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Supporting Information

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

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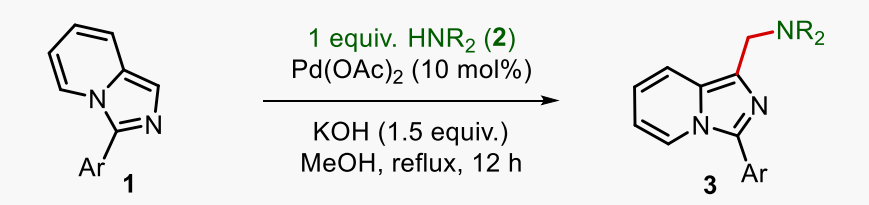
1. General Methods:

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 (^{1}H) 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 $CDCl_3$ (δ_H = 7.26 and δ_C = 77.16 ppm) and DMSO-d_6 (δH = 2.50 and δC = 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.

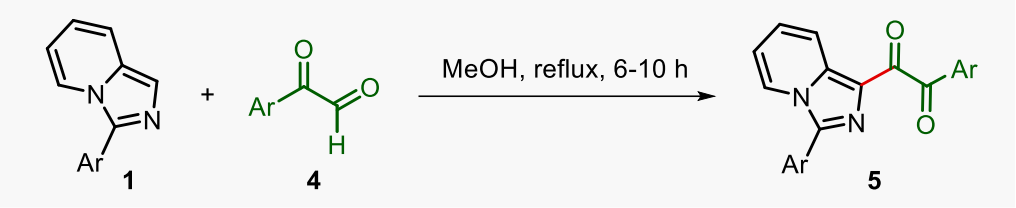
2. General Reaction Procedures:

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



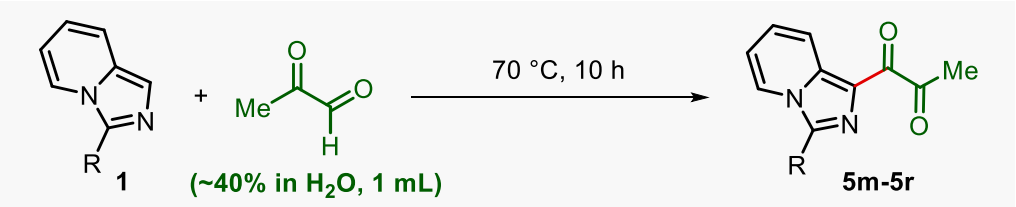
To the solution of 3-arylimidazo[1,5-*a*]pyridines **1** (1 equiv.) and secondary amines **2** (1 equiv.) in methanol was added KOH (1.5 quiv.). The mixture was allowed to stir at reflux temperature for 12 hours. After complete conversion (product monitored by TLC), methanol was removed by using a rotary 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.

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



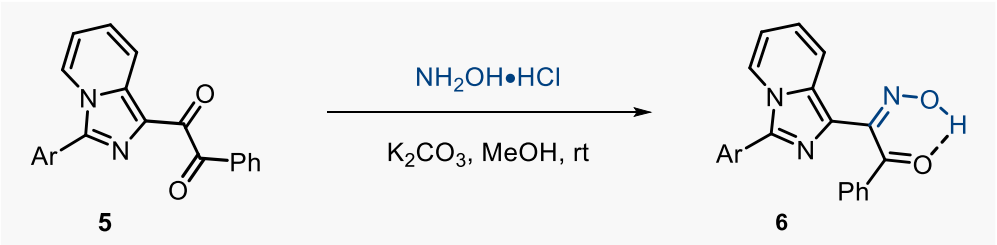
To the solution of 3-arylimidazo[1,5-*a*]pyridines **1** (1 equiv) in methanol, arylglyoxals **4** (1 equiv) was added. The mixture was then allowed to stir at reflux temperature. After complete conversion (product monitored by TLC), methanol was removed using a rotary evaporator. The residue was subjected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

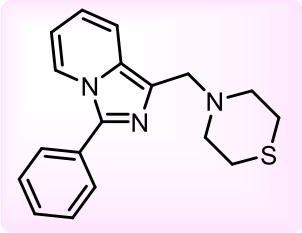
General Procedure for the Synthesis of oximes (GP4):



To the solution of 3-arylimidazo[1,5-*a*]pyridines (1 equiv) in methanol (1 mL), hydroxylamine hydrochloride (1.5 equiv) and K_2CO_3 (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.

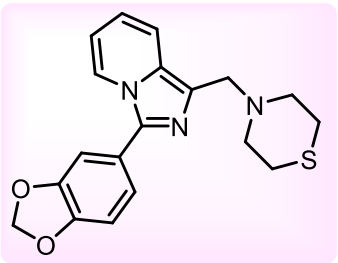
3. Characterization Data:

***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; **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{18}H_{19}N_3SNa$ $[M+Na]^+$: 332.1197, found: 332.1184; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{11}N_2$ $[M-C_4H_8NS]$: 207.0922, found: 207.0923

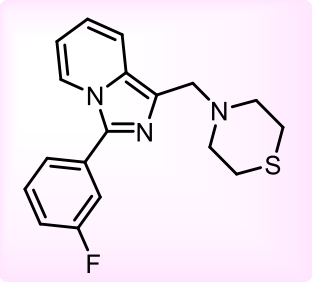
***4-((3-(benzo[d][1,3]dioxol-5-yl)imidazo[1,5-a]pyridin-1-yl)methyl)thiomorpholine* (3b)**



Following GP1, the compound **3b** was obtained as yellow solid (60 mg, 81%), m.p.= 180-182 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.12 (d, J = 7.25 Hz, 1H), 7.56 (d, J = 9.21, 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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-C_4H_8NS]: 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 ^oC; **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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; **^{19}F NMR (377 MHz, $CDCl_3$):** -110.97 to -110.99 (m) ppm; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{10}N_2F$ [M-C_4H_8NS]: 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%); **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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; **^{19}F NMR (377 MHz, $CDCl_3$):** -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-C_4H_8NS]: 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; **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{18}H_{19}N_4O_2S$ $[M+H]^+$: 355.1229, found: 355.1207; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{10}N_3O_2$ [M-C_4H_8NS]: 252.0773, found: 252.0770

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

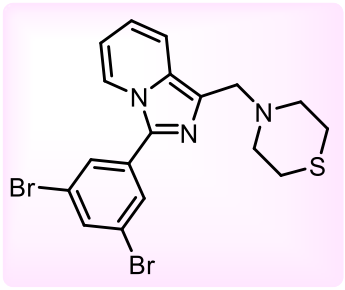
Following GP1, the compound **3f** was obtained as pale yellow semi-solid (59 mg, 80%); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.20 (d, J = 7.19 Hz, 1H), 7.69 (d, J = 8.32 Hz, 2H), 7.57 (d, J = 8.99 Hz, 1H), 7.36 (d, J = 7.99 Hz, 2H), 6.71-6.67 (m, 1H), 6.54-6.50 (m, 1H), 3.92 (s, 2H), 3.01-2.94 (m, 1H), 2.88-2.85 (m, 4H), 2.73-2.70 (m, 4H), 1.30 (s, 3H), 1.29 (s, 3H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{21}H_{26}N_3S$ $[M+H]^+$: 352.1847, found: 352.1827; **HRMS (ESI) m/z:** calcd. for $C_{17}H_{17}N_2$ [M-C_4H_8NS]: 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%); **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{19}H_{22}N_3OS$

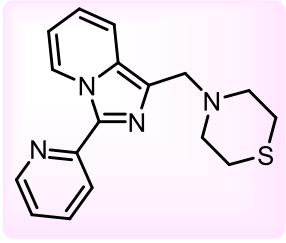
[M+H]$^+$: 340.1484, found: 340.1465; **HRMS (ESI) m/z:** calcd. for $C_{15}H_{13}N_2O$ [M-C_4H_8NS]: 237.1028, found: 237.1024

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



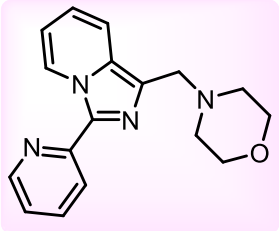
Following GP1, the compound **3h** was obtained as pale white solid (50 mg, 75%), m.p.= 108-110 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.19 (d, J = 7.15 Hz, 1H), 7.89 (d, J = 1.71 Hz, 2H), 7.70-7.69 (m, 1H), 7.62 (d, J = 9.09 Hz, 1H), 6.78 (t, J = 7.88 Hz, 1H), 6.66 (t, J = 6.70 Hz, 1H), 3.88 (s, 2H), 2.82-2.81 (m, 4H), 2.71-2.69 (m, 4H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{14}H_9N_2Br_2$ [M-C_4H_8NS]: 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 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{17}H_{18}N_4SNa$ [M+Na]$^+$: 333.1150, found: 333.1133; **HRMS (ESI) m/z:** calcd. for $C_{13}H_{10}N_3$ [M-C_4H_8NS]: 208.0875, found: 208.0875

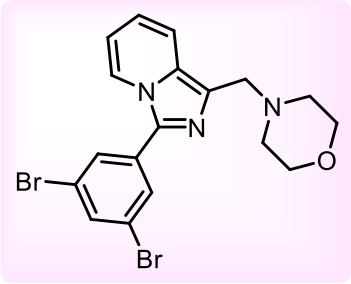
4-((3-(pyridin-2-yl)imidazo[1,5-a]pyridin-1-yl)methyl)morpholine **(3j)**



Following GP1, the compound **3j** was obtained as pale yellow solid (82 mg, 81%), m.p.= 122-124 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$):** 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),

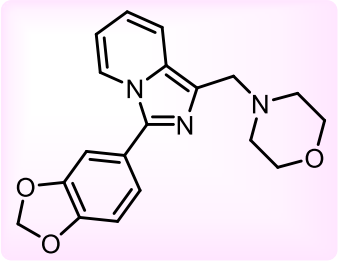
6.85-6.81 (m, 1H), 6.70 (t, *J* = 6.86 Hz, 1H), 3.88 (s, 2H), 3.72 (t, *J* = 4.64 Hz, 4H), 2.57 (m, 4H) ppm; **$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$):** *δ* 151.0, 148.1, 136.4, 134.4, 131.1, 128.9, 126.0, 122.0, 121.5, 119.8, 117.6, 113.5, 67.0, 55.8, 53.7 ppm; **HRMS (ESI) m/z:** calcd. for $C_{17}H_{18}N_4ONa$ $[M+Na]^+$: 317.1378, found: 317.1360; **HRMS (ESI) m/z:** calcd. for $C_{13}H_{10}N_3$ $[M-C_4H_8NO]$: 208.0875, found: 208.0881

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



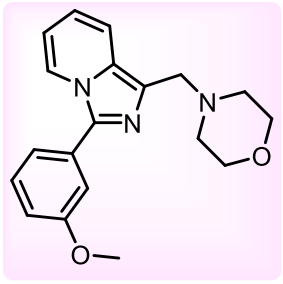
Following GP1, the compound **3k** was obtained as pale white solid (49 mg, 75%), m.p.= 114-116 °C; **^1H NMR (400 MHz, $CDCl_3$):** *δ* 8.20 (d, *J* = 7.20 Hz, 1H), 7.89 (d, *J* = 1.67 Hz, 2H), 7.71-7.67 (m, 2H), 6.83-6.79 (m, 1H), 6.68 (t, *J* = 6.76 Hz, 1H), 3.94 (s, 2H), 3.77 (t, *J* = 4.40 Hz, 4H), 2.66 (s, 4H) ppm; **$^{13}C\{^1H\}$ 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 $C_{18}H_{18}N_3Br_2O$ $[M+H]^+$: 449.9817, found: 449.9807; **HRMS (ESI) m/z:** calcd. for $C_{14}H_9N_2Br_2$ $[M-C_4H_8NO]$: 362.9132, found: 362.9124

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



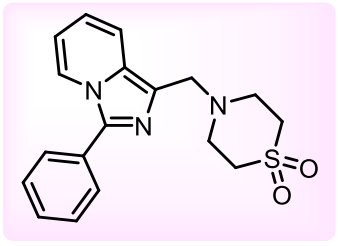
Following GP1, the compound **3l** was obtained as yellow solid (59 mg, 83%), m.p.= 188-190 °C; **^1H NMR (400 MHz, $CDCl_3$):** *δ* 8.11 (d, *J* = 7.31 Hz, 1H), 7.54 (tt, *J* = 9.18, 1.05 Hz, 1H), 7.22-7.20 (m, 2H), 6.92-6.89 (m, 1H), 6.69-6.65 (m, 1H), 6.52-6.48 (m, 1H), 6.01-6.00 (m, 2H), 3.86 (s, 2H), 3.71 (s, 4H), 2.59 (s, 4H) ppm; **$^{13}C\{^1H\}$ 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 $C_{19}H_{20}N_3O_3$ $[M+H]^+$: 338.1505, found: 338.1490; **HRMS (ESI) m/z:** calcd. for $C_{15}H_{11}N_2O_2$ $[M-C_4H_8NO]$: 251.0821, found: 251.0824

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



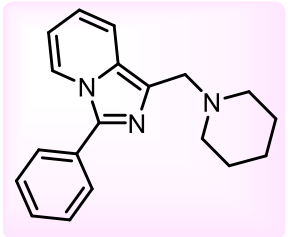
Following GP1, the compound **3m** was obtained as dark colored semi-solid (57 mg, 79%); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.20 (d, J = 7.27 Hz, 1H), 7.58 (dd, J = 9.21, 1.15 Hz, 1H), 7.39 (dt, J = 7.82, 1.25 Hz, 1H), 7.33-7.29 (m, 2H), 6.94 (dd, J = 8.20, 1.05 Hz, 1H), 6.72-6.68 (m, 1H), 6.54-6.50 (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}C{^{1}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 $C_{19}H_{22}N_3O_2$ $[M+H]^+$: 3241712, found: 334.1693; **HRMS (ESI) m/z:** calcd. for $C_{15}H_{13}N_2O$ $[M-C_4H_8NO]$: 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 ^{o}C; **^{1}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}C{^{1}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 $C_{18}H_{19}N_3O_2SNa$ $[M+Na]^+$: 364.1096, found: 364.1080; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{11}N_2$ $[M-C_4H_8NO_2S]$: 207.0922, found: 207.0922

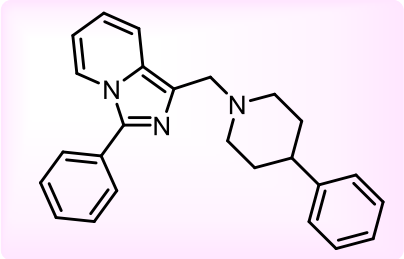
***3-phenyl-1-(piperidin-1-ylmethyl)imidazo[1,5-a]pyridine* (3o)**



Following GP1, the compound **3o** was obtained as pale yellow colored semi-solid (56 mg, 75%); **^{1}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}C{^{1}H} NMR**

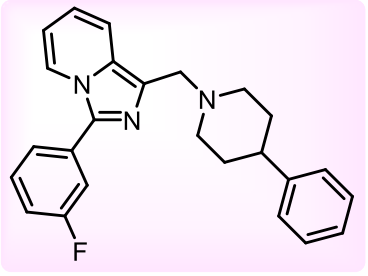
(101 MHz, $CDCl_3$): δ 137.2, 130.3, 129.9, 129.4, 128.9, 128.6, 128.4, 128.1, 121.3, 118.8, 118.4, 113.1, 55.8, 54.3, 25.7, 24.1 ppm; **HRMS (ESI) m/z:** calcd. for $C_{19}H_{22}N_3$ $[M+H]^+$: 292.1814, found: 292.1786; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{11}N_2$ [M-$C_5H_{10}N$]: 207.0922, found: 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%); **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{25}H_{26}N_3$ $[M+H]^+$: 368.2127, found: 368.2110; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{11}N_2$ [M-$C_{11}H_{14}N$]: 207.0922, found: 207.0925

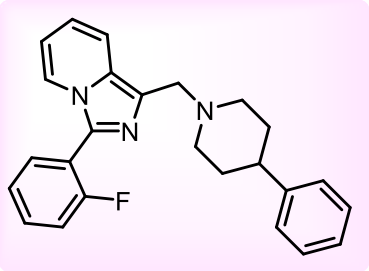
***3-(3-fluorophenyl)-1-((4-phenylpiperidin-1-yl)methyl)imidazo[1,5-a]pyridine* (3q)**



Following GP1, the compound **3q** was obtained as dark colored semi-solid (71 mg, 78%); **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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; **^{19}F NMR (377 MHz, $CDCl_3$):** -110.91 to -110.95 (m) ppm; **HRMS (ESI)**

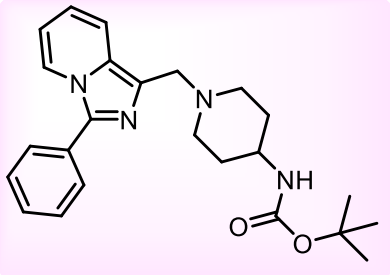
m/z: calcd. for $C_{25}H_{25}N_3F$ $[M+H]^+$: 386.2030, found: 386.2014; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{10}N_2F$ $[M-C_{11}H_{14}N]$: 225.0828, found: 225.0838

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



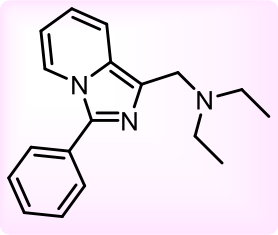
Following GP1, the compound **3r** was obtained as dark colored semi-solid (68 mg, 75%); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.18 (d, J = 7.19 Hz, 1H), 7.63 (d, J = 9.22 Hz, 1H), 7.56-7.54 (m, 1H), 7.50-7.46 (m, 1H), 7.46-7.40 (m, 2H), 7.24-7.22 (m, 2H), 7.19-7.17 (m, 1H), 7.16-7.12 (m, 1H), 7.09-7.04 (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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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; **^{19}F NMR (377 MHz, $CDCl_3$):** -110.91 to -110.95 (m) ppm; **HRMS (ESI) m/z:** calcd. for $C_{25}H_{25}N_3F$ $[M+H]^+$: 386.2033, found: 386.2015; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{10}N_2F$ $[M-C_{11}H_{14}N]$: 225.0828, found: 225.0824

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



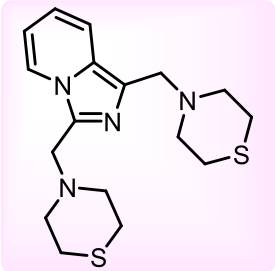
Following GP1, the compound **3s** was obtained as dark colored solid (80 mg, 76%), m.p.= 144-146 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 9.89 (d, J = 7.32 Hz, 1H), 8.61 (d, J = 4.82 Hz, 1H), 8.33 (d, J = 8.17 Hz, 1H), 7.74 (dt, J = 7.76, 1.71 Hz, 1H), 7.64 (d, J = 9.17 Hz, 1H), 7.18-7.15 (m, 1H), 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; **^{13}C{^{1}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 $C_{24}H_{31}N_4O_2$ $[M+H]^+$: 407.2447, found: 407.2435; **HRMS (ESI) m/z:** calcd. for $C_{14}H_{11}N_2$ $[M-C_{10}H_{19}N_2O_2]$: 207.0922, found: 207.0929

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



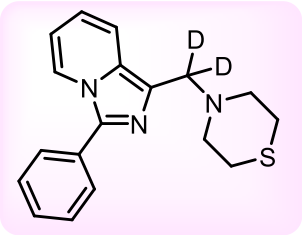
Following GP1, the compound **3t** was obtained as pale yellow semi-solid (60 mg, 83%); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.21 (d, J = 7.17 Hz, 1H), 7.88 (d, J = 8.91 Hz, 1H), 7.73 (d, J = 7.17 Hz, 2H), 7.52 (t, J = 7.51 Hz, 2H), 7.47-7.43 (m, 1H), 6.90-6.86 (m, 1H), 6.62 (t, J = 6.16 Hz, 1H), 4.68 (s, 2H), 3.20 (d, J = 6.42 Hz, 4H), 1.50 (t, J = 6.88 Hz, 6H) ppm; **^{13}C{^{1}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 $C_{14}H_{11}N_2$ [M-$C_4H_{10}N$]: 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}H NMR (400 MHz, $CDCl_3$):** δ 8.05 (d, J = 7.21 Hz, 1H), 7.42 (dd, J = 9.20, 0.66 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}C{^{1}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 $C_{17}H_{24}N_4S_2Na$ $[M+Na]^+$: 371.1340, found: 371.1312; **HRMS (ESI) m/z:** calcd. for $C_{13}H_{16}N_3S$ [M-C_4H_8NS]: 246.1065, found: 246.1082

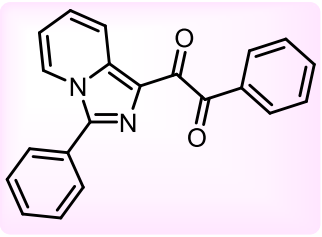
***4-((3-phenylimidazo[1,5-a]pyridin-1-yl)methyl-d_2)thiomorpholine* (3v)**



The compound **3v** was obtained as yellow semi-solid (52 mg, 65%); **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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.

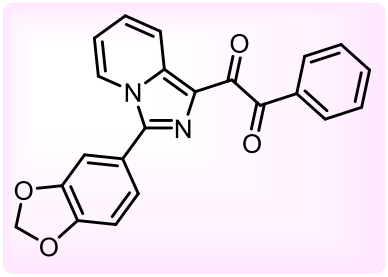
NOTE- During the HRMS analysis, it was observed that the molecular ion peak was undergoing fragmentation in the standard positive ESI mode. In some instances, the molecular ion peak was completely absent. Adjusting the temperature did not resolve this issue. To verify that the observed fragmented peak 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)**



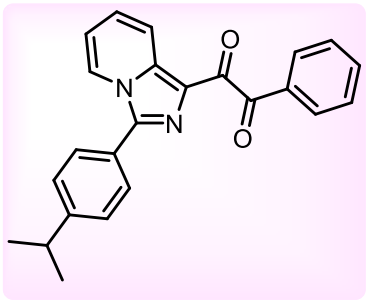
Following GP2, the compound **5a** was obtained as yellow colored solid (69 mg, 82%), m.p.= 160-162 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.46 (d, J = 9.06 Hz, 1H), 8.37 (td, J = 7.07, 1.05 Hz, 1H), 8.05 (d, J = 7.85 Hz, 2H), 7.69-7.67 (m, 2H), 7.60-7.56 (m, 1H), 7.48-7.44 (m, 5H), 7.38-7.33 (m, 1H), 6.97-6.93 (m, 1H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{21}H_{15}N_2O_2$ $[M+H]^+$: 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)**



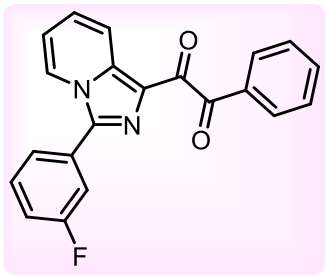
Following GP2, the compound **5b** was obtained as yellow solid (60 mg, 77%), m.p.= 186-188 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.48 (d, J = 9.15 Hz, 1H), 8.36 (d, J = 7.08 Hz, 1H), 8.07-8.05 (m, 2H), 7.60 (t, J = 7.41 Hz, 1H), 7.47 (t, J = 7.85 Hz, 2H), 7.39-7.35 (m, 1H), 7.19 (dd, J = 7.93, 1.64 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{22}H_{15}N_2O_4$ $[M+H]^+$: 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; **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{24}H_{21}N_2O_2$ $[M+H]^+$: 369.1603, found: 369.1611

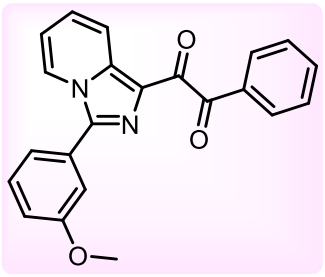
1-(3-(3-fluorophenyl)imidazo[1,5-a]pyridin-1-yl)-2-phenylethane-1,2-dione **(5d)**



Following GP2, the compound **5d** was obtained as yellow solid (62 mg, 76%), m.p.= 175-177 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** 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,

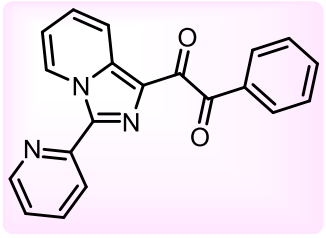
1H), 7.00 (dt, *J* = 6.88, 1.23 Hz, 1H) ppm; **$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$):** *δ* 194.8, 188.8, 161.4, 158.9, 136.6, 136.1, 134.2, 133.5, 132.9, 132.3 (d, *J* = 3.32 Hz), 130.1, 128.7, 128.3 (d, *J* = 14.74 Hz), 127.9 (d, *J* = 7.79 Hz), 127.6 (d, *J* = 8.42 Hz), 125.1 (d, *J* = 3.37 Hz), 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 $C_{21}H_{14}N_2O_2F$ $[M+H]^+$: 345.1039, found: 345.1047

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



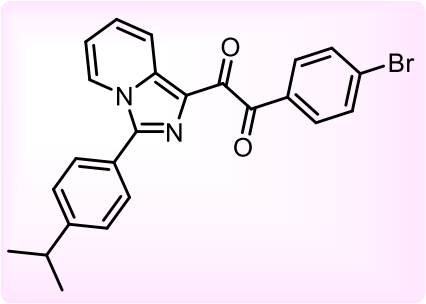
Following GP2, the compound **5e** was obtained as yellow solid (59 mg, 75%), m.p.= 148-150 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$):** *δ* 8.50 (d, *J* = 9.05 Hz, 1H), 8.41 (td, *J* = 7.13, 0.97 Hz, 1H), 8.08-8.05 (m, 2H), 7.62-7.58 (m, 1H), 7.47 (t, *J* = 7.63 Hz, 2H), 7.42-7.36 (m, 2H), 7.28 (t, *J* = 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; **$^{13}C\{^{1}H\}$ 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 $C_{22}H_{17}N_2O_3$ $[M+H]^+$: 357.1239, found: 357.1233

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



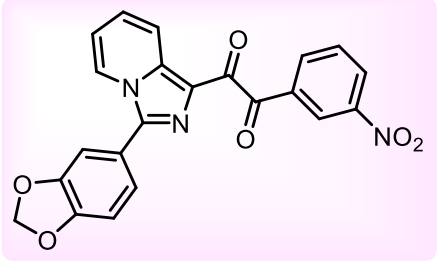
Following GP2, the compound **5f** was obtained as yellow solid (67 mg, 80%), m.p.= 167-169 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$):** *δ* 10.21 (dd, *J* = 7.12, 0.93 Hz, 1H), 8.61 (d, *J* = 4.14 Hz, 1H), 8.53 (d, *J* = 8.28 Hz, 1H), 8.26 (d, *J* = 8.10 Hz, 1H), 8.09-8.06 (m, 2H), 7.74-7.69 (m, 1H), 7.63-7.59 (m, 1H), 7.51-7.44 (m, 3H), 7.26-7.23 (m, 1H), 7.08 (t, *J* = 6.94 Hz, 1H) ppm; **$^{13}C\{^{1}H\}$ 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 $C_{20}H_{14}N_3O_2$ $[M+H]^+$: 328.1086, found: 328.1076

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



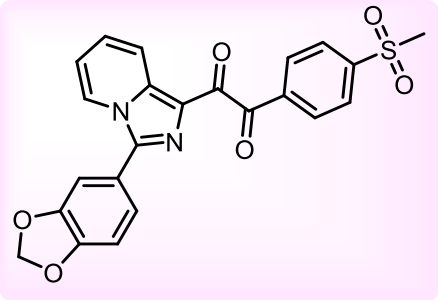
Following GP2, the compound **5g** was obtained as yellow solid (80 mg, 85%), m.p.= 130-132 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.50 (d, J = 9.08 Hz, 1H), 8.41 (d, J = 7.26 Hz, 1H), 7.93 (d, J = 7.40 Hz, 2H), 7.64-7.61 (m, 4H), 7.42-7.39 (m, 1H), 7.36 (d, J = 8.31 Hz, 2H), 7.27-7.26 (m, 1H), 6.97 (t, J = 6.88 Hz, 1H), 3.00-2.93 (m, 1H), 1.28 (s, 3H), 1.26 (s, 3H) ppm; **^{13}C{^{1}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 $C_{24}H_{20}N_2O_2Br$ $[M+H]^+$: 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)**



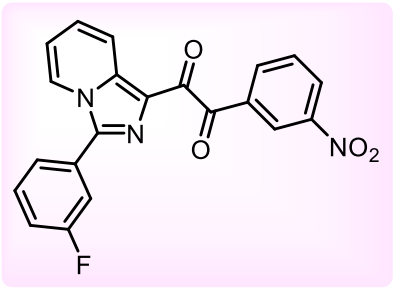
Following GP2, the compound **5h** was obtained as yellow solid (70 mg, 80%), m.p.= 188-190 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.85 (s, 1H), 8.53 (d, J = 8.71 Hz, 1H), 8.46 (d, J = 7.99 Hz, 1H), 8.41 (t, J = 6.94 Hz, 2H), 7.71 (t, J = 7.86 Hz, 1H), 7.46 (t, J = 7.74 Hz, 1H), 7.19 (d, J = 7.61 Hz, 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}C{^{1}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 $C_{22}H_{14}N_3O_6$ $[M+H]^+$: 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)**



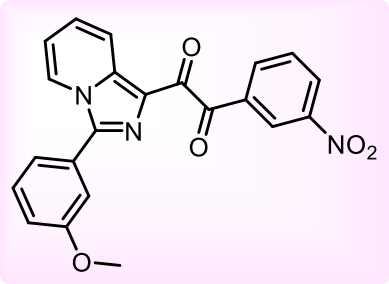
Following GP2, the compound **5i** was obtained as yellow solid (81 mg, 86%), m.p.= 180-182 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.51 (d, *J* = 8.98 Hz, 1H), 8.39 (td, *J* = 7.09, 0.95 Hz, 1H), 8.24 (td, *J* = 8.56, 1.77 Hz, 2H), 8.07-8.05 (m, 2H), 7.46-7.42 (m, 1H), 7.18 (dd, *J* = 8.01, 1.72 Hz, 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{23}H_{17}N_2O_6S$ $[M+H]^+$: 449.0807, found: 449.0796

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



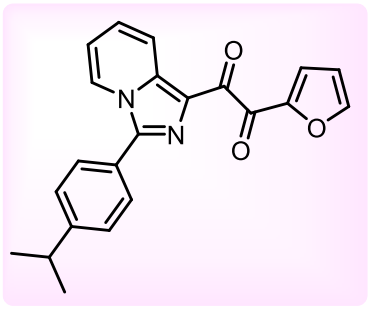
Following GP2, the compound **5j** was obtained as yellow solid (72 mg, 78%), m.p.= 157-159 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.85 (t, *J* = 1.77 Hz, 1H), 8.56 (d, *J* = 9.01 Hz, 1H), 8.48-8.41 (m, 3H), 7.71 (t, *J* = 7.88 Hz, 1H), 7.52-7.50 (m, 2H), 7.49-7.47 (m, 1H), 7.45-7.42 (m, 1H), 7.22-7.18 (m, 1H), 7.07 (dt, *J* = 6.88, 1.16 Hz, 1H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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; **^{19}F NMR (377 MHz, $CDCl_3$):** -110.77 to -110.83 (m) ppm; **HRMS (ESI) m/z:** calcd. for $C_{21}H_{13}N_3O_4F$ $[M+H]^+$: 390.0890, found: 390.0892

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



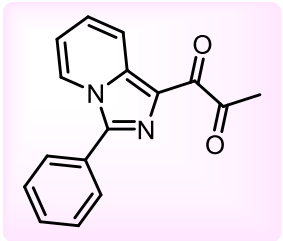
Following GP2, the compound **5k** was obtained as yellow solid (71 mg, 79%), m.p.= 149-151 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.86 (t, *J* = 1.68 Hz, 1H), 8.54 (d, *J* = 8.97 Hz, 1H), 8.47-8.44 (m, 2H), 8.43-8.41 (m, 1H), 7.71 (t, *J* = 7.98 Hz, 1H), 7.49-7.41 (m, 2H), 7.28-7.26 (m, 1H), 7.23-7.22 (m, 1H), 7.05-7.01 (m, 2H), 3.84 (s, 3H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{22}H_{16}N_3O_5$ $[M+H]^+$: 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; **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{22}H_{19}N_2O_3$ $[M+H]^+$: 359.1396, found: 359.1384

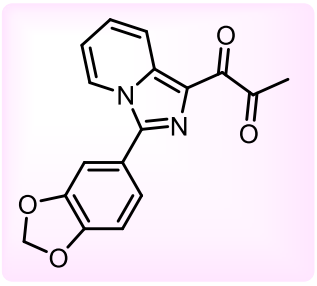
***1-(3-phenylimidazo[1,5-a]pyridin-1-yl)propane-1,2-dione* (5m)**



Following GP3, the compound **5m** was obtained as yellow semi-solid (54 mg, 79%); **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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,

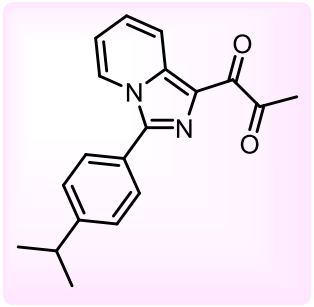
116.0, 27.3 ppm; **HRMS (ESI) m/z:** calcd. for $C_{16}H_{13}N_2O_2$ $[M+H]^+$: 265.0977, found: 265.0972

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



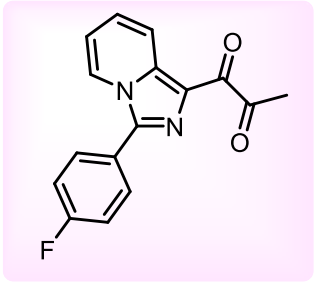
Following GP3, the compound **5n** was obtained as yellow semi-solid (54 mg, 83%); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.40 (d, J = 8.94 Hz, 1H), 8.35 (d, J = 7.05 Hz, 1H), 7.36-7.32 (m, 1H), 7.25-7.22 (m, 1H), 7.21 (d, J = 1.67 Hz, 1H), 6.97-6.93 (m, 2H), 6.02 (s, 2H), 2.59 (s, 3H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{17}H_{13}N_2O_4$ $[M+H]^+$: 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%); **^{1}H NMR (400 MHz, $CDCl_3$):** 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; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{19}H_{19}N_2O_2$ $[M+H]^+$: 307.1447 found: 307.1443

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



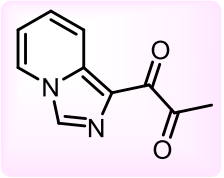
Following GP3, the compound **5p** was obtained as yellow solid (54 mg, 81%), m.p.= 114-116 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.44 (dd, J = 9.13, 0.85 Hz, 1H), 8.35 (td, J = 7.09, 1.05 Hz, 1H), 7.82-7.77 (m, 2H), 7.41-7.37 (m, 1H), 7.30-7.28 (m, 2H), 7.02-6.99 (m, 1H), 2.63 (s, 3H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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; **^{19}F NMR (377 MHz, $CDCl_3$):** -109.53 to -

109.60 (m) ppm; **HRMS (ESI) m/z:** calcd. for $C_{16}H_{12}N_2O_2F$ $[M+H]^+$: 283.0883, found: 283.0887

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

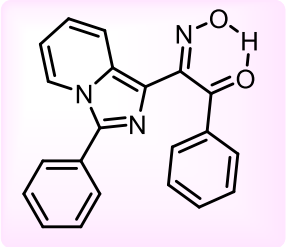
Following GP3, the compound **5q** was obtained as yellow solid (52 mg, 80%), m.p.= 108-110 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.43 (td, J = 9.05, 0.86 Hz, 1H), 8.36-8.34 (m, 1H), 7.75-7.71 (m, 2H), 7.56-7.52 (m, 2H), 7.39-7.35 (m, 1H), 7.00-6.96 (m, 1H), 2.60 (s, 3H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 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 $C_{16}H_{12}N_2O_2Cl$ $[M+H]^+$: 299.0587, found: 299.0585

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



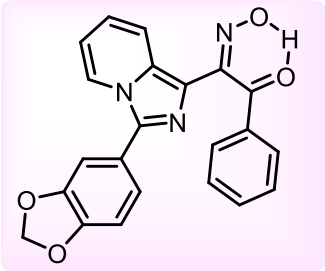
Following GP3, the compound **5r** was obtained as yellow semi-solid (68 mg, 85%); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 9.55 (dd, J = 7.03, 0.84 Hz, 1H), 7.76 (d, J = 8.86 Hz, 2H), 7.35-7.31 (m, 1H), 7.13 (t, J = 6.94 Hz, 1H), 2.60 (s, 3H) ppm; **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** δ 200.6, 181.1, 135.8, 131.7, 126.7, 126.4, 126.3, 118.4, 117.5, 27.1 ppm; **HRMS (ESI) m/z:** calcd. for $C_{10}H_9N_2O_2$ $[M+H]^+$: 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%); **^{1}H NMR (400 MHz, DMSO-d_6):** 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; **^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6):** 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 $C_{21}H_{16}N_3O_2$ $[M+H]^+$: 342.1243, found: 342.1252

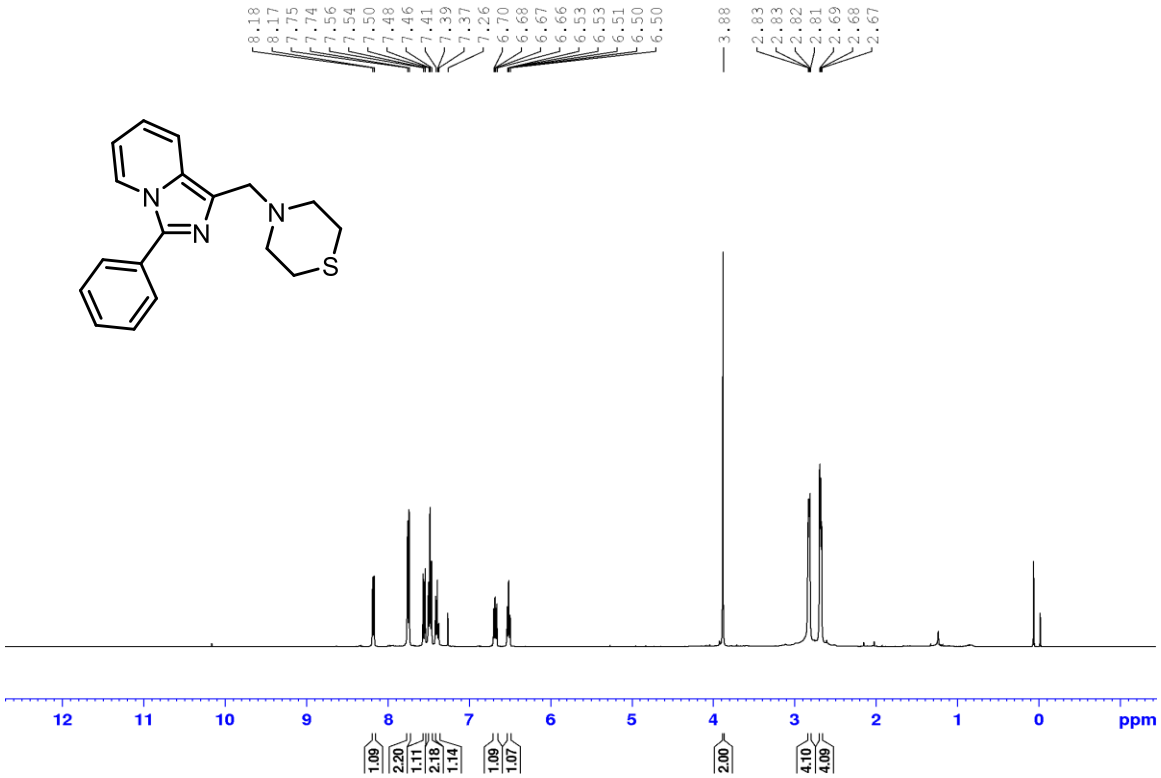
(Z)-2-(3-(benzo[d][1,3]dioxol-5-yl)imidazo[1,5-a]pyridin-1-yl)-2-(hydroxyimino)-1-phenylethan-1-one **(6b)**



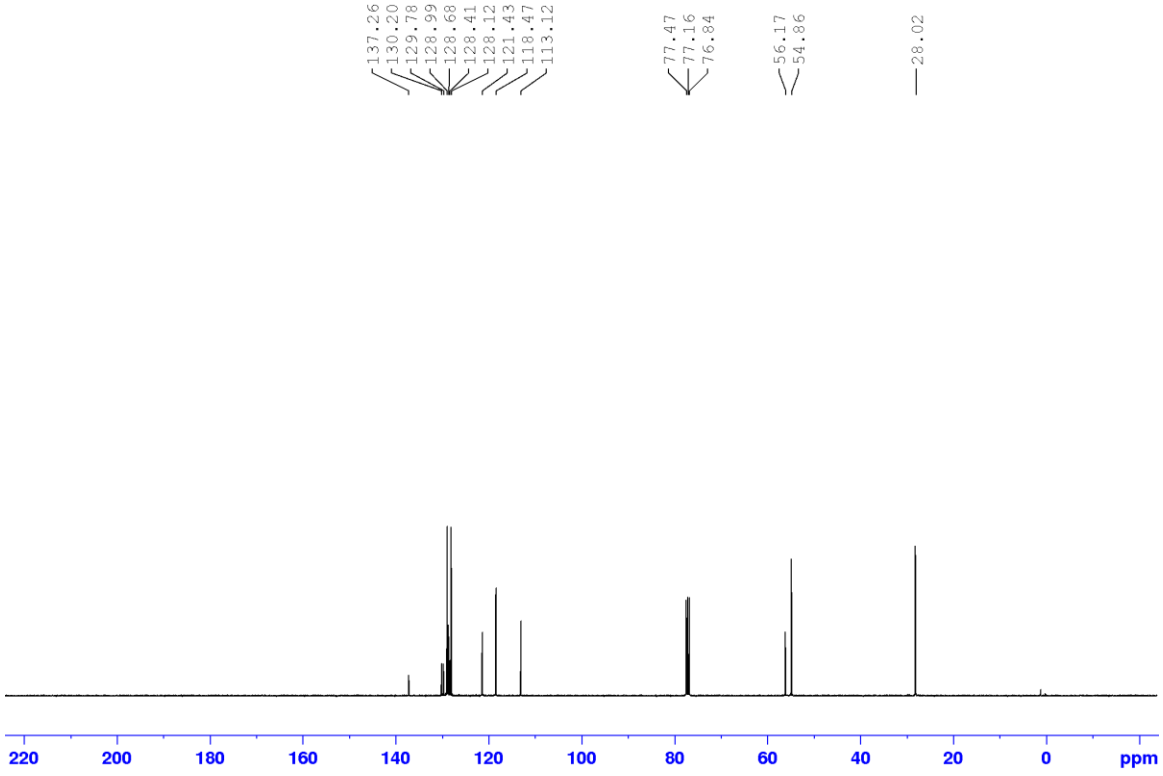
Following GP4, the compound **6b** was obtained as yellow solid (40 mg, 77%); **^{1}H NMR (400 MHz, $CDCl_3$ and DMSO-d_6):** δ 11.03 (d, J = 8.99 Hz, 1H), 8.33 (t, J = 6.18 Hz, 2H), 7.66-7.63 (m, 1H), 7.57-7.55 (m, 2H), 7.27-7.24 (m, 3H), 7.14-7.11 (m, 1H), 7.08-7.07 (m, 1H), 6.92-6.86 (m, 2H), 5.99-5.97 (m, 2H) ppm; **^{13}C{^{1}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 $C_{22}H_{16}N_3O_4$ $[M+H]^+$: 386.3790, found: 386.3792

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

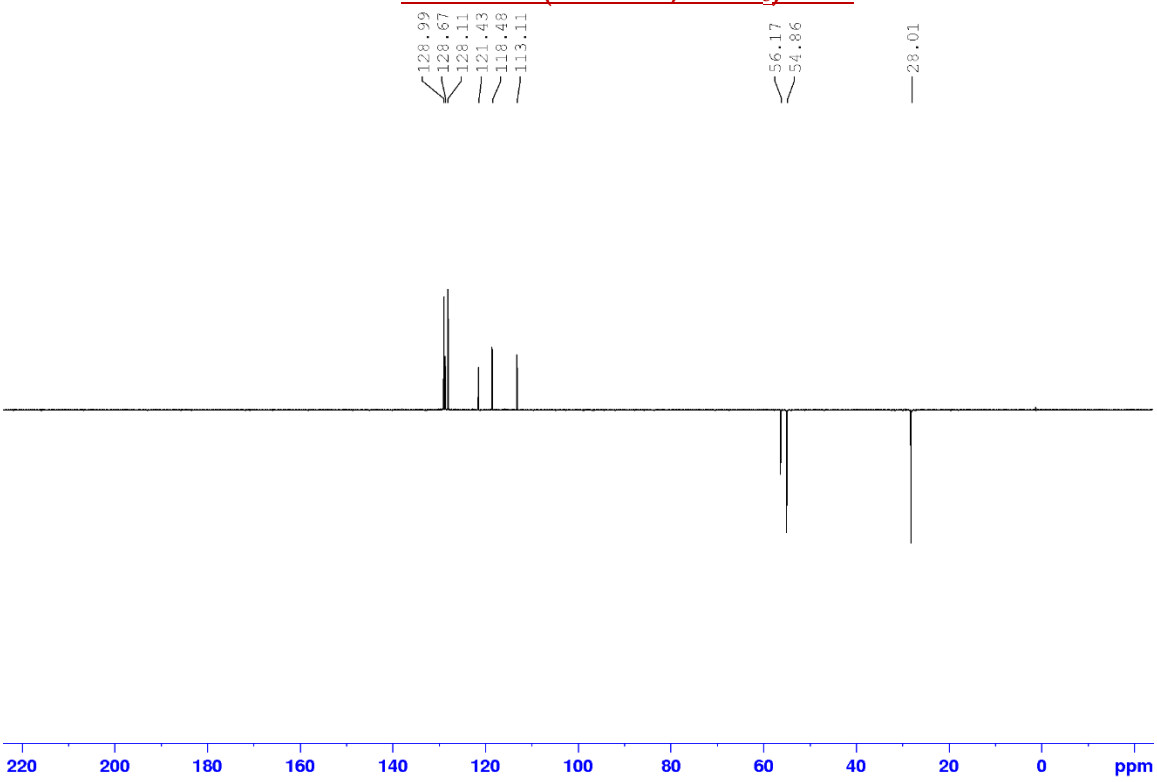
^{1}H NMR (400 MHz, $CDCl_3$) of 3a



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



DEPT-135 (101 MHz, $CDCl_3$) of 3a



HRMS of 3a

Elemental Composition Report **Page 1**

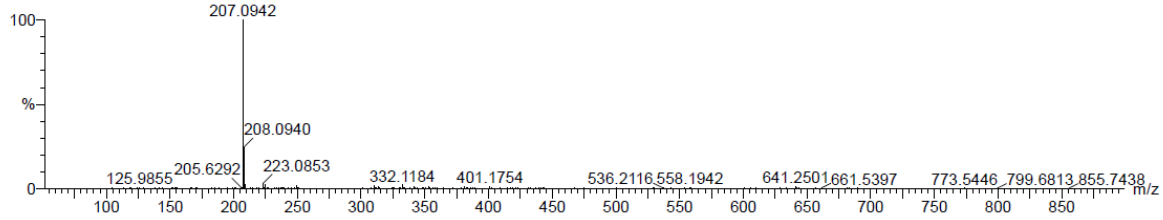
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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
230424_06 5 (0.121)

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

23-Apr-2024
12:22:54
1: TOF MS ES+
2.52e+007



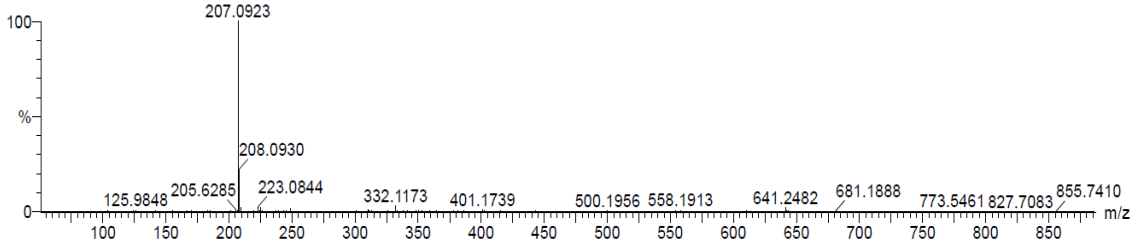
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
332.1184	332.1197	-1.3	-3.9	10.5	1145.4	n/a	n/a	C18 H19 N3 S Na

