

Supporting Information

Interrupted Borrowing Hydrogen Strategy Enabled Aminomethylation and Direct-Cross Dehydrogenative Coupling Strategy Enabled Dicarboxylation Reactions of Imidazo[1,5-*a*]pyridines

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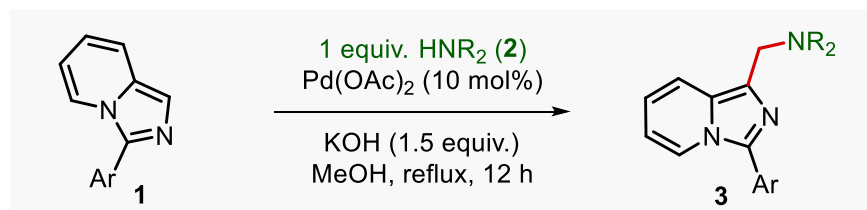
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1. General Methods:

All reactions were performed in an oven-dried glass apparatus. Solvents were distilled in the standard way, and commercial reagents were used without any purification. Analytical TLC was performed on 60 F254 plates, and visualized by exposure to ultraviolet light (UV-254 nm). Column chromatography was carried out with silica (100-200 mesh). NMR spectra for the characterization of compounds were recorded on Bruker Advance DPX FT-NMR 400 MHz instrument (^1H) at 400 MHz and (^{13}C) at 101 MHz, respectively. ^{19}F NMR was recorded at 377 MHz. Chemical shifts (δ) are reported in ppm, using the residual solvent peak in CDCl_3 ($\delta_{\text{H}} = 7.26$ and $\delta_{\text{C}} = 77.16$ ppm) and DMSO-d_6 ($\delta_{\text{H}} = 2.50$ and $\delta_{\text{C}} = 39.52$ ppm) as an internal reference and coupling constants (J) are given in hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet. High-Resolution Mass Spectra (HRMS) were recorded using a Waters XEVO-G2-XS-Q-TOF mass spectrometer.

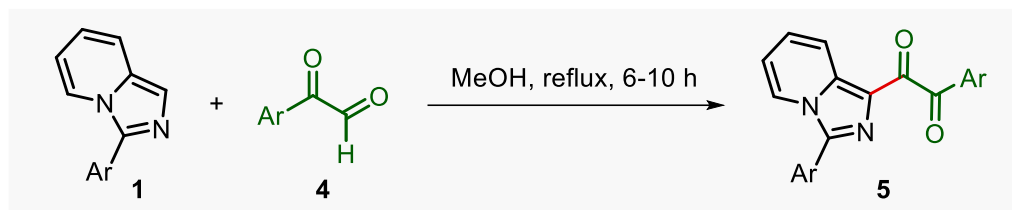
2. General Reaction Procedures:

General Procedure for the Synthesis of aminomethylated-[1,5-*a*]pyridins (GP1):



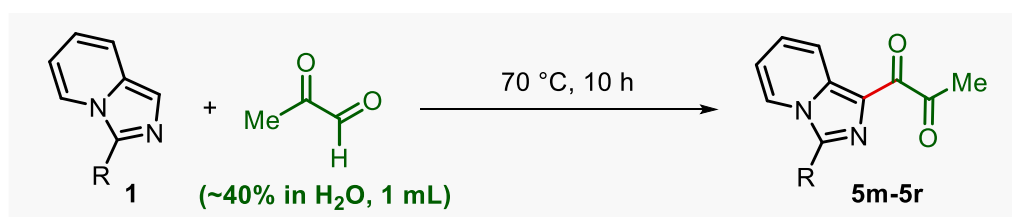
To the solution of 3-arylimidazo[1,5-*a*]pyridines **1** (1 equiv.) and secondary amines **2** (1 equiv.) in methanol was added KOH (1.5 equiv.). The mixture was allowed to stir at reflux temperature for 12 hours. After complete conversion (product monitored by TLC), methanol was removed by using a rotary evaporator. The crude residue was dissolved in dichloromethane. The organic layer was washed with water twice. The combined organic layers were dried over anhydrous sodium sulfate. After removal of the solvent in vacuo the residue was subjected to silica gel column chromatography by using $\text{EtOAc}/n\text{-Hexane}$ mixture as eluent.

General Procedure for the Synthesis of ethane-1,2-diones from aryl glyoxals (GP2):



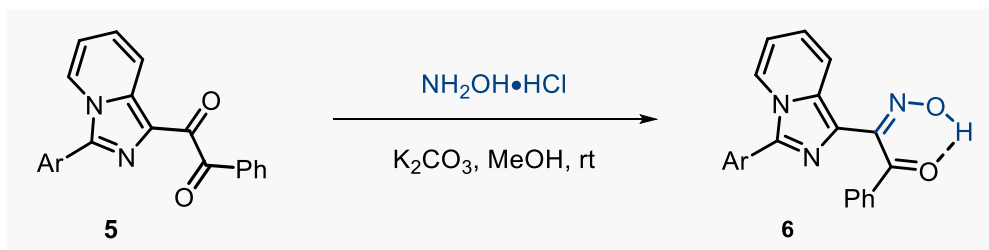
To the solution of 3-arylimidazo[1,5-*a*]pyridines **1** (1 equiv) in methanol, arylglyoxals **4** (1 equiv) was added. The mixture was then allowed to stir at reflux temperature. After complete conversion (product monitored by TLC), methanol was removed using a rotary evaporator. The residue was subjected to silica gel column chromatography using the EtOAc/*n*-hexane mixture as an eluent.

General Procedure for the Synthesis of propane-1,2-diones (GP3):



A mixture of the corresponding imidazo[1,5-*a*]pyridine (**1**) and pyruvaldehyde solution (40 wt% in water, 1 mL) was heated at 70 °C. After complete conversion (product monitored by TLC), the reaction was cooled down to room temperature. Dichloromethane was added. The phases were separated, and the aqueous phase was extracted with dichloromethane. The combined organic layers were dried with anhydrous sodium sulfate. After the removal of the solvents in vacuo, the residue was subjected to silica gel column chromatography using the EtOAc/*n*-hexane mixture as an eluent.

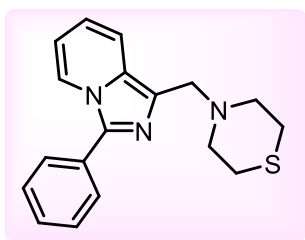
General Procedure for the Synthesis of oximes (GP4):



To the solution of 3-arylimidazo[1,5-*a*]pyridines (1 equiv) in methanol (1 mL), hydroxylamine hydrochloride (1.5 equiv) and K₂CO₃ (1 equiv) were added. The mixture was allowed to stir at room temperature until completion. After complete conversion (product monitored by TLC), methanol was removed using a rotary evaporator. The residue was dissolved in dichloromethane. Water was added. The phases were separated, and the aqueous phase was extracted with dichloromethane. The combined organic layers were dried with anhydrous sodium sulfate. After removal of the solvents in vacuo, the residue was subjected to silica gel column chromatography using the EtOAc/*n*-hexane mixture as an eluent.

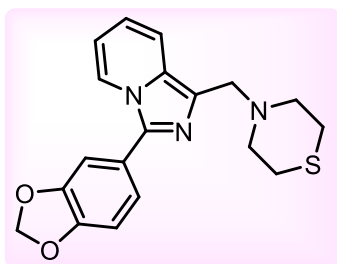
3. Characterization Data:

4-((3-phenylimidazo[1,5-*a*]pyridin-1-yl)methyl)thiomorpholine (**3a**)



Following GP1, the compound **3a** was obtained as yellow colored solid (68 mg, 85%), m.p.= 110-112 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.17 (d, *J* = 7.35 Hz, 1H), 7.74 (d, *J* = 7.09 Hz, 2H), 7.55 (d, *J* = 9.19 Hz, 1H), 7.48 (t, *J* = 7.69 Hz, 2H), 7.39 (t, *J* = 7.40 Hz, 1H), 6.70-6.66 (m, 1H), 6.53-6.50 (m, 1H), 3.88 (s, 2H), 2.83-2.81 (m, 4H), 2.69-2.67 (m, 4H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 137.2, 130.2, 129.7, 128.9, 128.6, 128.4, 128.1, 121.4, 118.4, 113.1, 56.1, 54.8, 28.0 ppm; HRMS (ESI) *m/z*: calcd. for C₁₈H₁₉N₃SNa [M+Na]⁺: 332.1197, found: 332.1184; HRMS (ESI) *m/z*: calcd. for C₁₄H₁₁N₂ [M-C₄H₈NS]: 207.0922, found: 207.0923

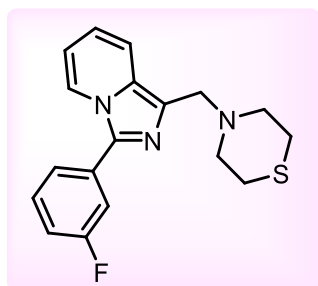
4-((3-(benzo[*d*][1,3]dioxol-5-yl)imidazo[1,5-*a*]pyridin-1-yl)methyl)thiomorpholine (**3b**)



Following GP1, the compound **3b** was obtained as yellow solid (60 mg, 81%), m.p.= 180-182 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.12 (d, *J* = 7.25 Hz, 1H), 7.56 (d, *J* = 9.21 Hz, 1H), 7.21 (s, 2H), 6.93 (d, *J* = 8.25 Hz, 1H), 6.72-6.68 (m, 1H), 6.53 (t, *J* = 6.80 Hz, 1H), 6.03 (s, 2H), 3.96 (s, 2H), 2.92-2.91 (m, 4H), 2.75-2.73 (m, 4H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 148.2 (2C), 137.3, 130.1, 126.1, 123.7, 122.2, 121.5,

118.9, 118.3, 113.2, 108.8, 101.5, 55.1, 54.2, 27.3 ppm; **HRMS (ESI) m/z**: calcd. for $C_{15}H_{11}N_2O_2$ [M-C₄H₈NS]: 251.0821, found: 251.0812

4-((3-(3-fluorophenyl)imidazo[1,5-a]pyridin-1-yl)methyl)thiomorpholine (3c)



Following GP1, the compound **3c** was obtained as dark colored solid (63 mg, 82%), m.p.= 126-128 °C; **¹H NMR (400 MHz, CDCl₃)**: δ 7.68-7.65 (m, 2H), 7.53 (dd, *J* = 9.18, 1.07 Hz, 1H), 7.40-7.35 (m, 1H), 7.25-7.20 (m, 1H), 7.18-7.13 (m, 1H), 6.70-6.66 (m, 1H), 6.52-6.49 (m, 1H), 3.85 (d, *J* = 0.84 Hz, 2H), 2.79-2.77 (m, 4H), 2.65-2.62 (m, 4H) ppm; **¹³C[¹H] NMR (101 MHz, CDCl₃)**: δ 160.9, 158.4, 132.2, 132.2 (d, *J* = 3.08 Hz), 130.7 (d, *J* = 8.21 Hz), 129.8, 128.5, 124.6 (d, *J* = 3.18 Hz), 122.1 (d, *J* = 6.82 Hz), 118.5, 117.9, 117.8, 115.9 (d, *J* = 21.48 Hz), 112.7, 55.9, 54.6, 27.7 ppm; **¹⁹F NMR (377 MHz, CDCl₃)**: -110.97 to -110.99 (m) ppm; **HRMS (ESI) m/z**: calcd. for $C_{14}H_{10}N_2F$ [M-C₄H₈NS]: 225.0828, found: 225.0827

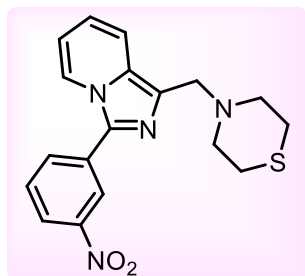
4-((3-(2-fluorophenyl)imidazo[1,5-a]pyridin-1-yl)methyl)thiomorpholine (3d)



Following GP1, the compound **3d** was obtained as dark colored semi-solid (60 mg, 78%); **¹H NMR (400 MHz, CDCl₃)**: δ 8.20 (d, *J* = 7.29 Hz, 1H), 7.61-7.55 (m, 2H), 7.51-7.43 (m, 2H), 7.12-7.08 (m, 1H), 6.75-6.71 (m, 1H), 6.60-6.57 (m, 1H), 3.89 (s, 2H), 2.85-2.82 (m, 4H), 2.71-2.68 (m, 4H) ppm; **¹³C[¹H] NMR (101 MHz, CDCl₃)**: δ 164.2, 161.8, 135.9 (d, *J* = 2.81 Hz), 132.1 (d, *J* = 8.36 Hz), 130.6 (d, *J* = 8.57 Hz), 130.3, 127.8, 123.5 (d, *J* = 2.83 Hz), 121.3, 119.0, 118.4, 115.6 (d, *J* = 21.09 Hz), 115.0 (d, *J* = 22.90 Hz), 113.6, 55.6, 55.5, 27.6 ppm; **¹⁹F NMR (377 MHz, CDCl₃)**: -111.86 to -111.92 (m) ppm; **HRMS (ESI) m/z**: calcd. for $C_{18}H_{18}N_3FS$ [M+H]⁺: 328.1284, found: 328.1273; **HRMS (ESI) m/z**: calcd. for $C_{14}H_{10}N_2F$ [M-C₄H₈NS]: 225.0828, found: 225.0825

4-((3-(3-nitrophenyl)imidazo[1,5-a]pyridin-1-yl)methyl)thiomorpholine (3e)

Following GP1, the compound **3e** was obtained as yellow solid (57 mg, 77%), m.p.= 170-

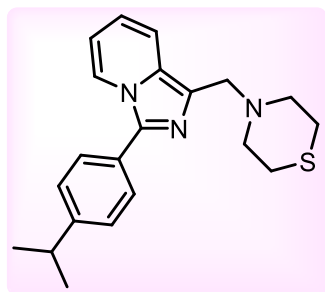


172 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.67 (t, J = 1.84 Hz, 1H), 7.28-7.24 (m, 2H), 8.19-8.17 (m, 1H), 7.72-7.65 (m, 2H), 6.83-6.79 (m, 1H), 6.69 (dt, J = 6.81, 1.23 Hz, 1H), 3.91 (s, 2H), 2.85-2.83 (m, 4H), 2.73-2.70 (m, 4H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 148.7, 134.6, 133.9, 132.0, 130.6, 130.2, 129.9, 123.0, 122.2, 120.9, 119.3, 118.9, 114.3, 56.3, 55.0, 28.1 ppm; HRMS (ESI) m/z: calcd.

for C₁₈H₁₉N₄O₂S [M+H]⁺: 355.1229, found: 355.1207; HRMS (ESI) m/z: calcd. for C₁₄H₁₀N₃O₂ [M-C₄H₈NS]: 252.0773, found: 252.0770

4-((3-(4-isopropylphenyl)imidazo[1,5-a]pyridin-1-yl)methyl)thiomorpholine (3f)

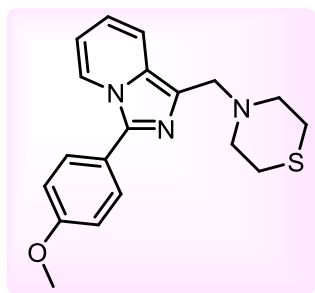
Following GP1, the compound **3f** was obtained as pale yellow semi-solid (59 mg, 80%);



¹H NMR (400 MHz, CDCl₃): δ 8.20 (d, J = 7.19 Hz, 1H), 7.69 (d, J = 8.32 Hz, 2H), 7.57 (d, J = 8.99 Hz, 1H), 7.36 (d, J = 7.99 Hz, 2H), 6.71-6.67 (m, 1H), 6.54-6.50 (m, 1H), 3.92 (s, 2H), 3.01-2.94 (m, 1H), 2.88-2.85 (m, 4H), 2.73-2.70 (m, 4H), 1.30 (s, 3H), 1.29 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 149.7, 137.6, 129.7, 128.2, 127.7, 127.6, 127.1, 126.8, 121.6, 118.5, 118.4, 112.9, 56.2,

54.8, 34.1, 28.0, 24.0 ppm; HRMS (ESI) m/z: calcd. for C₂₁H₂₆N₃S [M+H]⁺: 352.1847, found: 352.1827; HRMS (ESI) m/z: calcd. for C₁₇H₁₇N₂ [M-C₄H₈NS]: 249.1392, found: 249.1368

4-((3-(4-methoxyphenyl)imidazo[1,5-a]pyridin-1-yl)methyl)thiomorpholine (3g)

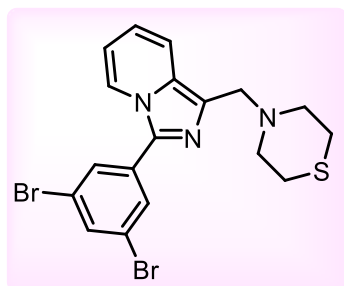


Following GP1, the compound **3g** was obtained as dark colored semi-solid (62 mg, 82%); ¹H NMR (400 MHz, CDCl₃): δ 8.11 (d, J = 7.27 Hz, 1H), 7.68 (d, J = 8.66 Hz, 2H), 7.54 (d, J = 9.14 Hz, 1H), 7.02 (d, J = 8.74 Hz, 2H), 6.68-6.64 (m, 1H), 6.52-6.48 (m, 1H), 3.88 (s, 2H), 3.86 (s, 3H), 2.85-2.82 (m, 4H), 2.71-2.68 (m, 4H) ppm;

¹³C{¹H} NMR (101 MHz, CDCl₃): δ 159.9, 137.4, 130.1, 129.6, 127.4, 122.6, 121.4, 118.3, 118.4, 114.4, 112.9, 56.0, 55.4, 54.7, 27.8 ppm; HRMS (ESI) m/z: calcd. for C₁₉H₂₂N₃OS

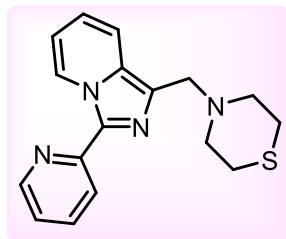
[M+H]⁺: 340.1484, found: 340.1465; **HRMS (ESI) m/z**: calcd. for C₁₅H₁₃N₂O [M-C₄H₈NS]: 237.1028, found: 237.1024

4-((3-(3,5-dibromophenyl)imidazo[1,5-a]pyridin-1-yl)methyl)thiomorpholine (3h)



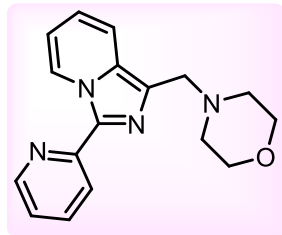
Following GP1, the compound **3h** was obtained as pale white solid (50 mg, 75%), m.p.= 108-110 °C; **¹H NMR (400 MHz, CDCl₃)**: δ 8.19 (d, *J* = 7.15 Hz, 1H), 7.89 (d, *J* = 1.71 Hz, 2H), 7.70-7.69 (m, 1H), 7.62 (d, *J* = 9.09 Hz, 1H), 6.78 (t, *J* = 7.88 Hz, 1H), 6.66 (t, *J* = 6.70 Hz, 1H), 3.88 (s, 2H), 2.82-2.81 (m, 4H), 2.71-2.69 (m, 4H) ppm; **¹³C{¹H} NMR (101 MHz, CDCl₃)**: δ 134.1, 133.8, 133.5, 130.6, 129.3, 123.5, 121.1, 119.3, 118.7, 114.1, 56.1, 54.9, 28.0 ppm; **HRMS (ESI) m/z**: calcd. for C₁₄H₉N₂Br₂ [M-C₄H₈NS]: 362.9132, found: 362.9135

4-((3-(pyridin-2-yl)imidazo[1,5-a]pyridin-1-yl)methyl)morpholine (3i)



Following GP1, the compound **3i** was obtained as pale white solid (65 mg, 82%), m.p.= 118-120 °C; **¹H NMR (400 MHz, CDCl₃)**: δ 9.88 (d, *J* = 7.31 Hz, 1H), 8.60-8.59 (m, 1H), 8.32 (d, *J* = 8.12 Hz, 1H), 7.73 (dt, *J* = 7.70, 1.71 Hz, 1H), 7.62 (m, *J* = 9.08 Hz, 1H), 7.17-7.13 (m, 1H), 6.83-6.79 (m, 1H), 6.71-6.67 (m, 1H), 3.89 (s, 2H), 2.82-2.80 (m, 4H), 2.69-2.67 (m, 4H) ppm; **¹³C{¹H} NMR (101 MHz, CDCl₃)**: δ 151.0, 148.1, 136.4, 134.3, 131.1, 129.0, 125.9, 121.9, 121.5, 119.7, 117.7, 113.5, 56.3, 54.9, 28.0 ppm; **HRMS (ESI) m/z**: calcd. for C₁₇H₁₈N₄SNa [M+Na]⁺: 333.1150, found: 333.1133; **HRMS (ESI) m/z**: calcd. for C₁₃H₁₀N₃ [M-C₄H₈NS]: 208.0875, found: 208.0875

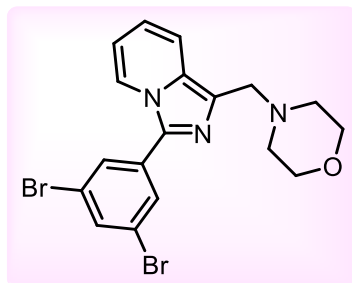
4-((3-(pyridin-2-yl)imidazo[1,5-a]pyridin-1-yl)methyl)morpholine (3j)



Following GP1, the compound **3j** was obtained as pale yellow solid (82 mg, 81%), m.p.= 122-124 °C; **¹H NMR (400 MHz, CDCl₃)**: δ 9.89 (d, *J* = 7.32 Hz, 1H), 8.60 (d, *J* = 4.82 Hz, 1H), 8.34 (d, *J* = 8.17 Hz, 1H), 7.76-7.72 (m, 1H), 7.65 (d, *J* = 9.17 Hz, 1H), 7.18-7.15 (m, 1H),

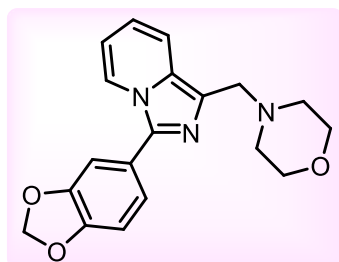
6.85-6.81 (m, 1H), 6.70 (t, $J = 6.86$ Hz, 1H), 3.88 (s, 2H), 3.72 (t, $J = 4.64$ Hz, 4H), 2.57 (m, 4H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 151.0, 148.1, 136.4, 134.4, 131.1, 128.9, 126.0, 122.0, 121.5, 119.8, 117.6, 113.5, 67.0, 55.8, 53.7 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{17}\text{H}_{18}\text{N}_4\text{ONa}$ $[\text{M}+\text{Na}]^+$: 317.1378, found: 317.1360; HRMS (ESI) m/z : calcd. for $\text{C}_{13}\text{H}_{10}\text{N}_3$ $[\text{M}-\text{C}_4\text{H}_8\text{NO}]$: 208.0875, found: 208.0881

4-((3-(3,5-dibromophenyl)imidazo[1,5-a]pyridin-1-yl)methyl)morpholine (3k)



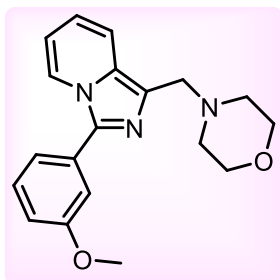
Following GP1, the compound **3k** was obtained as pale white solid (49 mg, 75%), m.p.= 114-116 °C; ^1H NMR (400 MHz, CDCl_3): δ 8.20 (d, $J = 7.20$ Hz, 1H), 7.89 (d, $J = 1.67$ Hz, 2H), 7.71-7.67 (m, 2H), 6.83-6.79 (m, 1H), 6.68 (t, $J = 6.76$ Hz, 1H), 3.94 (s, 2H), 3.77 (t, $J = 4.40$ Hz, 4H), 2.66 (s, 4H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 134.3, 133.9, 133.5, 130.8, 129.3, 127.8, 123.6, 121.2, 119.5, 118.6, 114.2, 66.7, 55.3, 53.4 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{18}\text{H}_{18}\text{N}_3\text{Br}_2\text{O}$ $[\text{M}+\text{H}]^+$: 449.9817, found: 449.9807; HRMS (ESI) m/z : calcd. for $\text{C}_{14}\text{H}_9\text{N}_2\text{Br}_2$ $[\text{M}-\text{C}_4\text{H}_8\text{NO}]$: 362.9132, found: 362.9124

4-((3-(benzo[d][1,3]dioxol-5-yl)imidazo[1,5-a]pyridin-1-yl)methyl)morpholine (3l)



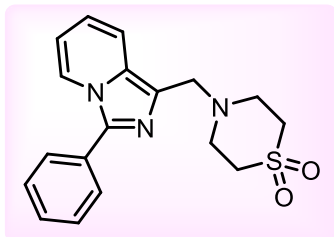
Following GP1, the compound **3l** was obtained as yellow solid (59 mg, 83%), m.p.= 188-190 °C; ^1H NMR (400 MHz, CDCl_3): δ 8.11 (d, $J = 7.31$ Hz, 1H), 7.54 (tt, $J = 9.18, 1.05$ Hz, 1H), 7.22-7.20 (m, 2H), 6.92-6.89 (m, 1H), 6.69-6.65 (m, 1H), 6.52-6.48 (m, 1H), 6.01-6.00 (m, 2H), 3.86 (s, 2H), 3.71 (s, 4H), 2.59 (s, 4H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 148.1, 148.0, 137.1, 129.6, 127.2, 123.9, 122.0, 121.3, 118.4, 118.2, 113.0, 108.7 (d, $J = 3.04$ Hz), 101.4, 66.7, 55.3, 53.3 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{19}\text{H}_{20}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$: 338.1505, found: 338.1490; HRMS (ESI) m/z : calcd. for $\text{C}_{15}\text{H}_{11}\text{N}_2\text{O}_2$ $[\text{M}-\text{C}_4\text{H}_8\text{NO}]$: 251.0821, found: 251.0824

4-((3-(3-methoxyphenyl)imidazo[1,5-a]pyridin-1-yl)methyl)morpholine (3m)



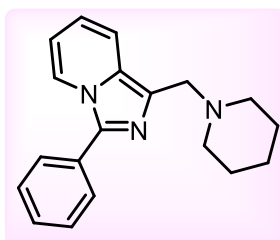
Following GP1, the compound **3m** was obtained as dark colored semi-solid (57 mg, 79%); $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.20 (d, $J = 7.27$ Hz, 1H), 7.58 (dd, $J = 9.21, 1.15$ Hz, 1H), 7.39 (dt, $J = 7.82, 1.25$ Hz, 1H), 7.33-7.29 (m, 2H), 6.94 (dd, $J = 8.20, 1.05$ Hz, 1H), 6.72-6.68 (m, 1H), 6.54-6.50 (m, 1H), 3.89 (s, 2H), 3.85 (d, $J = 1.70$ Hz, 3H), 3.74-3.71 (m, 4H), 2.61 (s, 4H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 160.1, 137.2, 131.3, 130.0, 127.6, 121.6, 120.2, 118.7, 118.4, 113.6, 113.1, 66.7, 55.5, 55.3, 53.3 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{19}\text{H}_{22}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$: 324.1712, found: 334.1693; HRMS (ESI) m/z : calcd. for $\text{C}_{15}\text{H}_{13}\text{N}_2\text{O}$ $[\text{M}-\text{C}_4\text{H}_8\text{NO}]$: 237.1028, found: 237.1033

4-((3-phenylimidazo[1,5-a]pyridin-1-yl)methyl)thiomorpholine 1,1-dioxide (3n)



Following GP1, the compound **3n** was obtained as pale white solid (70 mg, 80%), m.p.= 132-134 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.09-8.06 (m, 1H), 7.64-7.62 (m, 2H), 7.40-7.32 (m, 3H), 7.30-7.27 (m, 1H), 6.62-6.58 (m, 1H), 6.45-6.41 (m, 1H), 3.87 (d, $J = 11.62$ Hz, 2H), 2.97 (s, 4H), 2.95 (m, 4H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 137.1, 129.6, 129.4, 128.7, 128.4, 127.7, 127.3, 121.2, 118.8, 117.5, 113.0, 53.5, 51.0, 50.2 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{18}\text{H}_{19}\text{N}_3\text{O}_2\text{SNa}$ $[\text{M}+\text{Na}]^+$: 364.1096, found: 364.1080; HRMS (ESI) m/z : calcd. for $\text{C}_{14}\text{H}_{11}\text{N}_2$ $[\text{M}-\text{C}_4\text{H}_8\text{NO}_2\text{S}]$: 207.0922, found: 207.0922

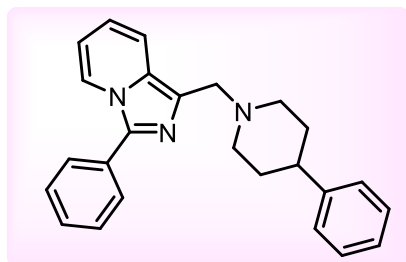
3-phenyl-1-(piperidin-1-ylmethyl)imidazo[1,5-a]pyridine (3o)



Following GP1, the compound **3o** was obtained as pale yellow colored semi-solid (56 mg, 75%); $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.19 (d, $J = 7.33$ Hz, 1H), 7.78-7.76 (m, 2H), 7.62 (d, $J = 9.21$ Hz, 1H), 7.50 (t, $J = 7.50$ Hz, 2H), 7.43-7.39 (m, 1H), 6.71-6.67 (m, 1H), 6.54-6.51 (m, 1H), 3.89 (s, 2H), 2.58 (s, 4H), 1.65-1.59 (m, 4H), 1.42 (s, 2H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR

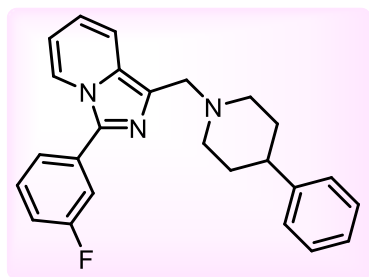
(101 MHz, CDCl₃): δ 137.2, 130.3, 129.9, 129.4, 128.9, 128.6, 128.4, 128.1, 121.3, 118.8, 118.4, 113.1, 55.8, 54.3, 25.7, 24.1 ppm; HRMS (ESI) m/z: calcd. for C₁₉H₂₂N₃ [M+H]⁺: 292.1814, found: 292.1786; HRMS (ESI) m/z: calcd. for C₁₄H₁₁N₂ [M-C₅H₁₀N]: 207.0922, found: 207.0908

3-phenyl-1-((4-phenylpiperidin-1-yl)methyl)imidazo[1,5-a]pyridine (3p)



Following GP1, the compound **3p** was obtained as dark colored semi-solid (76 mg, 80%); ¹H NMR (400 MHz, CDCl₃): δ 8.13 (d, *J* = 7.27 Hz, 1H), 7.73-7.71 (m, 2H), 7.56 (td, *J* = 9.24, 1.10 Hz, 1H), 7.45-7.41 (m, 2H), 7.36-7.32 (m, 1H), 7.22-7.18 (m, 2H), 7.16-7.13 (m, 2H), 7.12-7.08 (m, 1H), 6.65-6.61 (m, 1H), 6.48-6.44 (m, 1H), 3.88 (s, 2H), 3.57 (s, 1H), 3.11 (d, *J* = 11.72 Hz, 2H), 2.46-2.39 (m, 1H), 2.21-2.14 (m, 2H), 1.78-1.75 (m, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 146.5, 137.2, 130.3, 129.8, 129.0, 128.6, 128.4, 128.2, 127.0, 126.1, 121.4, 118.7, 118.4, 113.1, 70.6, 55.5, 55.4, 42.6, 33.4 ppm; HRMS (ESI) m/z: calcd. for C₂₅H₂₆N₃ [M+H]⁺: 368.2127, found: 368.2110; HRMS (ESI) m/z: calcd. for C₁₄H₁₁N₂ [M-C₁₁H₁₄N]: 207.0922, found: 207.0925

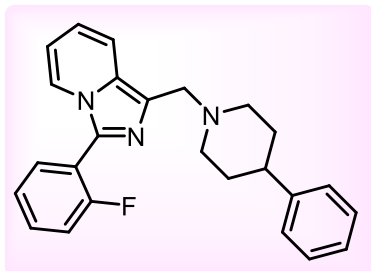
3-(3-fluorophenyl)-1-((4-phenylpiperidin-1-yl)methyl)imidazo[1,5-a]pyridine (3q)



Following GP1, the compound **3q** was obtained as dark colored semi-solid (71 mg, 78%); ¹H NMR (400 MHz, CDCl₃): δ 7.72-7.67 (m, 2H), 7.60 (d, *J* = 9.12 Hz, 1H), 7.40-7.36 (m, 1H), 7.22 (t, *J* = 7.45 Hz, 3H), 7.19-7.16 (m, 3H), 7.14-7.10 (m, 1H), 6.72-6.69 (m, 1H), 6.52 (t, *J* = 6.70 Hz, 1H), 3.93 (s, 2H), 3.15 (d, *J* = 11.60 Hz, 2H), 2.50-2.41 (m, 1H), 2.21 (dt, *J* = 11.10, 3.51 Hz, 2H), 1.84-1.77 (m, 4H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 161.1, 158.6, 146.3, 132.5, 132.4 (d, *J* = 3.19 Hz), 130.8 (d, *J* = 8.12 Hz), 130.1, 128.7, 128.3, 126.8, 126.1, 124.8 (d, *J* = 3.45 Hz), 122.3 (d, *J* = 6.89 Hz), 118.7, 118.1 (t, *J* = 7.09 Hz), 116.0 (d, *J* = 21.19 Hz), 112.8, 55.2, 54.0, 42.4, 33.2 ppm; ¹⁹F NMR (377 MHz, CDCl₃): -110.91 to -110.95 (m) ppm; HRMS (ESI)

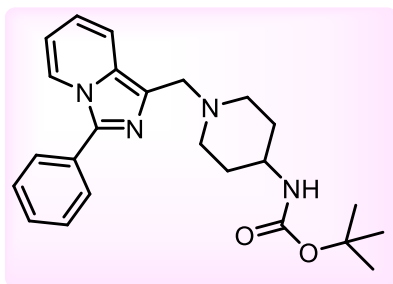
m/z: calcd. for C₂₅H₂₅N₃F [M+H]⁺: 386.2030, found: 386.2014; **HRMS (ESI) m/z:** calcd. for C₁₄H₁₀N₂F [M-C₁₁H₁₄N]: 225.0828, found: 225.0838

3-(2-fluorophenyl)-1-((4-phenylpiperidin-1-yl)methyl)imidazo[1,5-a]pyridine (3r)



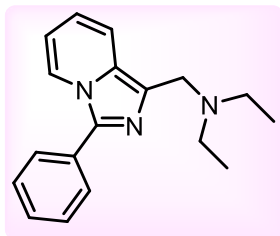
Following GP1, the compound **3r** was obtained as dark colored semi-solid (68 mg, 75%); **¹H NMR (400 MHz, CDCl₃):** δ 8.18 (d, *J* = 7.19 Hz, 1H), 7.63 (d, *J* = 9.22 Hz, 1H), 7.56-7.54 (m, 1H), 7.50-7.46 (m, 1H), 7.46-7.40 (m, 2H), 7.24-7.22 (m, 2H), 7.19-7.17 (m, 1H), 7.16-7.12 (m, 1H), 7.09-7.04 (m, 1H), 6.73-6.69 (m, 1H), 6.57-6.53 (m, 1H), 3.92 (s, 2H), 3.15 (d, *J* = 11.50 Hz, 2H), 2.51-2.43 (m, 1H), 2.22 (dt, *J* = 11.16, 3.30 Hz, 2H), 1.85-1.79 (m, 4H) ppm; **¹³C{¹H} NMR (101 MHz, CDCl₃):** δ 164.3, 161.9, 146.0, 136.0, 132.4 (d, *J* = 8.49 Hz), 130.6 (d, *J* = 8.42 Hz), 130.3, 128.5, 127.0, 126.2, 123.5 (d, *J* = 2.92 Hz), 121.3, 118.8 (d, *J* = 4.48 Hz), 115.5 (d, *J* = 21.14 Hz), 115.1 (d, *J* = 22.90 Hz), 113.6, 55.5, 54.2, 42.6, 33.3 ppm; **¹⁹F NMR (377 MHz, CDCl₃):** -110.91 to -110.95 (m) ppm; **HRMS (ESI) m/z:** calcd. for C₂₅H₂₅N₃F [M+H]⁺: 386.2033, found: 386.2015; **HRMS (ESI) m/z:** calcd. for C₁₄H₁₀N₂F [M-C₁₁H₁₄N]: 225.0828, found: 225.0824

tert-butyl (1-((3-phenylimidazo[1,5-a]pyridin-1-yl)methyl)piperidin-4-yl)carbamate (3s)



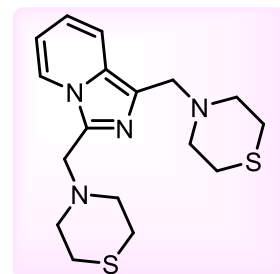
Following GP1, the compound **3s** was obtained as dark colored solid (80 mg, 76%), m.p. = 144-146 °C; **¹H NMR (400 MHz, CDCl₃):** δ 9.89 (d, *J* = 7.32 Hz, 1H), 8.61 (d, *J* = 4.82 Hz, 1H), 8.33 (d, *J* = 8.17 Hz, 1H), 7.74 (dt, *J* = 7.76, 1.71 Hz, 1H), 7.64 (d, *J* = 9.17 Hz, 1H), 7.18-7.15 (m, 1H), 6.86-6.82 (m, 1H), 6.71 (t, *J* = 6.86 Hz, 1H), 3.87 (s, 2H), 3.72 (t, *J* = 4.64 Hz, 4H), 2.56 (m, 4H) ppm; **¹³C{¹H} NMR (101 MHz, CDCl₃):** δ 151.0, 148.1, 136.4, 134.4, 131.1, 128.9, 126.0, 122.0, 121.5, 119.8, 117.6, 113.5, 67.0, 55.8, 53.7 ppm; **HRMS (ESI) m/z:** calcd. for C₂₄H₃₁N₄O₂ [M+H]⁺: 407.2447, found: 407.2435; **HRMS (ESI) m/z:** calcd. for C₁₄H₁₁N₂ [M-C₁₀H₁₉N₂O₂]: 207.0922, found: 207.0929

N-ethyl-*N*-((3-phenylimidazo[1,5-*a*]pyridin-1-yl)methyl)ethanamine (**3t**)



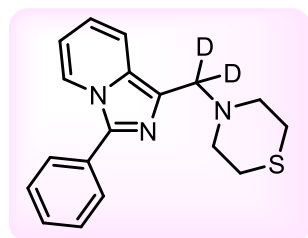
Following GP1, the compound **3t** was obtained as pale yellow semi-solid (60 mg, 83%); $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.21 (d, $J = 7.17$ Hz, 1H), 7.88 (d, $J = 8.91$ Hz, 1H), 7.73 (d, $J = 7.17$ Hz, 2H), 7.52 (t, $J = 7.51$ Hz, 2H), 7.47-7.43 (m, 1H), 6.90-6.86 (m, 1H), 6.62 (t, $J = 6.16$ Hz, 1H), 4.68 (s, 2H), 3.20 (d, $J = 6.42$ Hz, 4H), 1.50 (t, $J = 6.88$ Hz, 6H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 138.5, 132.3, 129.7, 129.2, 128.2, 121.6, 121.0, 120.6, 118.1, 113.8, 46.8, 9.9 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{14}\text{H}_{11}\text{N}_2$ [$\text{M}-\text{C}_4\text{H}_{10}\text{N}$]: 207.0922, found: 207.0922

4,4'-(imidazo[1,5-*a*]pyridine-1,3-diylbis(methylene))bis(thiomorpholine) (**3u**)



To the solution of imidazo[1,5-*a*]pyridine (0.42 mmol, 1 equiv.) in methanol, 0.84 mmol (2 equiv.) of thiomorpholine was added, followed by the addition of base KOH (0.84 mmol). The mixture was allowed to stir at reflux temperature for 12 hours. After complete conversion (product monitored by TLC), methanol was removed by using a rotary evaporator. The crude residue was dissolved in dichloromethane. The organic layer was washed with water twice. The combined organic layers were dried over anhydrous sodium sulfate. After removal of the solvent in vacuo the residue was subjected to silica gel column chromatography by using EtOAc/*n*-Hexane mixture as eluent. The compound **3u** was obtained as yellow semi-solid (120 mg, 82%); $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.05 (d, $J = 7.21$ Hz, 1H), 7.42 (dd, $J = 9.20, 0.66$ Hz, 1H), 6.65-6.61 (m, 1H), 6.46 (t, $J = 6.80$ Hz, 1H), 3.86 (s, 2H), 3.73 (s, 2H), 2.71-2.69 (m, 4H), 2.65-2.59 (m, 8H), 2.57-2.55 (m, 4H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 133.3, 129.4, 124.8, 122.0, 118.3, 117.3, 111.8, 55.4, 55.0, 54.3, 54.0, 27.5, 27.1 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{17}\text{H}_{24}\text{N}_4\text{S}_2\text{Na}$ [$\text{M}+\text{Na}$] $^+$: 371.1340, found: 371.1312; HRMS (ESI) m/z : calcd. for $\text{C}_{13}\text{H}_{16}\text{N}_3\text{S}$ [$\text{M}-\text{C}_4\text{H}_8\text{NS}$]: 246.1065, found: 246.1082

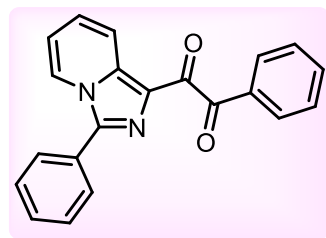
4-((3-phenylimidazo[1,5-a]pyridin-1-yl)methyl-*d*₂)thiomorpholine (3v)



The compound **3v** was obtained as yellow semi-solid (52 mg, 65%); ¹H NMR (400 MHz, CDCl₃): δ 8.15 (d, *J* = 7.32 Hz, 1H), 7.73 (d, *J* = 8.10, 2H), 7.53 (d, *J* = 9.21 Hz, 1H), 7.46 (t, *J* = 7.57 Hz, 2H), 7.38-7.35 (m, 1H), 6.65 (t, *J* = 7.80 Hz, 1H), 6.48 (t, *J* = 6.40 Hz, 1H), 2.80-2.79 (m, 4H), 2.66-2.66 (m, 4H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 136.8, 129.9, 129.4, 128.6, 128.3, 128.1, 127.7, 121.1, 118.1 (2C), 112.8, 54.5, 53.1, 27.7 ppm.

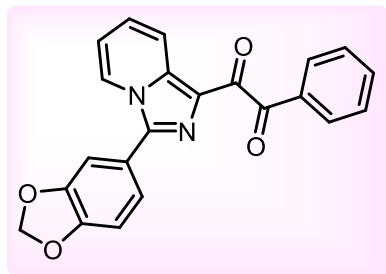
NOTE- During the HRMS analysis, it was observed that the molecular ion peak was undergoing fragmentation in the standard positive ESI mode. In some instances, the molecular ion peak was completely absent. Adjusting the temperature did not resolve this issue. To verify that the observed fragmented peak originated from the main molecular ion, Tandem Mass Spectroscopy (MS/MS) of **3s** was conducted. The results of the MS/MS analysis confirmed that the fragmented peak corresponded to the main molecular ion peak. This validation through MS/MS provided a clear confirmation of the initial observations.

1-Phenyl-2-(3-phenylimidazo[1,5-a]pyridin-1-yl)ethane-1,2-dione (5a)



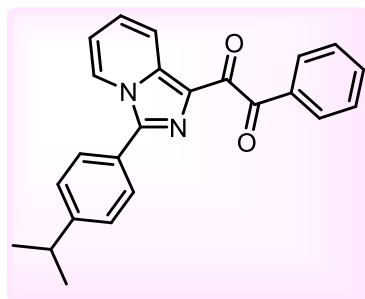
Following GP2, the compound **5a** was obtained as yellow colored solid (69 mg, 82%), m.p.= 160-162 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.46 (d, *J* = 9.06 Hz, 1H), 8.37 (td, *J* = 7.07, 1.05 Hz, 1H), 8.05 (d, *J* = 7.85 Hz, 2H), 7.69-7.67 (m, 2H), 7.60-7.56 (m, 1H), 7.48-7.44 (m, 5H), 7.38-7.33 (m, 1H), 6.97-6.93 (m, 1H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 194.9, 189.0, 140.5, 136.6, 134.2, 133.6, 130.1, 129.9, 129.1, 128.9, 128.7, 128.5, 127.6 (2C), 123.2, 120.3, 116.0 ppm; HRMS (ESI) *m/z*: calcd. for C₂₁H₁₅N₂O₂ [M+H]⁺: 327.1134, found: 327.1133

1-(3-(benzo[d][1,3]dioxol-5-yl)imidazo[1,5-a]pyridin-1-yl)-2-phenylethane-1,2-dione (5b)



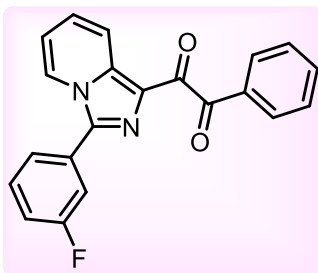
Following GP2, the compound **5b** was obtained as yellow solid (60 mg, 77%), m.p.= 186-188 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.48 (d, *J* = 9.15 Hz, 1H), 8.36 (d, *J* = 7.08 Hz, 1H), 8.07-8.05 (m, 2H), 7.60 (t, *J* = 7.41 Hz, 1H), 7.47 (t, *J* = 7.85 Hz, 2H), 7.39-7.35 (m, 1H), 7.19 (dd, *J* = 7.93, 1.64 Hz, 1H), 7.15 (d, *J* = 1.55 Hz, 1H), 6.96 (t, *J* = 6.85 Hz, 1H), 6.91 (d, *J* = 8.02 Hz, 1H), 6.02 (s, 2H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 194.9, 189.0, 149.1, 148.4, 140.3, 136.6, 134.2, 133.7, 130.2, 128.8, 127.4, 123.2, 123.1, 122.2, 120.5, 115.9, 109.5, 108.9, 101.7 ppm; HRMS (ESI) *m/z*: calcd. for C₂₂H₁₅N₂O₄ [M+H]⁺: 371.1032, found: 371.1016

1-(3-(4-isopropylphenyl)imidazo[1,5-a]pyridin-1-yl)-2-phenylethane-1,2-dione (5c)



Following GP2, the compound **5c** was obtained as yellow solid (58 mg, 74%), m.p.= 154-156 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.50 (d, *J* = 9.05 Hz, 1H), 8.40 (d, *J* = 7.17 Hz, 1H), 8.08-8.05 (m, 2H), 7.63 (d, *J* = 8.20 Hz, 2H), 7.59 (d, *J* = 7.51 Hz, 1H), 7.47 (t, *J* = 7.85 Hz, 2H), 7.40-7.34 (m, 3H), 6.95 (t, *J* = 6.86 Hz, 1H), 3.00-2.93 (m, 1H), 1.28 (s, 3H), 1.26 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 195.0, 189.1, 151.1, 136.7, 134.2, 133.7, 130.2, 129.0, 128.8, 127.4, 127.3, 123.4, 120.5, 115.8, 34.2, 23.9 ppm; HRMS (ESI) *m/z*: calcd. for C₂₄H₂₁N₂O₂ [M+H]⁺: 369.1603, found: 369.1611

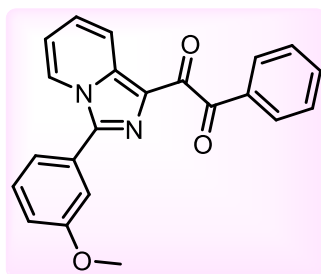
1-(3-(3-fluorophenyl)imidazo[1,5-a]pyridin-1-yl)-2-phenylethane-1,2-dione (5d)



Following GP2, the compound **5d** was obtained as yellow solid (62 mg, 76%), m.p.= 175-177 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.51 (d, *J* = 9.01 Hz, 1H), 8.08-8.05 (m, 2H), 7.98-7.95 (m, 1H), 7.67 (dt, *J* = 7.44, 1.47 Hz, 1H), 7.61-7.57 (m, 1H), 7.49-7.45 (m, 3H), 7.44-7.40 (m, 1H), 7.27 (dt, *J* = 7.61, 1.06 Hz, 1H), 7.24-7.19 (m,

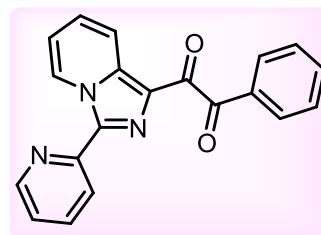
1H), 7.00 (dt, $J = 6.88, 1.23$ Hz, 1H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 194.8, 188.8, 161.4, 158.9, 136.6, 136.1, 134.2, 133.5, 132.9, 132.3 (d, $J = 3.32$ Hz), 130.1, 128.7, 128.3 (d, $J = 14.74$ Hz), 127.9 (d, $J = 7.79$ Hz), 127.6 (d, $J = 8.42$ Hz), 125.1 (d, $J = 3.37$ Hz), 123.9 (d, $J = 6.53$ Hz), 119.9, 116.5 (d, $J = 14.34$ Hz), 116.2, 115.9 (d, $J = 13.81$ Hz) ppm; ^{19}F NMR (377 MHz, CDCl_3): -110.65 to -110.73 (m) ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{21}\text{H}_{14}\text{N}_2\text{O}_2\text{F}$ $[\text{M}+\text{H}]^+$: 345.1039, found: 345.1047

1-(3-(3-methoxyphenyl)imidazo[1,5-a]pyridin-1-yl)-2-phenylethane-1,2-dione (5e)



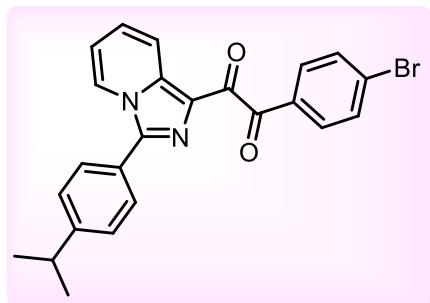
Following GP2, the compound **5e** was obtained as yellow solid (59 mg, 75%), m.p. = 148-150 °C; ^1H NMR (400 MHz, CDCl_3): δ 8.50 (d, $J = 9.05$ Hz, 1H), 8.41 (td, $J = 7.13, 0.97$ Hz, 1H), 8.08-8.05 (m, 2H), 7.62-7.58 (m, 1H), 7.47 (t, $J = 7.63$ Hz, 2H), 7.42-7.36 (m, 2H), 7.28 (t, $J = 1.27$ Hz, 1H), 7.24-7.23 (m, 1H), 7.02-6.99 (m, 1H), 6.96 (dt, $J = 6.86, 0.98$ Hz, 1H), 3.83 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 194.8, 189.0, 160.2, 140.4, 136.8, 134.2, 133.7, 130.2, 129.8, 128.8, 128.5, 127.7, 127.5, 123.4, 120.9, 120.5, 115.9 (d, $J = 3.03$ Hz), 114.6, 55.6 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{22}\text{H}_{17}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$: 357.1239, found: 357.1233

1-phenyl-2-(3-(pyridin-2-yl)imidazo[1,5-a]pyridin-1-yl)ethane-1,2-dione (5f)



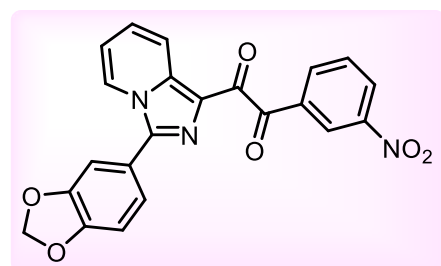
Following GP2, the compound **5f** was obtained as yellow solid (67 mg, 80%), m.p. = 167-169 °C; ^1H NMR (400 MHz, CDCl_3): δ 10.21 (dd, $J = 7.12, 0.93$ Hz, 1H), 8.61 (d, $J = 4.14$ Hz, 1H), 8.53 (d, $J = 8.28$ Hz, 1H), 8.26 (d, $J = 8.10$ Hz, 1H), 8.09-8.06 (m, 2H), 7.74-7.69 (m, 1H), 7.63-7.59 (m, 1H), 7.51-7.44 (m, 3H), 7.26-7.23 (m, 1H), 7.08 (t, $J = 6.94$ Hz, 1H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 195.0, 189.0, 149.9, 148.1, 137.5, 137.2, 136.8, 134.2, 133.8, 130.1, 128.8, 128.3, 128.1, 127.4, 123.3, 123.2, 119.6, 116.2 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{20}\text{H}_{14}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$: 328.1086, found: 328.1076

1-(4-bromophenyl)-2-(3-(4-isopropylphenyl)imidazo[1,5-a]pyridin-1-yl)ethane-1,2-dione (5g)



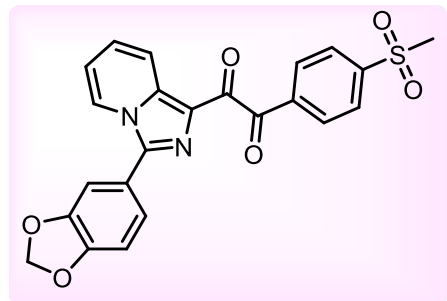
Following GP2, the compound **5g** was obtained as yellow solid (80 mg, 85%), m.p.= 130-132 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.50 (d, $J = 9.08$ Hz, 1H), 8.41 (d, $J = 7.26$ Hz, 1H), 7.93 (d, $J = 7.40$ Hz, 2H), 7.64-7.61 (m, 4H), 7.42-7.39 (m, 1H), 7.36 (d, $J = 8.31$ Hz, 2H), 7.27-7.26 (m, 1H), 6.97 (t, $J = 6.88$ Hz, 1H), 3.00-2.93 (m, 1H), 1.28 (s, 3H), 1.26 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 193.9, 188.3, 146.3, 151.2, 140.9, 136.8, 132.5, 132.1, 131.6, 129.6, 129.0, 127.7, 127.5, 127.4, 125.9, 123.4, 120.4, 115.9, 34.2, 23.9 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_2\text{Br}$ $[\text{M}+\text{H}]^+$: 447.0708, found: 447.0697

1-(3-(benzo[d][1,3]dioxol-5-yl)imidazo[1,5-a]pyridin-1-yl)-2-(3-nitrophenyl)ethane-1,2-dione (5h)



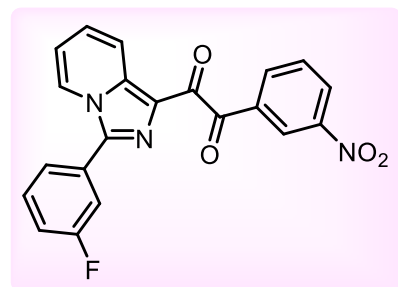
Following GP2, the compound **5h** was obtained as yellow solid (70 mg, 80%), m.p.= 188-190 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.85 (s, 1H), 8.53 (d, $J = 8.71$ Hz, 1H), 8.46 (d, $J = 7.99$ Hz, 1H), 8.41 (t, $J = 6.94$ Hz, 2H), 7.71 (t, $J = 7.86$ Hz, 1H), 7.46 (t, $J = 7.74$ Hz, 1H), 7.19 (d, $J = 7.61$ Hz, 1H), 7.14 (s, 1H), 7.03 (t, $J = 6.55$ Hz, 1H), 6.93 (d, $J = 7.97$ Hz, 1H), 6.04 (s, 2H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 192.4, 187.0, 149.3, 148.5, 140.6, 137.1, 135.4, 135.1, 130.1, 128.3, 128.2, 127.1, 125.0, 123.5, 123.1, 121.9, 120.5, 116.3, 109.4, 109.0, 101.8 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{22}\text{H}_{14}\text{N}_3\text{O}_6$ $[\text{M}+\text{H}]^+$: 416.0883, found: 416.0890

1-(3-(benzo[d][1,3]dioxol-5-yl)imidazo[1,5-a]pyridin-1-yl)-2-(4-(methylsulfonyl)phenyl)ethane-1,2-dione (5i)



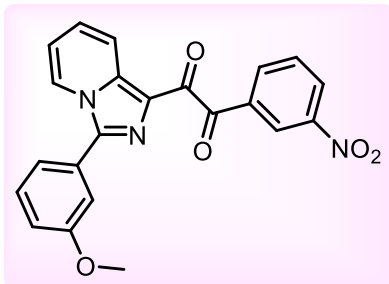
Following GP2, the compound **5i** was obtained as yellow solid (81 mg, 86%), m.p.= 180-182 °C; **¹H NMR (400 MHz, CDCl₃):** δ 8.51 (d, *J* = 8.98 Hz, 1H), 8.39 (td, *J* = 7.09, 0.95 Hz, 1H), 8.24 (td, *J* = 8.56, 1.77 Hz, 2H), 8.07-8.05 (m, 2H), 7.46-7.42 (m, 1H), 7.18 (dd, *J* = 8.01, 1.72 Hz, 1H), 7.14 (d, *J* = 1.66 Hz, 1H), 7.02 (dt, *J* = 6.89, 1.09 Hz, 1H), 6.93 (d, *J* = 8.04 Hz, 1H), 6.04 (s, 2H), 3.08 (s, 3H) ppm; **¹³C{¹H} NMR (101 MHz, CDCl₃):** δ 193.3, 187.4, 149.3, 148.5, 144.8, 140.6, 137.7, 137.0, 130.9, 128.1, 127.9, 127.1, 123.5, 123.1, 121.9, 120.4, 116.3, 109.4, 109.0, 101.8, 44.5 ppm; **HRMS (ESI) m/z:** calcd. for C₂₃H₁₇N₂O₆S [M+H]⁺: 449.0807, found: 449.0796

1-(3-(3-fluorophenyl)imidazo[1,5-a]pyridin-1-yl)-2-(3-nitrophenyl)ethane-1,2-dione (5j)



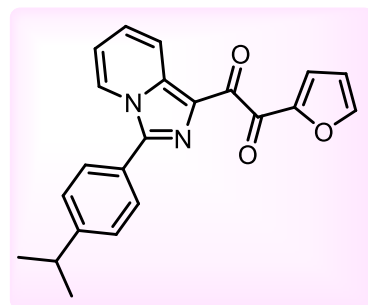
Following GP2, the compound **5j** was obtained as yellow solid (72 mg, 78%), m.p.= 157-159 °C; **¹H NMR (400 MHz, CDCl₃):** δ 8.85 (t, *J* = 1.77 Hz, 1H), 8.56 (d, *J* = 9.01 Hz, 1H), 8.48-8.41 (m, 3H), 7.71 (t, *J* = 7.88 Hz, 1H), 7.52-7.50 (m, 2H), 7.49-7.47 (m, 1H), 7.45-7.42 (m, 1H), 7.22-7.18 (m, 1H), 7.07 (dt, *J* = 6.88, 1.16 Hz, 1H) ppm; **¹³C{¹H} NMR (101 MHz, CDCl₃):** δ 192.2, 187.1, 164.3, 161.8, 148.5, 139.4 (d, *J* = 2.92 Hz), 137.2, 135.4, 135.0, 131.0 (d, *J* = 8.43 Hz), 130.3 (d, *J* = 8.22 Hz), 130.1, 128.4 (d, *J* = 4.73 Hz), 127.4, 125.0, 124.4 (d, *J* = 3.08 Hz), 123.3, 120.5, 117.3 (d, *J* = 21.17 Hz), 116.7, 116.1 (d, *J* = 23.44 Hz) ppm; **¹⁹F NMR (377 MHz, CDCl₃):** -110.77 to -110.83 (m) ppm; **HRMS (ESI) m/z:** calcd. for C₂₁H₁₃N₃O₄F [M+H]⁺: 390.0890, found: 390.0892

1-(3-(3-methoxyphenyl)imidazo[1,5-a]pyridin-1-yl)-2-(3-nitrophenyl)ethane-1,2-dione (5k)



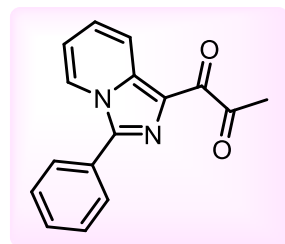
Following GP2, the compound **5k** was obtained as yellow solid (71 mg, 79%), m.p.= 149-151 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.86 (t, J = 1.68 Hz, 1H), 8.54 (d, J = 8.97 Hz, 1H), 8.47-8.44 (m, 2H), 8.43-8.41 (m, 1H), 7.71 (t, J = 7.98 Hz, 1H), 7.49-7.41 (m, 2H), 7.28-7.26 (m, 1H), 7.23-7.22 (m, 1H), 7.05-7.01 (m, 2H), 3.84 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 192.3, 187.1, 160.2, 148.5, 140.8, 137.2, 135.4, 135.1, 130.3, 130.1, 129.5, 128.3, 127.3, 125.0, 123.6, 120.9, 120.5, 116.4, 116.0, 114.6, 55.6 ppm; HRMS (ESI) m/z: calcd. for C₂₂H₁₆N₃O₅ [M+H]⁺: 402.1090, found: 402.1070

1-(furan-2-yl)-2-(3-(4-isopropylphenyl)imidazo[1,5-a]pyridin-1-yl)ethane-1,2-dione (5l)



Following GP2, the compound **5l** was obtained as yellow solid (64 mg, 84%), m.p.= 148-150 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.44 (d, J = 9.06 Hz, 1H), 8.40 (d, J = 7.10 Hz, 1H), 7.69 (s, 1H), 7.65 (d, J = 8.08 Hz, 2H), 7.37-7.35 (m, 4H), 6.95 (t, J = 6.80 Hz, 1H), 6.57-6.56 (m, 1H), 2.99-2.93 (m, 1H), 1.28 (s, 3H), 1.26 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 186.2, 182.1, 151.1, 150.5, 148.3, 140.8, 137.1, 128.9, 127.6, 127.3, 127.1, 126.0, 123.4, 122.0, 120.4, 115.9, 112.7, 34.2, 23.9 ppm HRMS (ESI) m/z: calcd. for C₂₂H₁₉N₂O₃ [M+H]⁺: 359.1396, found: 359.1384

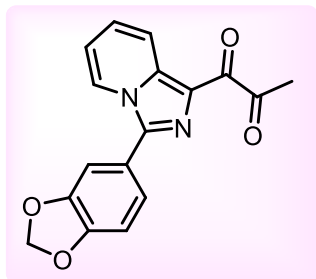
1-(3-phenylimidazo[1,5-a]pyridin-1-yl)propane-1,2-dione (5m)



