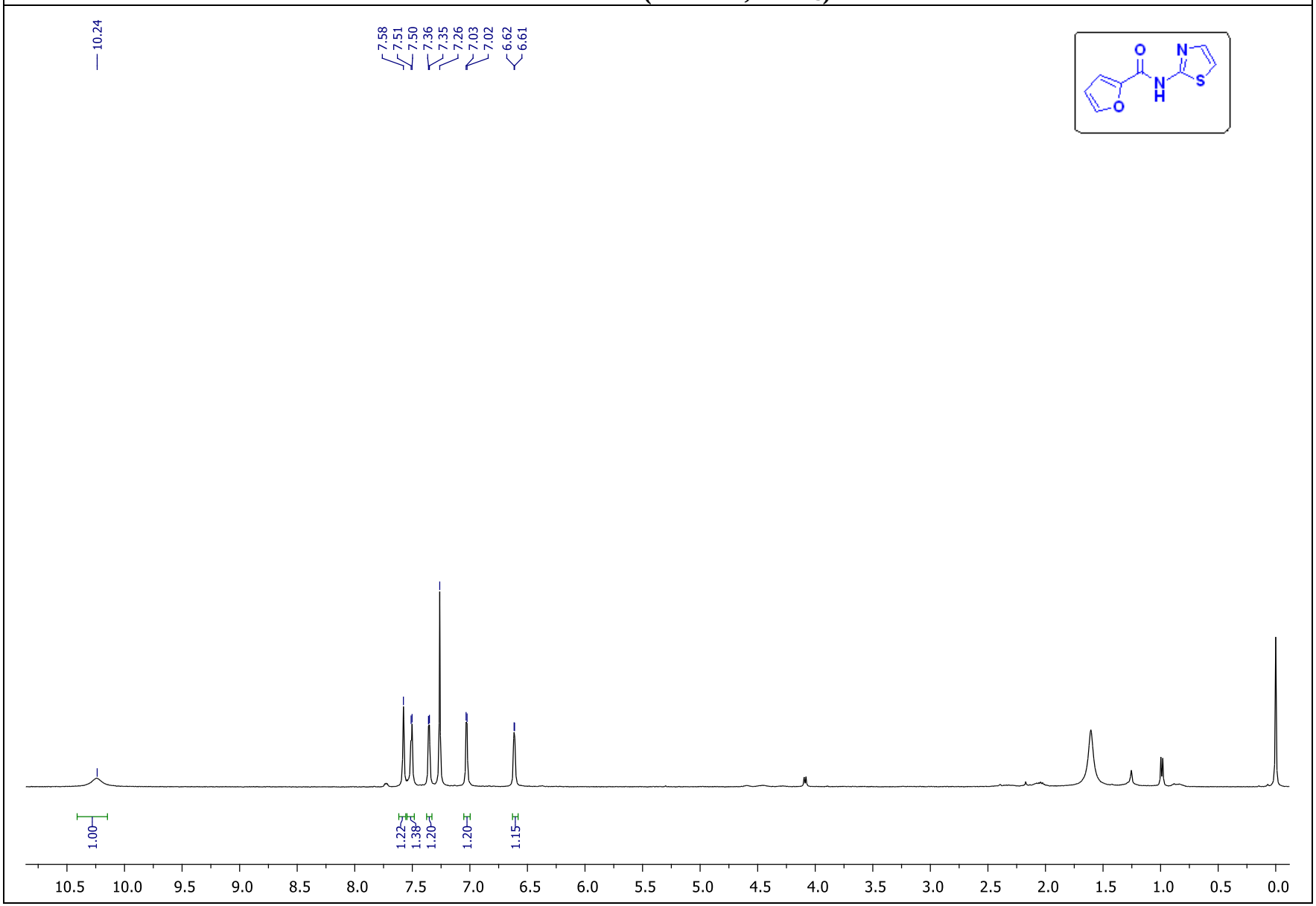
Data File	SUR-RR-2CL-4ME.d	**Sample Name**	
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	CSIR-IICT\Analyst
Acq Method	hrms-pos-method.m	**Acquired Time**	03-09-2021 12:15:47
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra