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

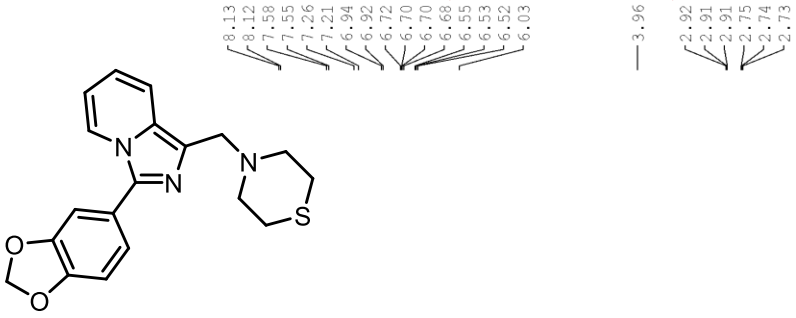
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2

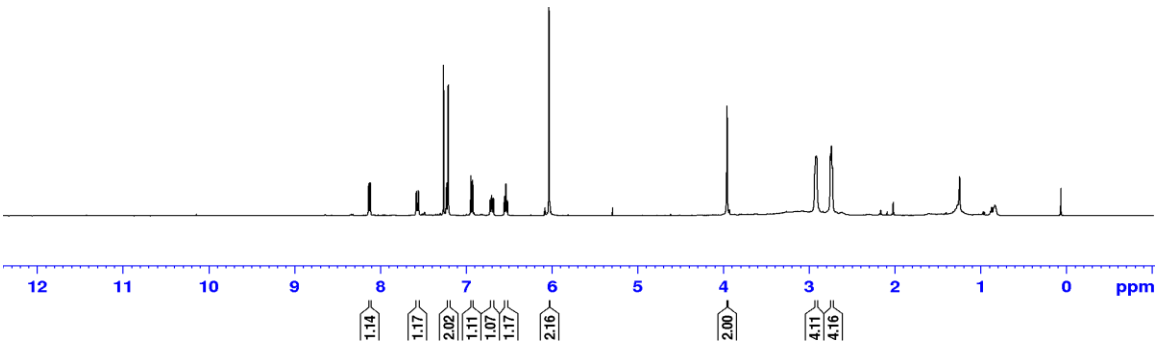
SM-334 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:22:54
230424_06 7 (0.155) 1: TOF MS ES+
2.44e+007



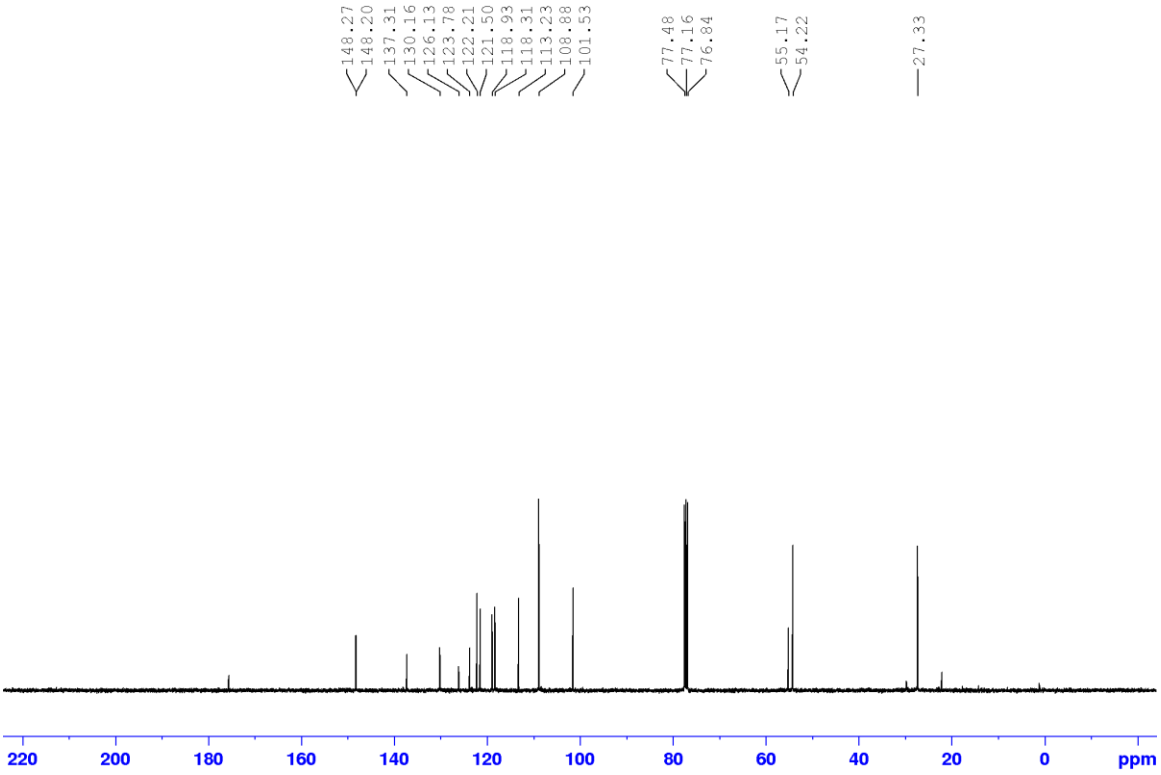
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
207.0923	207.0922	0.1	0.5	10.5	1517.9	n/a	n/a	C14 H11 N2

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

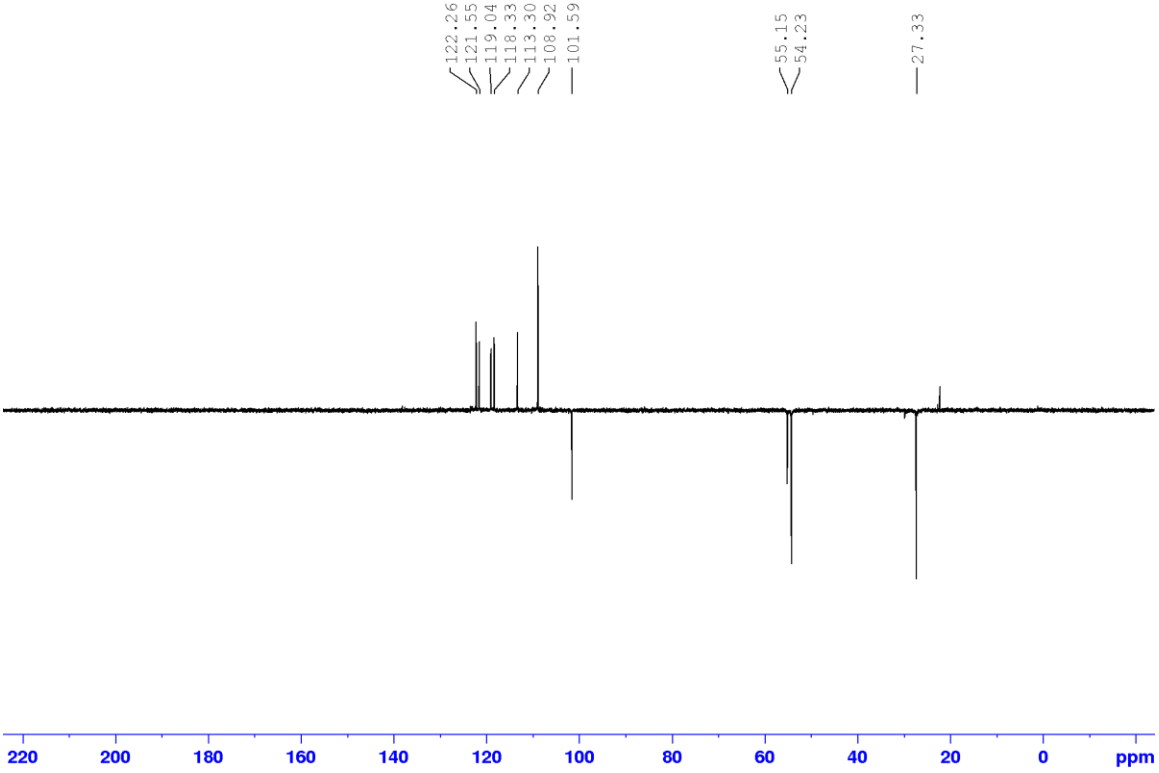




$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3b



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



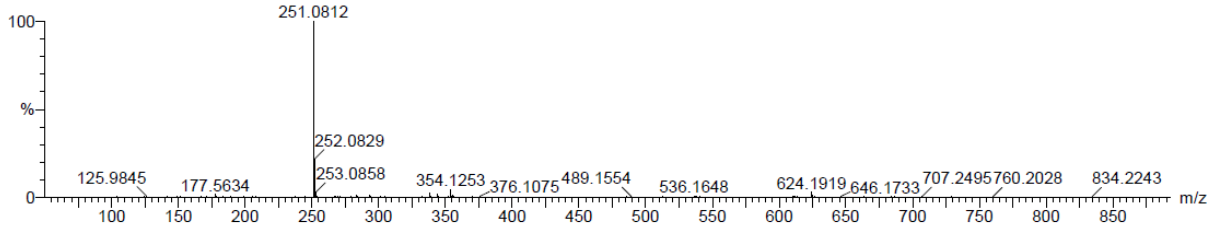
HRMS of 3b

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

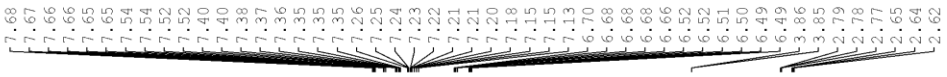
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-2 O: 0-2

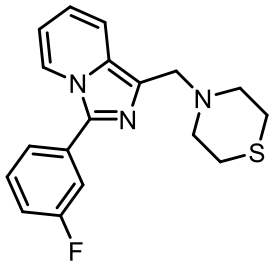
SM-520 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 14:31:09
070524_36 5 (0.121) 1: TOF MS ES+
1.76e+007

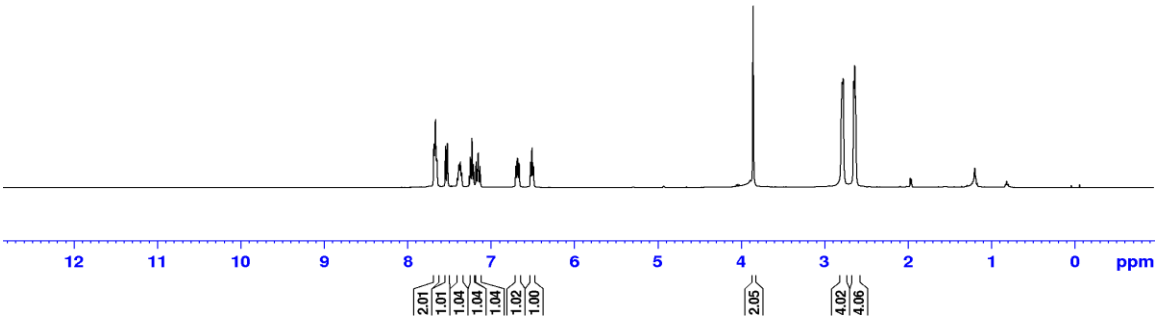


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
251.0812	251.0821	-0.9	-3.6	11.5	1201.2	n/a	n/a	C15 H11 N2 O2

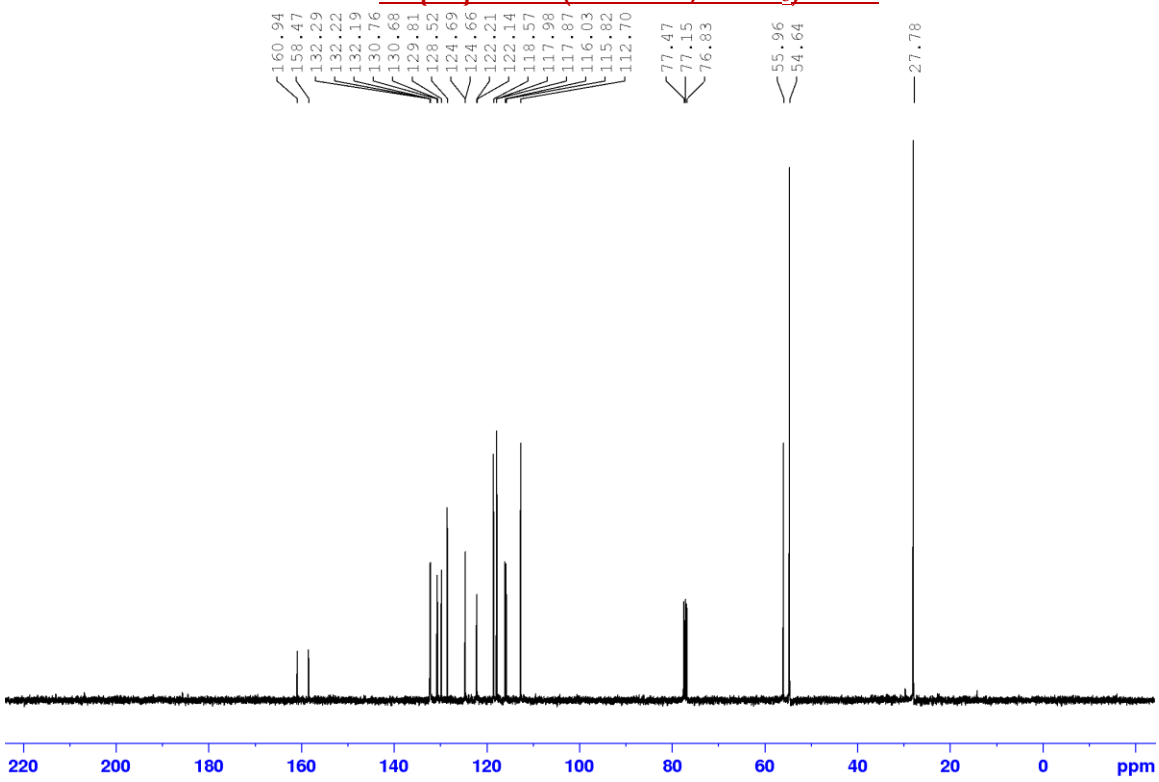
^{1}H NMR (400 MHz, $CDCl_3$) of 3c



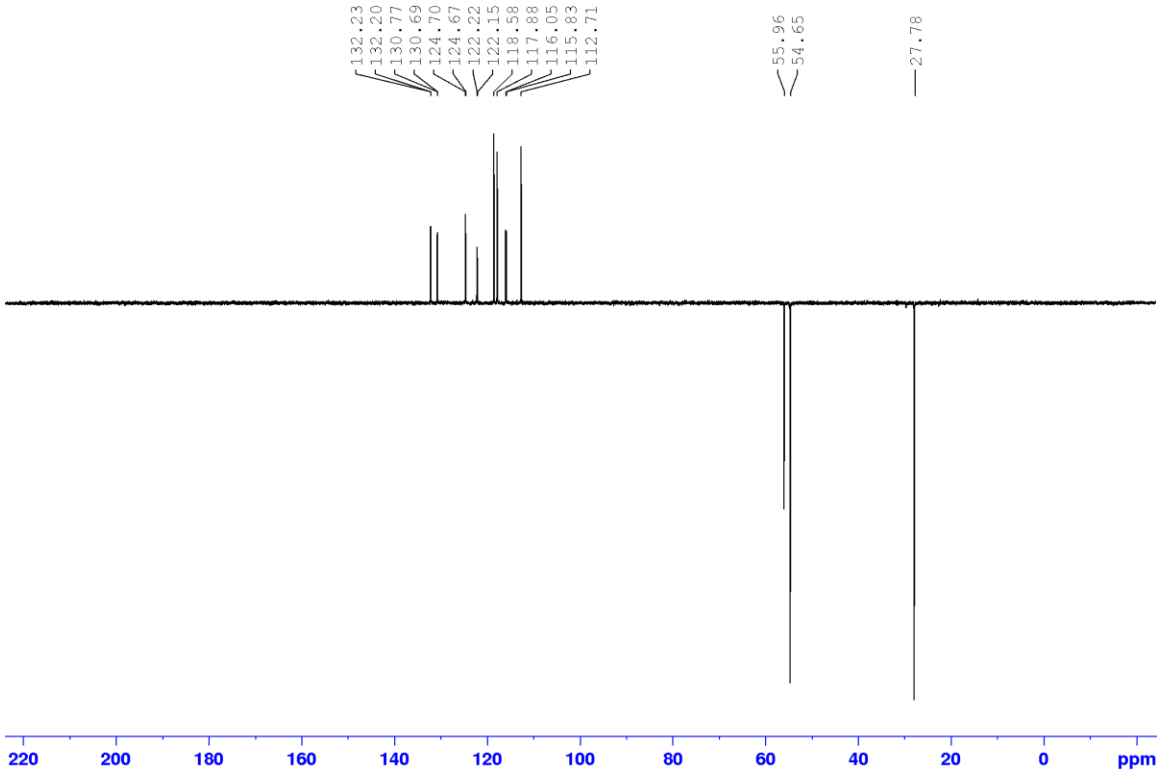




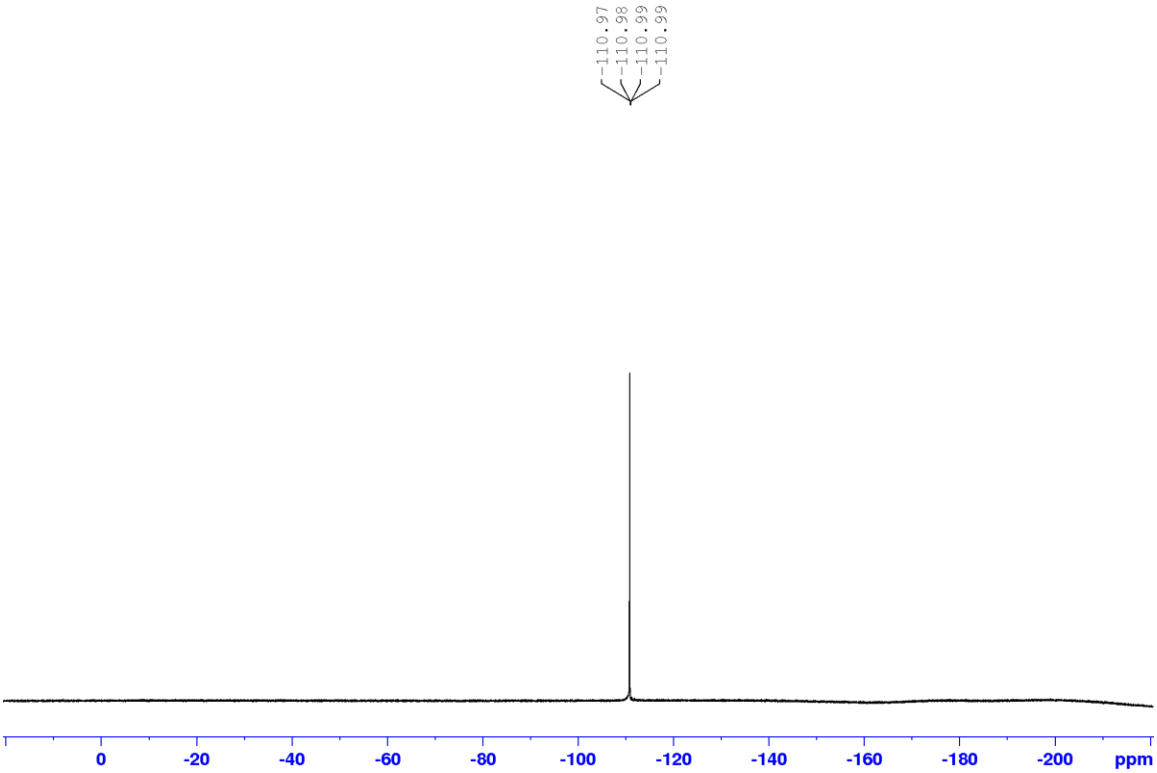
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3c



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



^{19}F NMR (377 MHz, $CDCl_3$) of 3c



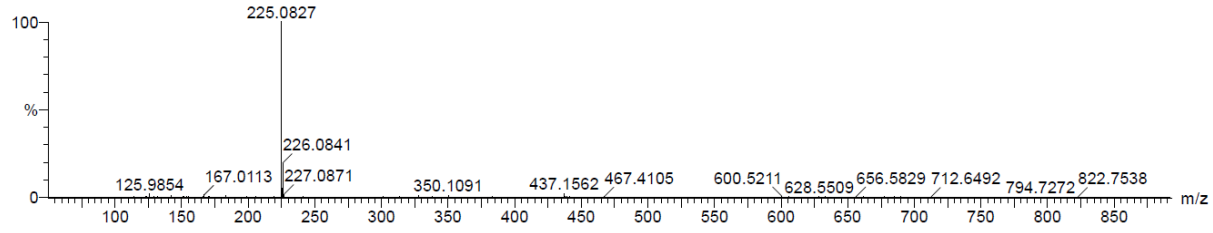
HRMS of 3c

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

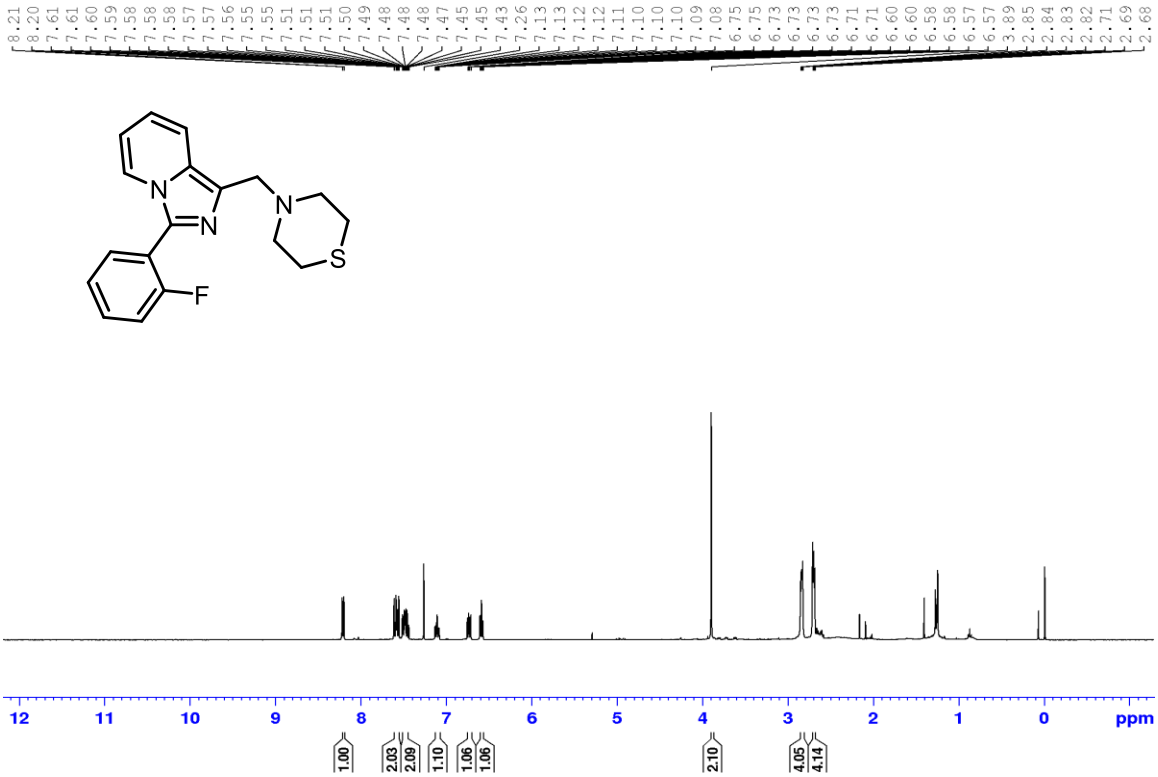
Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2 F: 0-1

SM-378 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:33:19
230424_10 4 (0.104) 1: TOF MS ES+
9.41e+006

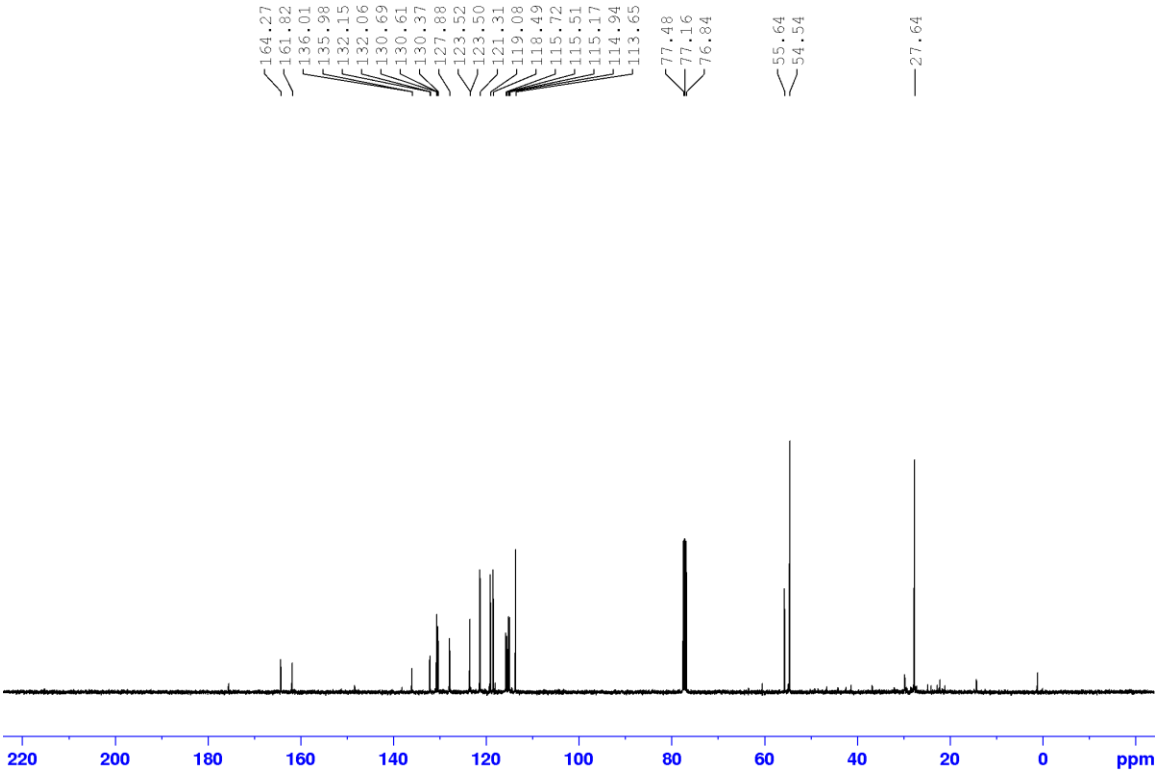


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
225.0827	225.0828	-0.1	-0.4	10.5	1384.3	n/a	n/a	C14 H10 N2 F

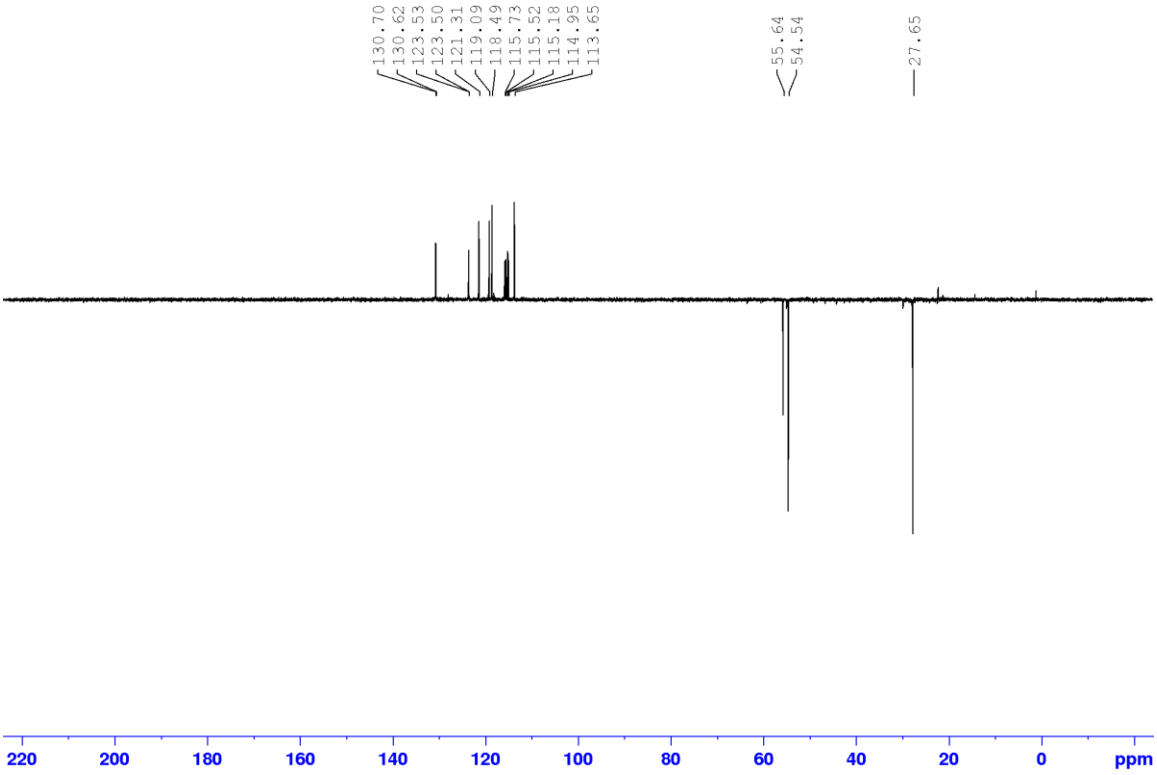
^{1}H NMR (400 MHz, $CDCl_3$) of 3d



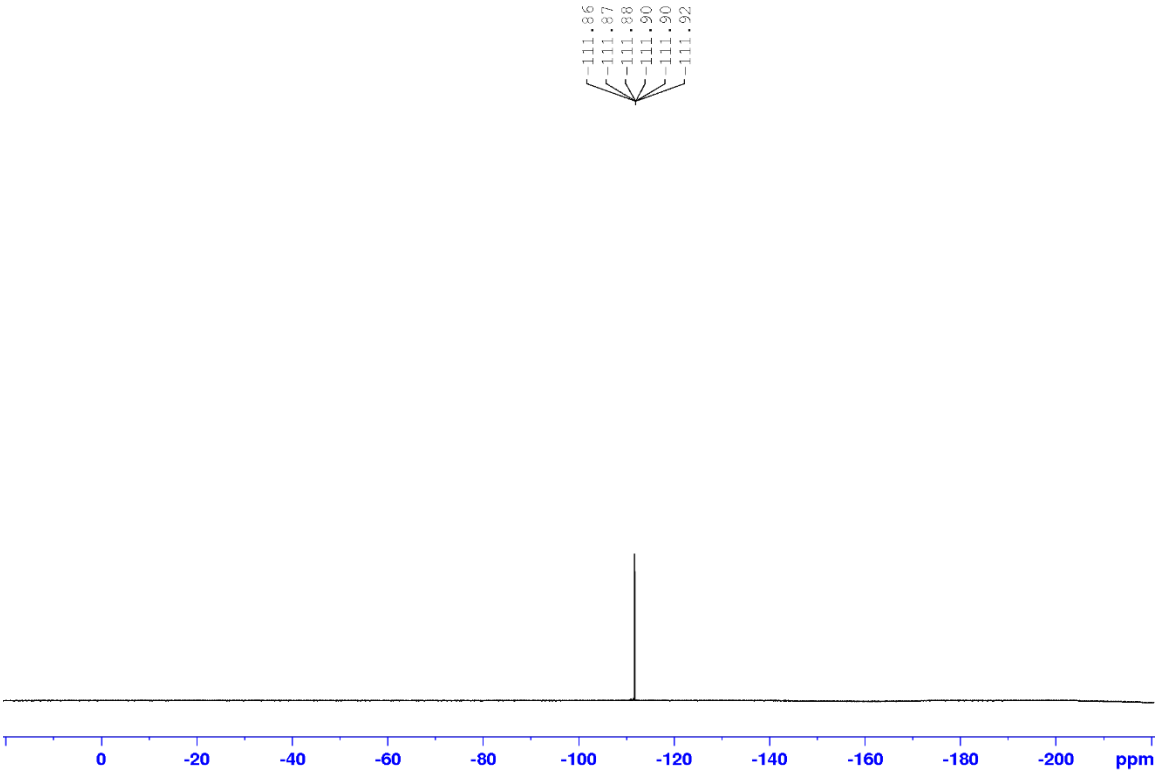
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3d



DEPT-135 (400 MHz, $CDCl_3$) of 3d



^{19}F NMR (377 MHz, $CDCl_3$) of 3d



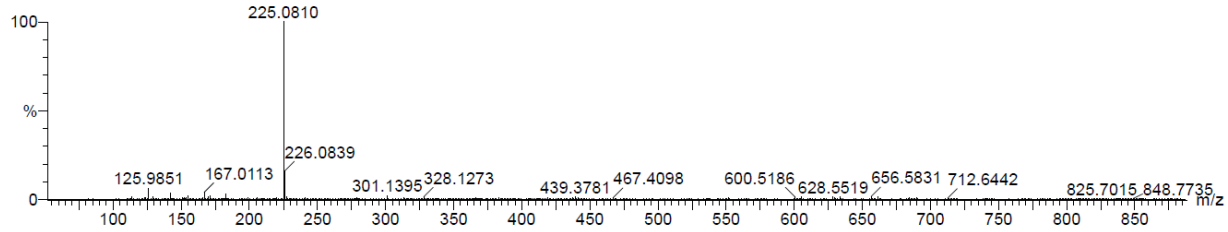
HRMS of 3d

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 23-Apr-2024
Xevo G2-XS QTOF YFC2015 13:00:06
230424_20 4 (0.104) 1: TOF MS ES+
3.02e+006



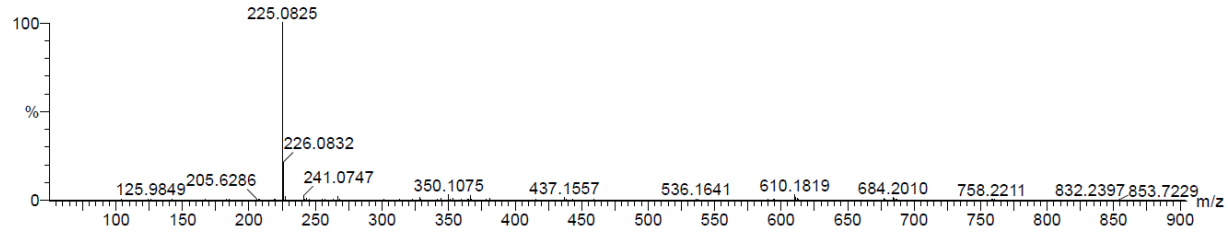
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
328.1273	328.1284	-1.1	-3.4	10.5	1134.8	n/a	n/a	C18 H19 N3 S F

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

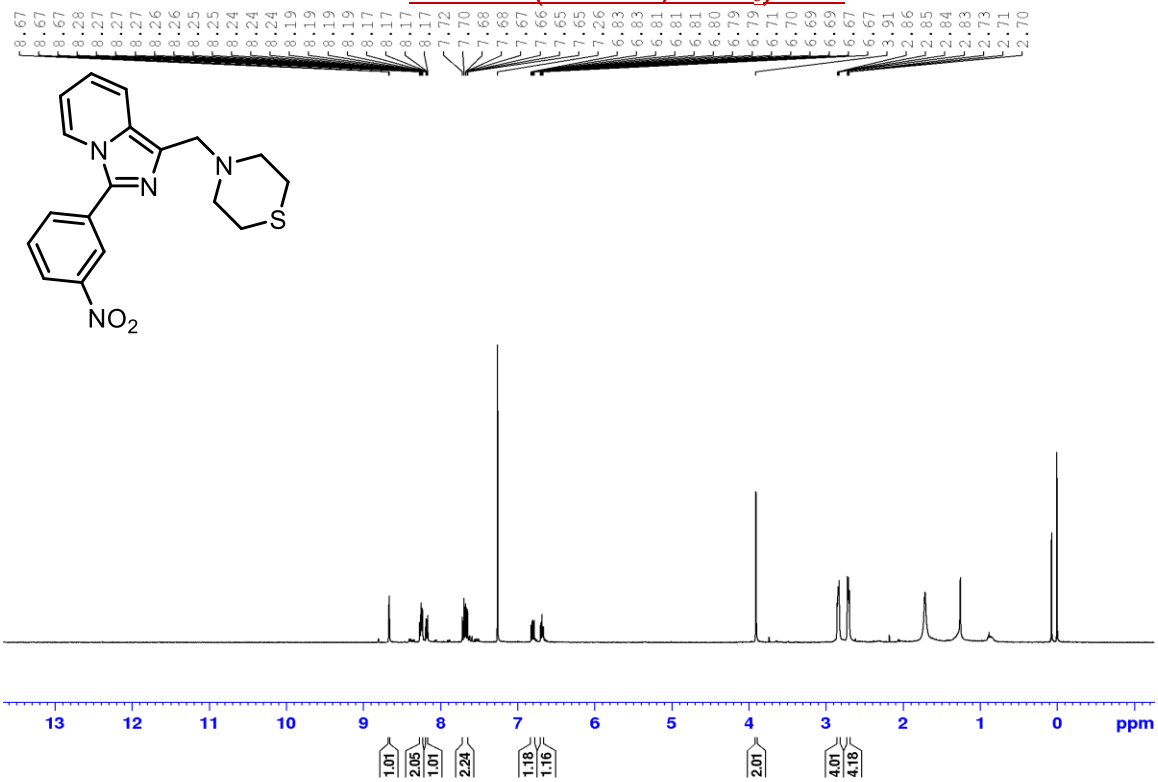
Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2 F: 0-1

SM-379 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 13:00:06
230424_20 7 (0.155) 1: TOF MS ES+
2.28e+007

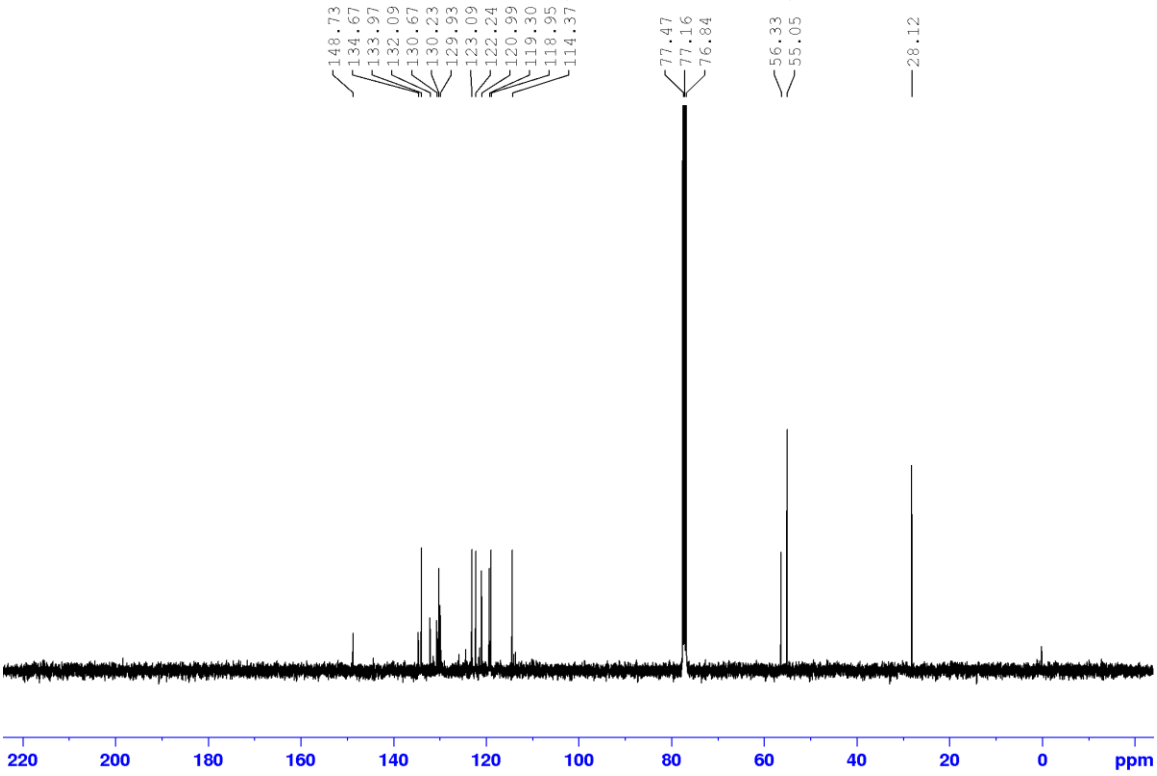


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
225.0825	225.0828	-0.3	-1.3	10.5	1403.5	n/a	n/a	C14 H10 N2 F

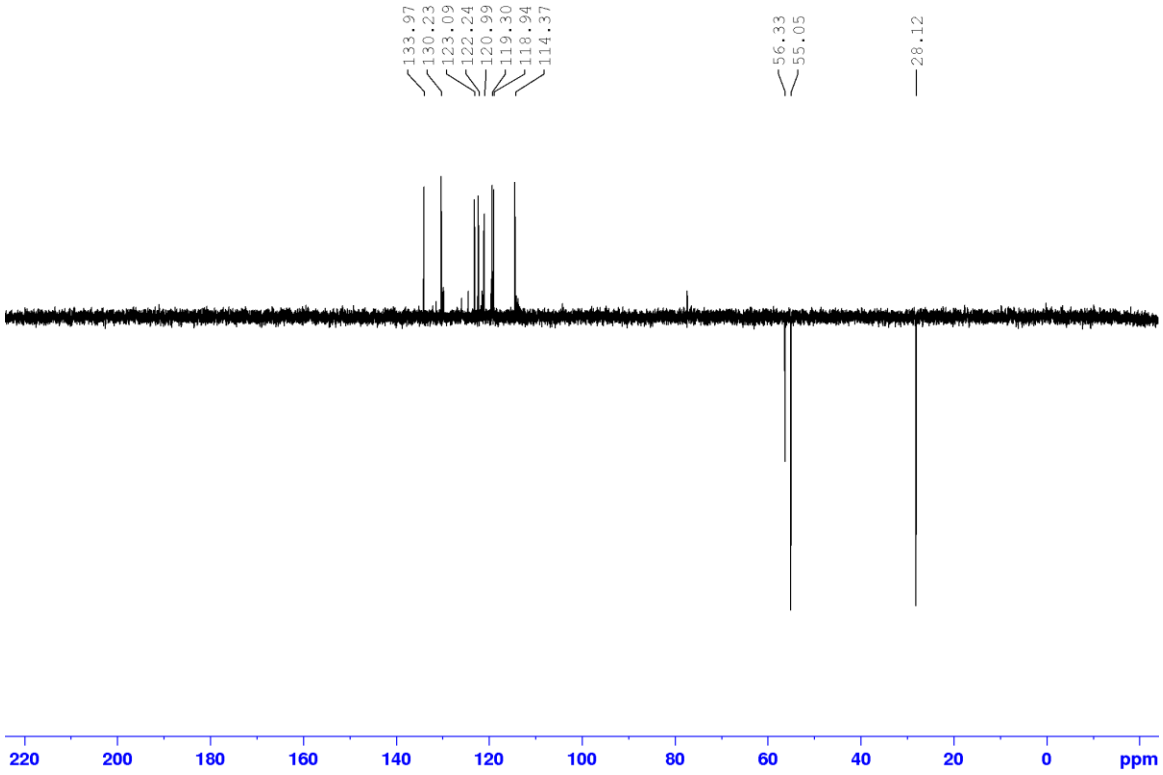
^{1}H NMR (400 MHz, $CDCl_3$) of 3e



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



DEPT-135 (400 MHz, $CDCl_3$) of 3e



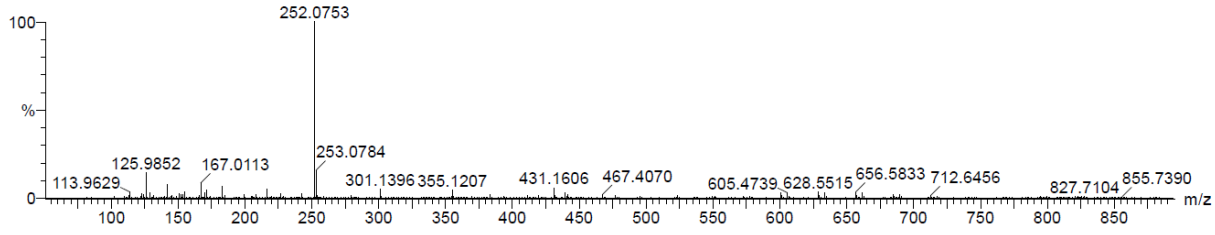
HRMS of 3e

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 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:52:14
230424_17 4 (0.104) 1: TOF MS ES+
1.38e+006



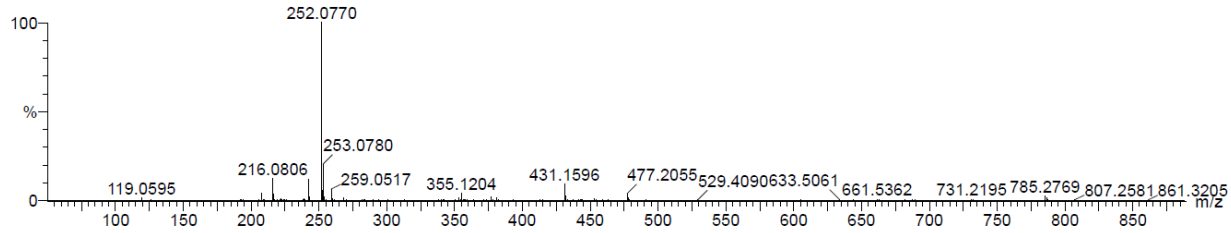
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
355.1207	355.1229	-2.2	-6.2	11.5	1058.2	n/a	n/a	C18 H19 N4 O2 S

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

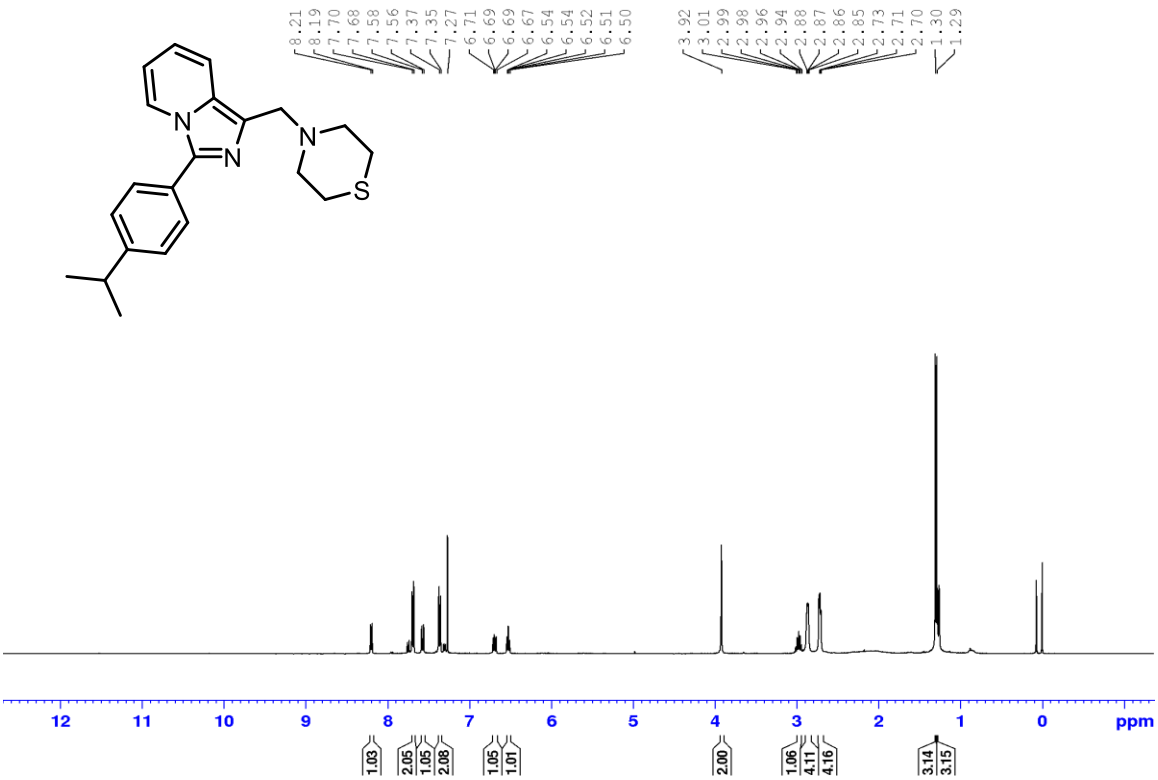
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3 O: 0-2

SM-392 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:52:14
230424_17 6 (0.138) 1: TOF MS ES+
2.66e+007