Following GP3, the compound **5m** was obtained as yellow semi-solid (54 mg, 79%); ¹H NMR (400 MHz, CDCl₃): δ 8.45-8.39 (m, 2H), 7.79-7.77 (m, 2H), 7.59-7.52 (m, 3H), 7.39-7.34 (m, 1H), 6.96 (dt, J = 6.88, 1.20 Hz, 1H), 2.62 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 202.5, 187.7, 140.5, 137.2, 130.1, 129.3, 128.9, 128.7, 127.5, 126.3, 123.2, 120.5,

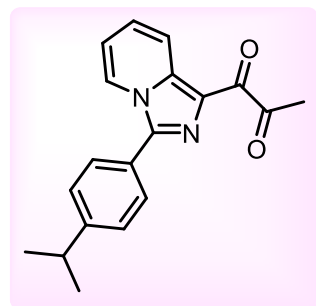
116.0, 27.3 ppm; **HRMS (ESI) m/z**: calcd. for C₁₆H₁₃N₂O₂ [M+H]⁺: 265.0977, found: 265.0972

1-(3-(benzo[d][1,3]dioxol-5-yl)imidazo[1,5-a]pyridin-1-yl)propane-1,2-dione (5n)



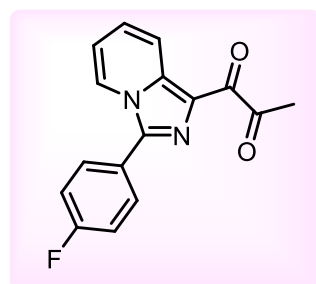
Following GP3, the compound **5n** was obtained as yellow semi-solid (54 mg, 83%); ¹H NMR (400 MHz, CDCl₃): δ 8.40 (d, J = 8.94 Hz, 1H), 8.35 (d, J = 7.05 Hz, 1H), 7.36-7.32 (m, 1H), 7.25-7.22 (m, 1H), 7.21 (d, J = 1.67 Hz, 1H), 6.97-6.93 (m, 2H), 6.02 (s, 2H), 2.59 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 202.5, 187.6, 149.2, 148.5, 140.2, 137.1, 127.4, 126.0, 123.3, 123.1, 122.2, 120.5, 115.9, 109.4, 109.0, 101.8, 27.3 ppm; **HRMS (ESI) m/z**: calcd. for C₁₇H₁₃N₂O₄ [M+H]⁺: 309.0875, found: 309.0858

1-(3-(4-isopropylphenyl)imidazo[1,5-a]pyridin-1-yl)propane-1,2-dione (5o)



Following GP3, the compound **5o** was obtained as yellow semi-solid (53 mg, 82%); ¹H NMR (400 MHz, CDCl₃): δ 8.41-8.38 (m, 2H), 7.68 (d, J = 8.27 Hz, 2H), 7.40 (d, J = 7.99 Hz, 2H), 7.36-7.31 (m, 1H), 6.95-6.91 (m, 1H), 3.03-2.96 (m, 1H), 2.60 (s, 3H), 1.31 (s, 3H), 1.29 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 202.6, 187.8, 151.2, 140.7, 137.1, 128.9, 127.4, 126.2, 126.1, 123.4, 120.4, 115.8, 34.2, 27.3, 23.9 ppm; **HRMS (ESI) m/z**: calcd. for C₁₉H₁₉N₂O₂ [M+H]⁺: 307.1447 found: 307.1443

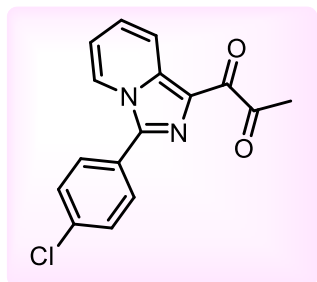
1-(3-(4-fluorophenyl)imidazo[1,5-a]pyridin-1-yl)propane-1,2-dione (5p)



Following GP3, the compound **5p** was obtained as yellow solid (54 mg, 81%), m.p. = 114-116 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.44 (dd, J = 9.13, 0.85 Hz, 1H), 8.35 (td, J = 7.09, 1.05 Hz, 1H), 7.82-7.77 (m, 2H), 7.41-7.37 (m, 1H), 7.30-7.28 (m, 2H), 7.02-6.99 (m, 1H), 2.63 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 202.4, 187.6, 164.9, 162.4, 139.4, 137.1, 131.0 (d, J = 8.66 Hz), 127.5, 126.2, 124.8 (d, J = 3.50 Hz), 123.0, 120.5, 116.6, 116.4, 116.1, 27.5 ppm; ¹⁹F NMR (377 MHz, CDCl₃): -109.53 to -

109.60 (m) ppm; **HRMS (ESI) m/z**: calcd. for C₁₆H₁₂N₂O₂F [M+H]⁺: 283.0883, found: 283.0887

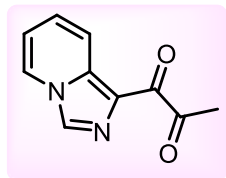
1-(3-(4-chlorophenyl)imidazo[1,5-a]pyridin-1-yl)propane-1,2-dione (5q)



Following GP3, the compound **5q** was obtained as yellow solid (52 mg, 80%), m.p.= 108-110 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.43 (td, J = 9.05, 0.86 Hz, 1H), 8.36-8.34 (m, 1H), 7.75-7.71 (m, 2H), 7.56-7.52 (m, 2H), 7.39-7.35 (m, 1H), 7.00-6.96 (m, 1H), 2.60 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 202.3, 187.6,

139.3, 137.2, 136.2, 130.1, 129.6, 127.5, 127.1, 126.4, 123.0, 120.6, 116.3, 27.2 ppm; **HRMS (ESI) m/z**: calcd. for C₁₆H₁₂N₂O₂Cl [M+H]⁺: 299.0587, found: 299.0585

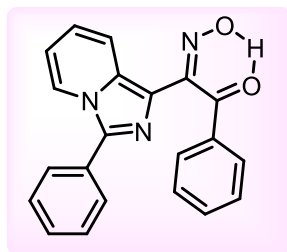
1-(imidazo[1,5-a]pyridin-1-yl)propane-1,2-dione (5r)



Following GP3, the compound **5r** was obtained as yellow semi-solid (68 mg, 85%); ¹H NMR (400 MHz, CDCl₃): δ 9.55 (dd, J = 7.03, 0.84 Hz, 1H), 7.76 (d, J = 8.86 Hz, 2H), 7.35-7.31 (m, 1H), 7.13 (t, J = 6.94 Hz, 1H),

2.60 (s, 3H) ppm; ¹³C{¹H} NMR (101 MHz, CDCl₃): δ 200.6, 181.1, 135.8, 131.7, 126.7, 126.4, 126.3, 118.4, 117.5, 27.1 ppm; **HRMS (ESI) m/z**: calcd. for C₁₀H₉N₂O₂ [M+H]⁺: 189.0664, found: 189.0665

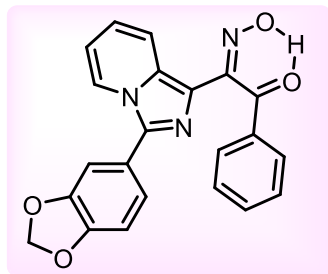
(Z)-2-(hydroxyimino)-1-phenyl-2-(3-phenylimidazo[1,5-a]pyridin-1-yl)ethan-1-one (6a)



Following GP4, the compound **6a** was obtained as yellow colored solid (42 mg, 81%); ¹H NMR (400 MHz, DMSO-d₆): δ 11.40 (s, 1H), 8.62 (d, J = 7.01 Hz, 1H), 8.35 (d, J = 6.26 Hz, 1H), 7.75 (d, J = 6.40 Hz, 2H), 7.58-7.51 (m, 6H), 7.39-7.37 (m, 3H), 7.12 (t, J = 6.63 Hz,

1H) ppm; ¹³C{¹H} NMR (101 MHz, DMSO-d₆): δ 155.7, 139.1, 135.0, 132.7, 129.6, 129.3, 129.0, 128.7, 128.5, 128.4, 128.3 (d, J = 2.73 Hz), 125.8, 124.3, 118.7, 116.1 ppm; **HRMS (ESI) m/z**: calcd. for C₂₁H₁₆N₃O₂ [M+H]⁺: 342.1243, found: 342.1252

(Z)-2-(3-(benzo[d][1,3]dioxol-5-yl)imidazo[1,5-a]pyridin-1-yl)-2-(hydroxyimino)-1-phenylethan-1-one (6b)

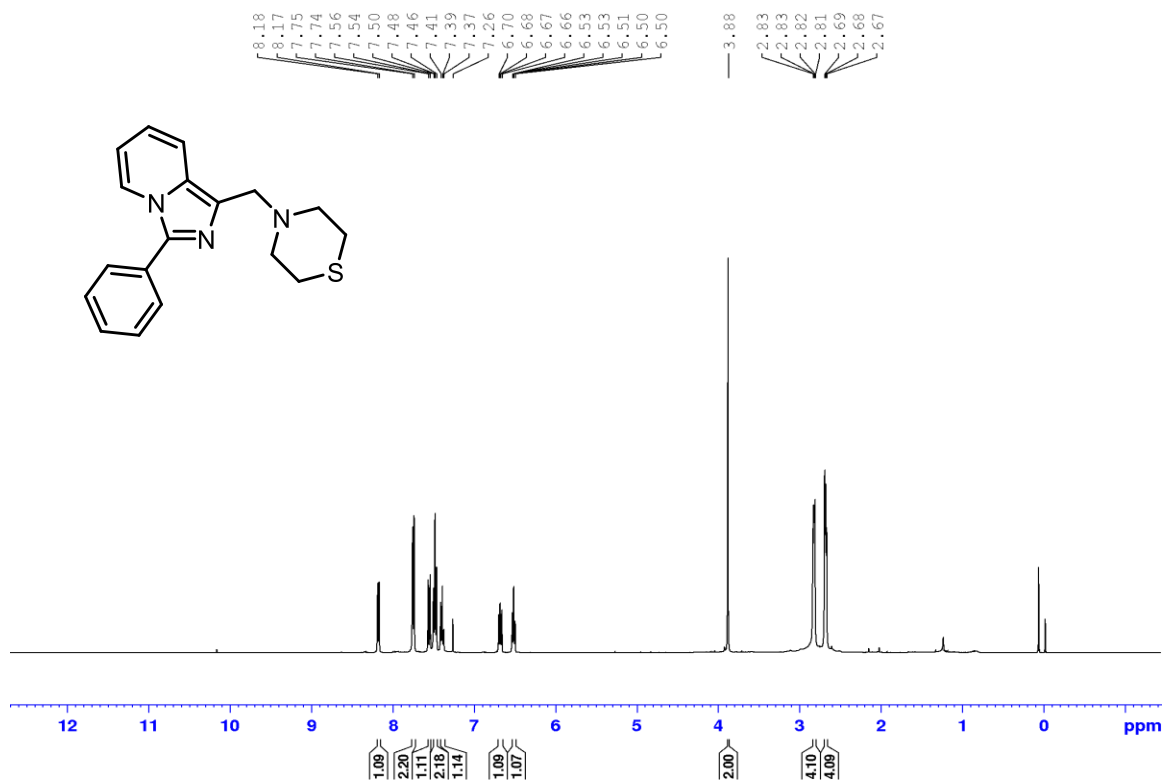


Following GP4, the compound **6b** was obtained as yellow solid (40 mg, 77%); ^1H NMR (400 MHz, CDCl_3 and DMSO-d_6): δ 11.03 (d, $J = 8.99$ Hz, 1H), 8.33 (t, $J = 6.18$ Hz, 2H), 7.66-7.63 (m, 1H), 7.57-7.55 (m, 2H), 7.27-7.24 (m, 3H), 7.14-7.11 (m, 1H), 7.08-7.07 (m, 1H), 6.92-6.86 (m, 2H), 5.99-5.97 (m, 2H) ppm; $^{13}\text{C}\{^1\text{H}\}$

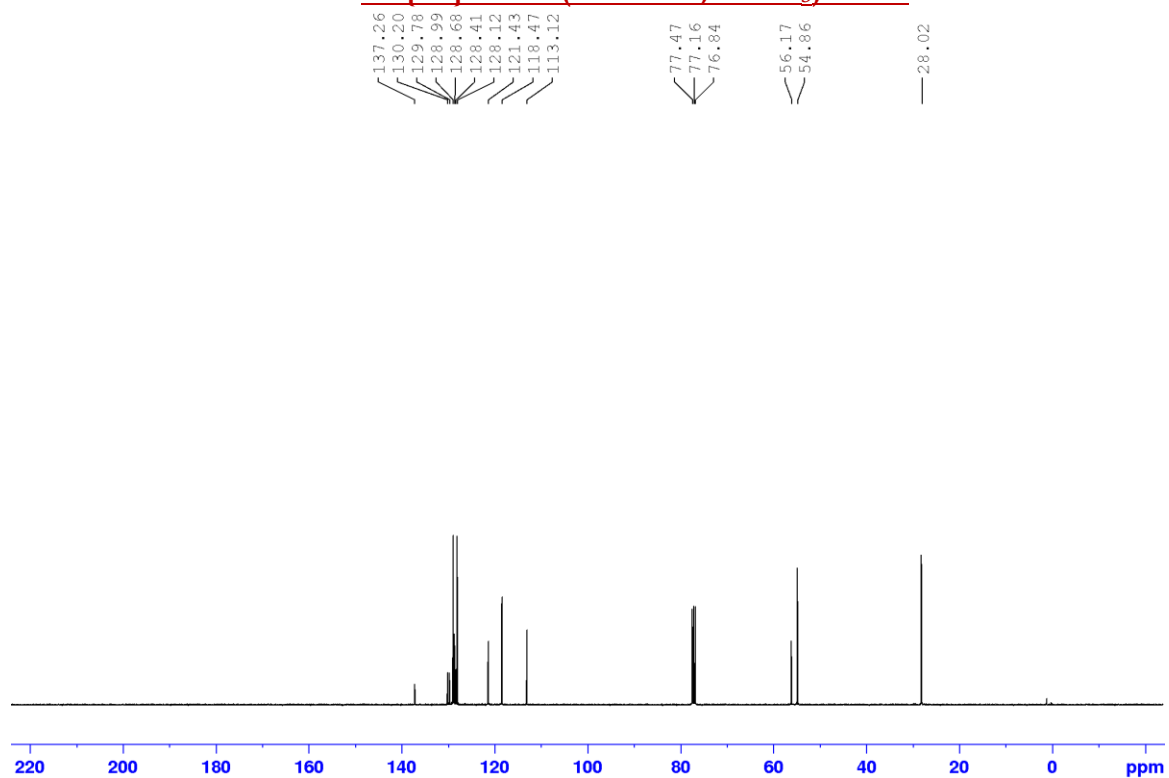
NMR (101 MHz, CDCl_3 and DMSO-d_6): δ 155.5, 147.9, 147.3, 138.5, 134.5, 132.1, 128.6, 128.3, 127.8, 127.5, 127.0, 126.1, 125.3, 122.4, 121.9, 121.4, 118.8, 114.7, 108.2, 107.8, 100.7 ppm; HRMS (ESI) m/z : calcd. for $\text{C}_{22}\text{H}_{16}\text{N}_3\text{O}_4$ $[\text{M}+\text{H}]^+$: 386.3790, found: 386.3792

4. Copies of NMR, HRMS, GC-MS, MS-MS Spectra

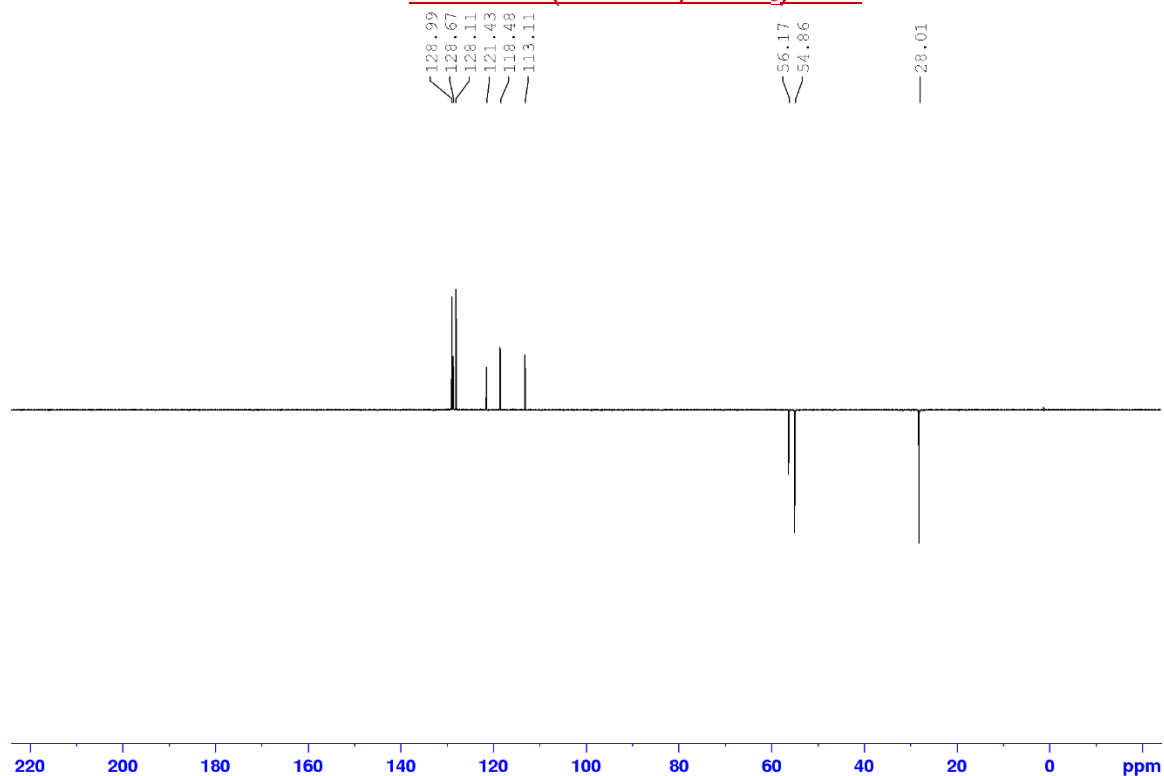
^1H NMR (400 MHz, CDCl_3) of 3a



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



DEPT-135 (101 MHz, CDCl₃) of 3a



HRMS of 3a

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-18 H: 0-100 N: 0-3 S: 0-1 Na: 0-1

SM-334

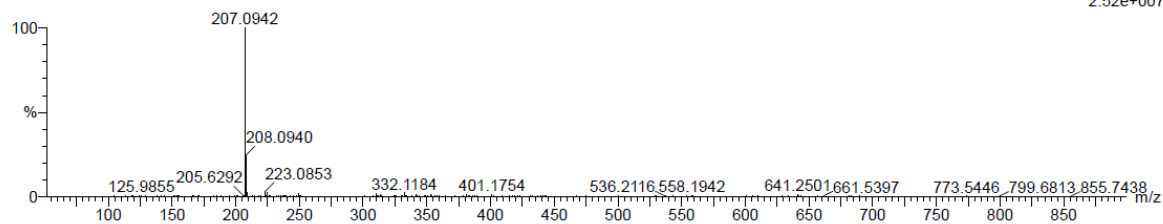
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Apr-2024

12:22:54

230424_06 5 (0.121)

1: TOF MS ES+
2.52e+007



Minimum: -1.5
Maximum: 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|-----------------|
| 332.1184 | 332.1197 | -1.3 | -3.9 | 10.5 | 1145.4 | n/a | n/a | C18 H19 N3 S Na |

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2

SM-334

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

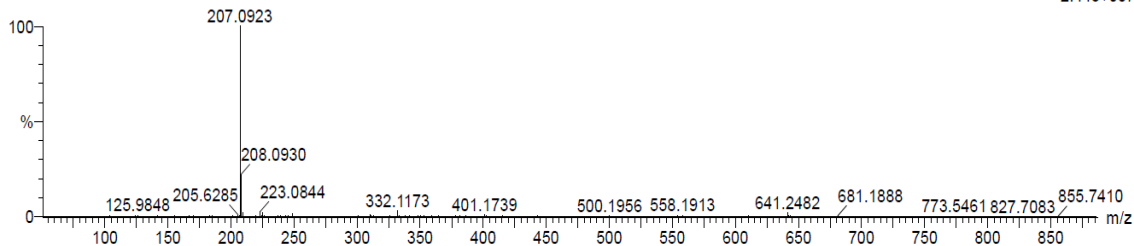
23-Apr-2024

12:22:54

1: TOF MS ES+

2.44e+007

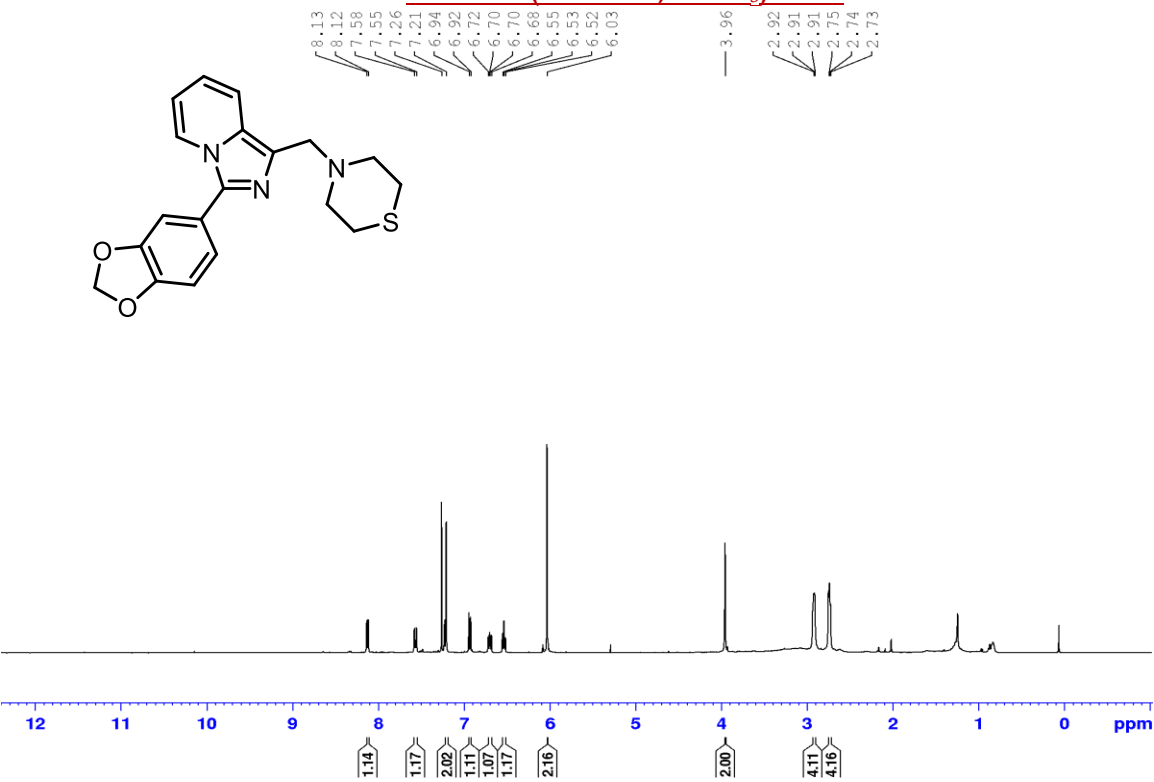
230424_06 7 (0.155)



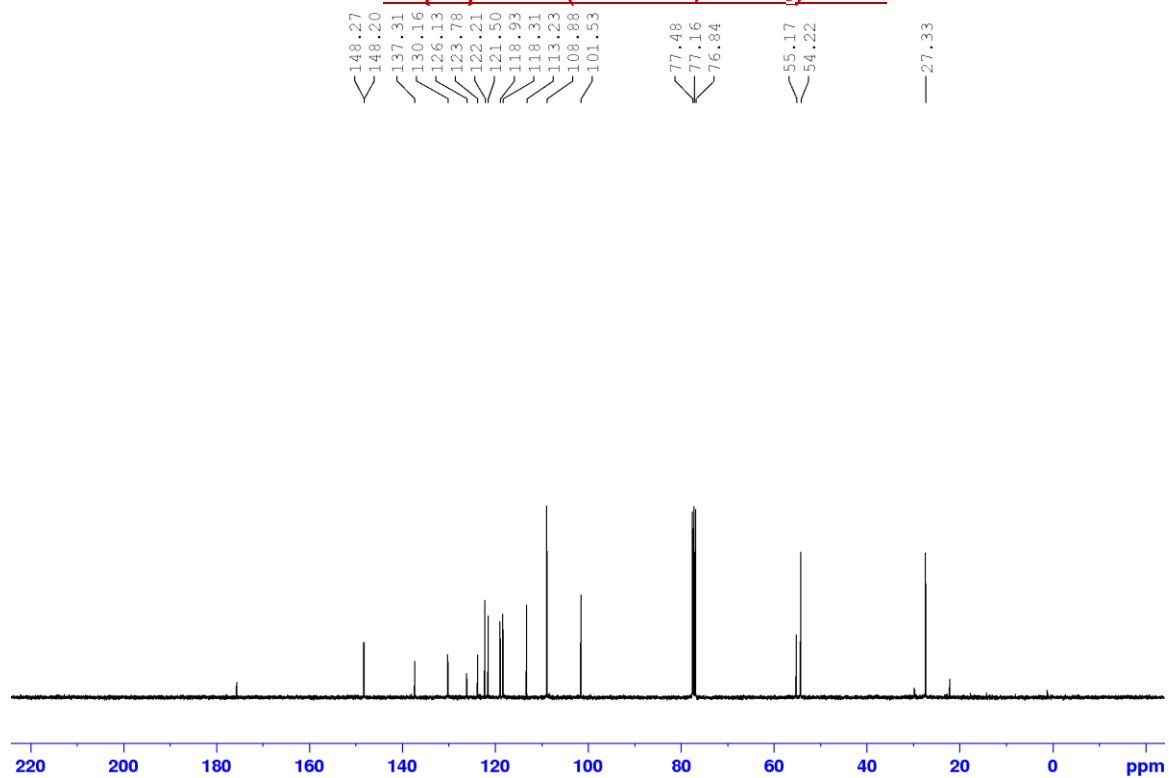
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|------------|
| 207.0923 | 207.0922 | 0.1 | 0.5 | 10.5 | 1517.9 | n/a | n/a | C14 H11 N2 |

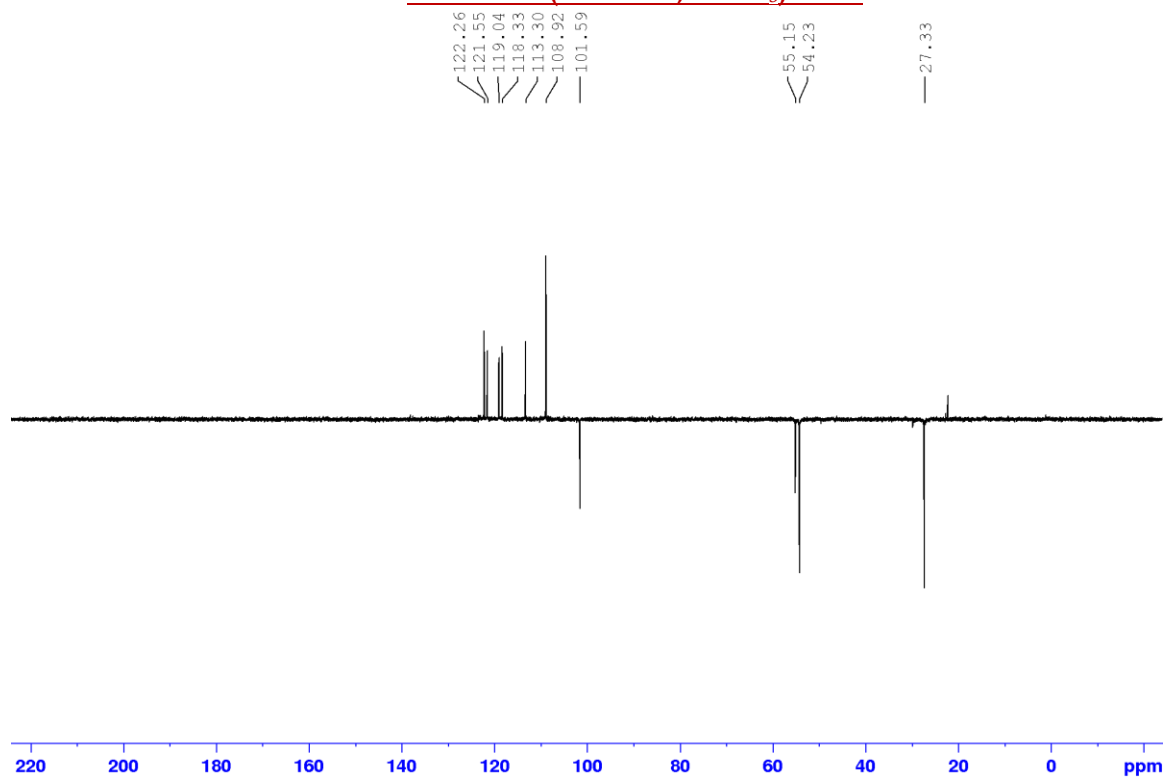
¹H NMR (400 MHz, CDCl₃) of 3b



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3b



DEPT-135 (400 MHz, CDCl_3) of 3b



HRMS of 3b

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-15 H: 0-100 N: 0-2 O: 0-2

SM-520

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

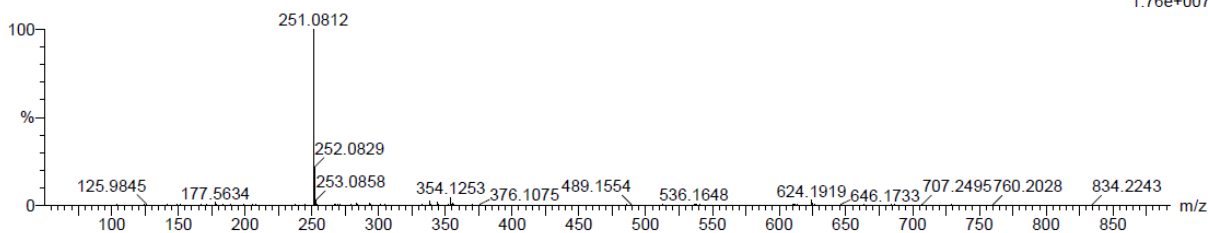
07-May-2024

14:31:09

1: TOF MS ES+

1.76e+007

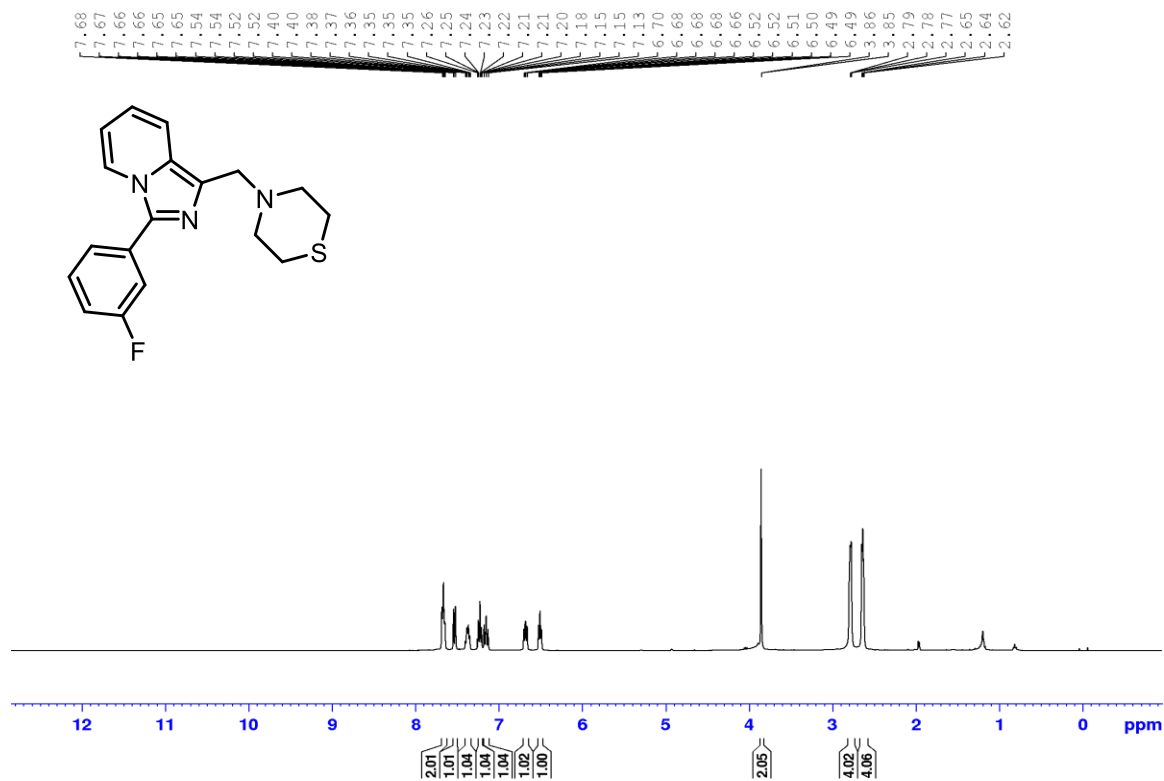
070524_36 5 (0.121)



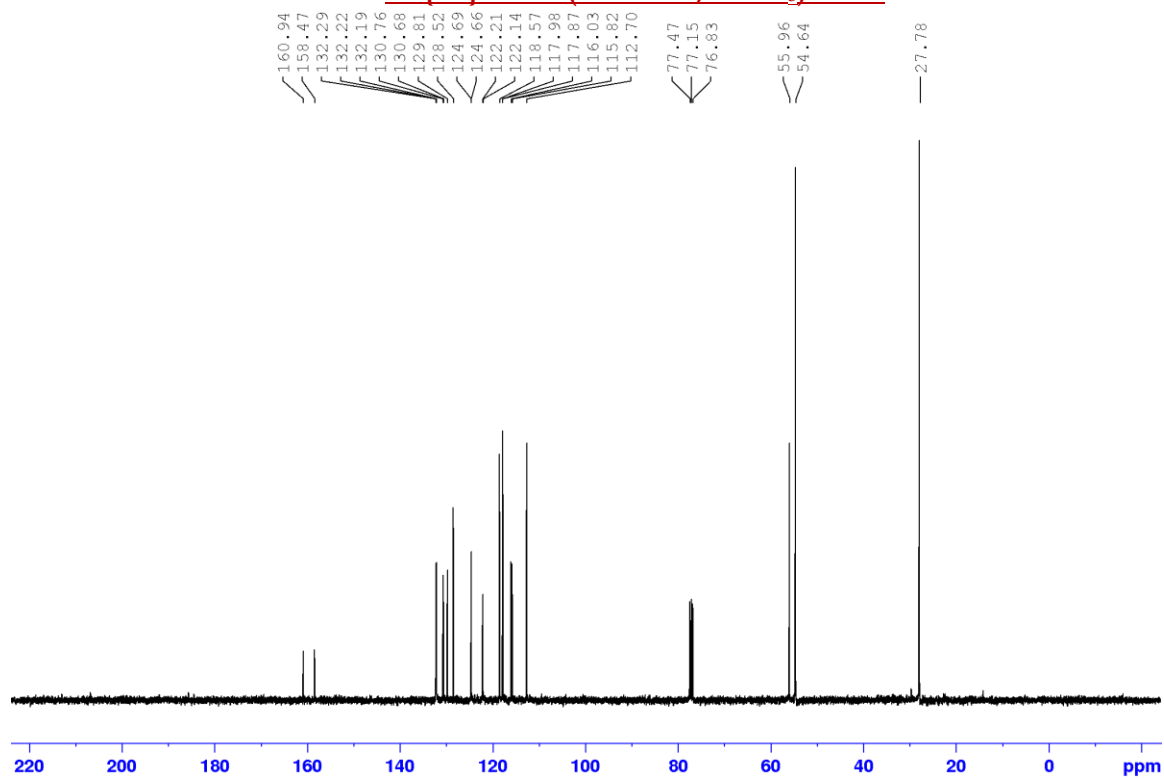
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|---------------|
| 251.0812 | 251.0821 | -0.9 | -3.6 | 11.5 | 1201.2 | n/a | n/a | C15 H11 N2 O2 |

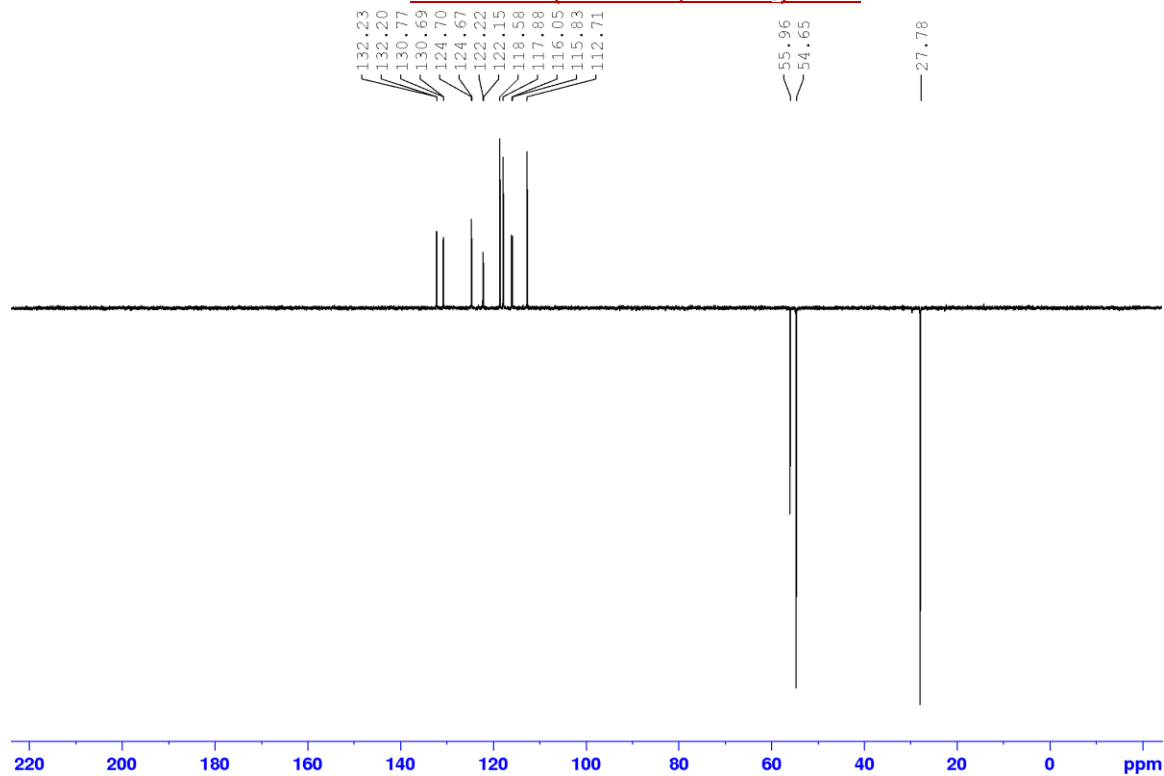
¹H NMR (400 MHz, CDCl₃) of 3c



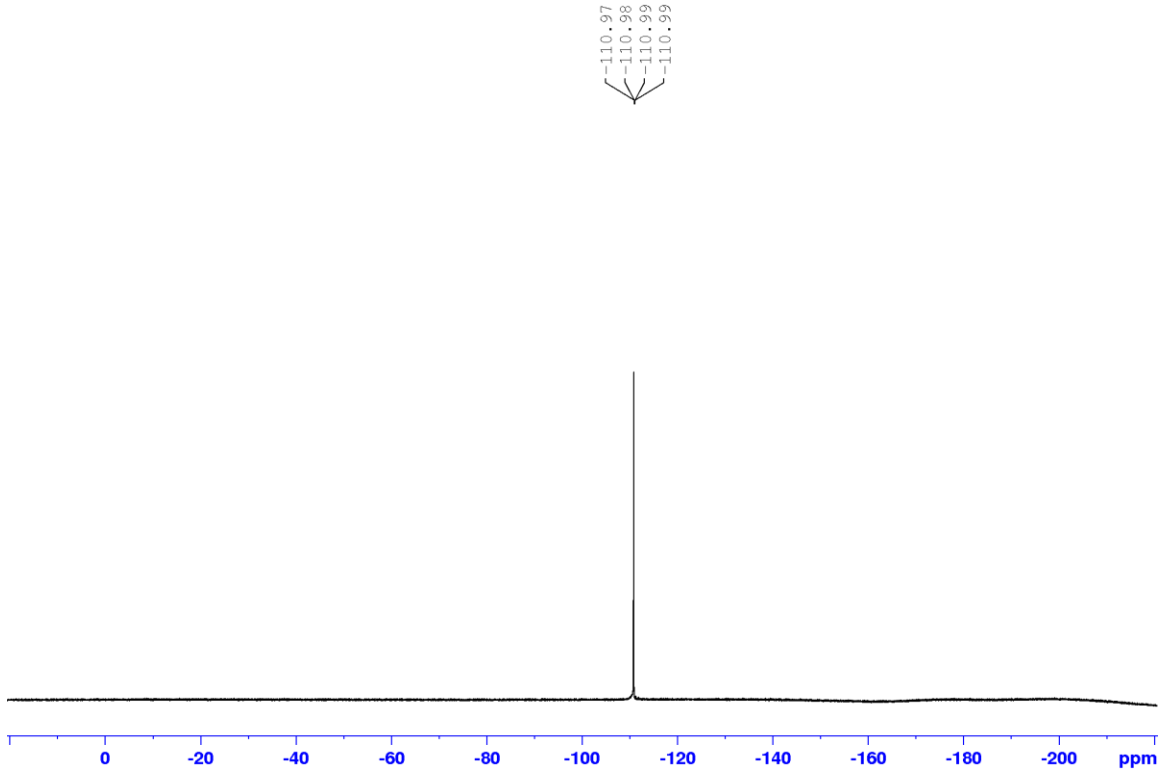
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3c



DEPT-135 (400 MHz, CDCl_3) of 3c



¹⁹F NMR (377 MHz, CDCl₃) of 3c



HRMS of 3c

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2 F: 0-1

SM-378

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

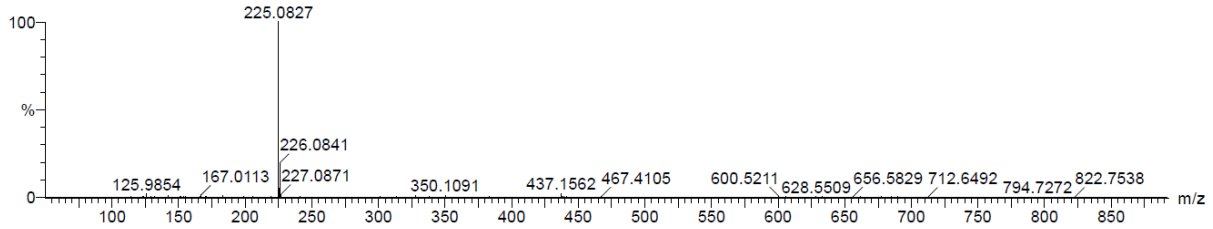
23-Apr-2024

12:33:19

1: TOF MS ES+

9.41e+006

230424_10 4 (0.104)

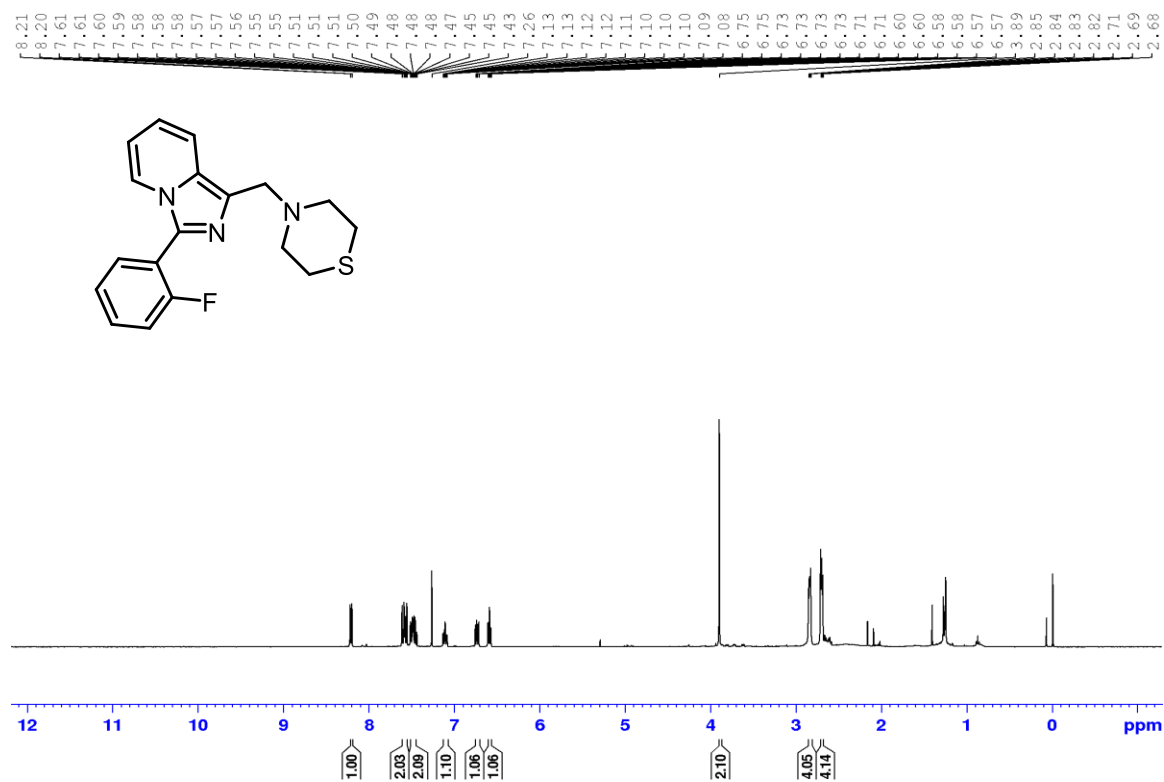


Minimum: -1.5

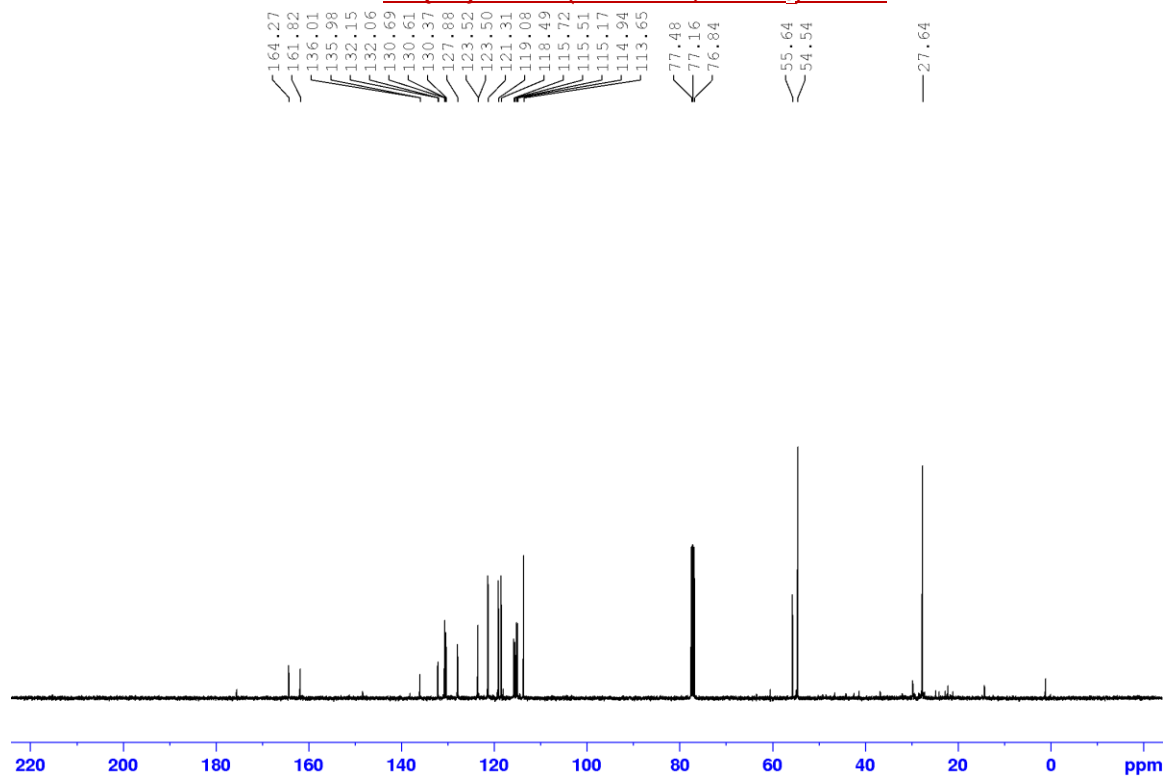
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|--------------|
| 225.0827 | 225.0828 | -0.1 | -0.4 | 10.5 | 1384.3 | n/a | n/a | C14 H10 N2 F |

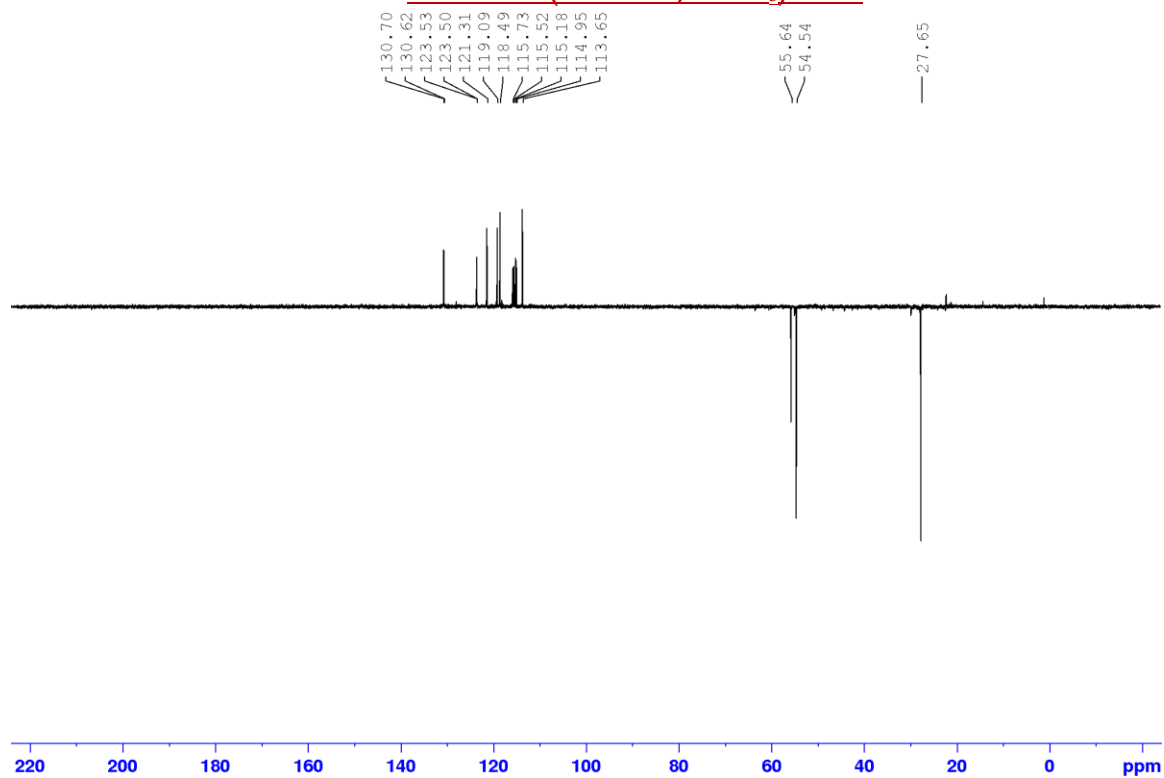
^1H NMR (400 MHz, CDCl_3) of 3d



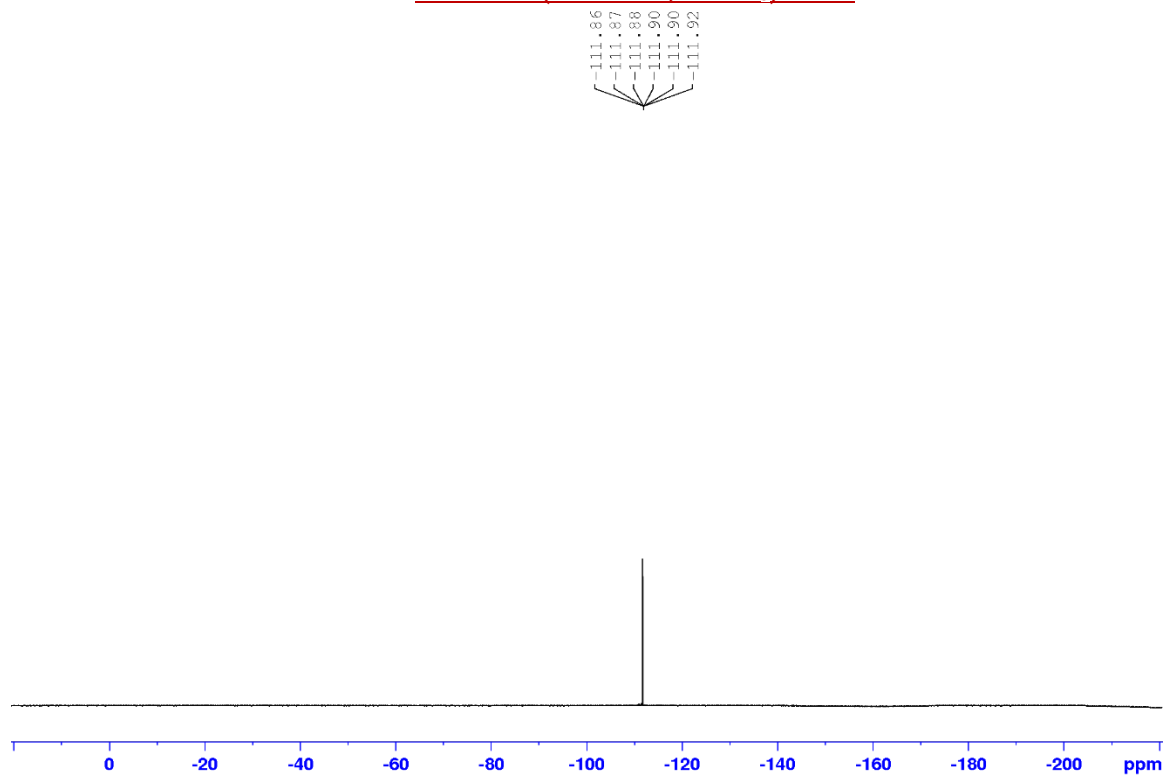
^{13}C NMR (101 MHz, CDCl_3) of 3d



DEPT-135 (400 MHz, CDCl₃) of 3d



¹⁹F NMR (377 MHz, CDCl₃) of 3d



HRMS of 3d

Elemental Composition Report

Page 1

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions

29 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-18 H: 0-100 N: 0-4 S: 0-1 F: 0-1

SM-379

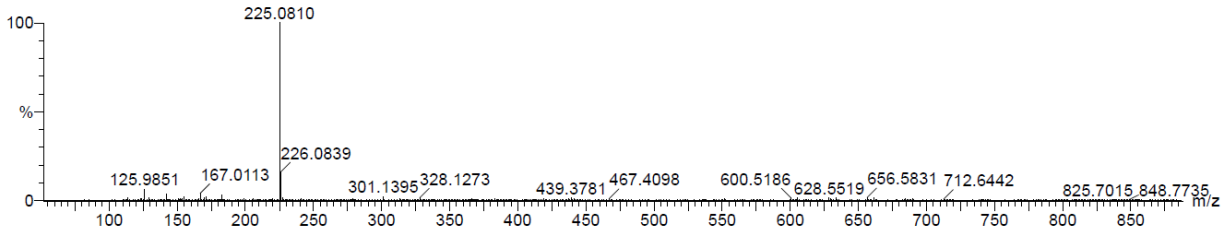
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Apr-2024

13:00:06

230424_20 4 (0.104)

1: TOF MS ES+
3.02e+006



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|----------------|
| 328.1273 | 328.1284 | -1.1 | -3.4 | 10.5 | 1134.8 | n/a | n/a | C18 H19 N3 S F |

Elemental Composition Report

Page 1

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2 F: 0-1

SM-379

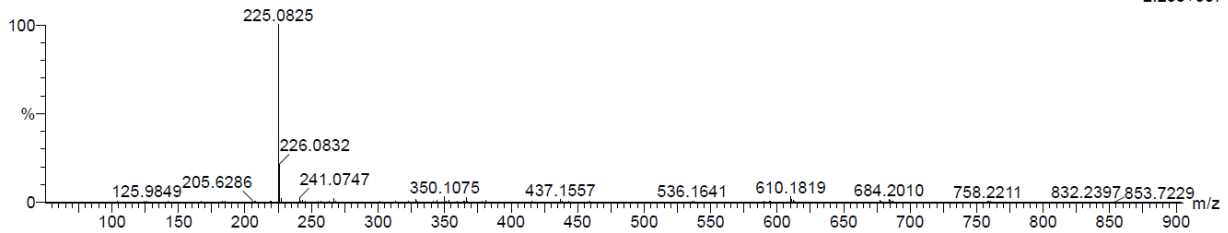
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Apr-2024

13:00:06

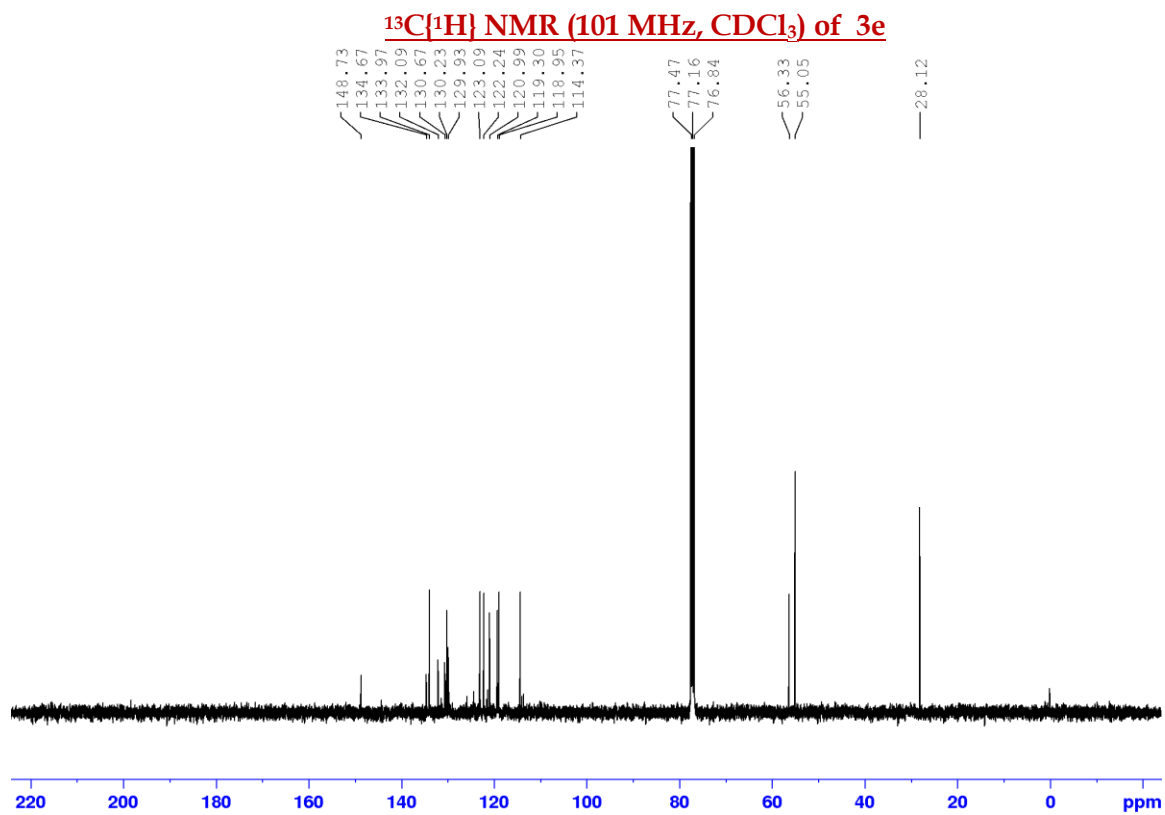
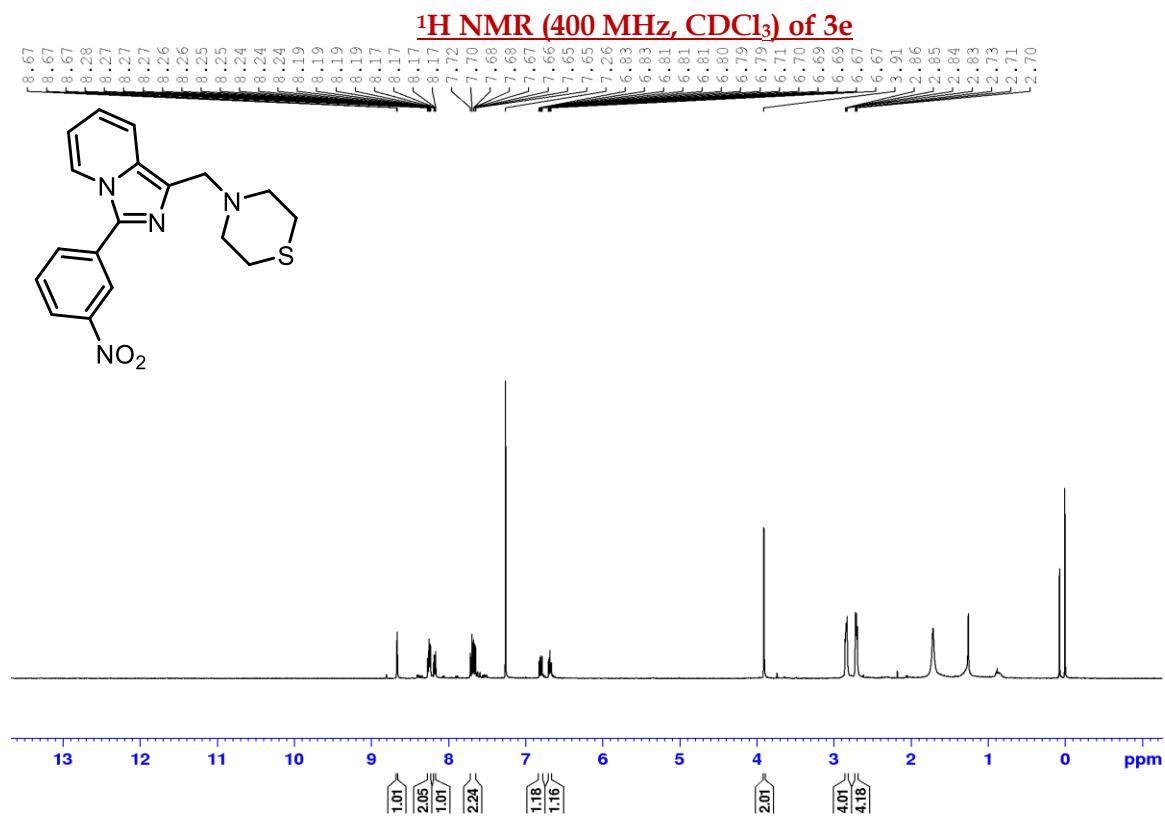
230424_20 7 (0.155)