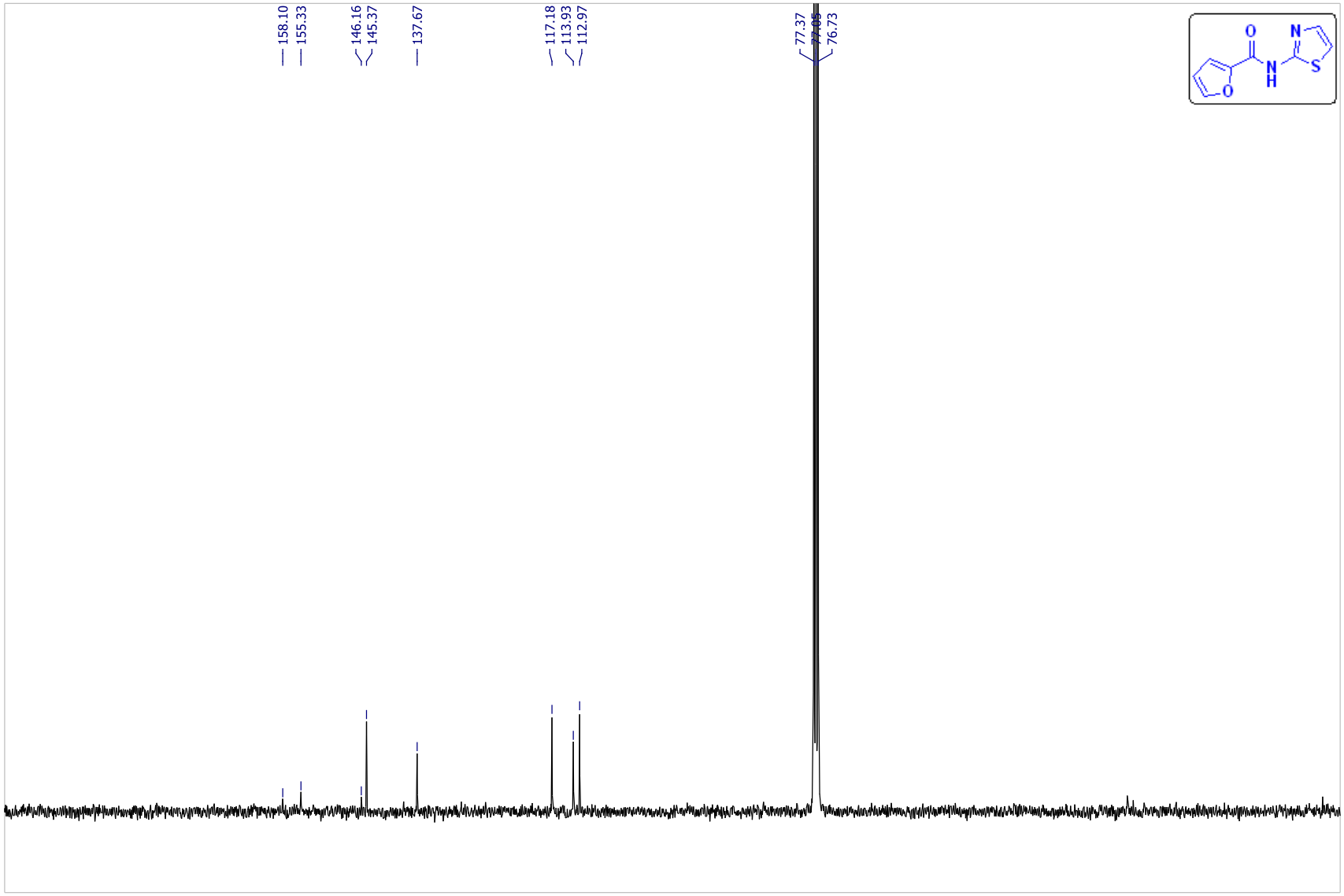
Fragmentor Voltage	Collision Energy	Ionization Mode
60	0	ESI



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



$^{13}C\{^{1}H\}$NMR of 4af (101 MHz, $CDCl_3$)