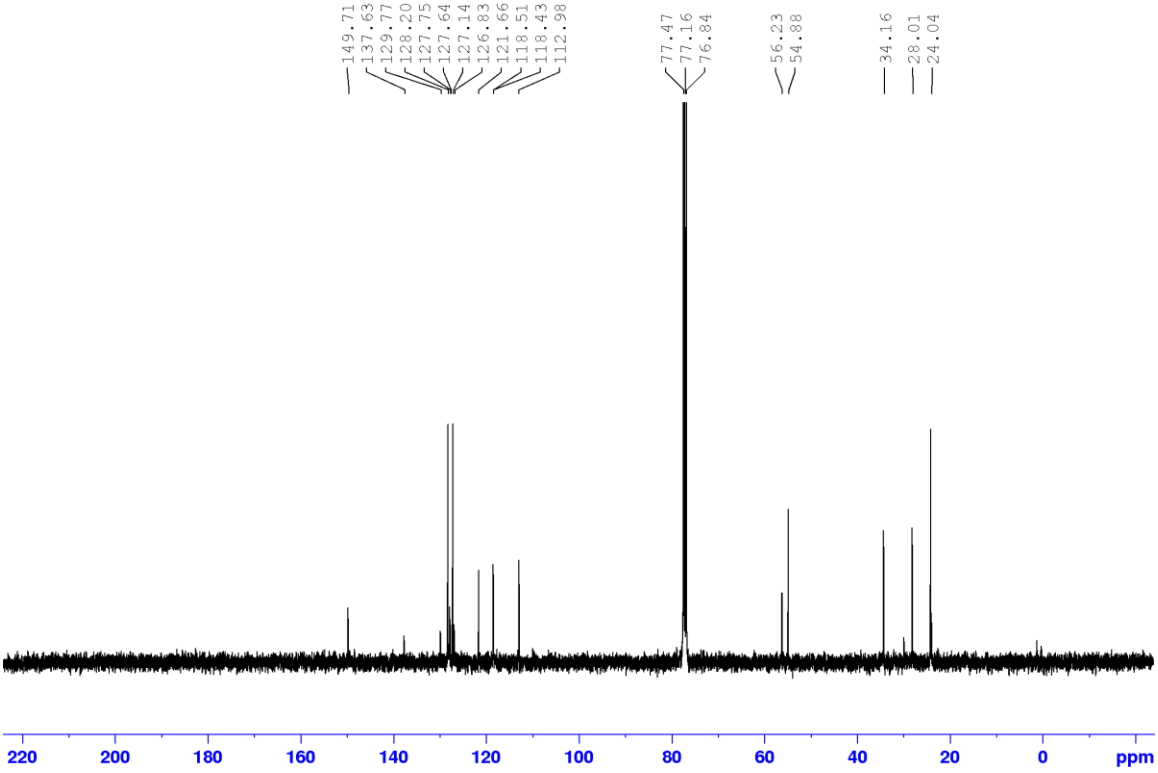


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
252.0770	252.0773	-0.3	-1.2	11.5	1342.3	n/a	n/a	C14 H10 N3 O2

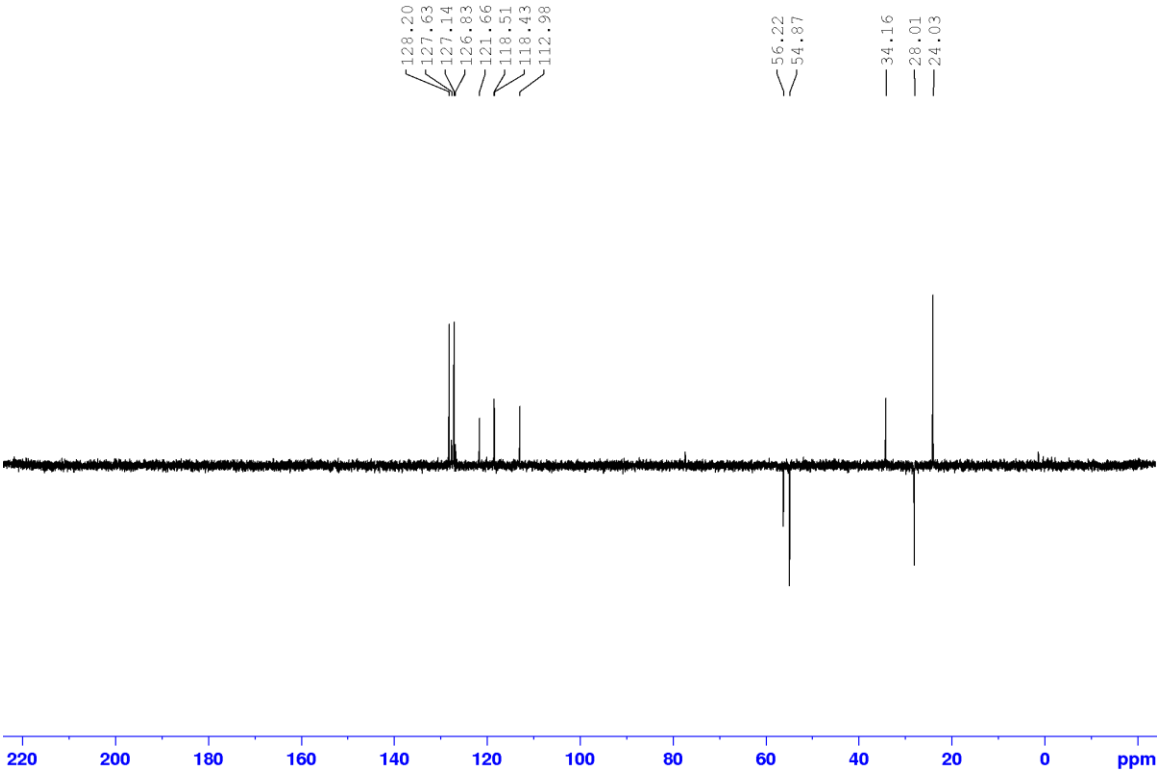
^{1}H NMR (400 MHz, $CDCl_3$) of 3f



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



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



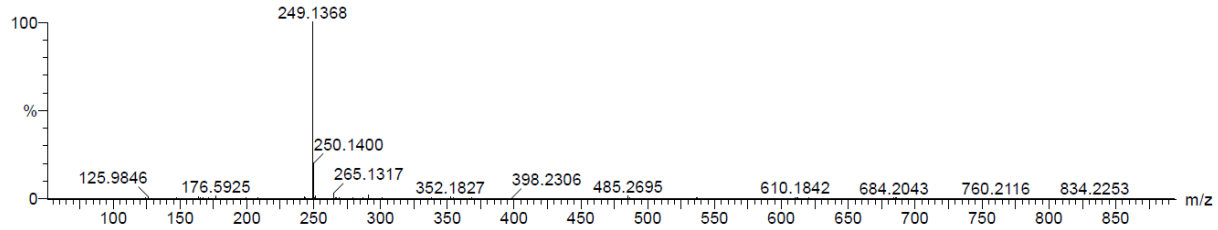
HRMS of 3f

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 07-May-2024
Xevo G2-XS QTOF YFC2015 15:16:22
070524_53 5 (0.121) 1: TOF MS ES+
6.97e+006



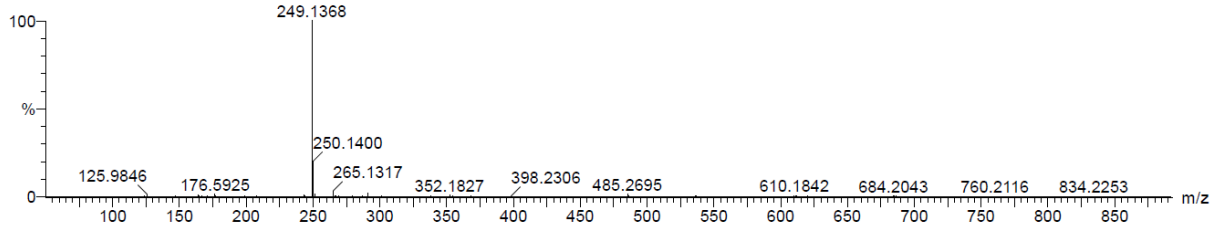
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
352.1827	352.1847	-2.0	-5.7	10.5	891.0	n/a	n/a	C21 H26 N3 S

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

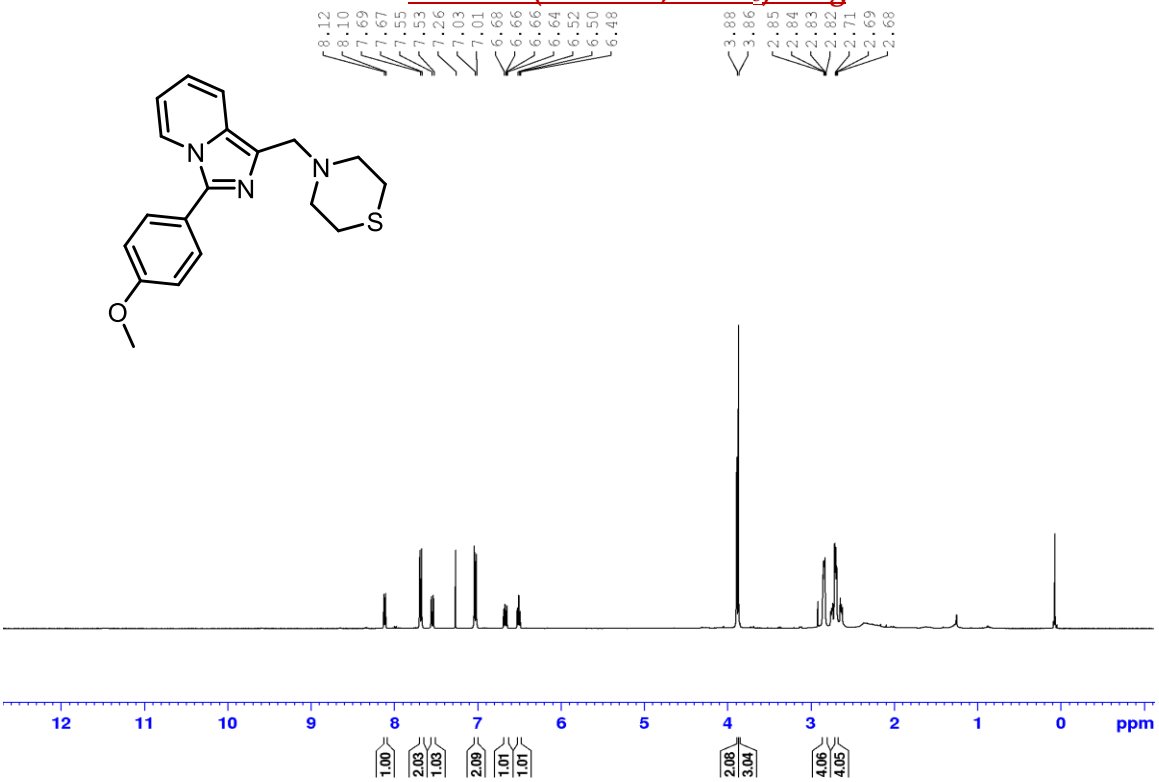
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-17 H: 0-100 N: 0-2

SM-396 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 15:16:22
070524_53 5 (0.121) 1: TOF MS ES+
6.97e+006

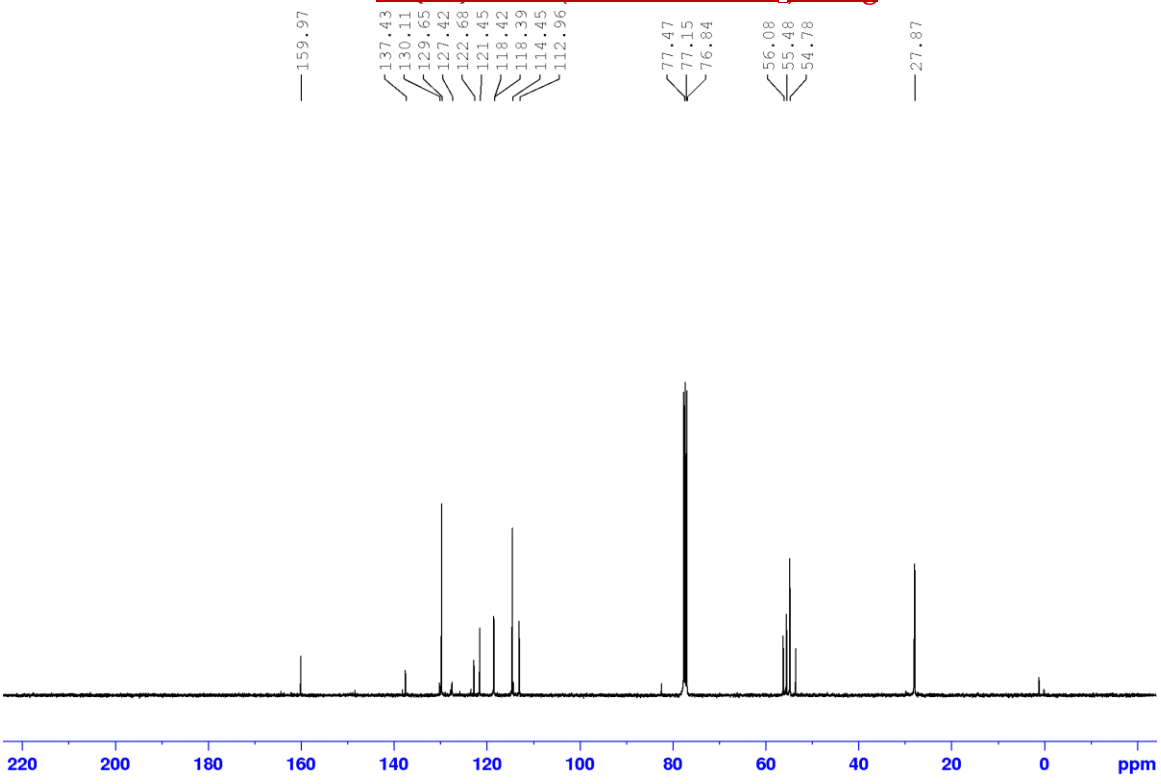


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
249.1368	249.1392	-2.4	-9.6	10.5	1207.6	n/a	n/a	C17 H17 N2

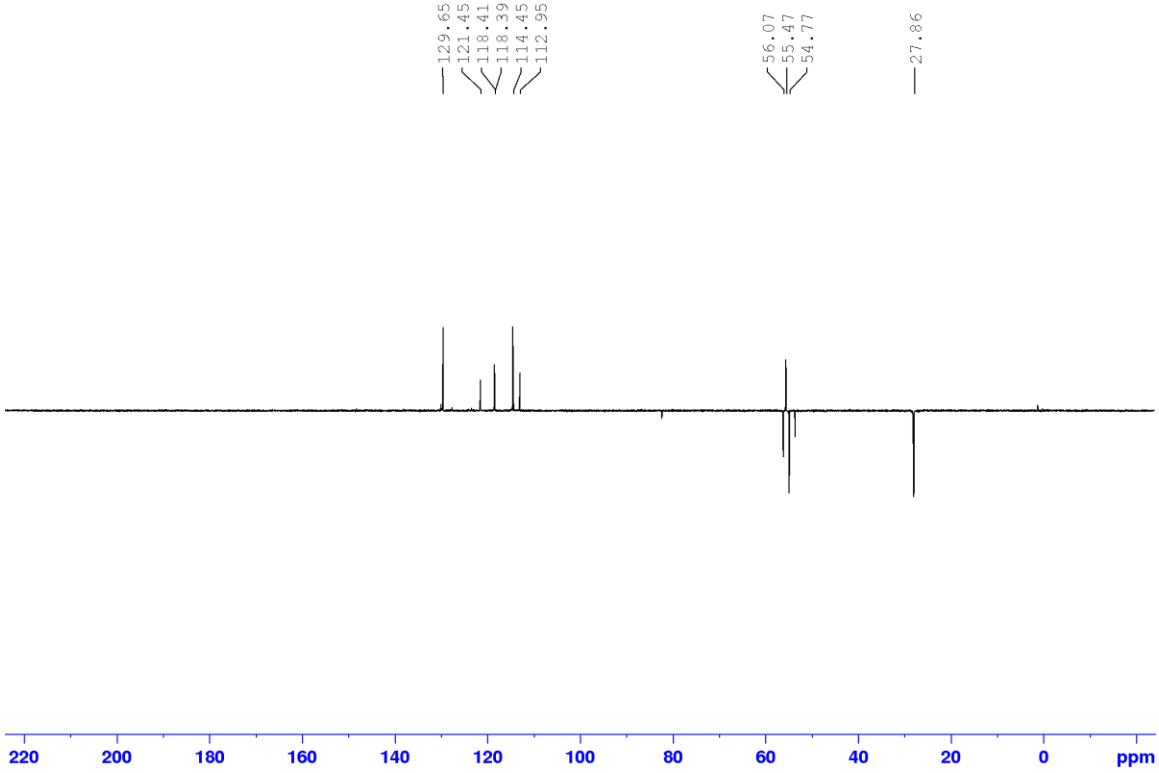
^{1}H NMR (400 MHz, $CDCl_3$) of 3g



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



DEPT-135 (400 MHz, $CDCl_3$) of 3g



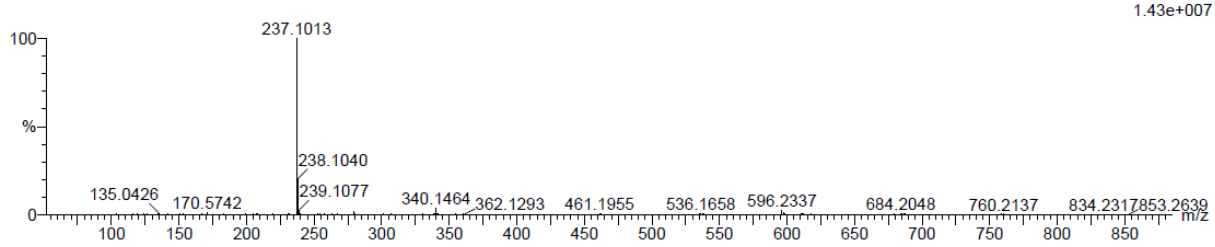
HRMS of 3g

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: 0-1 S: 0-1

SM-477 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 15:24:04
070524_56 5 (0.121) 1: TOF MS ES+
1.43e+007



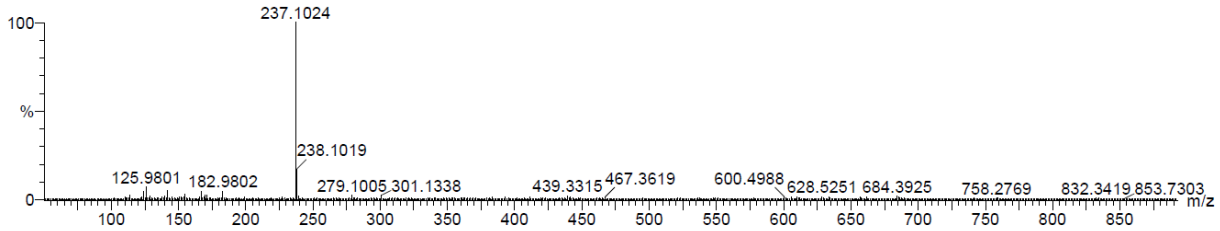
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
340.1464	340.1484	-2.0	-5.9	10.5	976.8	n/a	n/a	C19 H22 N3 O S

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

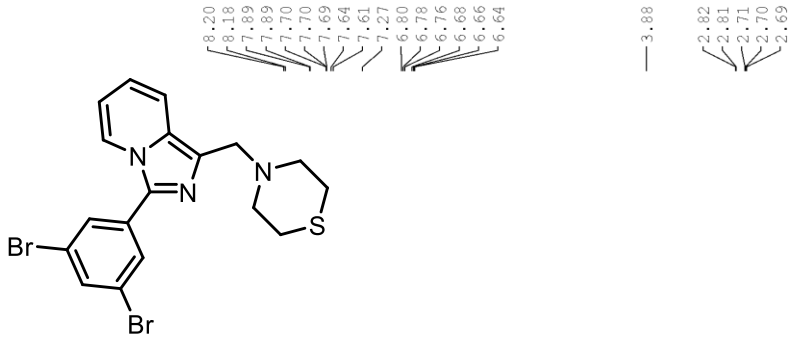
Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-2 O: 0-1

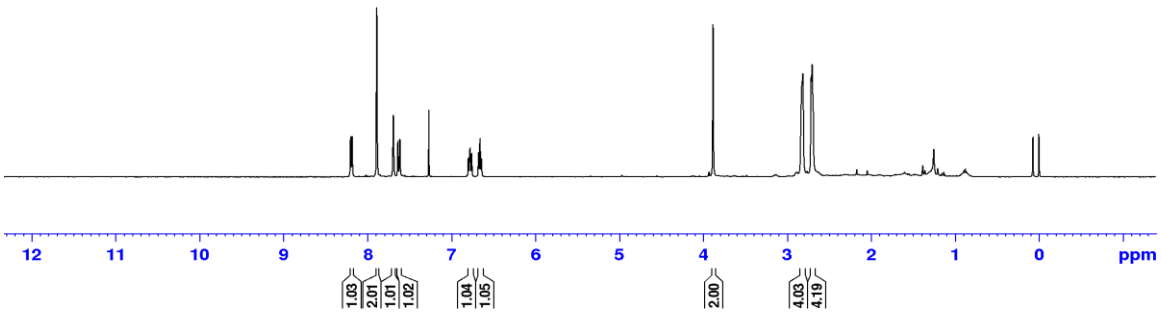
SM-477 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:12:30
230424_02 9 (0.208) Cm (9) 1: TOF MS ES+
3.40e+006



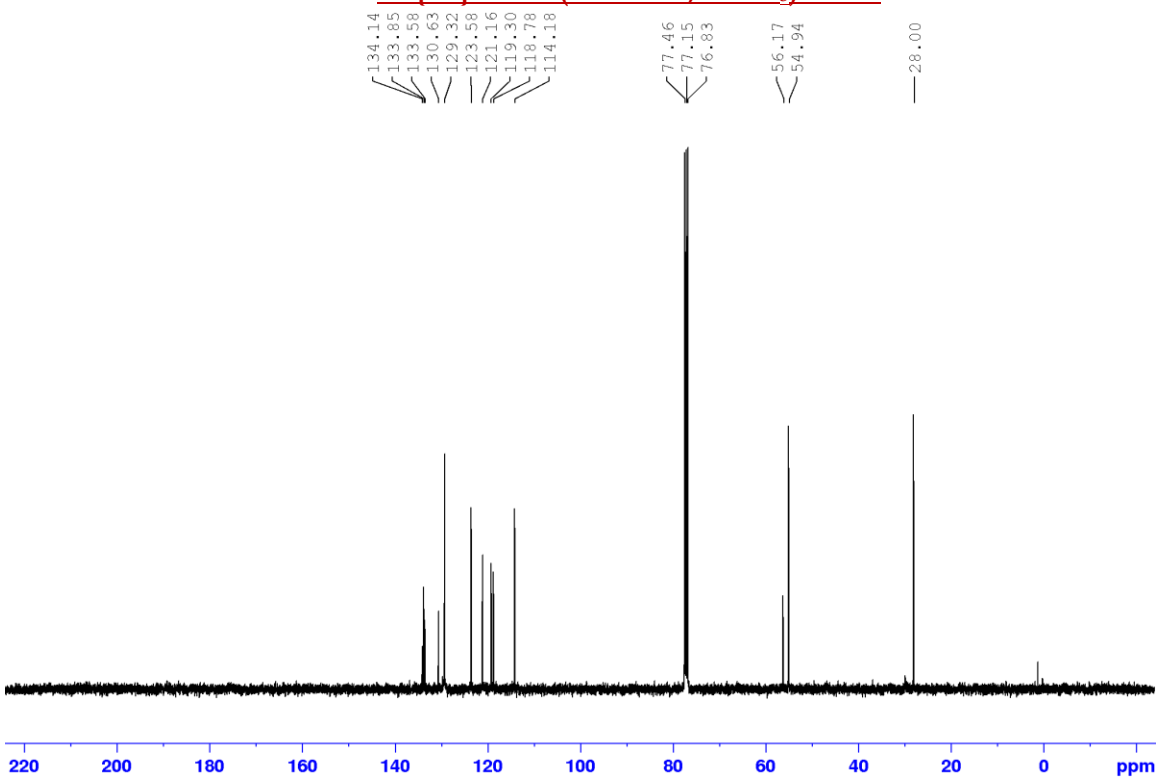
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
237.1024	237.1028	-0.4	-1.7	10.5	46.3	n/a	n/a	C15 H13 N2 O

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

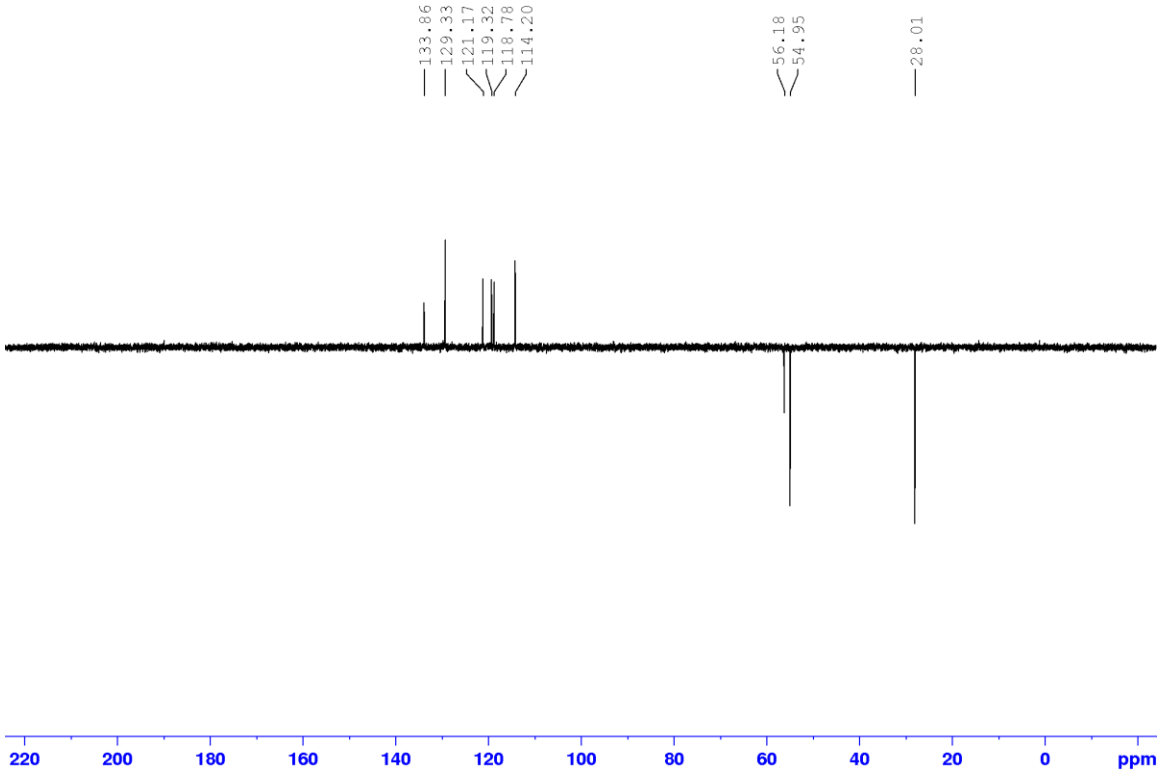




$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3h



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



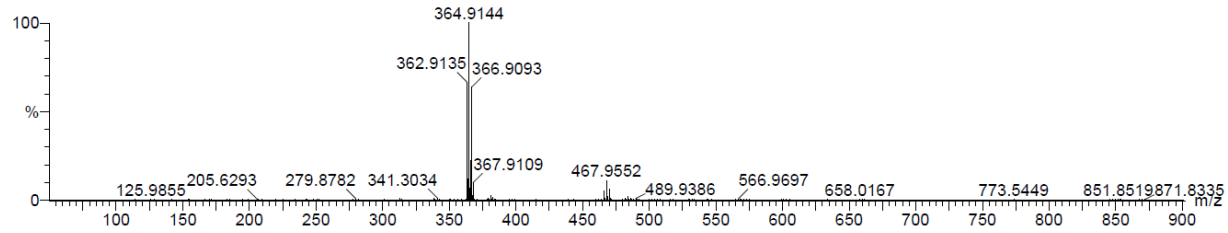
HRMS of 3h

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

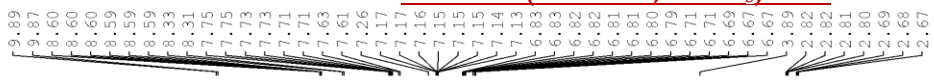
Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2 Br: 0-2

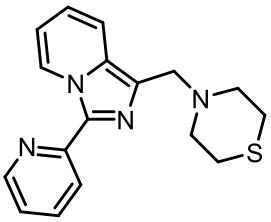
SM-381 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:43:52
230424_14 5 (0.121) 1: TOF MS ES+
2.93e+007

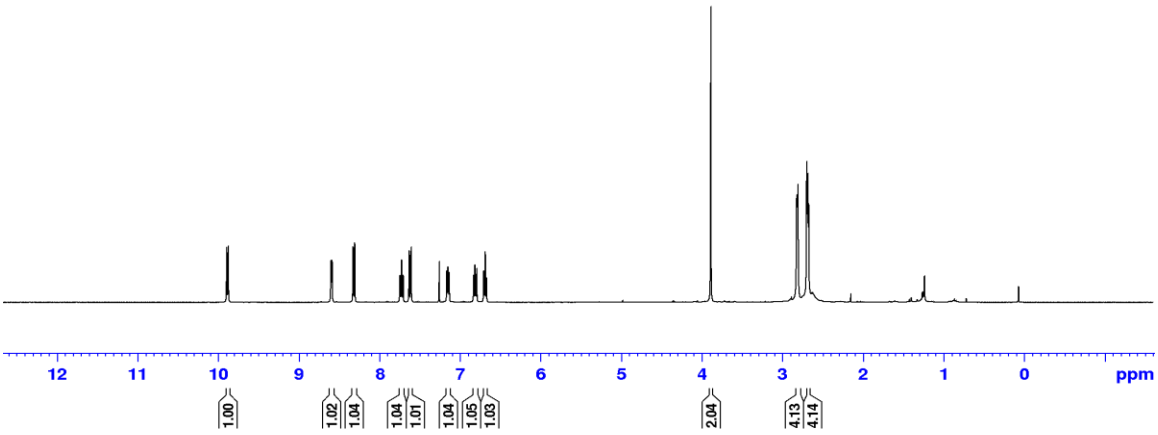


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
362.9135	362.9132	0.3	0.8	10.5	1191.1	n/a	n/a	C14 H9 N2 Br2

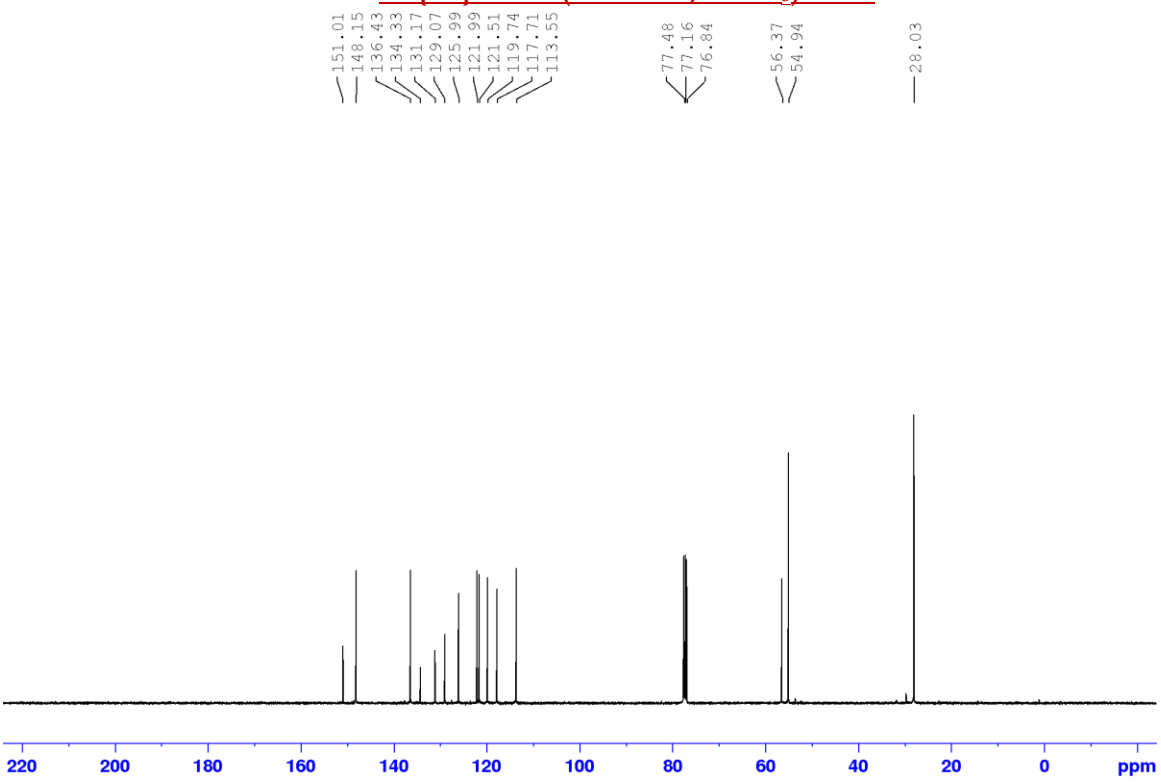
^{1}H NMR (400 MHz, $CDCl_3$) of 3i



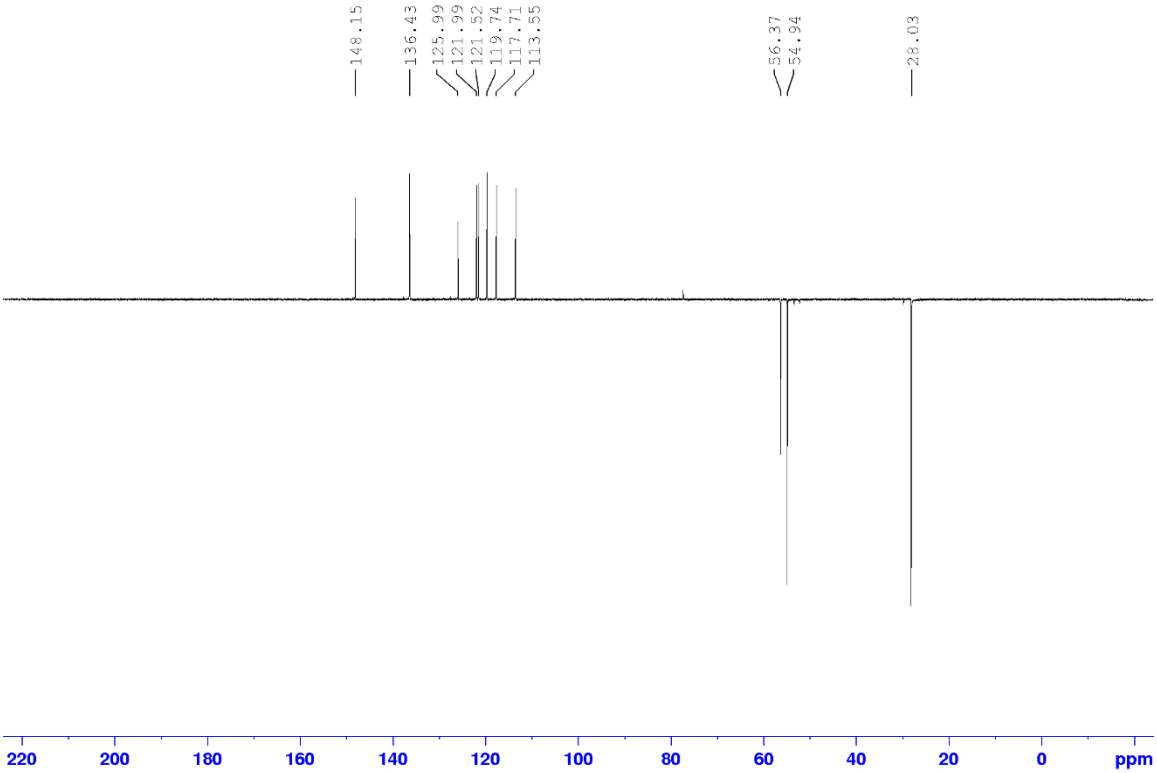




$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3i



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



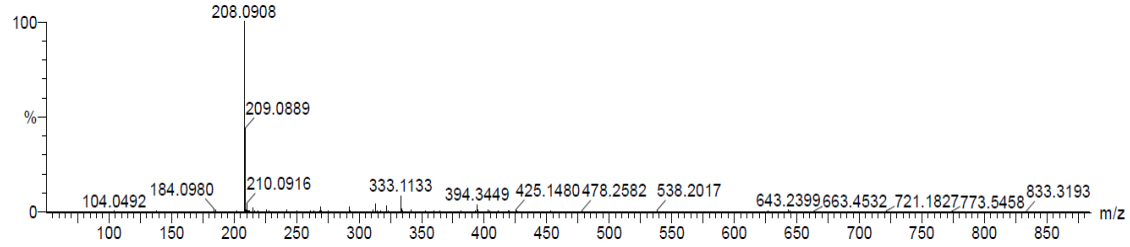
HRMS of 3i

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

SM-402 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:17:47
230424_04 5 (0.121) 1: TOF MS ES+
3.66e+007



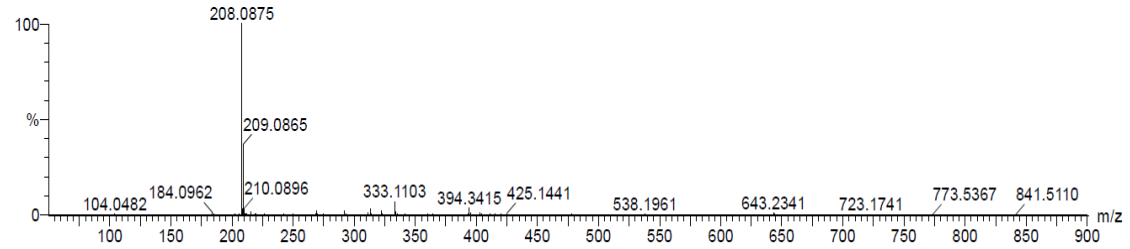
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
333.1133	333.1150	-1.7	-5.1	10.5	1204.8	n/a	n/a	C17 H18 N4 Na S

Elemental Composition Report **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

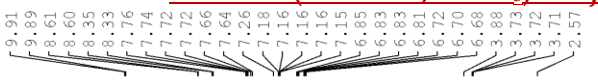
Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 N: 0-3

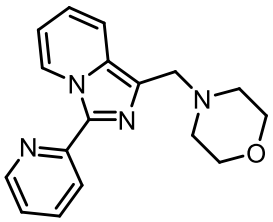
SM-402 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:17:47
230424_04 7 (0.155) 1: TOF MS ES+
4.08e+007

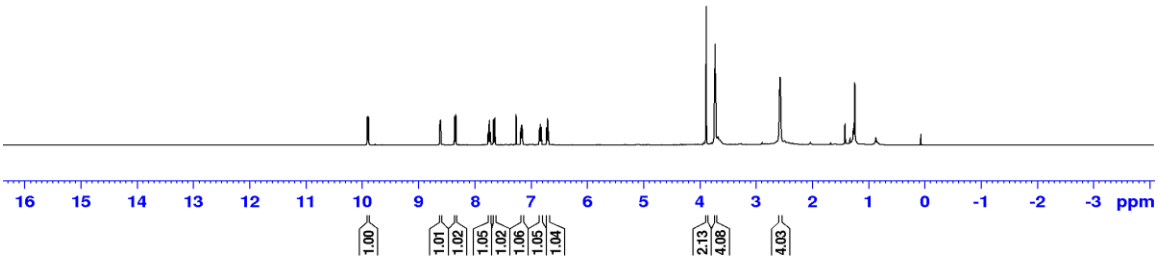


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
208.0875	208.0875	0.0	0.0	10.5	1321.5	n/a	n/a	C13 H10 N3

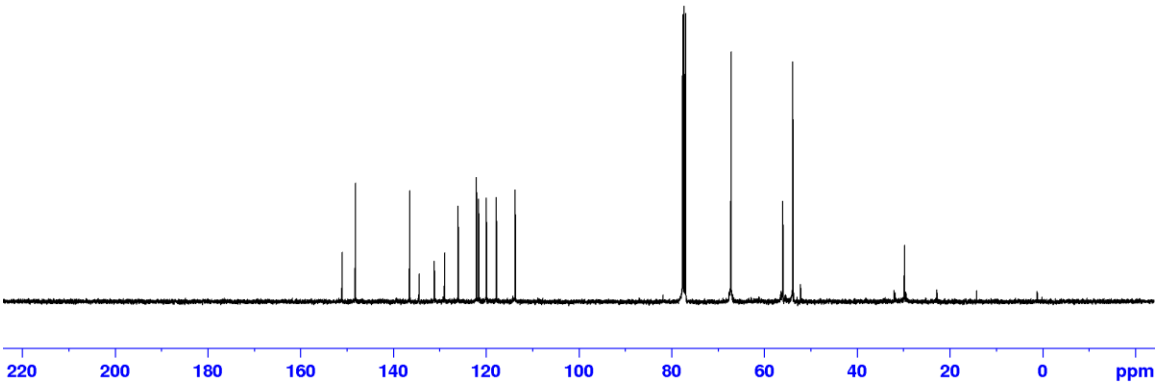
^{1}H NMR (400 MHz, $CDCl_3$) of 3j



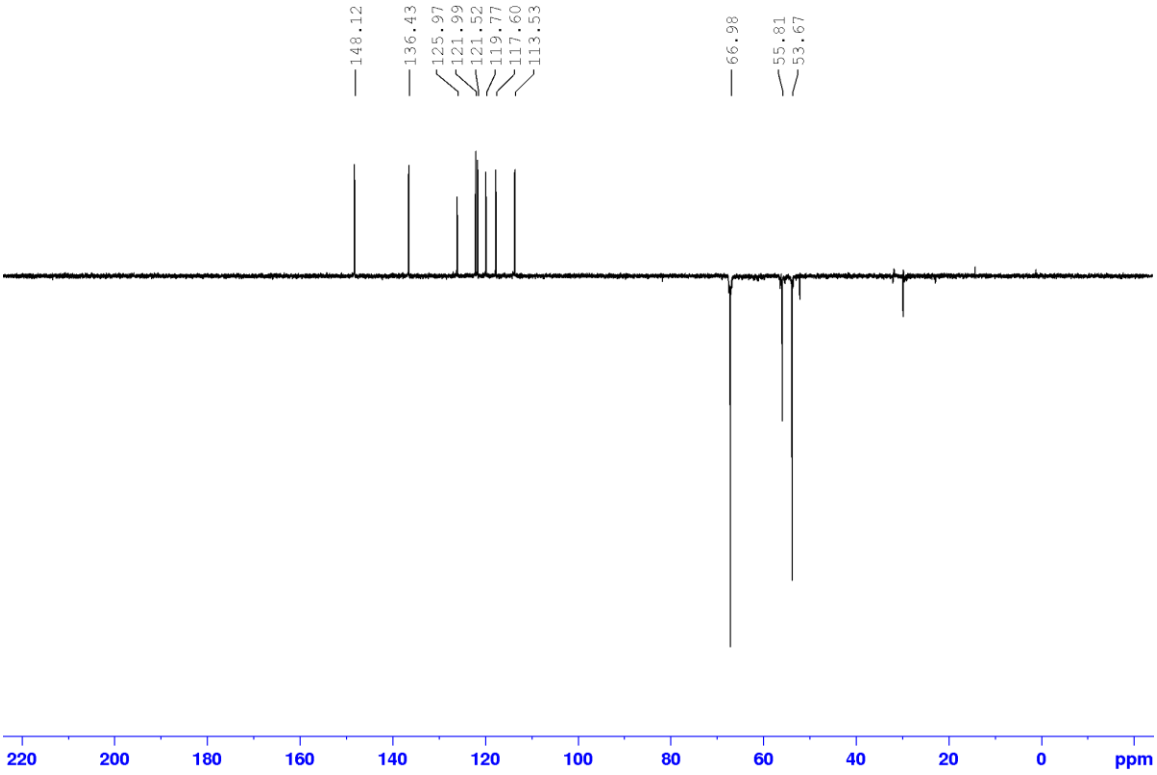




$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3j



DEPT-135 (400 MHz, $CDCl_3$) of 3j



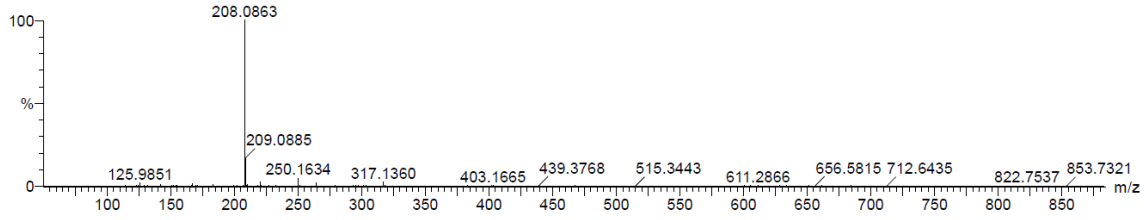
HRMS of 3j

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 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:38:36
230424_12 4 (0.104) 1: TOF MS ES+
8.96e+006



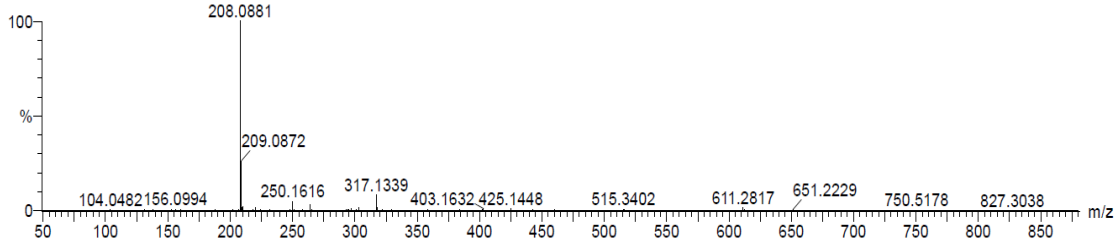
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
317.1360	317.1378	-1.8	-5.7	10.5	1133.8	n/a	n/a	C17 H18 N4 O Na

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

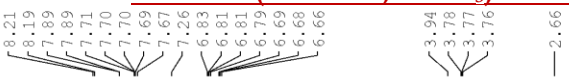
Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 N: 0-3

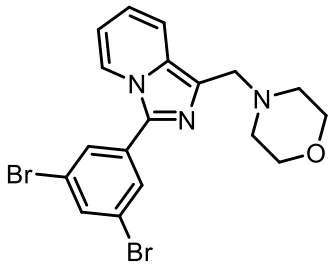
SM-484 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:38:36
230424_12 7 (0.155) 1: TOF MS ES+
4.75e+007

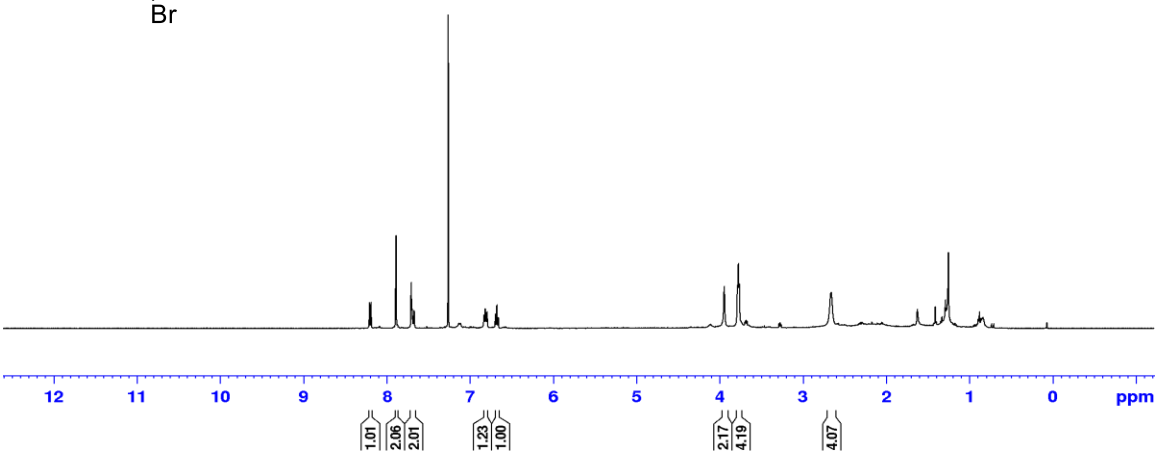


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
208.0881	208.0875	0.6	2.9	10.5	1545.5	n/a	n/a	C13 H10 N3