1: TOF MS ES+
2.28e+007

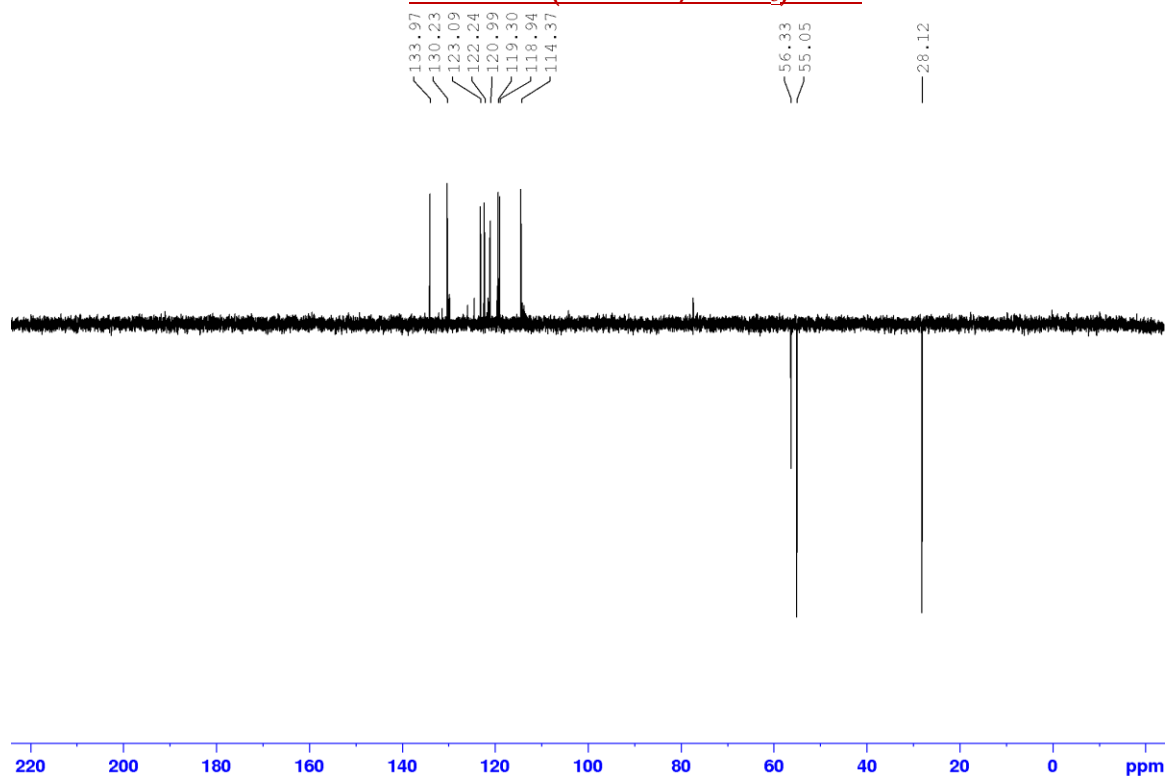


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|--------------|
| 225.0825 | 225.0828 | -0.3 | -1.3 | 10.5 | 1403.5 | n/a | n/a | C14 H10 N2 F |



DEPT-135 (400 MHz, CDCl₃) of 3e



HRMS of 3e

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

34 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-18 H: 0-100 N: 0-4 O: 0-2 S: 0-1

SM-392

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

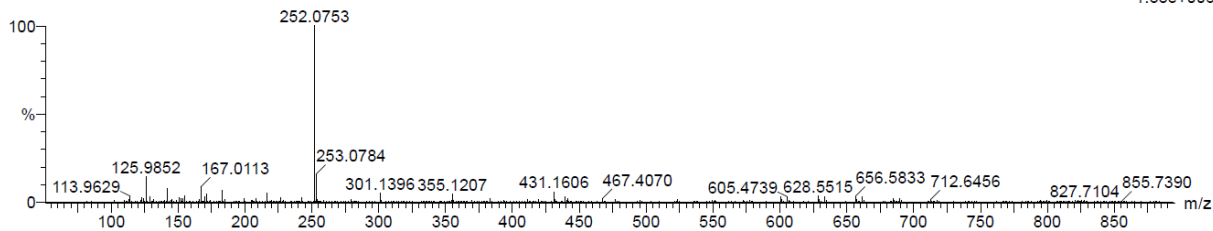
23-Apr-2024

12:52:14

1: TOF MS ES+

1.38e+006

230424_17 4 (0.104)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|-----------------|
| 355.1207 | 355.1229 | -2.2 | -6.2 | 11.5 | 1058.2 | n/a | n/a | C18 H19 N4 O2 S |

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-3 O: 0-2

SM-392

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

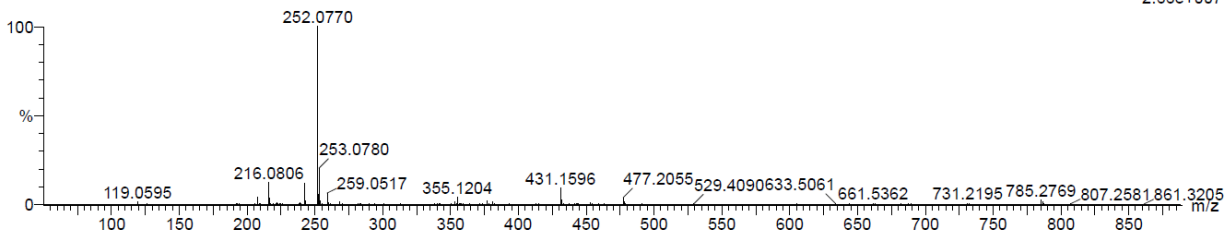
23-Apr-2024

12:52:14

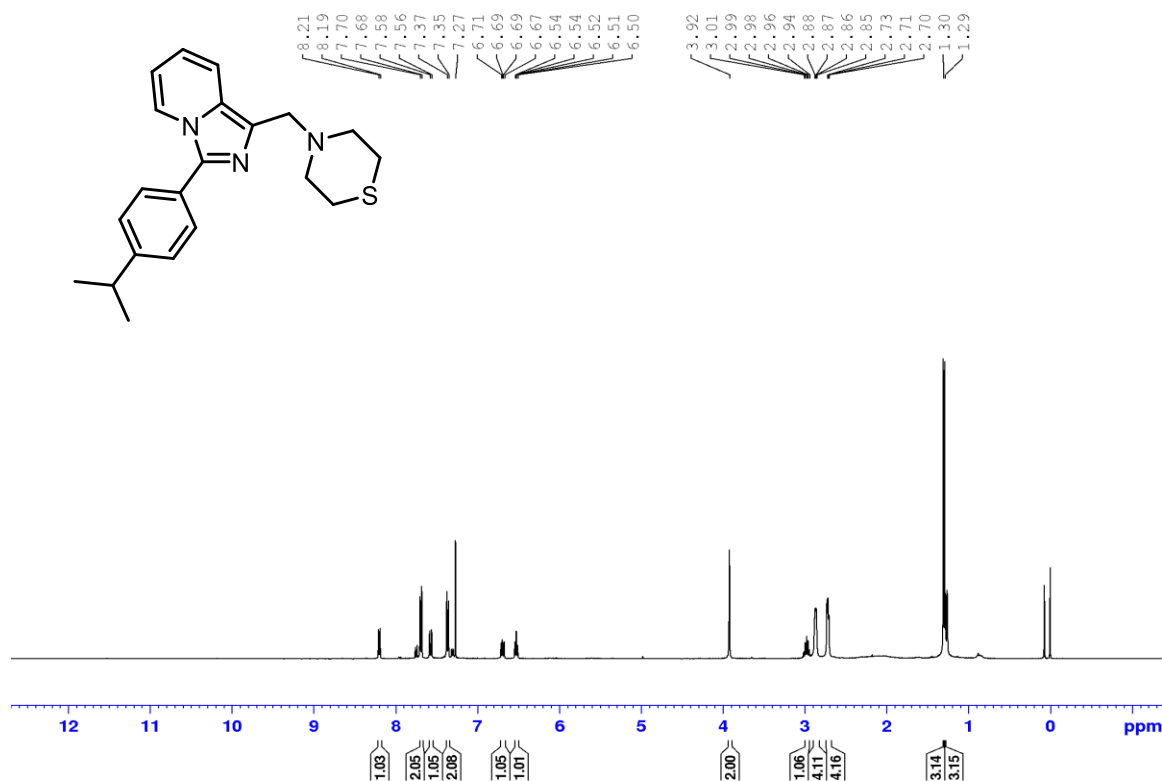
1: TOF MS ES+

2.66e+007

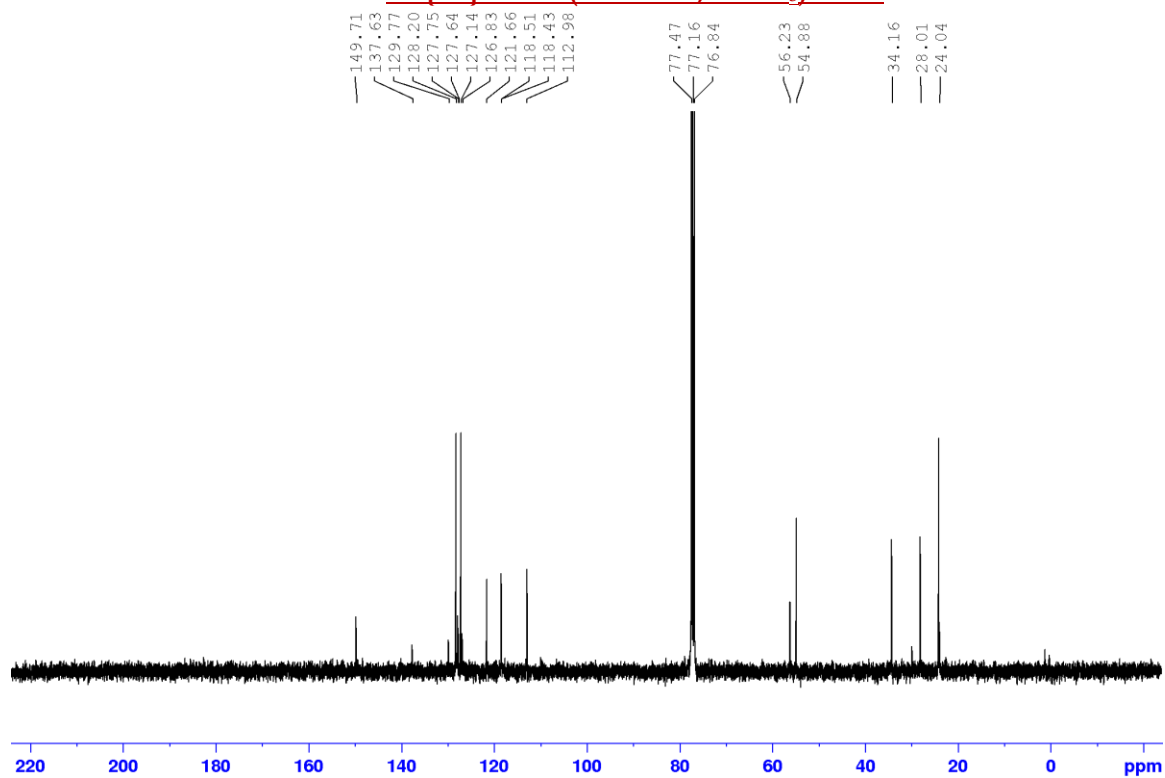
230424_17 6 (0.138)

Minimum: -1.5
Maximum: 2.0 50.0 50.0

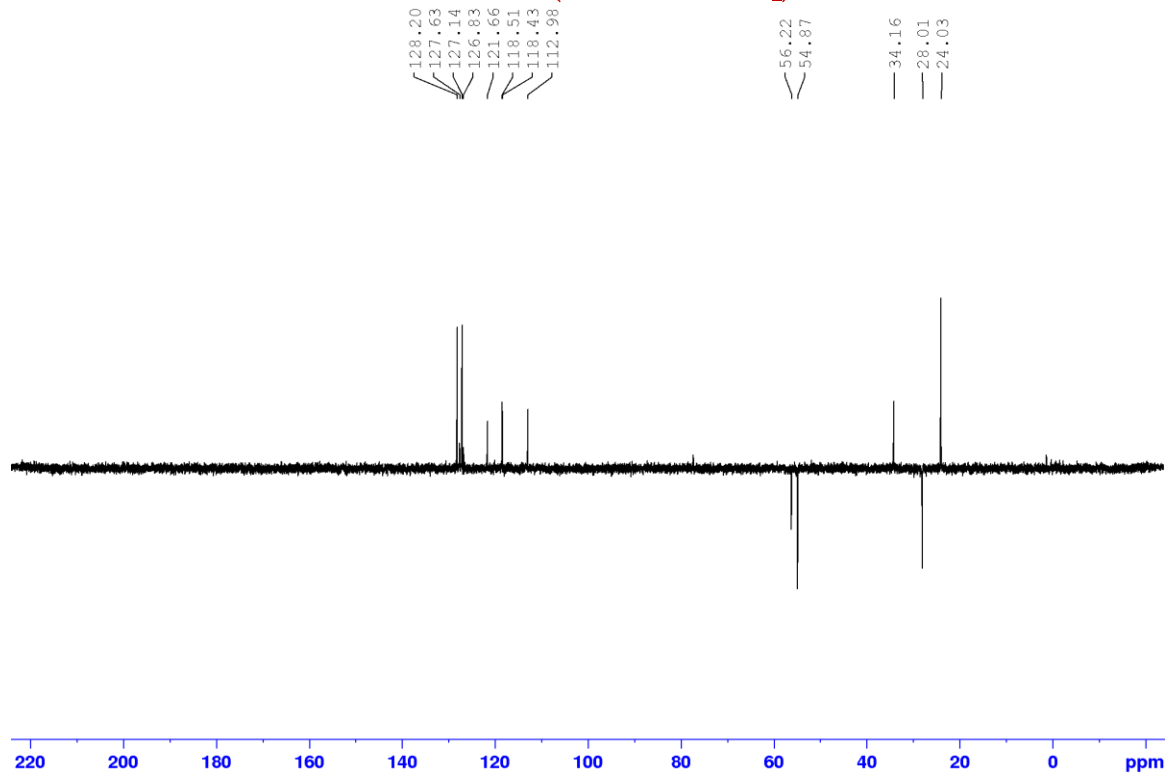
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|---------------|
| 252.0770 | 252.0773 | -0.3 | -1.2 | 11.5 | 1342.3 | n/a | n/a | C14 H10 N3 O2 |

¹H NMR (400 MHz, CDCl₃) of 3f

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3f



DEPT-135 (400 MHz, CDCl_3) of 3f



HRMS of 3f

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-21 H: 0-100 N: 0-3 S: 0-1

SM-396

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

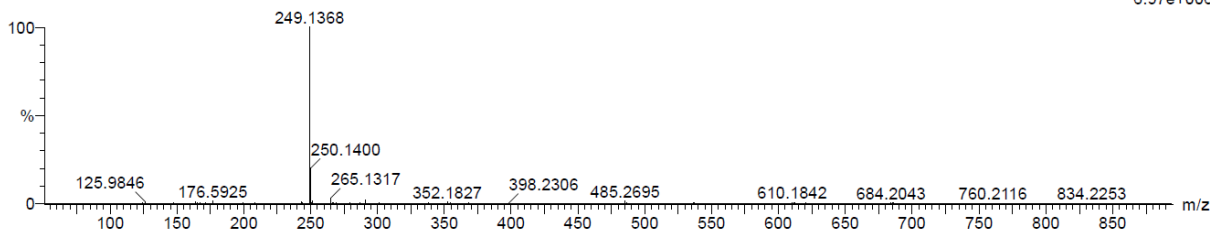
07-May-2024

15:16:22

1: TOF MS ES+

6.97e+006

070524_53 5 (0.121)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|-------|------|----------|--------------|
| 352.1827 | 352.1847 | -2.0 | -5.7 | 10.5 | 891.0 | n/a | n/a | C21 H26 N3 S |

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-17 H: 0-100 N: 0-2

SM-396

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

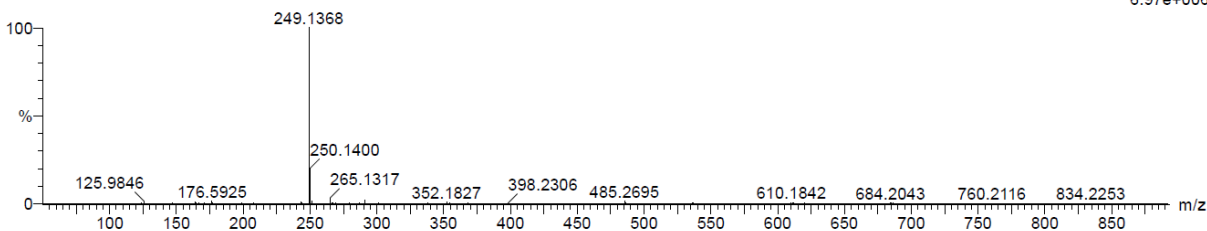
07-May-2024

15:16:22

1: TOF MS ES+

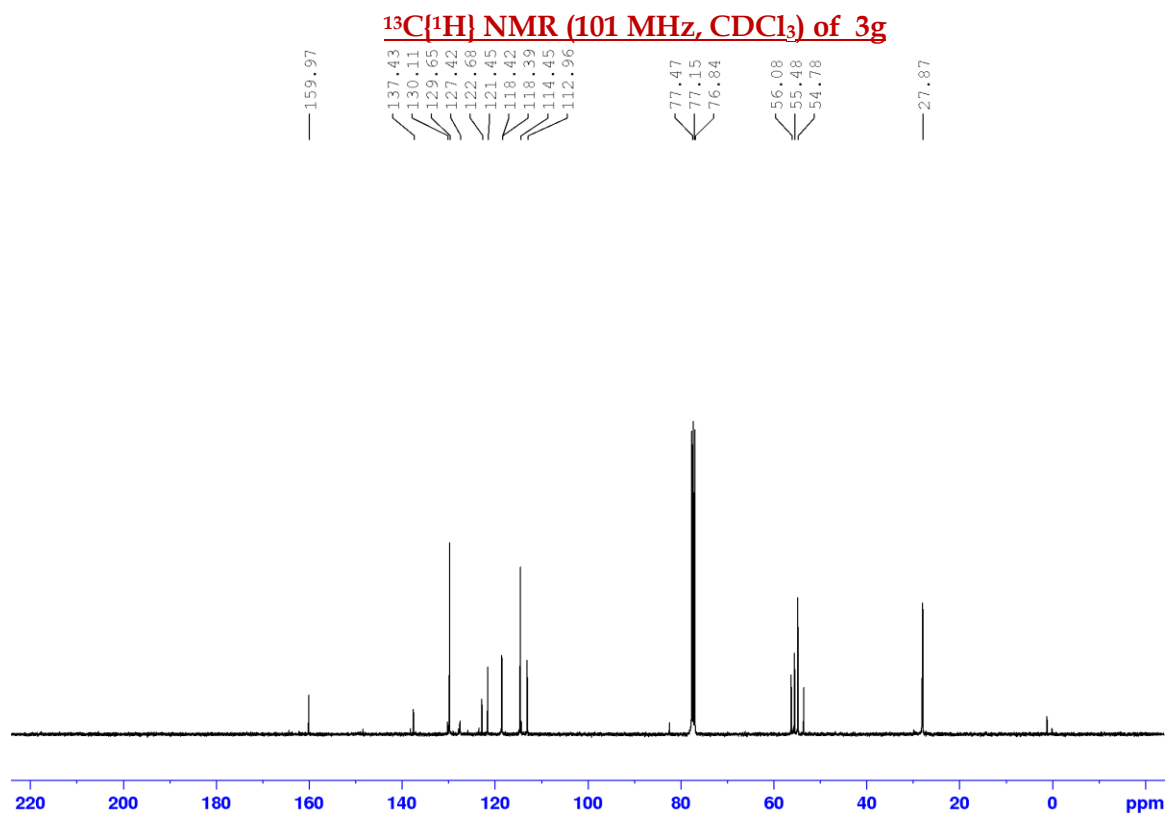
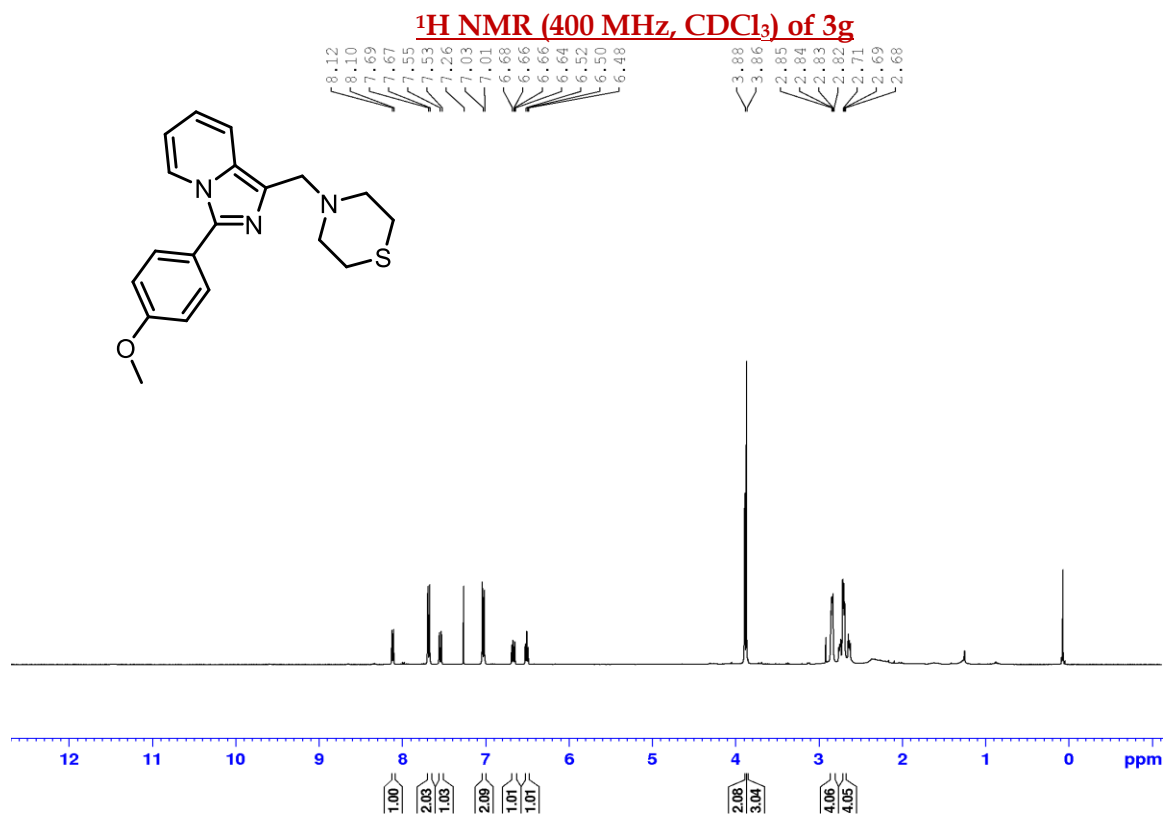
6.97e+006

070524_53 5 (0.121)

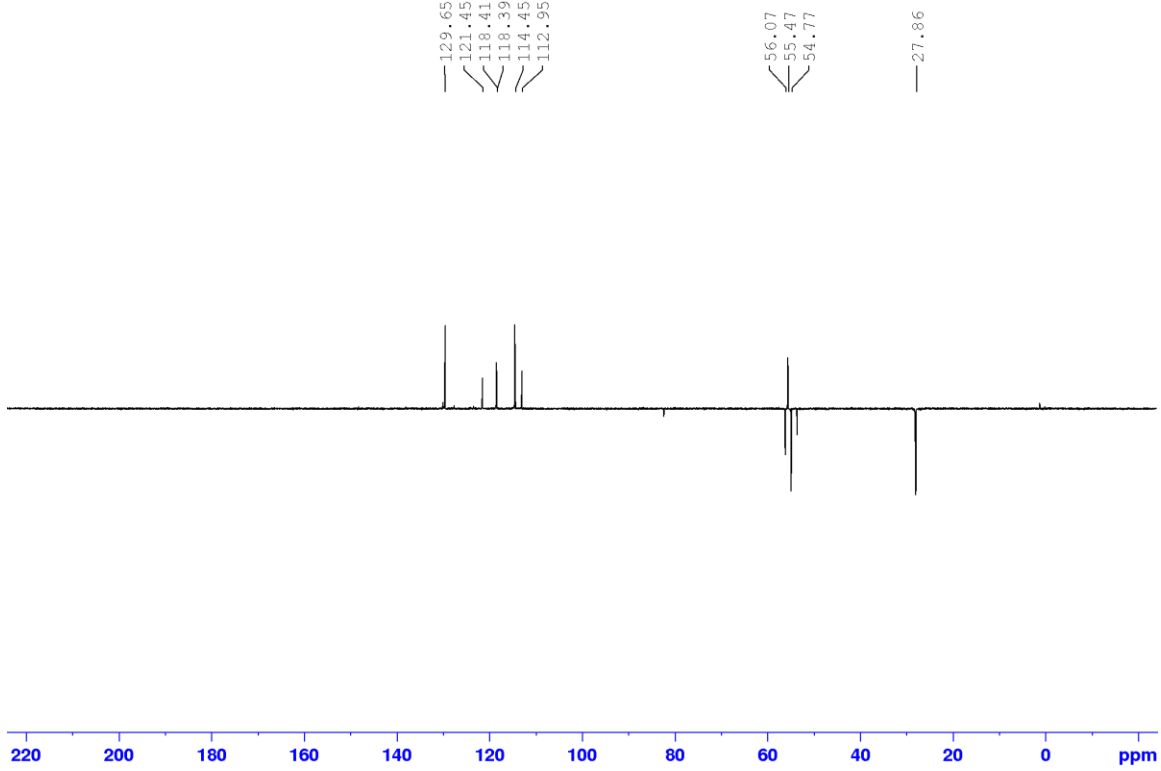


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|------------|
| 249.1368 | 249.1392 | -2.4 | -9.6 | 10.5 | 1207.6 | n/a | n/a | C17 H17 N2 |



DEPT-135 (400 MHz, CDCl₃) of 3g



HRMS of 3g

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

20 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-19 H: 0-100 N: 0-3 O: 0-1 S: 0-1

SM-477

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

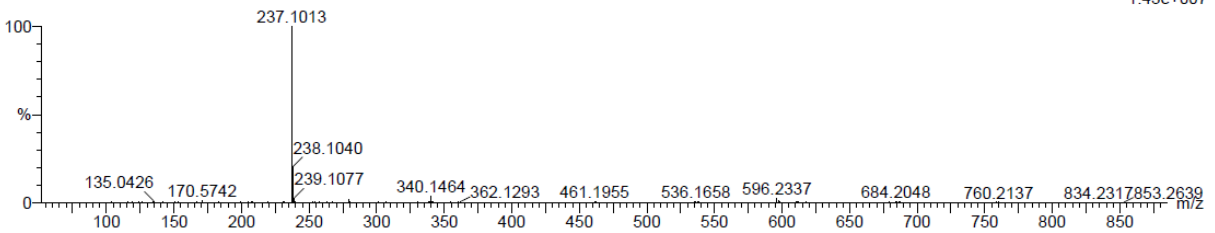
07-May-2024

15:24:04

1: TOF MS ES+

1.43e+007

070524_56 5 (0.121)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PEM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|-------|------|---------|----------------|
| 340.1464 | 340.1484 | -2.0 | -5.9 | 10.5 | 976.8 | n/a | n/a | C19 H22 N3 O S |

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-15 H: 0-100 N: 0-2 O: 0-1

SM-477

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

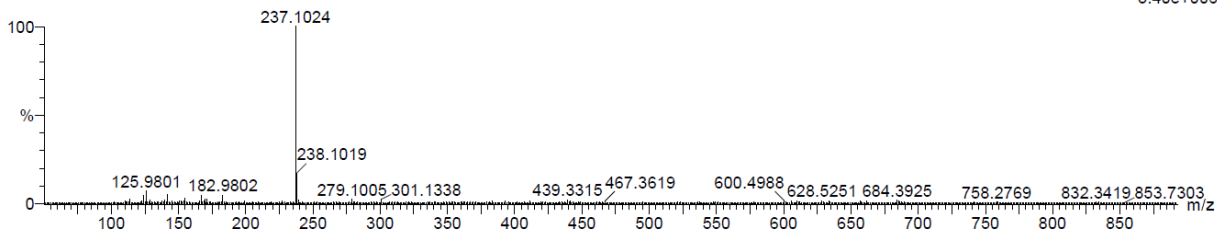
23-Apr-2024

12:12:30

1: TOF MS ES+

3.40e+006

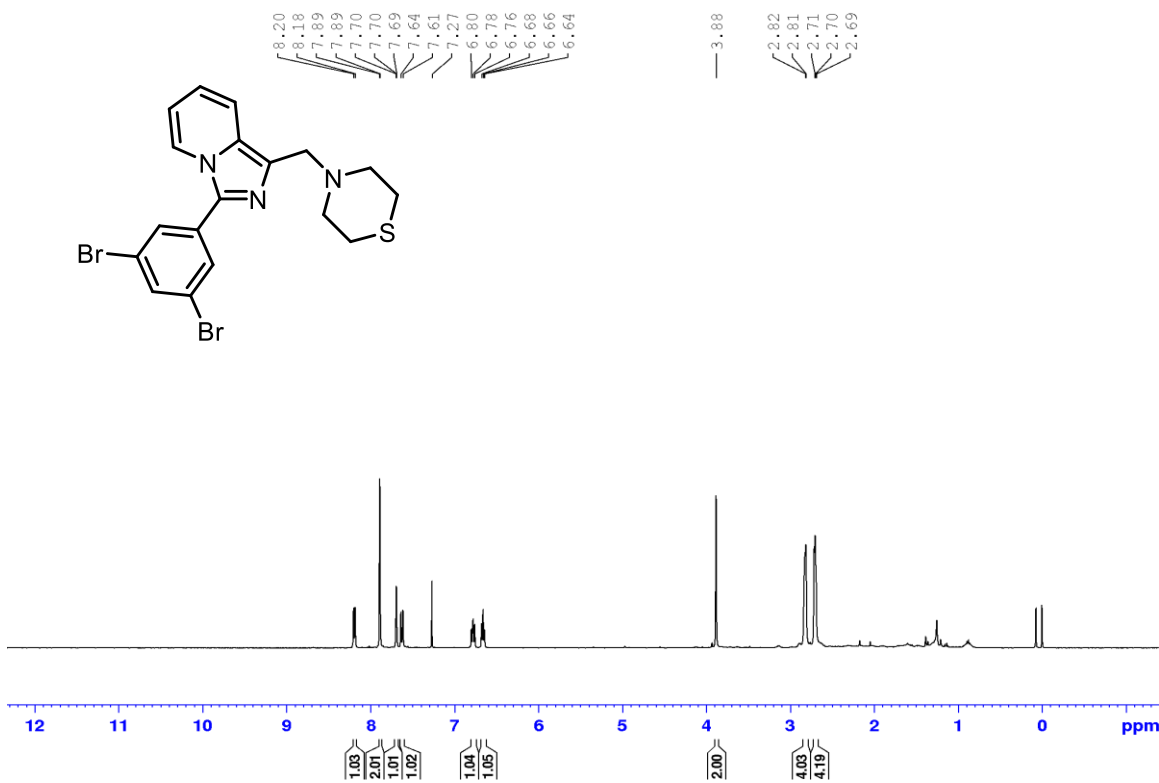
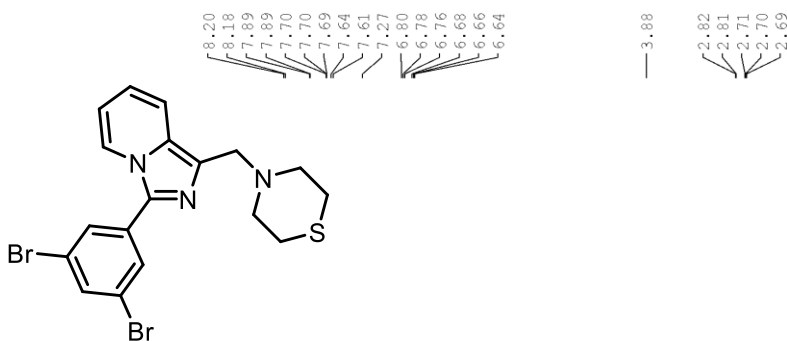
230424_02 9 (0.208) Cm (9)



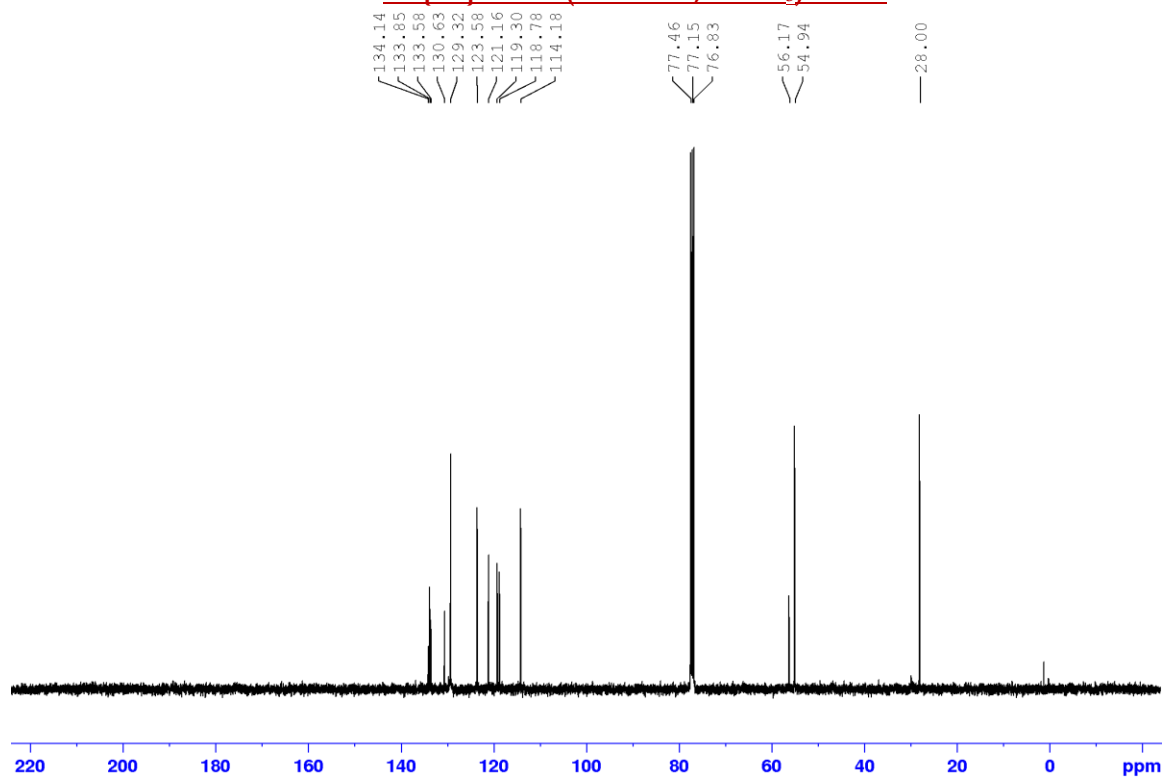
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|-------|------|----------|--------------|
| 237.1024 | 237.1028 | -0.4 | -1.7 | 10.5 | 46.3 | n/a | n/a | C15 H13 N2 O |

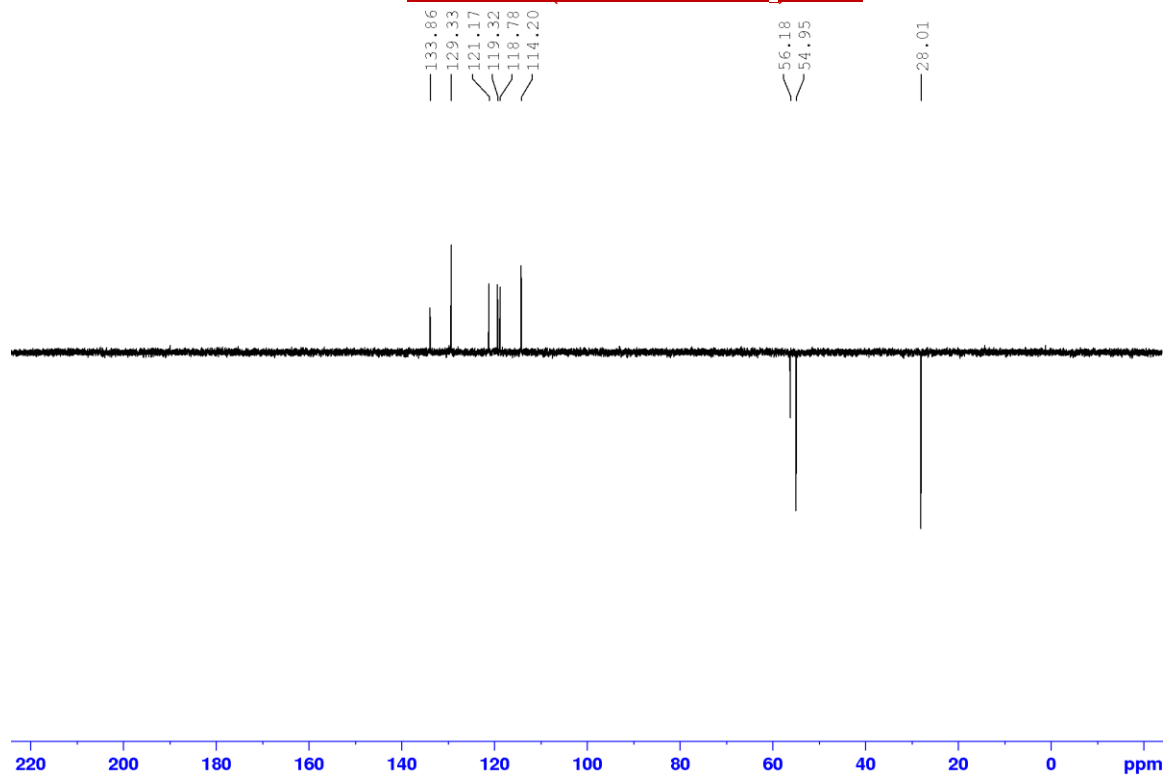
¹H NMR (400 MHz, CDCl₃) of 3h



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3h



DEPT-135 (400 MHz, CDCl_3) of 3h



HRMS of 3h

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2 Br: 0-2

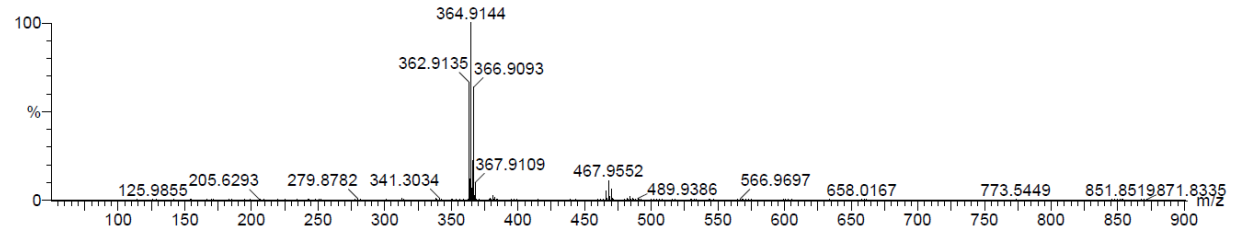
SM-381

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Apr-2024

230424_14 5 (0.121)

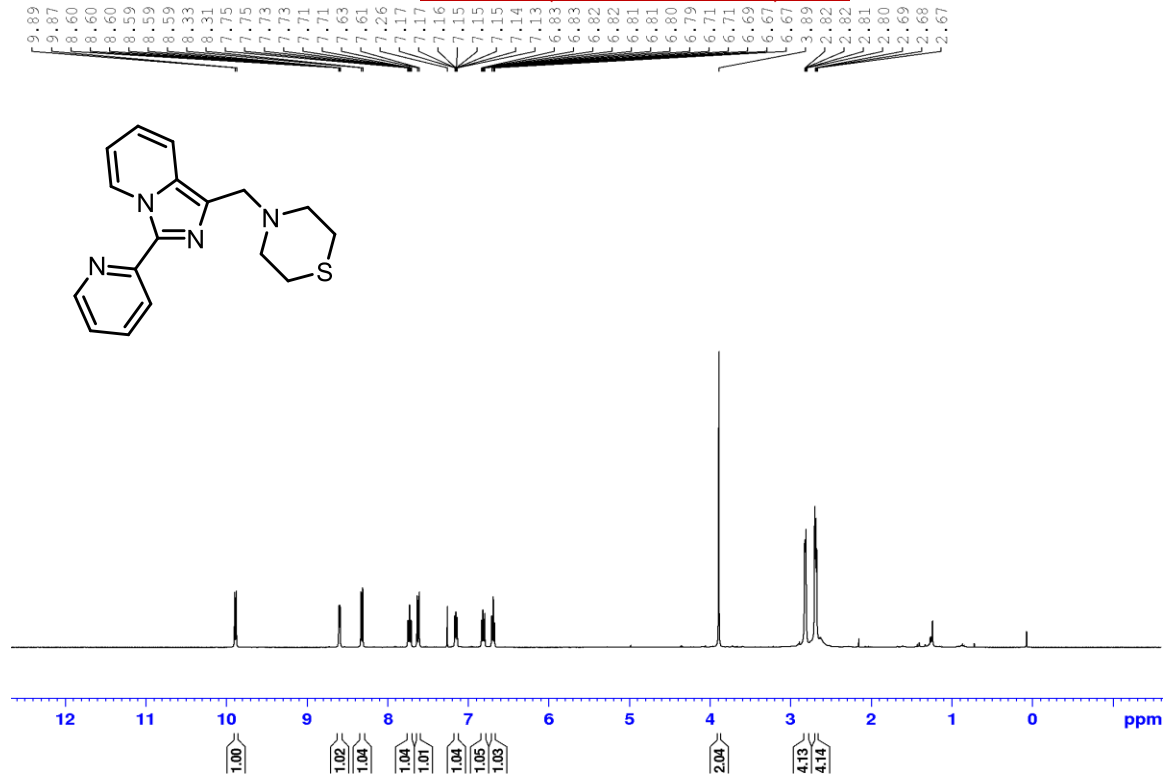
12:43:52
1: TOF MS ES+
2.93e+007



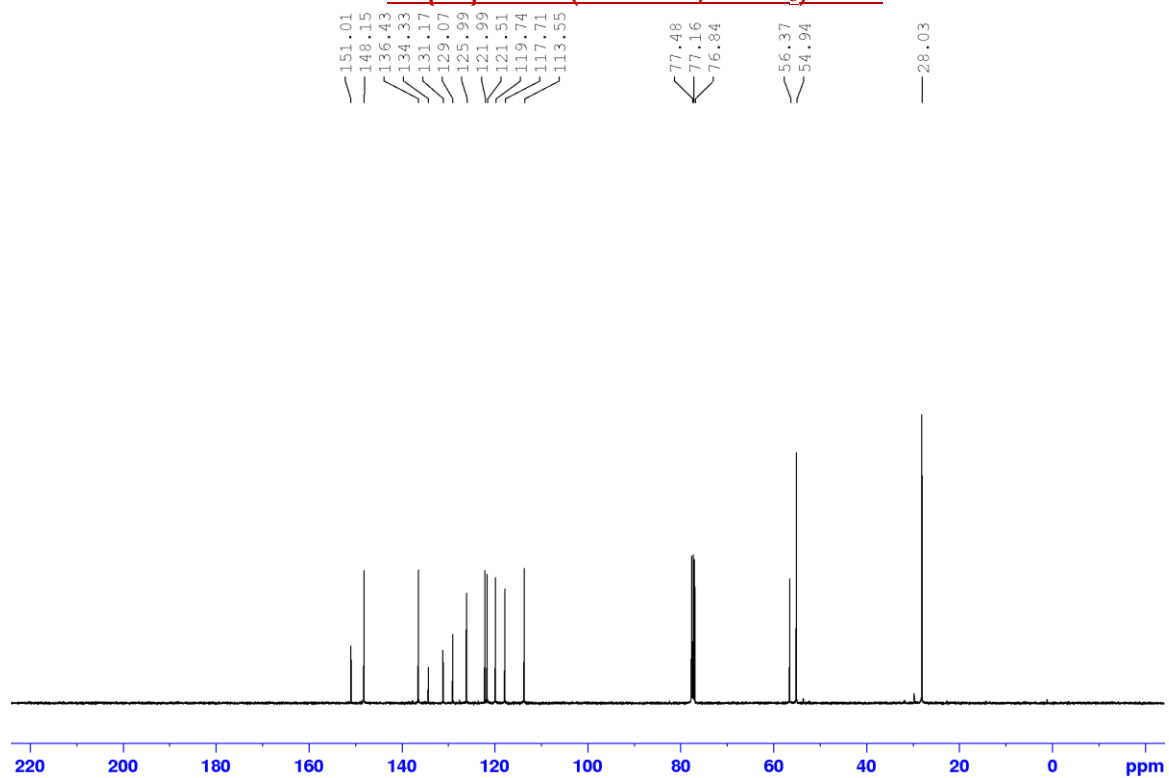
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|-----|-----|------|--------|------|---------|---------------|
| 362.9135 | 362.9132 | 0.3 | 0.8 | 10.5 | 1191.1 | n/a | n/a | C14 H9 N2 Br2 |

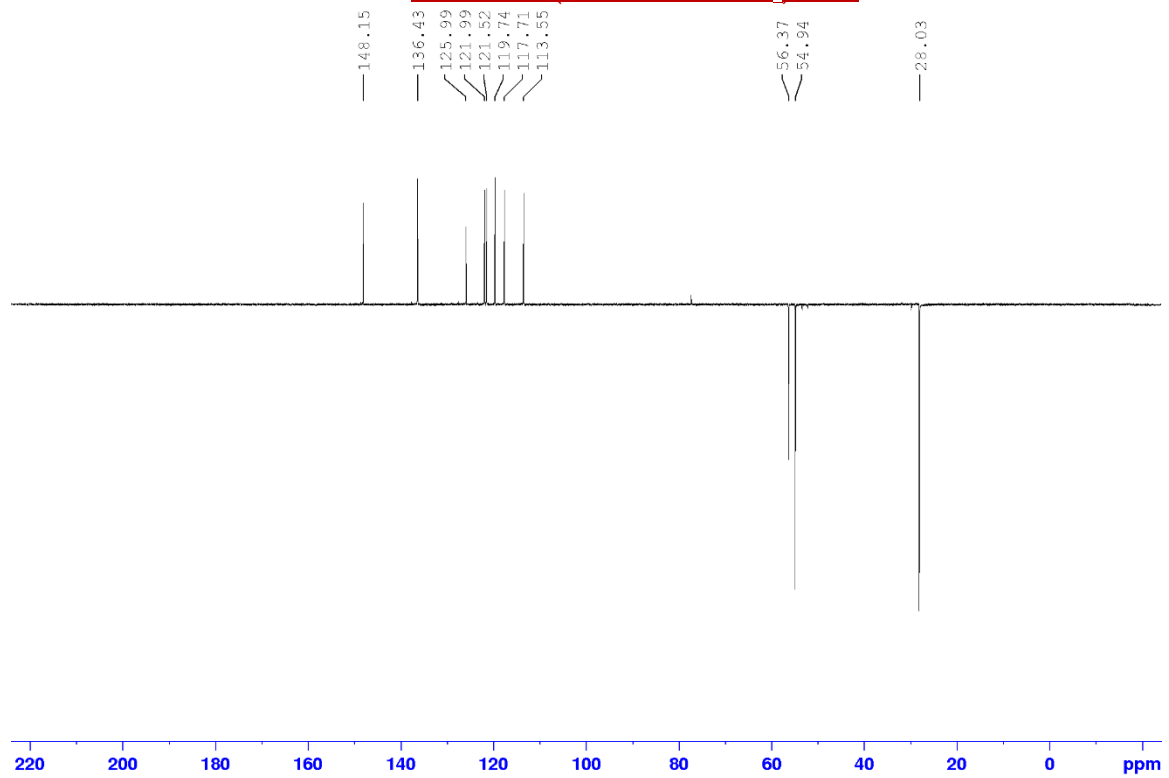
¹H NMR (400 MHz, CDCl₃) of 3i



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3i



DEPT-135 (101 MHz, CDCl_3) of 3i



HRMS of 3i

Elemental Composition Report

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:

C: 0-17 H: 0-100 N: 0-4 Na: 0-1 S: 0-1

SM-402

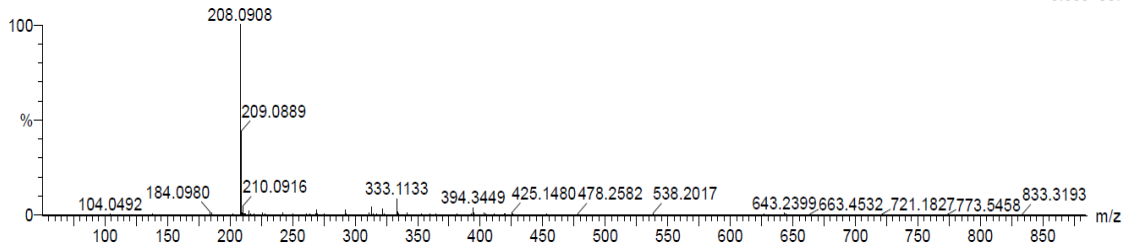
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Apr-2024

12:17:47

1: TOF MS ES+
3.66e+007

230424_04 5 (0.121)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|-----------------|
| 333.1133 | 333.1150 | -1.7 | -5.1 | 10.5 | 1204.8 | n/a | n/a | C17 H18 N4 Na S |

Elemental Composition Report

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:

C: 0-13 H: 0-100 N: 0-3

SM-402

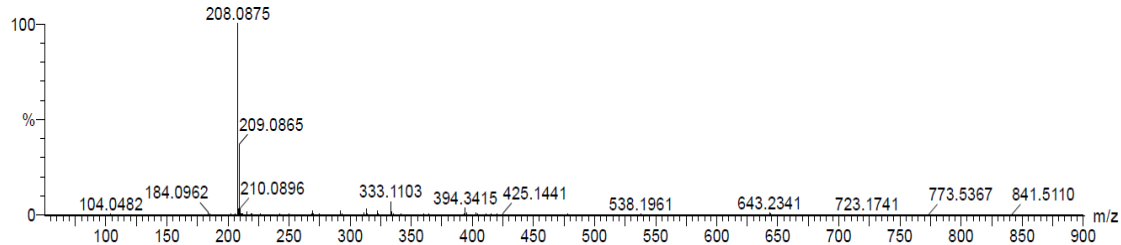
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Apr-2024

12:17:47

1: TOF MS ES+
4.08e+007

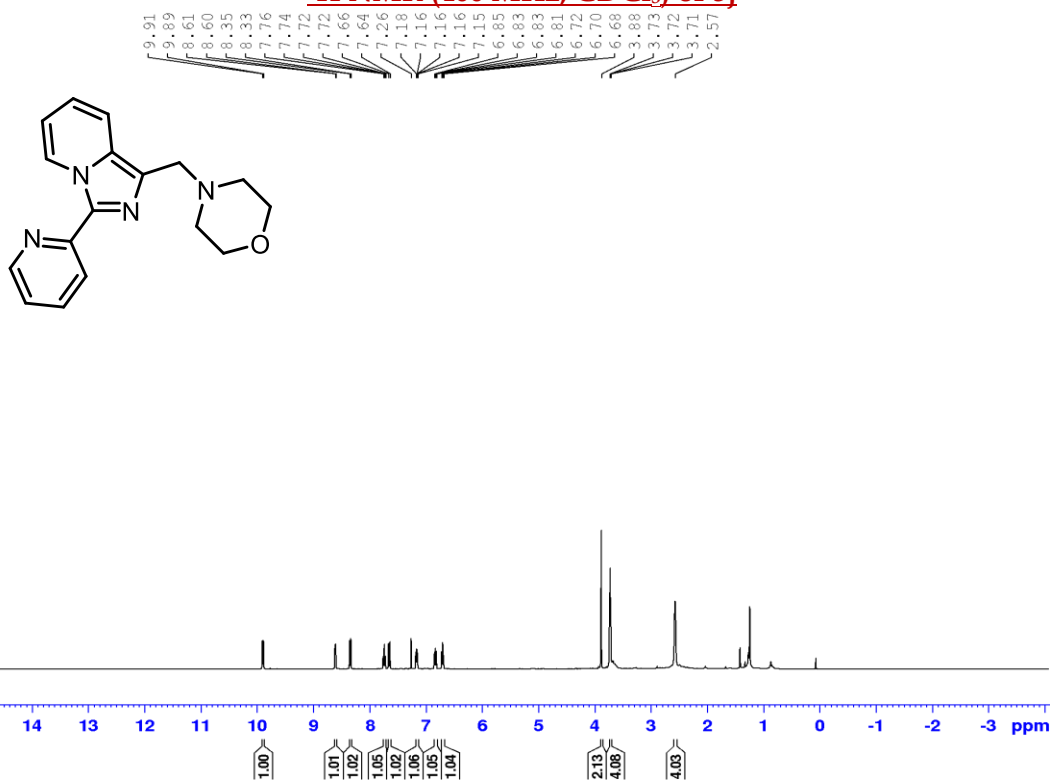
230424_04 7 (0.155)



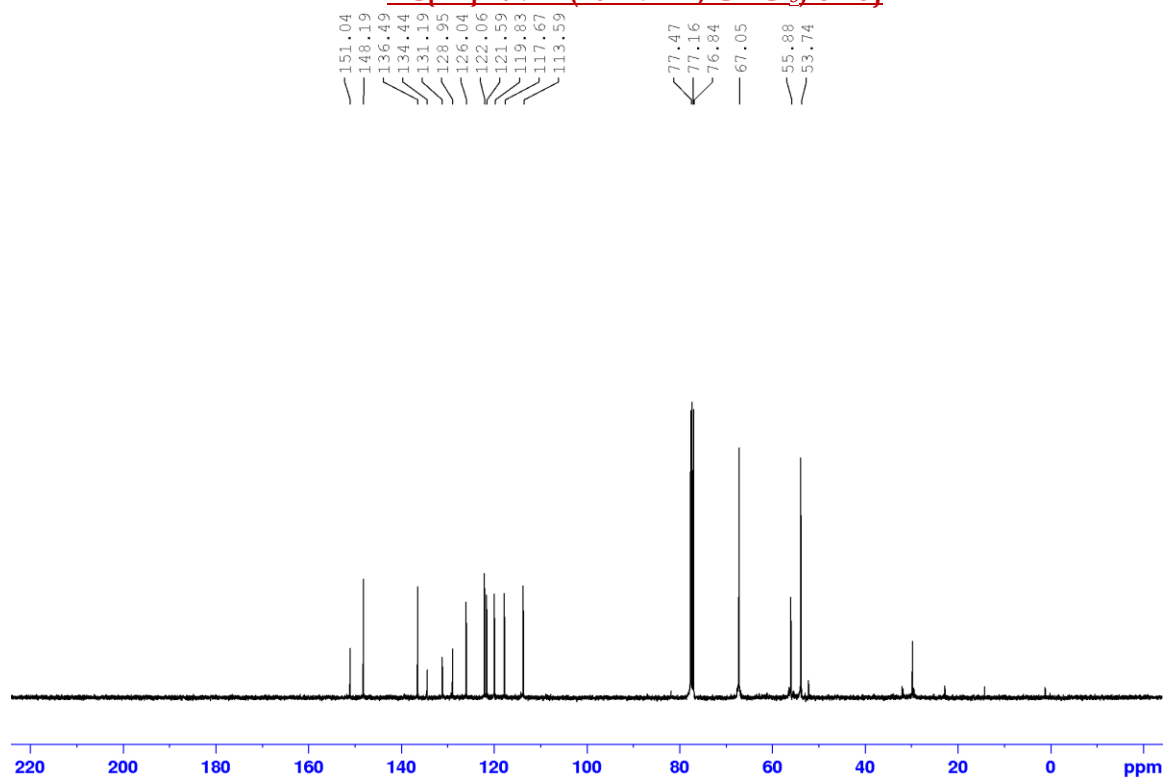
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|------------|
| 208.0875 | 208.0875 | 0.0 | 0.0 | 10.5 | 1321.5 | n/a | n/a | C13 H10 N3 |

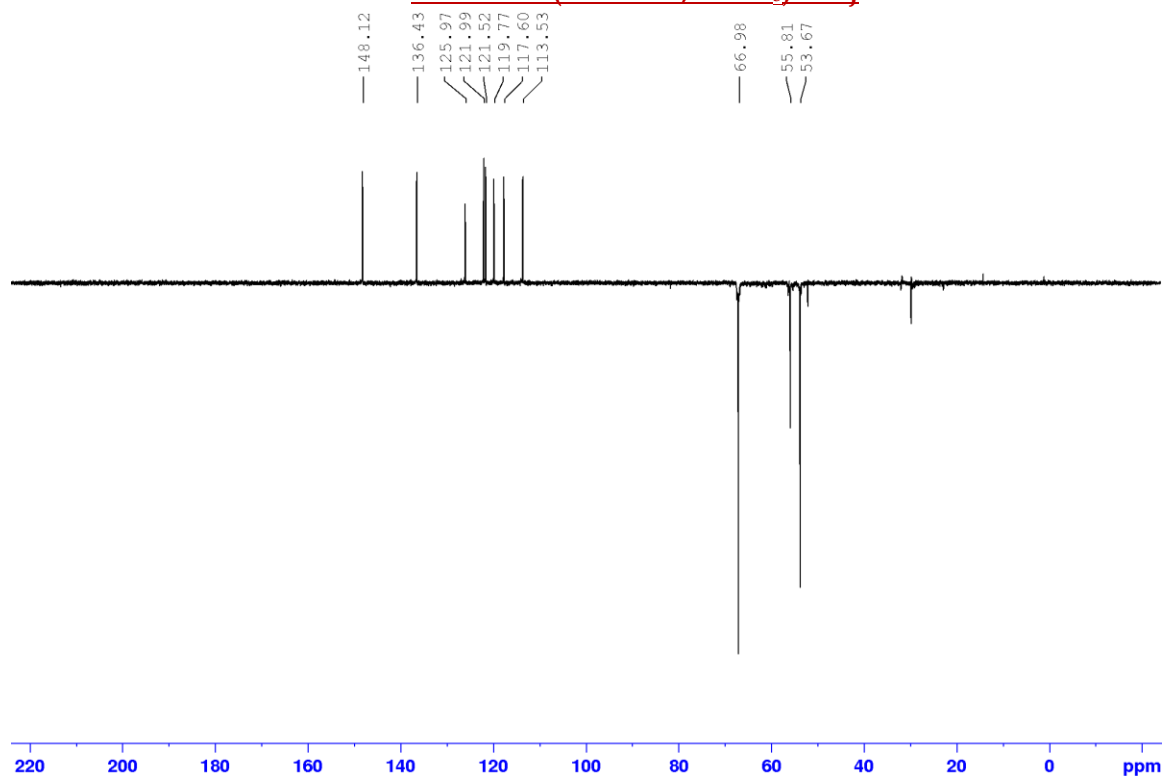
¹H NMR (400 MHz, CDCl₃) of 3j



¹³C[¹H] NMR (101 MHz, CDCl₃) of 3j



DEPT-135 (400 MHz, CDCl₃) of 3j



HRMS of 3j

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-17 H: 0-100 N: 0-4 O: 0-1 Na: 0-1

SM-484

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

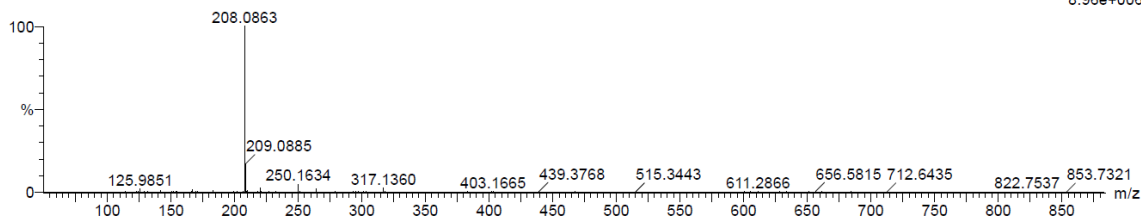
23-Apr-2024

12:38:36

1: TOF MS ES+

8.96e+006

230424_12 4 (0.104)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|-----------------|
| 317.1360 | 317.1378 | -1.8 | -5.7 | 10.5 | 1133.8 | n/a | n/a | C17 H18 N4 O Na |