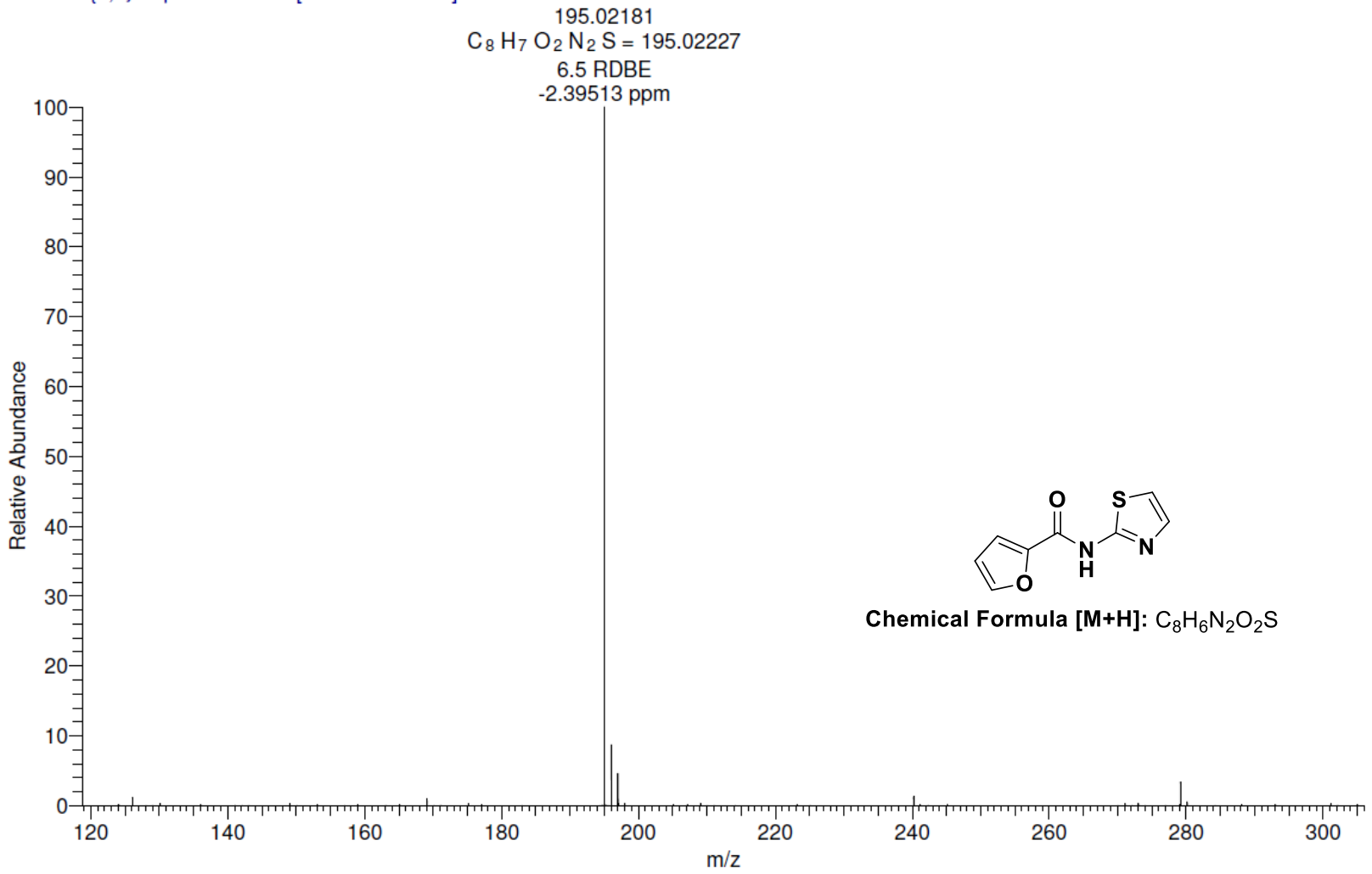
HRMS of 4af

D:\Sai krishna Important\...\SUR-RR-THAM

CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
DEPARTMENT OF ANALYTICAL& STRUCTURAL CHEMISTRY

3/23/2021 7:56:35 PM
ThermoScientific EXACTIVE ORBITRAP
Analysed By G SaiKrishna

SUR-RR-THAM #8-25 RT: 0.06-0.18 AV: 18 NL: 3.30E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



Chemical Formula [M+H]: $C_8H_6N_2O_2S$