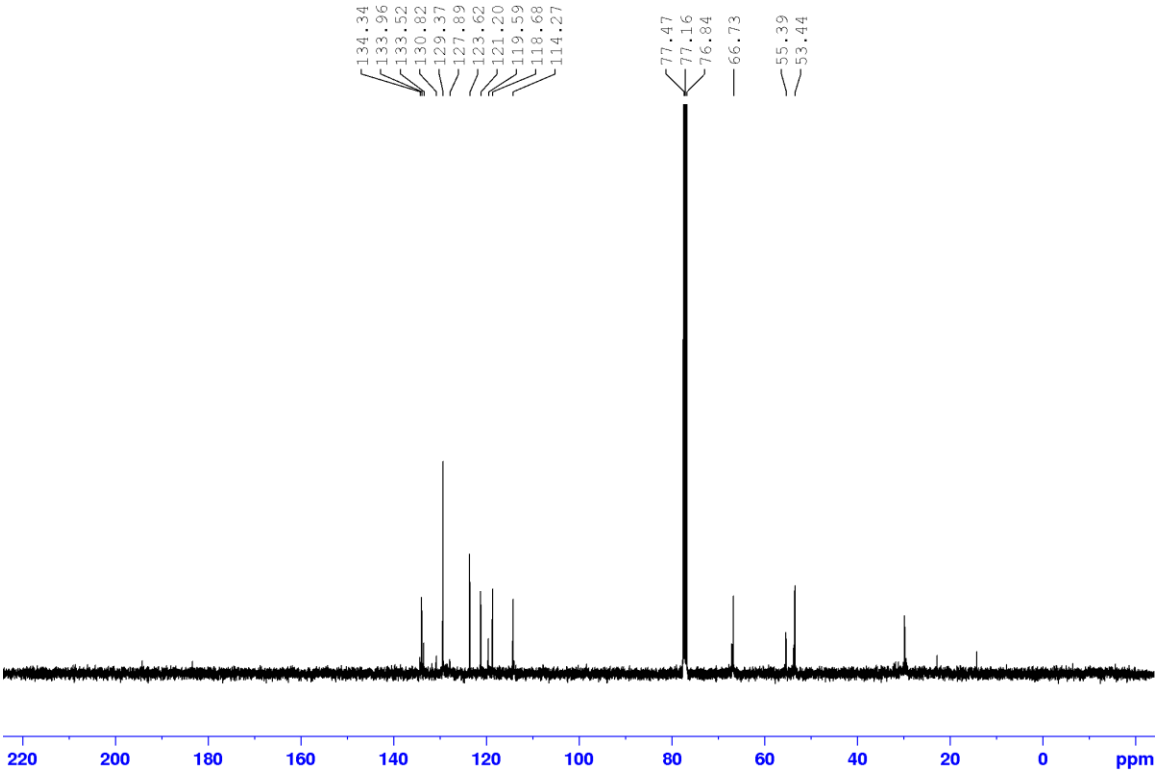
^{1}H NMR (400 MHz, $CDCl_3$) of 3k



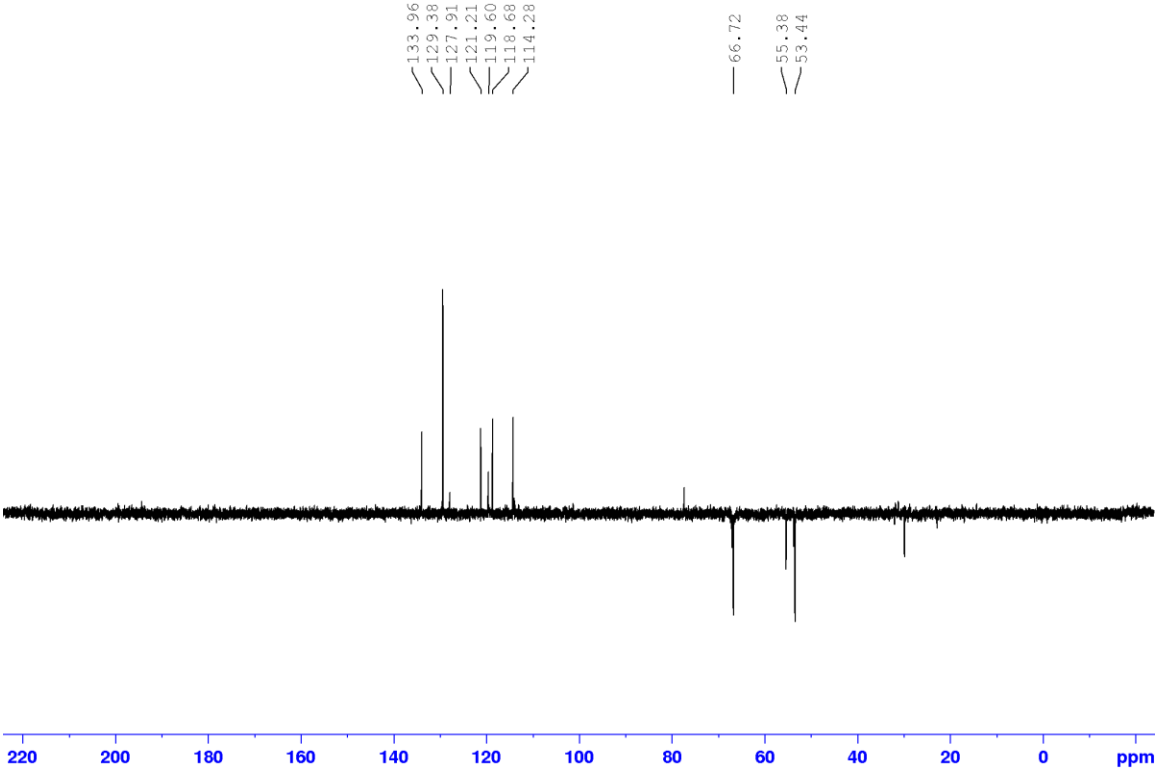




$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3k



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

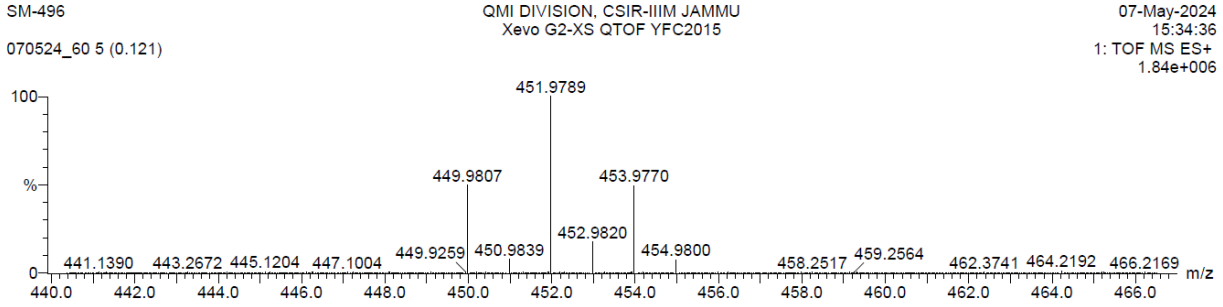


HRMS of 3k

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
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

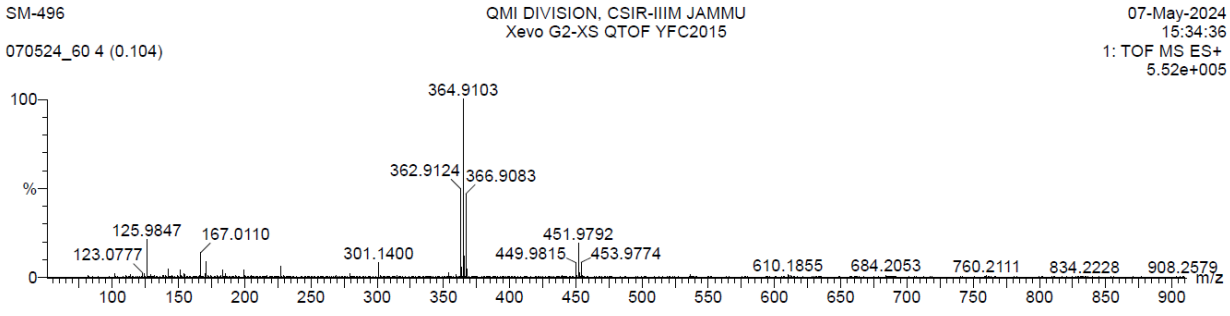


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
449.9807	449.9817	-1.0	-2.2	10.5	924.5	n/a	n/a	C18 H18 N3 O Br2

Elemental Composition Report **Page 1**

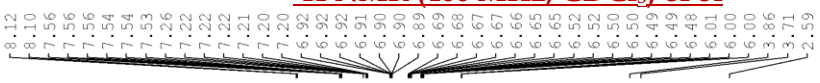
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

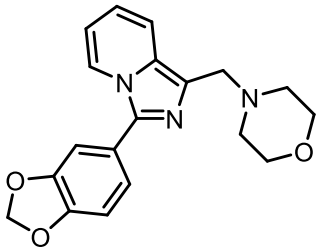
Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2 Br: 0-2

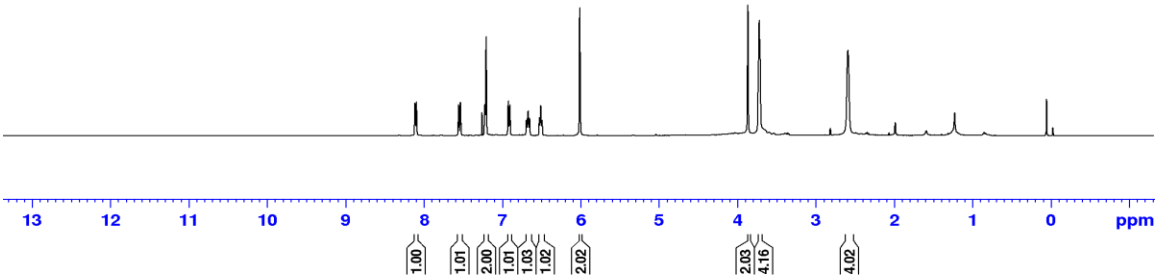


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
362.9124	362.9132	-0.8	-2.2	10.5	805.1	n/a	n/a	C14 H9 N2 Br2

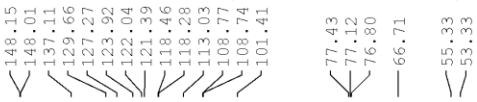
^{1}H NMR (400 MHz, $CDCl_3$) of 3l

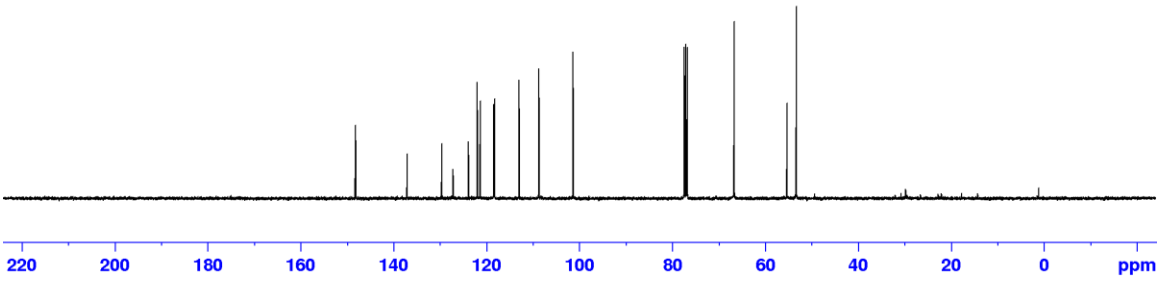




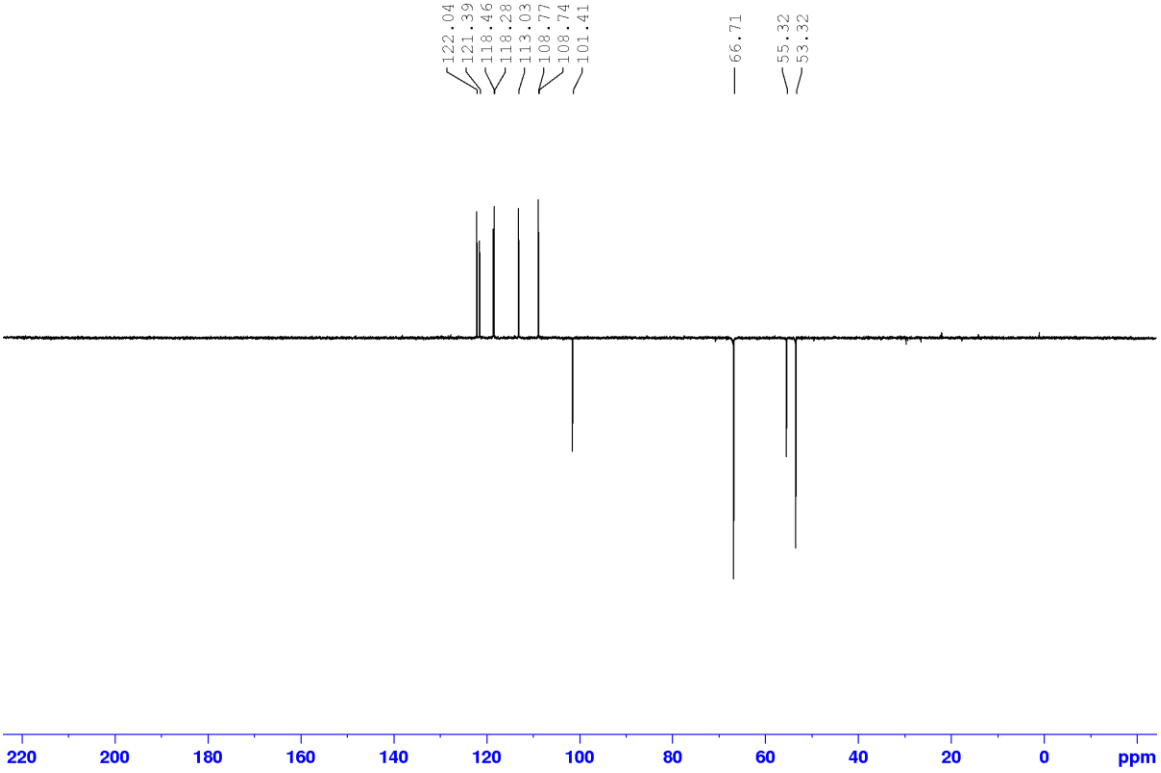


$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3l





DEPT-135 (400 MHz, $CDCl_3$) of 3l



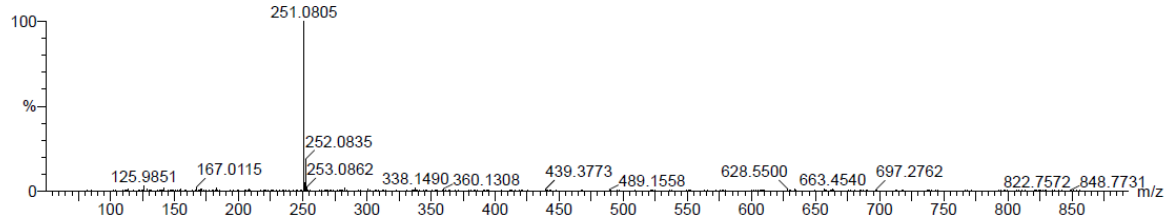
HRMS of 3l

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 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:30:44
230424_09 4 (0.104) 1: TOF MS ES+
6.35e+006



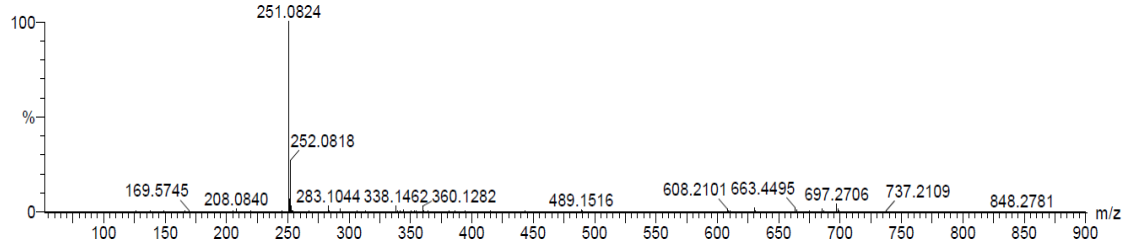
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
338.1490	338.1505	-1.5	-4.4	11.5	1206.1	n/a	n/a	C19 H20 N3 O3

Elemental Composition Report **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

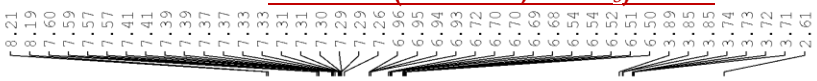
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-2 O: 0-2

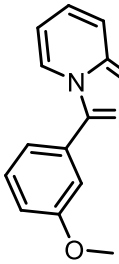
SM-497 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:30:44
230424_09 7 (0.155) 1: TOF MS ES+
3.52e+007

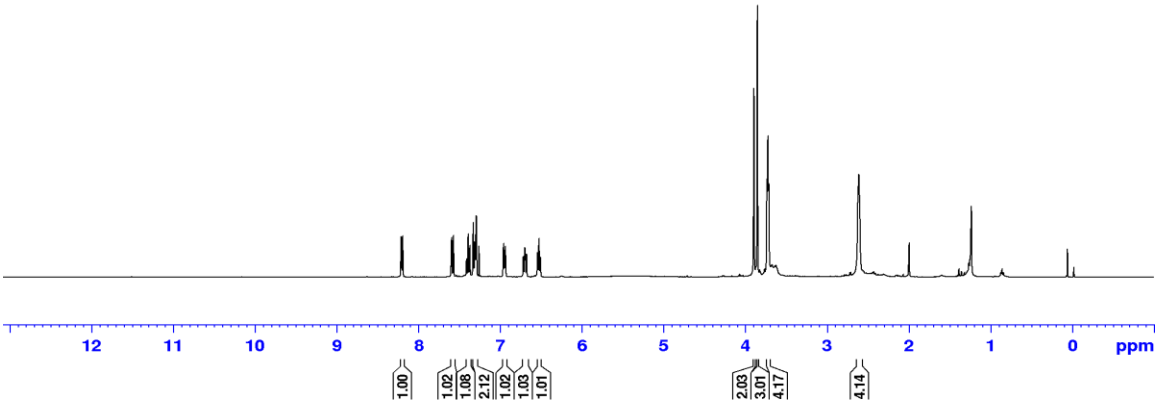


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
251.0824	251.0821	0.3	1.2	11.5	1366.5	n/a	n/a	C15 H11 N2 O2

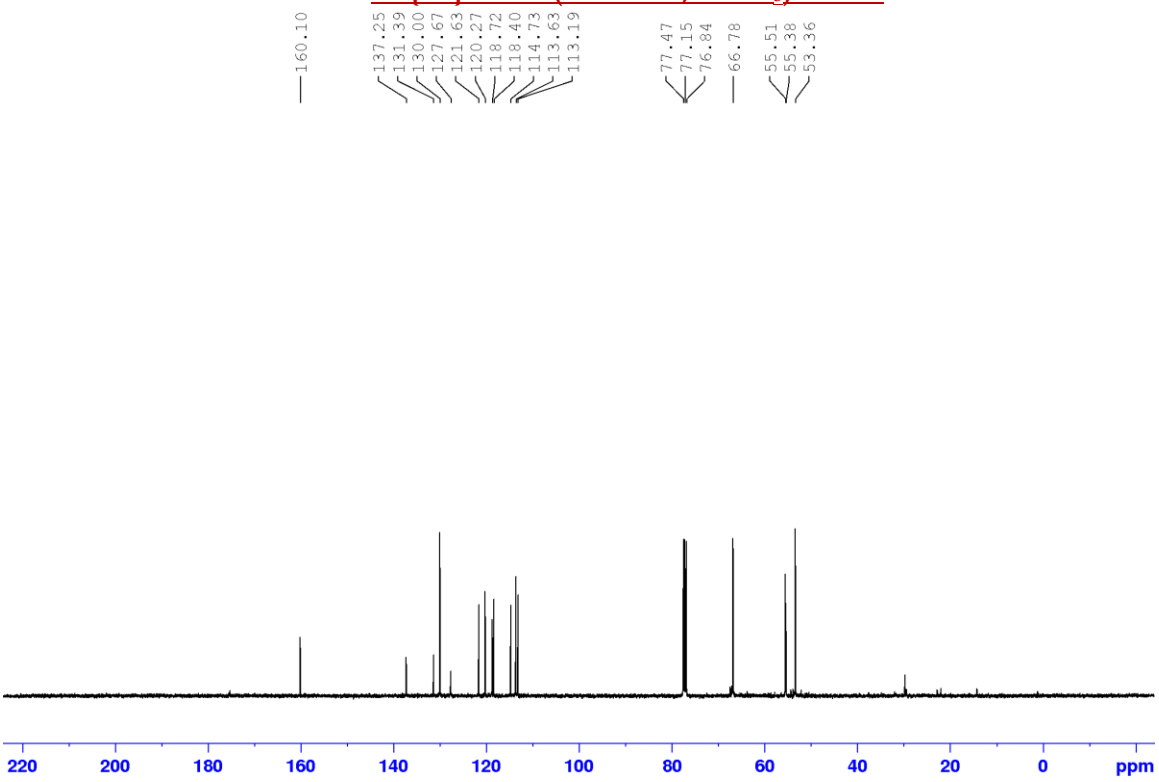
^{1}H NMR (400 MHz, $CDCl_3$) of 3m



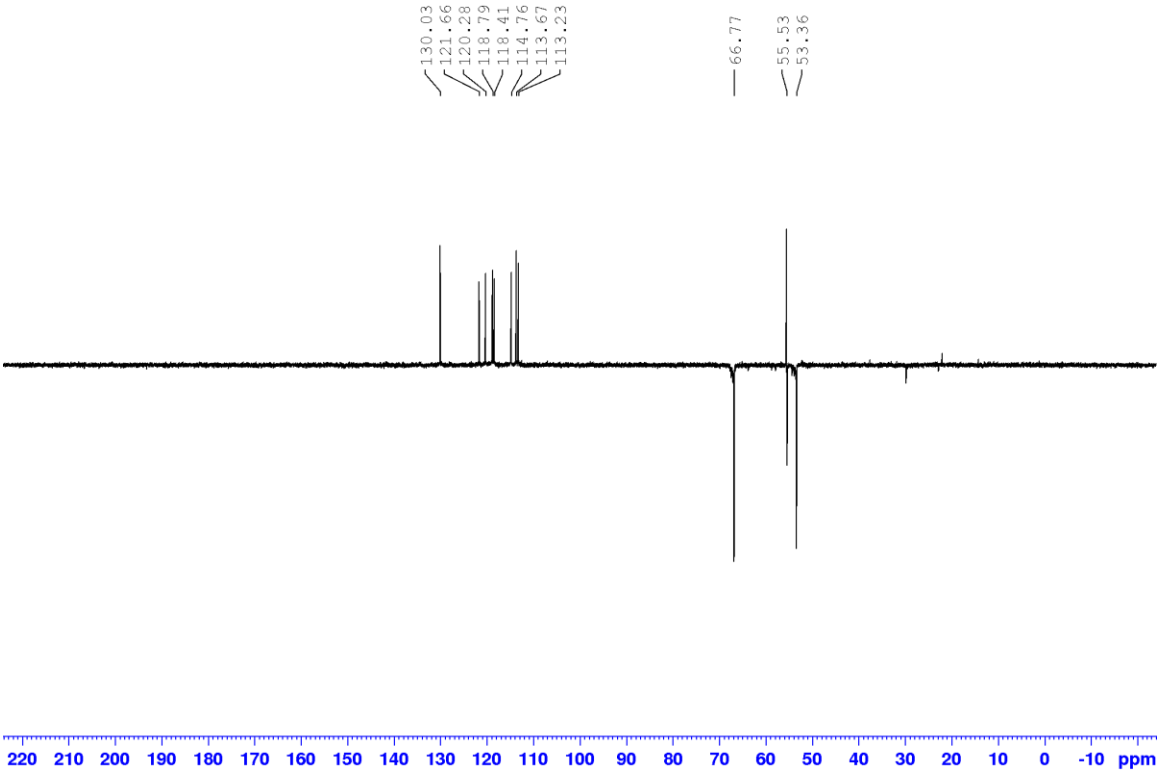




$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3m



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



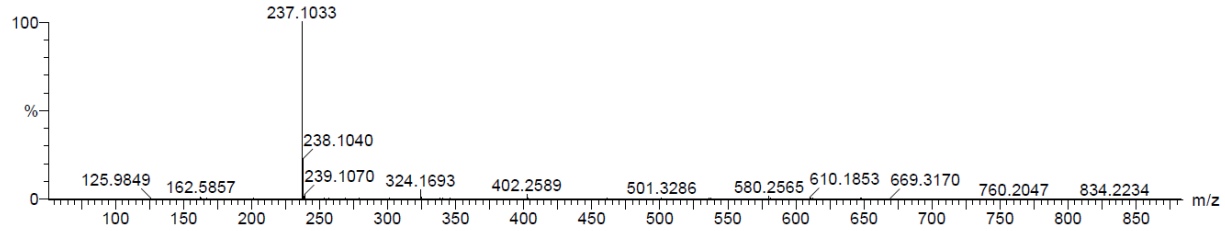
HRMS of 3m

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
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 07-May-2024
Xevo G2-XS QTOF YFC2015 15:39:45
070524_62 5 (0.121) 1: TOF MS ES+
1.96e+007



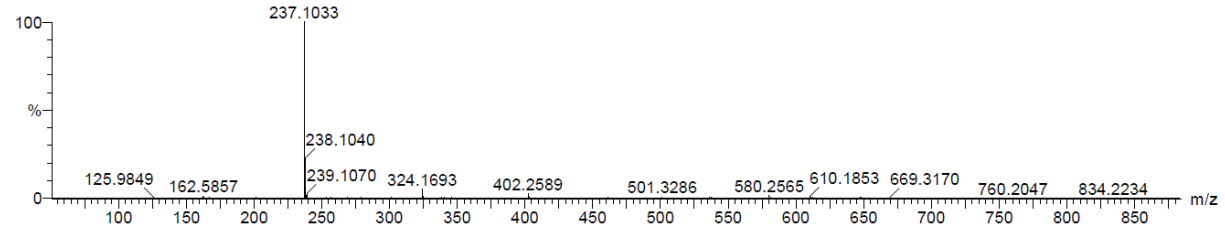
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
324.1693	324.1712	-1.9	-5.9	10.5	1034.0	n/a	n/a	C19 H22 N3 O2

Elemental Composition Report **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

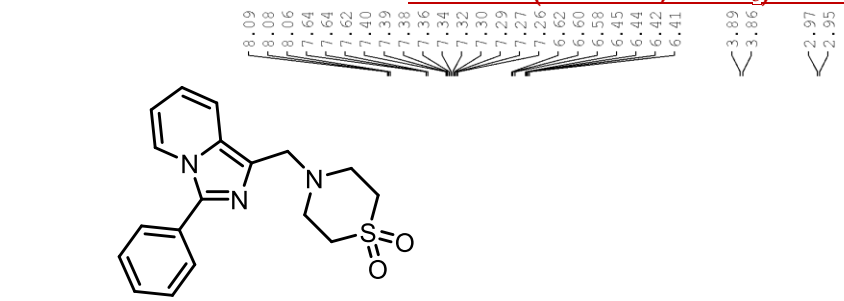
Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-3 O: 0-3

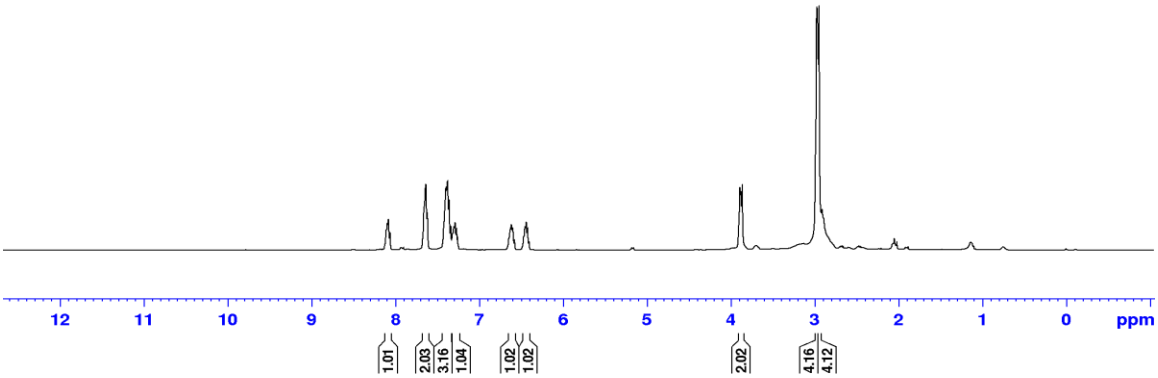
SM-498 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 15:39:45
070524_62 5 (0.121) 1: TOF MS ES+
1.96e+007



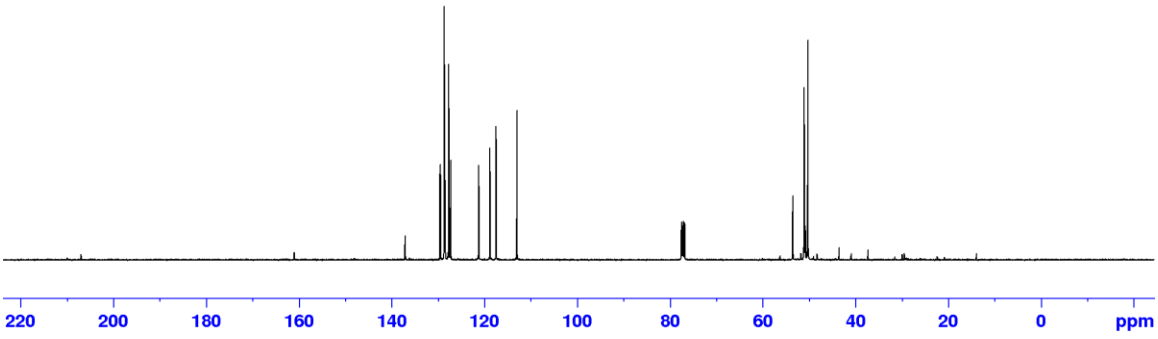
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
324.1693	324.1712	-1.9	-5.9	10.5	1034.0	n/a	n/a	C19 H22 N3 O2

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

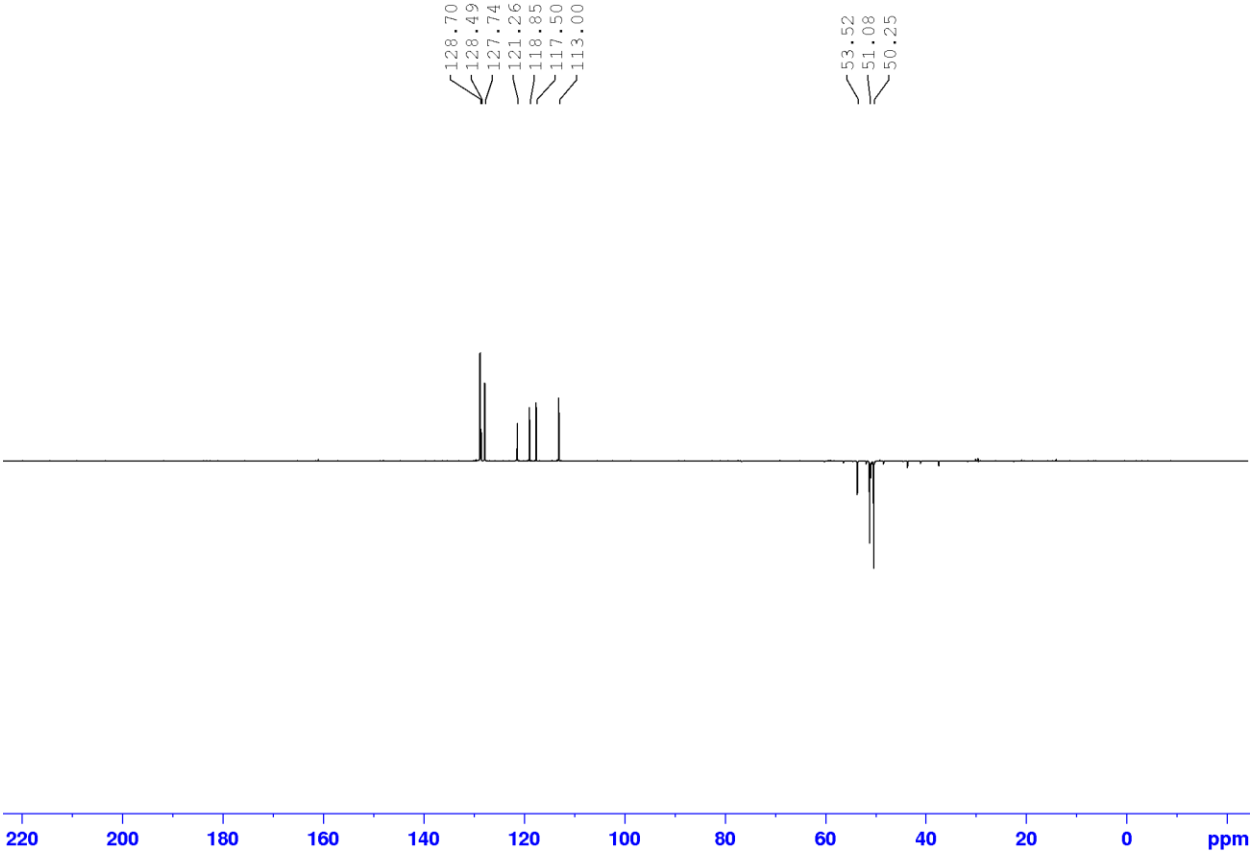




$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3n



DEPT-135 (400 MHz, $CDCl_3$) of 3n



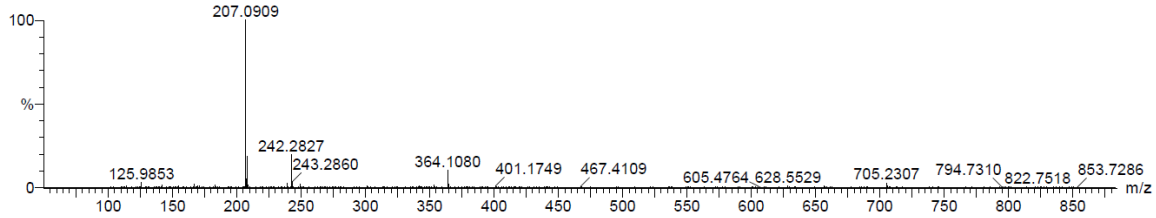
HRMS of 3n

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
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 23-Apr-2024
Xevo G2-XS QTOF YFC2015 13:02:49
230424_21 4 (0.104) 1: TOF MS ES+
6.28e+006



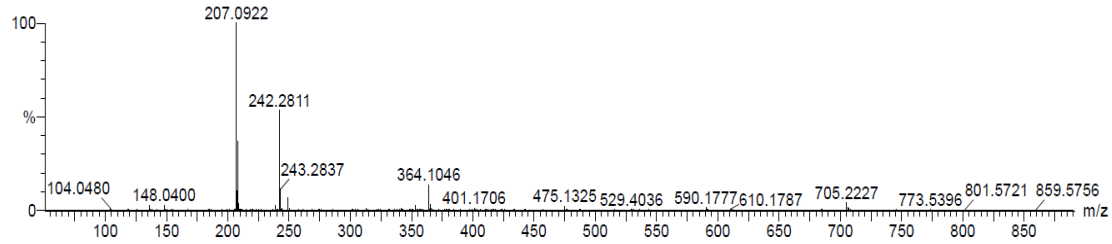
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
364.1080	364.1096	-1.6	-4.4	10.5	1124.1	n/a	n/a	C18 H19 N3 O2 S Na

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

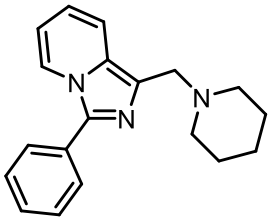
Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2 Br: 0-2

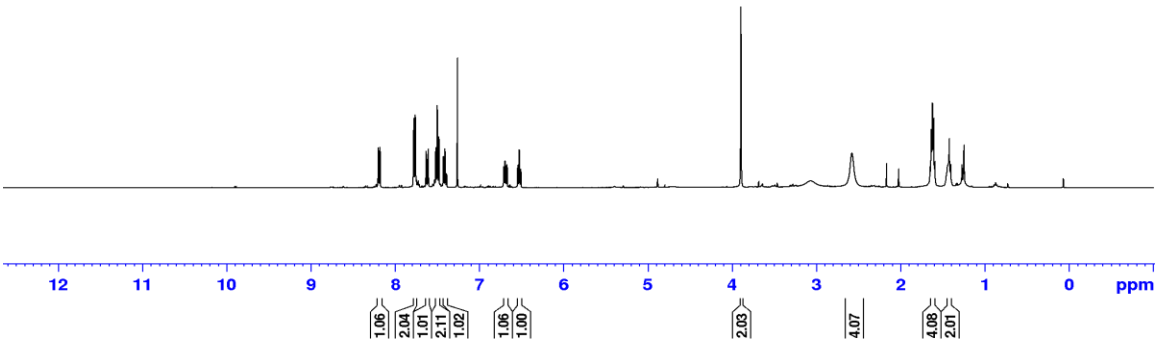
SM-384 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 13:02:49
230424_21 7 (0.155) 1: TOF MS ES+
3.41e+007



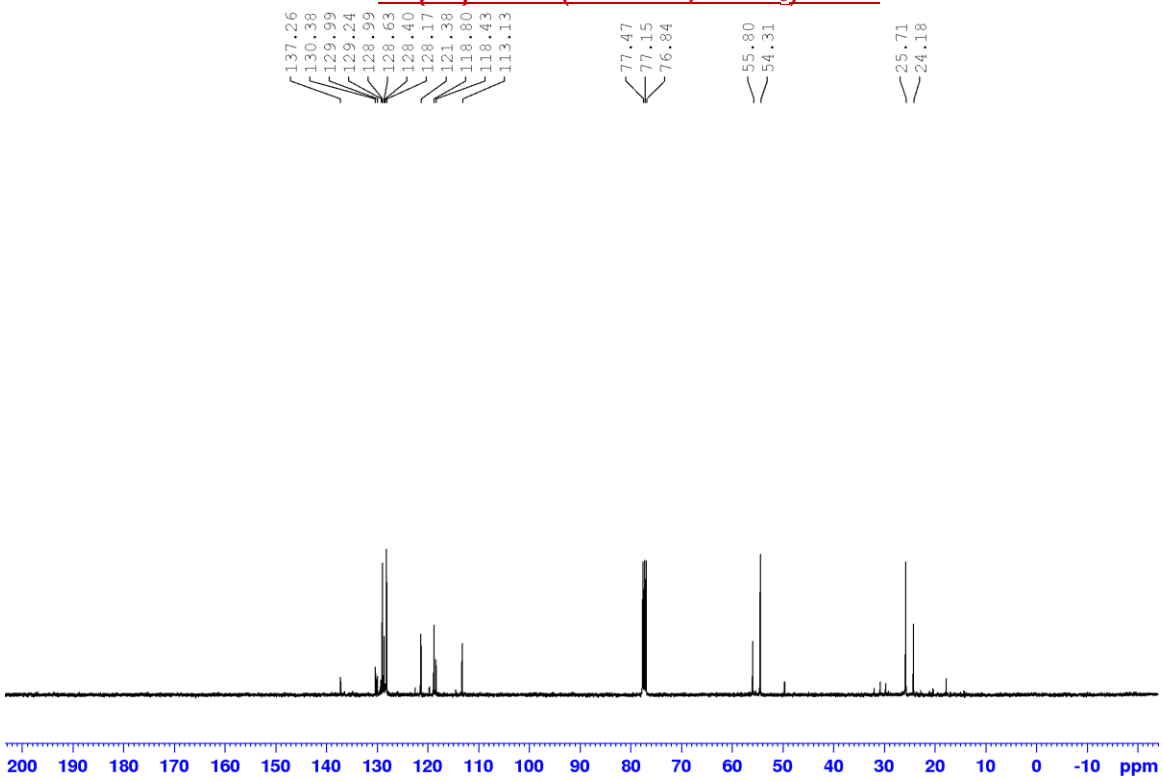
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
207.0922	207.0922	0.0	0.0	10.5	1352.3	n/a	n/a	C14 H11 N2

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

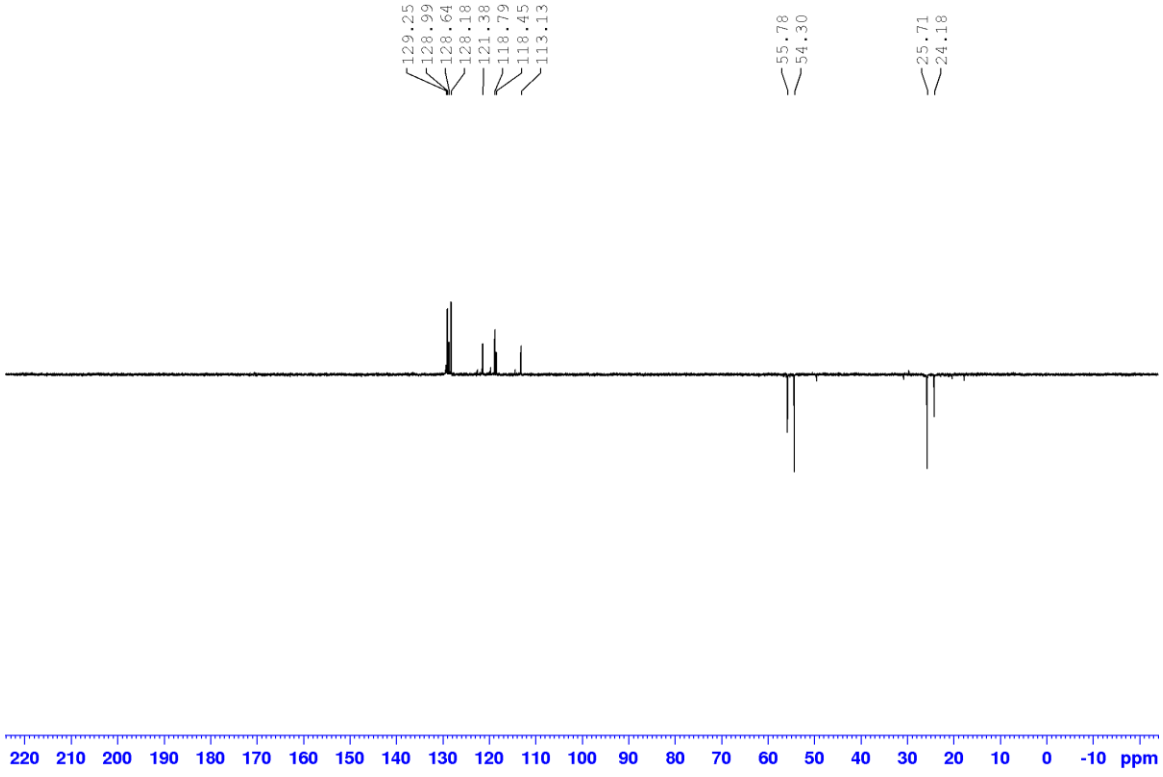




$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3o



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



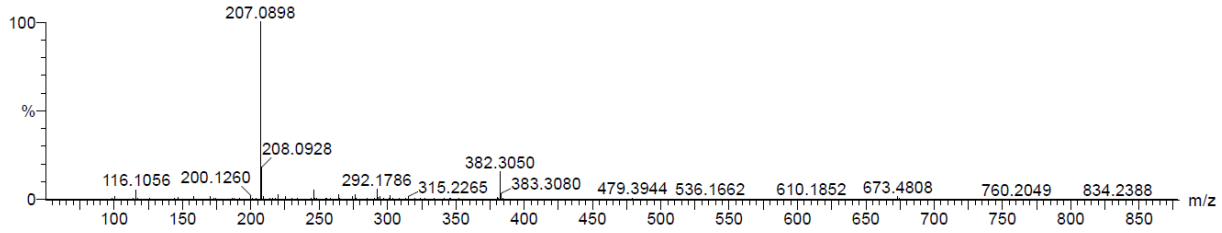
HRMS of 3o

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 07-May-2024
Xevo G2-XS QTOF YFC2015 15:21:30
070524_55 5 (0.121) 1: TOF MS ES+
1.04e+007



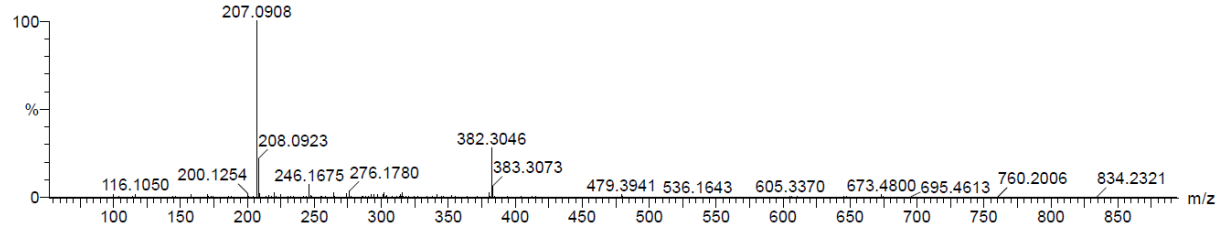
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
292.1786	292.1814	-2.8	-9.6	10.5	916.5	n/a	n/a	C19 H22 N3

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

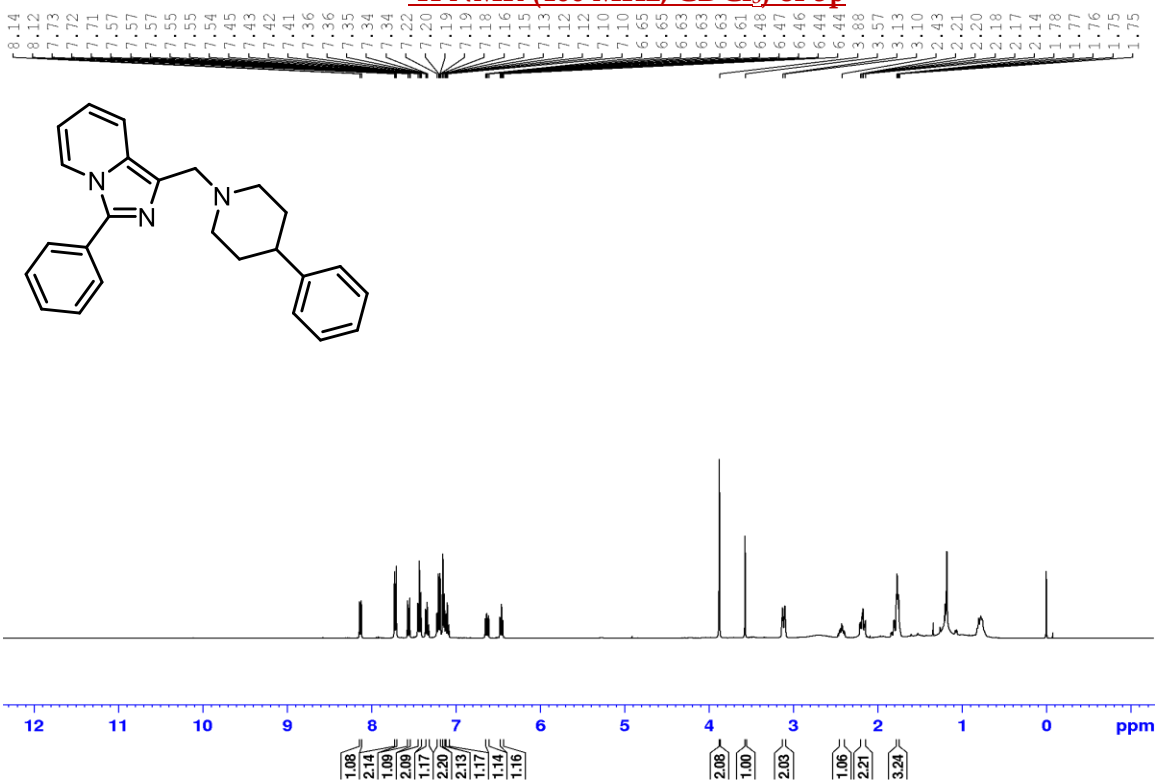
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2

SM-430 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 13:54:45
070524_26 6 (0.138) 1: TOF MS ES+
1.99e+007