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

7 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-13 H: 0-100 N: 0-3

SM-484

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

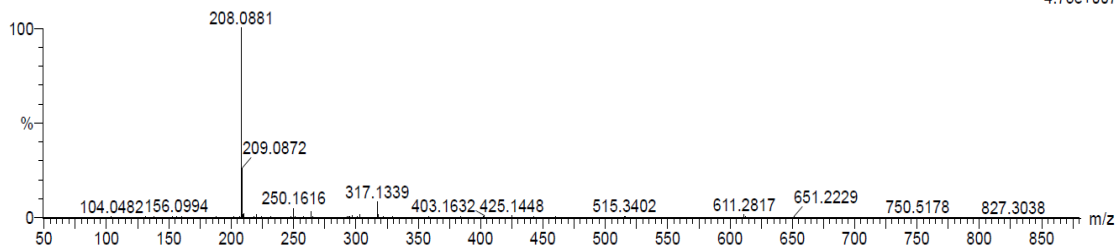
23-Apr-2024

12:38:36

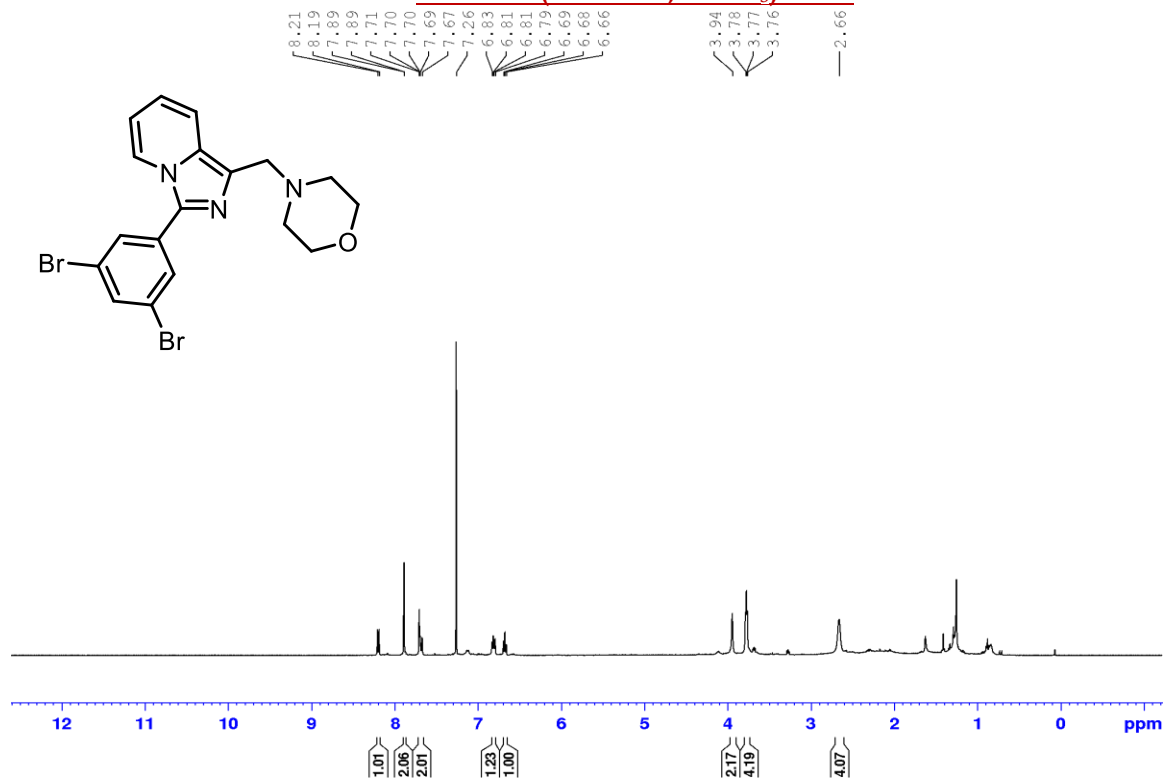
1: TOF MS ES+

4.75e+007

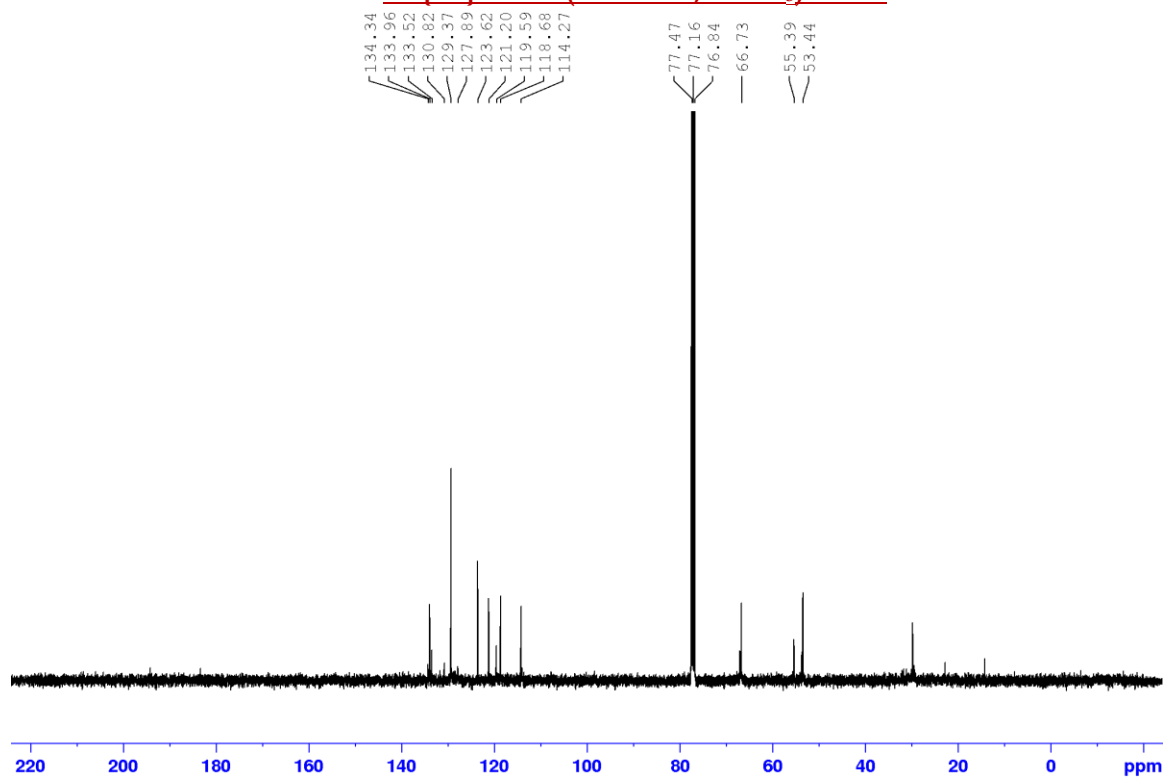
230424_12.7 (0.155)

Minimum: -1.5
Maximum: 2.0 50.0 50.0

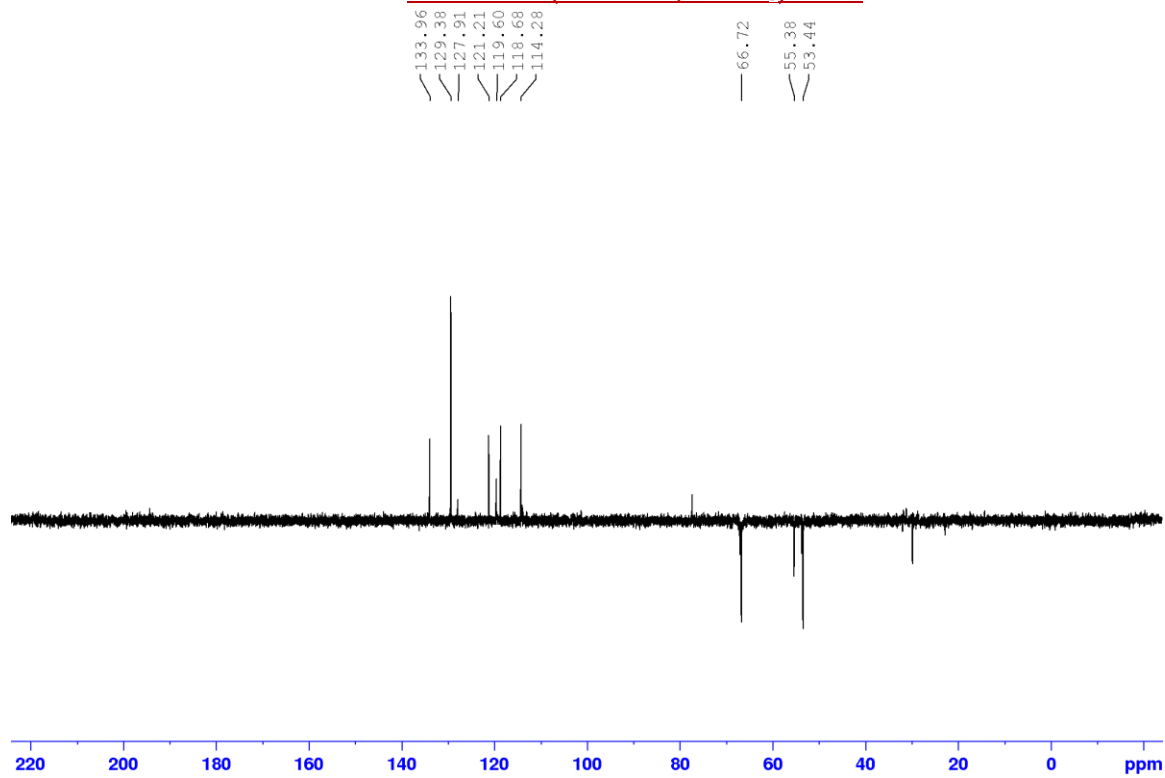
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|------------|
| 208.0881 | 208.0875 | 0.6 | 2.9 | 10.5 | 1545.5 | n/a | n/a | C13 H10 N3 |

¹H NMR (400 MHz, CDCl₃) of 3k

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3k



DEPT-135 (400 MHz, CDCl_3) of 3k



HRMS of 3k

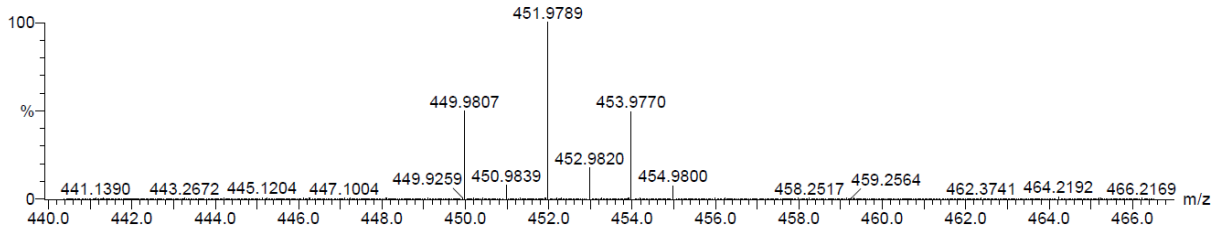
Elemental Composition Report

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-18 H: 0-100 N: 0-3 O: 0-1 Br: 0-2

SM-496 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 15:34:36
070524_60 5 (0.121) 1: TOF MS ES+ 1.84e+006



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|-------|------|----------|------------------|
| 449.9807 | 449.9817 | -1.0 | -2.2 | 10.5 | 924.5 | n/a | n/a | C18 H18 N3 O Br2 |

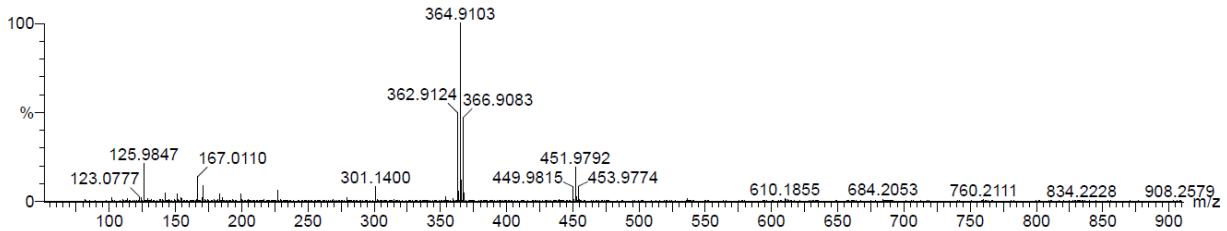
Elemental Composition Report

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2 Br: 0-2

SM-496 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 15:34:36
070524_60 4 (0.104) 1: TOF MS ES+ 5.52e+005

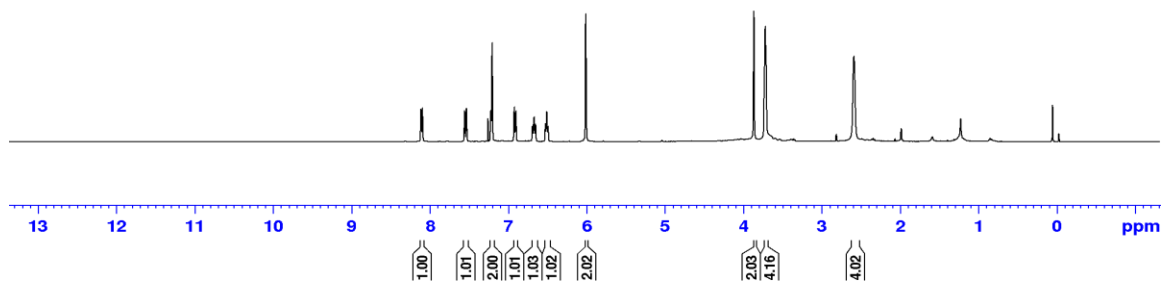
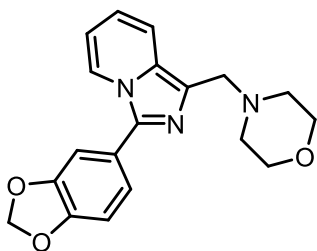


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|-------|------|----------|---------------|
| 362.9124 | 362.9132 | -0.8 | -2.2 | 10.5 | 805.1 | n/a | n/a | C14 H9 N2 Br2 |

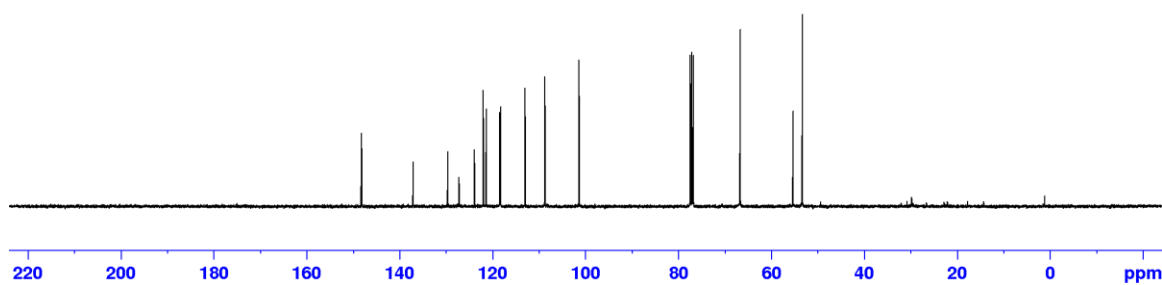
^1H NMR (400 MHz, CDCl_3) of 31

8.12
8.10
7.56
7.56
7.54
7.54
7.53
7.26
7.22
7.22
7.21
7.20
7.20
6.92
6.92
6.91
6.90
6.90
6.89
6.69
6.68
6.67
6.66
6.65
6.65
6.52
6.52
6.50
6.50
6.49
6.48
6.01
6.00
6.00
3.86
3.71
2.59

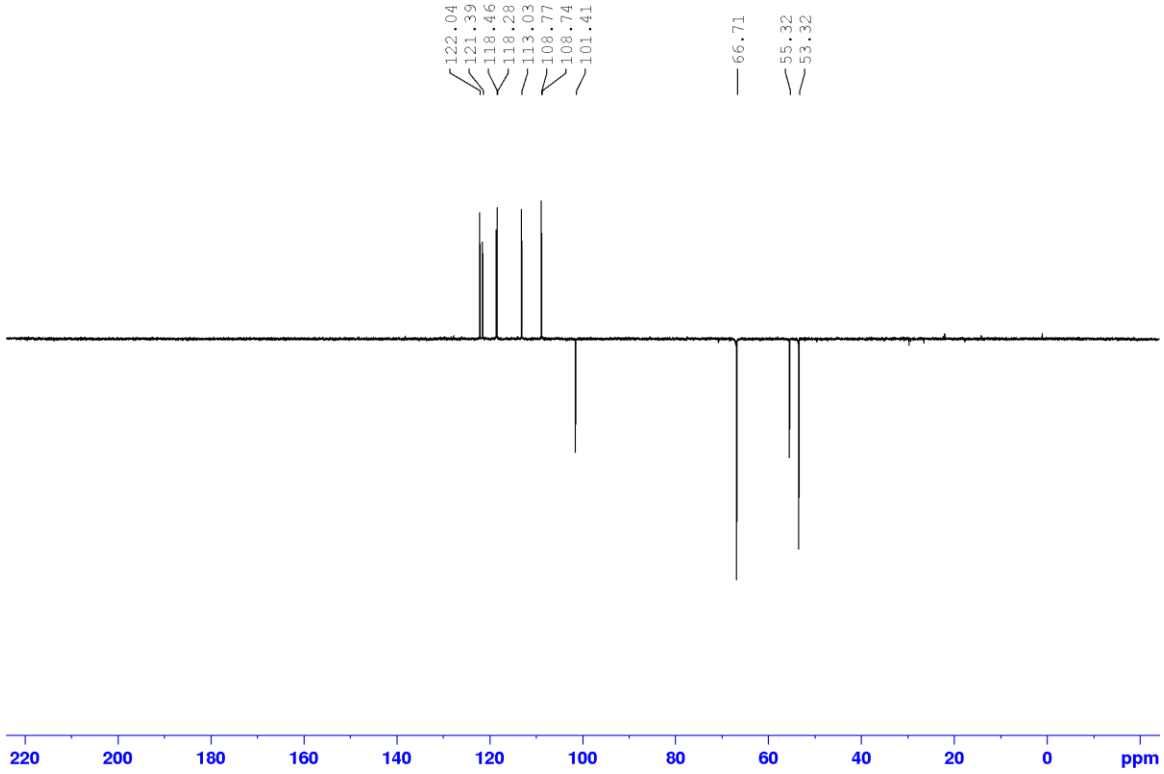


$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 31

148.15
148.01
137.11
129.66
127.27
123.92
122.04
121.39
118.46
118.28
113.03
108.77
108.74
101.41
77.43
77.12
76.80
66.71
55.33
53.33



DEPT-135 (400 MHz, CDCl₃) of 3l



HRMS of 3l

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

20 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-19 H: 0-100 N: 0-3 O: 0-3

SM-497

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

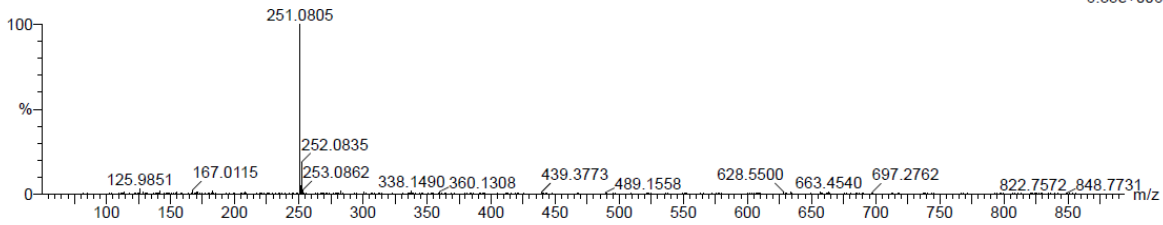
23-Apr-2024

12:30:44

1: TOF MS ES+

6.35e+006

230424_09 4 (0.104)



Minimum: -1.5

Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|---------------|
| 338.1490 | 338.1505 | -1.5 | -4.4 | 11.5 | 1206.1 | n/a | n/a | C19 H20 N3 O3 |

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-15 H: 0-100 N: 0-2 O: 0-2

SM-497

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

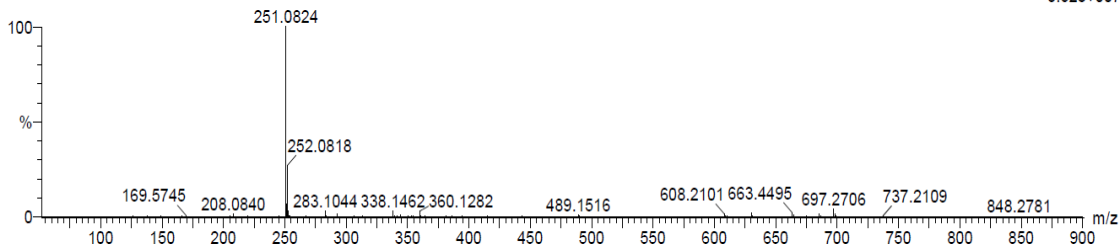
23-Apr-2024

12:30:44

1: TOF MS ES+

3.52e+007

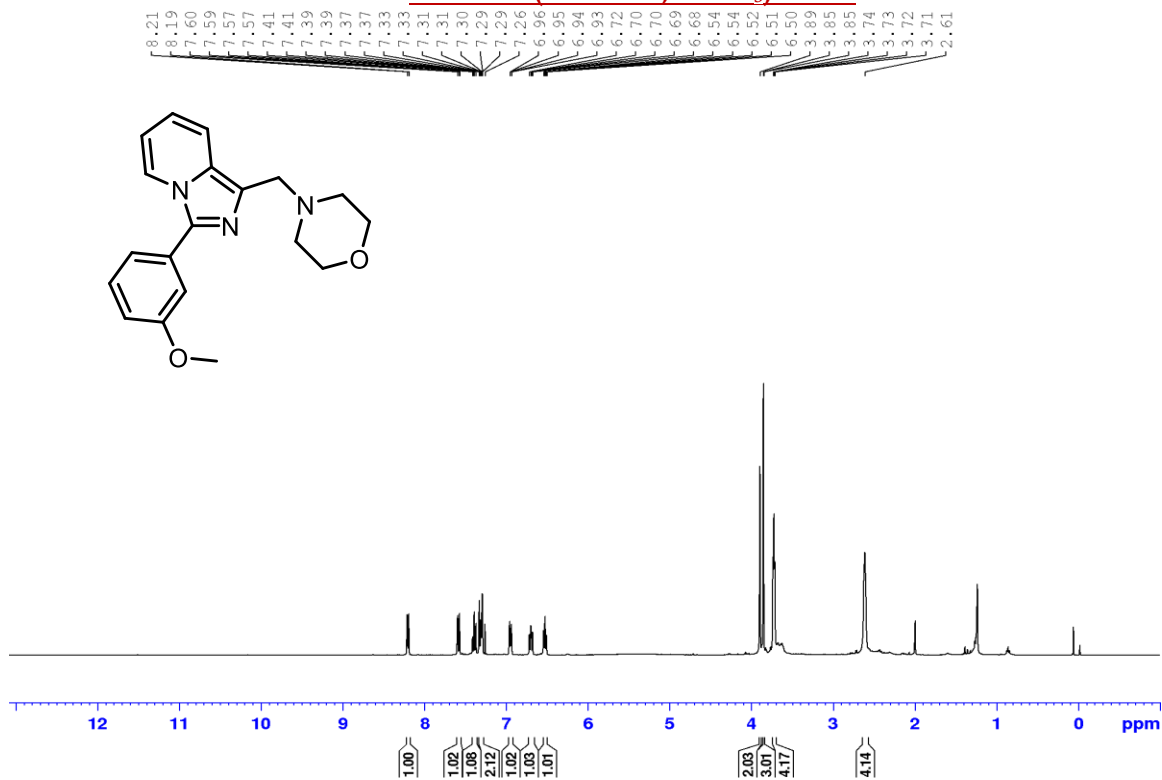
230424_09 7 (0.155)



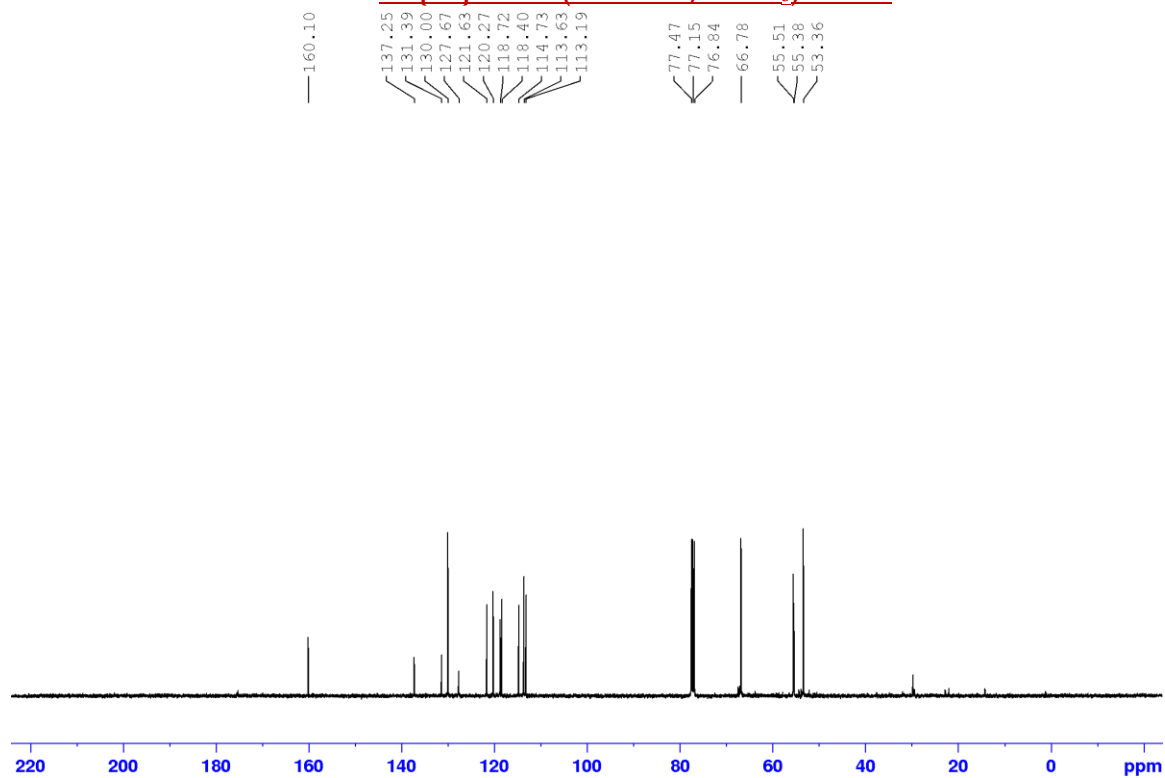
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|---------------|
| 251.0824 | 251.0821 | 0.3 | 1.2 | 11.5 | 1366.5 | n/a | n/a | C15 H11 N2 O2 |

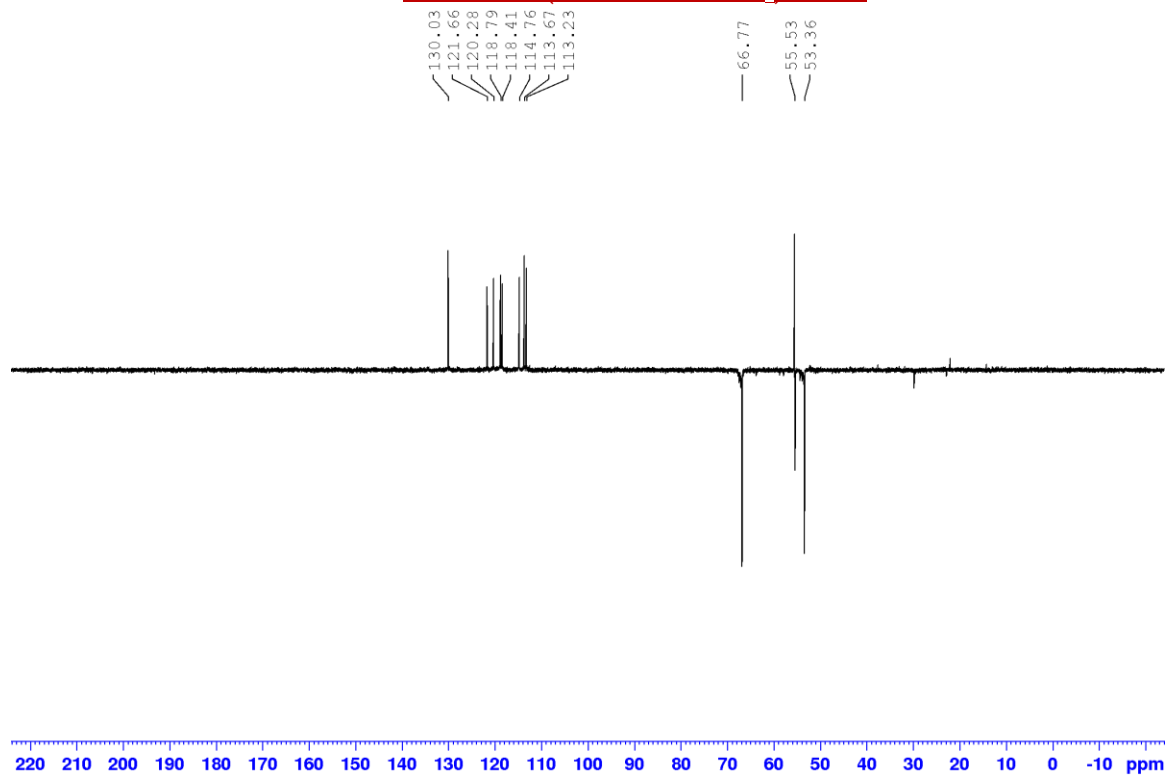
¹H NMR (400 MHz, CDCl₃) of 3m



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3m



DEPT-135 (400 MHz, CDCl_3) of 3m



HRMS of 3m

Elemental Composition Report

Single Mass Analysis

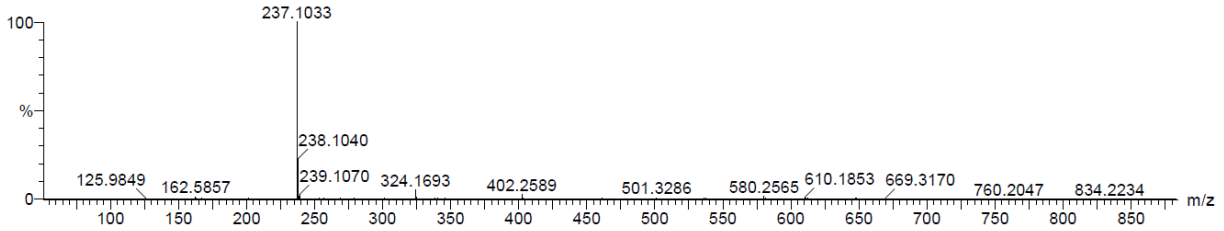
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-3 O: 0-3
SM-498

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

07-May-2024
15:39:45
1: TOF MS ES+
1.96e+007

070524_62 5 (0.121)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|---------------|
| 324.1693 | 324.1712 | -1.9 | -5.9 | 10.5 | 1034.0 | n/a | n/a | C19 H22 N3 O2 |

Elemental Composition Report

Single Mass Analysis

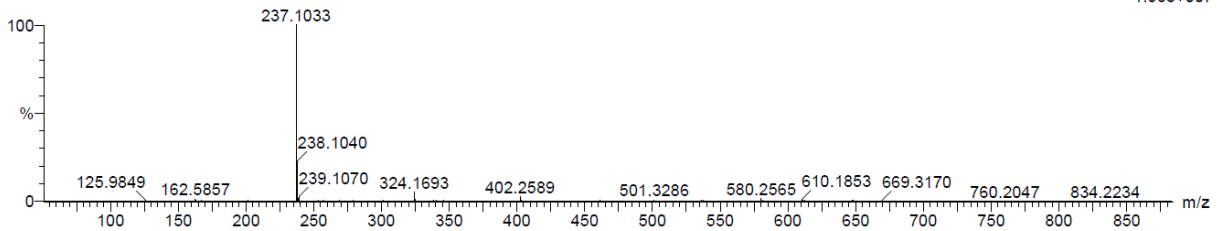
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-3 O: 0-3
SM-498

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

07-May-2024
15:39:45
1: TOF MS ES+
1.96e+007

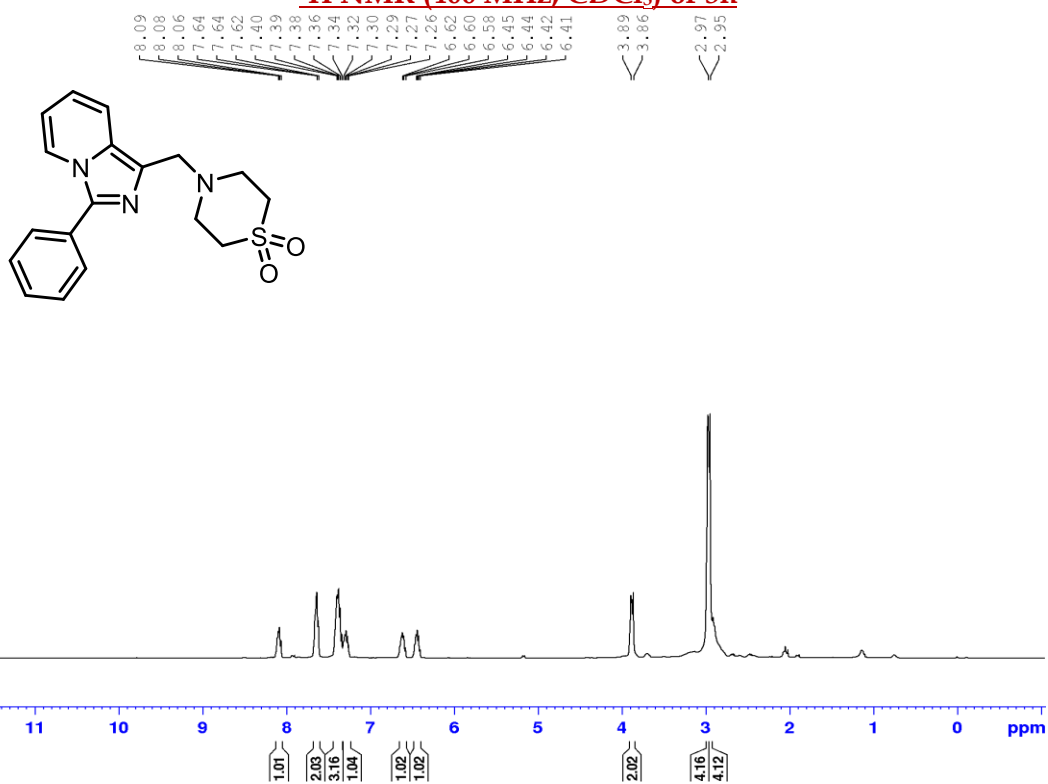
070524_62 5 (0.121)



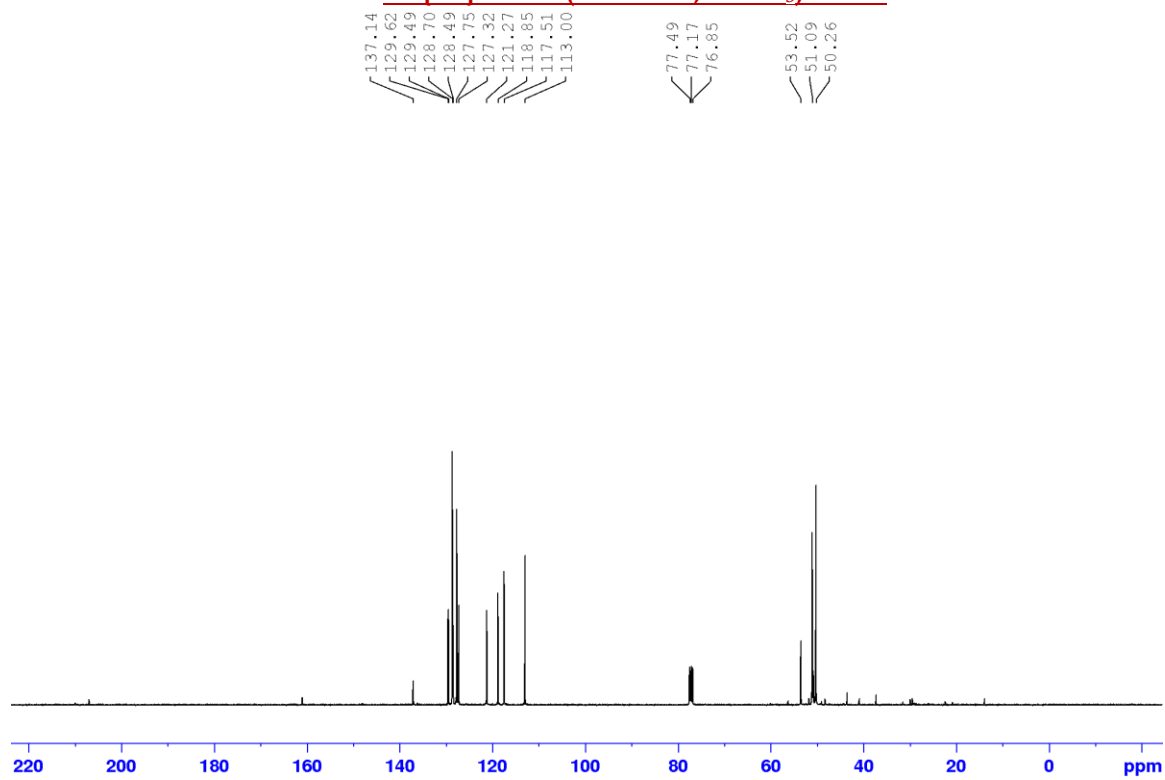
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|---------------|
| 324.1693 | 324.1712 | -1.9 | -5.9 | 10.5 | 1034.0 | n/a | n/a | C19 H22 N3 O2 |

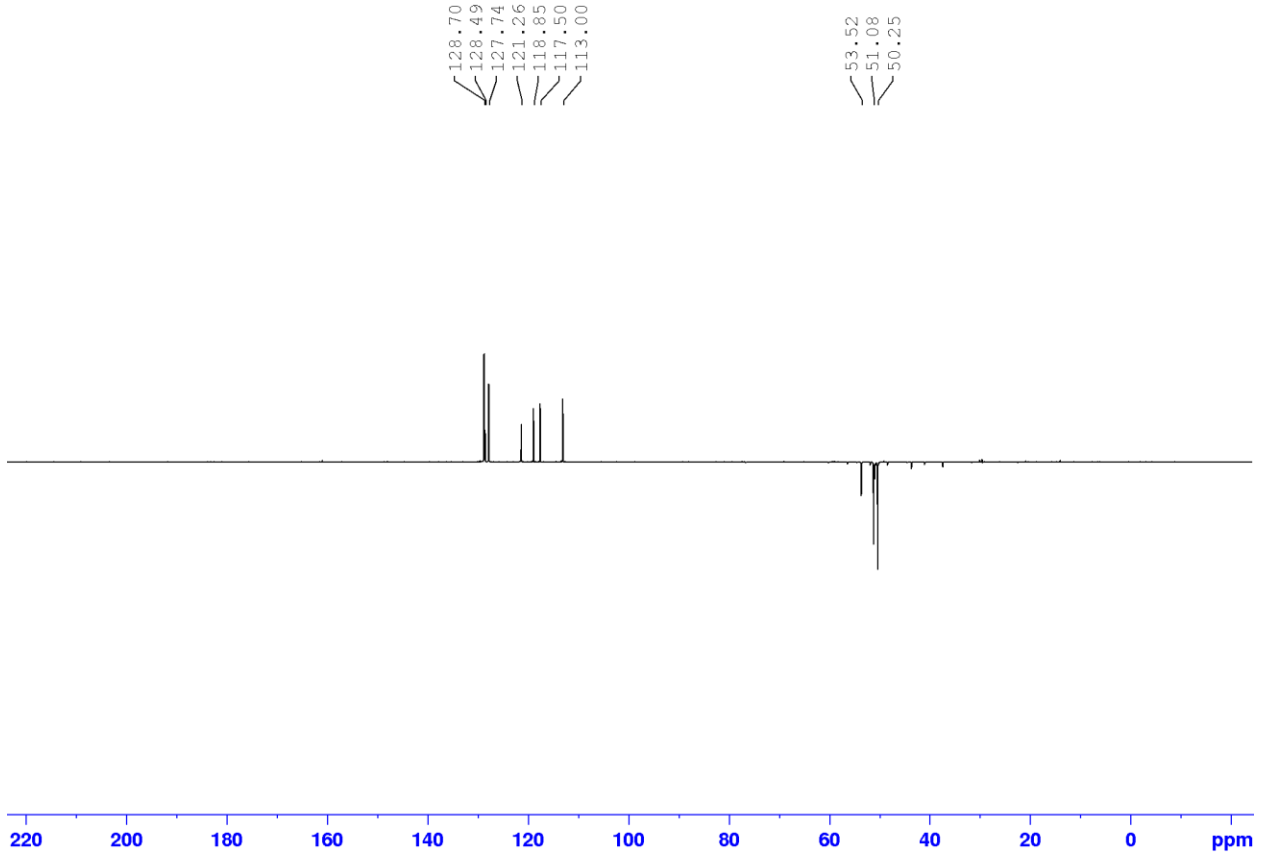
¹H NMR (400 MHz, CDCl₃) of 3n



¹³C{¹H} NMR (101 MHz, CDCl₃) of 3n



DEPT-135 (400 MHz, CDCl₃) of 3n



HRMS of 3n

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

52 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-18 H: 0-100 N: 0-3 O: 0-2 S: 0-1 Na: 0-1

SM-384

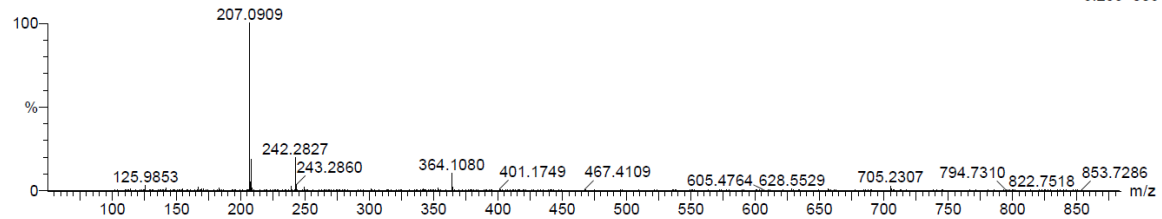
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Apr-2024

13:02:49

230424_21 4 (0.104)

1: TOF MS ES+
6.28e+006



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|--------------------|
| 364.1080 | 364.1096 | -1.6 | -4.4 | 10.5 | 1124.1 | n/a | n/a | C18 H19 N3 O2 S Na |

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2 Br: 0-2

SM-384

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

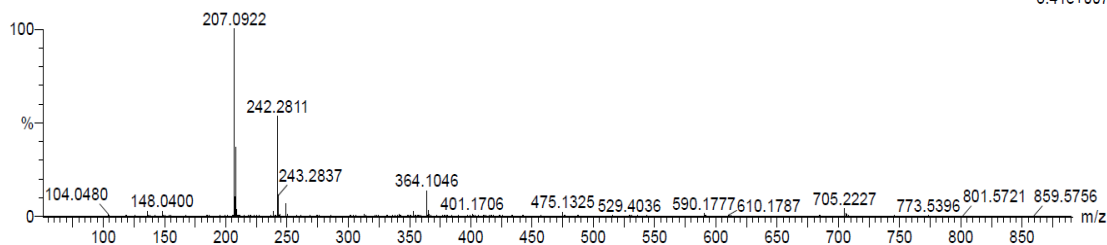
23-Apr-2024

13:02:49

230424_21 7 (0.155)

1: TOF MS ES+

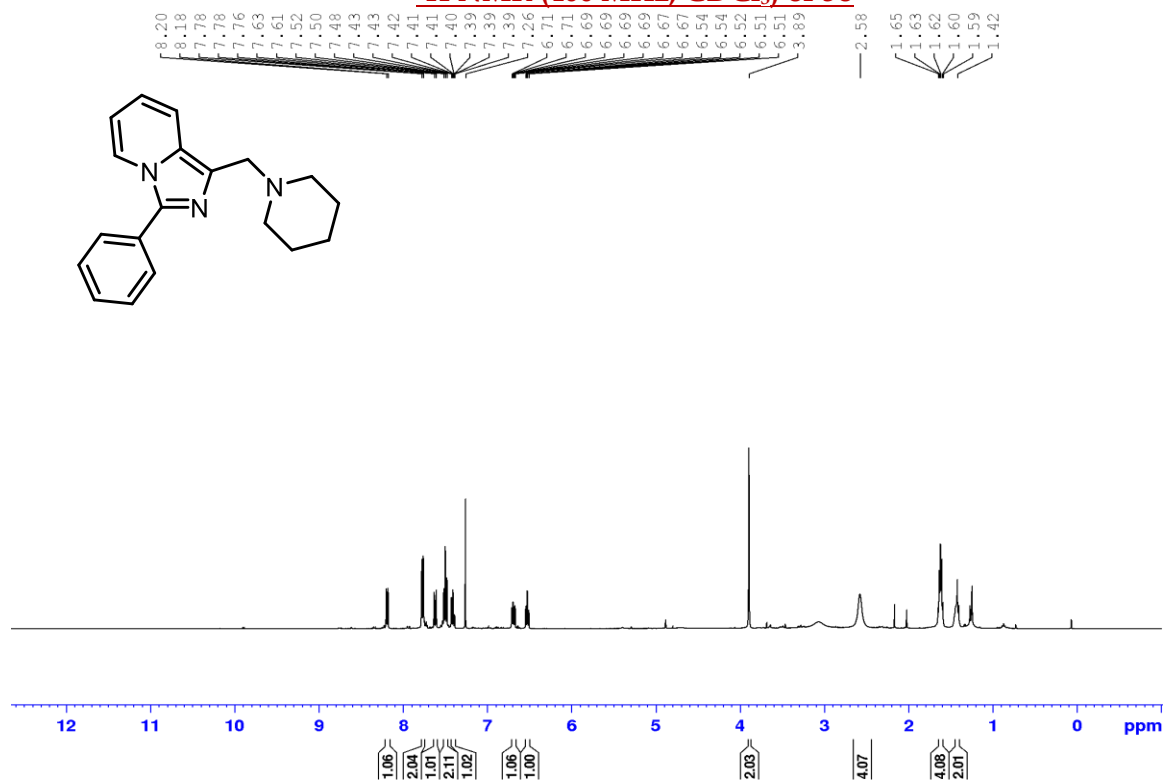
3.41e+007



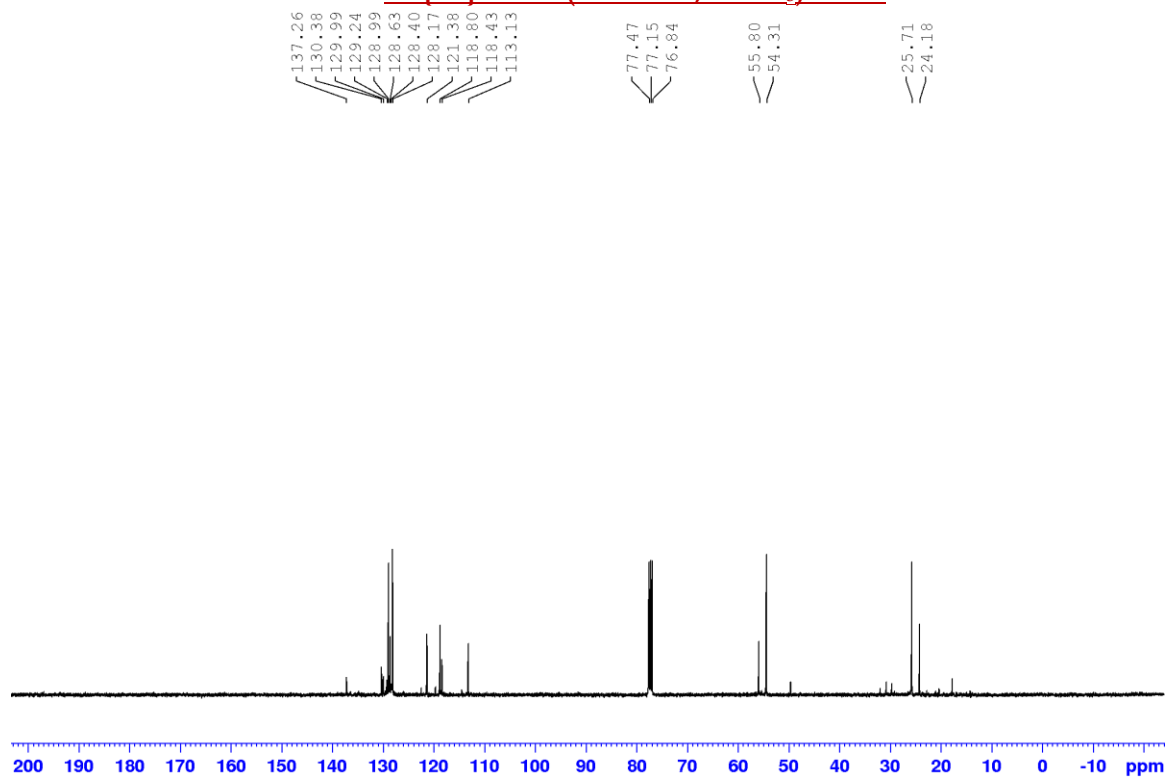
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|-----|-----|------|--------|------|---------|------------|
| 207.0922 | 207.0922 | 0.0 | 0.0 | 10.5 | 1352.3 | n/a | n/a | C14 H11 N2 |

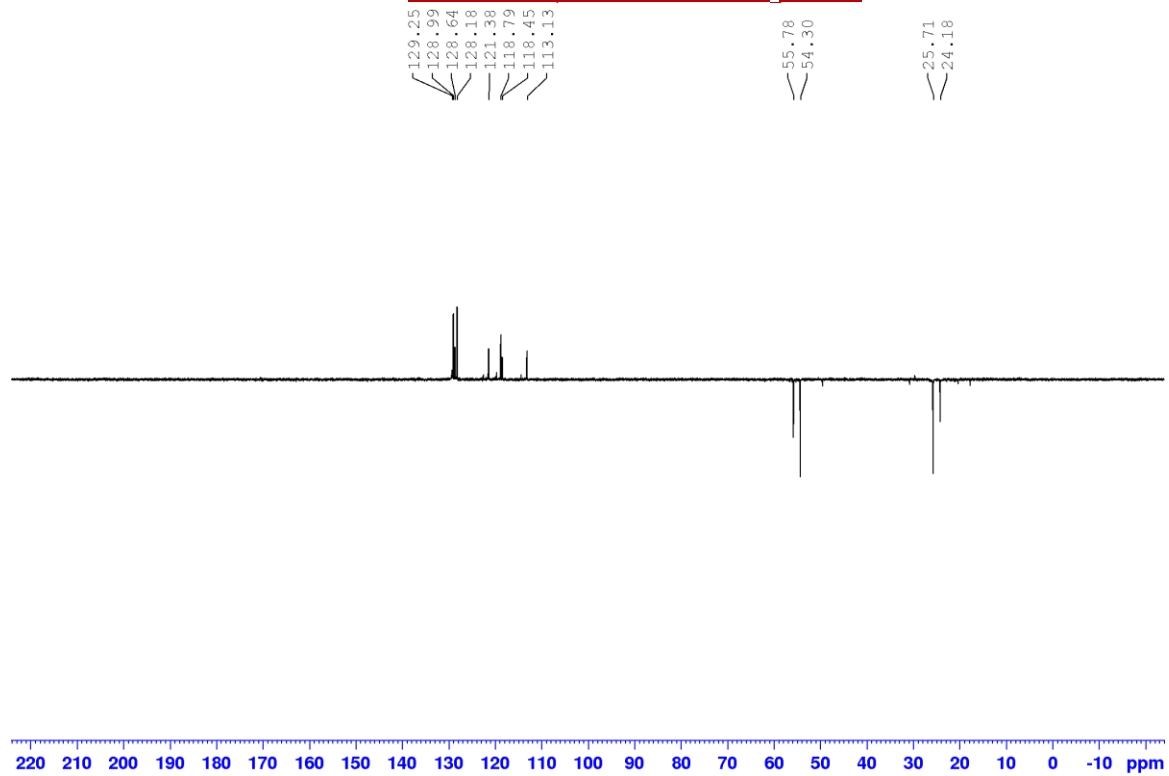
¹H NMR (400 MHz, CDCl₃) of 3o



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3o



DEPT-135 (400 MHz, CDCl_3) of 3o



HRMS of 3o

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

7 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-19 H: 0-100 N: 0-3

SM-430

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

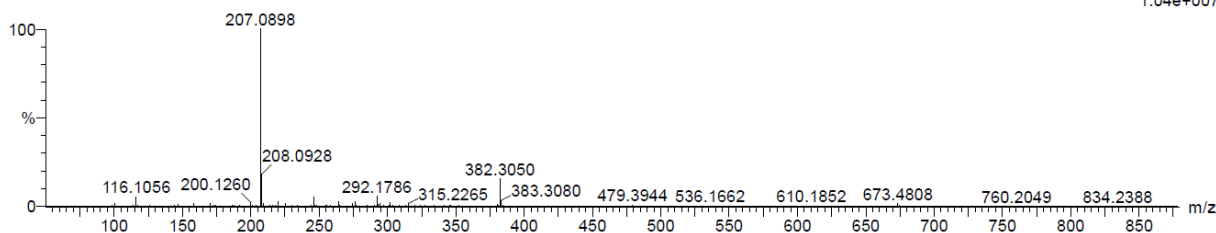
07-May-2024

15:21:30

1: TOF MS ES+

1.04e+007

070524_55 5 (0.121)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|-------|------|----------|------------|
| 292.1786 | 292.1814 | -2.8 | -9.6 | 10.5 | 916.5 | n/a | n/a | C19 H22 N3 |

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2

SM-430

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

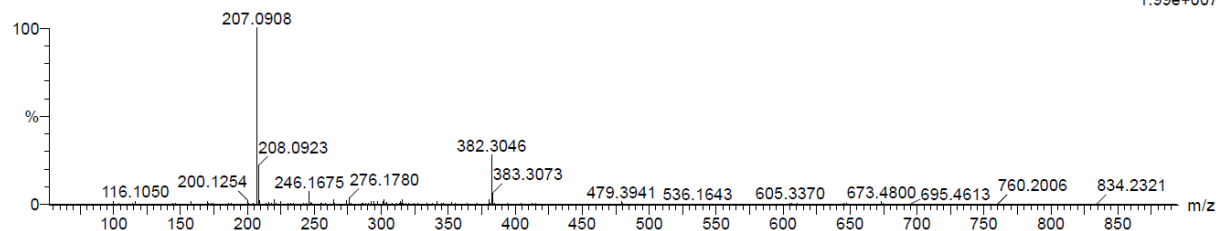
07-May-2024

13:54:45

1: TOF MS ES+

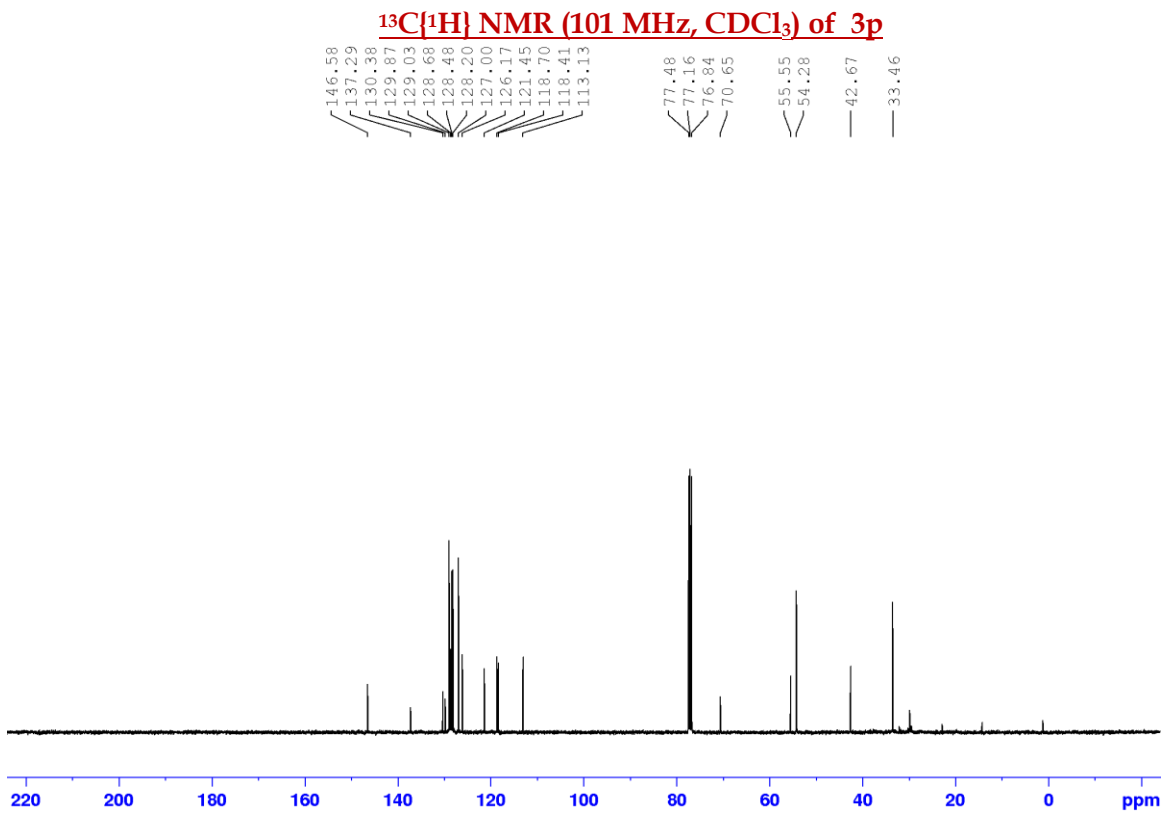
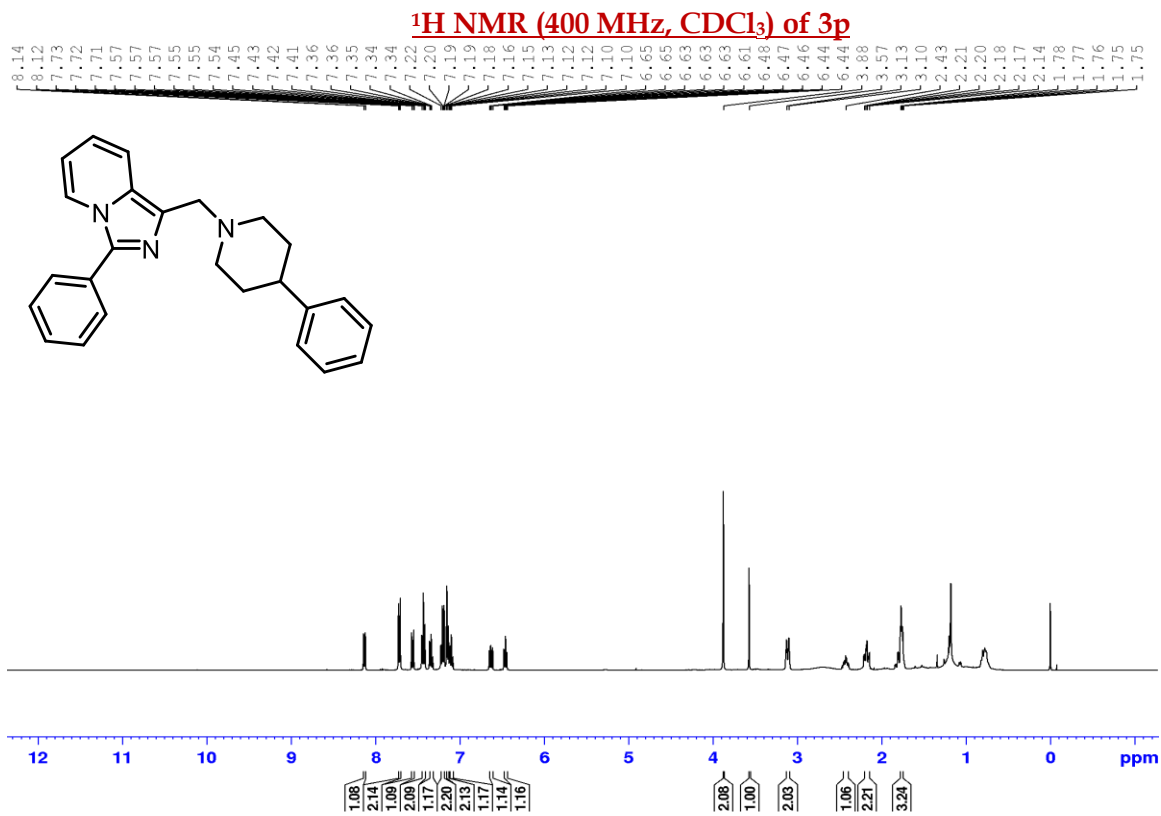
1.99e+007

070524_26 6 (0.138)

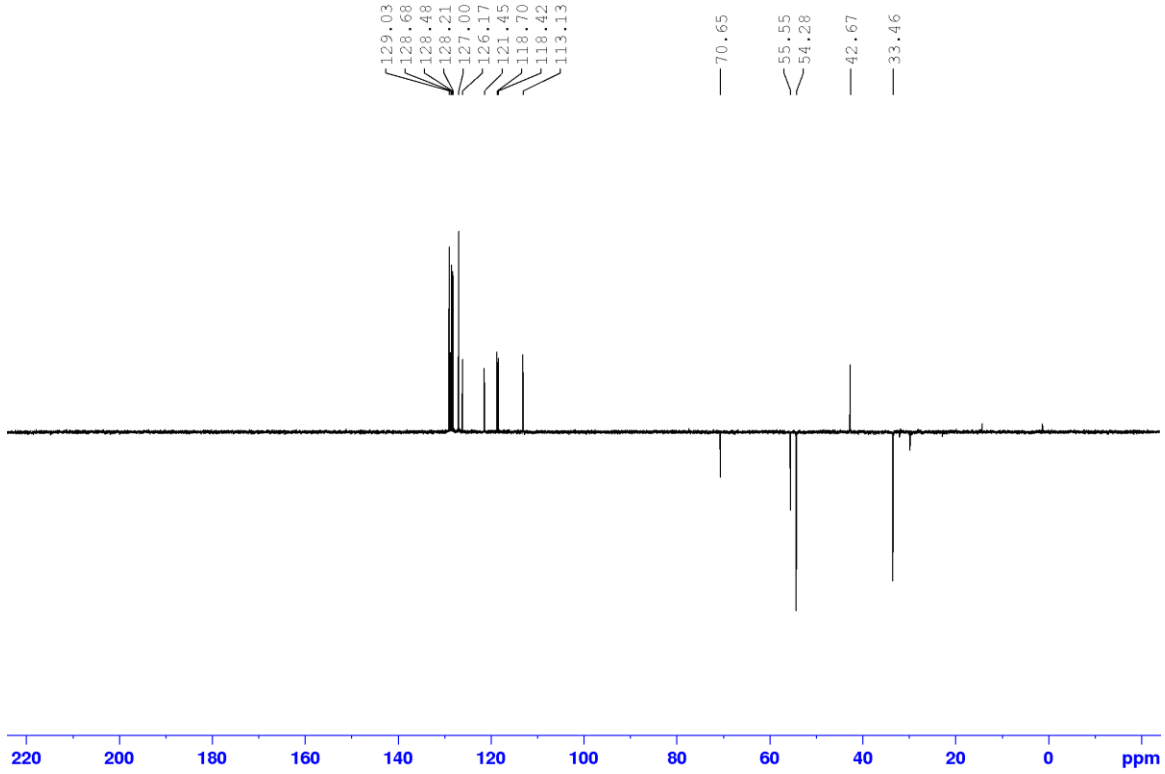


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|------------|
| 207.0908 | 207.0922 | -1.4 | -6.8 | 10.5 | 1342.7 | n/a | n/a | C14 H11 N2 |



DEPT-135 (400 MHz, CDCl₃) of 3p



HRMS of 3p

Elemental Composition Report

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions

7 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-25 H: 0-100 N: 0-3

SM-341

QMI DIVISION, CSIR-IIIM JAMMU
 Xevo G2-XS QTOF YFC2015

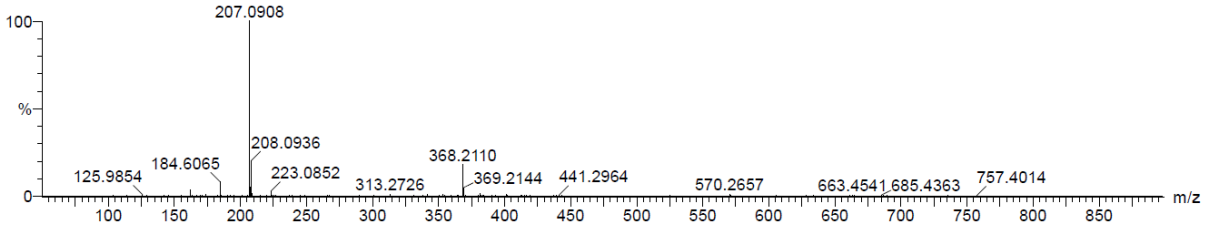
23-Apr-2024

12:20:20

1: TOF MS ES+

1.47e+007

230424_05 5 (0.121)



Minimum: -1.5
 Maximum: 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|--|
| 368.2110 | 368.2127 | -1.7 | -4.6 | 14.5 | 1152.7 | n/a | n/a | C ₂₅ H ₂₆ N ₃ |

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2

SM-341

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

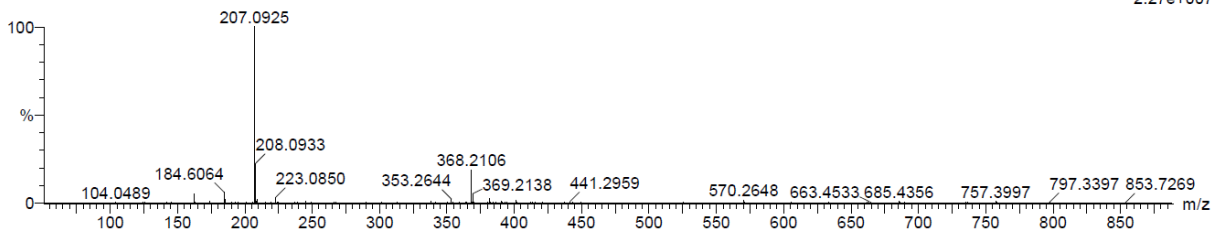
23-Apr-2024

12:20:20

1: TOF MS ES+

2.27e+007

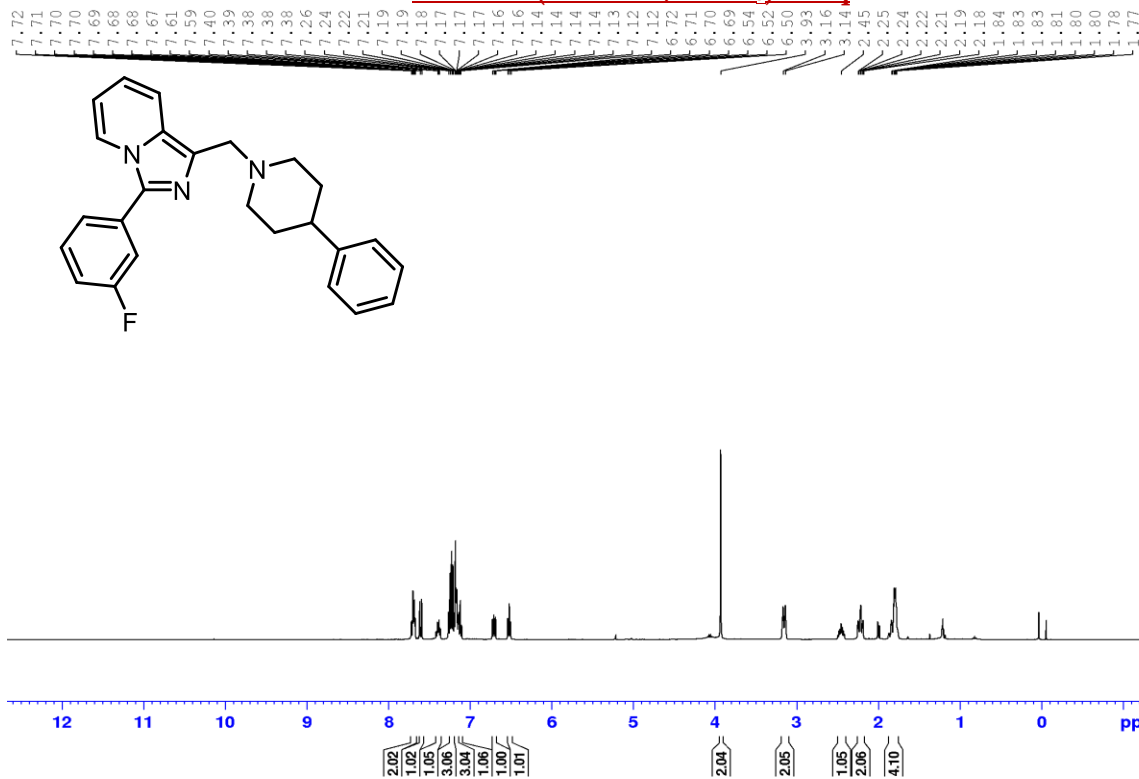
230424_05 6 (0.138)



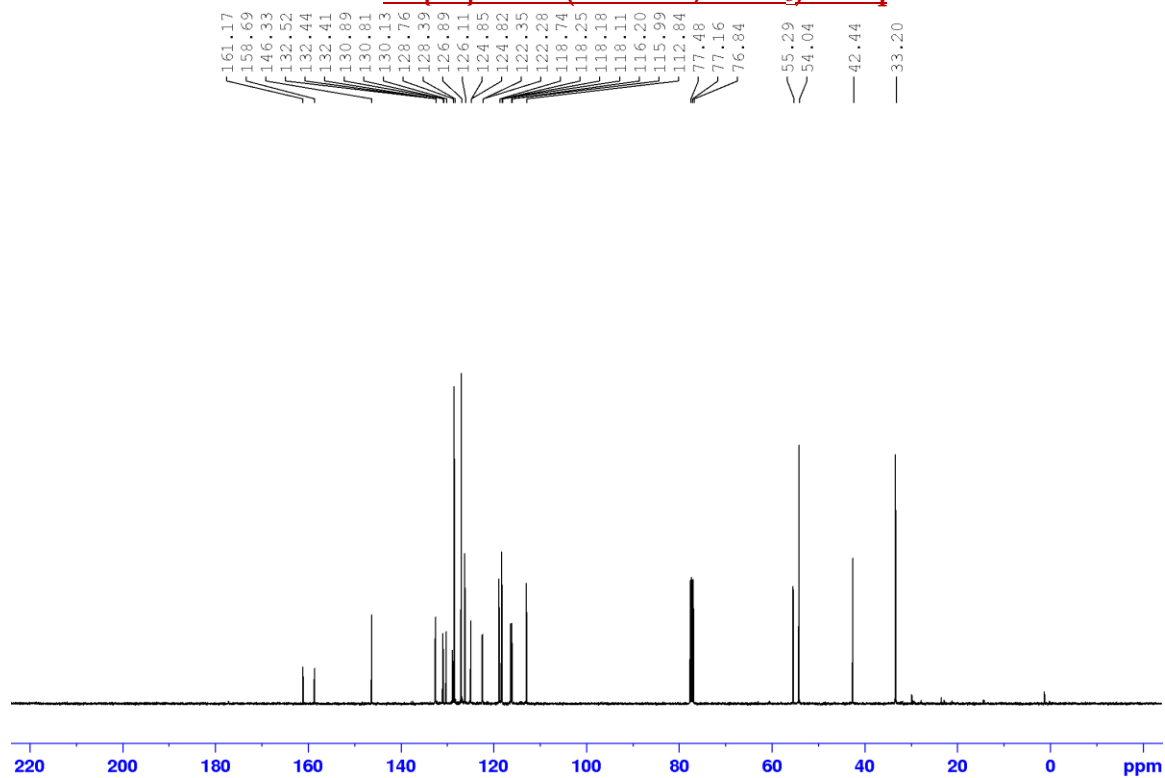
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|------------|
| 207.0925 | 207.0922 | 0.3 | 1.4 | 10.5 | 1532.3 | n/a | n/a | C14 H11 N2 |

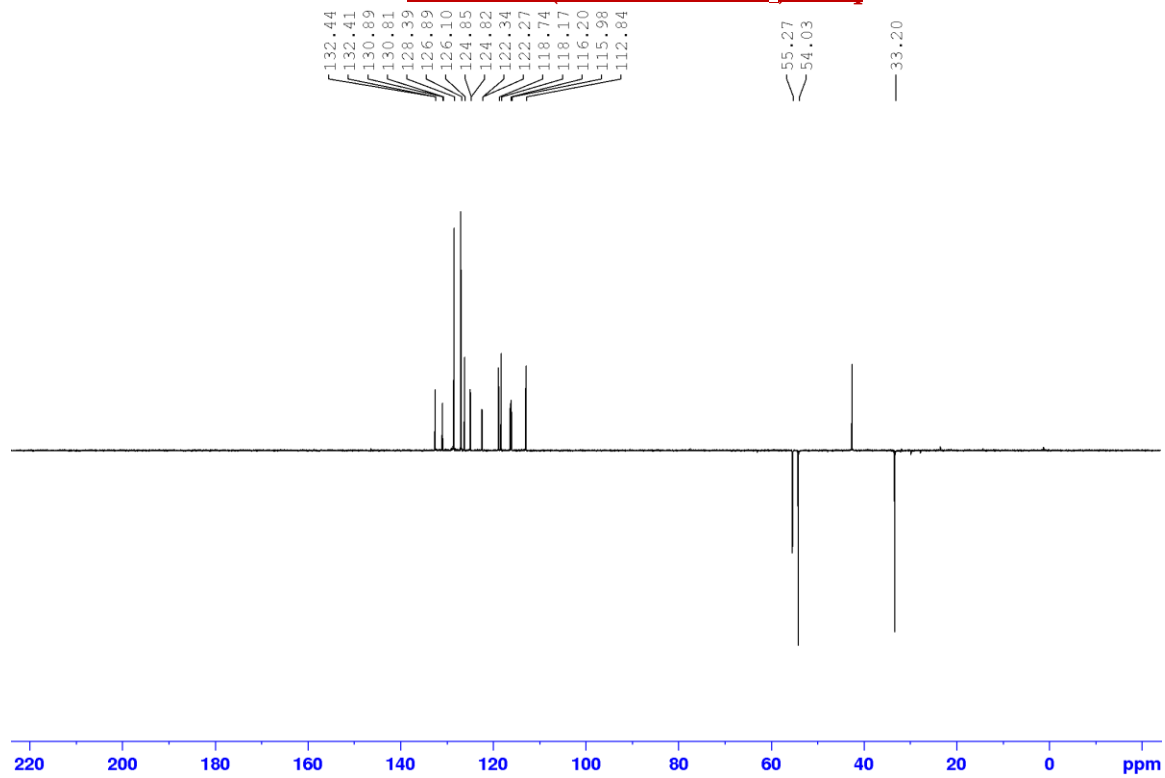
¹H NMR (400 MHz, CDCl₃) of 3q



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3q

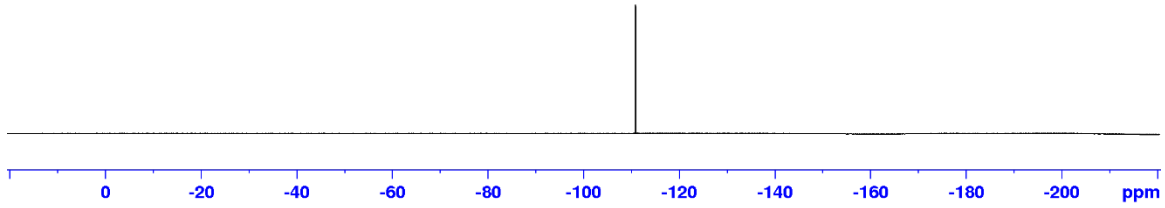


DEPT-135 (400 MHz, CDCl_3) of 3q



¹⁹F NMR (377 MHz, CDCl₃) of 3q

-110.91
-110.92
-110.94
-110.95



HRMS of 3q

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-25 H: 0-100 N: 0-4 F: 0-1

SM-389

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

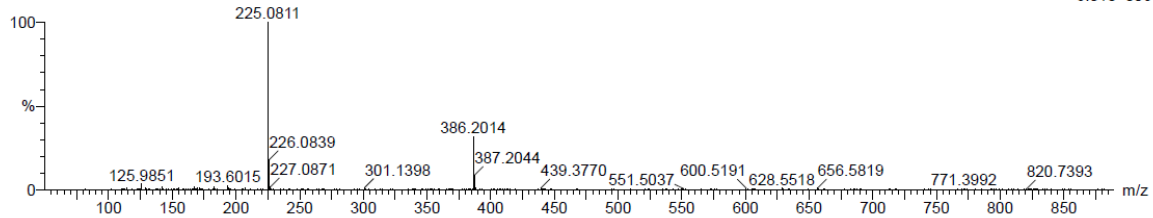
23-Apr-2024

12:54:49

1: TOF MS ES+

6.01e+006

230424_18.4 (0.104)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|--------------|
| 386.2014 | 386.2033 | -1.9 | -4.9 | 14.5 | 1005.5 | n/a | n/a | C25 H25 N3 F |

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2 F: 0-1

SM-389

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

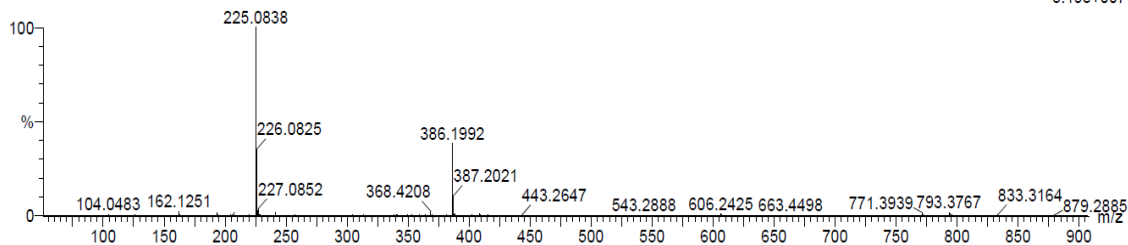
23-Apr-2024

12:54:49

1: TOF MS ES+

3.19e+007

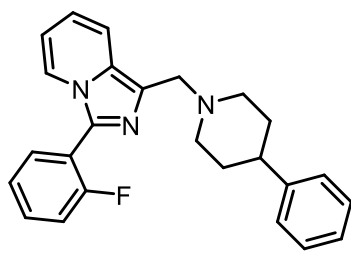
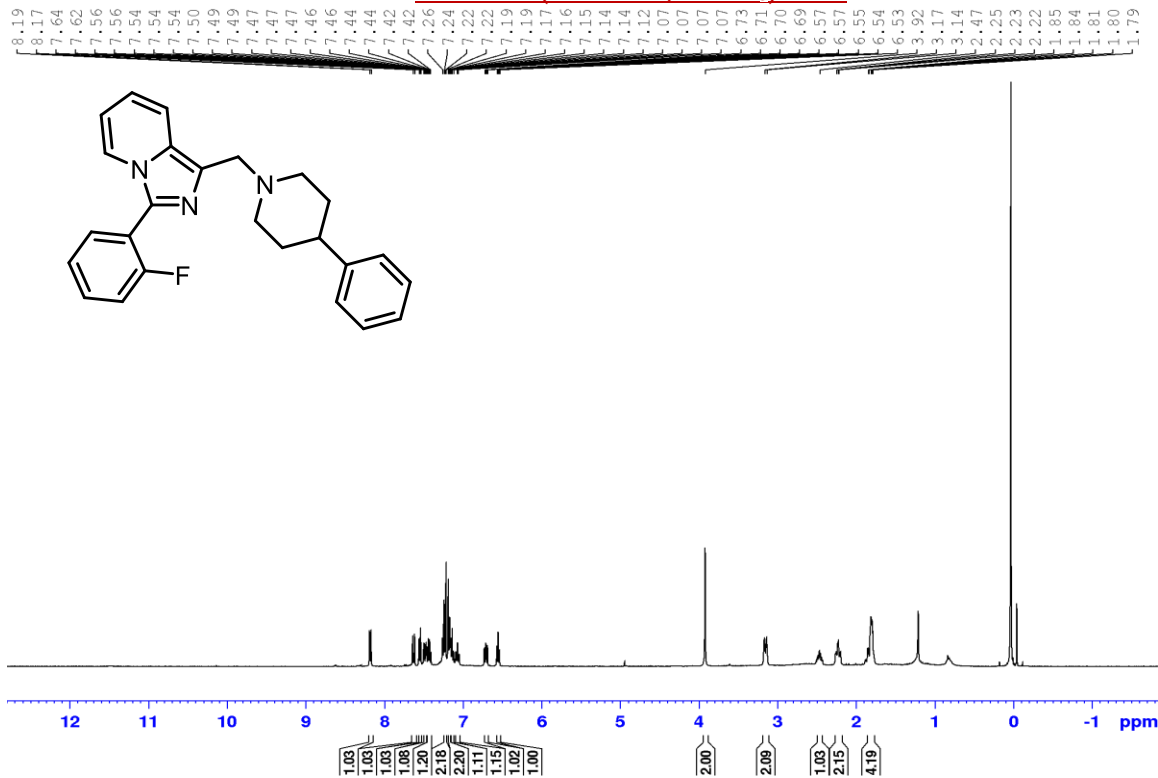
230424_187 (0.155)



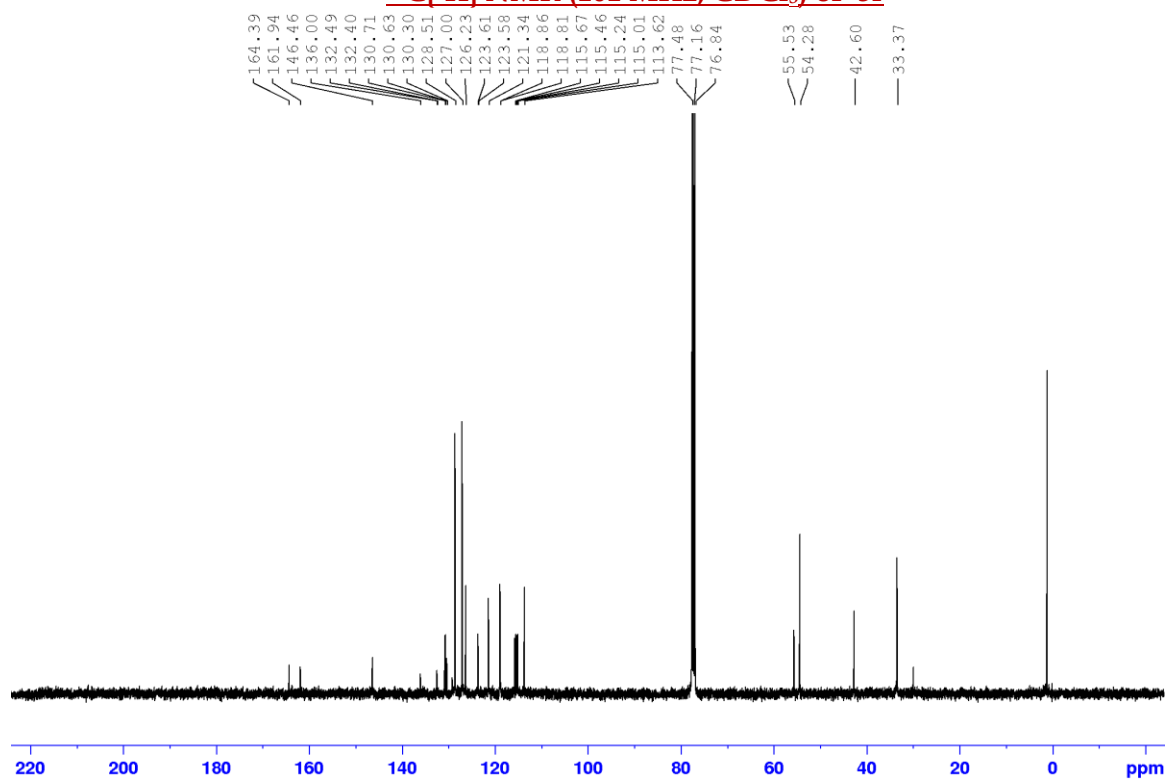
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|--------------|
| 225.0838 | 225.0828 | 1.0 | 4.4 | 10.5 | 1350.8 | n/a | n/a | C14 H10 N2 F |

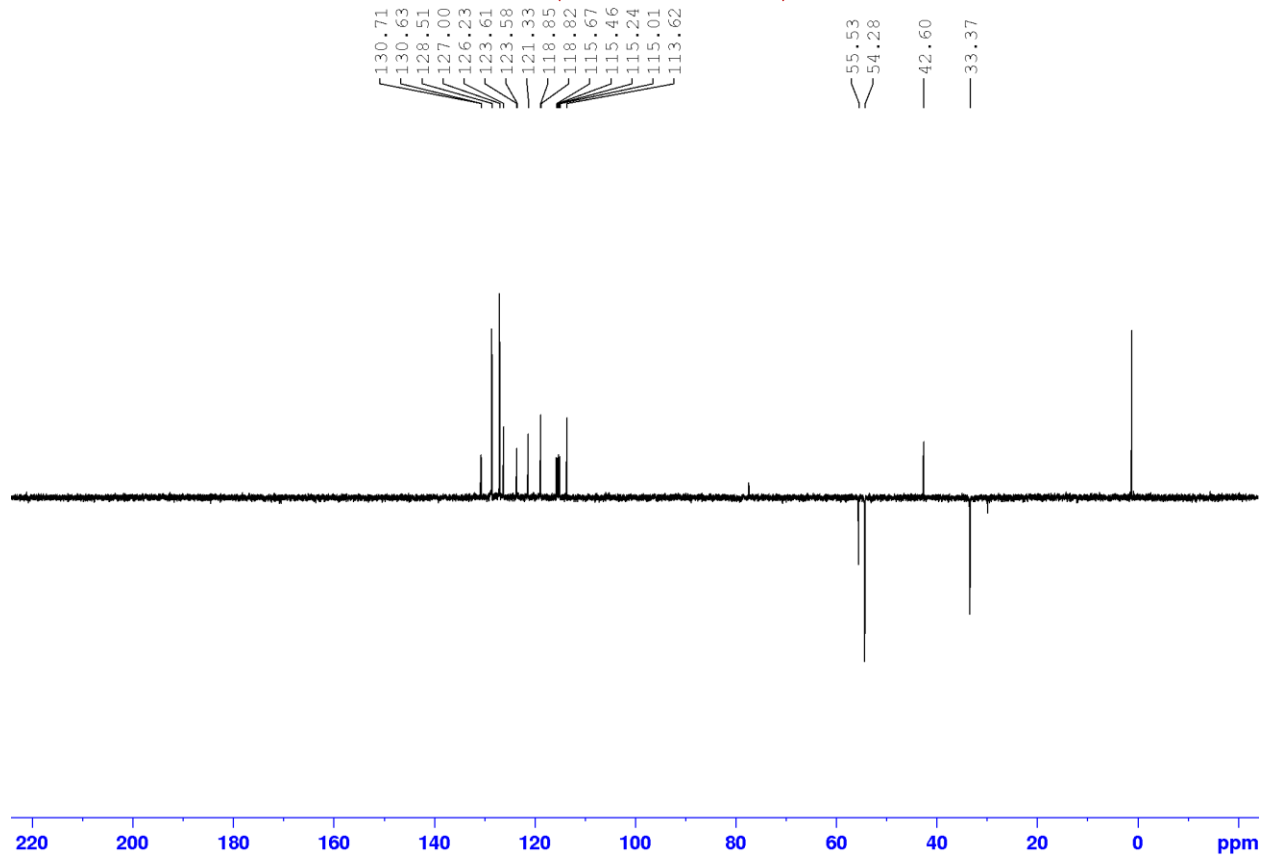
¹H NMR (400 MHz, CDCl₃) of 3r



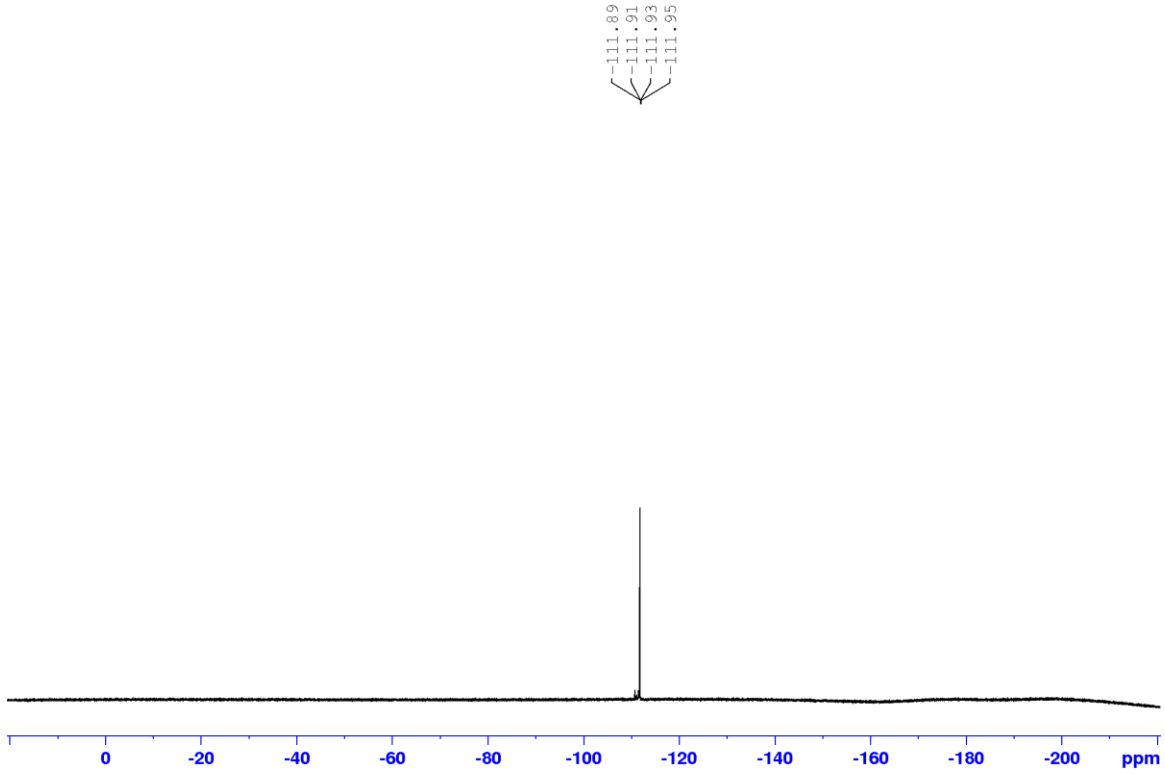
¹³C{¹H} NMR (101 MHz, CDCl₃) of 3r



DEPT-135 (400 MHz, CDCl₃) of 3r



¹⁹F NMR (377 MHz, CDCl₃) of 3r



HRMS of 3r

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-25 H: 0-100 N: 0-3 F: 0-1

SM-390

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

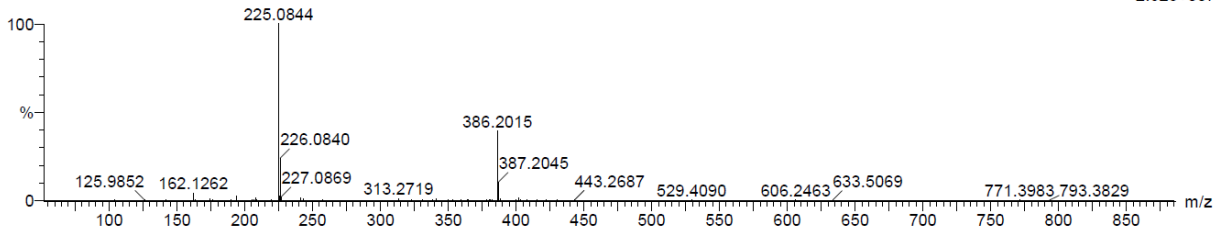
23-Apr-2024

12:41:11

1: TOF MS ES+

2.52e+007

230424_13 5 (0.121)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|--------------|
| 386.2015 | 386.2033 | -1.8 | -4.7 | 14.5 | 1088.1 | n/a | n/a | C25 H25 N3 F |

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2 F: 0-1

SM-390

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

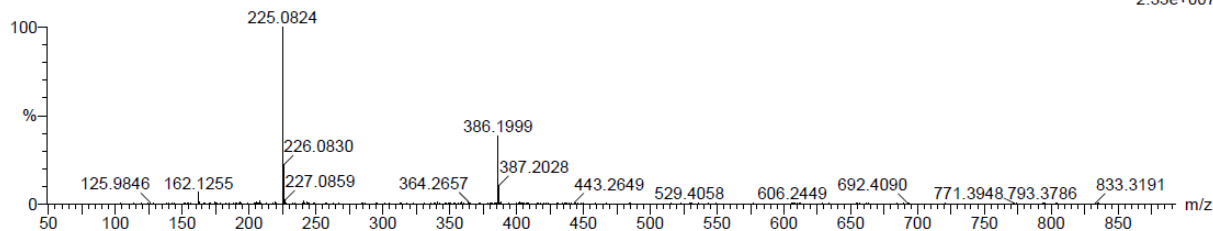
23-Apr-2024

12:41:11

1: TOF MS ES+

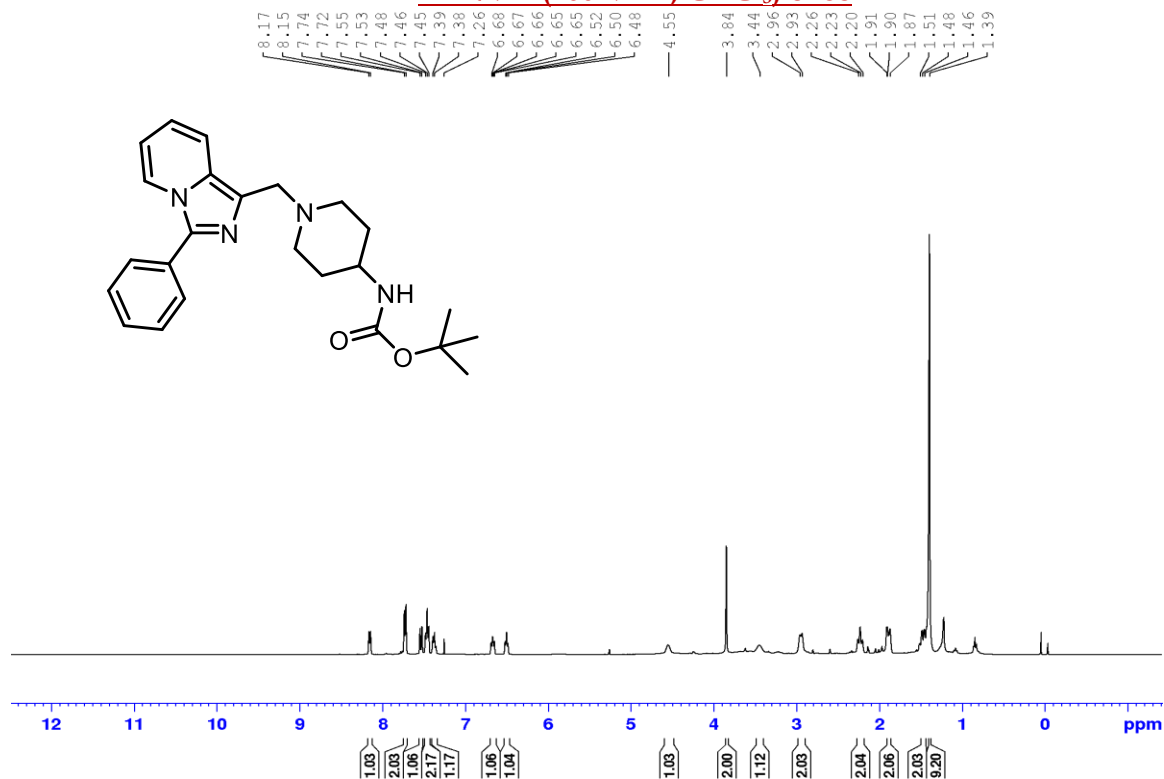
2.33e+007

230424_13 7 (0.155)

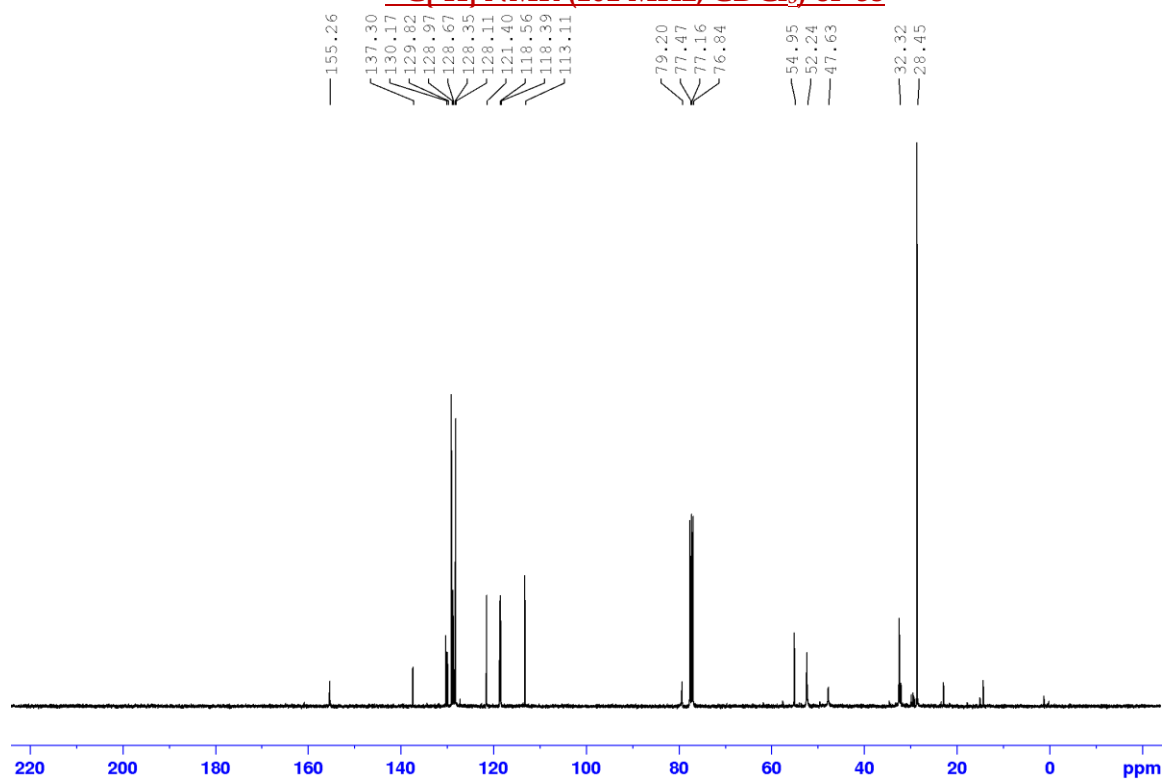


Minimum: -1.5
Maximum: 2.0 50.0 50.0

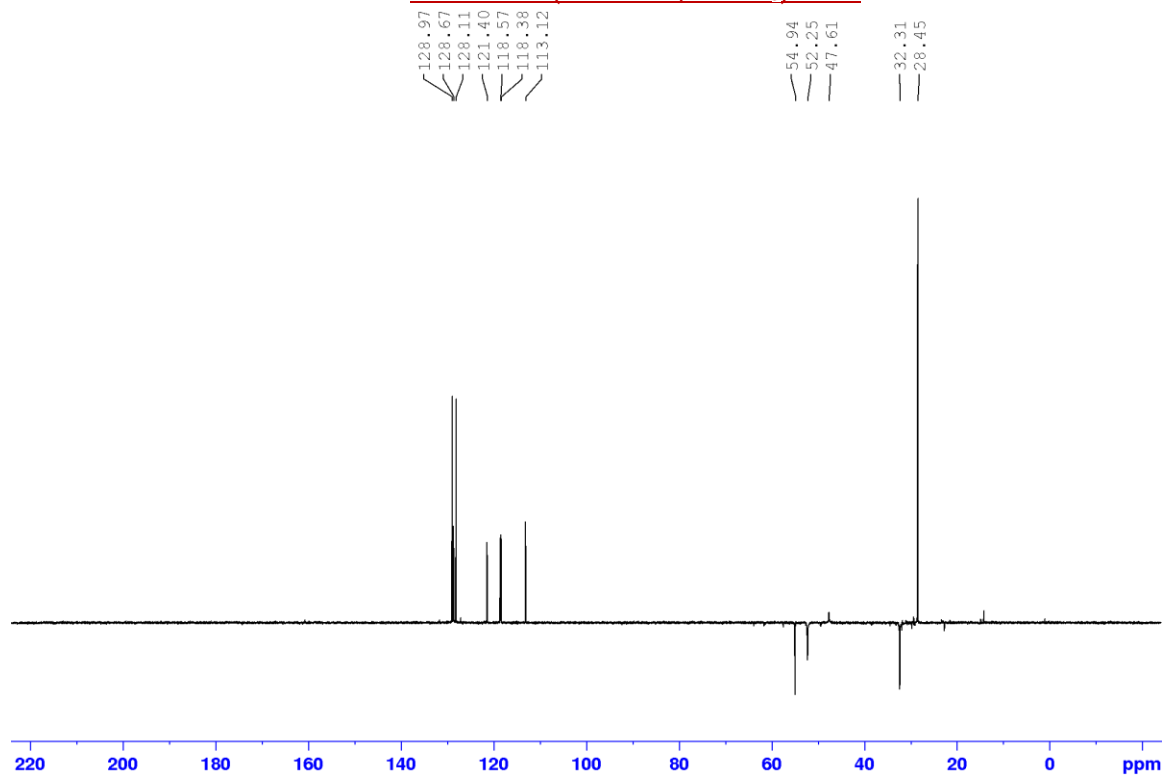
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|--------------|
| 225.0824 | 225.0828 | -0.4 | -1.8 | 10.5 | 1408.5 | n/a | n/a | C14 H10 N2 F |

¹H NMR (400 MHz, CDCl₃) of 3s

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3s



DEPT-135 (400 MHz, CDCl_3) of 3s



HRMS of 3s

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-24 H: 0-100 N: 0-4 O: 0-2

SM-376

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

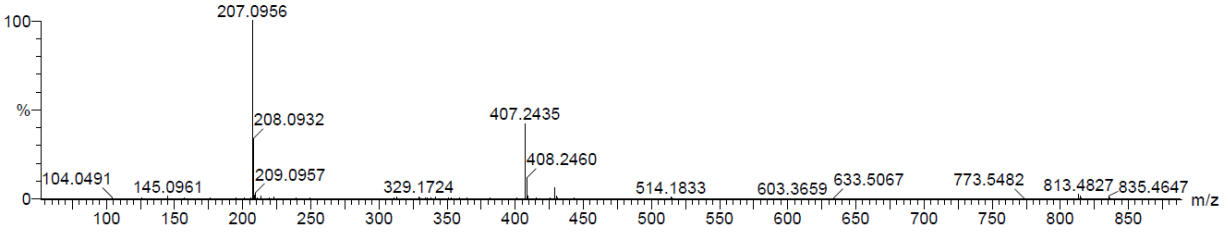
23-Apr-2024

12:15:12

1: TOF MS ES+

3.19e+007

230424_03 5 (0.121)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|---------------|
| 407.2435 | 407.2447 | -1.2 | -2.9 | 11.5 | 1078.5 | n/a | n/a | C24 H31 N4 O2 |

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-2

SM-376

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

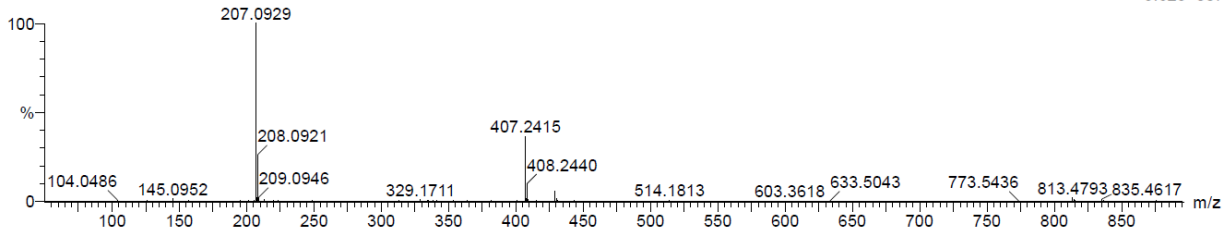
23-Apr-2024

12:15:12

1: TOF MS ES+

3.62e+007

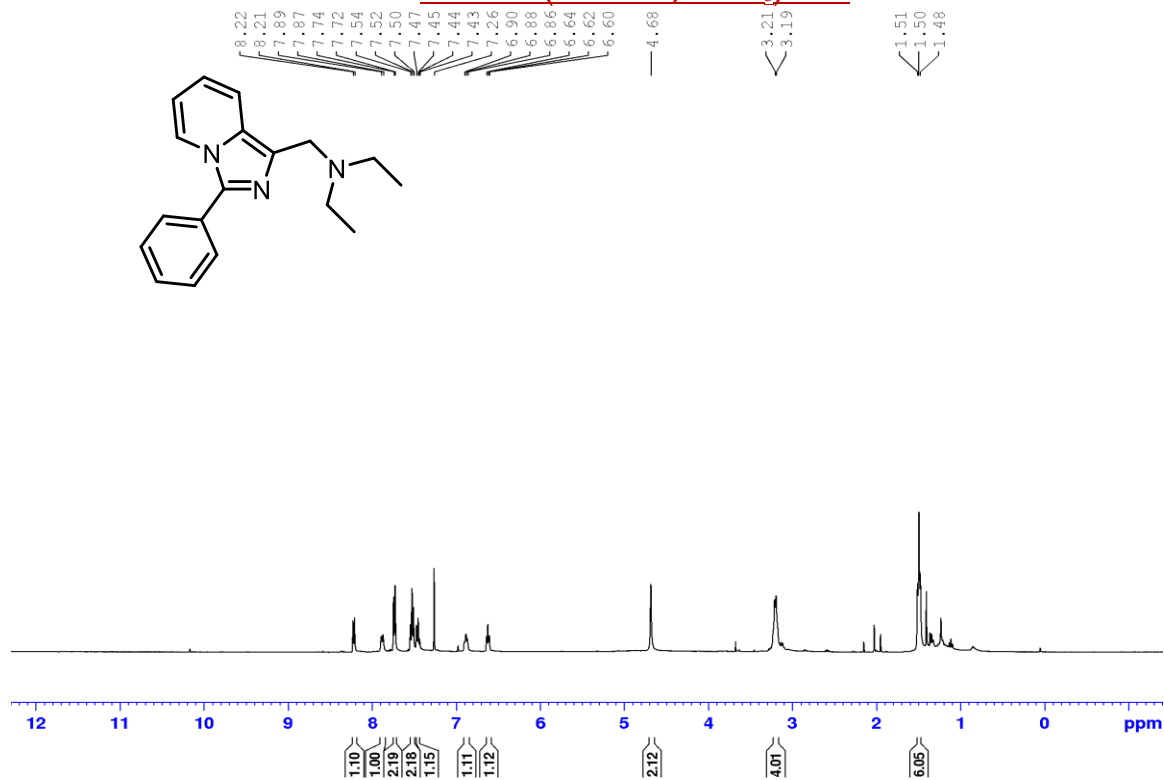
230424_03 7 (0.155)



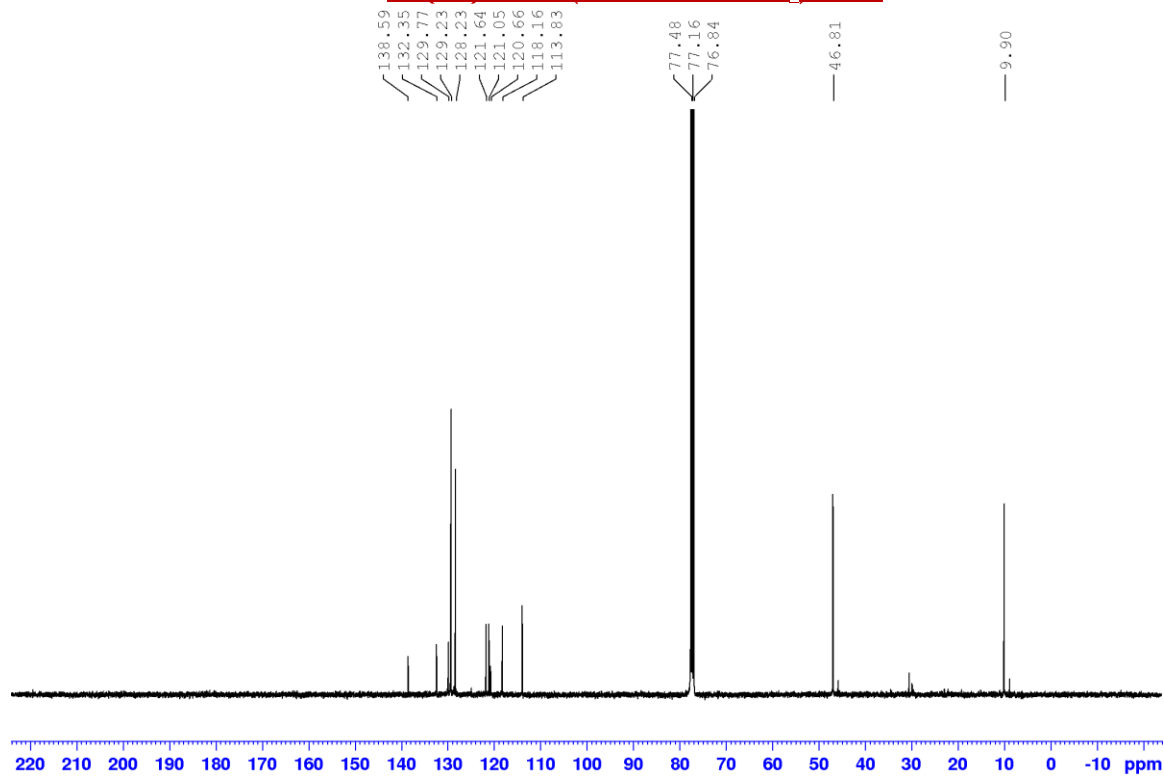
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|-----|-----|------|--------|------|---------|------------|
| 207.0929 | 207.0922 | 0.7 | 3.4 | 10.5 | 1510.8 | n/a | n/a | C14 H11 N2 |

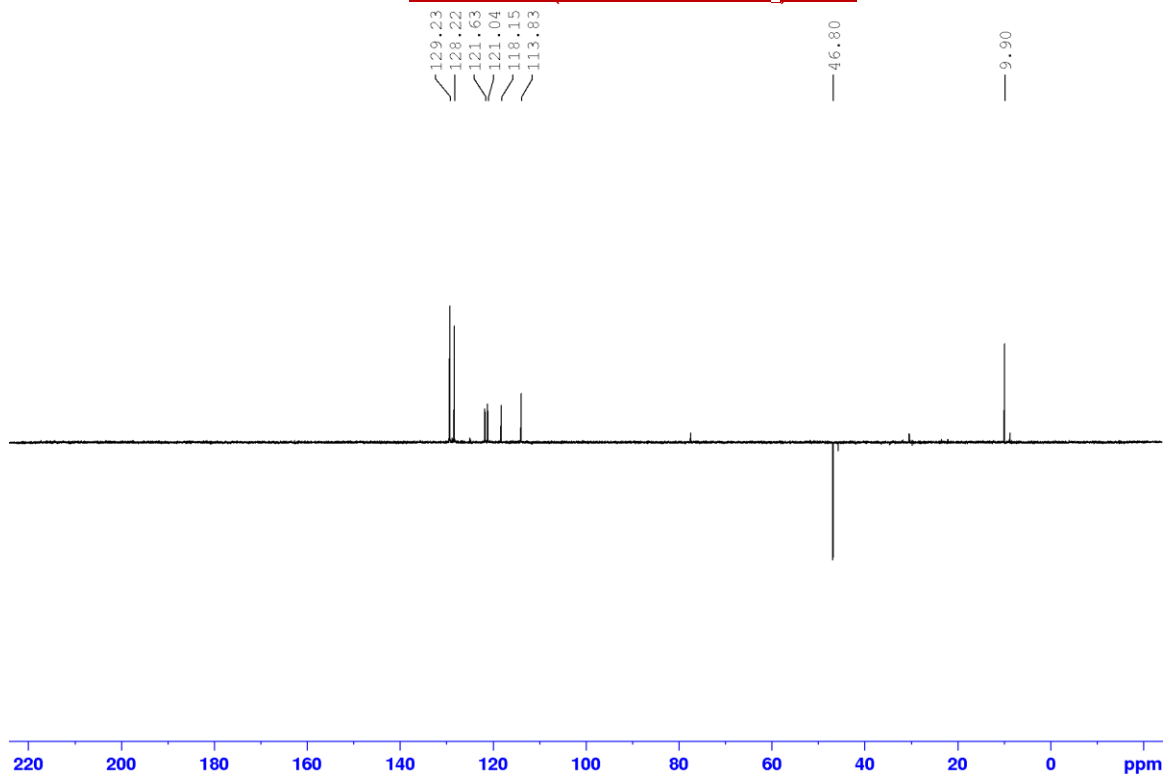
¹H NMR (400 MHz, CDCl₃) of 3t



¹³C[¹H] NMR (101 MHz, CDCl₃) of 3t



DEPT-135 (400 MHz, CDCl₃) of 3t



HRMS of 3t

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-14 H: 0-100 N: 0-3

SM-486

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

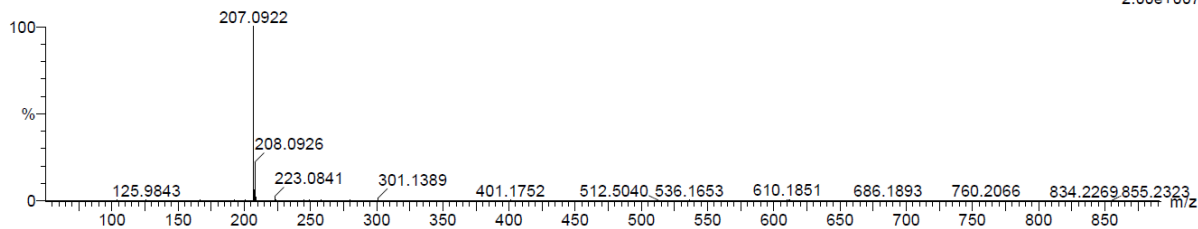
07-May-2024

14:05:00

070524_30 5 (0.121)

1: TOF MS ES+

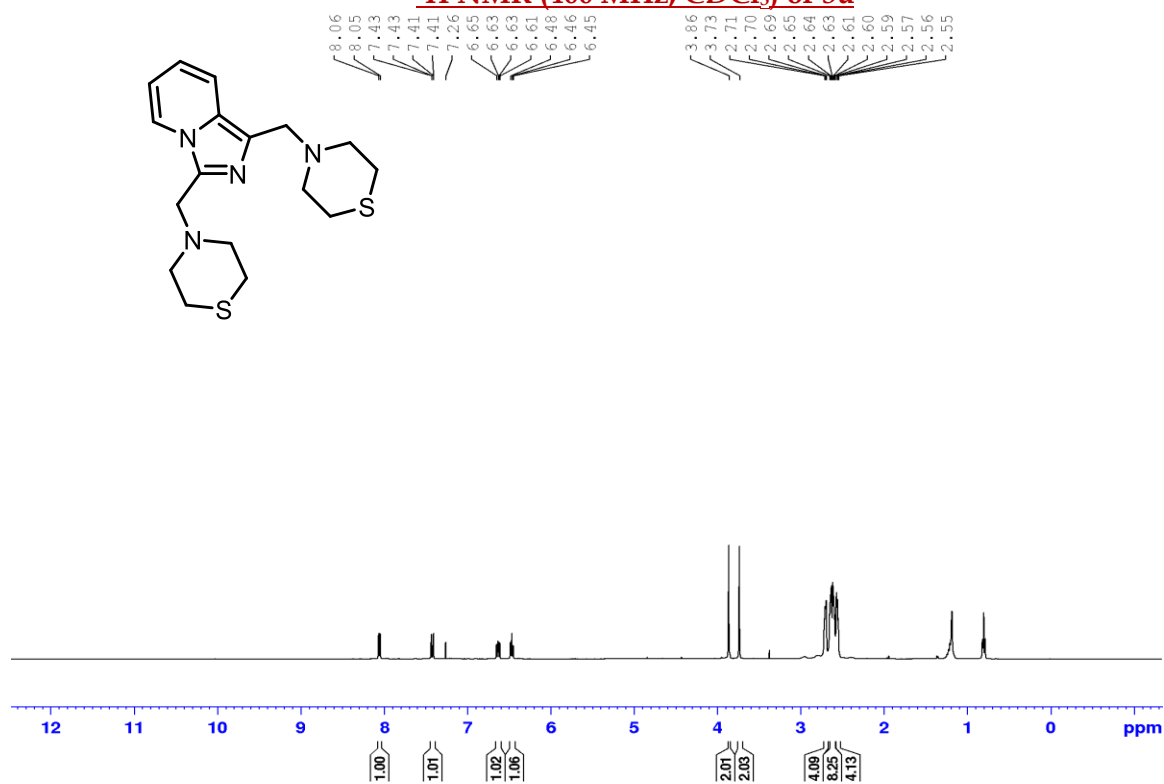
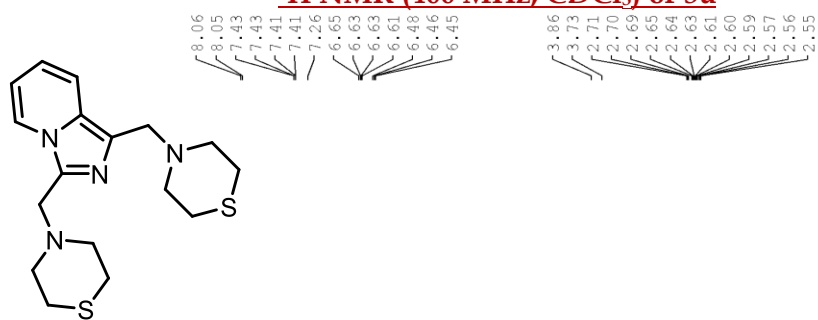
2.00e+007



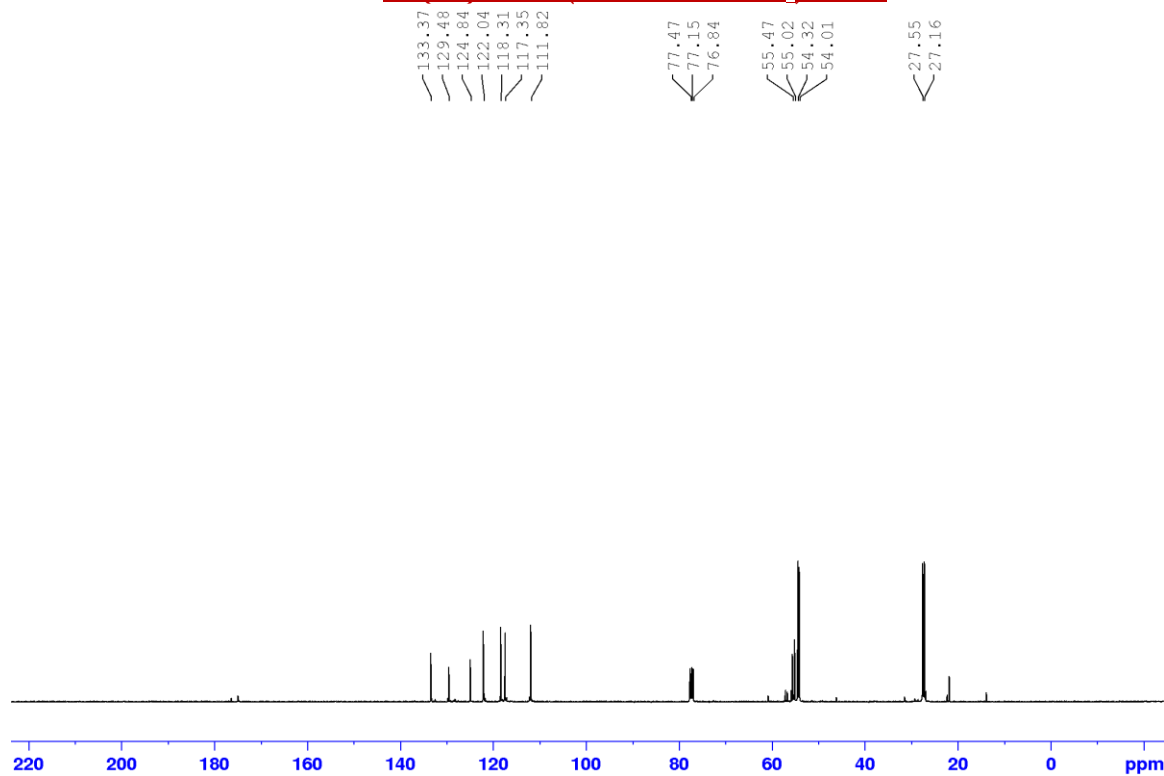
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|-----|-----|------|--------|------|---------|------------|
| 207.0922 | 207.0922 | 0.0 | 0.0 | 10.5 | 1350.9 | n/a | n/a | C14 H11 N2 |

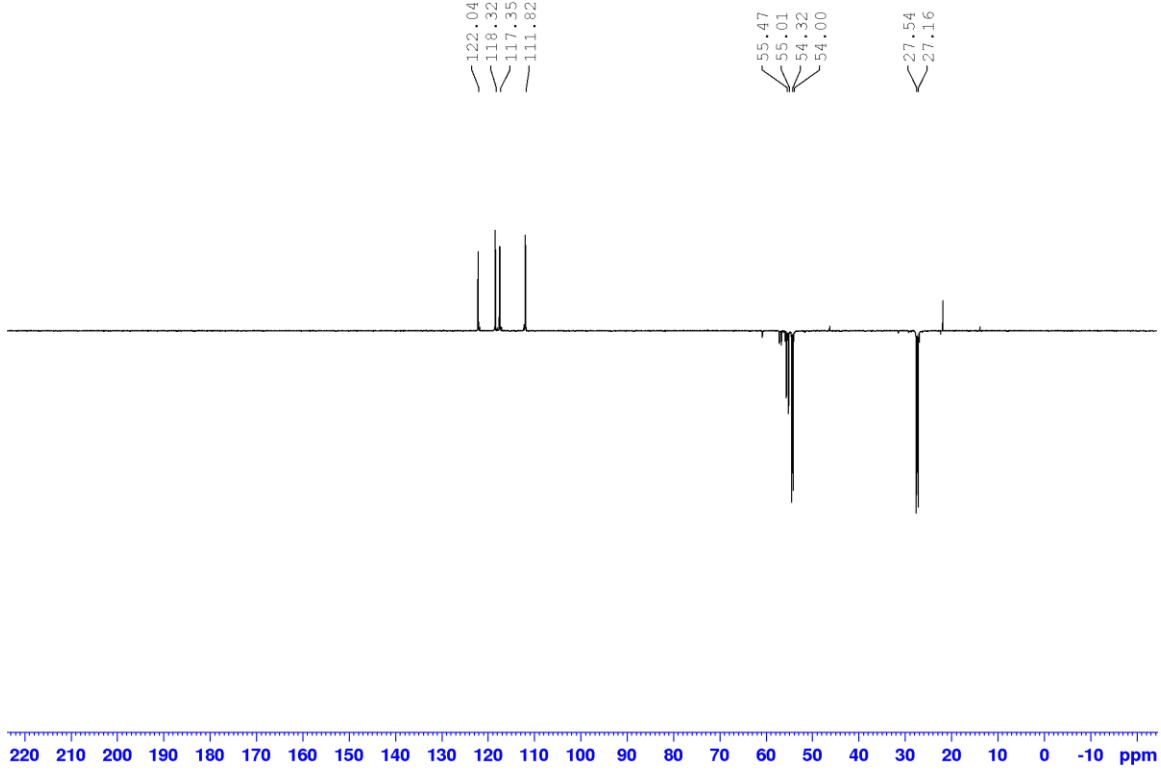
¹H NMR (400 MHz, CDCl₃) of 3u



¹³C[¹H] NMR (101 MHz, CDCl₃) of 3u



DEPT-135 (400 MHz, CDCl₃) of 3u



HRMS of 3u

Elemental Composition Report

Page 1

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions

31 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

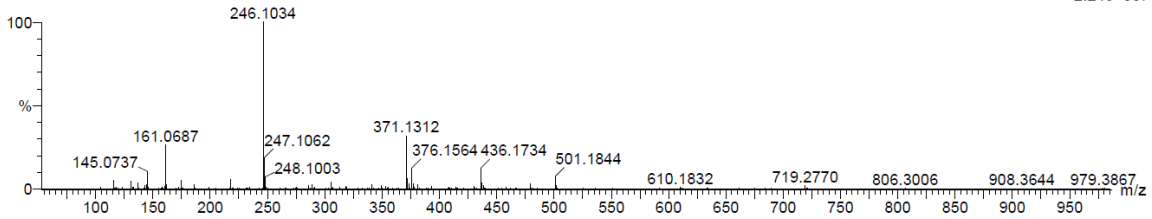
C: 0-17 H: 0-100 N: 0-4 Na: 0-1 S: 0-2

SM-524

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

02-May-2024
13:29:15
1: TOF MS ES+
2.24e+007

020524_32 6 (0.138)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|-----|--------|------|----------|------------------|
| 371.1312 | 371.1340 | -2.8 | -7.5 | 7.5 | 1133.0 | n/a | n/a | C17 H24 N4 Na S2 |