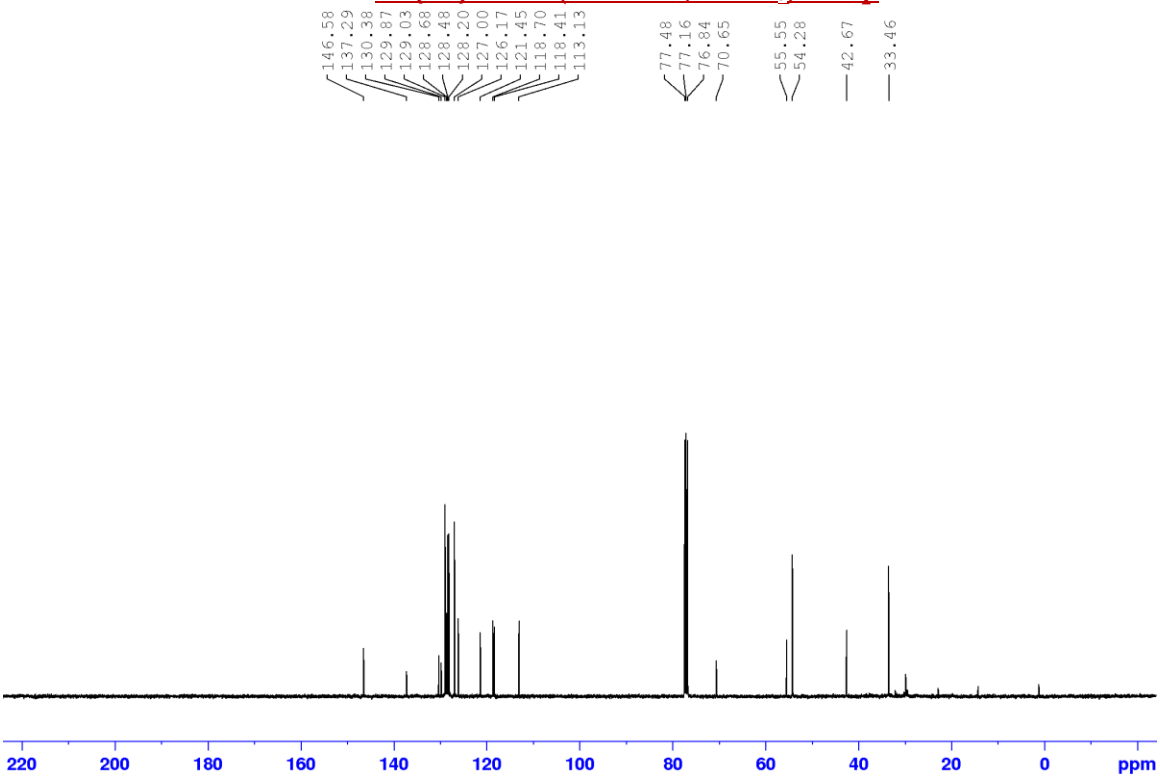


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
207.0908	207.0922	-1.4	-6.8	10.5	1342.7	n/a	n/a	C14 H11 N2

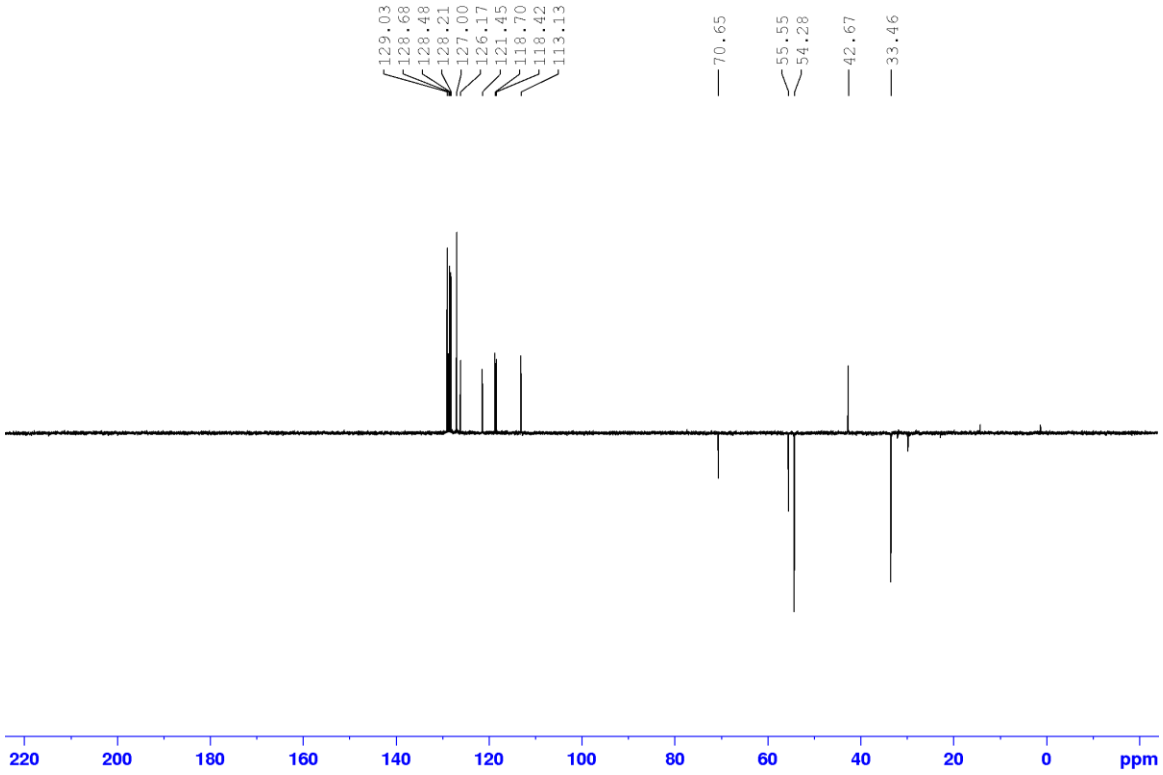
^{1}H NMR (400 MHz, $CDCl_3$) of 3p



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



DEPT-135 (400 MHz, $CDCl_3$) of 3p



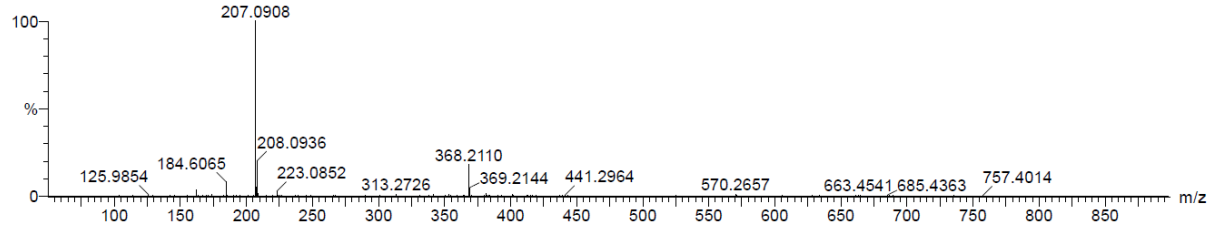
HRMS of 3p

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

SM-341 — QMI DIVISION, CSIR-IIIM JAMMU — 23-Apr-2024 12:20:20
230424_05 5 (0.121) — Xevo G2-XS QTOF YFC2015 — 1: TOF MS ES+ 1.47e+007



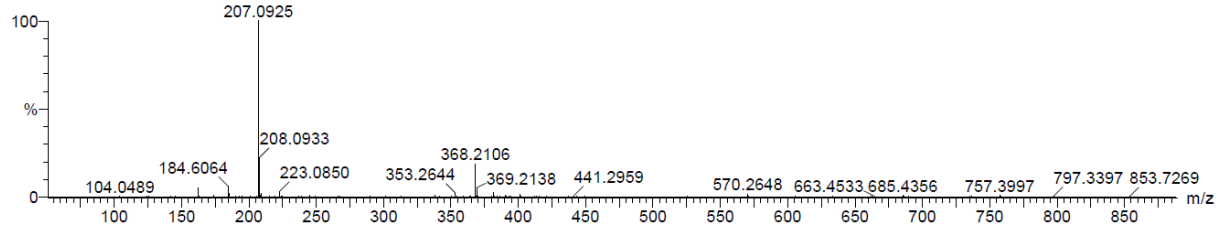
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
368.2110	368.2127	-1.7	-4.6	14.5	1152.7	n/a	n/a	C25 H26 N3

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

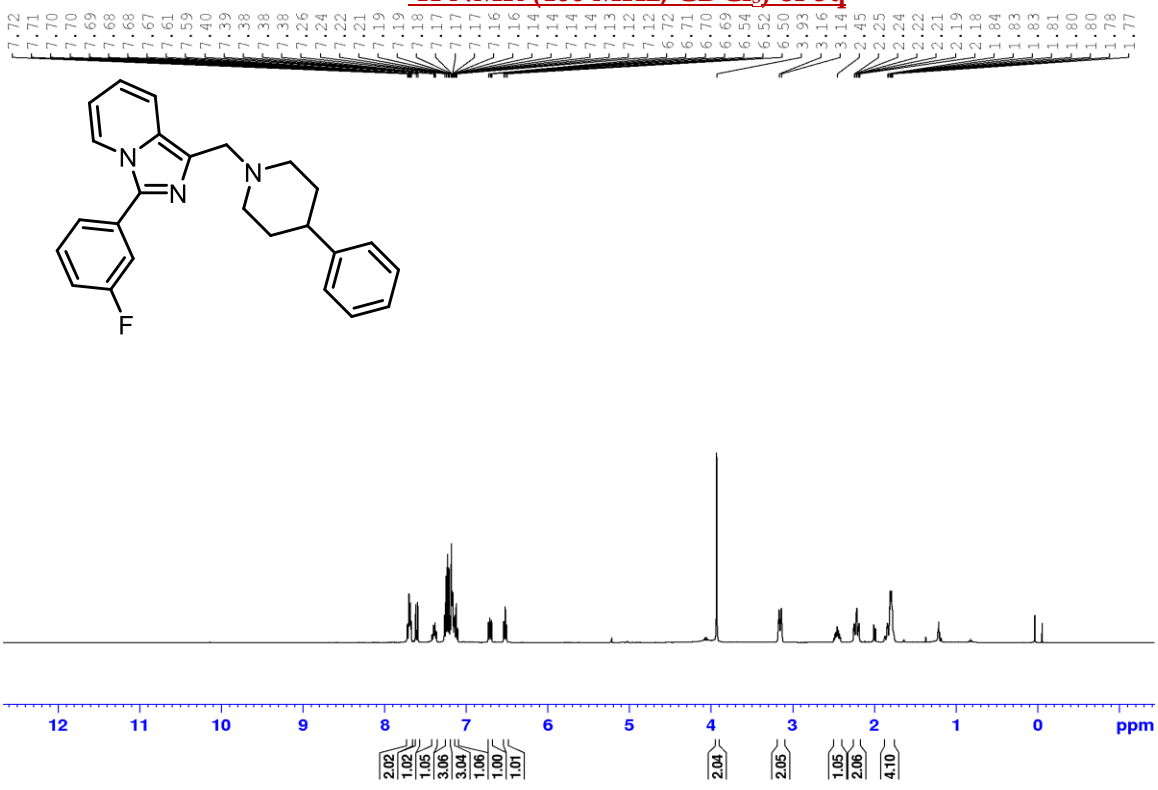
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2

SM-341 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:20:20
230424_05 6 (0.138) 1: TOF MS ES+
2.27e+007

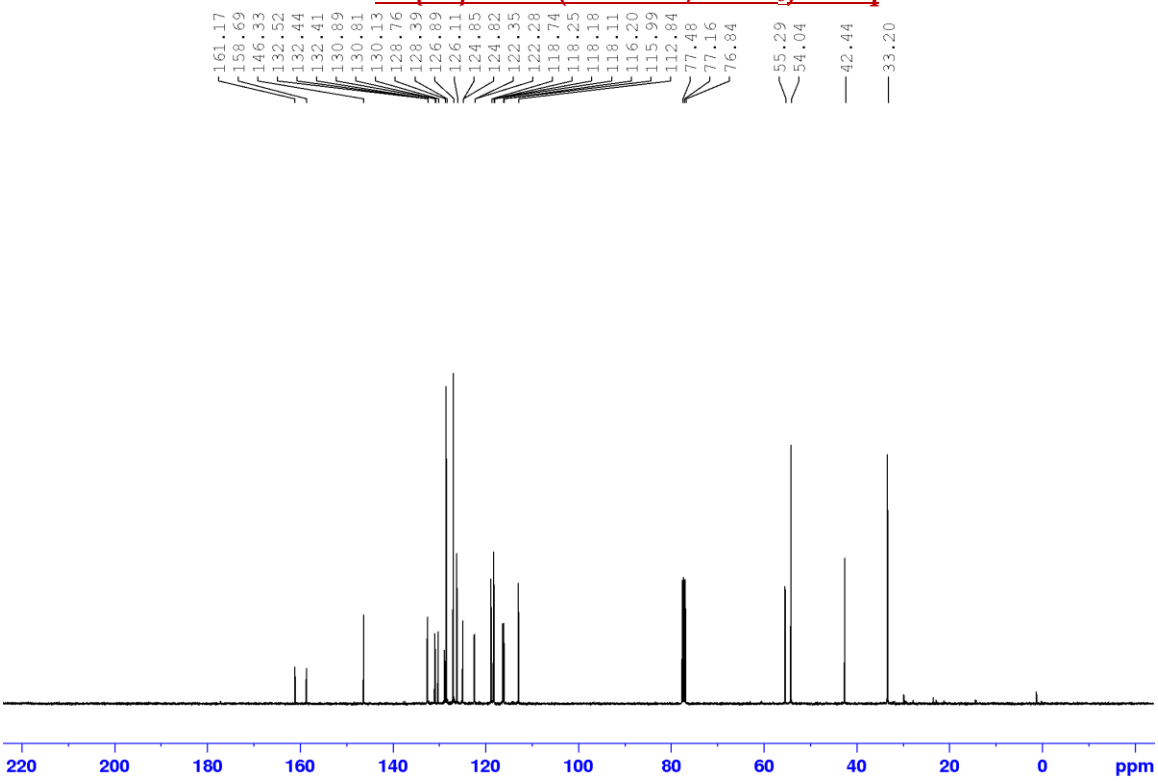


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
207.0925	207.0922	0.3	1.4	10.5	1532.3	n/a	n/a	C14 H11 N2

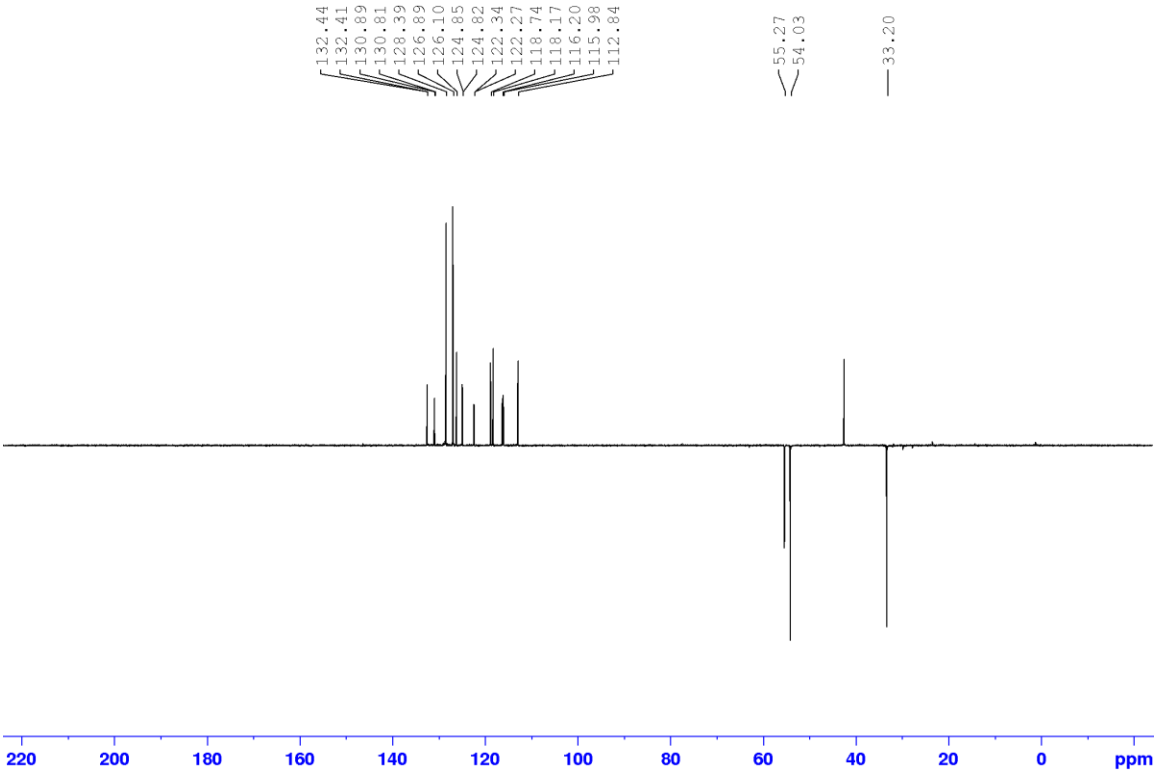
^{1}H NMR (400 MHz, $CDCl_3$) of 3q



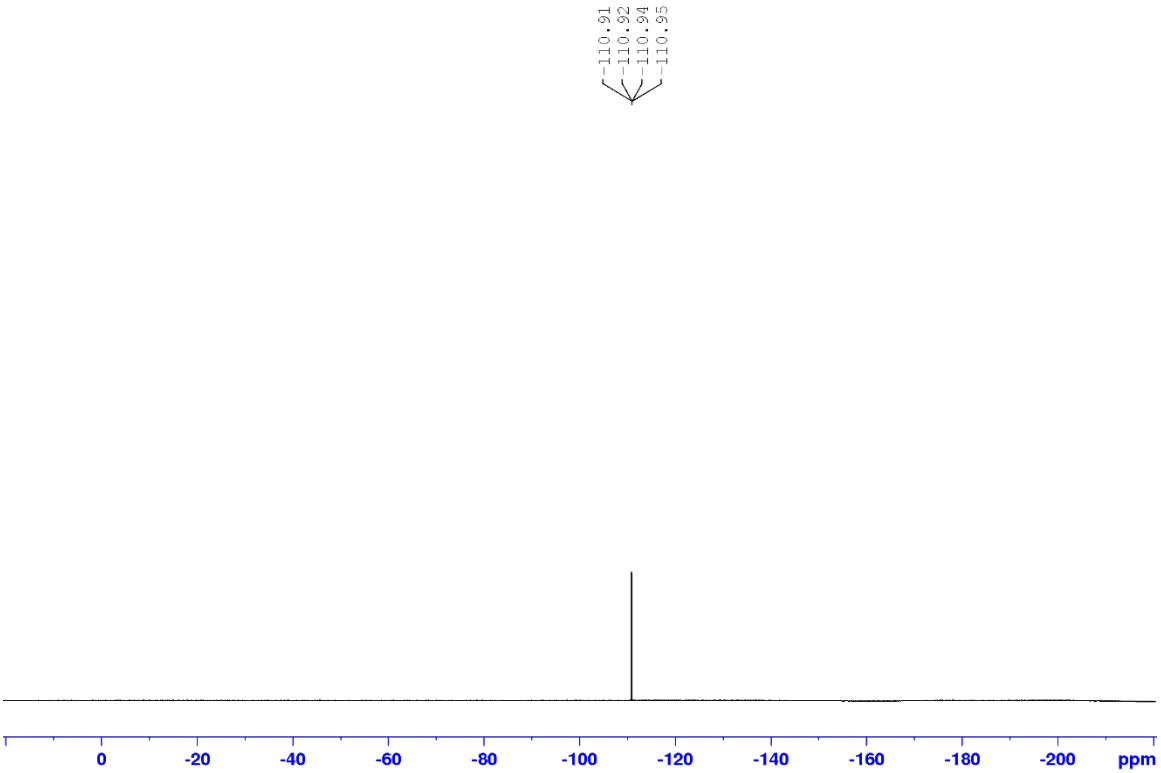
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3q



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



^{19}F NMR (377 MHz, $CDCl_3$) of 3q



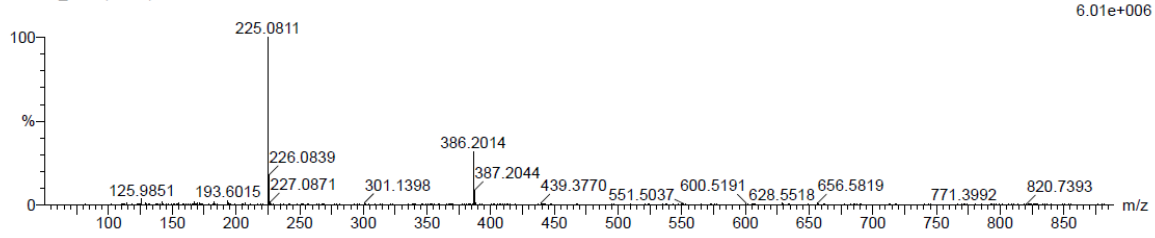
HRMS of 3q

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 23-Apr-2024
230424_18 4 (0.104) Xevo G2-XS QTOF YFC2015 12:54:49
1: TOF MS ES+
6.01e+006



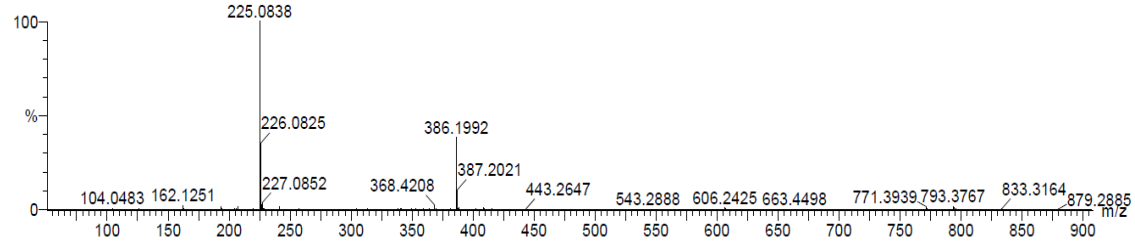
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
386.2014	386.2033	-1.9	-4.9	14.5	1005.5	n/a	n/a	C25 H25 N3 F

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

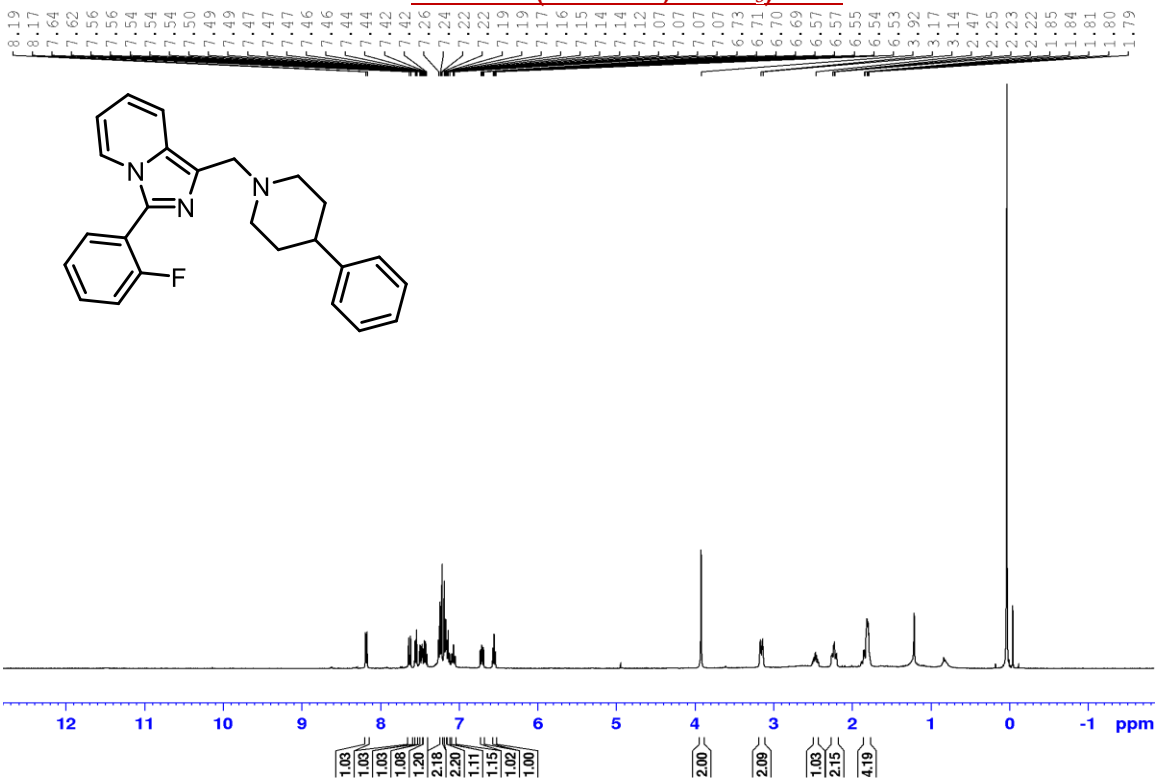
Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2 F: 0-1

SM-389 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024 12:54:49
230424_18 7 (0.155) Xevo G2-XS QTOF YFC2015 1: TOF MS ES+ 3.19e+007

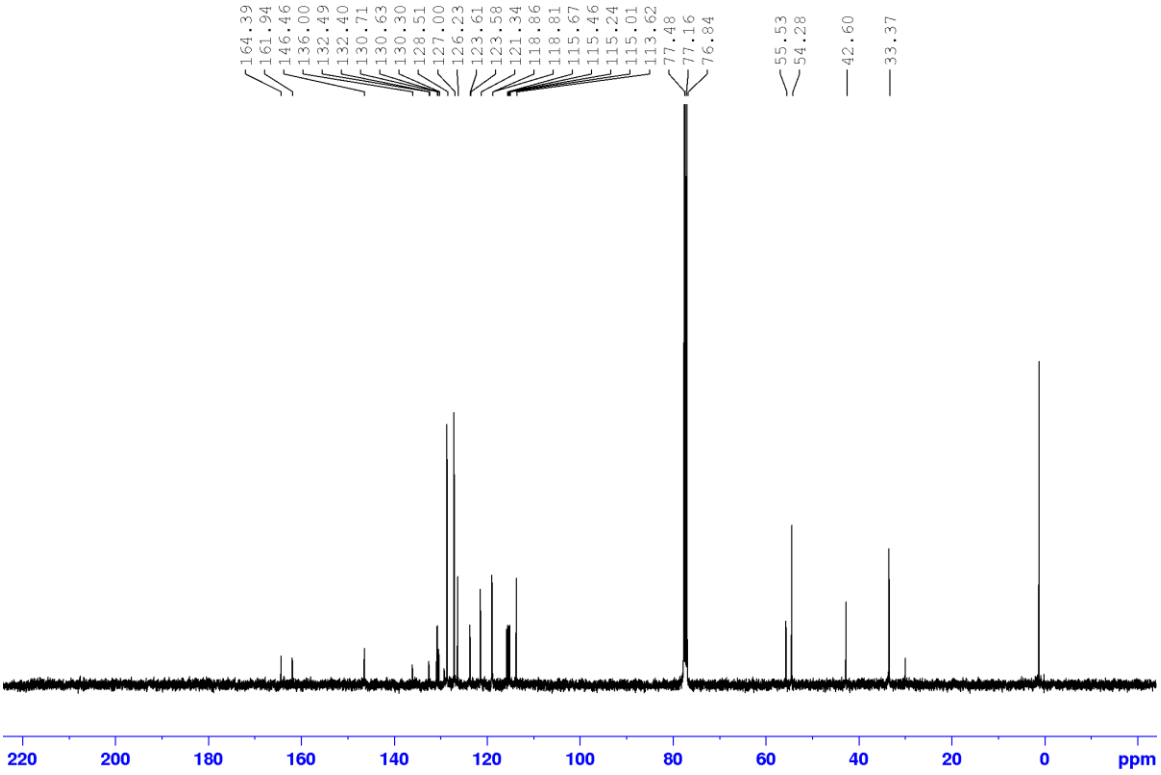


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
225.0838	225.0828	1.0	4.4	10.5	1350.8	n/a	n/a	C14 H10 N2 F

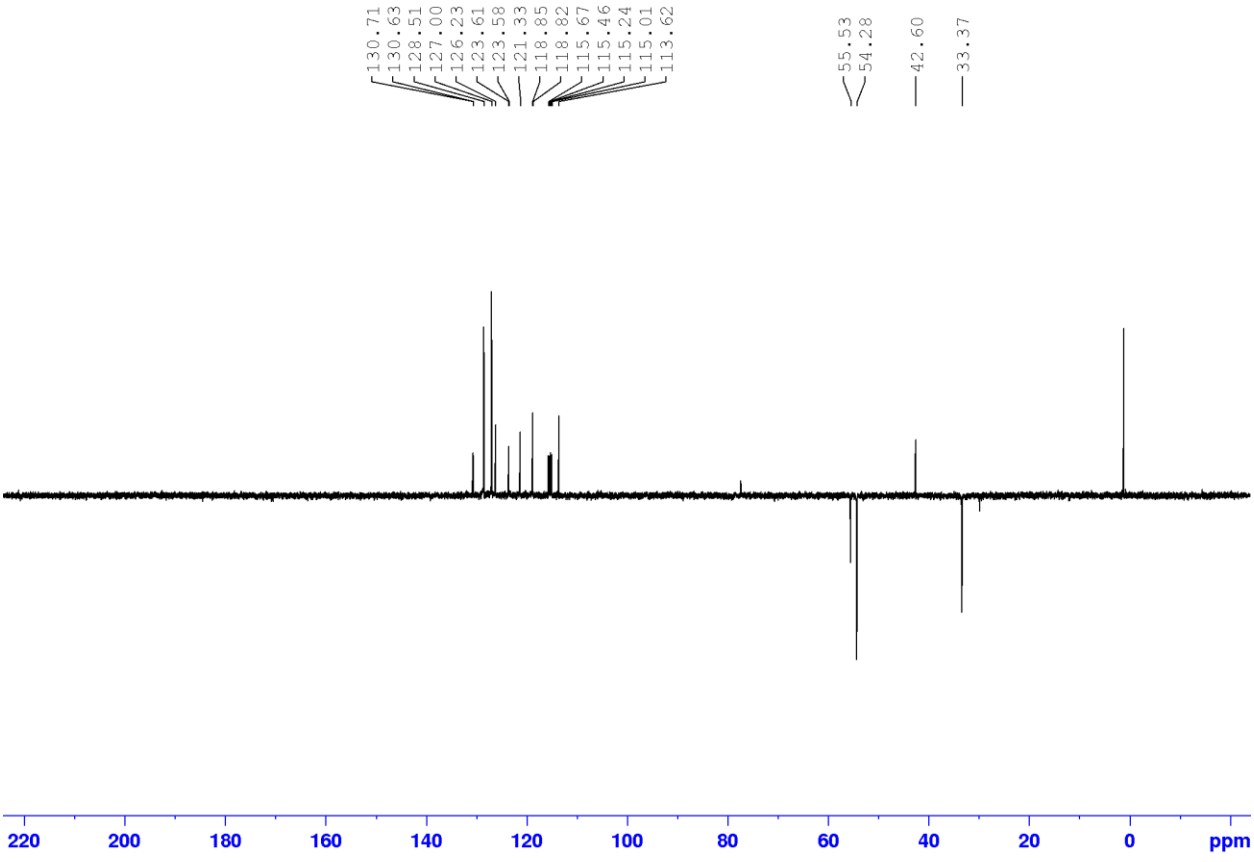
^{1}H NMR (400 MHz, $CDCl_3$) of 3r



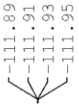
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3r

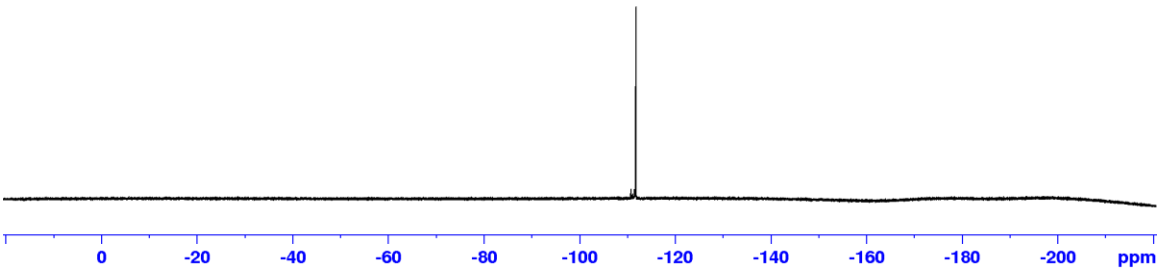


DEPT-135 (400 MHz, $CDCl_3$) of 3r



^{19}F NMR (377 MHz, $CDCl_3$) of 3r





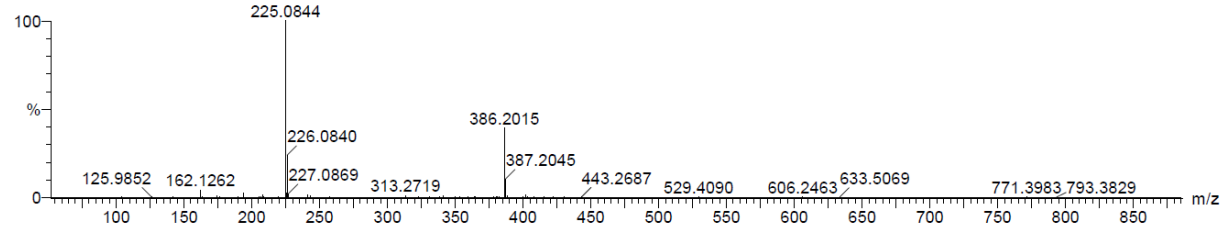
HRMS of 3r

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

SM-390 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:41:11
230424_13 5 (0.121) 1: TOF MS ES+
2.52e+007



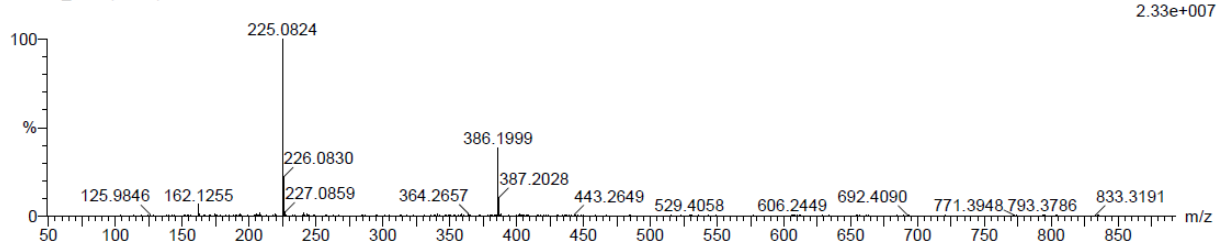
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
386.2015	386.2033	-1.8	-4.7	14.5	1088.1	n/a	n/a	C25 H25 N3 F

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

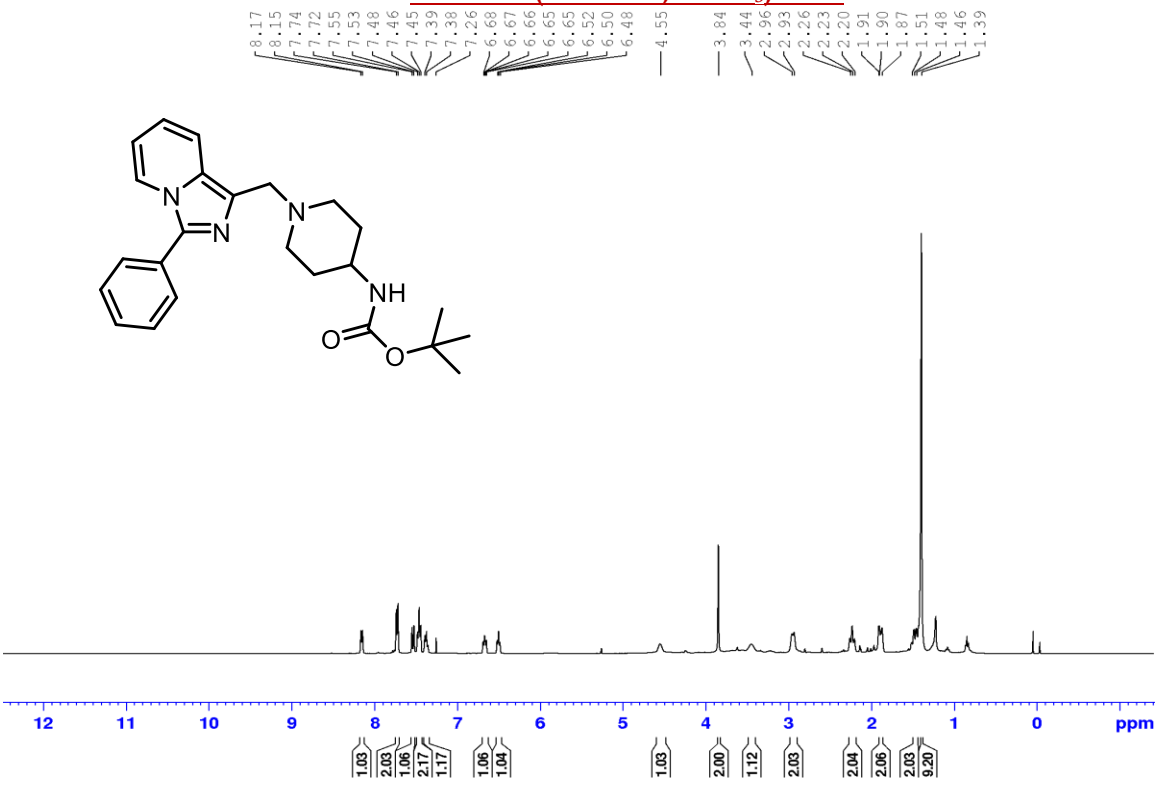
Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2 F: 0-1

SM-390 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024 12:41:11
230424_13 7 (0.155) Xevo G2-XS QTOF YFC2015 1: TOF MS ES+ 2.33e+007

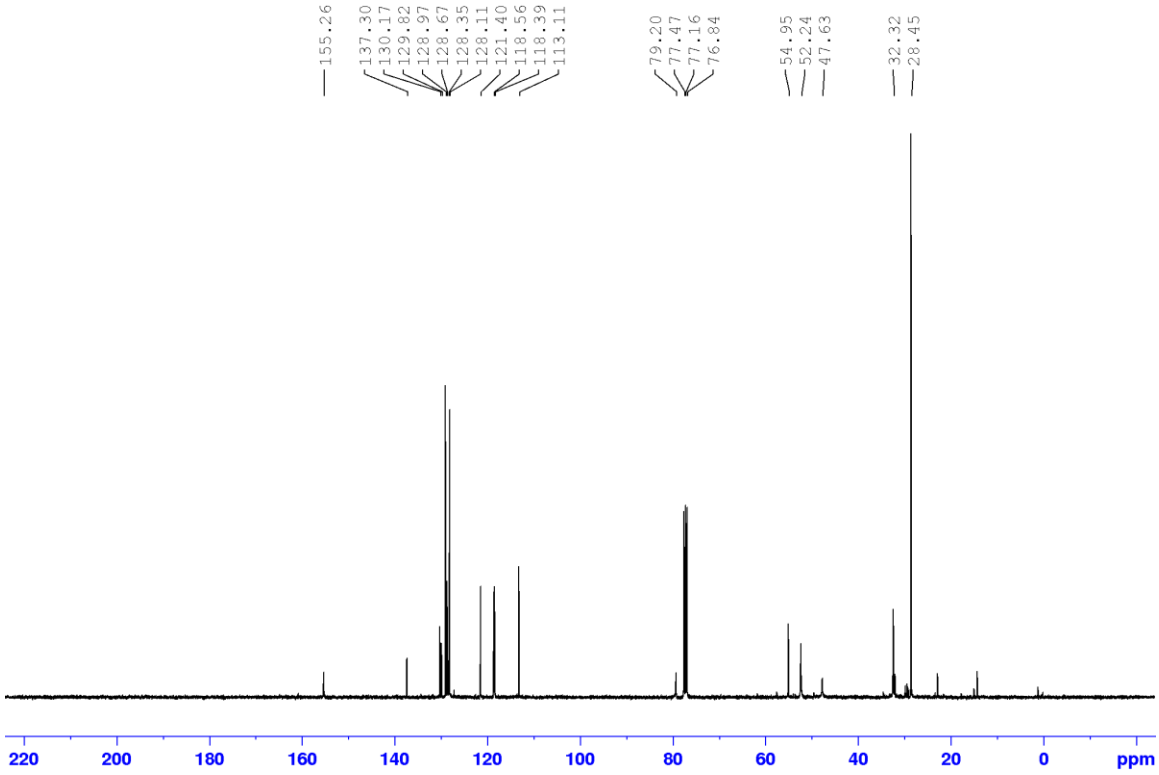


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
225.0824	225.0828	-0.4	-1.8	10.5	1408.5	n/a	n/a	C14 H10 N2 F

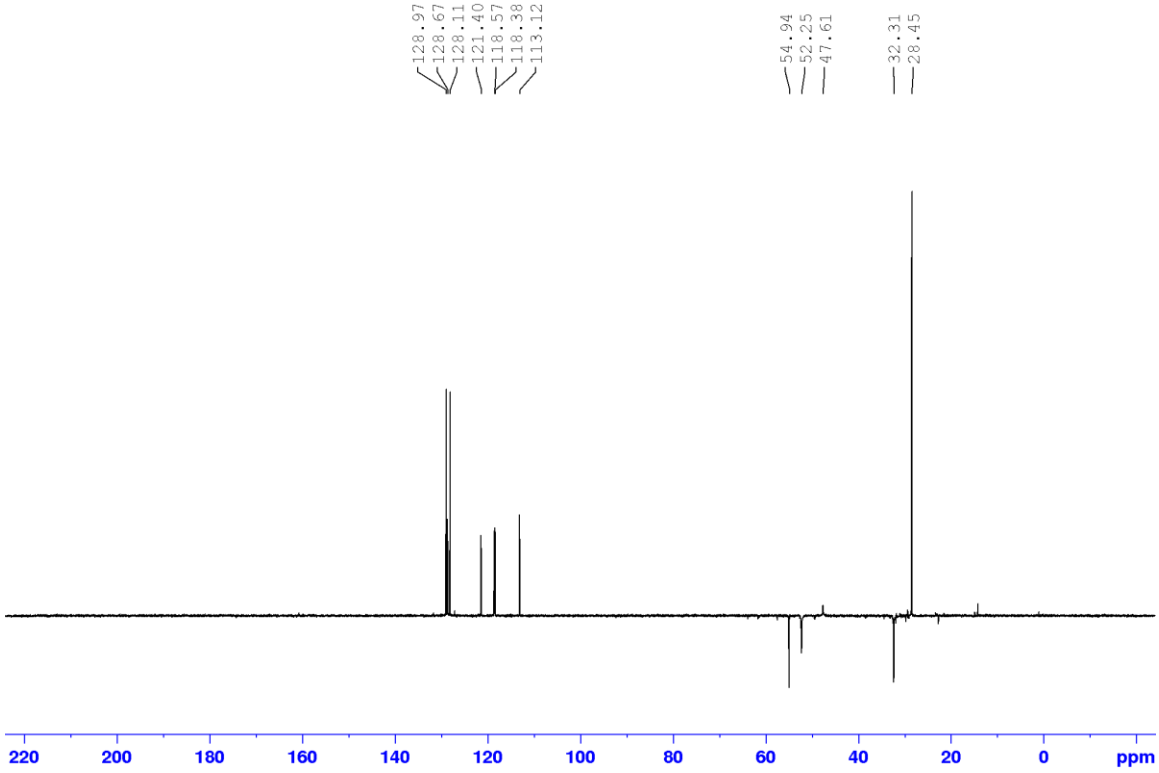
^{1}H NMR (400 MHz, $CDCl_3$) of 3s



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



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



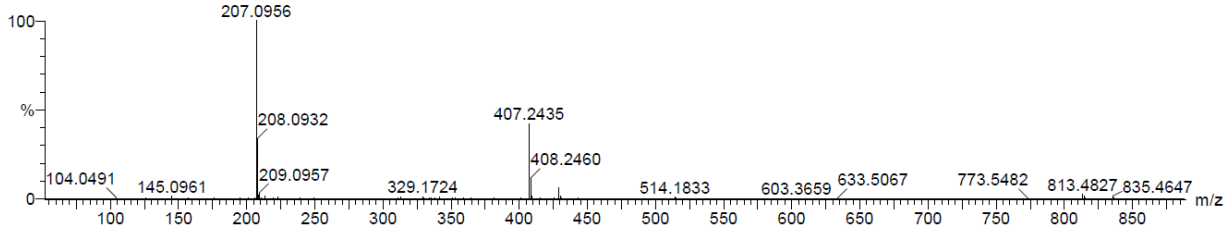
HRMS of 3s

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 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:15:12
230424_03 5 (0.121) 1: TOF MS ES+
3.19e+007



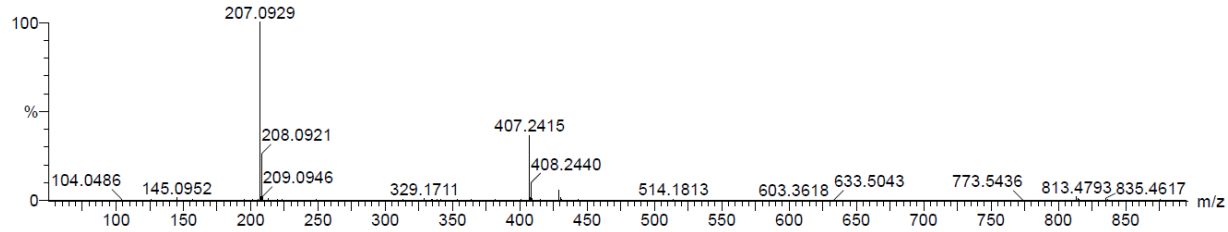
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
407.2435	407.2447	-1.2	-2.9	11.5	1078.5	n/a	n/a	C24 H31 N4 O2

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

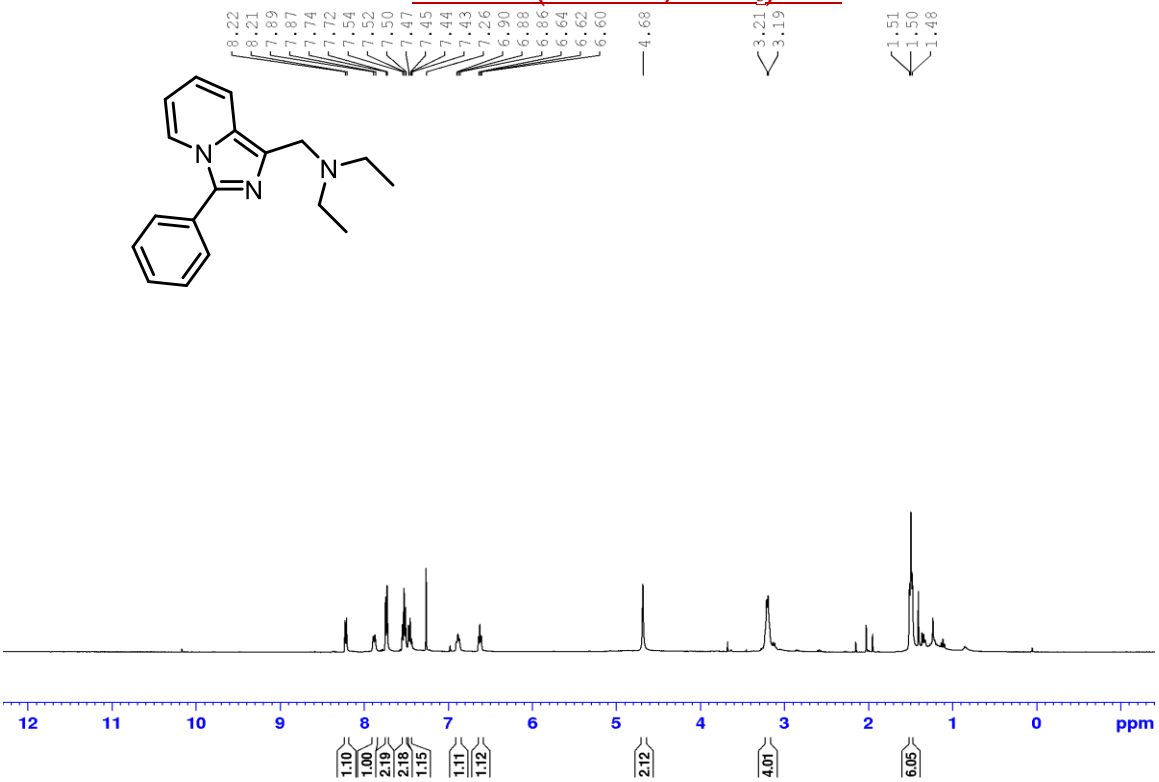
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-2

SM-376 QMI DIVISION, CSIR-IIIM JAMMU 23-Apr-2024
Xevo G2-XS QTOF YFC2015 12:15:12
230424_03 7 (0.155) 1: TOF MS ES+
3.62e+007