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-13 H: 0-100 N: 0-3 S: 0-1

SM-524

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

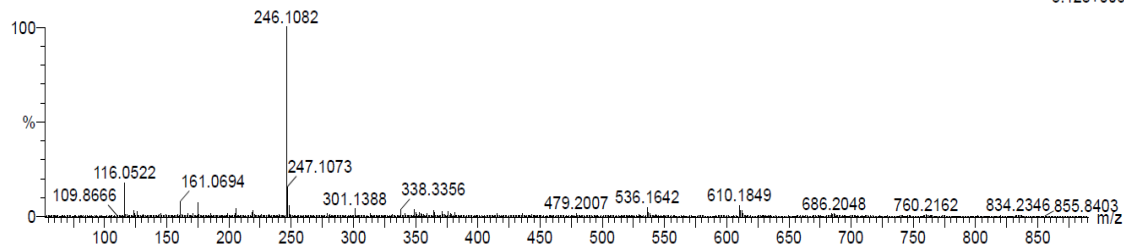
07-May-2024

14:33:46

1: TOF MS ES+

3.12e+006

070524_37 5 (0.121) Cm (5)

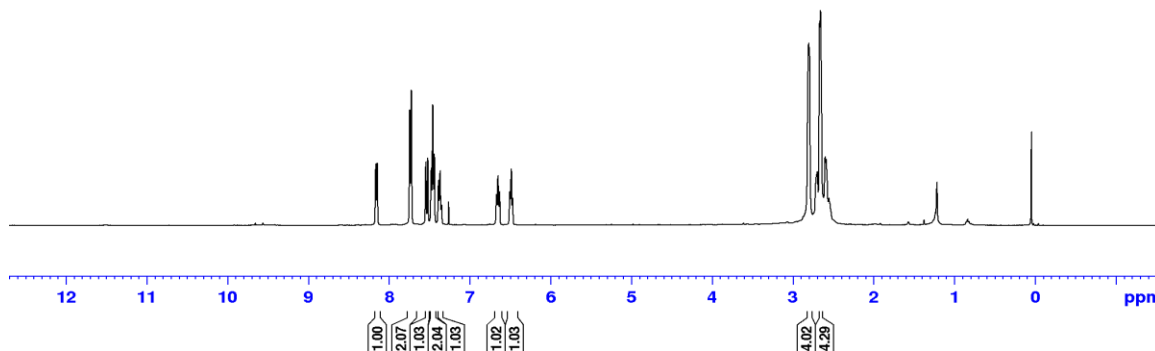
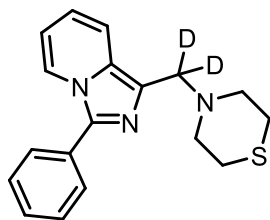


Minimum: -1.5
Maximum: 2.0 50.0 50.0

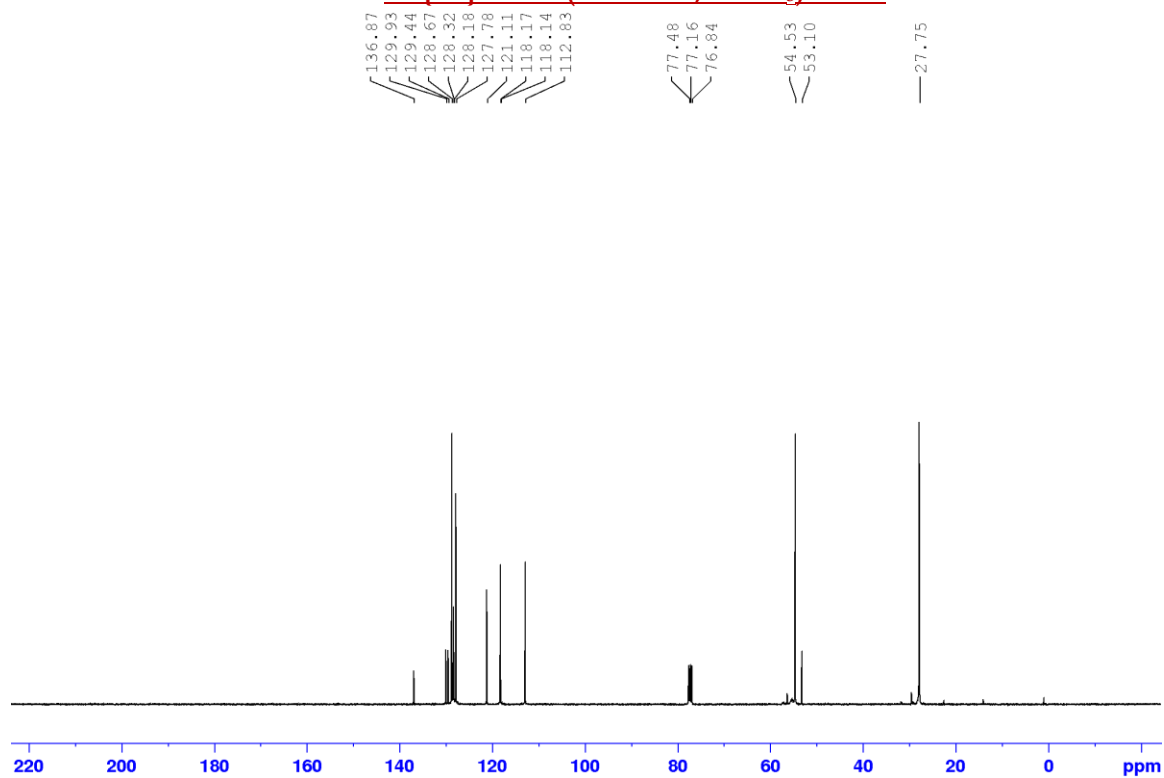
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|-----|-----|-----|-------|------|---------|--------------|
| 246.1082 | 246.1065 | 1.7 | 6.9 | 7.5 | 27.1 | n/a | n/a | C13 H16 N3 S |

¹H NMR (400 MHz, CDCl₃) of 3v

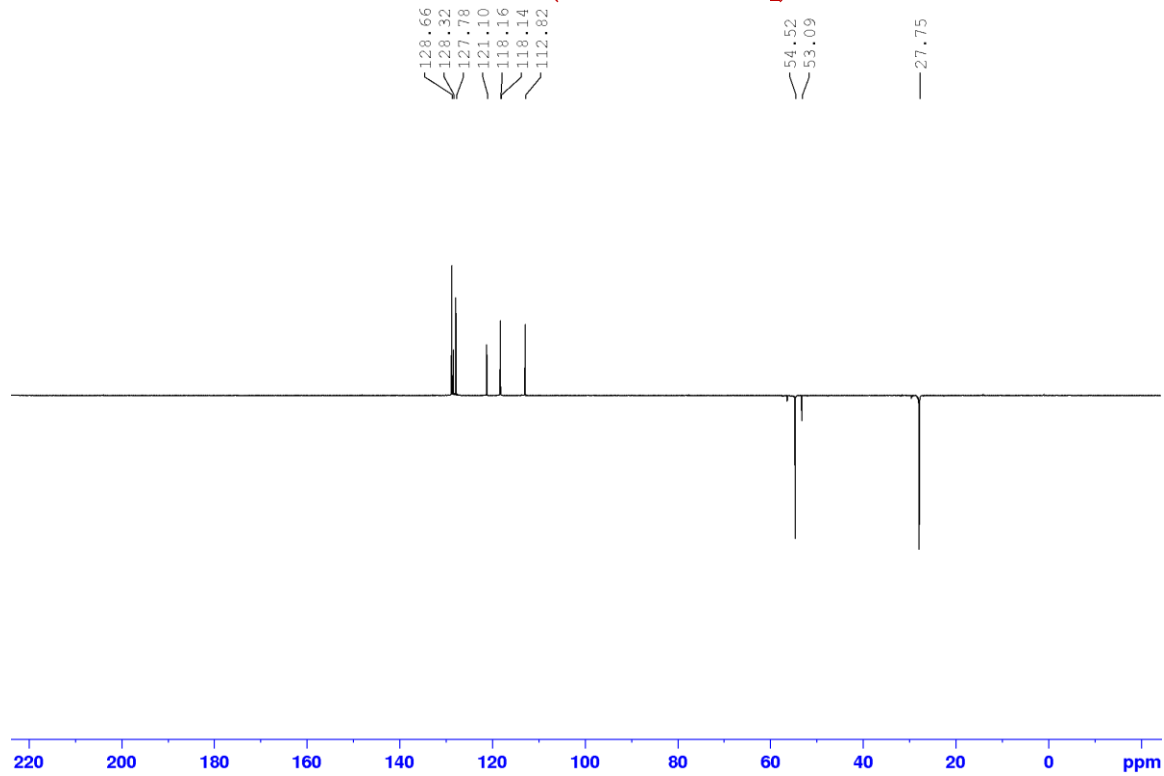
8.16, 8.14, 7.74, 7.72, 7.54, 7.52, 7.47, 7.46, 7.44, 7.38, 7.36, 7.35, 7.35, 7.26, 6.87, 6.65, 6.63, 6.50, 6.48, 6.47, 2.80, 2.79, 2.66, 2.66



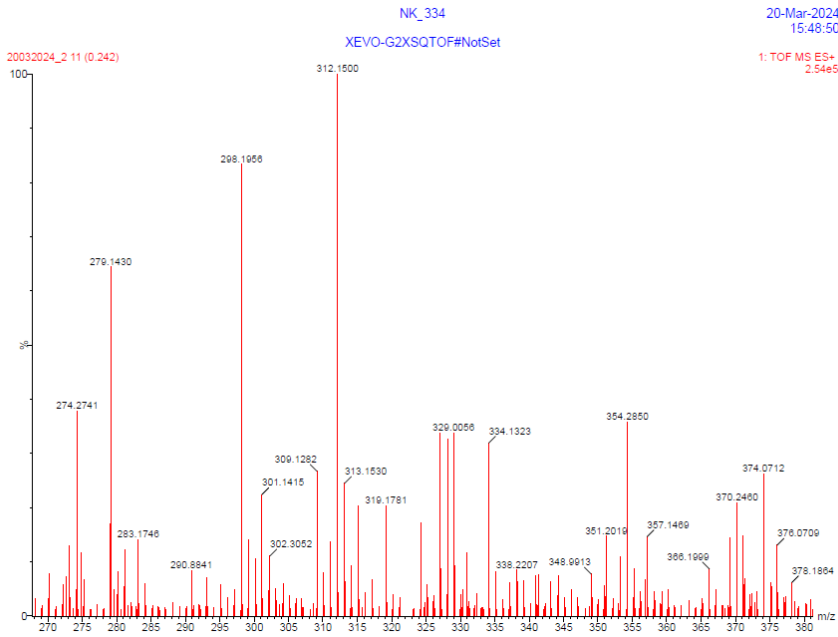
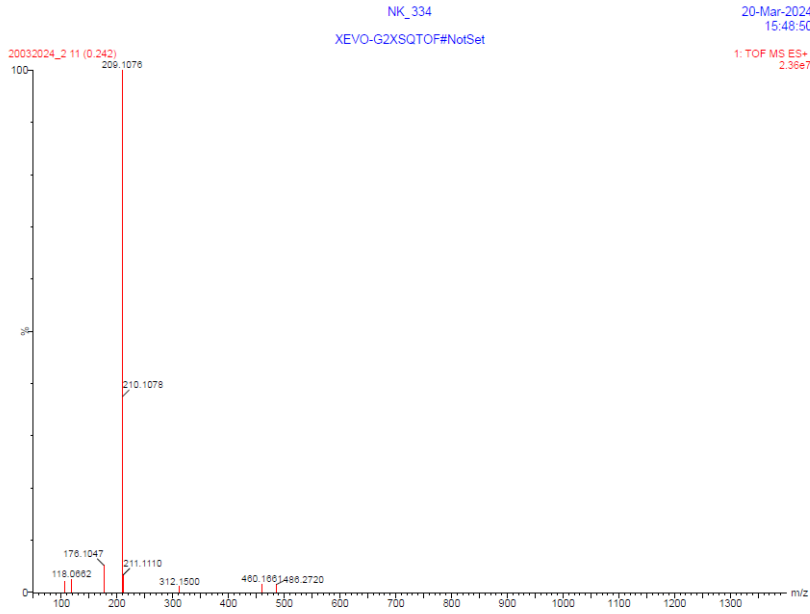
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 3v



DEPT-135 (101 MHz, CDCl_3) of 3v



HRMS of 3v

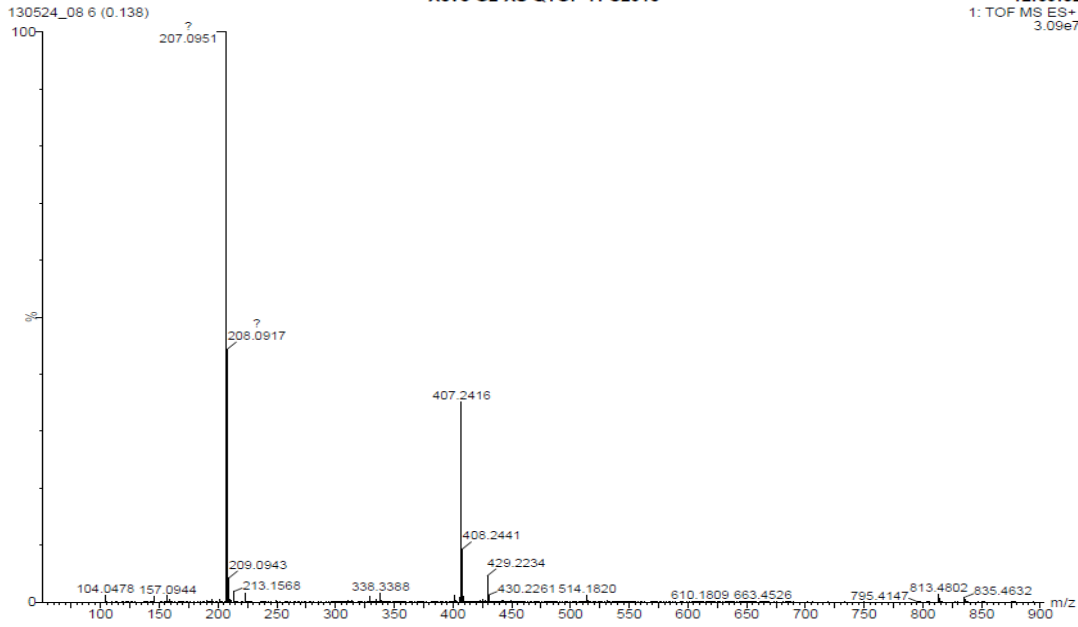


MS/MS Spectra of 3s

SM-376

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

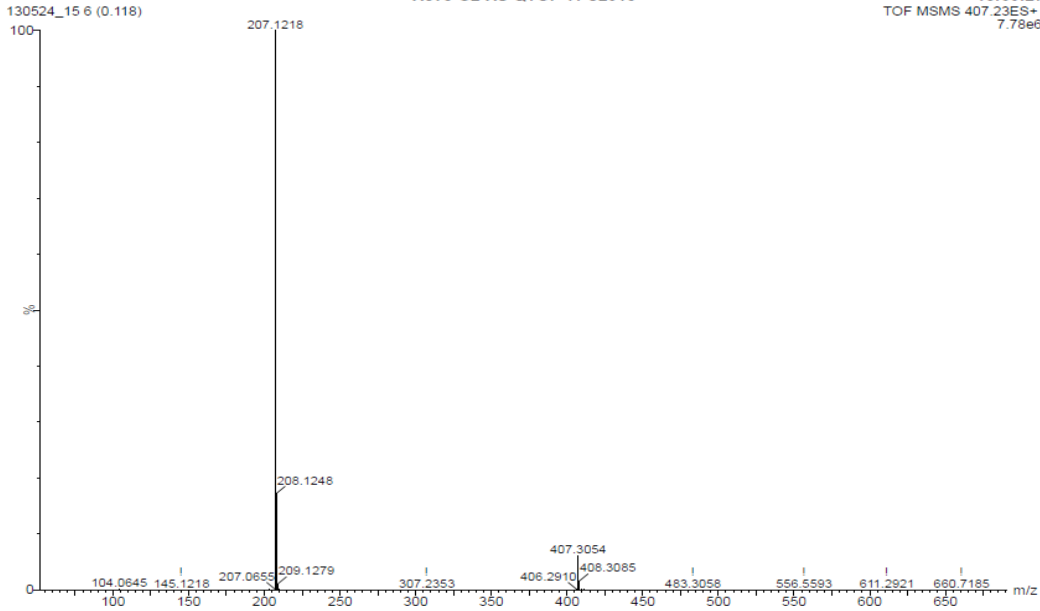
13-May-2024
12:39:52
1: TOF MS ES+
3.09e7



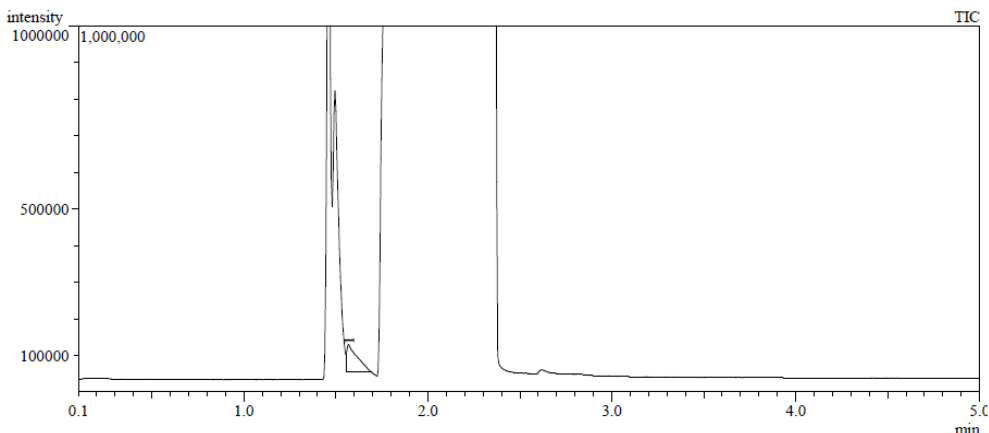
SM-376 MSMS 10V

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

13-May-2024
15:00:27
TOF MSMS 407.23ES+
7.78e6



GC-MS for Standard HCHO

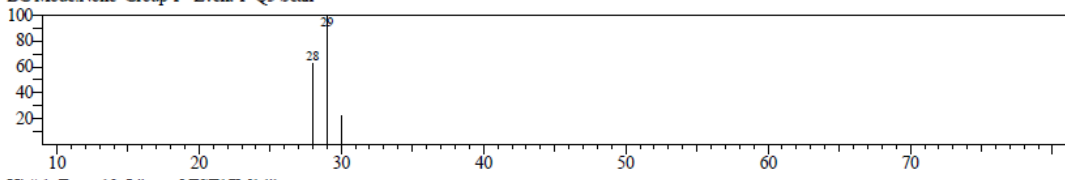


| Peak Report TIC | | | | | |
|-----------------|---------|--------|--------|------------|--------------------|
| Peak# | R. Time | Area | Area% | Similarity | Base m/z Name |
| 1 | 1.569 | 289295 | 100.00 | 0 | 29.00 Formaldehyde |
| | | 289295 | 100.00 | | |

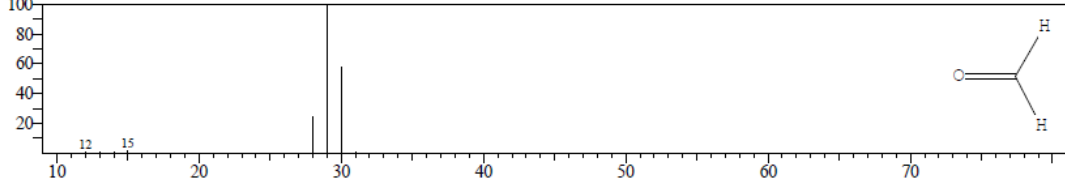
Library

<< Target >>

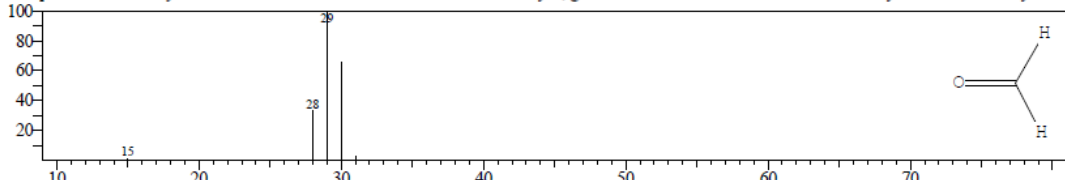
Line#:1 R. Time:1.570(Scan#:315) MassPeaks:3
 RawMode:Averaged 1.560-1.590(313-319) BasePeak:29.00(65222)
 BG Mode:None Group 1 - Event 1 Q3 Scan



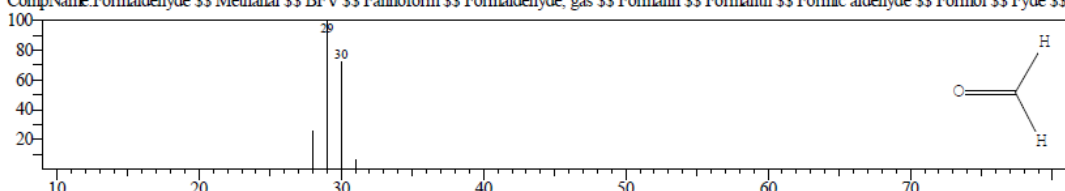
Hit#:1 Entry:12 Library:NIST17M1.lib
 SI:90 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0
 CompName:Formaldehyde \$\$ Methanal \$\$ BFV \$\$ Fannoform \$\$ Formaldehyde, gas \$\$ Formalin \$\$ Formalith \$\$ Formic aldehyde \$\$ Formol \$\$ Fyde \$\$



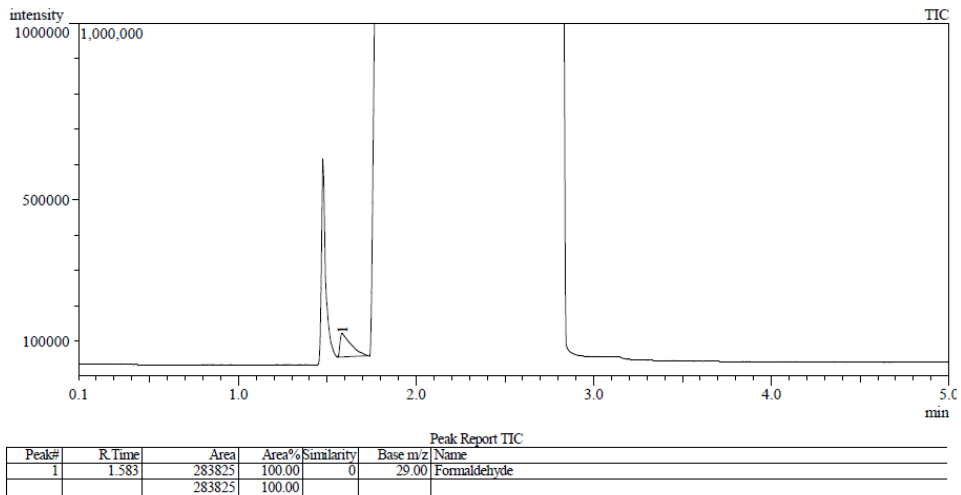
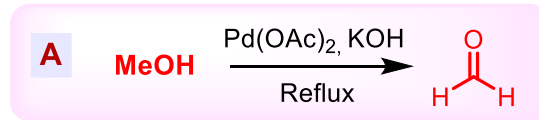
Hit#:2 Entry:10 Library:NIST17R.lib
 SI:90 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0
 CompName:Formaldehyde \$\$ Methanal \$\$ BFV \$\$ Fannoform \$\$ Formaldehyde, gas \$\$ Formalin \$\$ Formalith \$\$ Formic aldehyde \$\$ Formol \$\$ Fyde \$\$



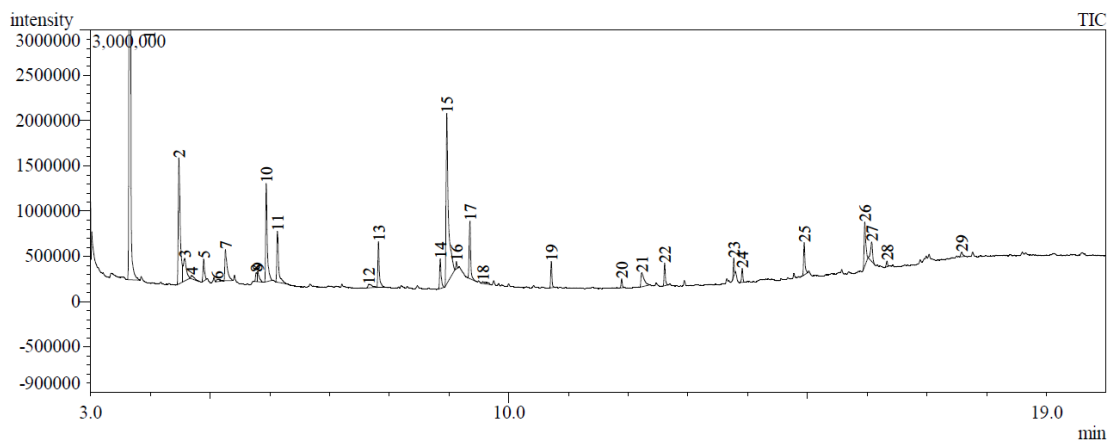
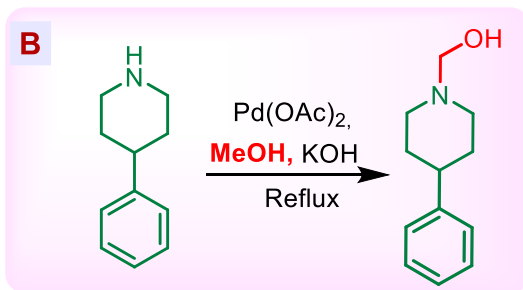
Hit#:3 Entry:11 Library:NIST17R.lib
 SI:87 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0
 CompName:Formaldehyde \$\$ Methanal \$\$ BFV \$\$ Fannoform \$\$ Formaldehyde, gas \$\$ Formalin \$\$ Formalith \$\$ Formic aldehyde \$\$ Formol \$\$ Fyde \$\$



GC-MS for reaction A



GCMS for reaction B

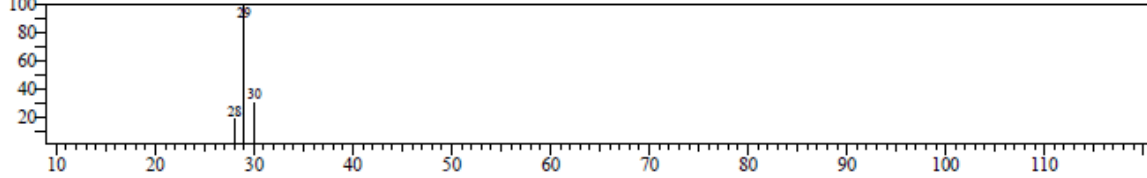


Library for reaction A

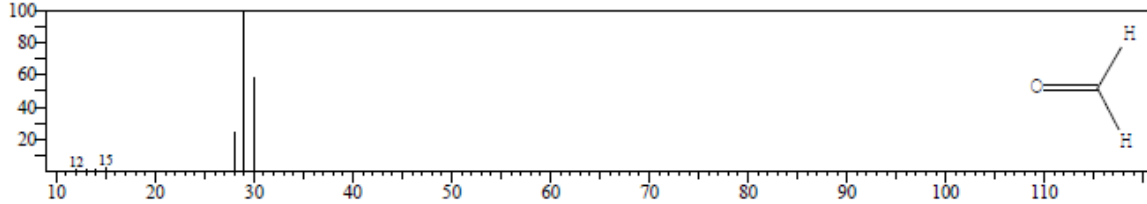
Library

<< Target >>

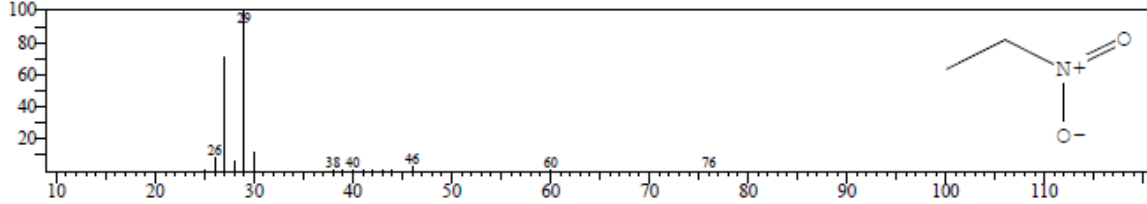
Line# 1 RTime: 1.585 (Scan# 318) MassPeaks: 3
RawMode: Averaged 1.565-1.605 (314-322) BasePeak: 29.00 (30142)
BG Mode: 1.715 (344) Group 1 - Event 1 Q3 Scan



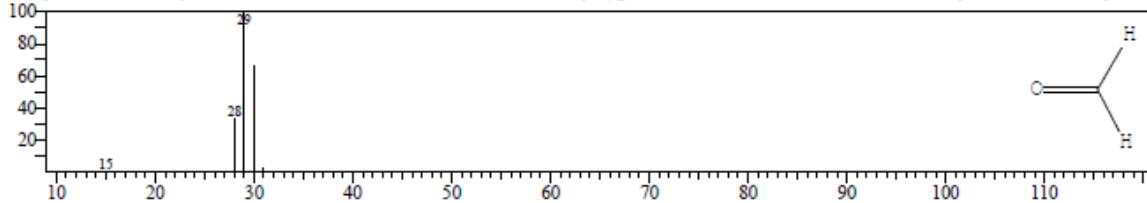
Hit# 1 Entry: 12 Library: NIST17M1.lib
SI: 95 Formula: CH2O CAS: 50-00-0 MolWeight: 30 RetIndex: 0
CompName: Formaldehyde \$\$ Methanal \$\$ BFV \$\$ Fannoform \$\$ Formaldehyde, gas \$\$ Formalin \$\$ Formalith \$\$ Formic aldehyde \$\$ Formol \$\$ Fyde \$\$



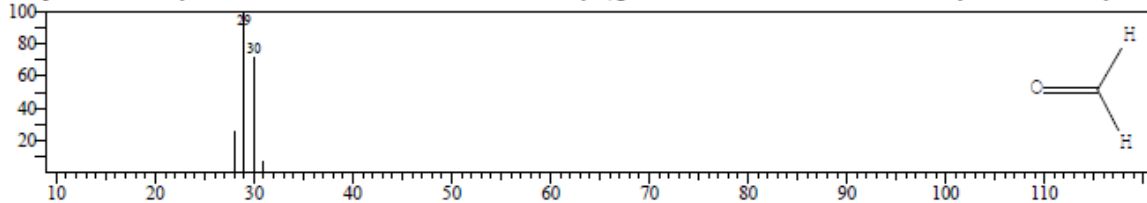
Hit# 2 Entry: 584 Library: NIST17R.lib
SI: 92 Formula: C2H5NO2 CAS: 79-24-3 MolWeight: 75 RetIndex: 602
CompName: Ethane, nitro- \$\$ Nitroethane \$\$ C2H5NO2 \$\$ Nitroetan \$\$ UN 2842 \$\$ NE \$\$ Nitroparaffin \$\$ 1-Nitroethane #



Hit# 3 Entry: 10 Library: NIST17R.lib
SI: 92 Formula: CH2O CAS: 50-00-0 MolWeight: 30 RetIndex: 0
CompName: Formaldehyde \$\$ Methanal \$\$ BFV \$\$ Fannoform \$\$ Formaldehyde, gas \$\$ Formalin \$\$ Formalith \$\$ Formic aldehyde \$\$ Formol \$\$ Fyde \$\$



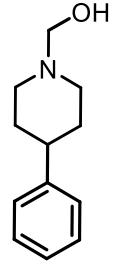
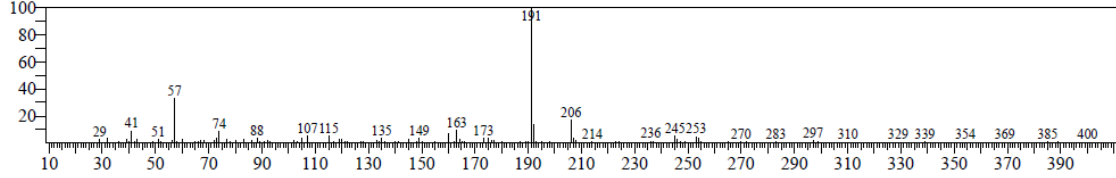
Hit# 4 Entry: 11 Library: NIST17R.lib
SI: 91 Formula: CH2O CAS: 50-00-0 MolWeight: 30 RetIndex: 0
CompName: Formaldehyde \$\$ Methanal \$\$ BFV \$\$ Fannoform \$\$ Formaldehyde, gas \$\$ Formalin \$\$ Formalith \$\$ Formic aldehyde \$\$ Formol \$\$ Fyde \$\$



Library for reaction B

<< Target >>

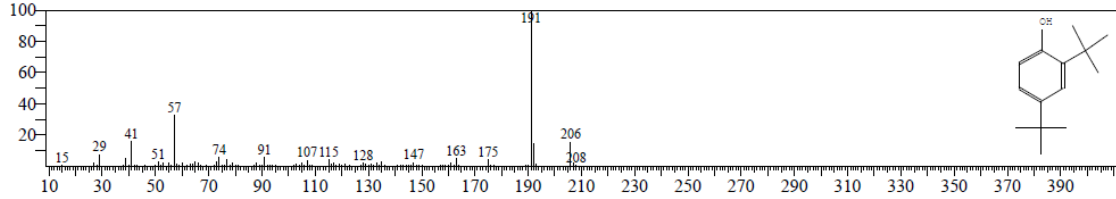
Line#:18 R.Time:9.565(Scan#:1314) MassPeaks:221
RawMode:Averaged 9.560-9.570(1313-1315) BasePeak:191.10(6936)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#1 Entry:54577 Library:NIST17M1.lib

SI:80 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555

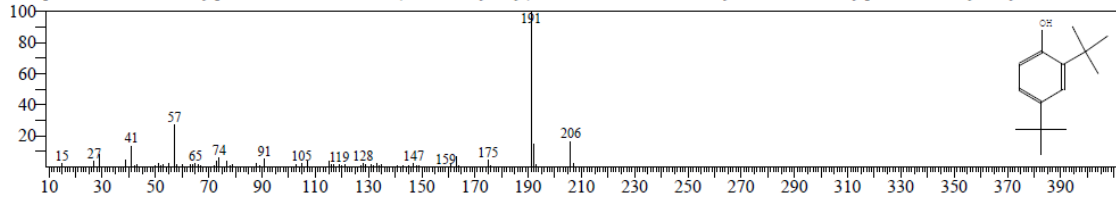
CompName:2,4-Di-tert-butylphenol \$\$ Phenol, 2,4-bis(1,1-dimethylethyl)- \$\$ Phenol, 2,4-di-tert-butyl- \$\$ 2,4-di-t-Butylphenol \$\$ 1-Hydroxy-2,4-di-tert-bu



Hit#2 Entry:22784 Library:NIST17R.lib

SI:79 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555

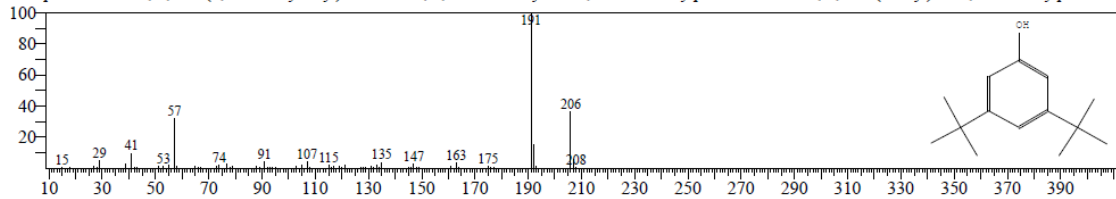
CompName:2,4-Di-tert-butylphenol \$\$ Phenol, 2,4-bis(1,1-dimethylethyl)- \$\$ Phenol, 2,4-di-tert-butyl- \$\$ 2,4-di-t-Butylphenol \$\$ 1-Hydroxy-2,4-di-tert-bu



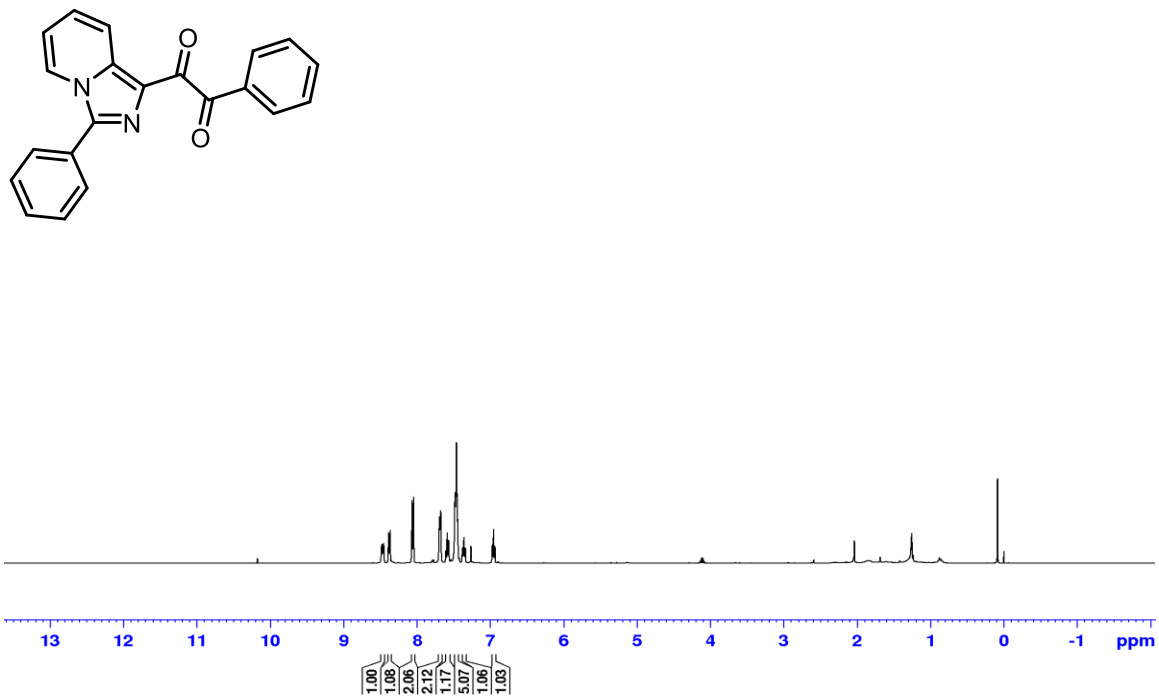
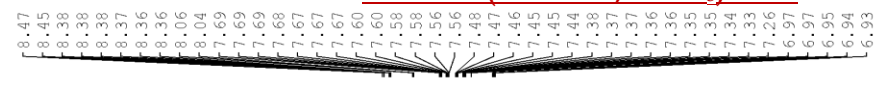
Hit#3 Entry:22787 Library:NIST17R.lib

SI:79 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555

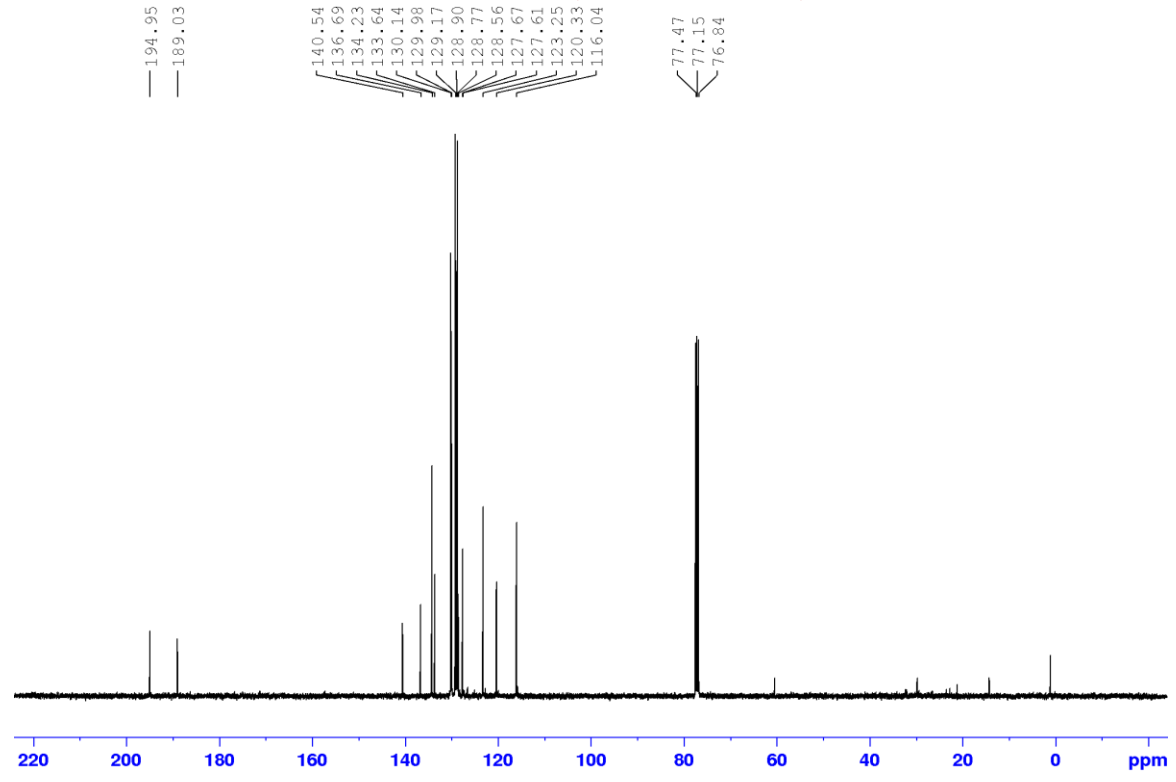
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- \$\$ Phenol, 3,5-di-tert-butyl- \$\$ 3,5-Di-tert-butylphenol \$\$ Phenol, 3,5-bis(t-butyl) \$\$ 3,5-Di-t-butylphenol \$



¹H NMR (400 MHz, CDCl₃) of 5a



¹³C(¹H) NMR (101 MHz, CDCl₃) of 5a



HRMS of 5a

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-21 H: 0-100 N: 0-2 O: 0-2

SM-339

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

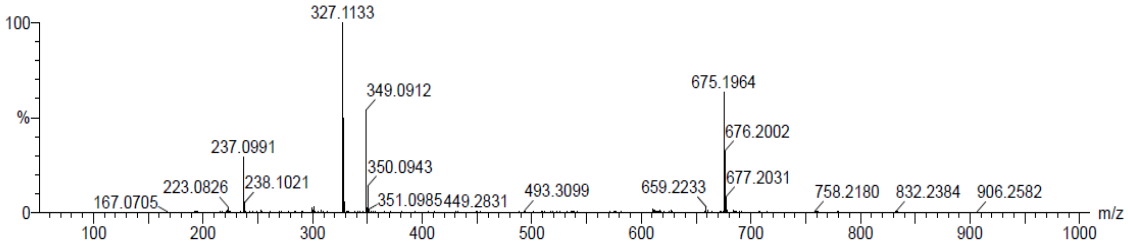
02-May-2024

13:13:03

1: TOF MS ES+

4.95e+007

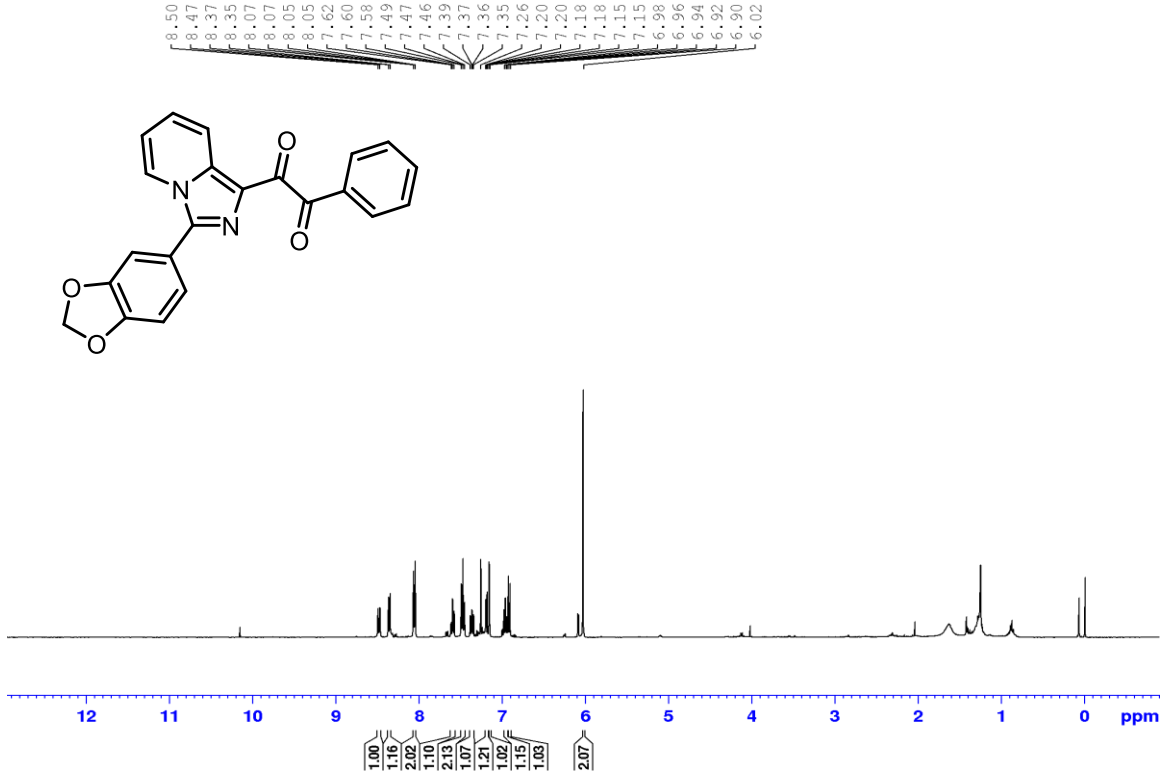
020524_26 6 (0.138)



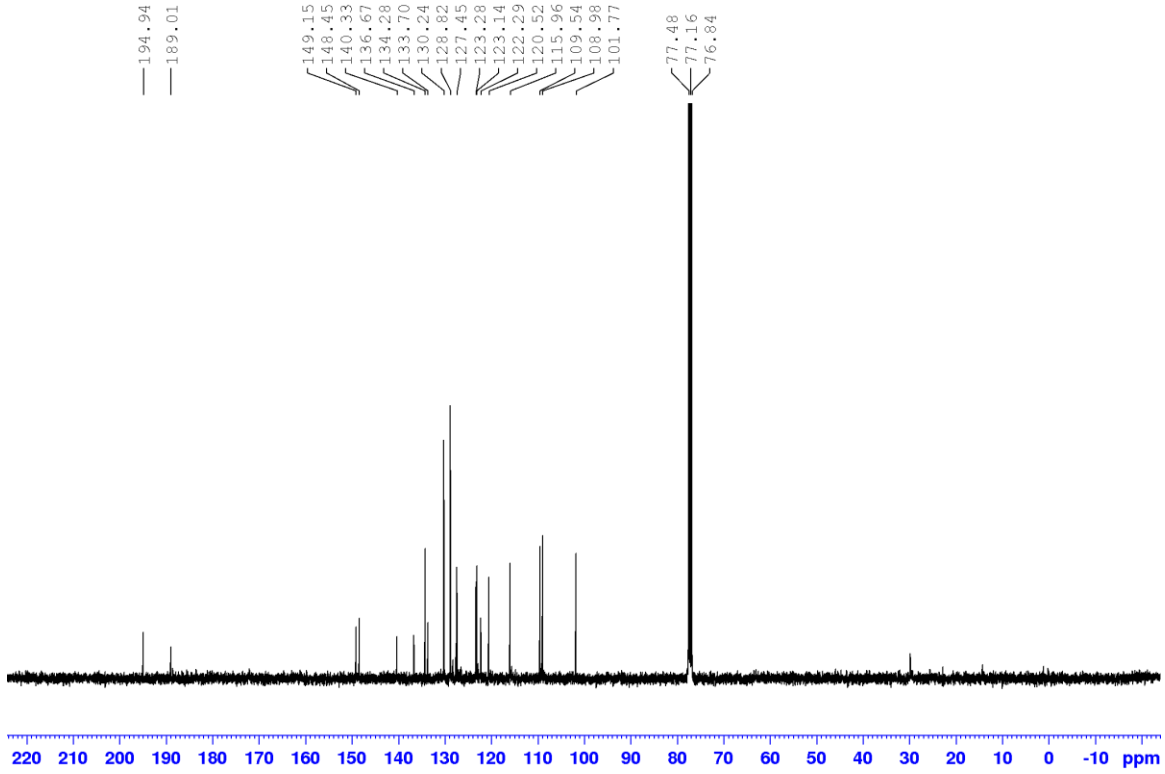
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|---------------|
| 327.1133 | 327.1134 | -0.1 | -0.3 | 15.5 | 1061.9 | n/a | n/a | C21 H15 N2 O2 |

¹H NMR (400 MHz, CDCl₃) of 5b



¹³C{¹H} NMR (101 MHz, CDCl₃) of 5b



HRMS of 5b

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

21 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-22 H: 0-100 N: 0-2 O: 0-4

SM-502

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

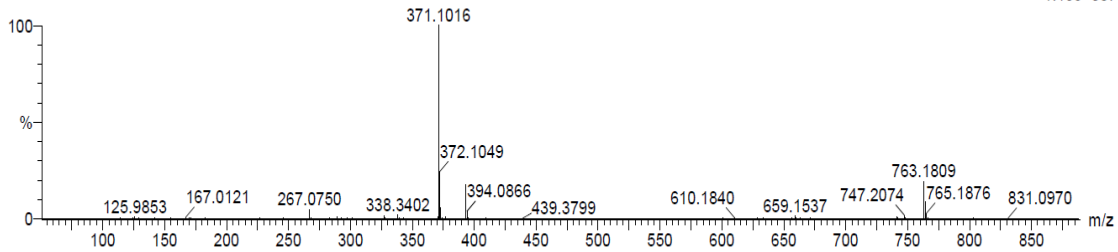
30-Apr-2024

12:00:41

1: TOF MS ES+

1.18e+007

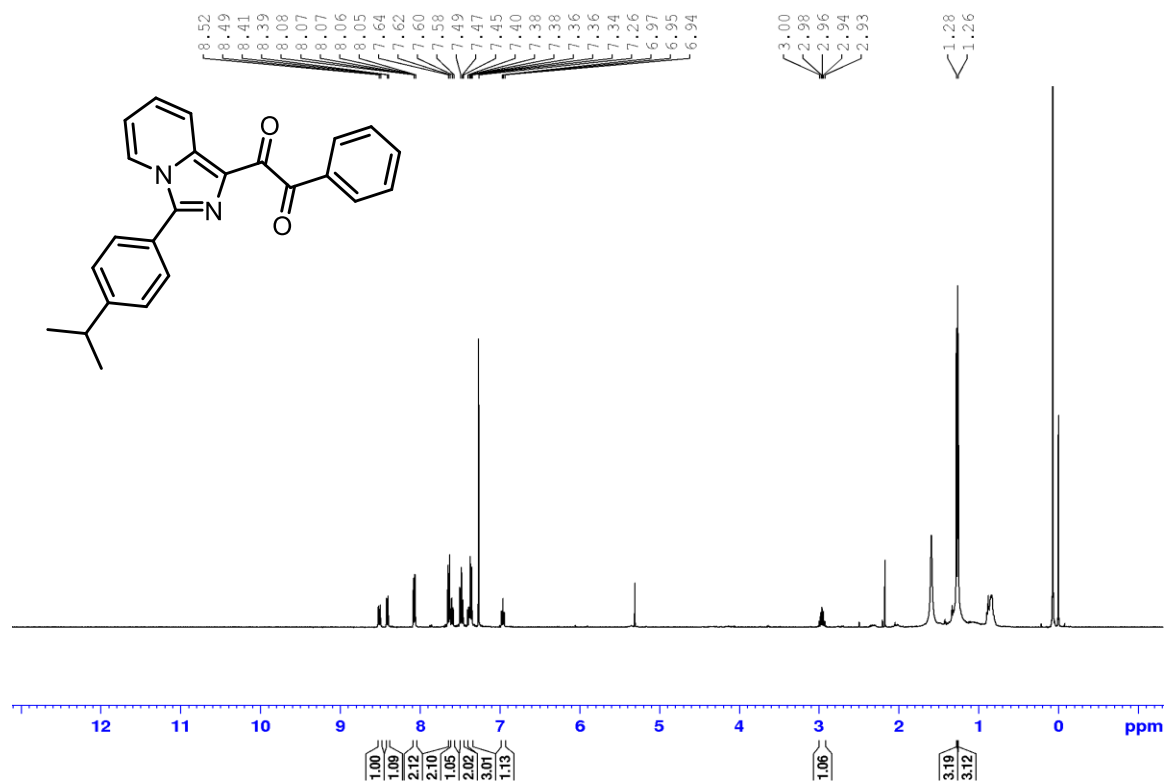
300424_10 5 (0.121)



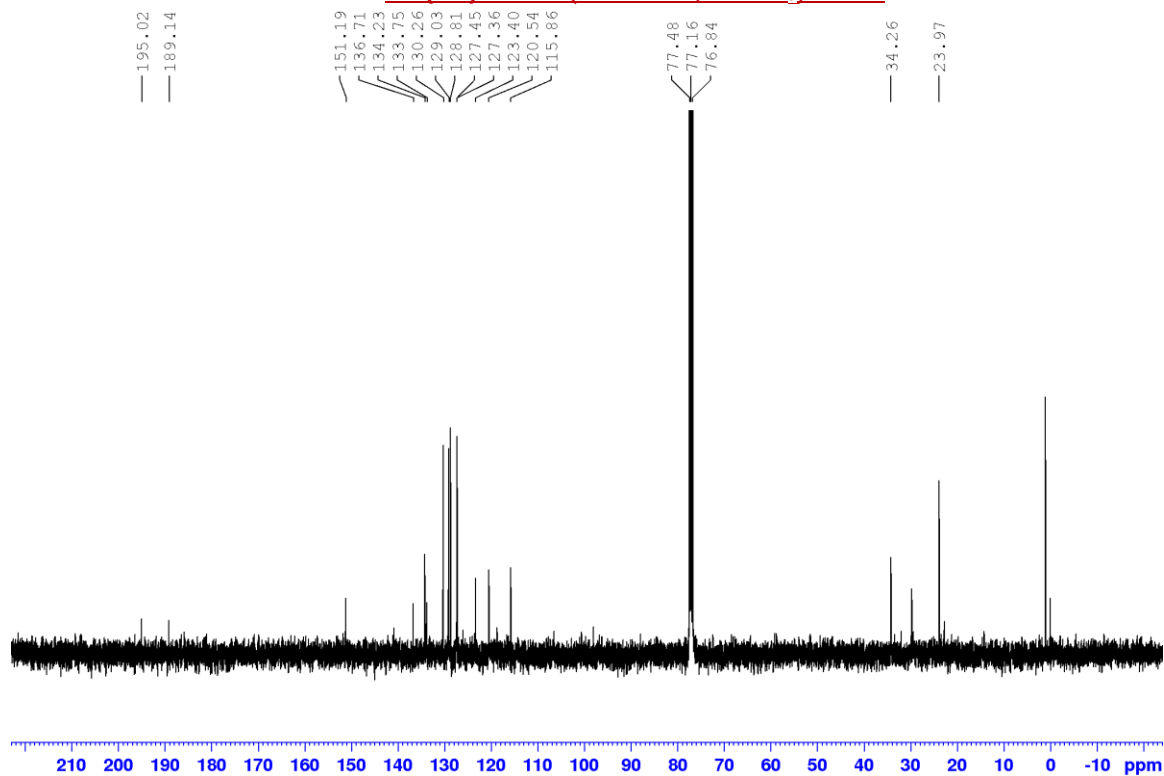
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|---------------|
| 371.1016 | 371.1032 | -1.6 | -4.3 | 16.5 | 1090.3 | n/a | n/a | C22 H15 N2 O4 |

¹H NMR (400 MHz, CDCl₃) of 5c



¹³C[¹H] NMR (101 MHz, CDCl₃) of 5c



HRMS of 5c

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-24 H: 0-100 N: 0-2 O: 0-2

SM-395

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

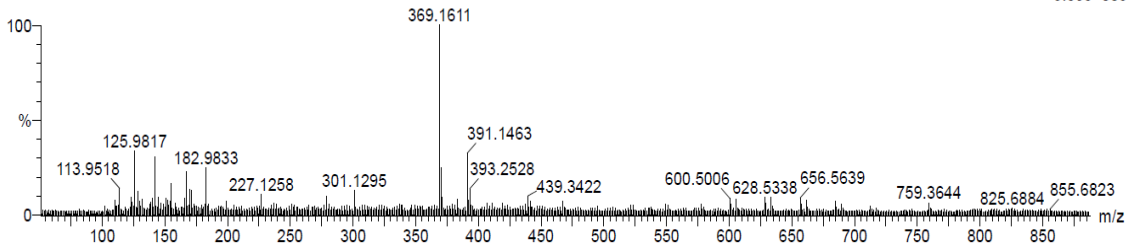
30-Apr-2024

11:42:36

1: TOF MS ES+

5.83e+005

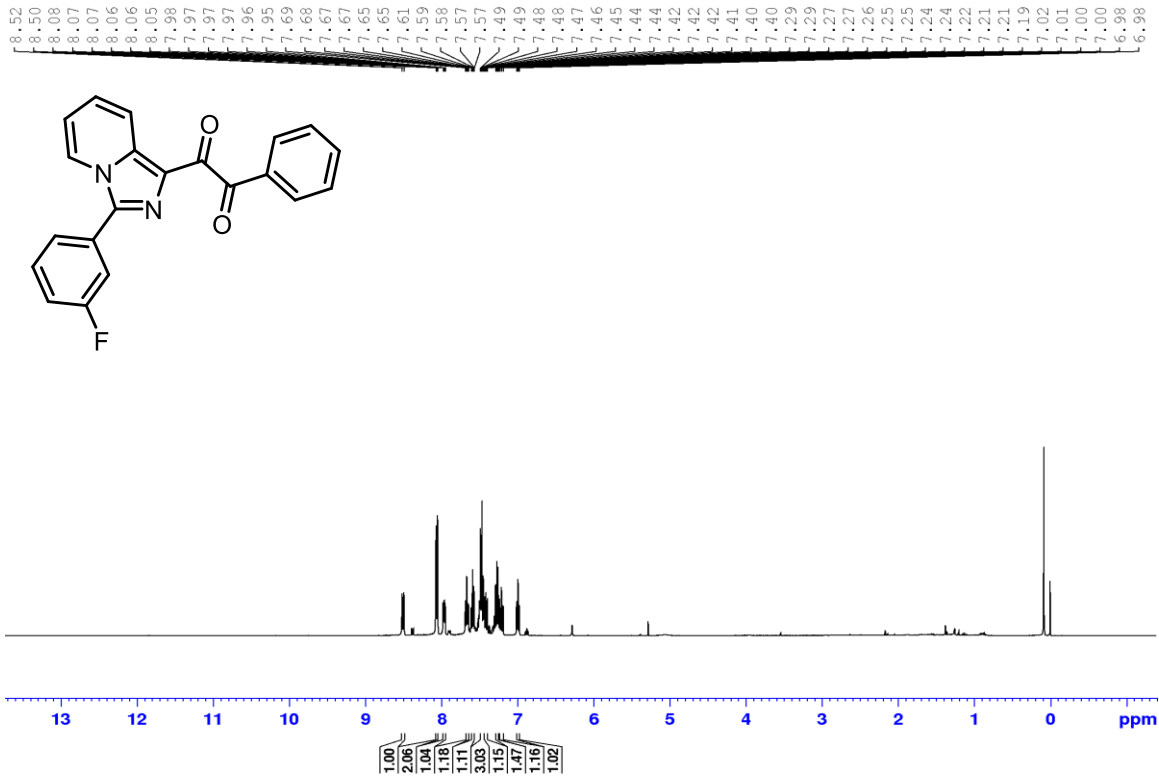
300424_03 4 (0.104) Cm (4)



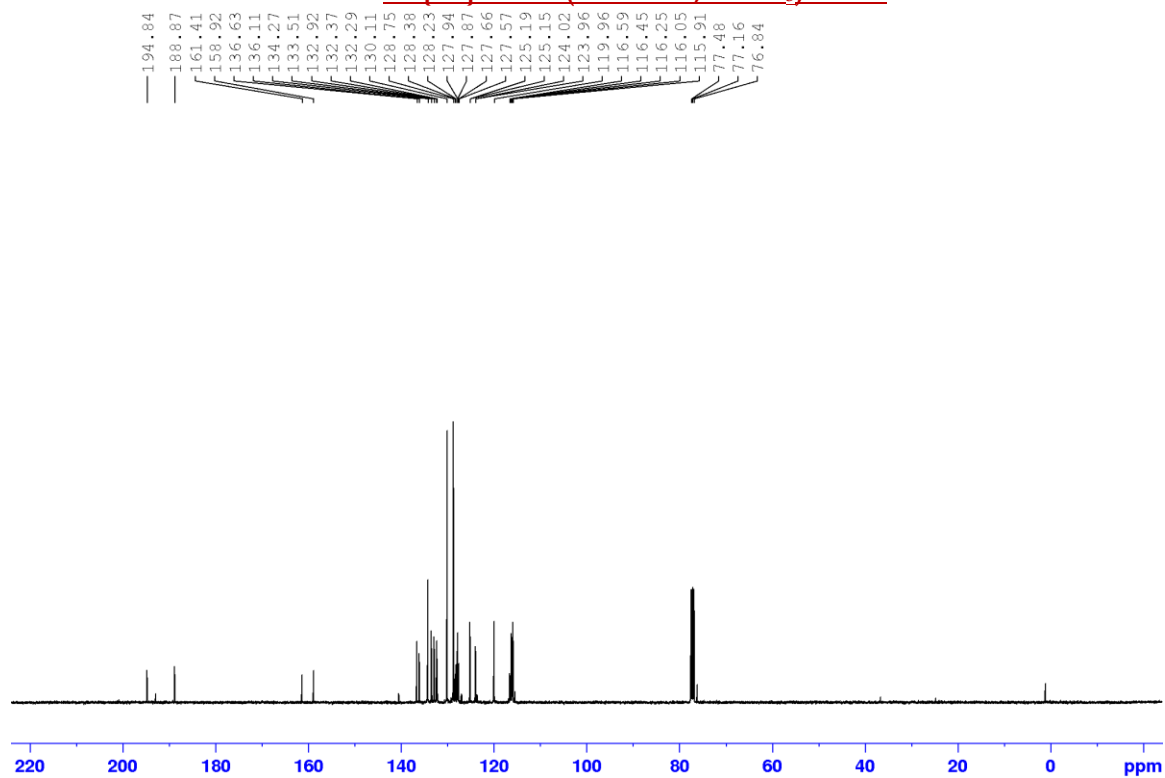
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|-------|------|----------|---------------|
| 369.1611 | 369.1603 | 0.8 | 2.2 | 15.5 | 57.3 | n/a | n/a | C24 H21 N2 O2 |