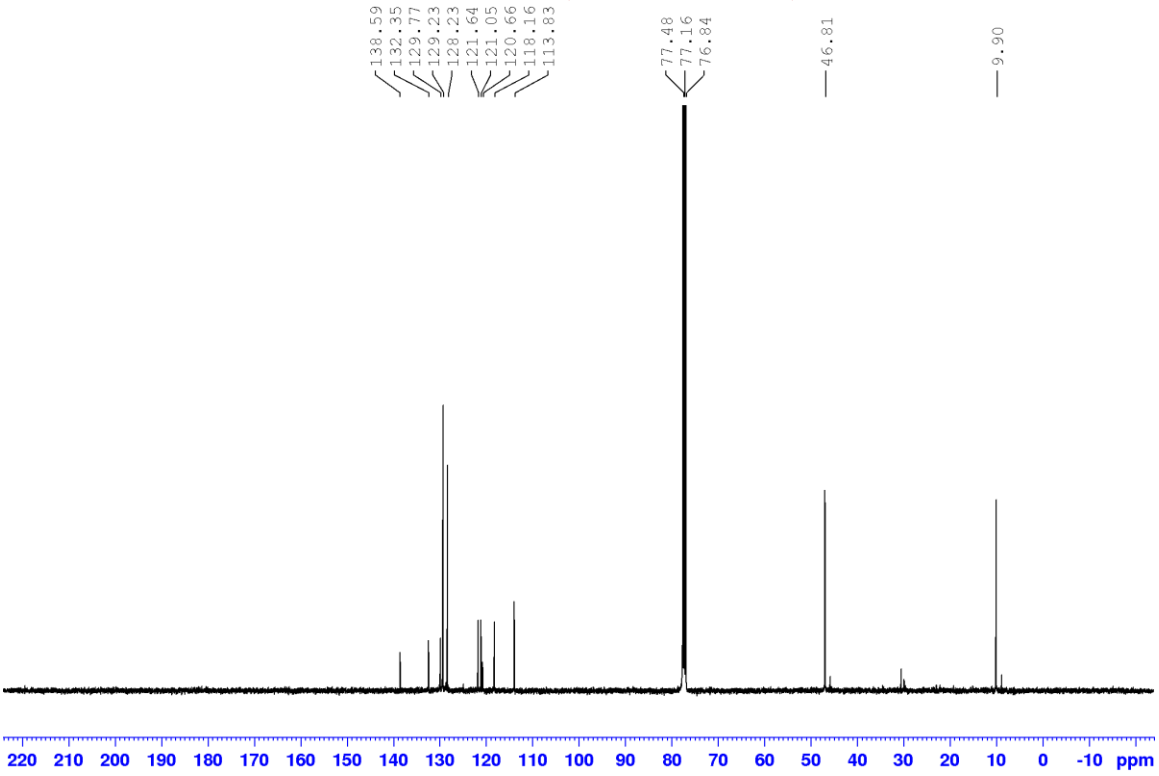


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
207.0929	207.0922	0.7	3.4	10.5	1510.8	n/a	n/a	C14 H11 N2

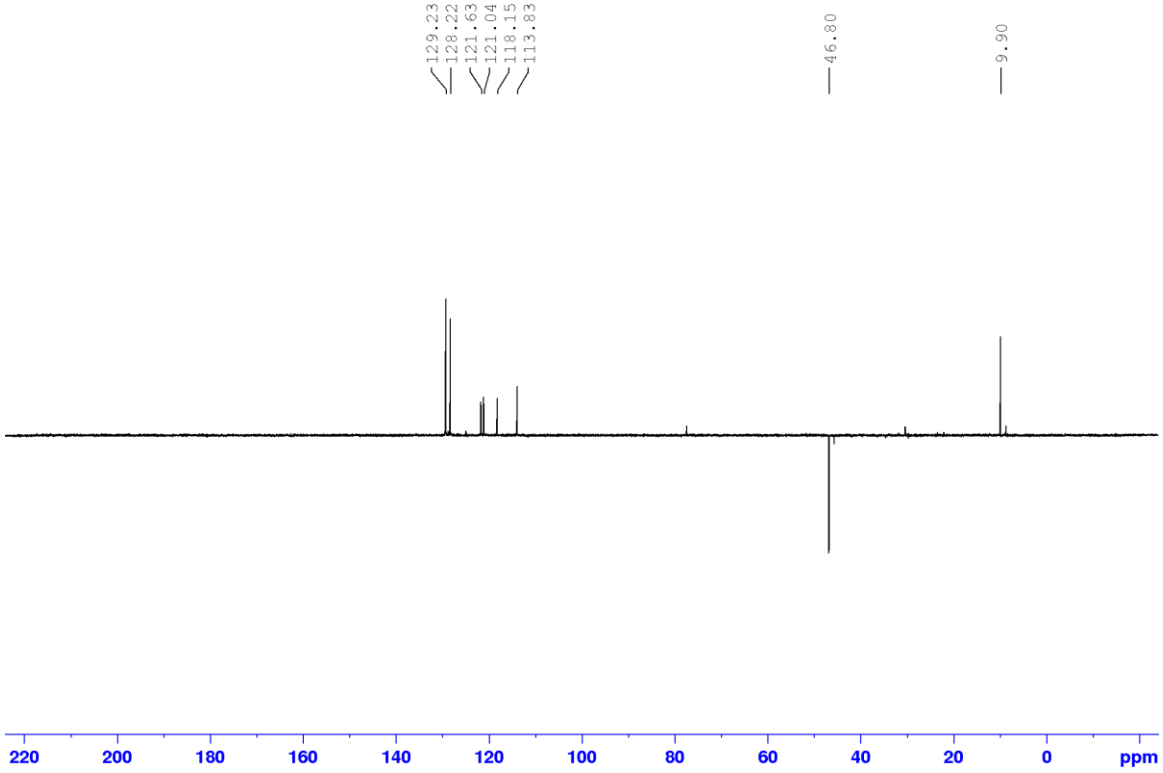
^{1}H NMR (400 MHz, $CDCl_3$) of 3t



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



DEPT-135 (400 MHz, $CDCl_3$) of 3t



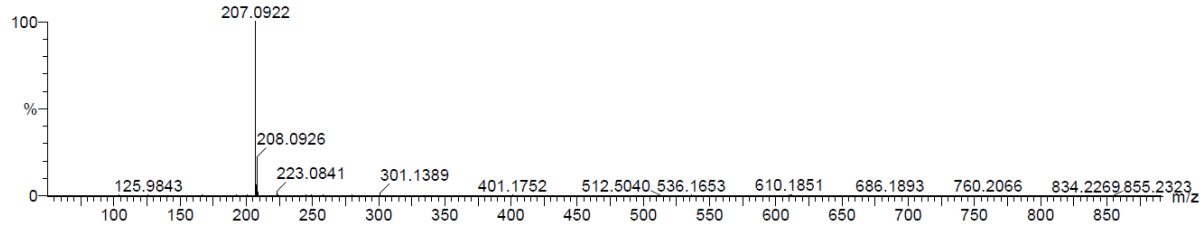
HRMS of 3t

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

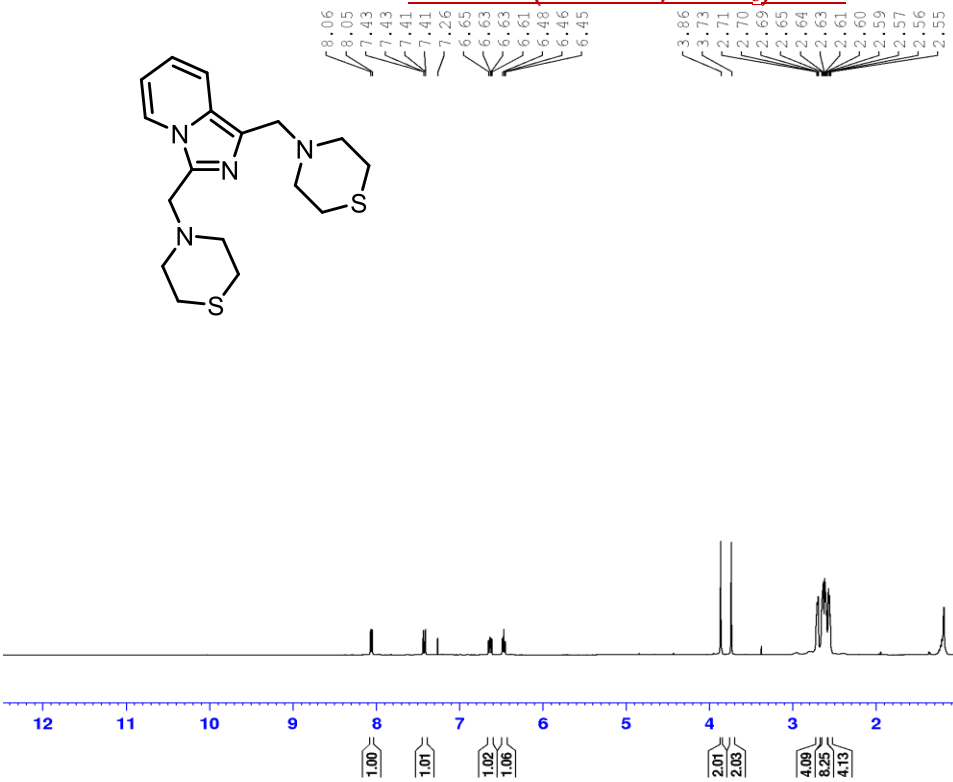
Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3

SM-486 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
070524_30 5 (0.121) Xevo G2-XS QTOF YFC2015 14:05:00
1: TOF MS ES+
2.00e+007

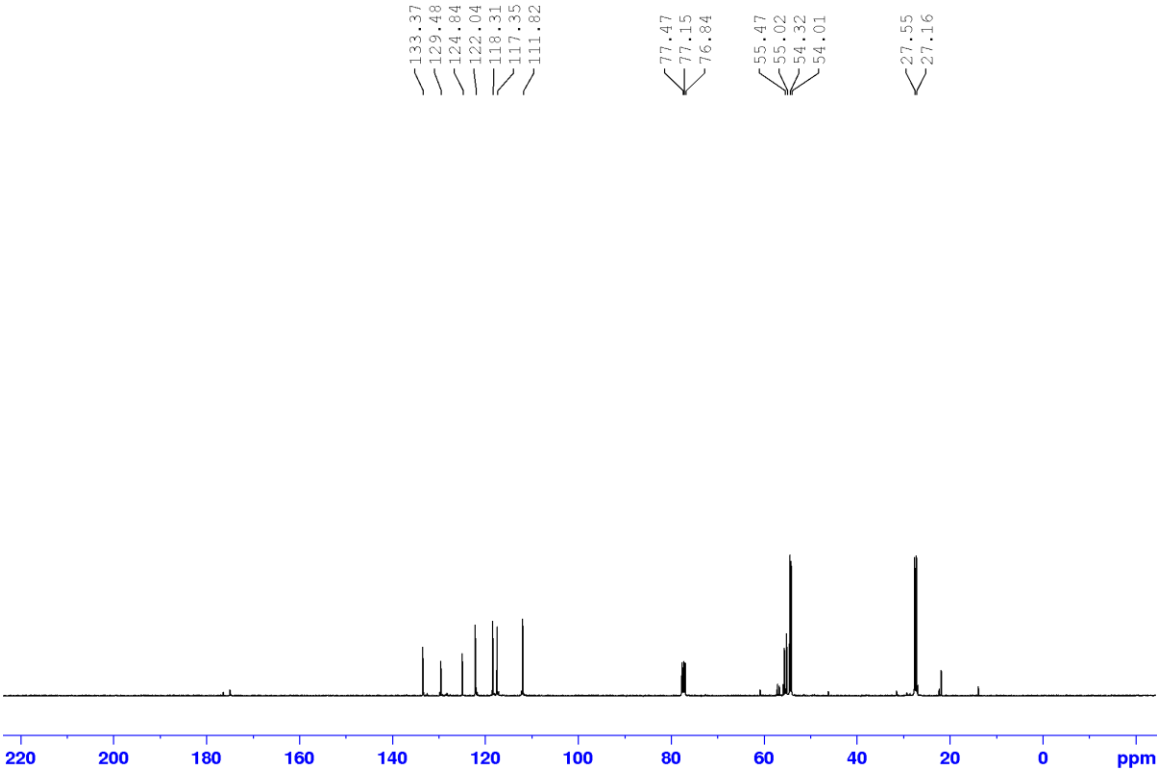


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
207.0922	207.0922	0.0	0.0	10.5	1350.9	n/a	n/a	C14 H11 N2

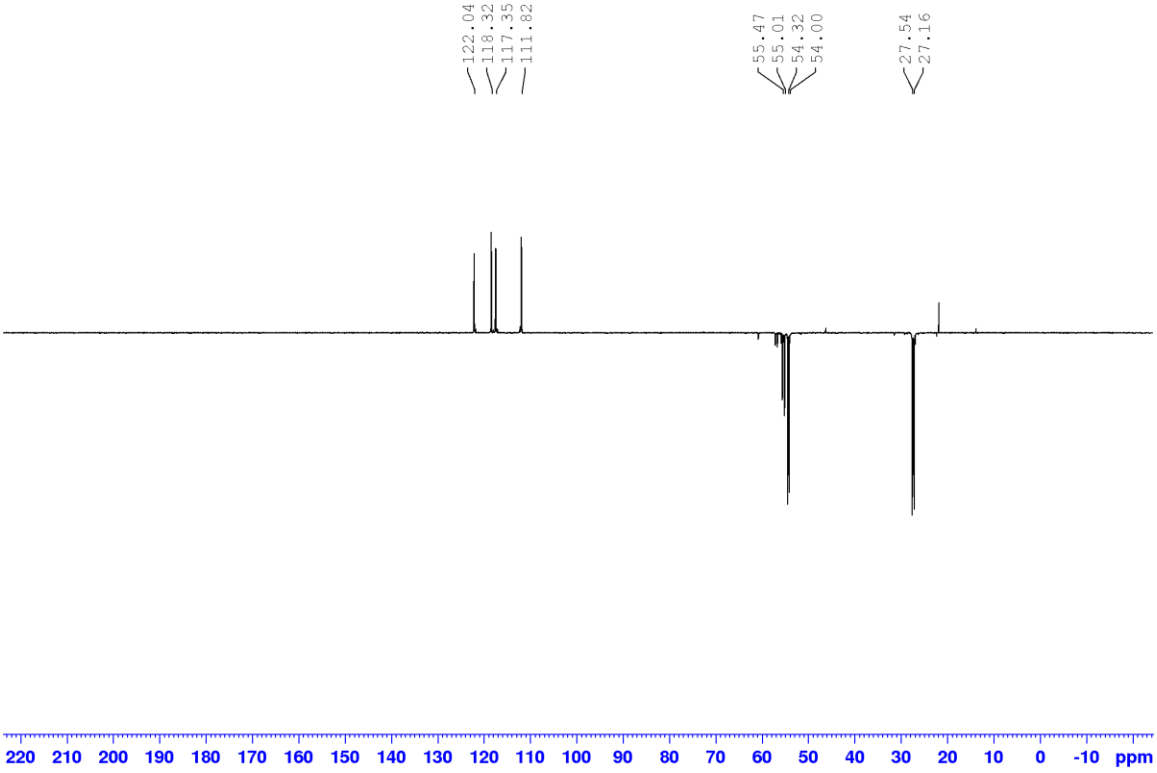
^{1}H NMR (400 MHz, $CDCl_3$) of 3u



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



DEPT-135 (400 MHz, $CDCl_3$) of 3u



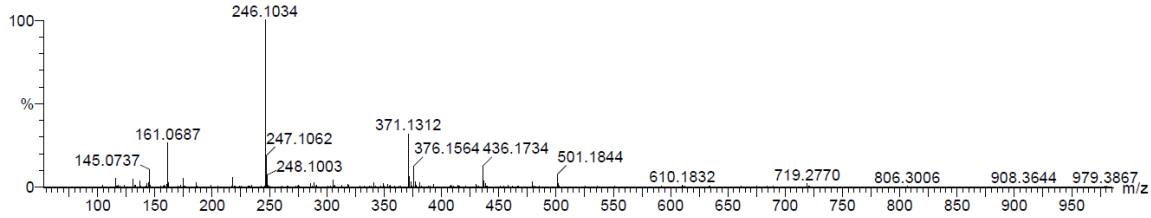
HRMS of 3u

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 02-May-2024
Xevo G2-XS QTOF YFC2015 13:29:15
020524_32 6 (0.138) 1: TOF MS ES+
2.24e+007



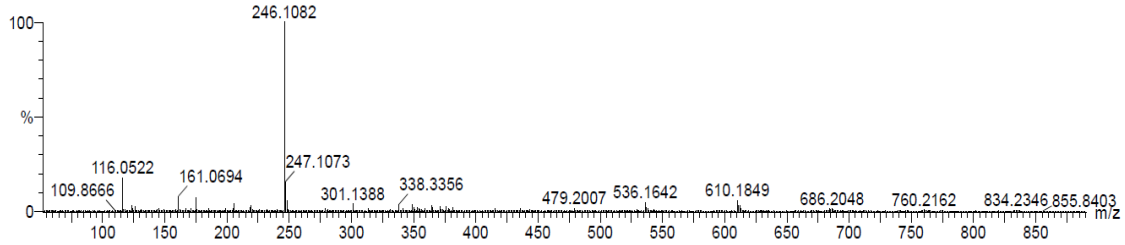
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
371.1312	371.1340	-2.8	-7.5	7.5	1133.0	n/a	n/a	C17 H24 N4 Na S2

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

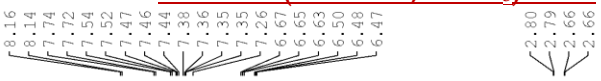
Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 N: 0-3 S: 0-1

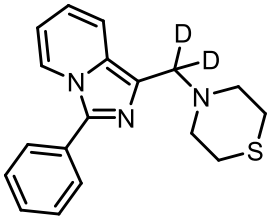
SM-524 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024 14:33:46
070524_37 5 (0.121) Cm (5) Xevo G2-XS QTOF YFC2015 1: TOF MS ES+ 3.12e+006

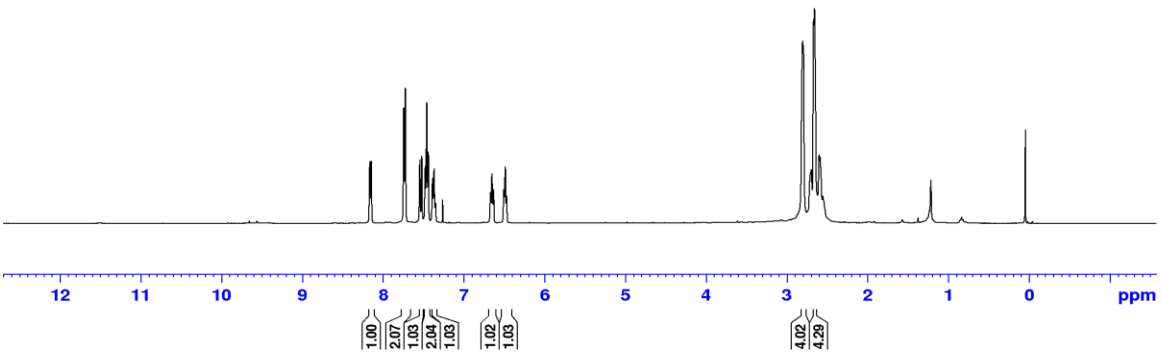


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
246.1082	246.1065	1.7	6.9	7.5	27.1	n/a	n/a	C13 H16 N3 S

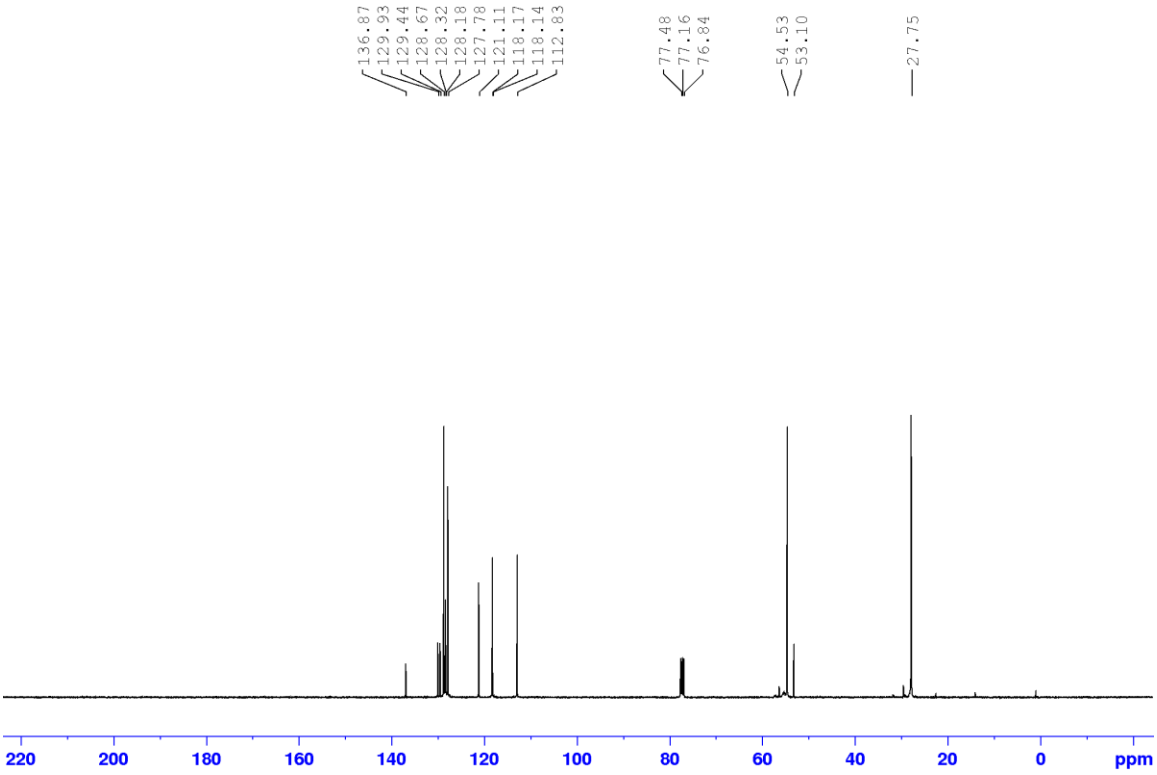
^{1}H NMR (400 MHz, $CDCl_3$) of 3v



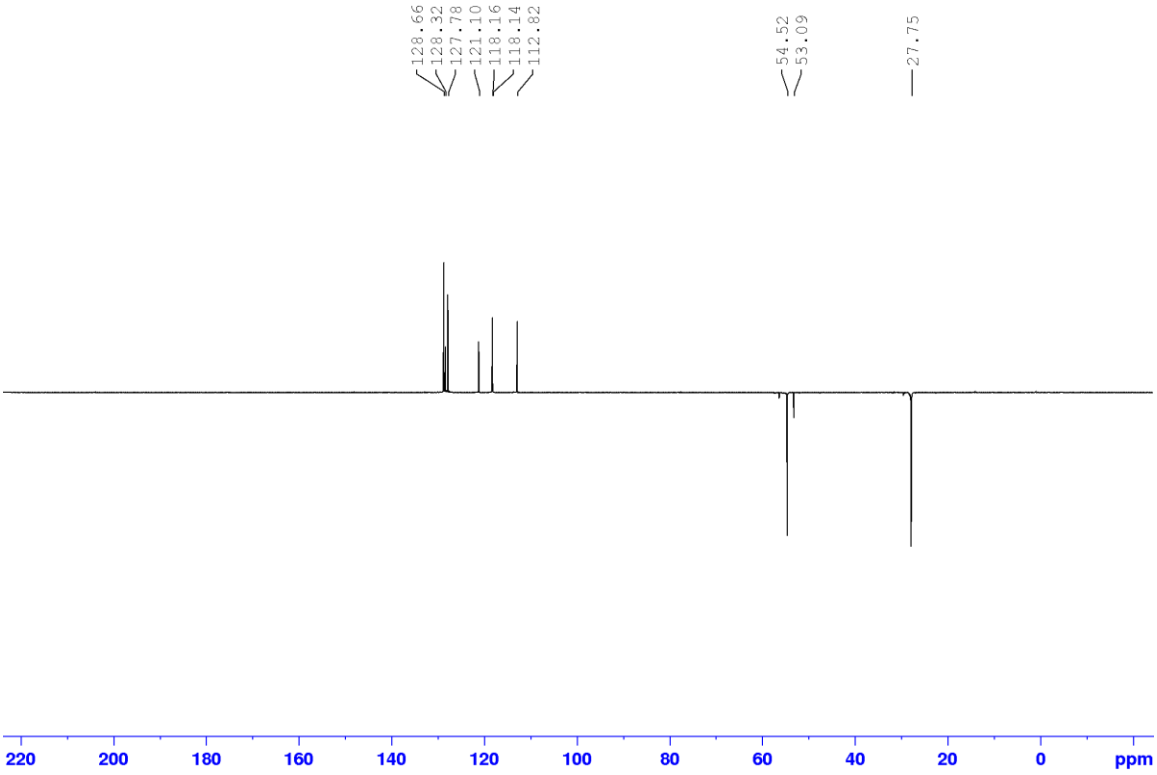




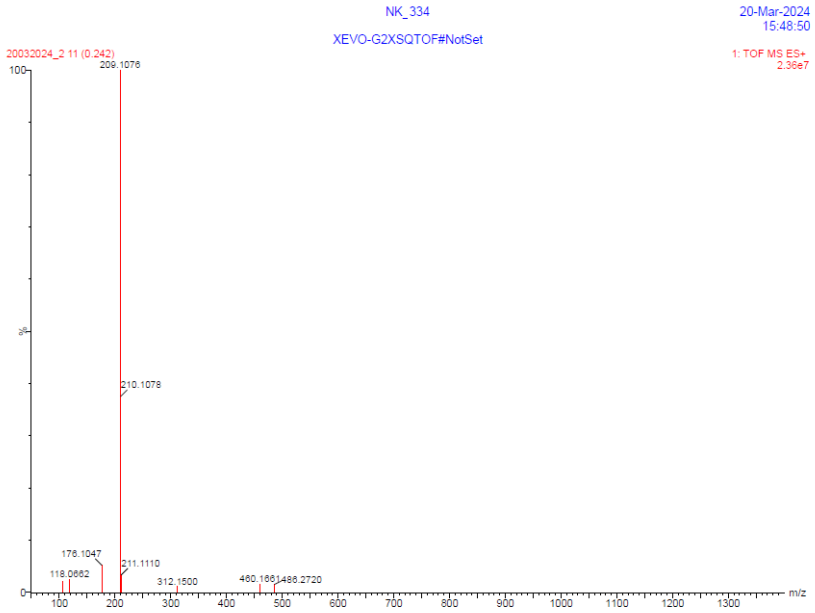
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 3v

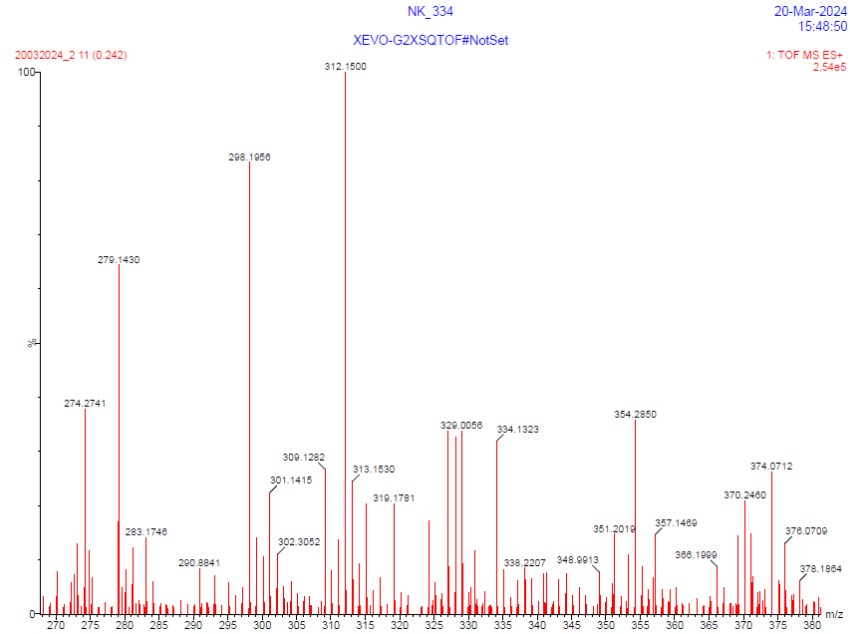


DEPT-135 (101 MHz, $CDCl_3$) of 3v

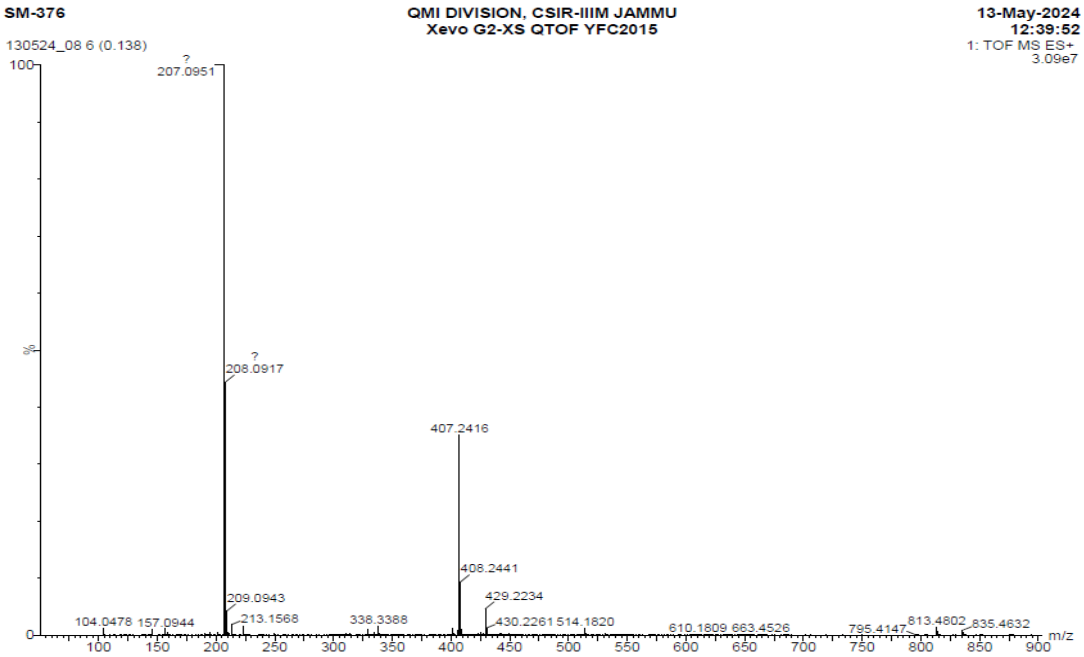


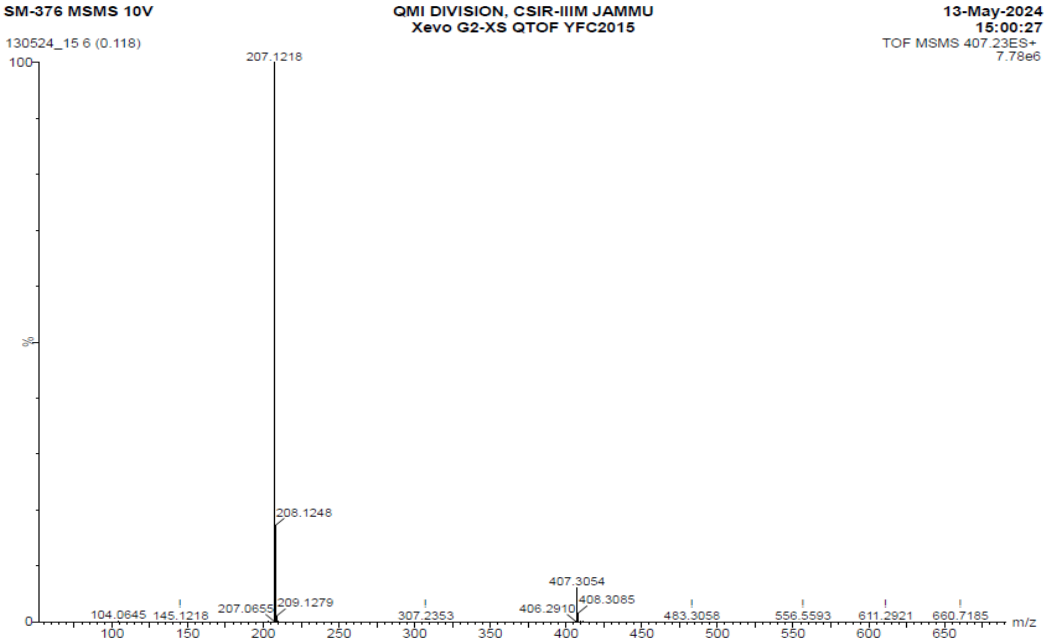
HRMS of 3v


NK_334
XEVO-G2XSQTOF#NotSet
20-Mar-2024
15:48:50
20032024_2 11 (0.242)
1: TOF MS ES+
2.36e7
209.1076
210.1078
176.1047
118.0862
211.1110
312.1500
460.1661
486.2720
%
m/z

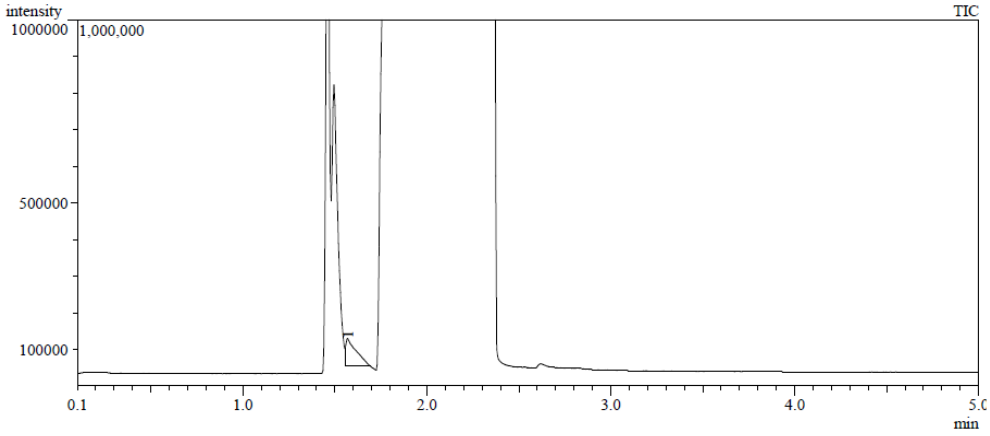

NK_334
XEVO-G2XSQTOF#NotSet
20-Mar-2024
15:48:50
20032024_2 11 (0.242)
1: TOF MS ES+
2.54e5
312.1500
298.1956
279.1430
274.2741
329.0056
334.1323
354.2850
309.1282
313.1530
301.1415
319.1781
374.0712
370.2460
283.1746
351.2019
357.1469
376.0709
302.3052
366.1999
290.8841
338.2207
348.9913
378.1864
%
m/z

MS/MS Spectra of 3s





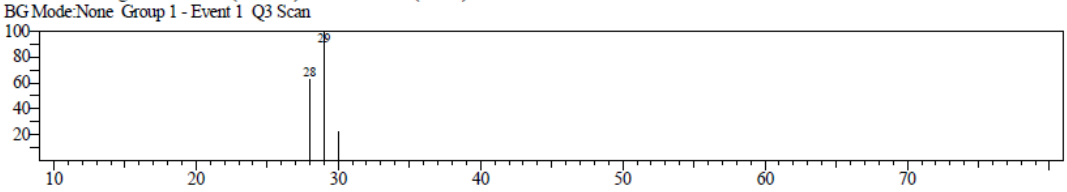
GC-MS for Standard HCHO



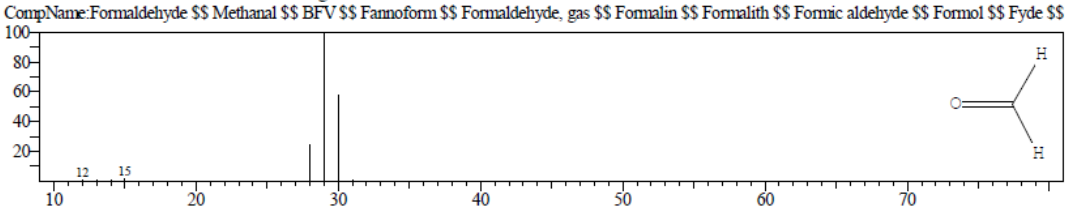
Peak Report TIC

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

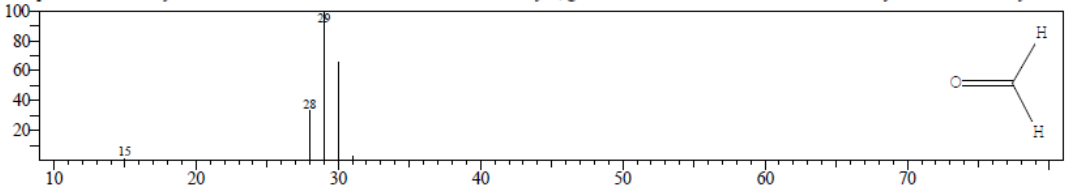
Library
<< Target >>
Line#:1 R.Time:1.570(Scan#:315) MassPeaks:3
RawMode:Averaged 1.560-1.590(313-319) BasePeak:29.00(65222)
BG Mode:None Group 1 - Event 1 Q3 Scan



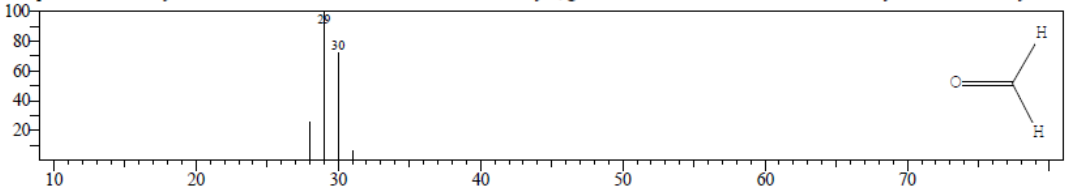
Hit#:1 Entry:12 Library:NIST17M1.lib
SI:90 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0
CompName:Formaldehyde $$ Methanal $$ BFV $$ Fannoform $$ Formaldehyde, gas $$ Formalin $$ Formalith $$ Formic aldehyde $$ Formol $$ Fyde $$



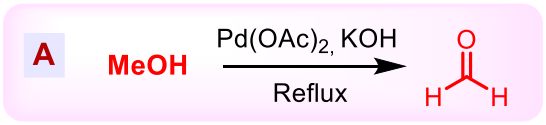
Hit#:2 Entry:10 Library:NIST17R.lib
SI:90 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0
CompName:Formaldehyde $$ Methanal $$ BFV $$ Fannoform $$ Formaldehyde, gas $$ Formalin $$ Formalith $$ Formic aldehyde $$ Formol $$ Fyde $$

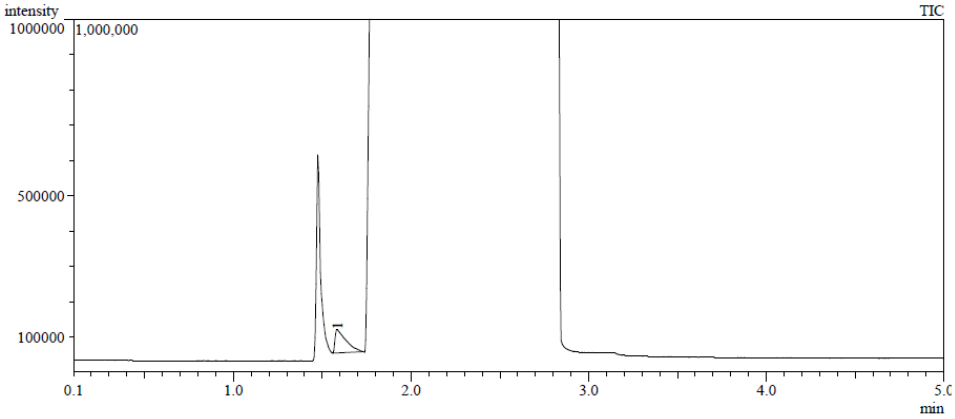


Hit#:3 Entry:11 Library:NIST17R.lib
SI:87 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0
CompName:Formaldehyde $$ Methanal $$ BFV $$ Fannoform $$ Formaldehyde, gas $$ Formalin $$ Formalith $$ Formic aldehyde $$ Formol $$ Fyde $$



GC-MS for reaction A

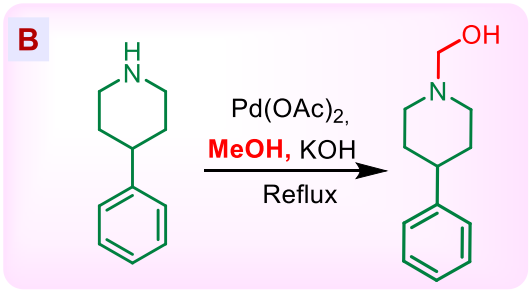


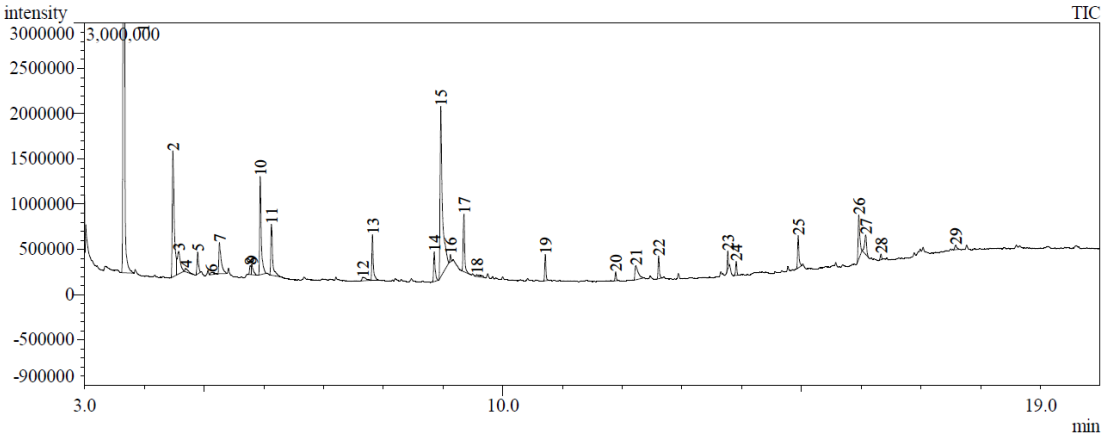


Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	1.583	283825	100.00	0	29.00	Formaldehyde
		283825	100.00			

GCMS for reaction B





Library for reaction A

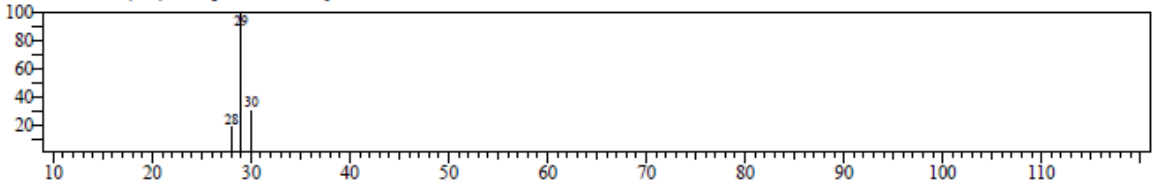
Library

<< Target >>

Line#:1 R.Time:1.585(Scan#:318) MassPeaks:3

RawMode:Averaged 1.565-1.605(314-322) BasePeak:29.00(30142)

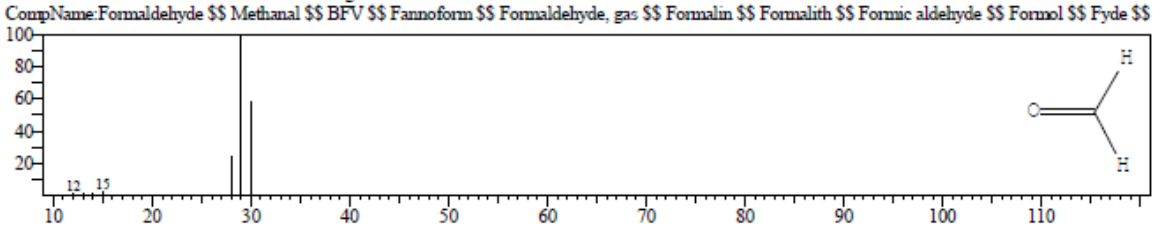
BG Mode:1.715(344) Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:12 Library:NIST17M1.lib

SI:95 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0

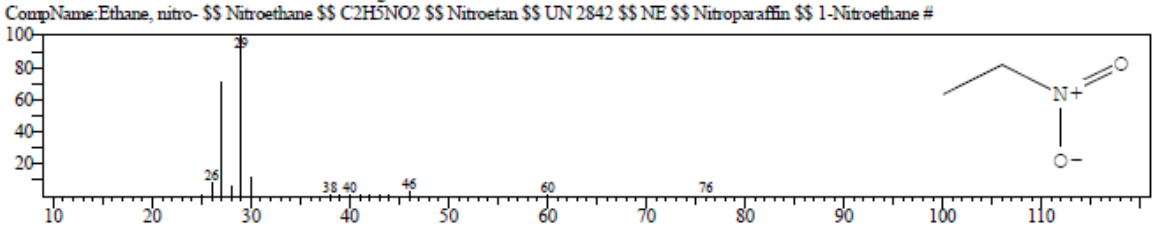
CompName:Formaldehyde $$ Methanal $$ BFV $$ Fannoform $$ Formaldehyde, gas $$ Formalin $$ Formalith $$ Formic aldehyde $$ Formol $$ Fyde $$



Hit#:2 Entry:584 Library:NIST17R.lib

SI:92 Formula:C2H5NO2 CAS:79-24-3 MolWeight:75 RetIndex:602

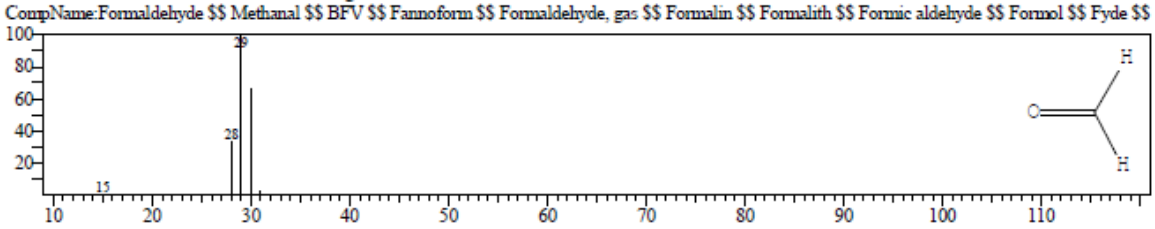
CompName:Ethane, nitro- $$ Nitroethane $$ C2H5NO2 $$ Nitroetan $$ UN 2842 $$ NE $$ Nitroparaffin $$ 1-Nitroethane #



Hit#:3 Entry:10 Library:NIST17R.lib

SI:92 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0

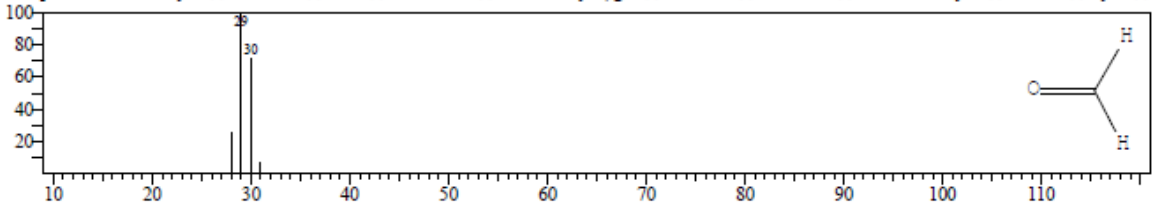
CompName:Formaldehyde $$ Methanal $$ BFV $$ Fannoform $$ Formaldehyde, gas $$ Formalin $$ Formalith $$ Formic aldehyde $$ Formol $$ Fyde $$



Hit#:4 Entry:11 Library:NIST17R.lib

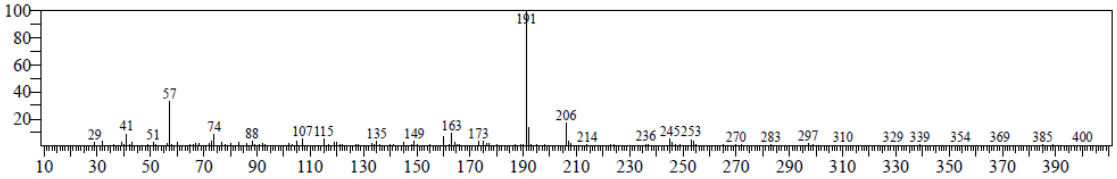
SI:91 Formula:CH2O CAS:50-00-0 MolWeight:30 RetIndex:0

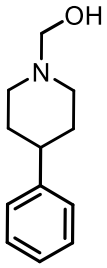
CompName:Formaldehyde $$ Methanal $$ BFV $$ Fannoform $$ Formaldehyde, gas $$ Formalin $$ Formalith $$ Formic aldehyde $$ Formol $$ Fyde $$