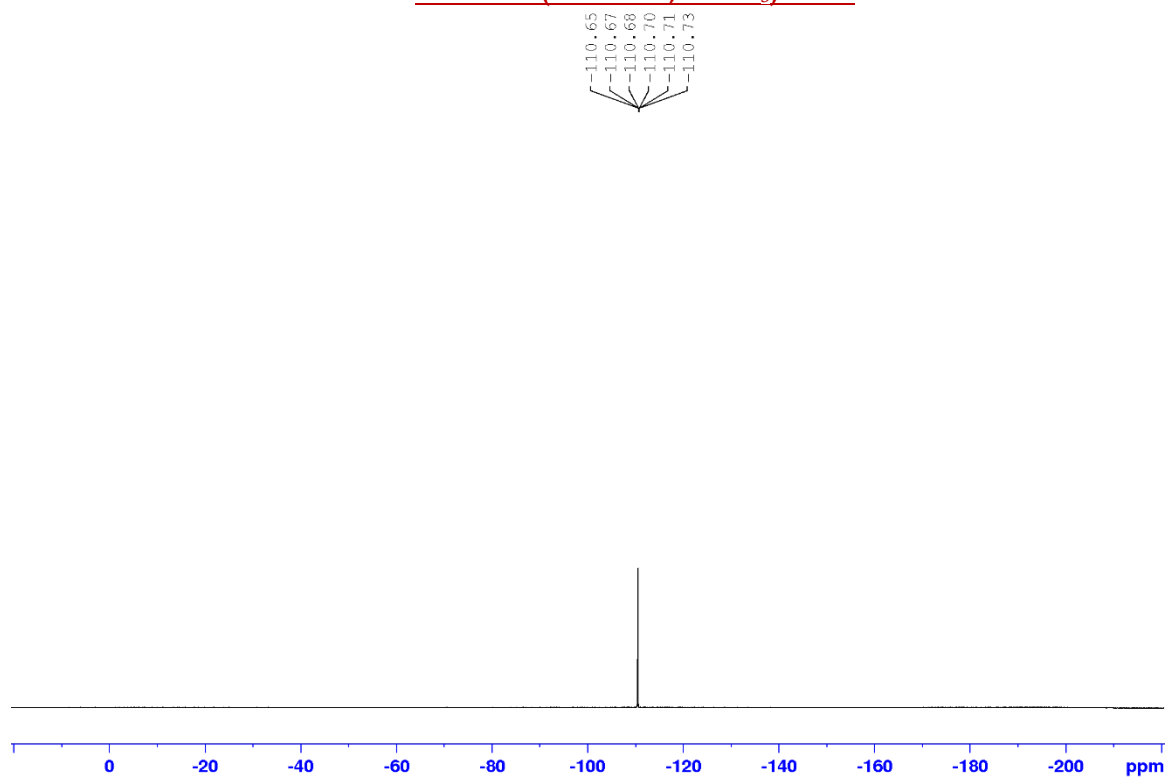
¹H NMR (400 MHz, CDCl₃) of 5d



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 5d



^{19}F NMR (377 MHz, CDCl_3) of 5d



HRMS of 5d

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

23 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-21 H: 0-100 N: 0-2 O: 0-2 F: 0-1

SM-386

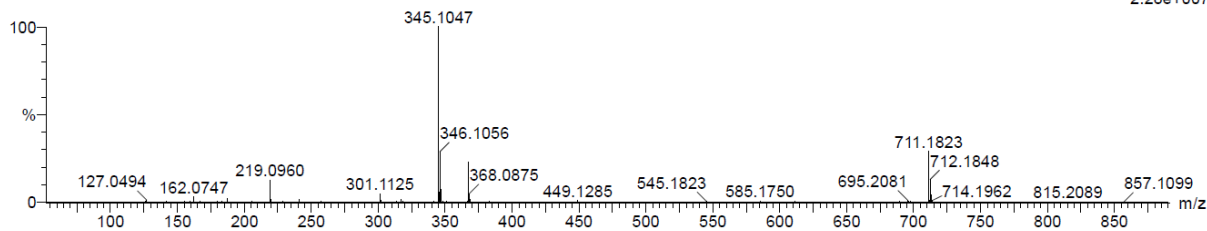
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

30-Apr-2024

11:52:52

1: TOF MS ES+
2.28e+007

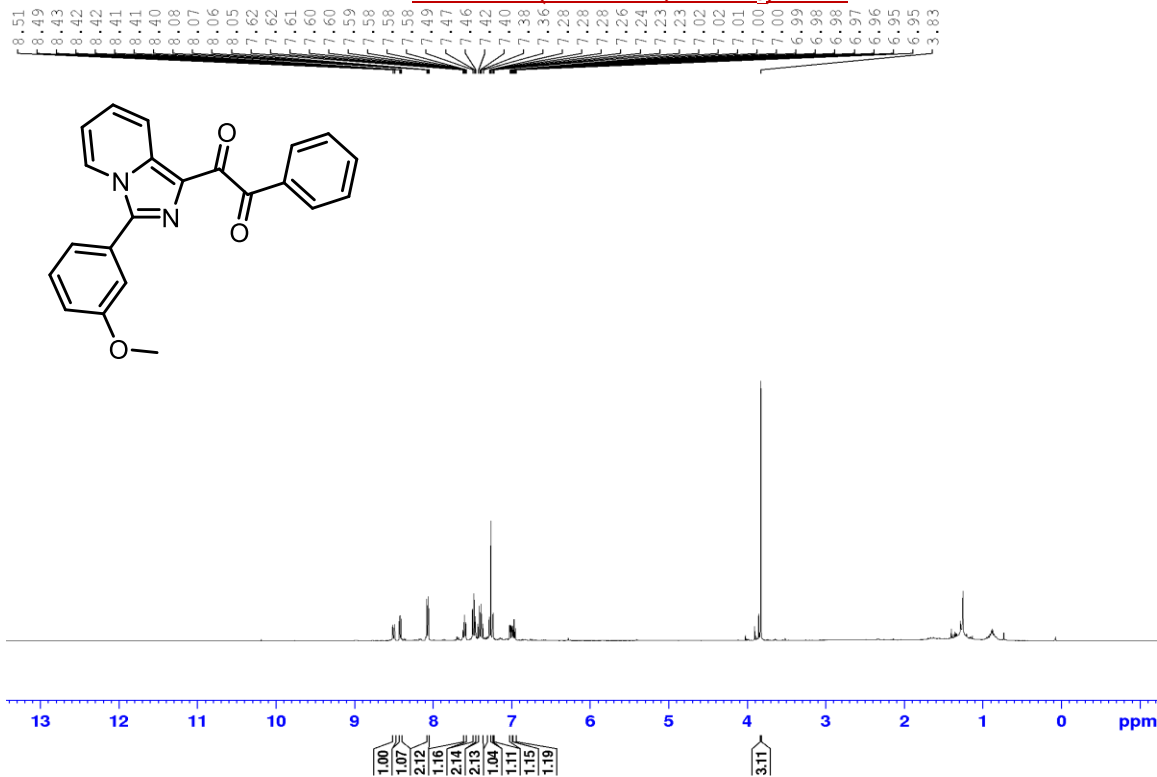
300424_07 5 (0.121)

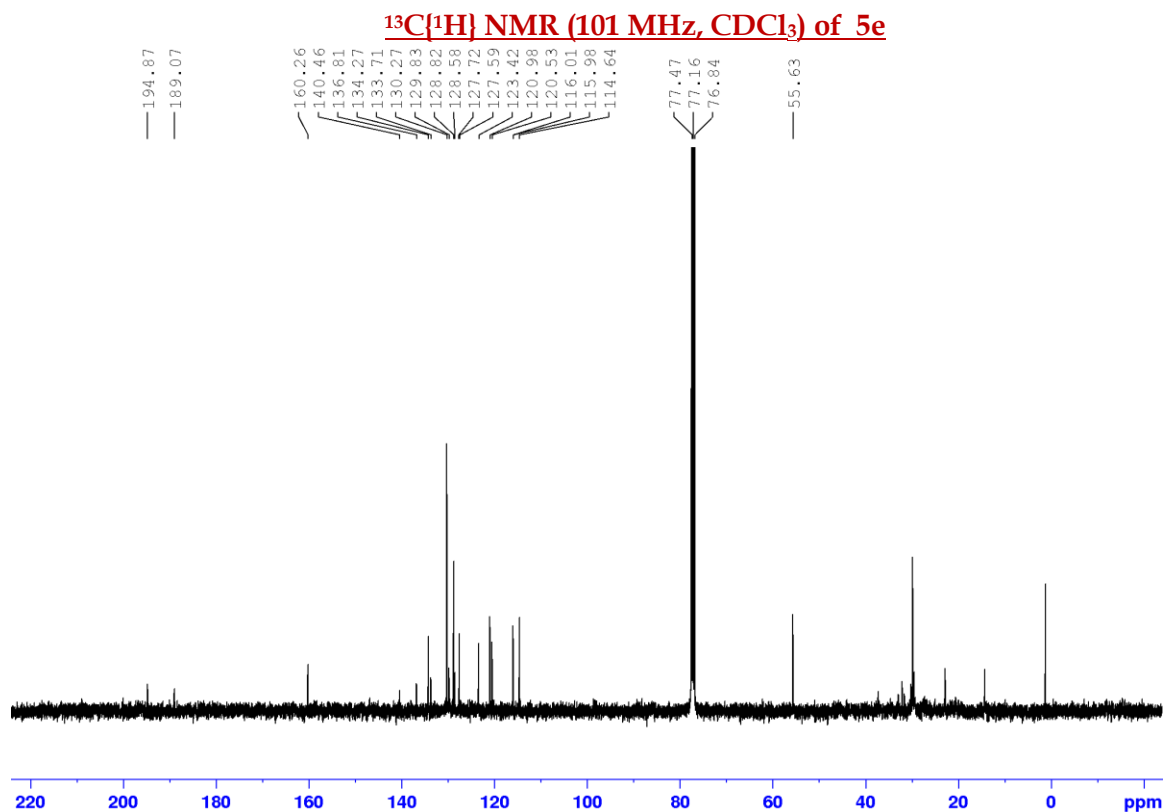


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|-----------------|
| 345.1047 | 345.1039 | 0.8 | 2.3 | 15.5 | 1171.1 | n/a | n/a | C21 H14 N2 O2 F |

¹H NMR (400 MHz, CDCl₃) of 5e





HRMS of 5e

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-22 H: 0-100 N: 0-2 O: 0-3

SM-413

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

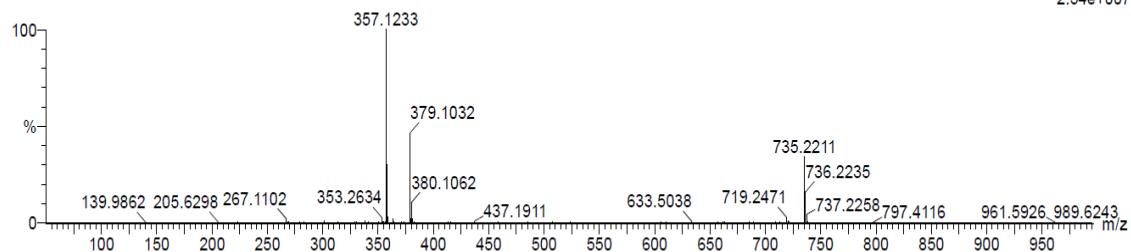
02-May-2024

13:15:46

1: TOF MS ES+

2.54e+007

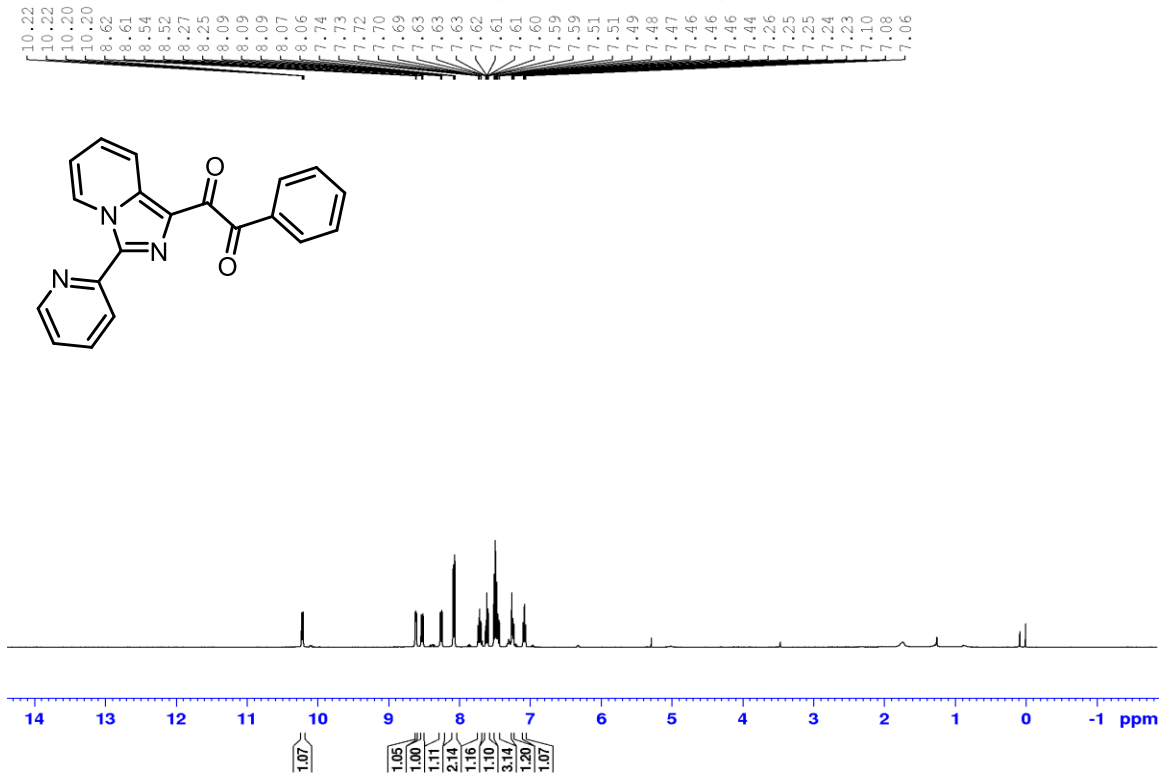
020524_27 6 (0.138)



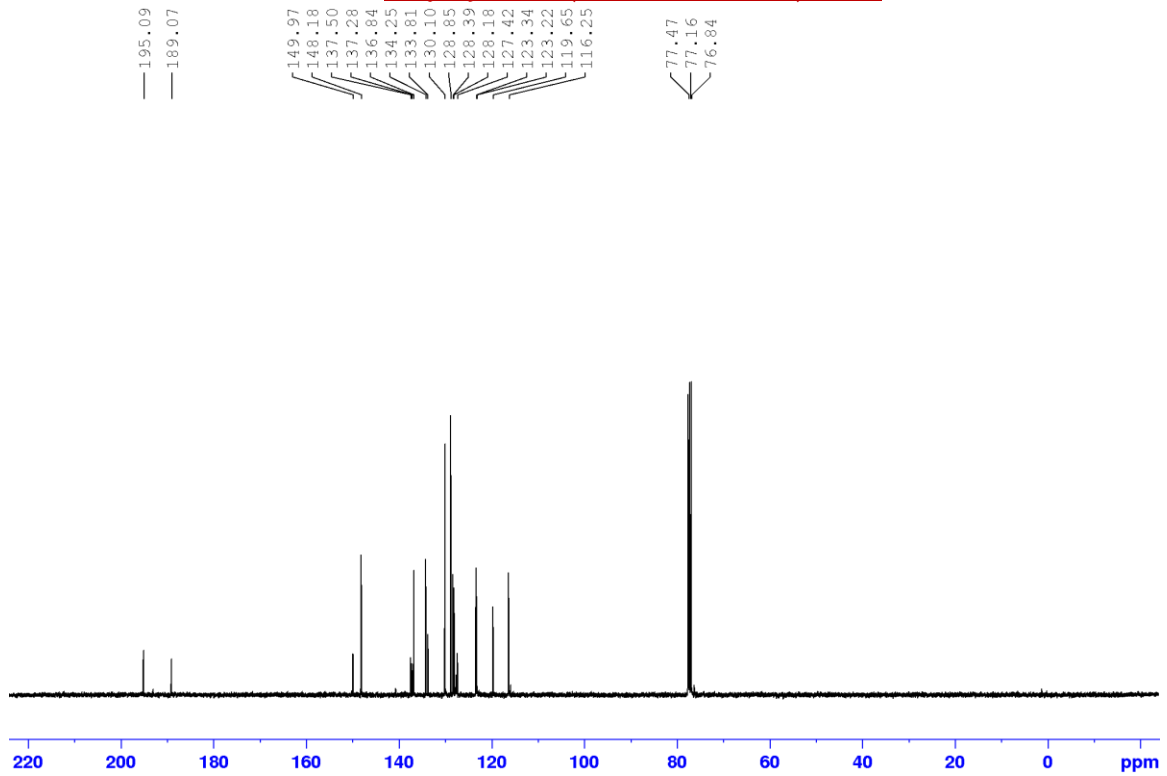
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|---------------|
| 357.1233 | 357.1239 | -0.6 | -1.7 | 15.5 | 1087.1 | n/a | n/a | C22 H17 N2 O3 |

^1H NMR (400 MHz, CDCl_3) of 5f



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of 5f



HRMS of 5f

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-20 H: 0-100 N: 0-3 O: 0-2

SM-387

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

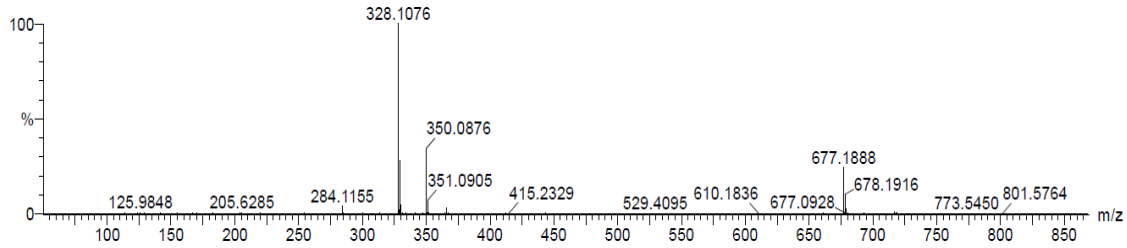
30-Apr-2024

11:50:17

1: TOF MS ES+

2.32e+007

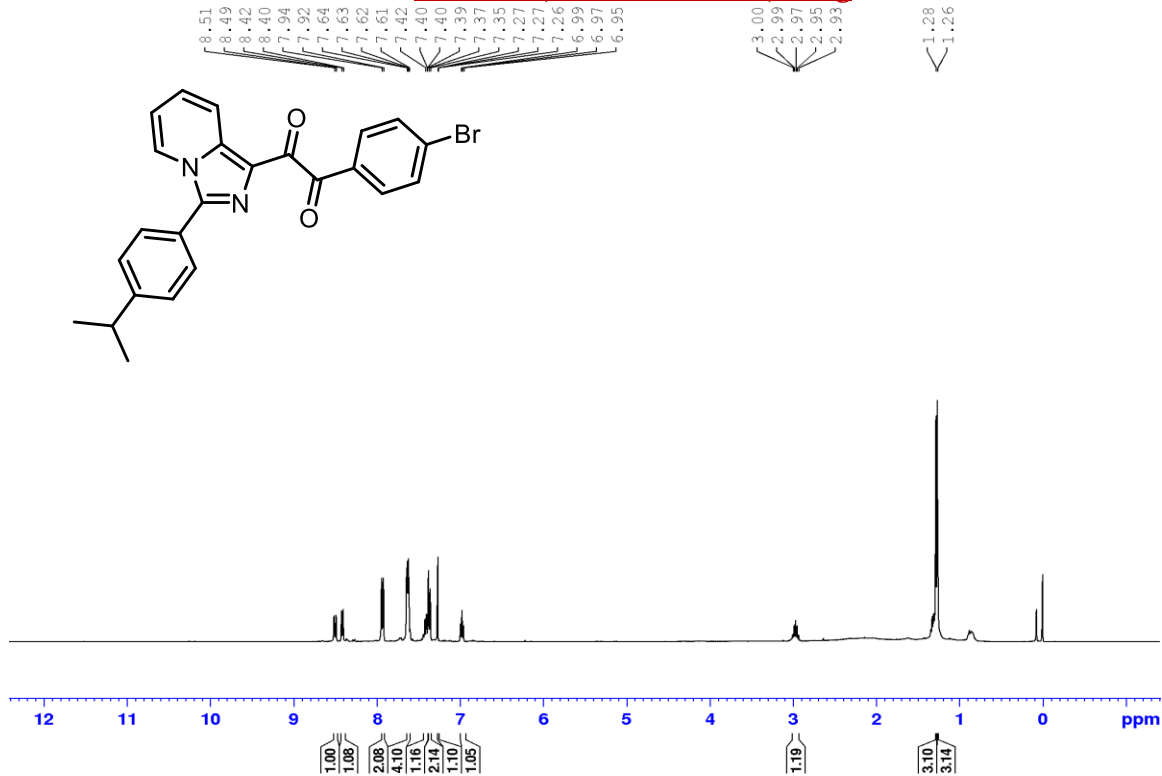
300424_06 7 (0.155)



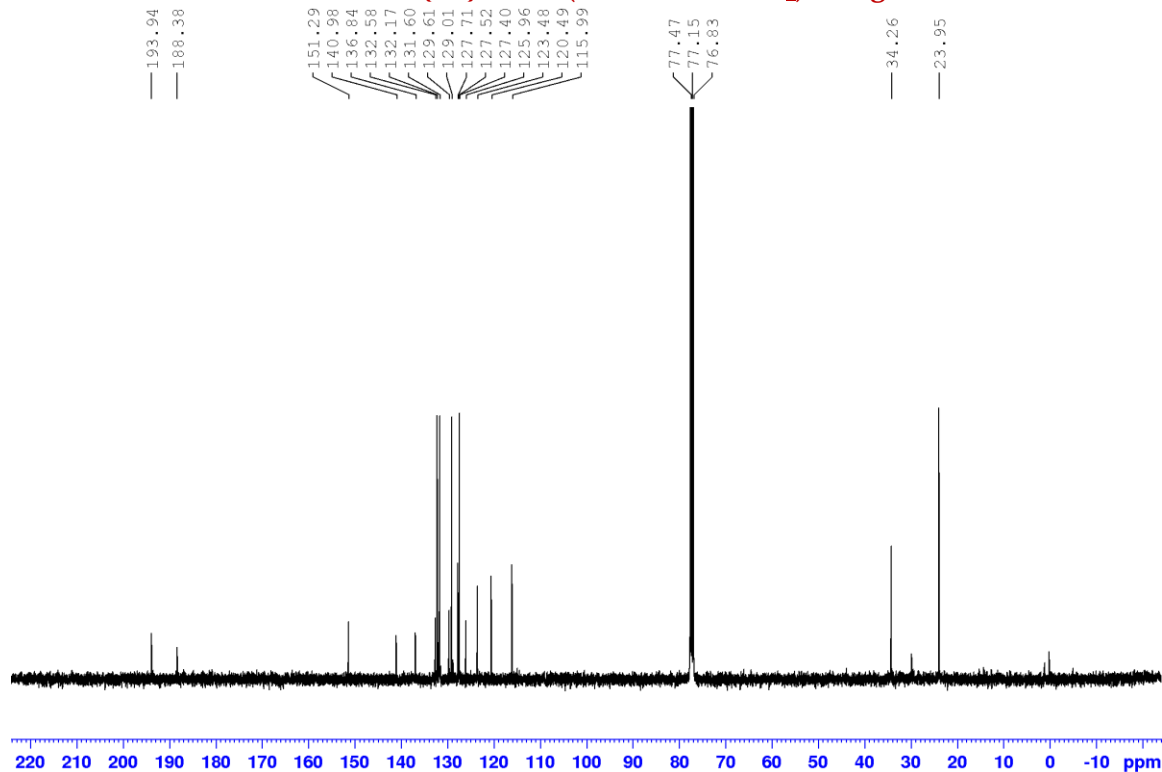
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|---------------|
| 328.1076 | 328.1086 | -1.0 | -3.0 | 15.5 | 1253.3 | n/a | n/a | C20 H14 N3 O2 |

¹H NMR (400 MHz, CDCl₃) of 5g



¹³C{¹H} NMR (101 MHz, CDCl₃) of 5g



HRMS of 5g

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

22 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-24 H: 0-100 N: 0-2 O: 0-2 Br: 0-1

SM-439

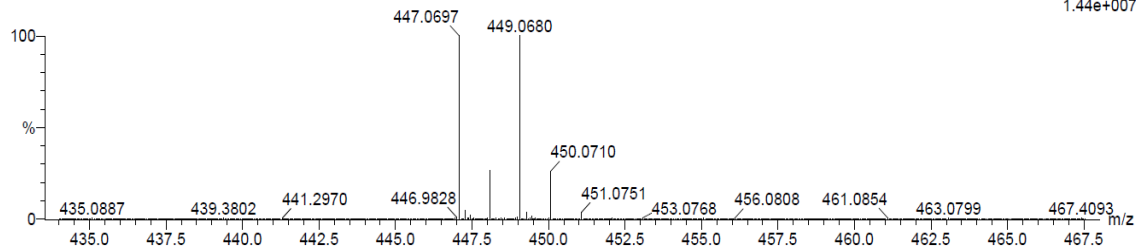
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

30-Apr-2024

11:55:25

300424_08 5 (0.121)

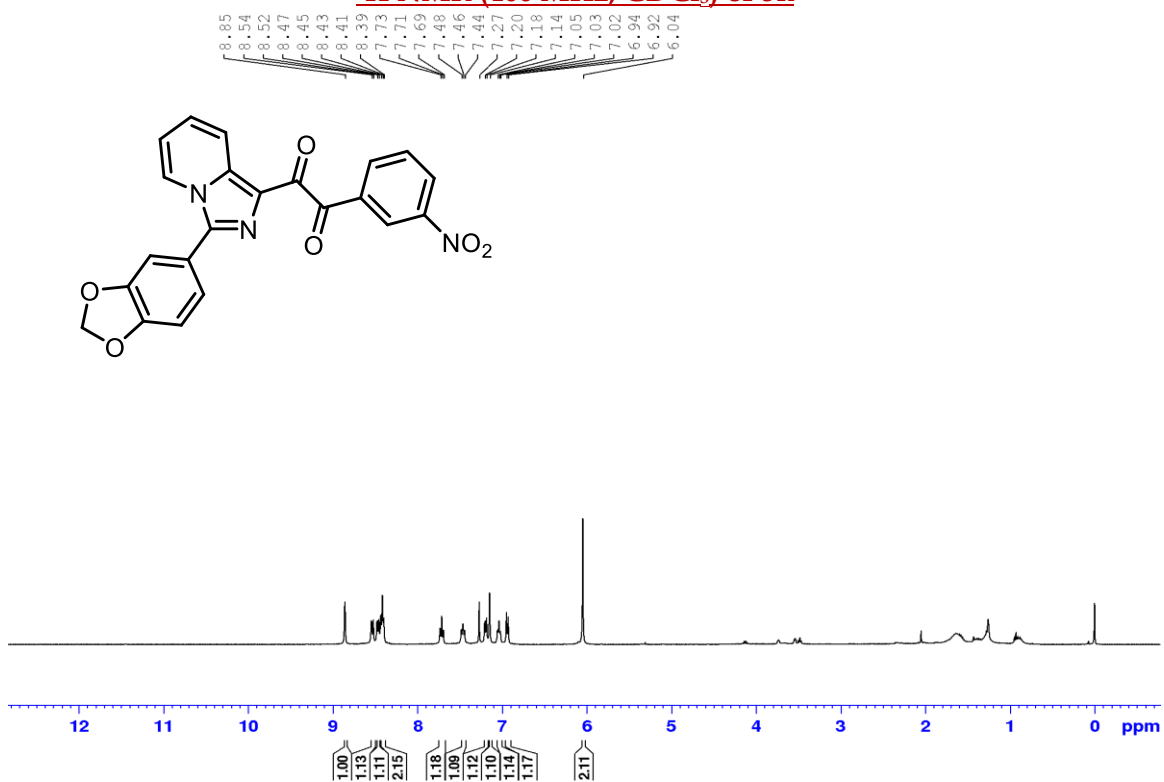
1: TOF MS ES+
1.44e+007



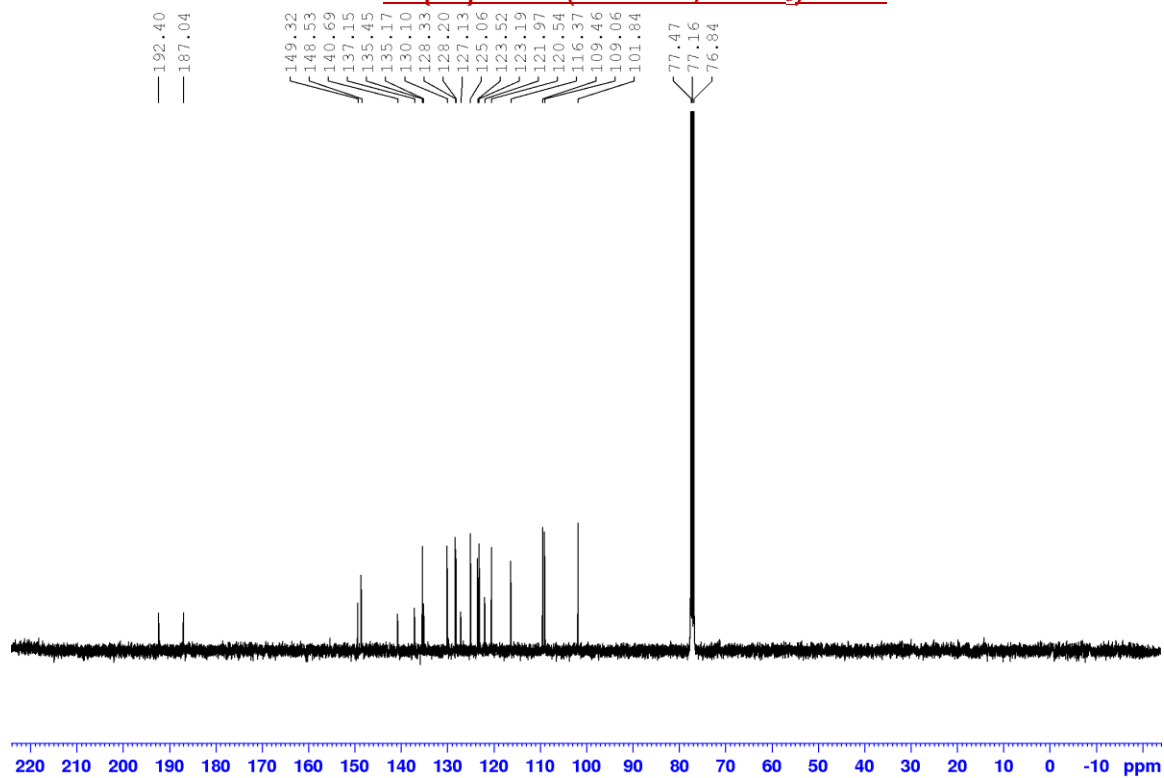
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|-------|------|----------|--|
| 447.0697 | 447.0708 | -1.1 | -2.5 | 15.5 | 997.6 | n/a | n/a | C ₂₄ H ₂₀ N ₂ O ₂ Br |

¹H NMR (400 MHz, CDCl₃) of 5h



¹³C[¹H] NMR (101 MHz, CDCl₃) of 5h



HRMS of 5h

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

37 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-22 H: 0-150 N: 0-3 O: 0-6

SM-515

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

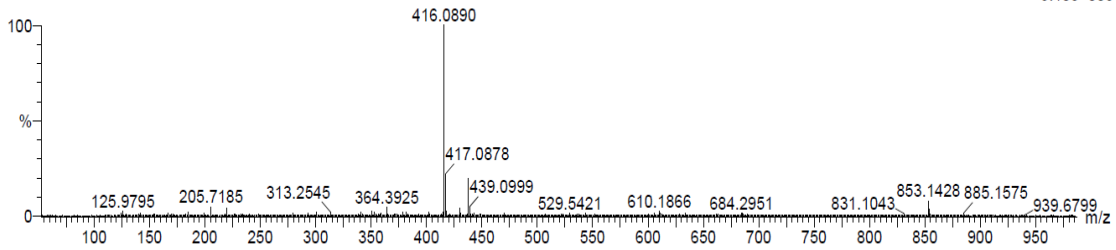
02-May-2024

13:09:40

1: TOF MS ES+

5.10e+006

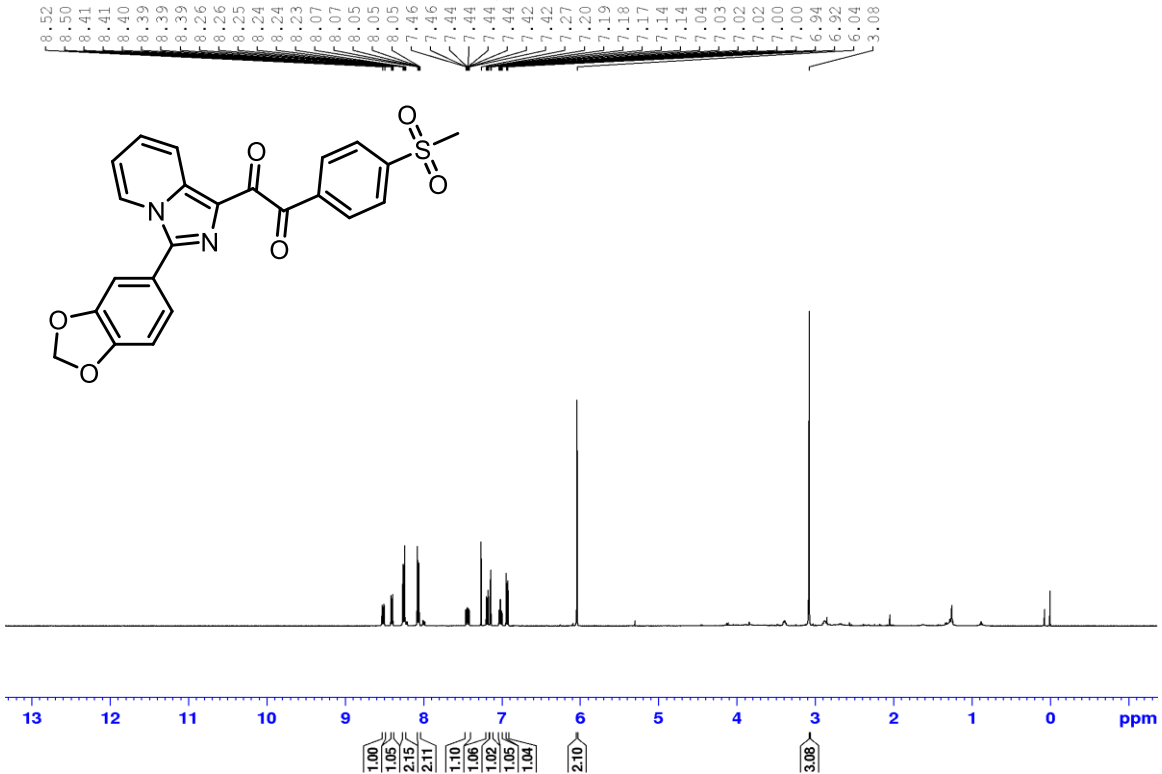
020524_25 8 (0.172) Cm (8)

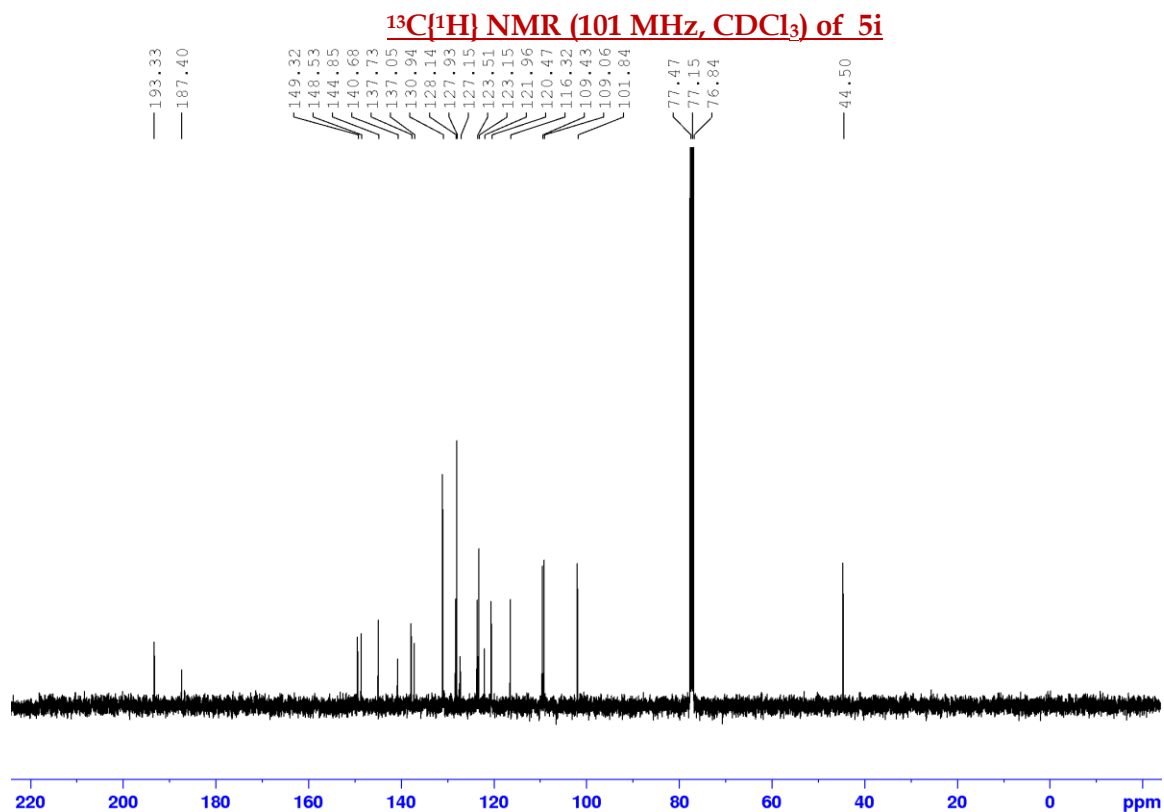


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|-----|-----|------|-------|------|---------|---------------|
| 416.0890 | 416.0883 | 0.7 | 1.7 | 17.5 | 37.8 | n/a | n/a | C22 H14 N3 O6 |

¹H NMR (400 MHz, CDCl₃) of 5i





HRMS of 5i

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

48 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-23 H: 0-100 N: 0-2 O: 0-6 S: 0-1

SM-527

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

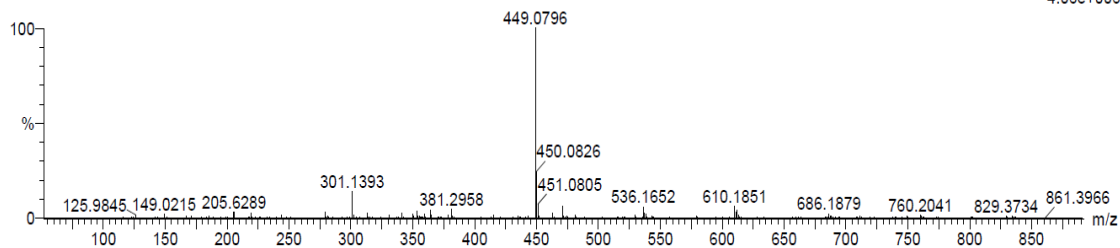
07-May-2024

14:47:00

1: TOF MS ES+

4.06e+006

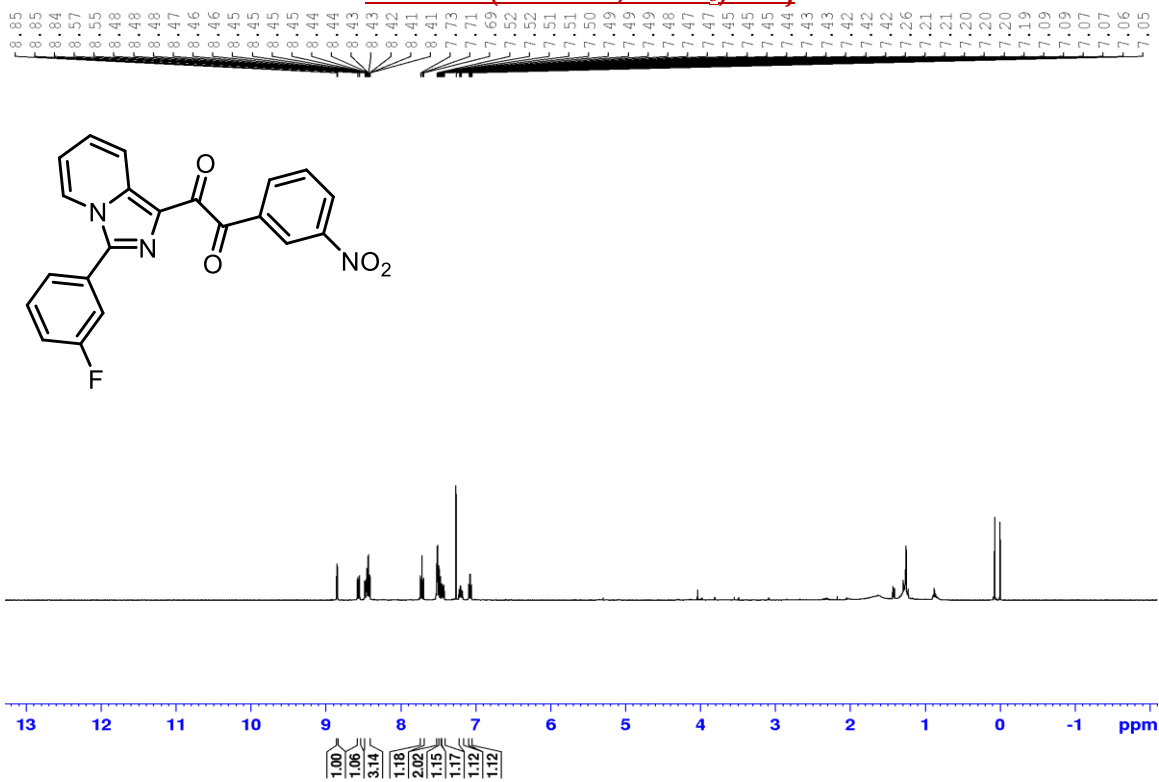
070524_42 5 (0.121)



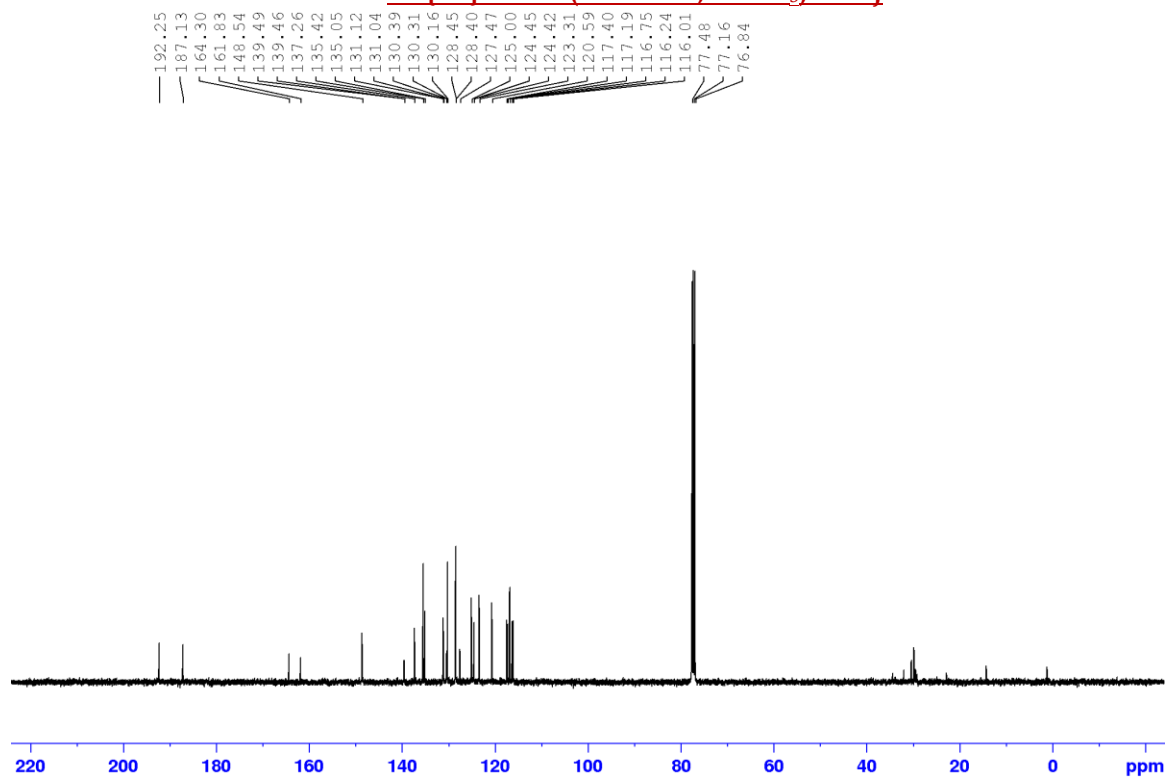
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|-------|------|---------|-----------------|
| 449.0796 | 449.0807 | -1.1 | -2.4 | 16.5 | 894.5 | n/a | n/a | C23 H17 N2 O6 S |

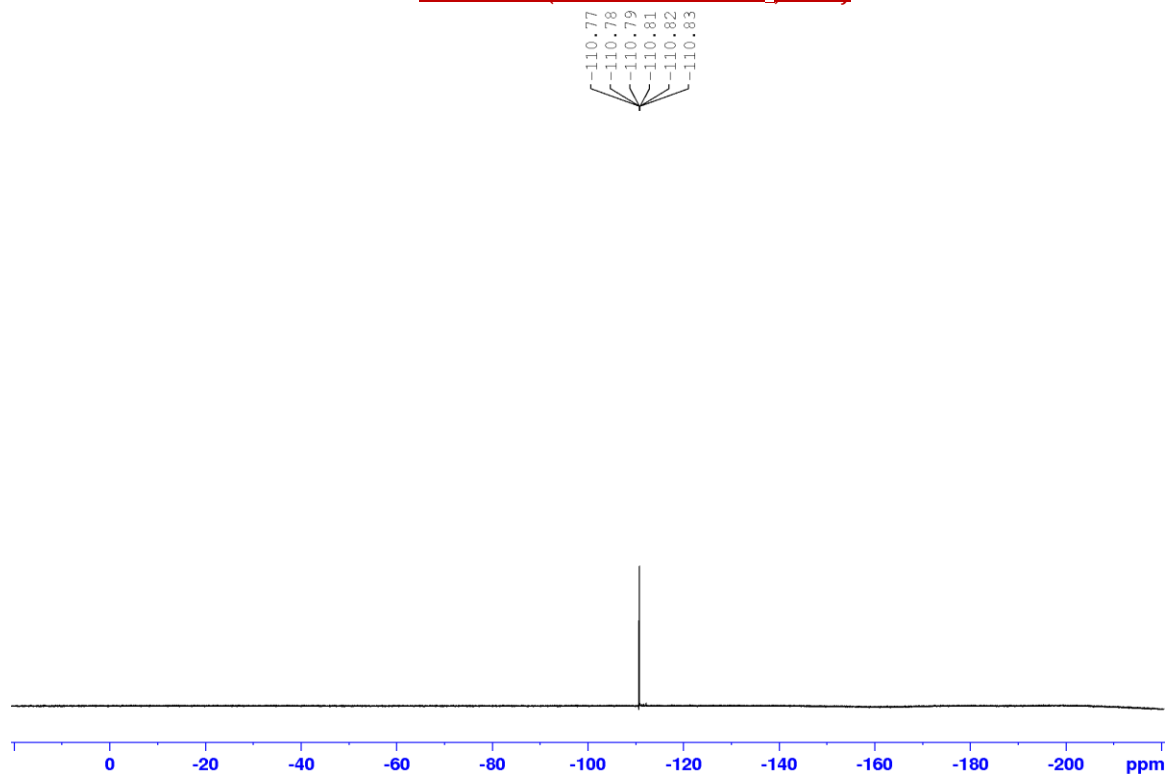
¹H NMR (400 MHz, CDCl₃) of 5j



¹³C[¹H] NMR (101 MHz, CDCl₃) of 5j



¹⁹F NMR (377 MHz, CDCl₃) of 5j



HRMS of 5j

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

47 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-21 H: 0-100 N: 0-3 O: 0-4 F: 0-1

SM-516

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

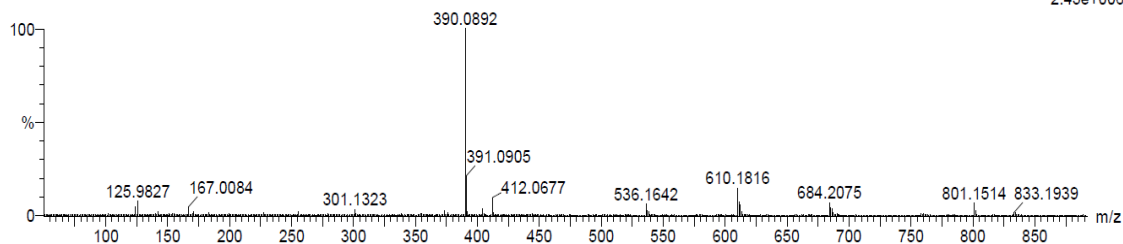
07-May-2024

14:36:27

1: TOF MS ES+

2.45e+006

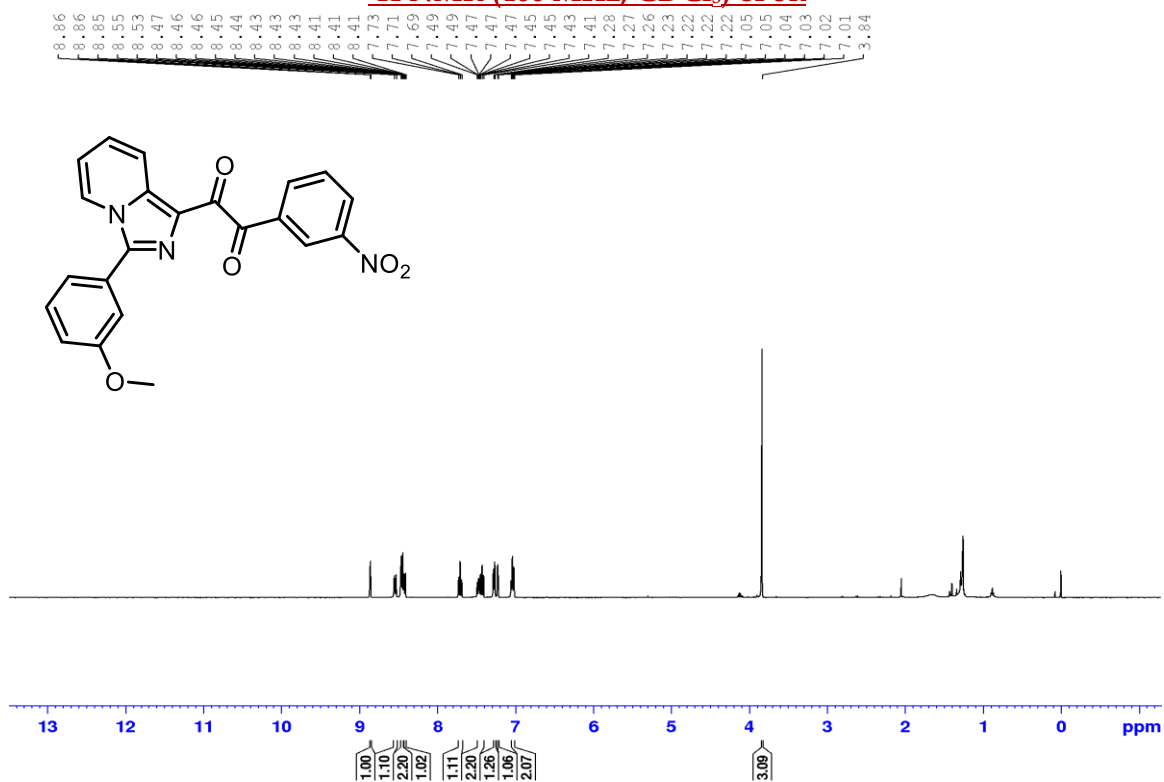
070524_38 8 (0.172) Cm (8)



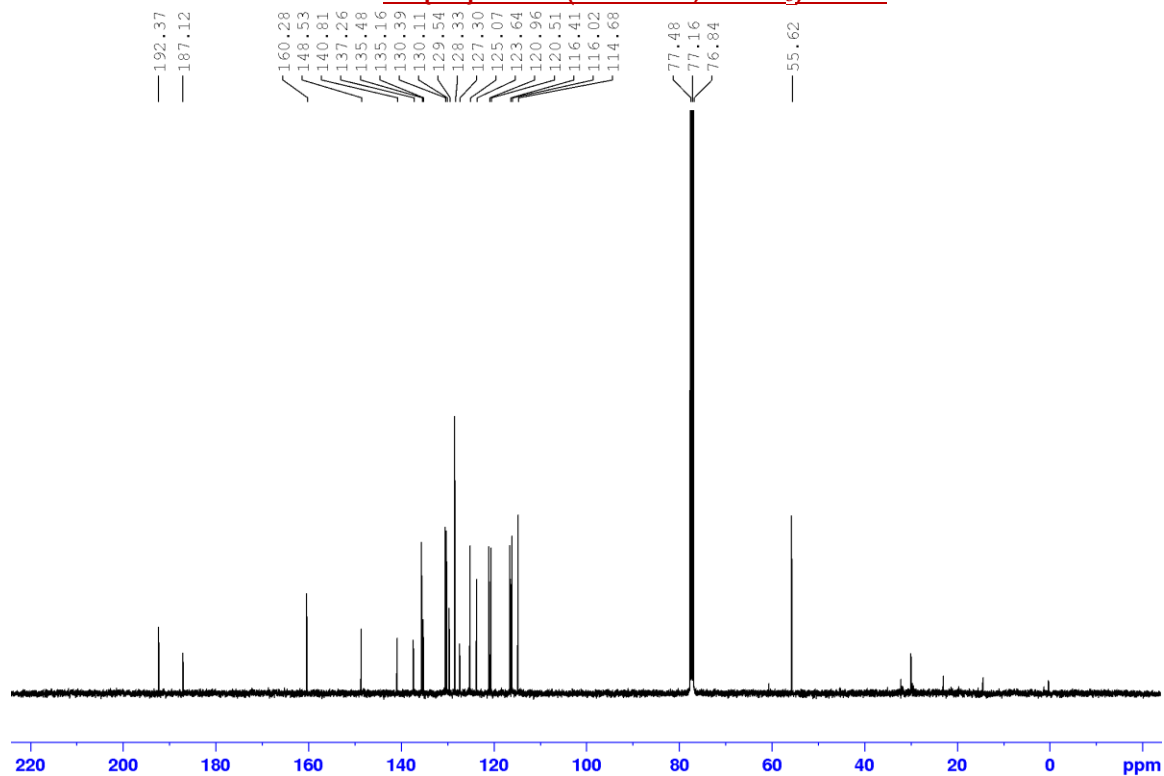
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|-------|------|----------|-----------------|
| 390.0892 | 390.0890 | 0.2 | 0.5 | 16.5 | 38.4 | n/a | n/a | C21 H13 N3 O4 F |

¹H NMR (400 MHz, CDCl₃) of 5k



¹³C{¹H} NMR (101 MHz, CDCl₃) of 5k



HRMS of 5k

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

30 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-22 H: 0-100 N: 0-3 O: 0-5

SM-514

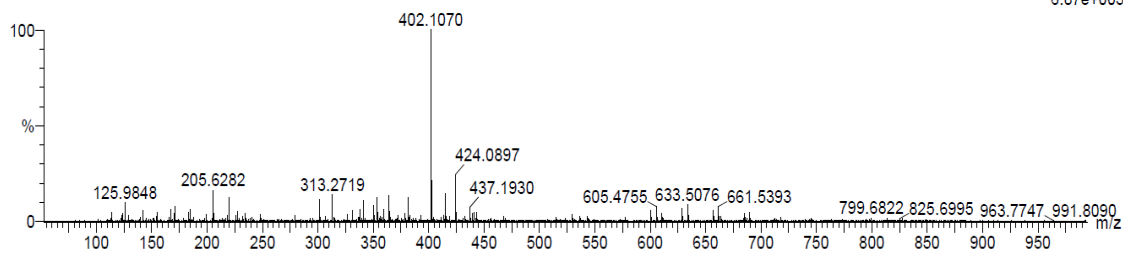
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

02-May-2024

11:50:21

1: TOF MS ES+
6.87e+005

020524_06 5 (0.121)

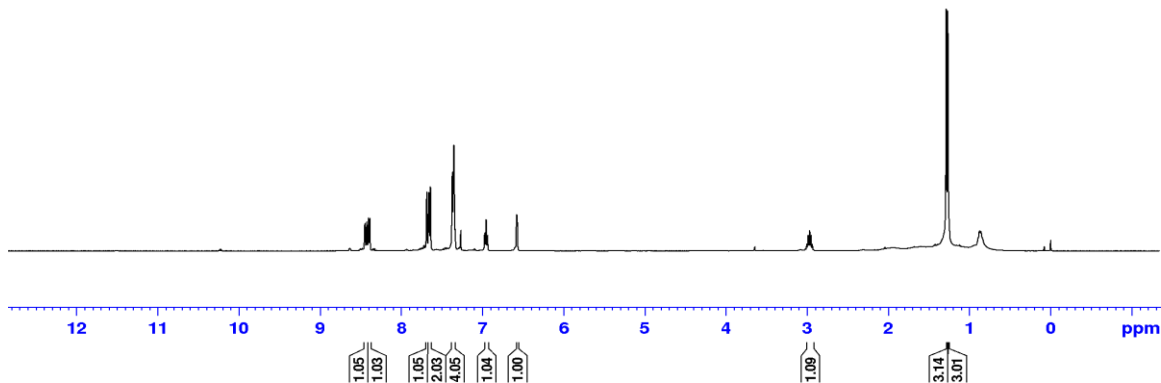
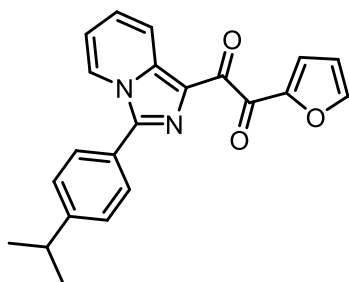


Minimum: -1.5
Maximum: 2.0 50.0 50.0

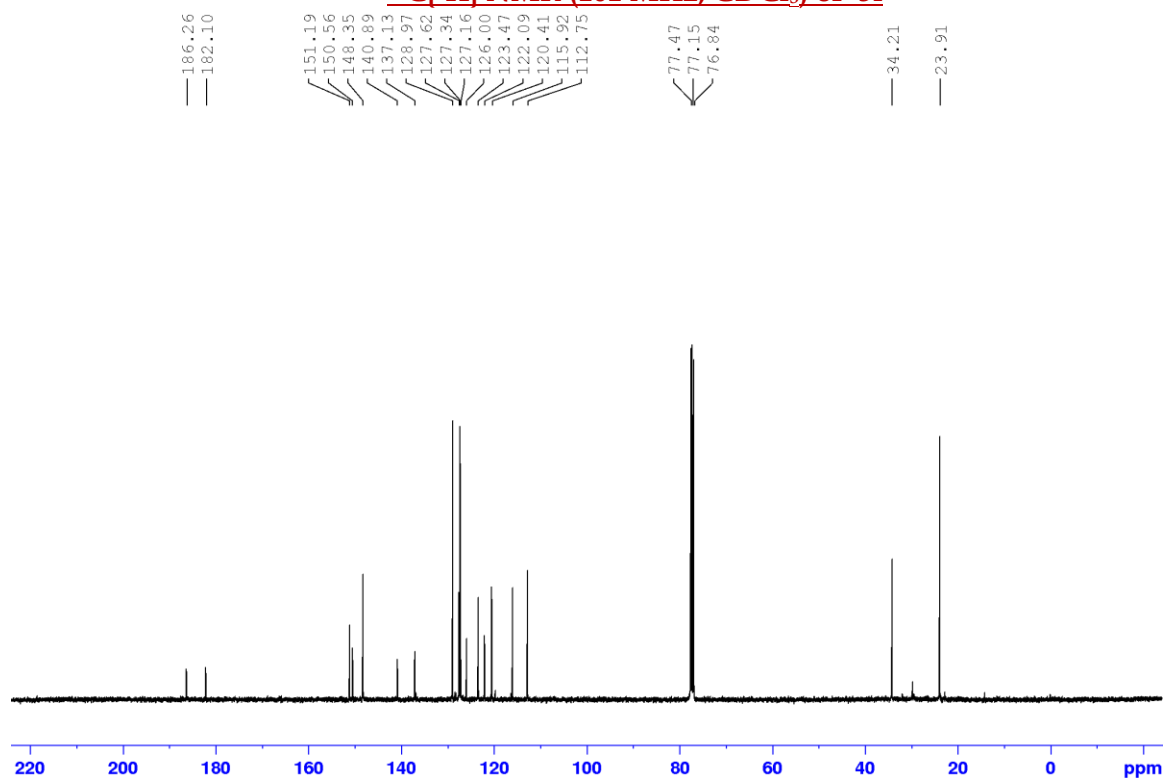
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|---------------|
| 402.1070 | 402.1090 | -2.0 | -5.0 | 16.5 | 1043.6 | n/a | n/a | C22 H16 N3 O5 |