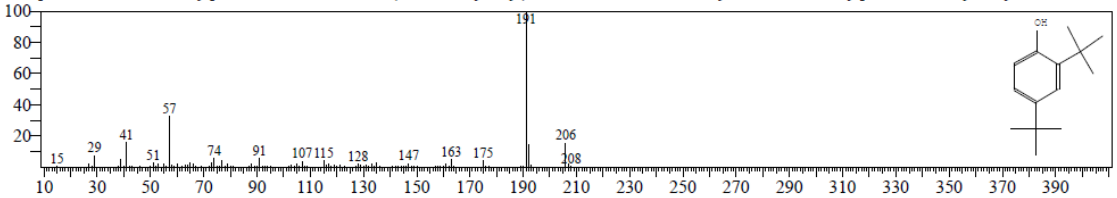
Library for reaction B

<< 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

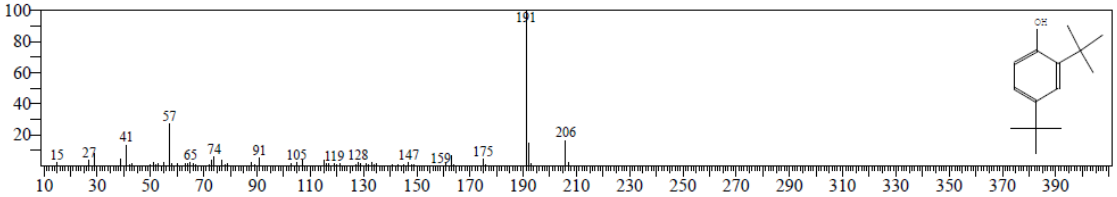




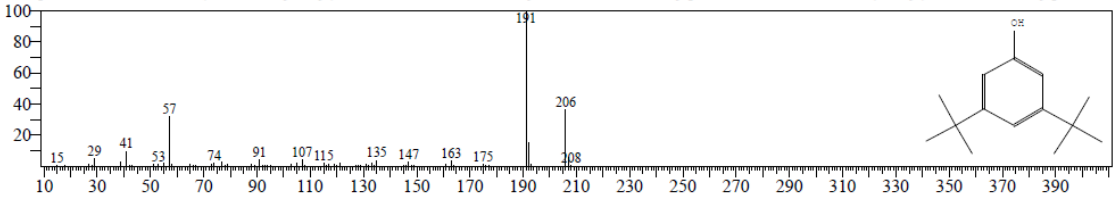
Hit#:1 Entry:54577 Library:NIST17M1.lib
SI:80 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



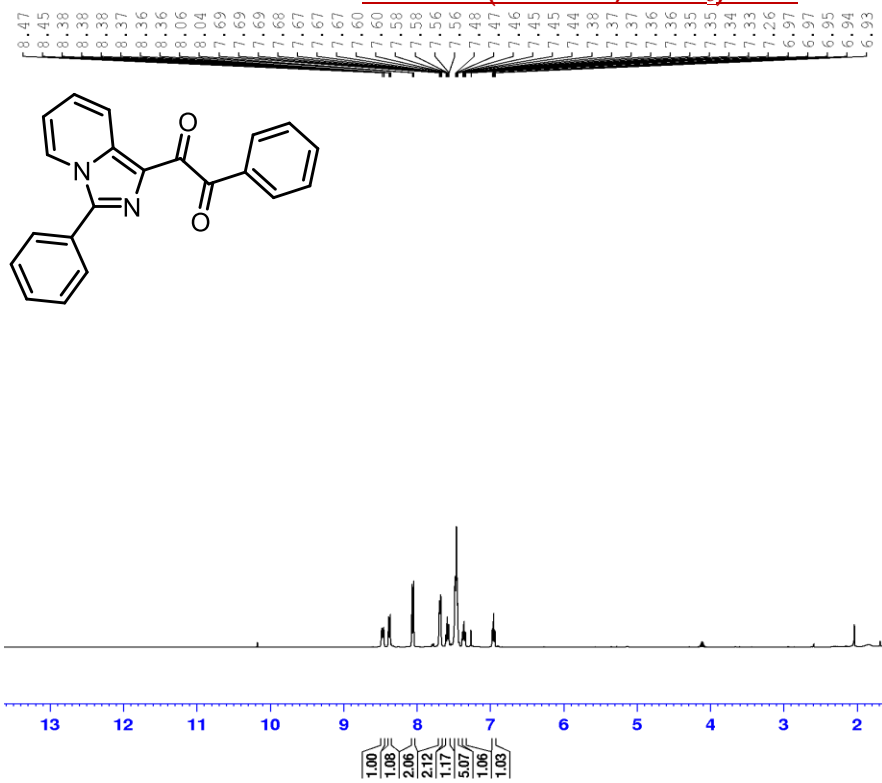
Hit#:2 Entry:22784 Library:NIST17R.lib
SI:79 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



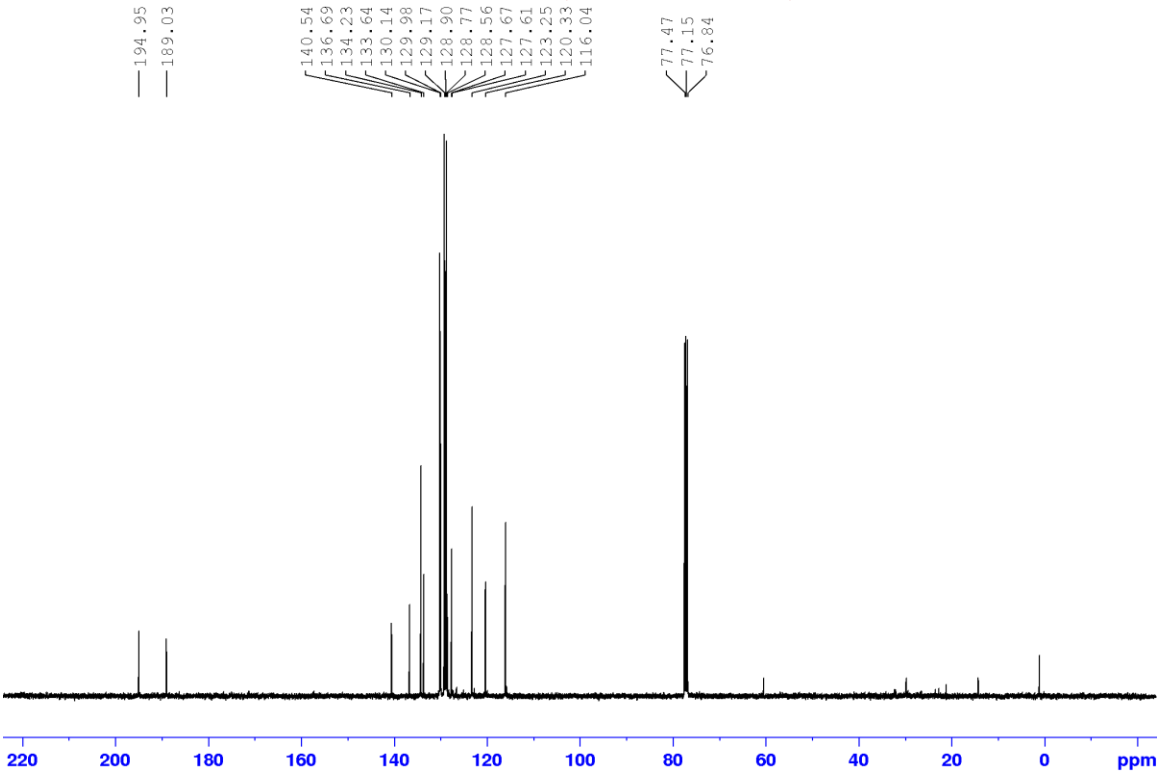
Hit#:3 Entry:22787 Library:NIST17R.lib
SI:79 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



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



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



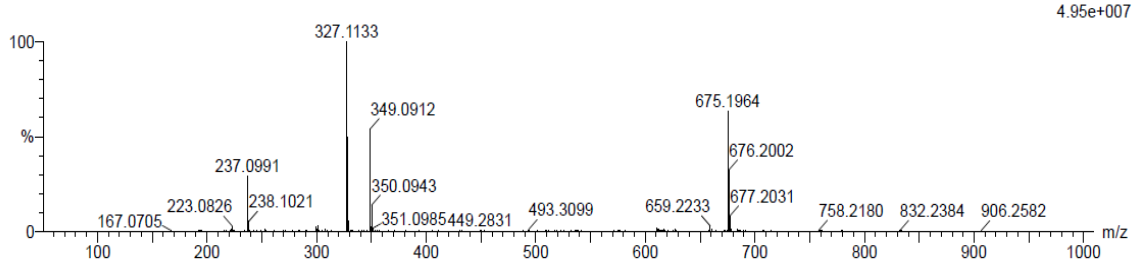
HRMS of 5a

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

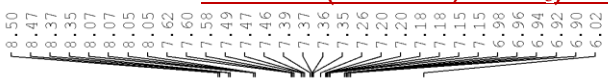
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-21 H: 0-100 N: 0-2 O: 0-2

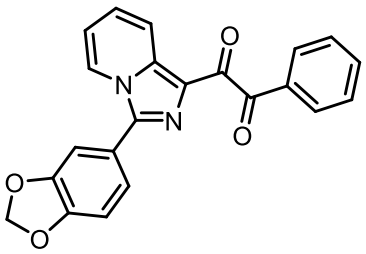
SM-339 QMI DIVISION, CSIR-IIIM JAMMU 02-May-2024
Xevo G2-XS QTOF YFC2015 13:13:03
020524_26 6 (0.138) 1: TOF MS ES+
4.95e+007

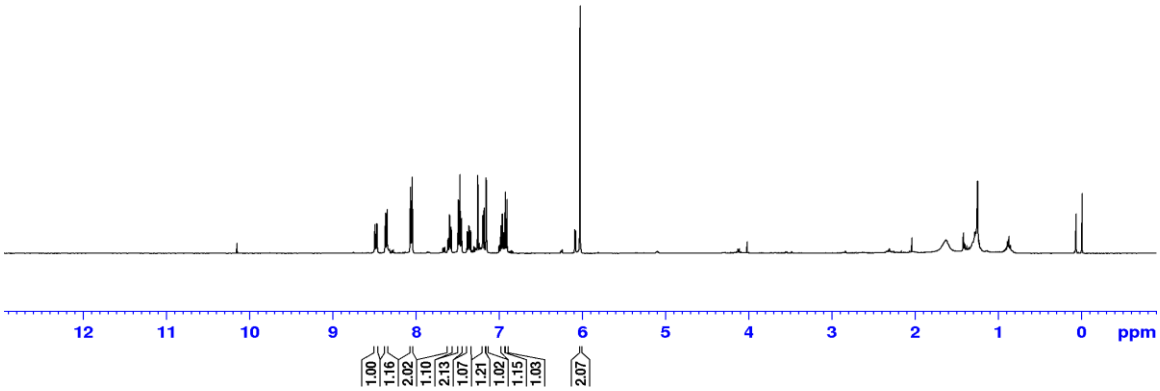


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
327.1133	327.1134	-0.1	-0.3	15.5	1061.9	n/a	n/a	C21 H15 N2 O2

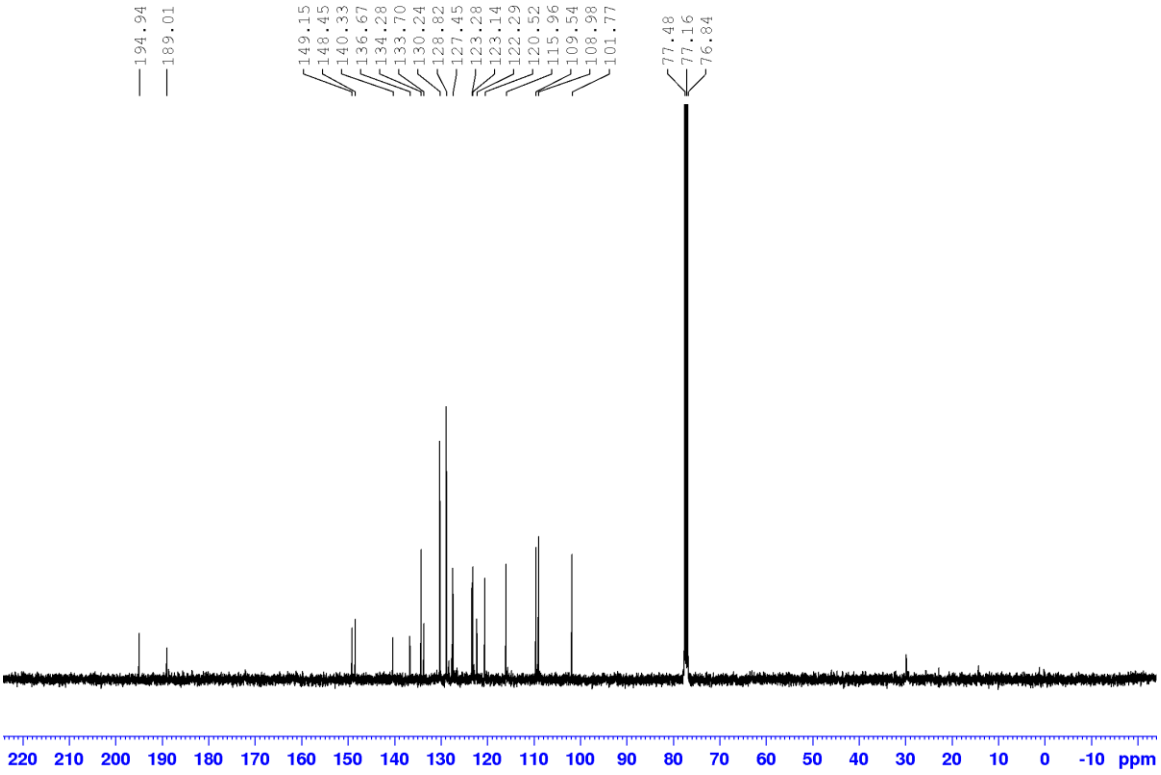
^{1}H NMR (400 MHz, $CDCl_3$) of 5b







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



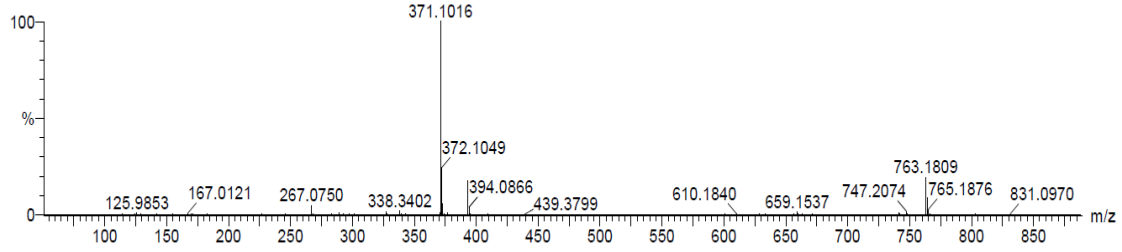
HRMS of 5b

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

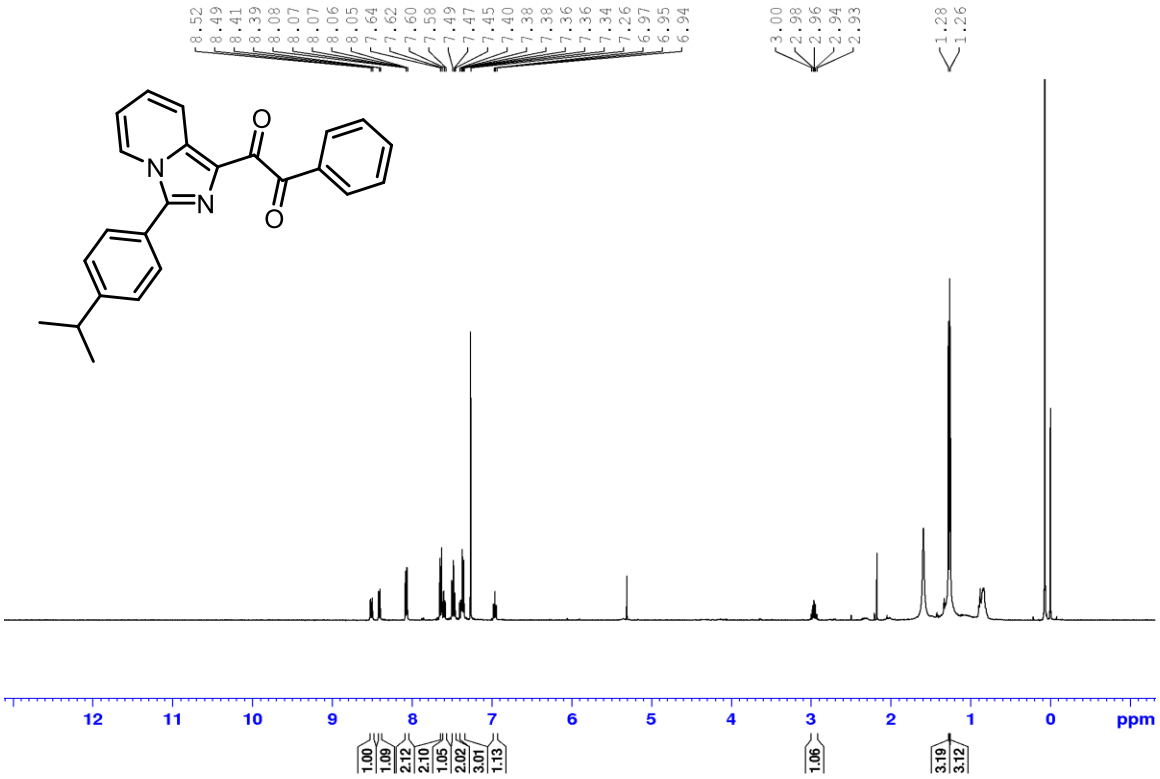
Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-22 H: 0-100 N: 0-2 O: 0-4

SM-502 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 12:00:41
300424_10 5 (0.121) 1: TOF MS ES+
1.18e+007

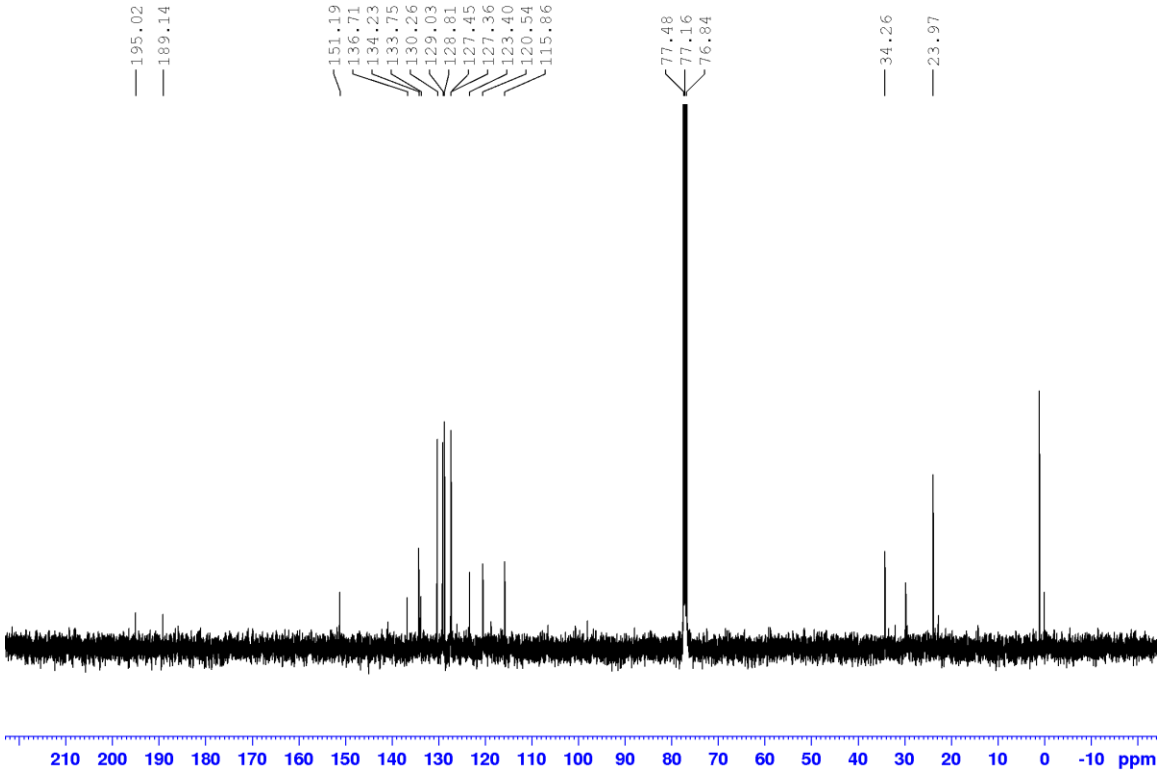


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
371.1016	371.1032	-1.6	-4.3	16.5	1090.3	n/a	n/a	C22 H15 N2 O4

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



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



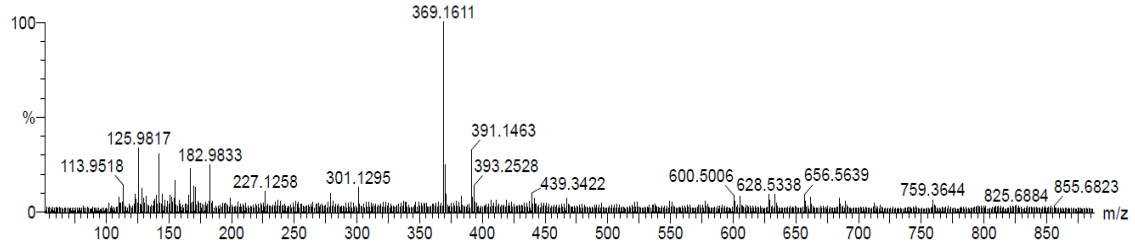
HRMS of 5c

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

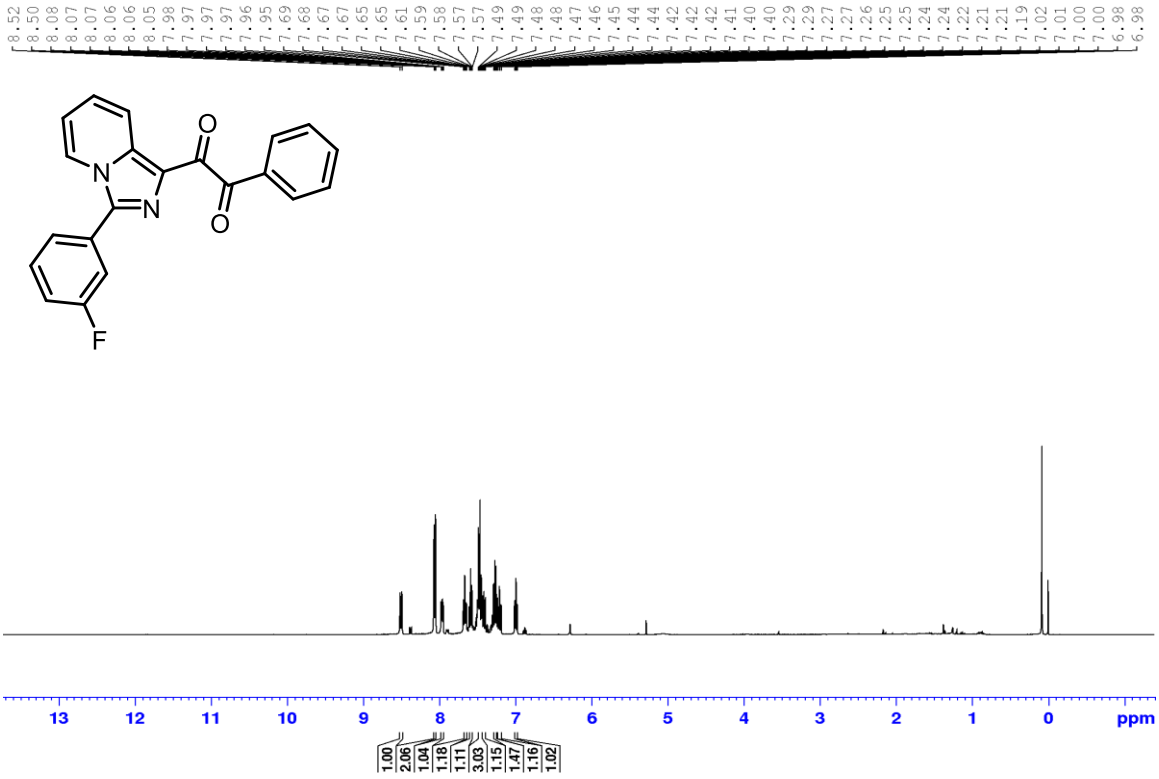
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-24 H: 0-100 N: 0-2 O: 0-2

SM-395 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 11:42:36
300424_03 4 (0.104) Cm (4) 1: TOF MS ES+
5.83e+005

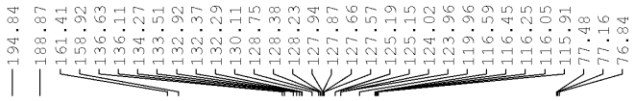


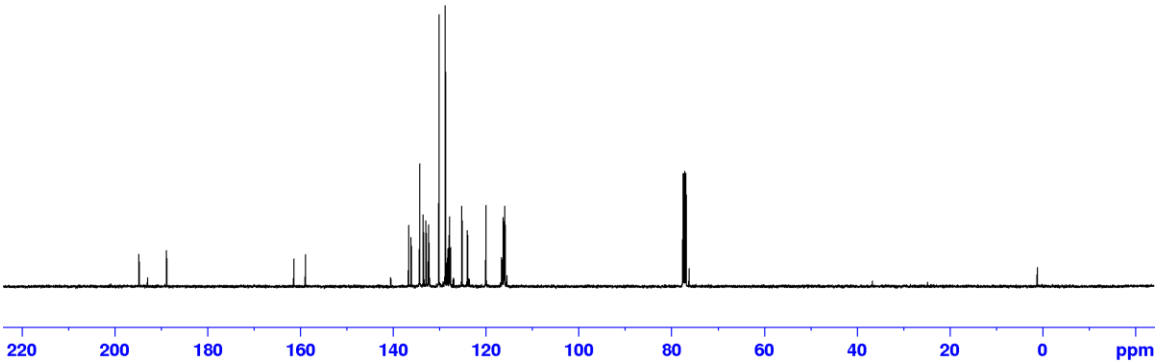
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
369.1611	369.1603	0.8	2.2	15.5	57.3	n/a	n/a	C24 H21 N2 O2

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

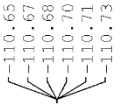


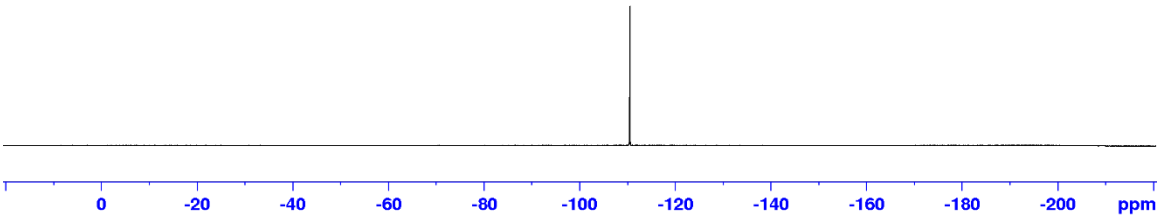
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of 5d





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





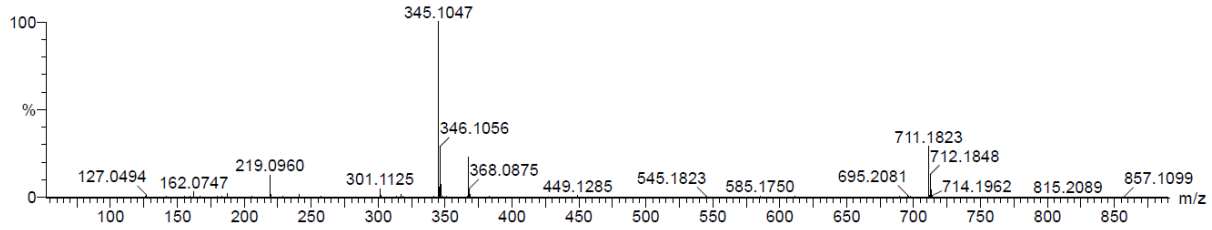
HRMS of 5d

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

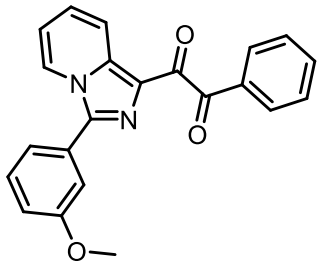
Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-21 H: 0-100 N: 0-2 O: 0-2 F: 0-1

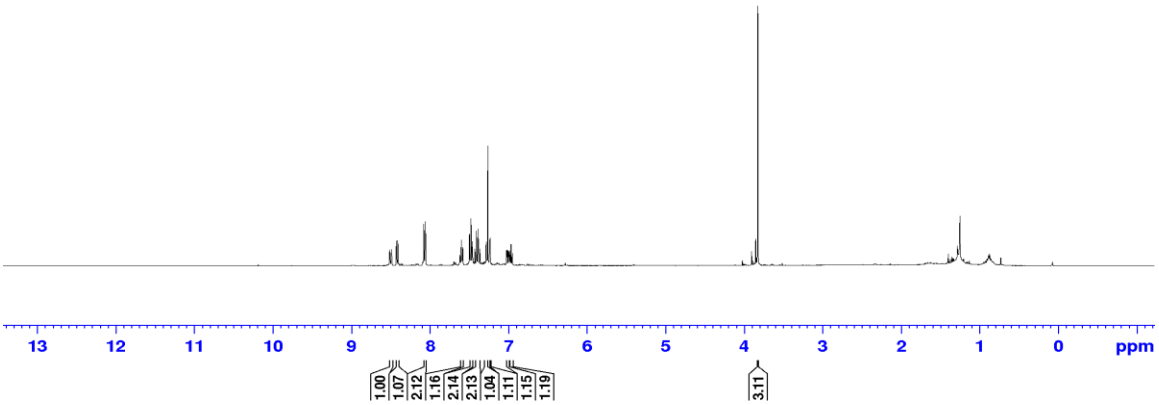
SM-386 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 11:52:52
300424_07 5 (0.121) 1: TOF MS ES+
2.28e+007



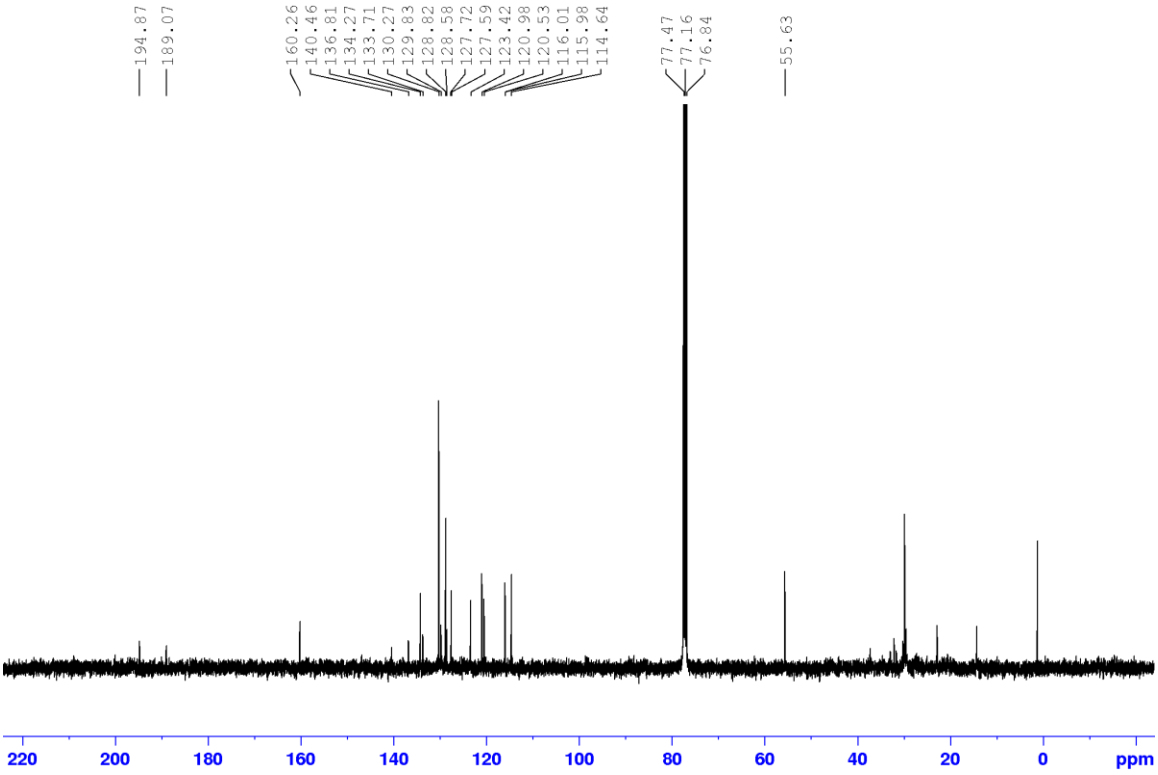
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
345.1047	345.1039	0.8	2.3	15.5	1171.1	n/a	n/a	C21 H14 N2 O2 F

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





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



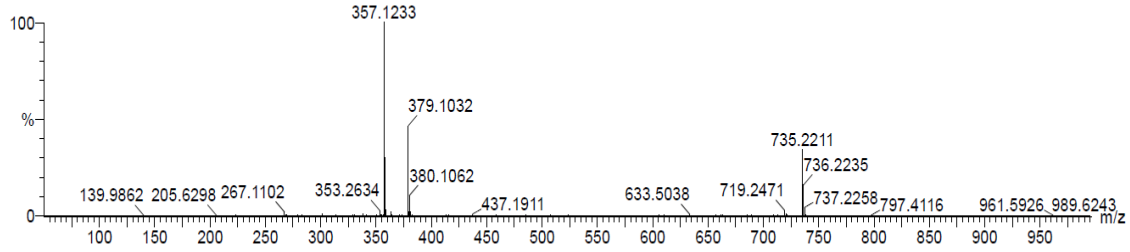
HRMS of 5e

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

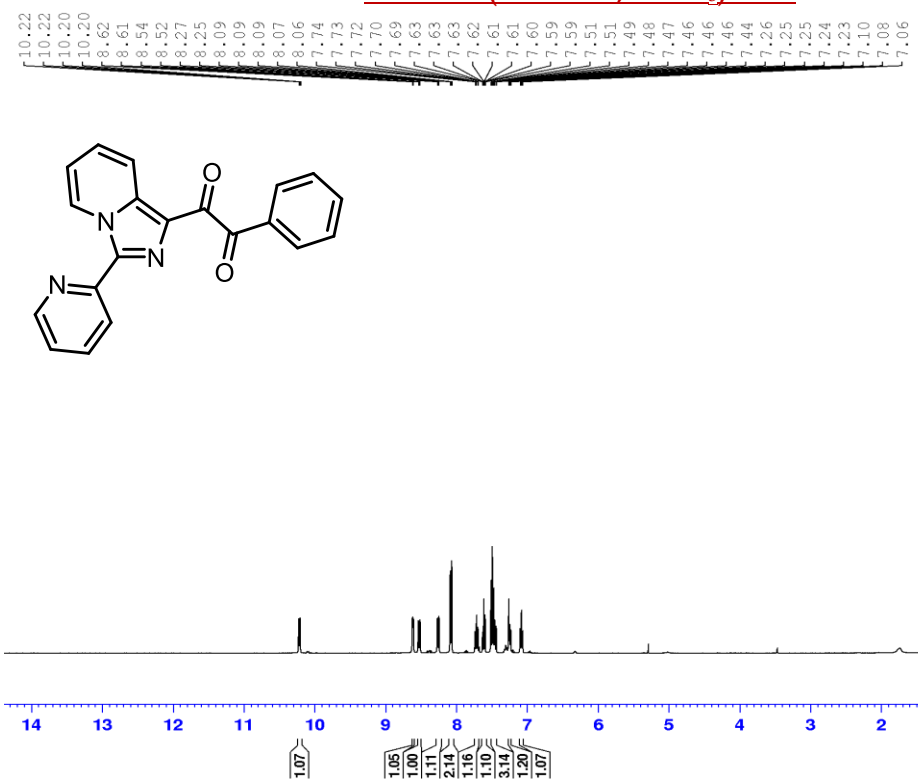
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-22 H: 0-100 N: 0-2 O: 0-3

SM-413 QMI DIVISION, CSIR-IIIM JAMMU 02-May-2024
Xevo G2-XS QTOF YFC2015 13:15:46
020524_27 6 (0.138) 1: TOF MS ES+
2.54e+007

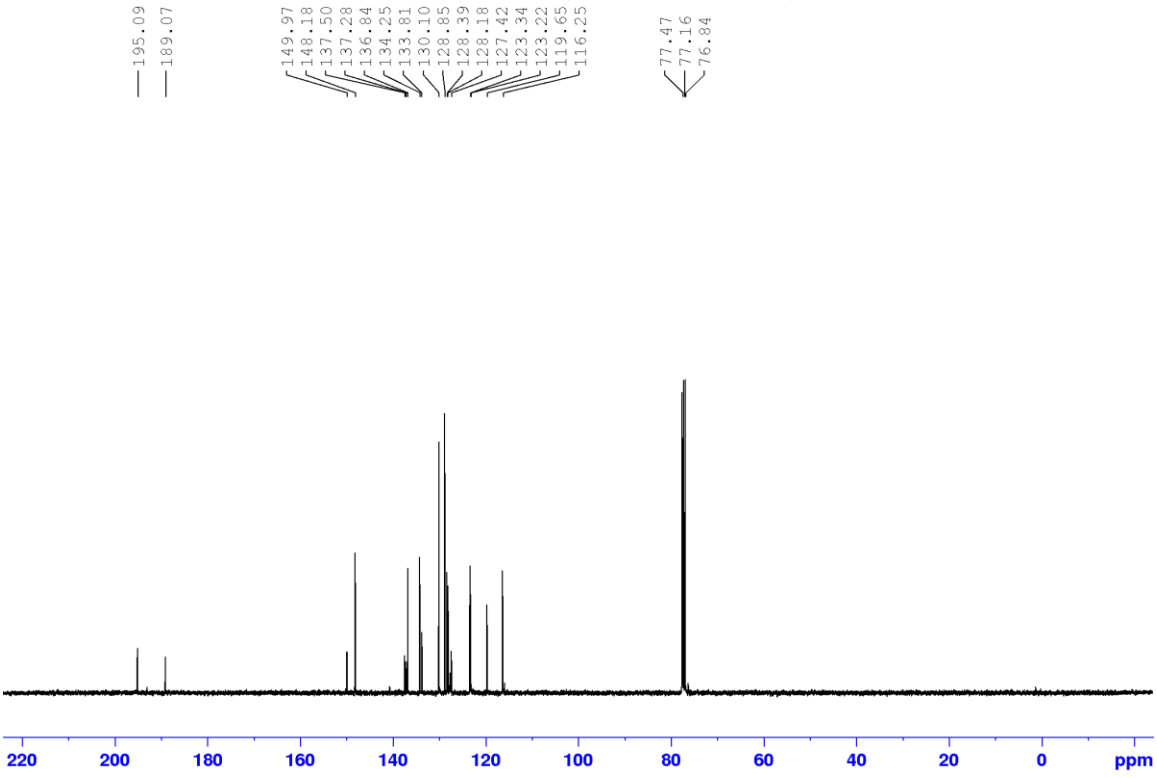


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
357.1233	357.1239	-0.6	-1.7	15.5	1087.1	n/a	n/a	C22 H17 N2 O3

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



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



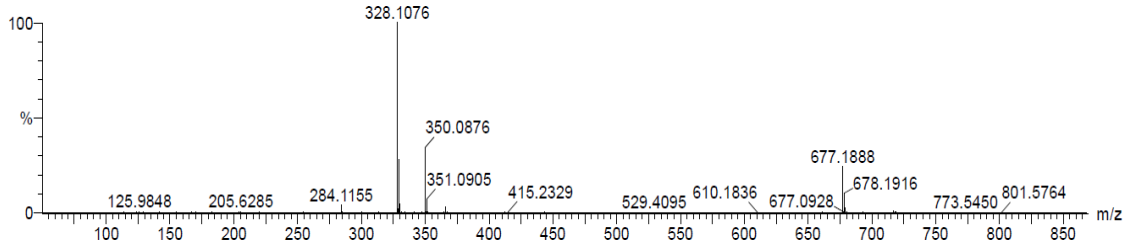
HRMS of 5f

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

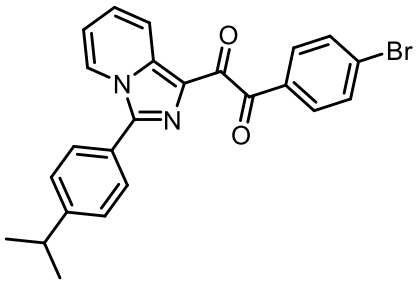
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-20 H: 0-100 N: 0-3 O: 0-2

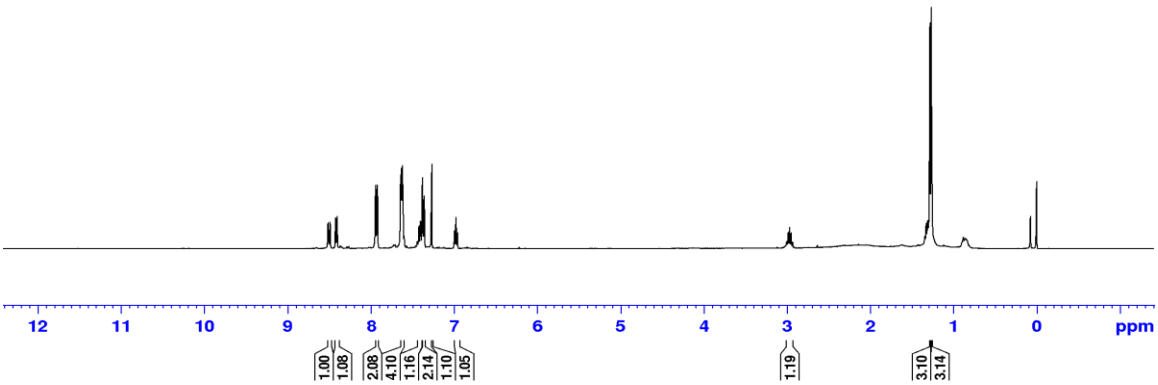
SM-387 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 11:50:17
300424_06 7 (0.155) 1: TOF MS ES+
2.32e+007



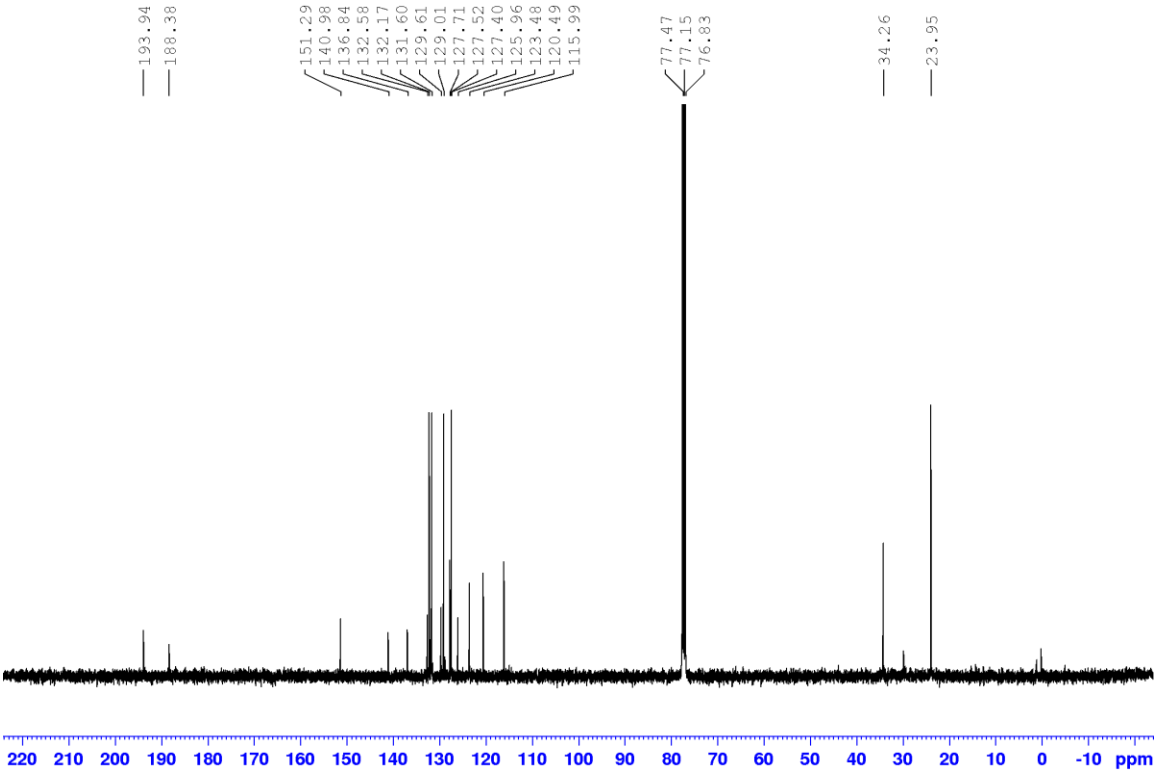
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
328.1076	328.1086	-1.0	-3.0	15.5	1253.3	n/a	n/a	C20 H14 N3 O2

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





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



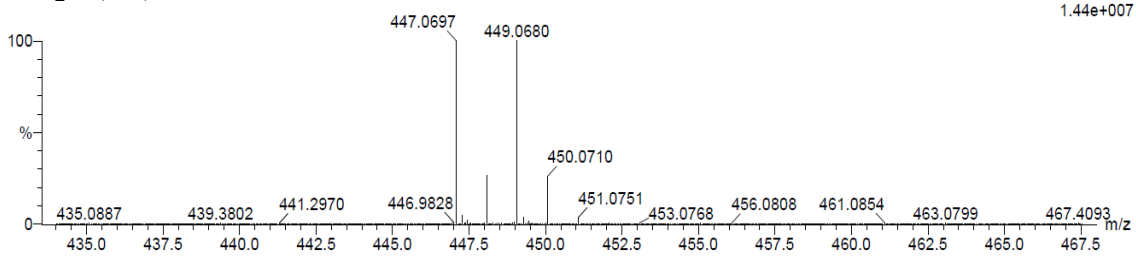
HRMS of 5g

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

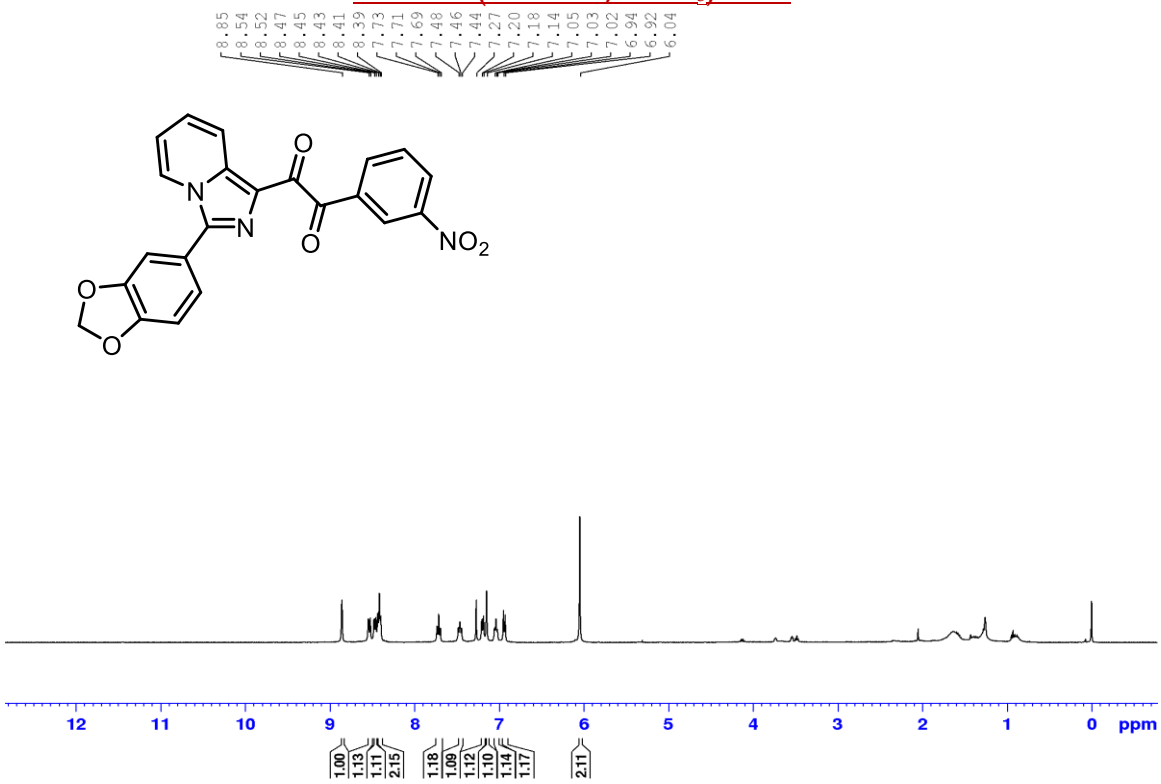
Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-24 H: 0-100 N: 0-2 O: 0-2 Br: 0-1

SM-439 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 11:55:25
300424_08 5 (0.121) 1: TOF MS ES+
1.44e+007