¹H NMR (400 MHz, CDCl₃) of 5l

8.45, 8.43, 8.41, 8.39, 7.69, 7.66, 7.64, 7.37, 7.35, 7.35, 7.35, 7.26, 6.96, 6.95, 6.93, 6.57, 6.57, 6.57, 6.56, 2.99, 2.96, 2.94, 2.93, 1.28, 1.26



¹³C{¹H} NMR (101 MHz, CDCl₃) of 51



HRMS of 51

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-22 H: 0-100 N: 0-2 O: 0-3

SM-440

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

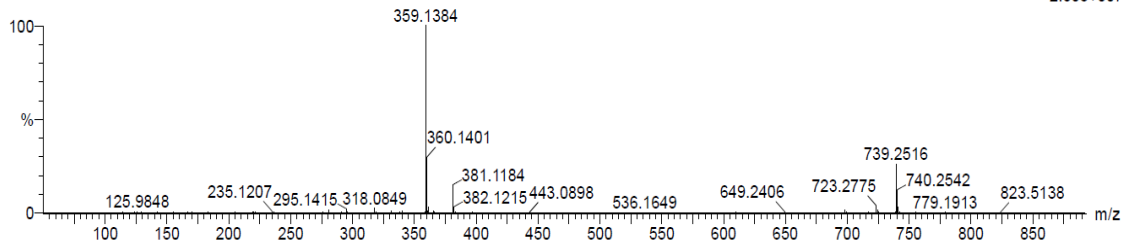
30-Apr-2024

11:40:02

1: TOF MS ES+

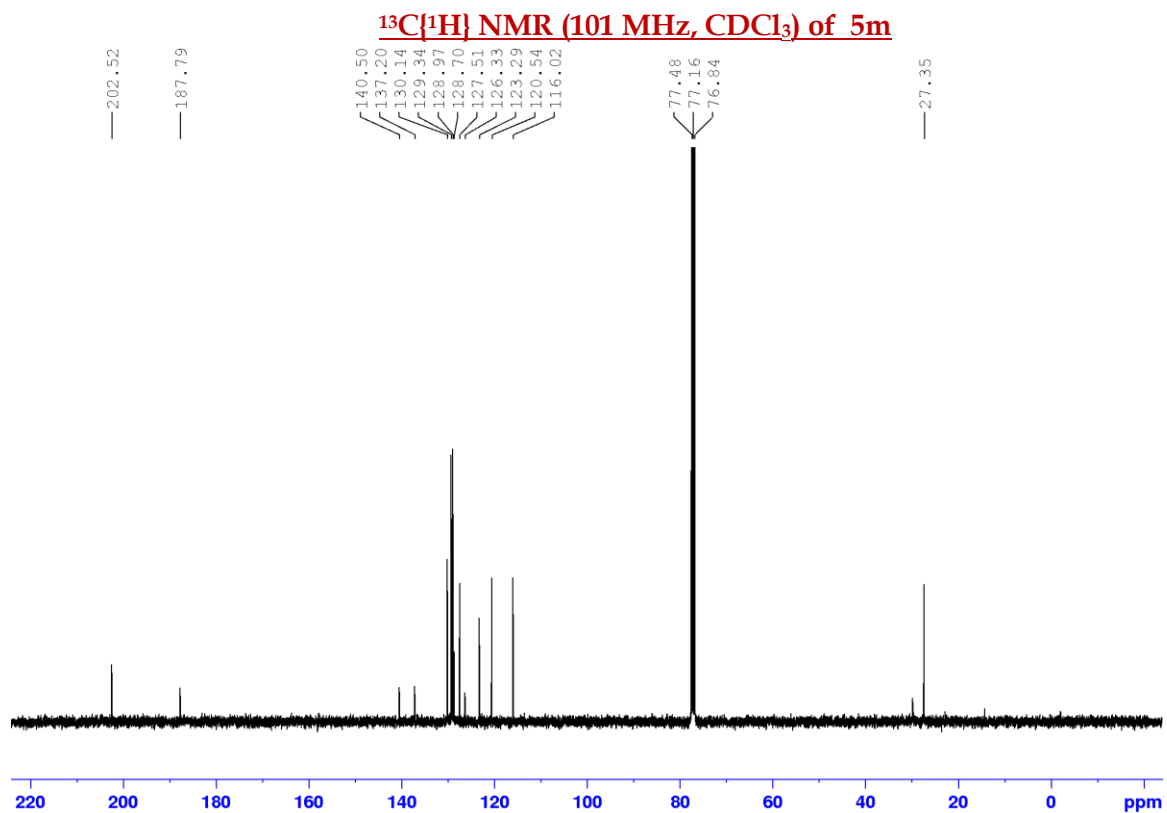
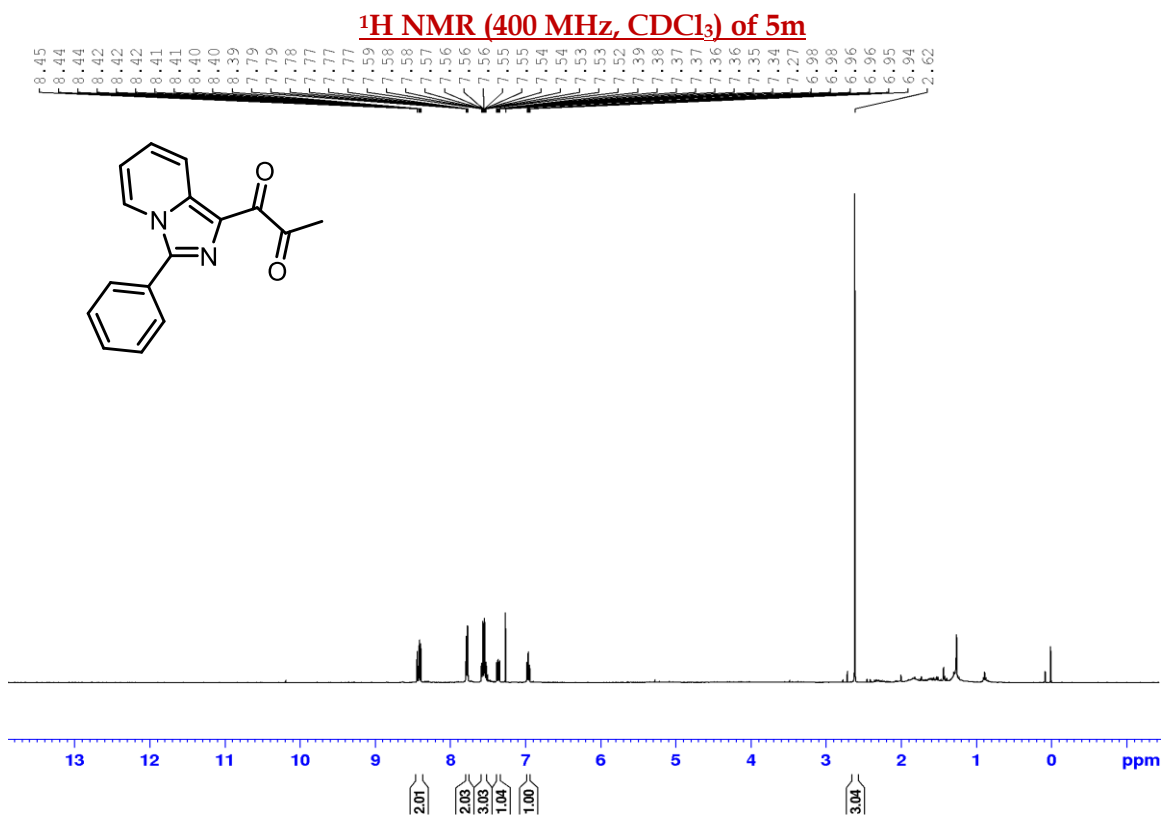
2.30e+007

300424_02.7 (0.155)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|--------|------|----------|---------------|
| 359.1384 | 359.1396 | -1.2 | -3.3 | 14.5 | 1132.6 | n/a | n/a | C22 H19 N2 O3 |



HRMS of 5m

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-16 H: 0-100 N: 0-2 O: 0-2

SM-522

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

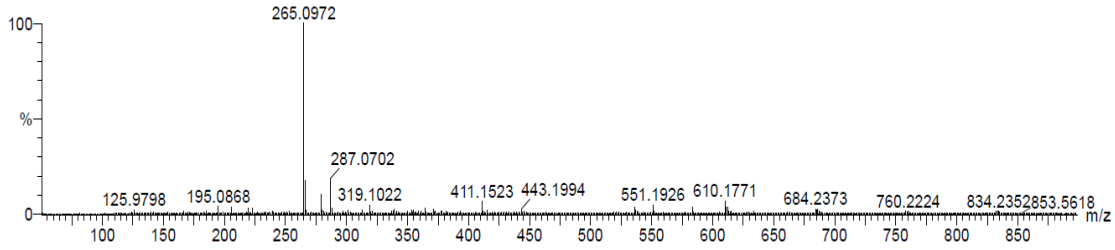
02-May-2024

13:21:09

1: TOF MS ES+

5.30e+006

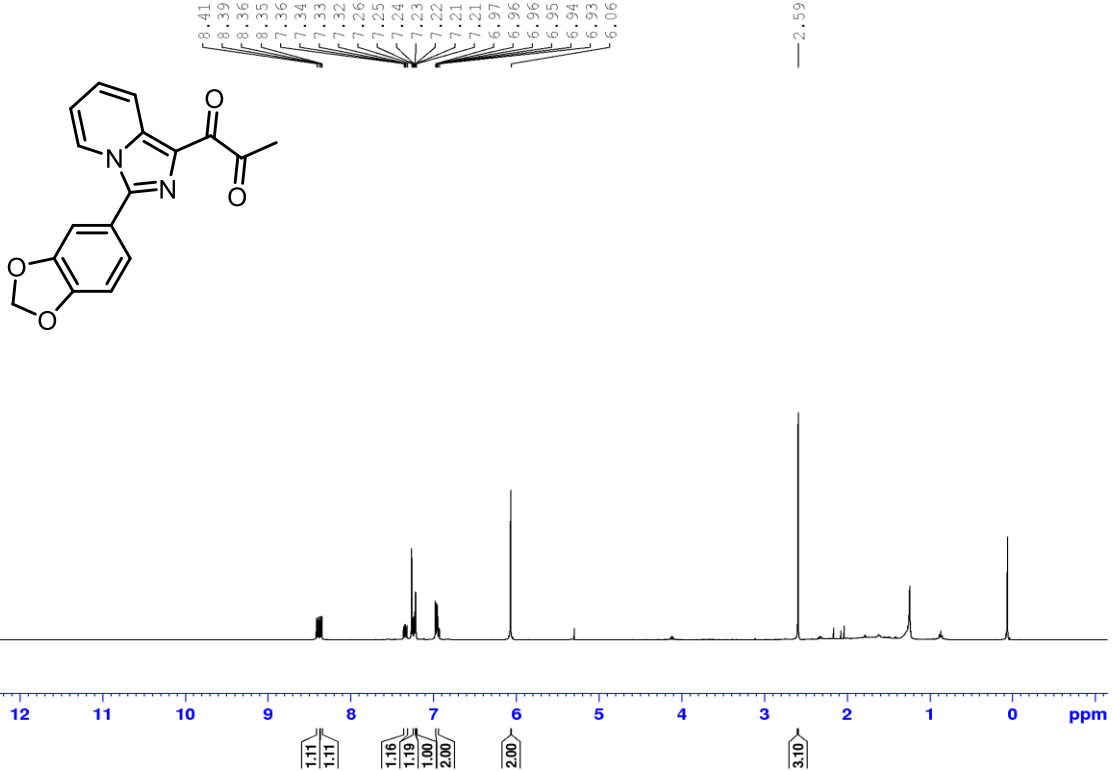
020524_29 8 (0.172) Cm (8)

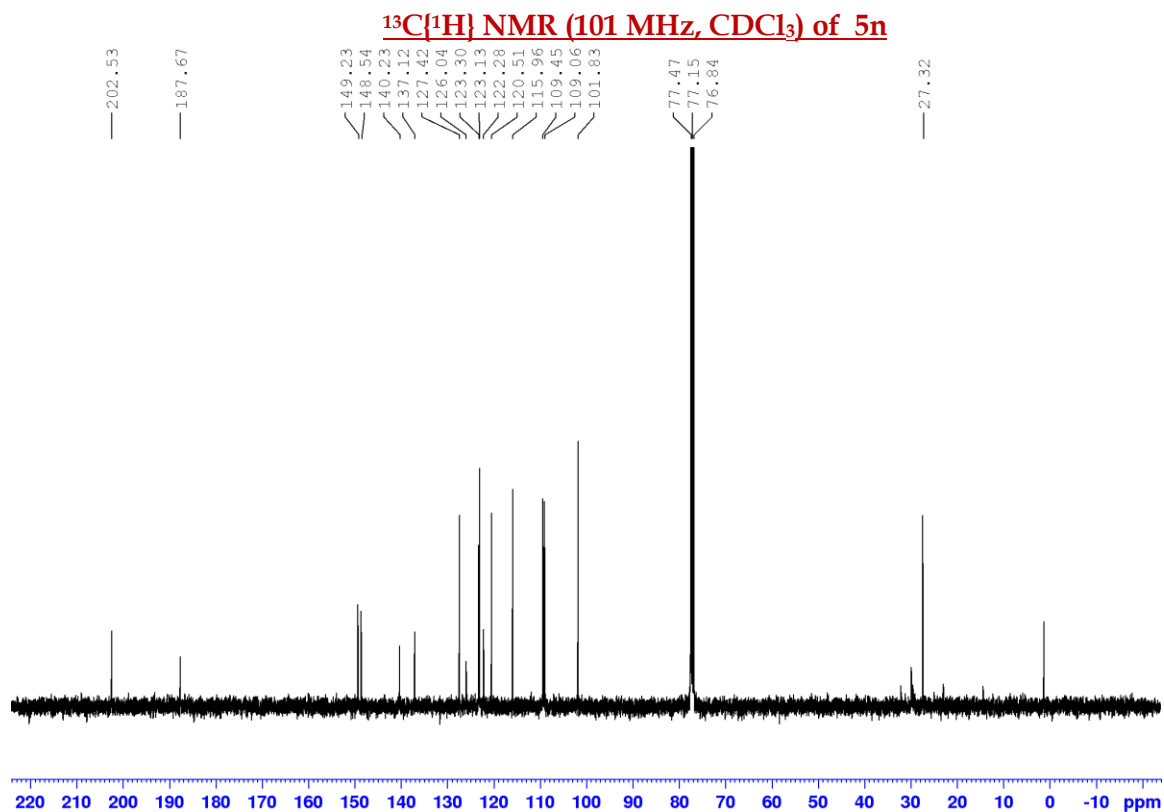


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|-------|------|---------|---------------|
| 265.0972 | 265.0977 | -0.5 | -1.9 | 11.5 | 48.5 | n/a | n/a | C16 H13 N2 O2 |

¹H NMR (400 MHz, CDCl₃) of 5n





HRMS of 5n

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-17 H: 0-100 N: 0-2 O: 0-4

SM-470

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

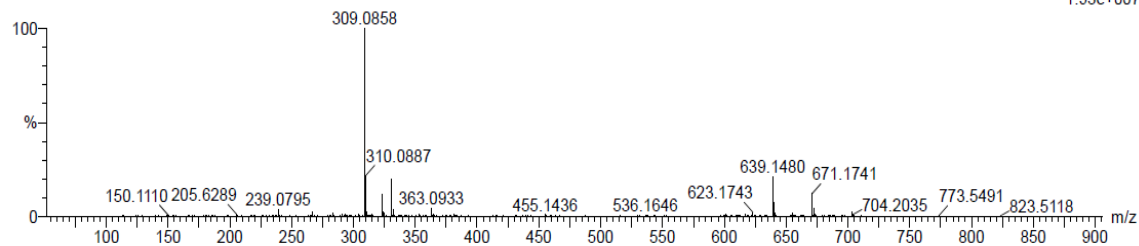
30-Apr-2024

12:03:16

1: TOF MS ES+

1.93e+007

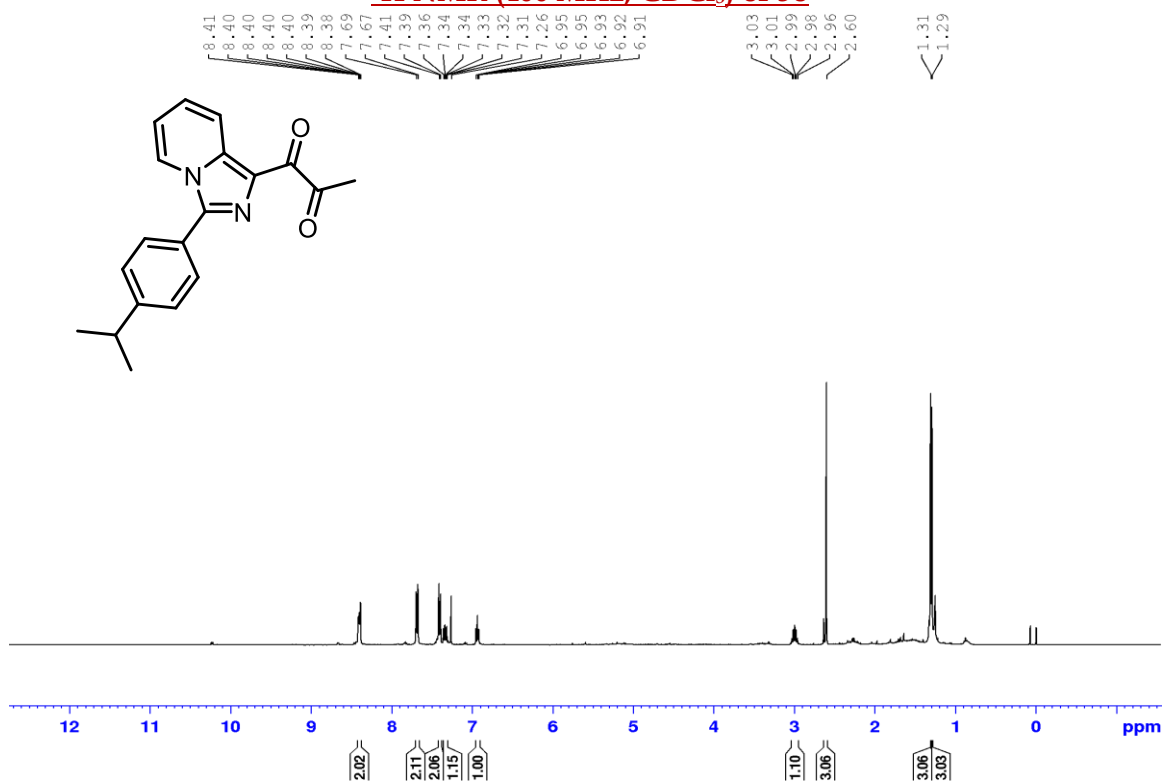
300424_11 6 (0.138)



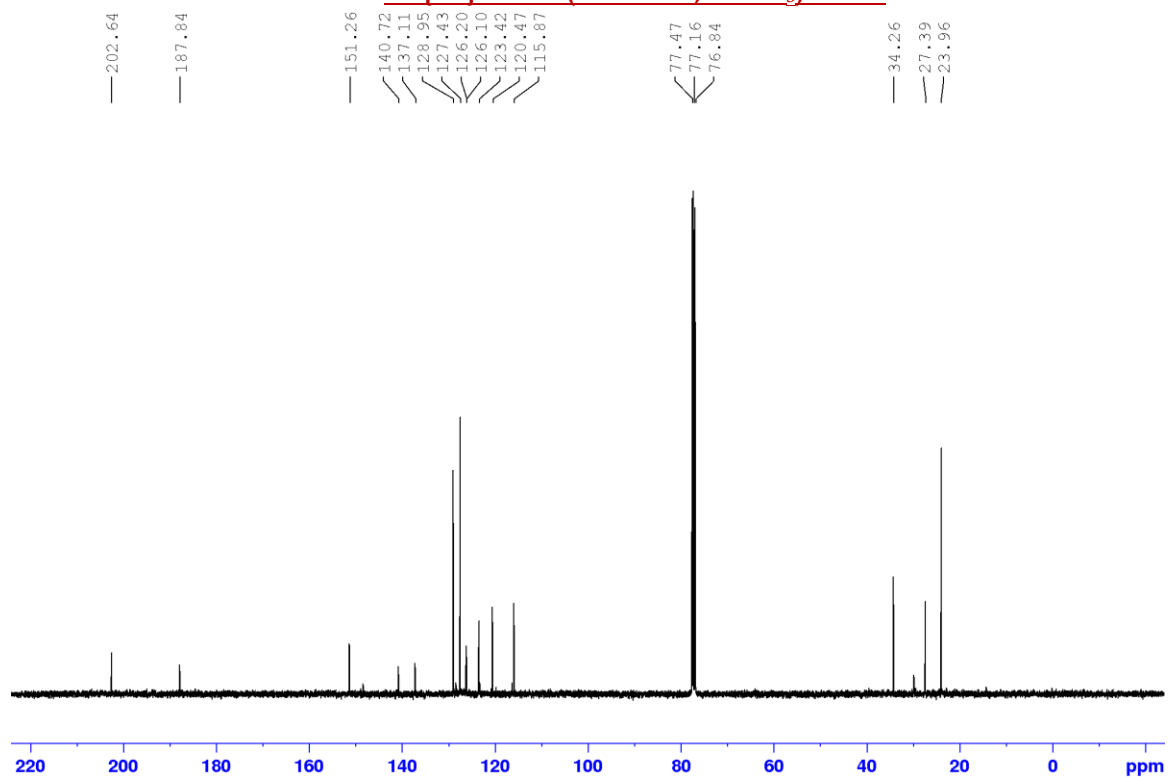
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|--------|------|---------|---------------|
| 309.0858 | 309.0875 | -1.7 | -5.5 | 12.5 | 1203.4 | n/a | n/a | C17 H13 N2 O4 |

^1H NMR (400 MHz, CDCl_3) of 5o



^{13}C [^1H] NMR (101 MHz, CDCl_3) of 5o



HRMS of 5o

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-19 H: 0-100 N: 0-2 O: 0-2

SM-428

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

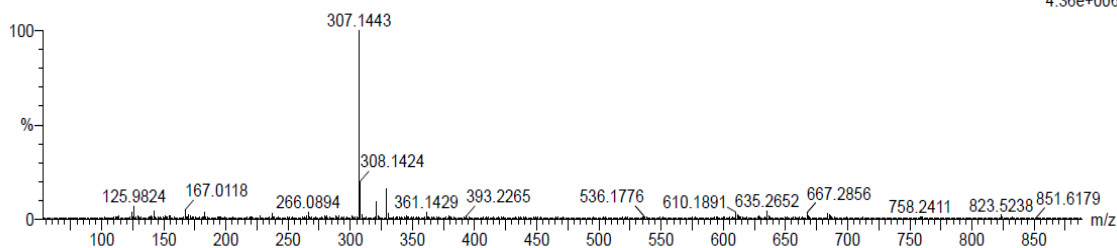
30-Apr-2024

11:47:43

1: TOF MS ES+

4.36e+006

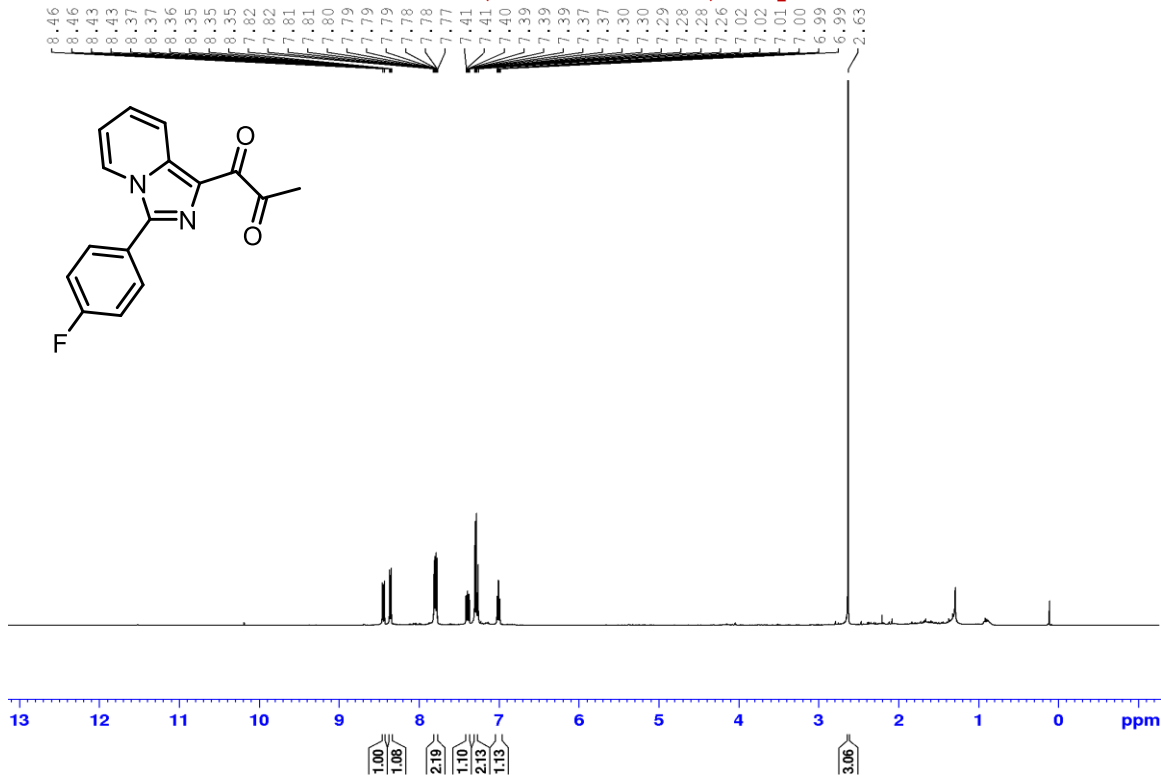
300424_05 8 (0.172) Cm (8)

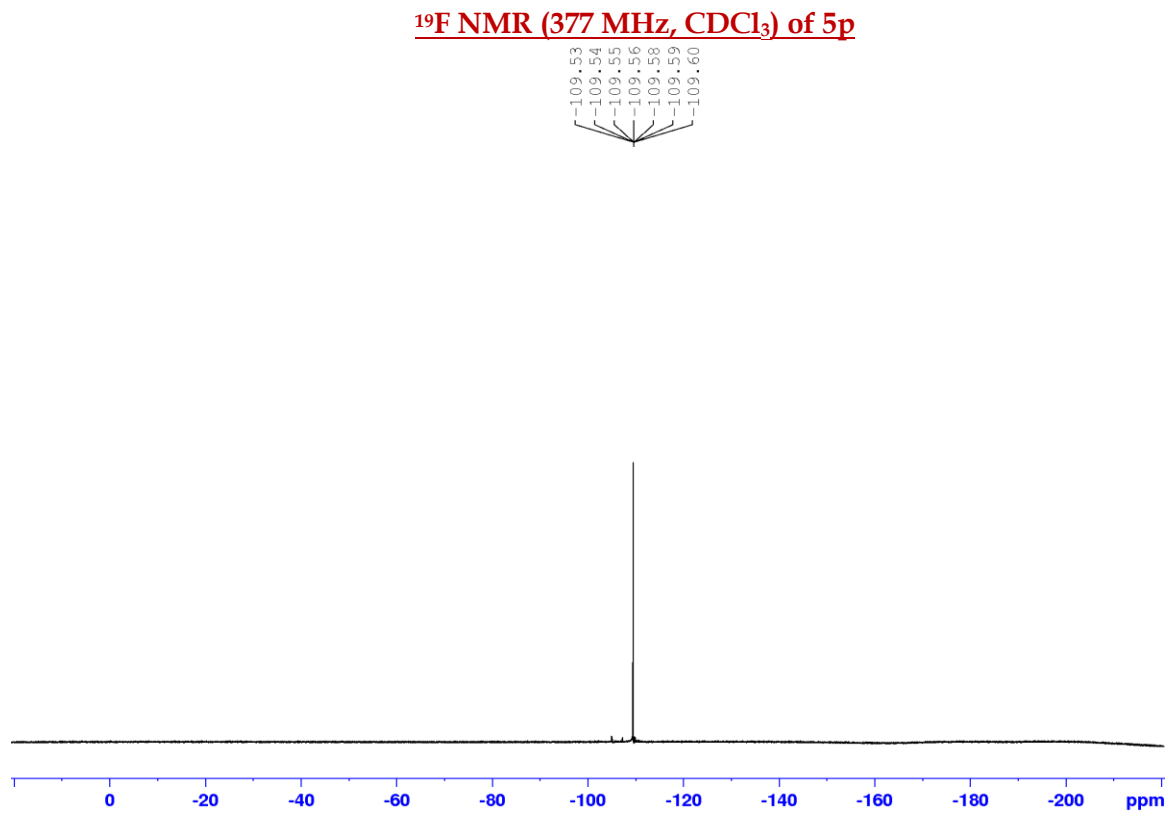
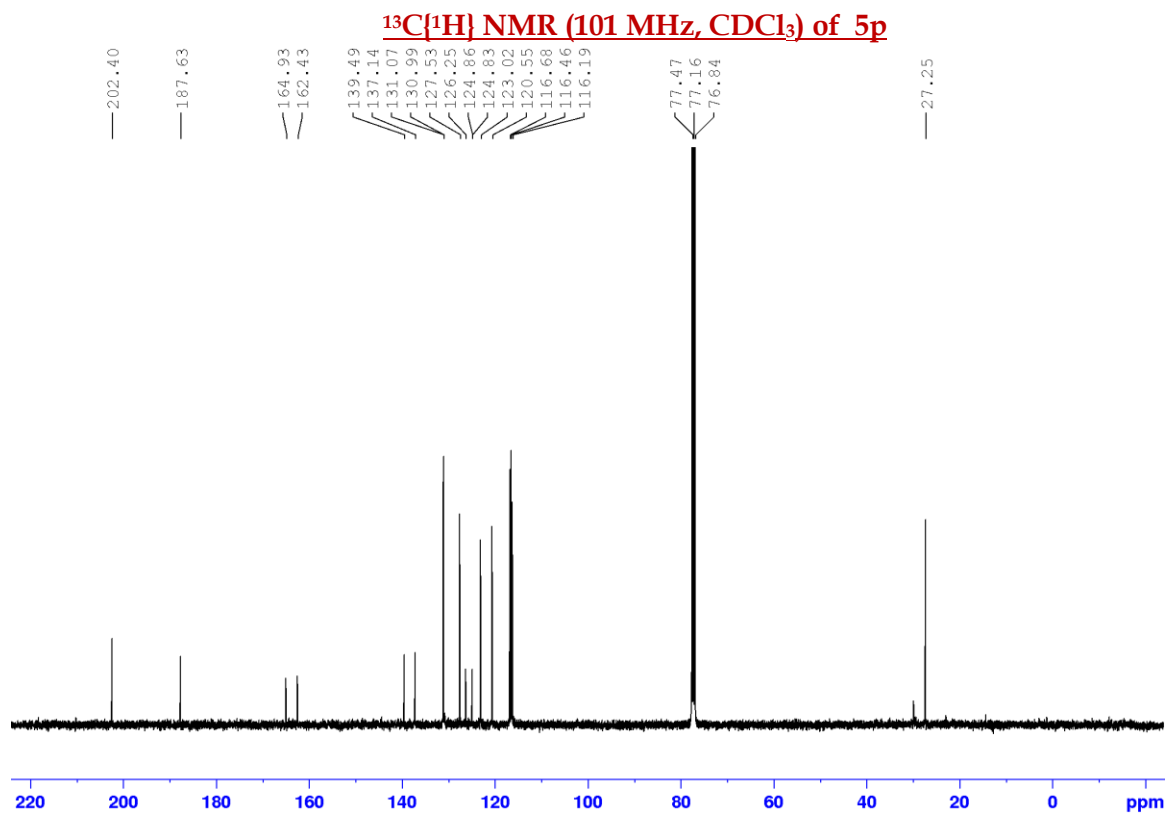


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|------|------|------|-------|------|---------|---------------|
| 307.1443 | 307.1447 | -0.4 | -1.3 | 11.5 | 35.9 | n/a | n/a | C19 H19 N2 O2 |

¹H NMR (400 MHz, CDCl₃) of 5p





HRMS of 5p

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

23 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-16 H: 0-100 N: 0-2 O: 0-2 F: 0-1

SM-469

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

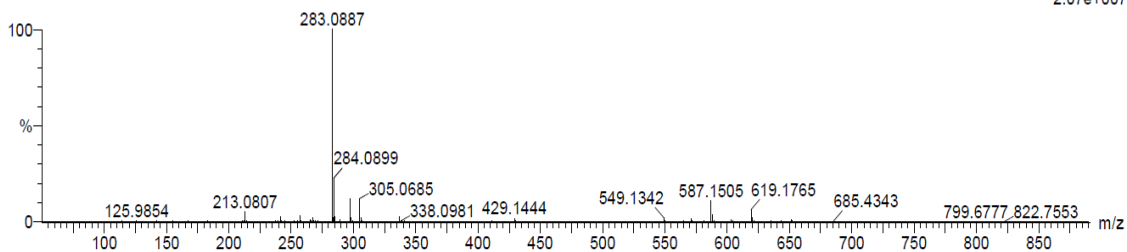
30-Apr-2024

11:57:59

1: TOF MS ES+

2.07e+007

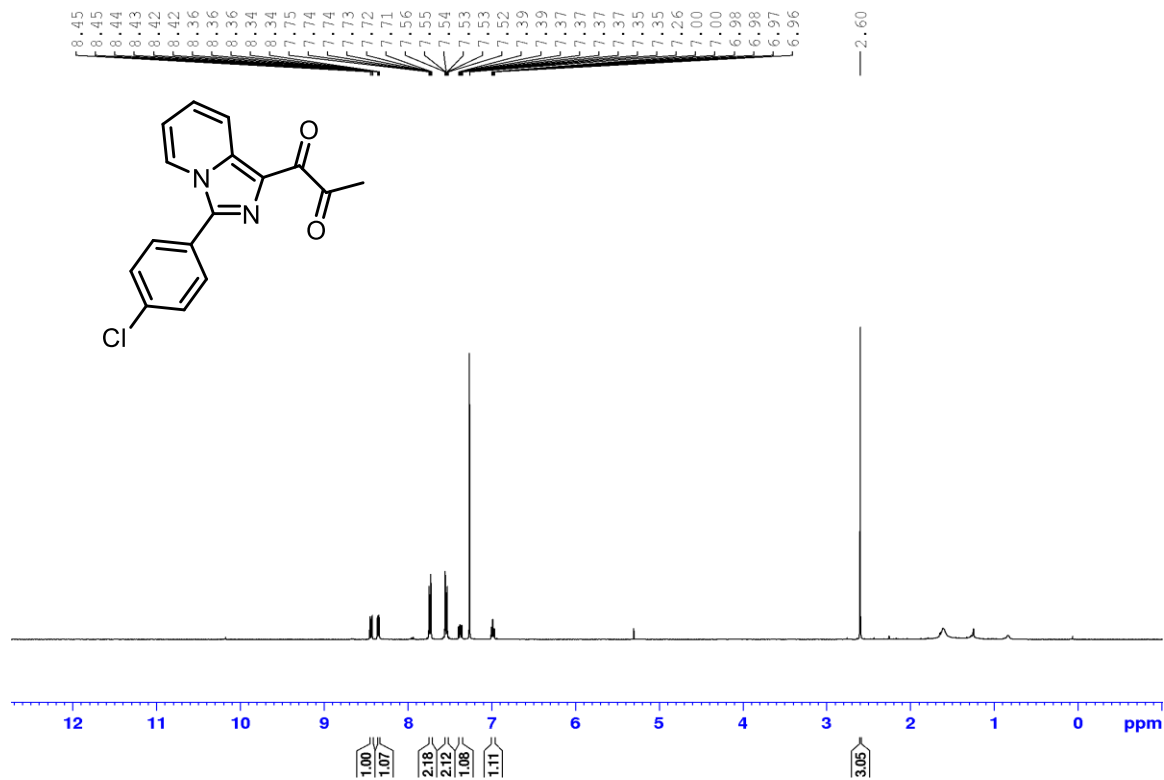
300424_09 5 (0.121)

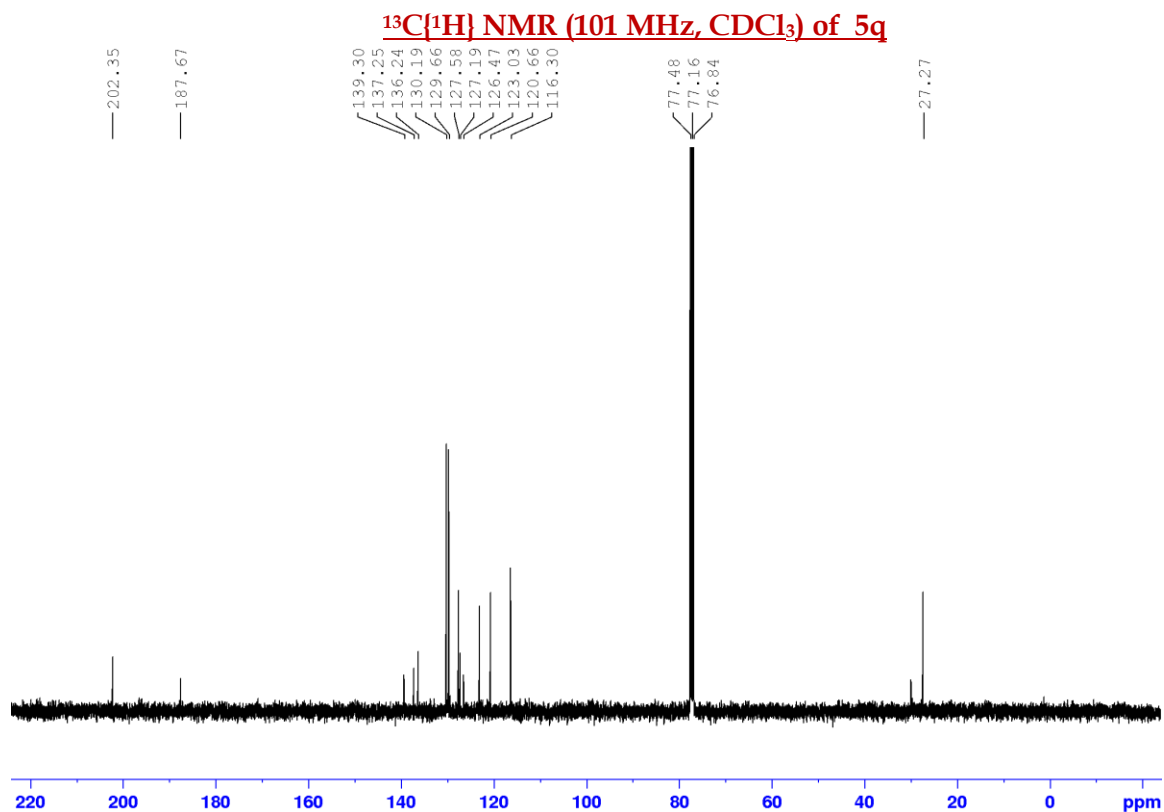


Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
|----------|------------|-----|-----|------|--------|------|---------|-----------------|
| 283.0887 | 283.0883 | 0.4 | 1.4 | 11.5 | 1274.1 | n/a | n/a | C16 H12 N2 O2 F |

¹H NMR (400 MHz, CDCl₃) of 5q





HRMS of 5q

Elemental Composition Report

Page 1

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
 22 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-16 H: 0-100 N: 0-2 O: 0-2 Cl: 0-1

SM-385

QMI DIVISION, CSIR-IIIM JAMMU
 Xevo G2-XS QTOF YFC2015

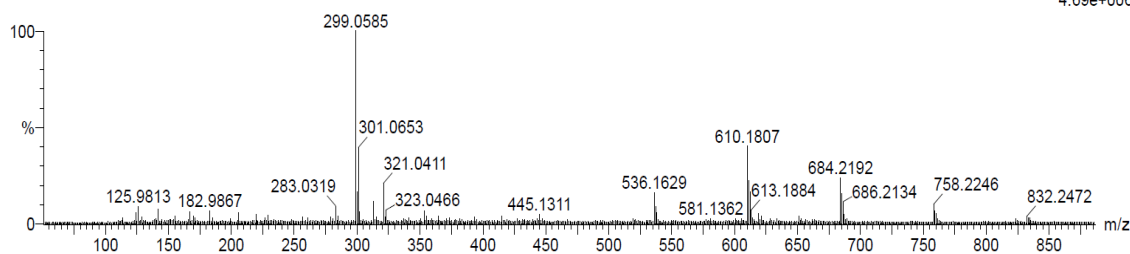
30-Apr-2024

11:45:10

1: TOF MS ES+

4.69e+006

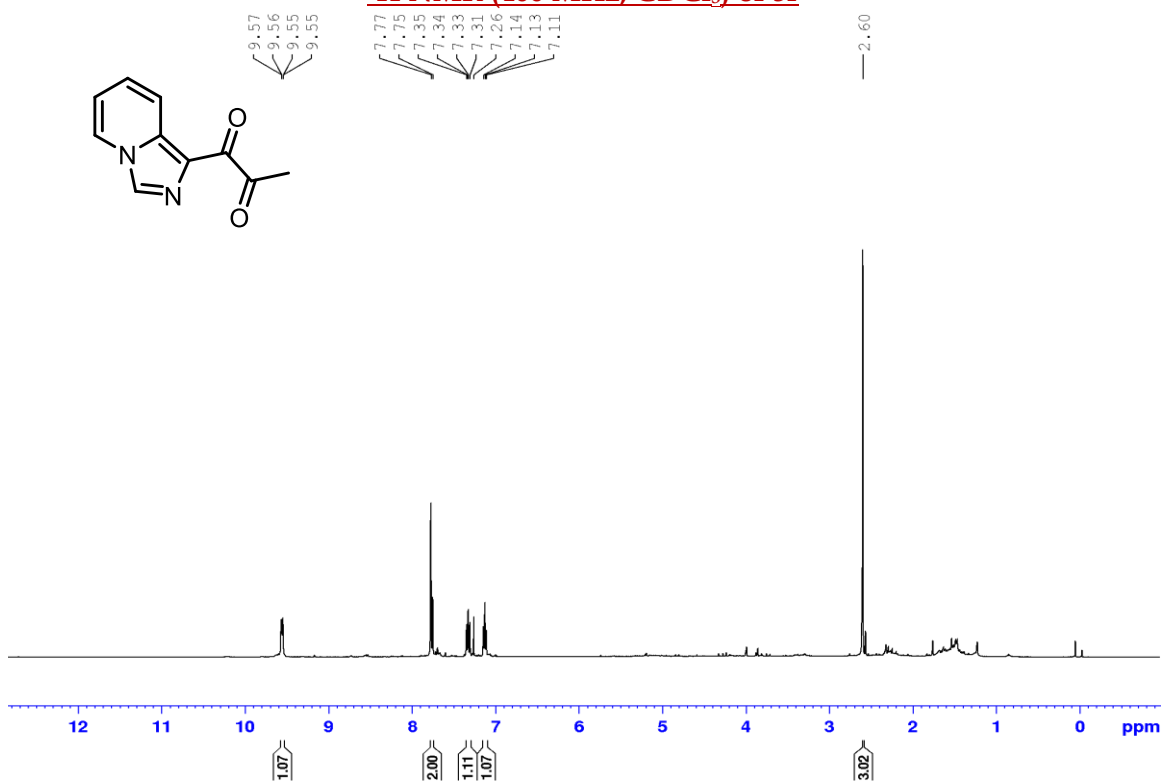
300424_04 7 (0.155) Cm (7:8)



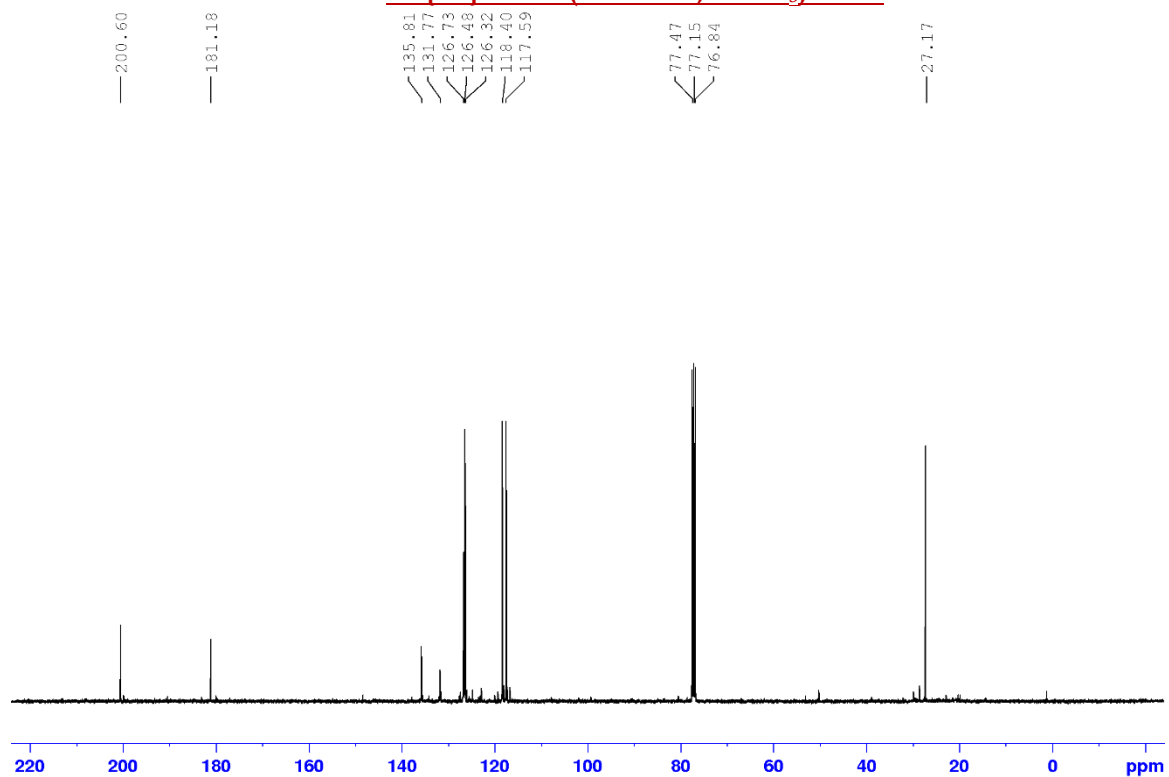
Minimum: -1.5
 Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|-------|------|----------|------------------|
| 299.0585 | 299.0587 | -0.2 | -0.7 | 11.5 | 54.8 | n/a | n/a | C16 H12 N2 O2 Cl |

¹H NMR (400 MHz, CDCl₃) of 5r



¹³C[¹H] NMR (101 MHz, CDCl₃) of 5r



HRMS of 5r

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-10 H: 0-100 N: 0-2 O: 0-2

SM-521

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

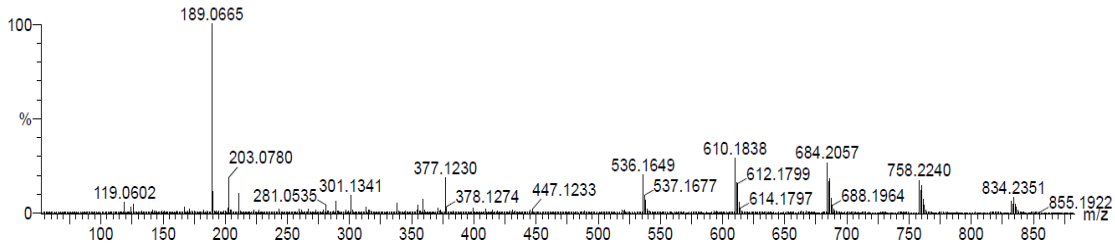
07-May-2024

14:41:43

1: TOF MS ES+

6.87e+006

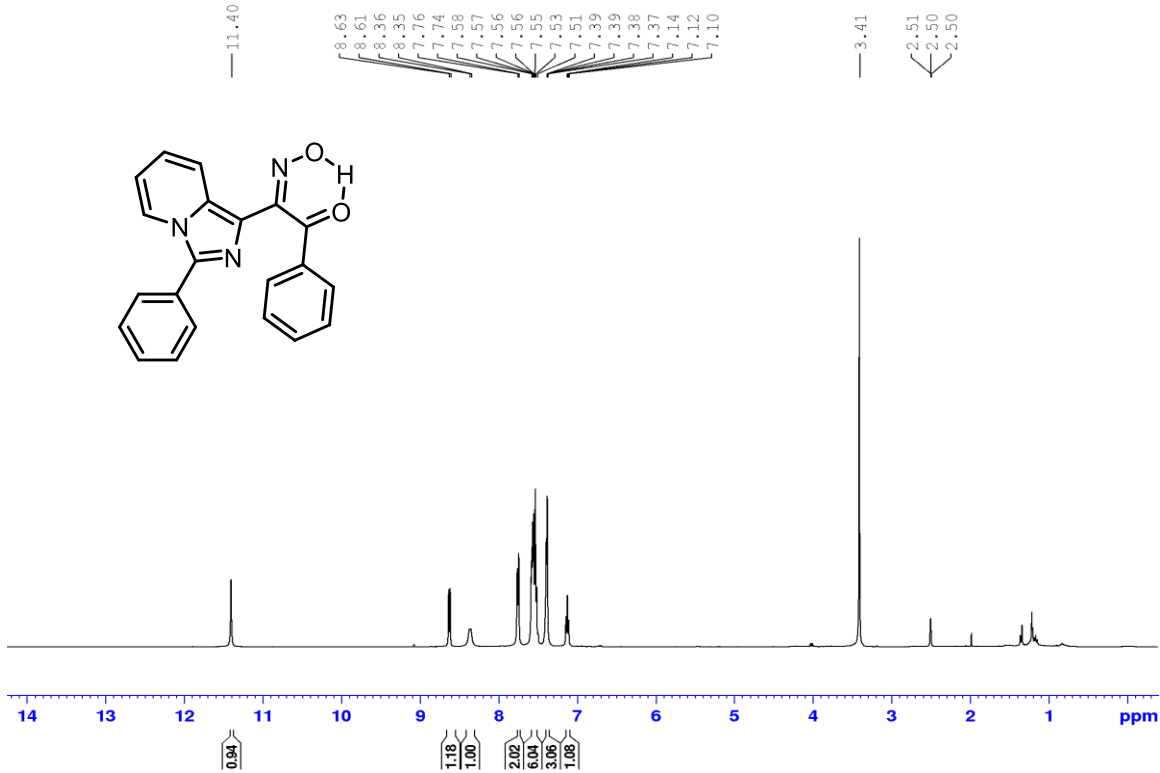
070524_40 6 (0.138) Cm (5:7)



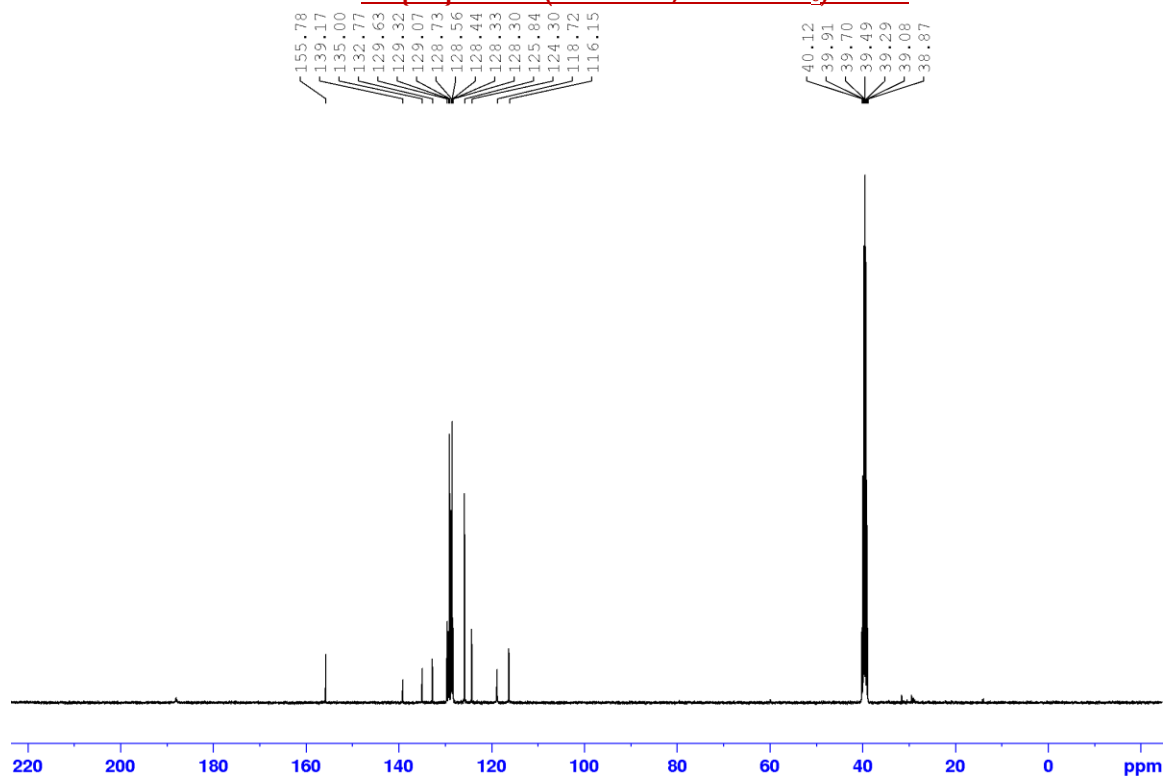
Minimum: -1.5
Maximum: 2.0 50.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 189.0665 | 189.0664 | 0.1 | 0.5 | 7.5 | 27.7 | n/a | n/a | C10 H9 N2 O2 |

¹H NMR (400 MHz, DMSO-d₆) of 6a



¹³C[¹H] NMR (101 MHz, DMSO-d₆) of 6a



HRMS of 6a

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-21 H: 0-100 N: 0-3 O: 0-2

SM-Ph-OX

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

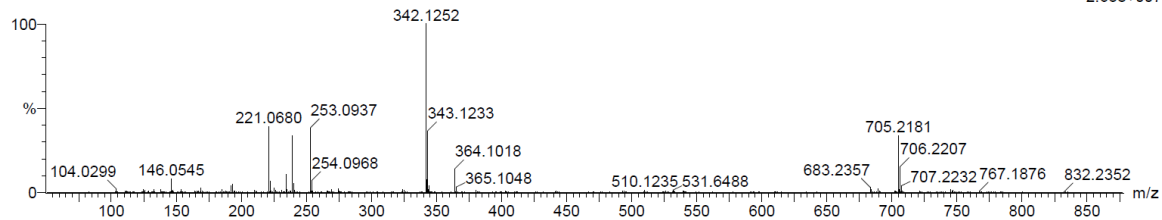
19-Mar-2024

14:10:43

1: TOF MS ES+

2.68e+007

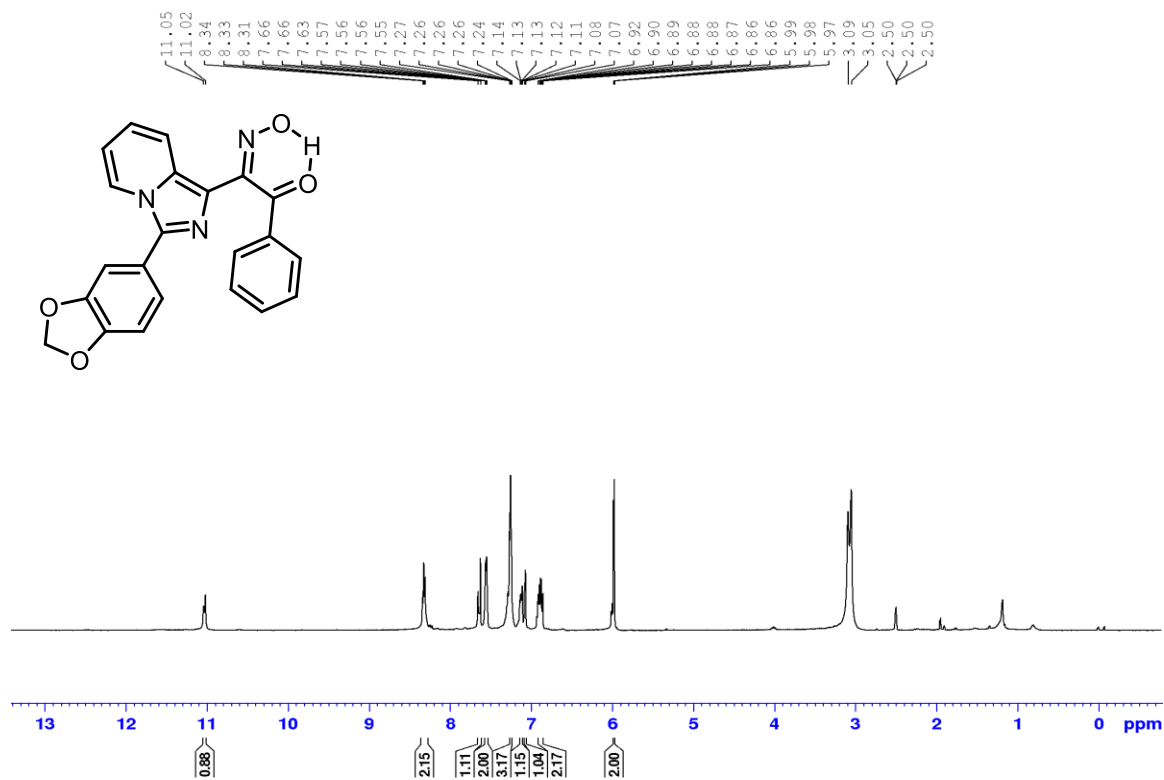
190324_17 8 (0.172)



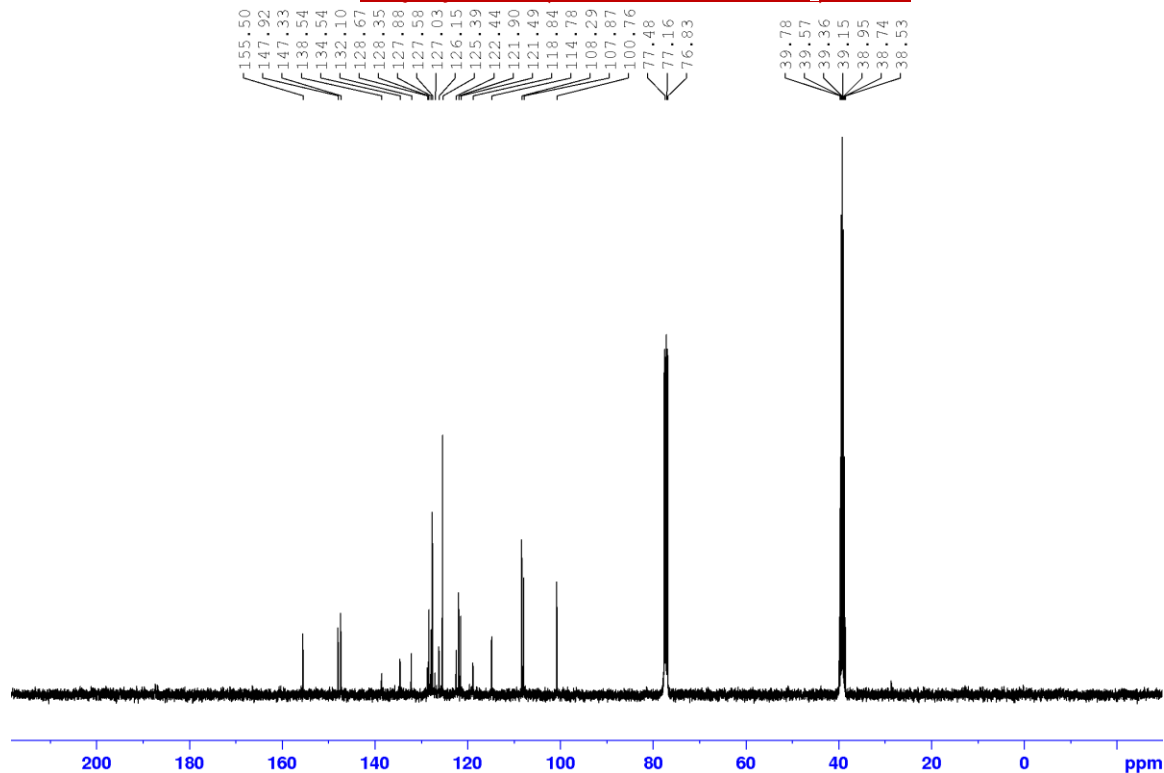
Minimum: -1.5
Maximum: 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|---------------|
| 342.1252 | 342.1243 | 0.9 | 2.6 | 15.5 | 1205.1 | n/a | n/a | C21 H16 N3 O2 |

¹H NMR (400 MHz, DMSO-d₆) of 6b



¹³C{¹H} NMR (101 MHz, DMSO-d₆) of 6b



HRMS of 6b

Elemental Composition Report

Single Mass Analysis

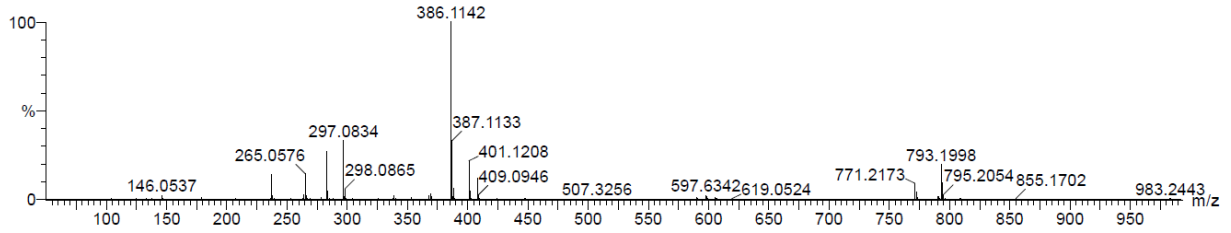
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-22 H: 0-100 N: 0-3 O: 0-4
SM-528

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

17-May-2024
13:41:34
1: TOF MS ES+
4.08e+007

170524_02 6 (0.138)



Minimum: -1.5
Maximum: 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|------|--------|------|----------|---------------|
| 386.1142 | 386.1141 | 0.1 | 0.3 | 16.5 | 1030.3 | n/a | n/a | C22 H16 N3 O4 |