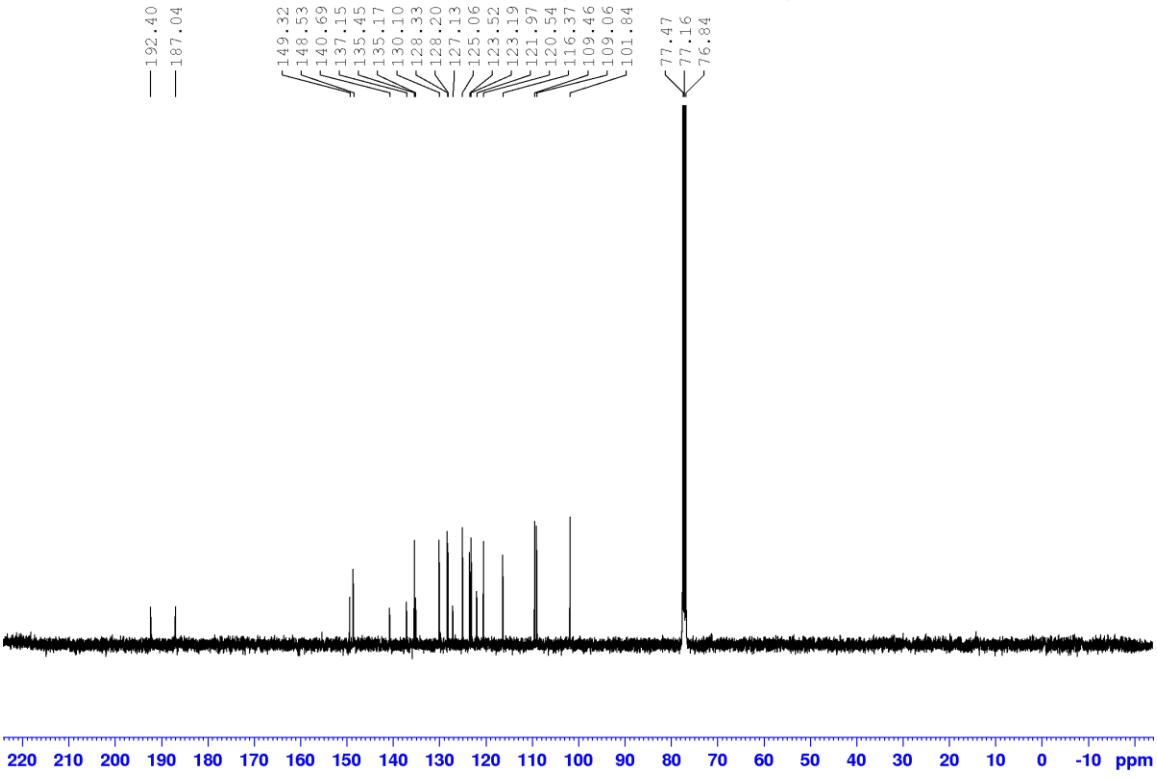


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
447.0697	447.0708	-1.1	-2.5	15.5	997.6	n/a	n/a	C24 H20 N2 O2 Br

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



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



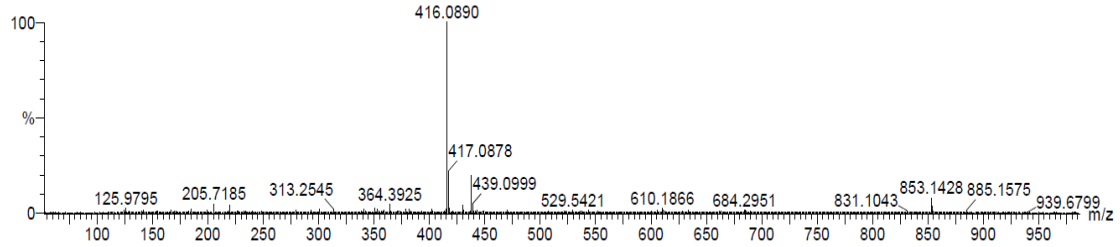
HRMS of 5h

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

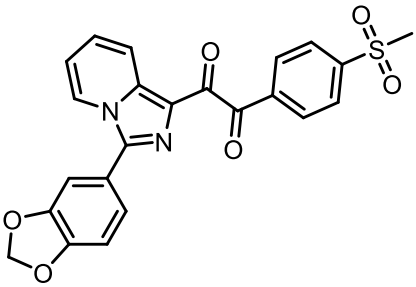
Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-22 H: 0-150 N: 0-3 O: 0-6

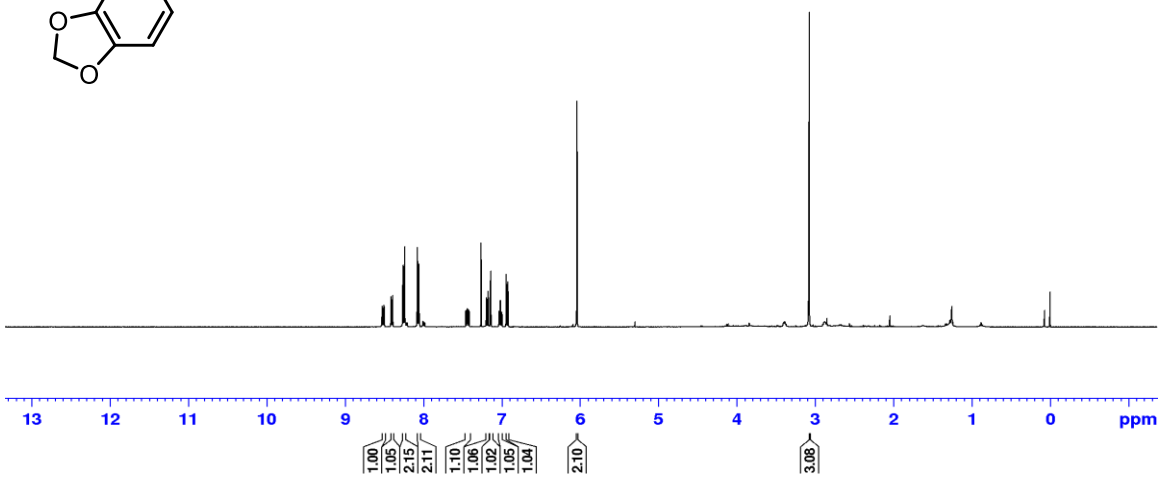
SM-515 QMI DIVISION, CSIR-IIIM JAMMU 02-May-2024
Xevo G2-XS QTOF YFC2015 13:09:40
020524_25 8 (0.172) Cm (8) 1: TOF MS ES+
5.10e+006



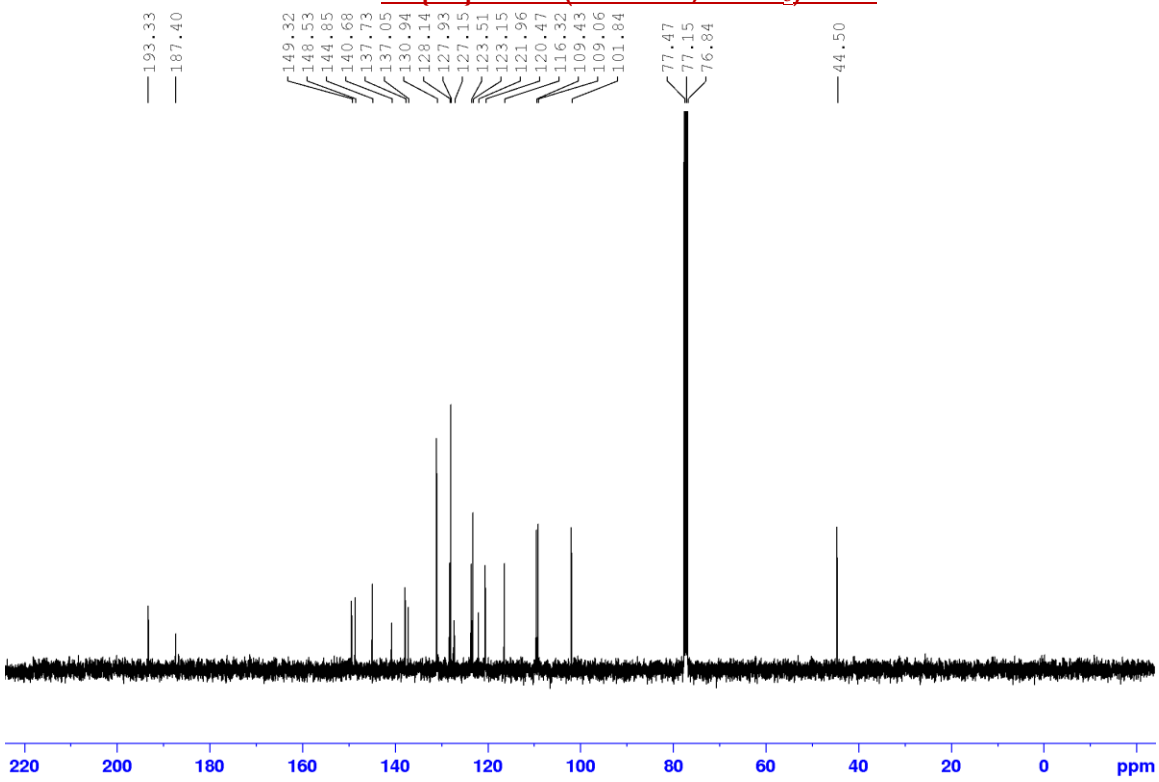
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
416.0890	416.0883	0.7	1.7	17.5	37.8	n/a	n/a	C22 H14 N3 O6

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





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



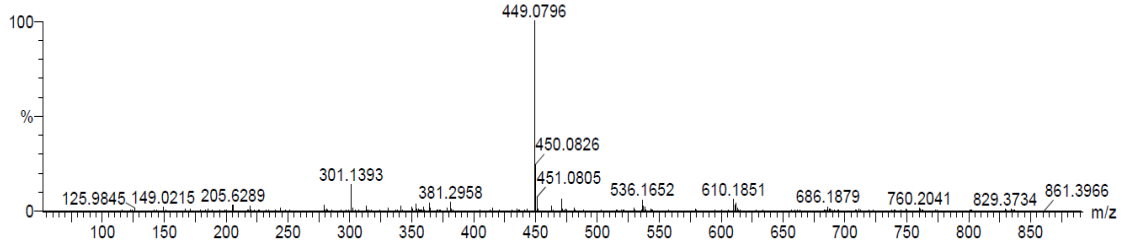
HRMS of 5i

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

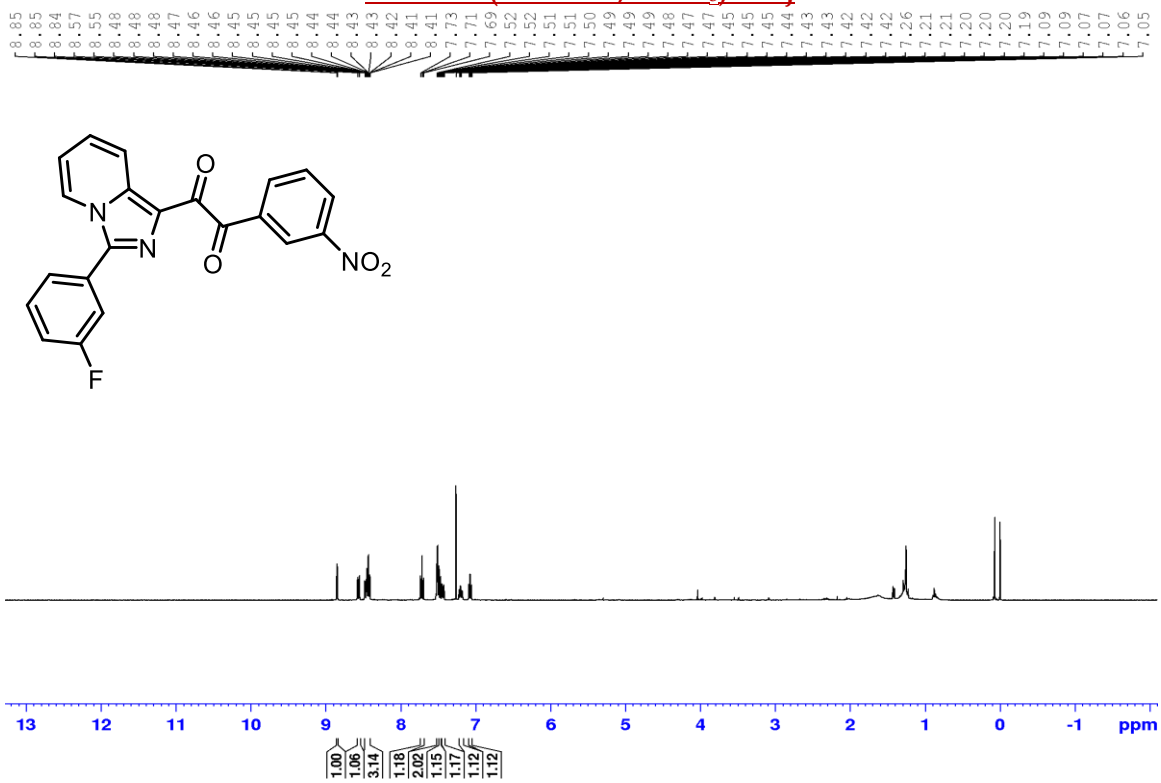
Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-23 H: 0-100 N: 0-2 O: 0-6 S: 0-1

SM-527 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 14:47:00
070524_42 5 (0.121) 1: TOF MS ES+
4.06e+006

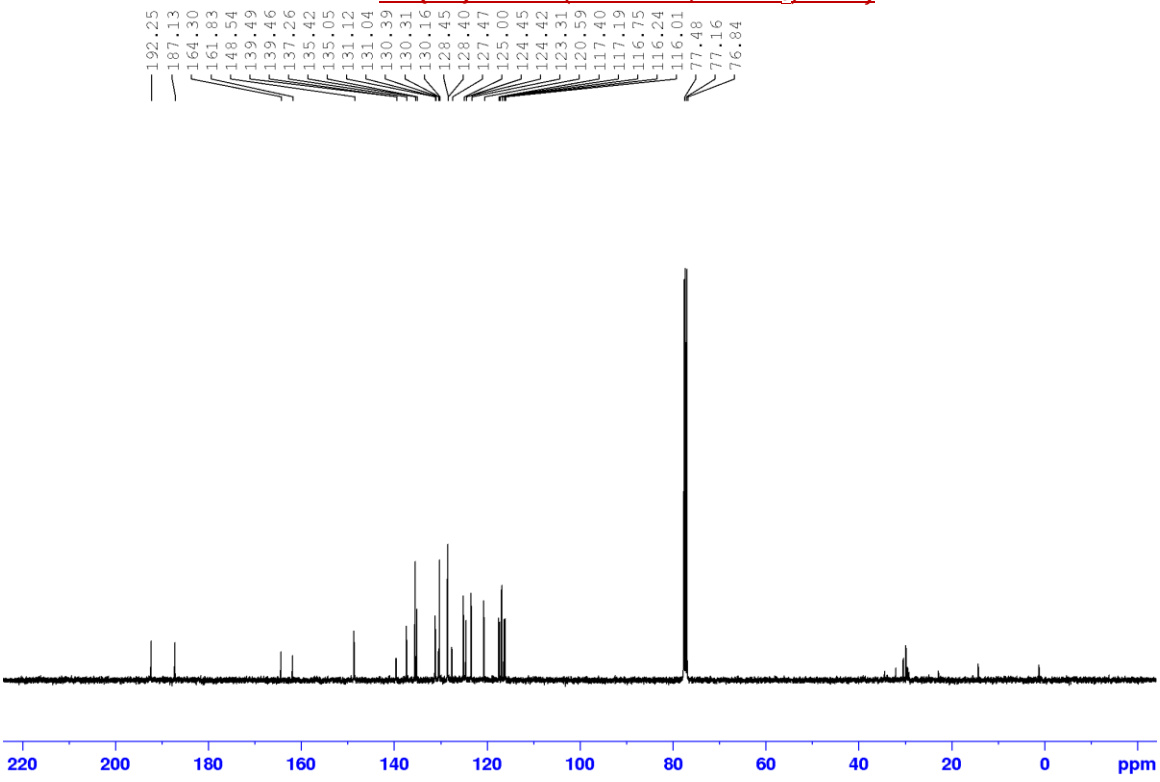


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
449.0796	449.0807	-1.1	-2.4	16.5	894.5	n/a	n/a	C23 H17 N2 O6 S

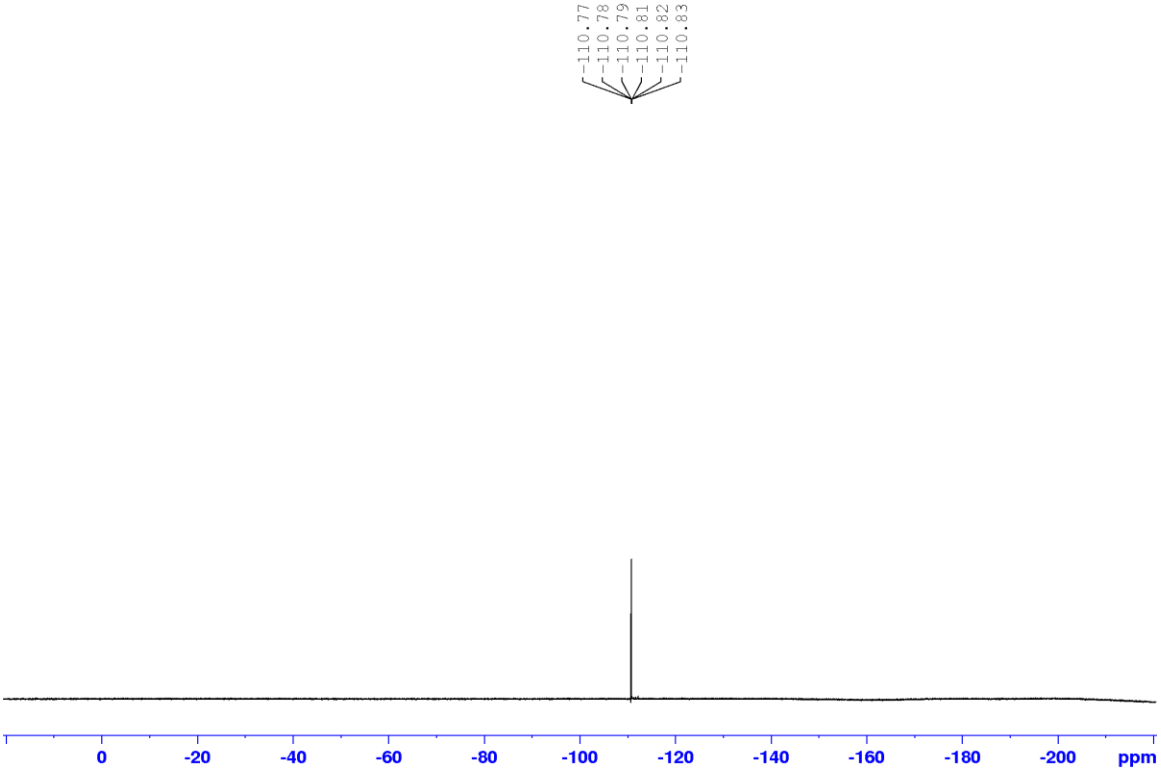
^{1}H NMR (400 MHz, $CDCl_3$) of 5j



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



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



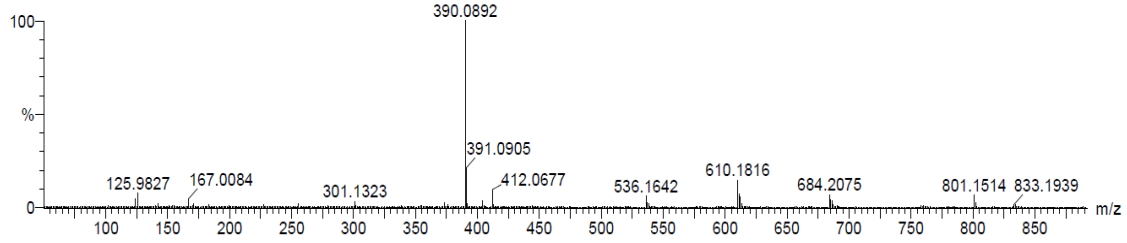
HRMS of 5j

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

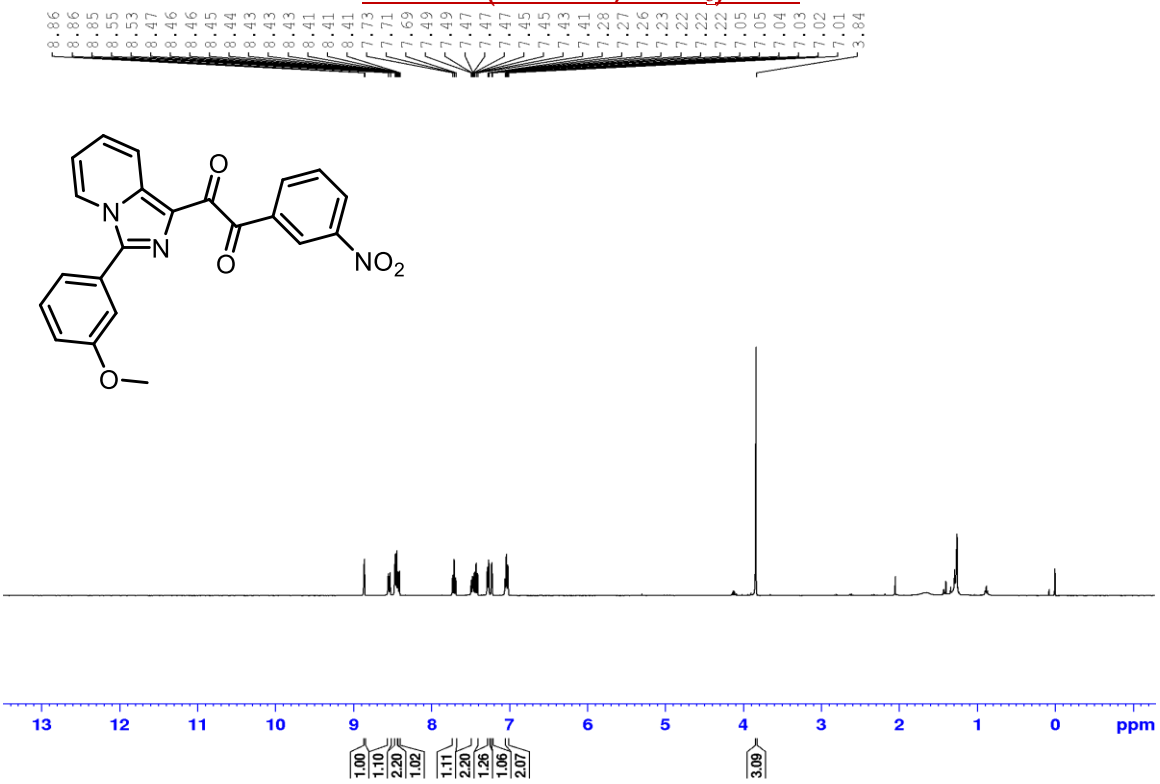
Monoisotopic Mass, Even Electron Ions
47 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-21 H: 0-100 N: 0-3 O: 0-4 F: 0-1

SM-516 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 14:36:27
070524_38 8 (0.172) Cm (8) 1: TOF MS ES+
2.45e+006

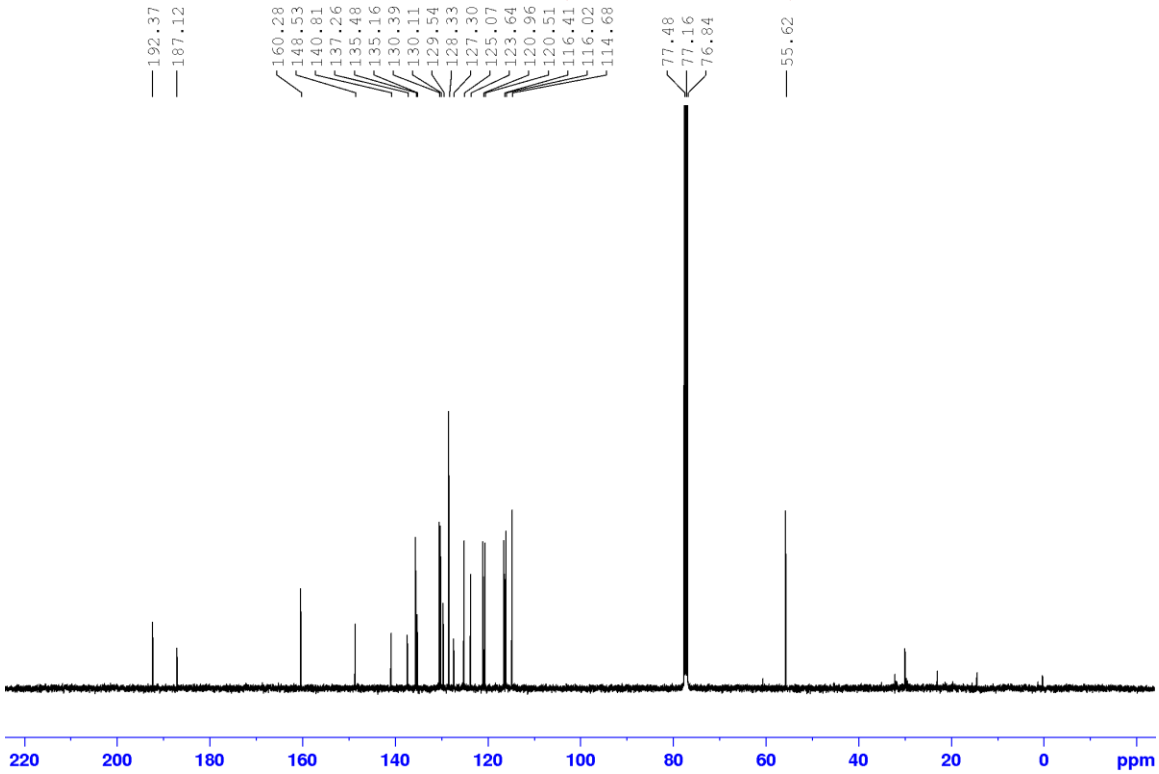


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
390.0892	390.0890	0.2	0.5	16.5	38.4	n/a	n/a	C21 H13 N3 O4 F

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



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



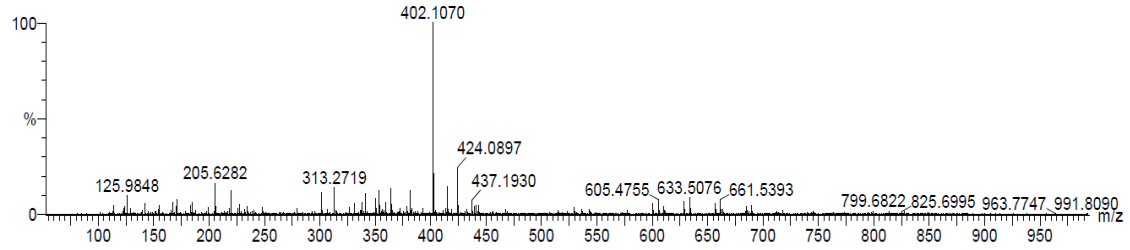
HRMS of 5k

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

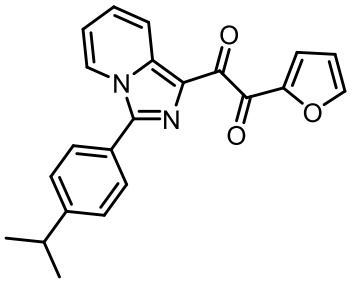
Monoisotopic Mass, Even Electron Ions
30 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-22 H: 0-100 N: 0-3 O: 0-5

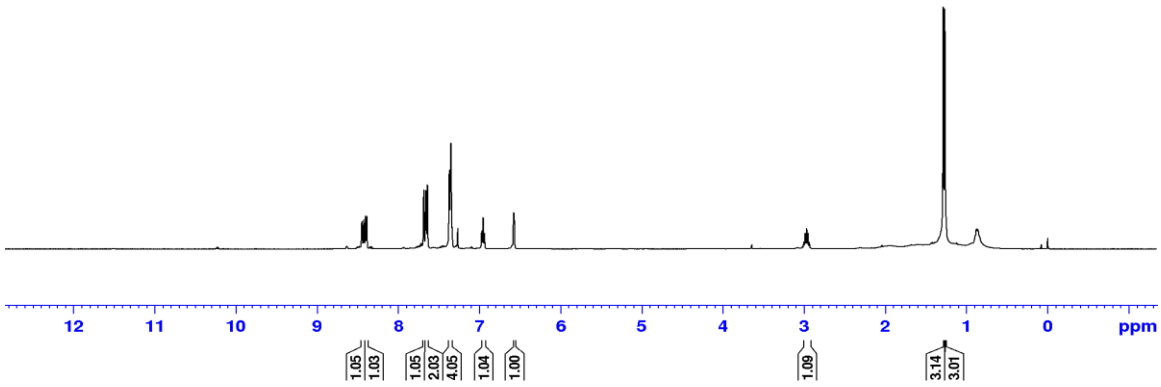
SM-514 QMI DIVISION, CSIR-IIIM JAMMU 02-May-2024
Xevo G2-XS QTOF YFC2015 11:50:21
020524_06 5 (0.121) 1: TOF MS ES+
6.87e+005



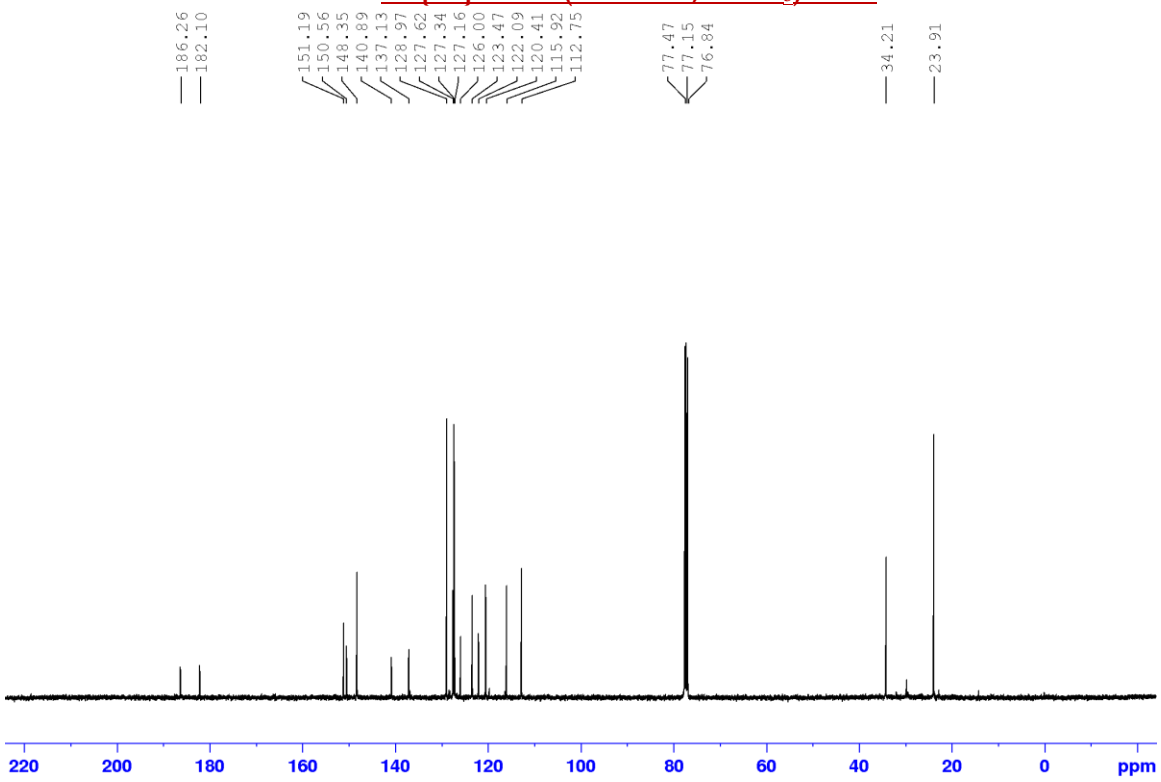
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
402.1070	402.1090	-2.0	-5.0	16.5	1043.6	n/a	n/a	C22 H16 N3 O5

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





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



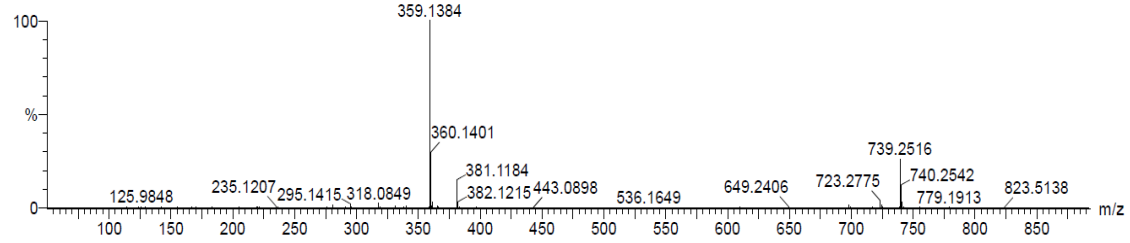
HRMS of 5l

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

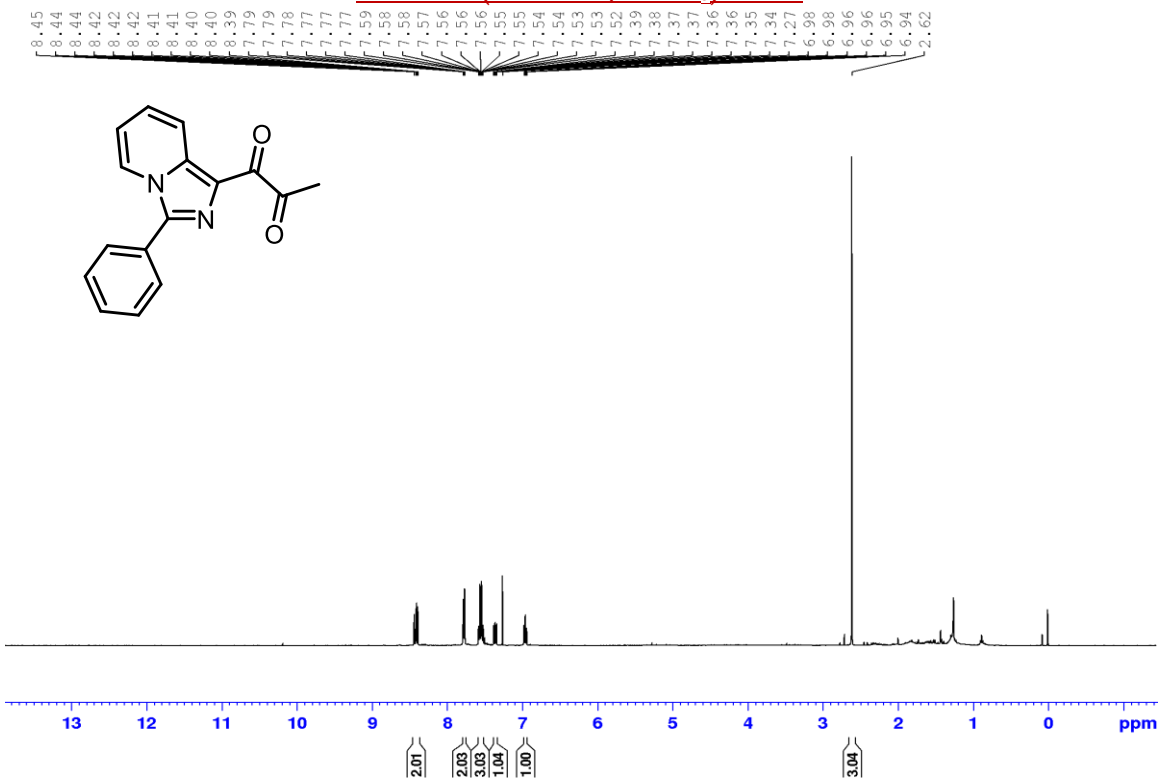
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-22 H: 0-100 N: 0-2 O: 0-3

SM-440 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 11:40:02
300424_02 7 (0.155) 1: TOF MS ES+
2.30e+007

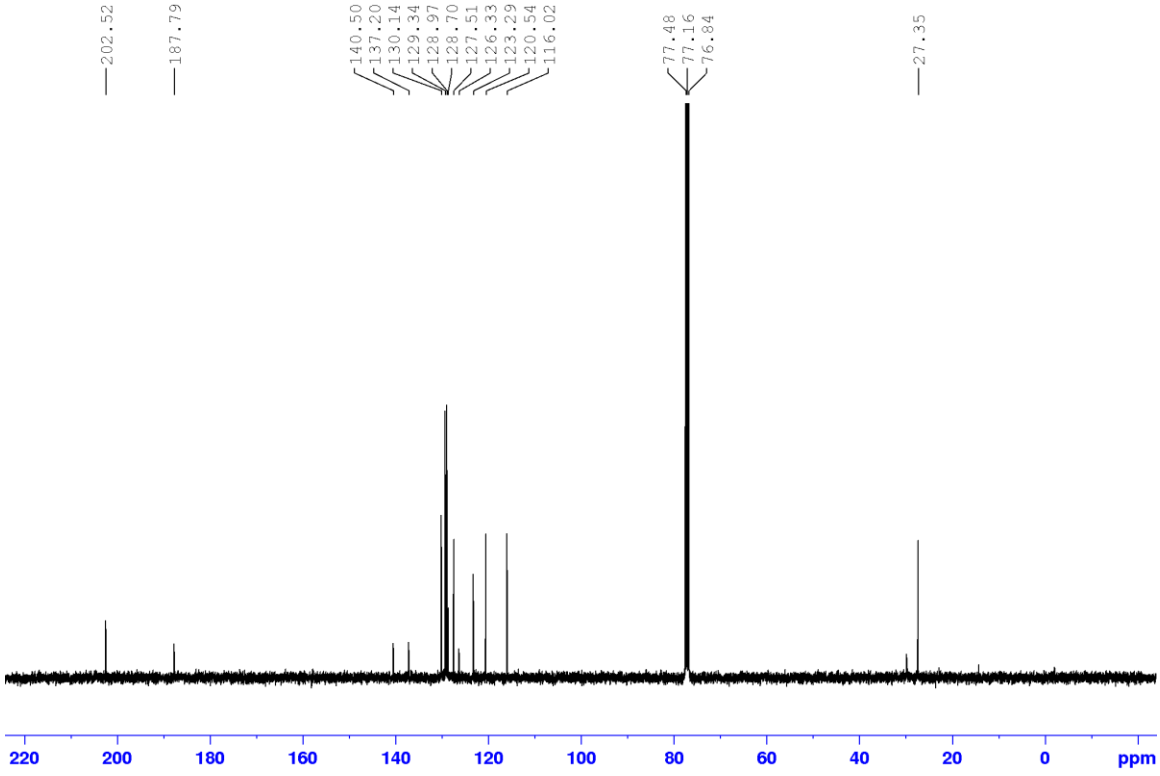


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
359.1384	359.1396	-1.2	-3.3	14.5	1132.6	n/a	n/a	C22 H19 N2 O3

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



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



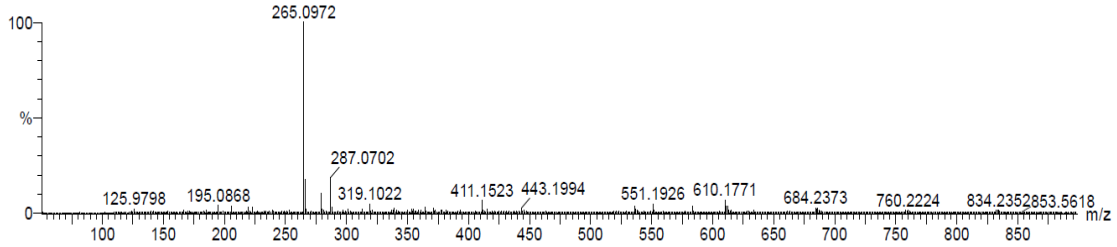
HRMS of 5m

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

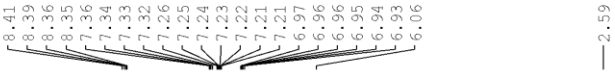
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-16 H: 0-100 N: 0-2 O: 0-2

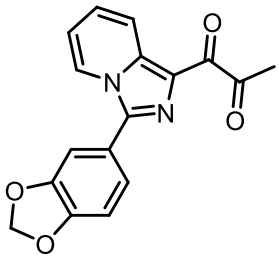
SM-522 QMI DIVISION, CSIR-IIIM JAMMU 02-May-2024
Xevo G2-XS QTOF YFC2015 13:21:09
020524_29 8 (0.172) Cm (8) 1: TOF MS ES+
5.30e+006

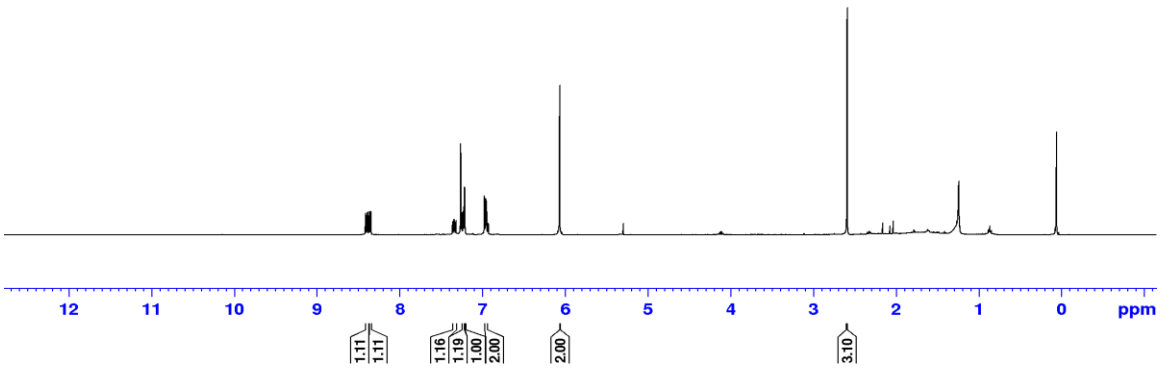


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
265.0972	265.0977	-0.5	-1.9	11.5	48.5	n/a	n/a	C16 H13 N2 O2

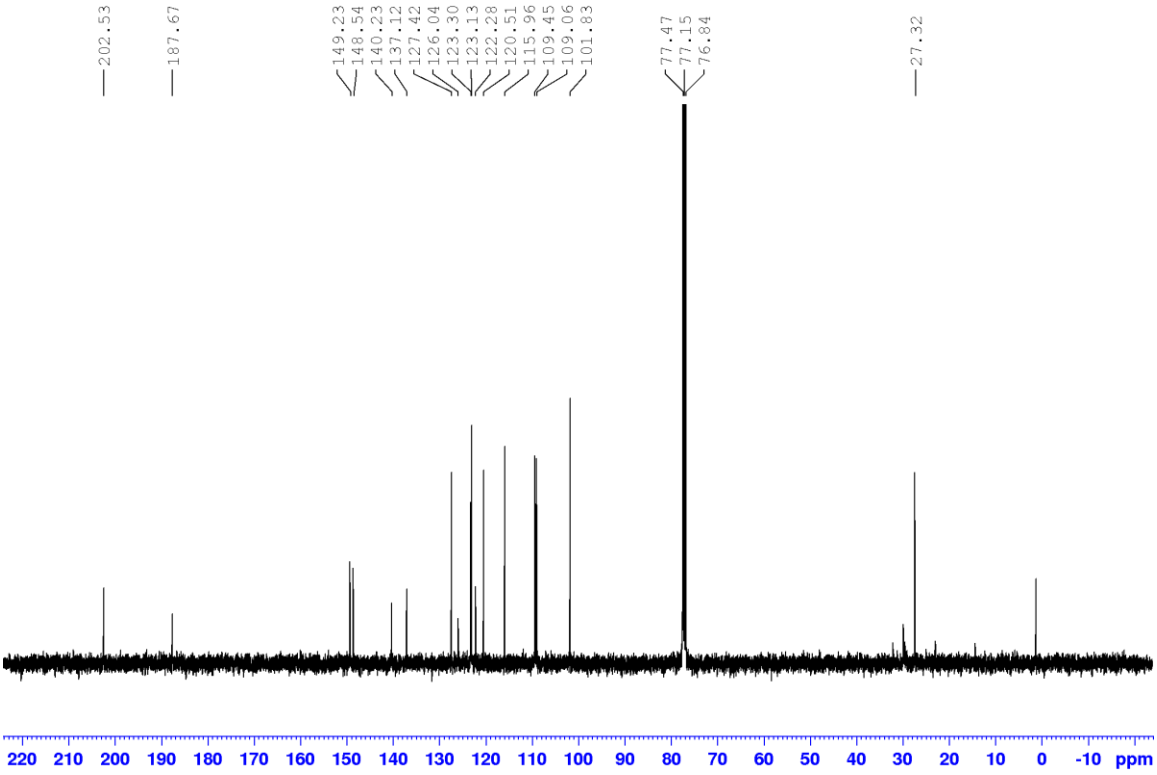
^{1}H NMR (400 MHz, $CDCl_3$) of 5n







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



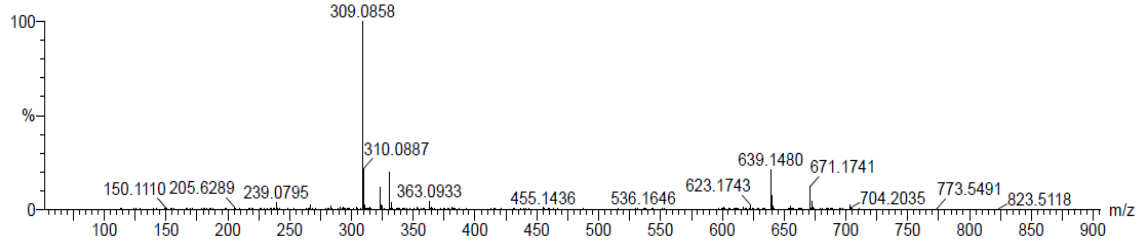
HRMS of 5n

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

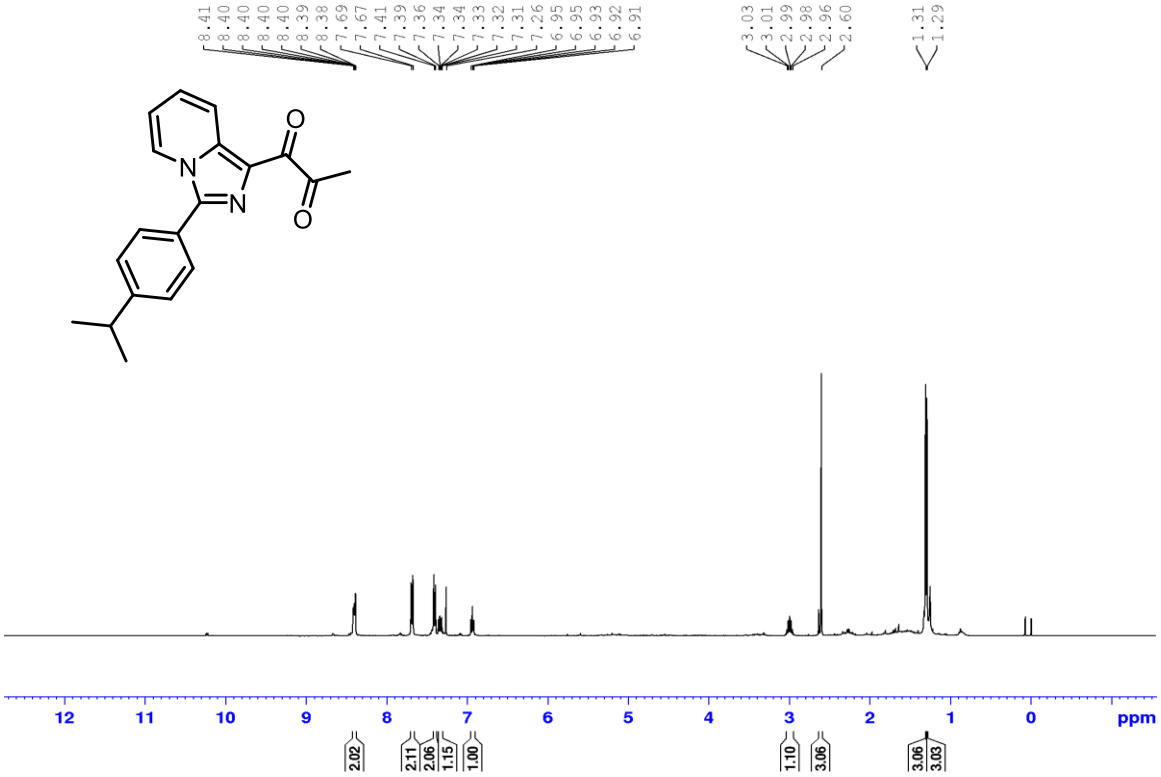
Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-17 H: 0-100 N: 0-2 O: 0-4

SM-470 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 12:03:16
300424_11 6 (0.138) 1: TOF MS ES+
1.93e+007

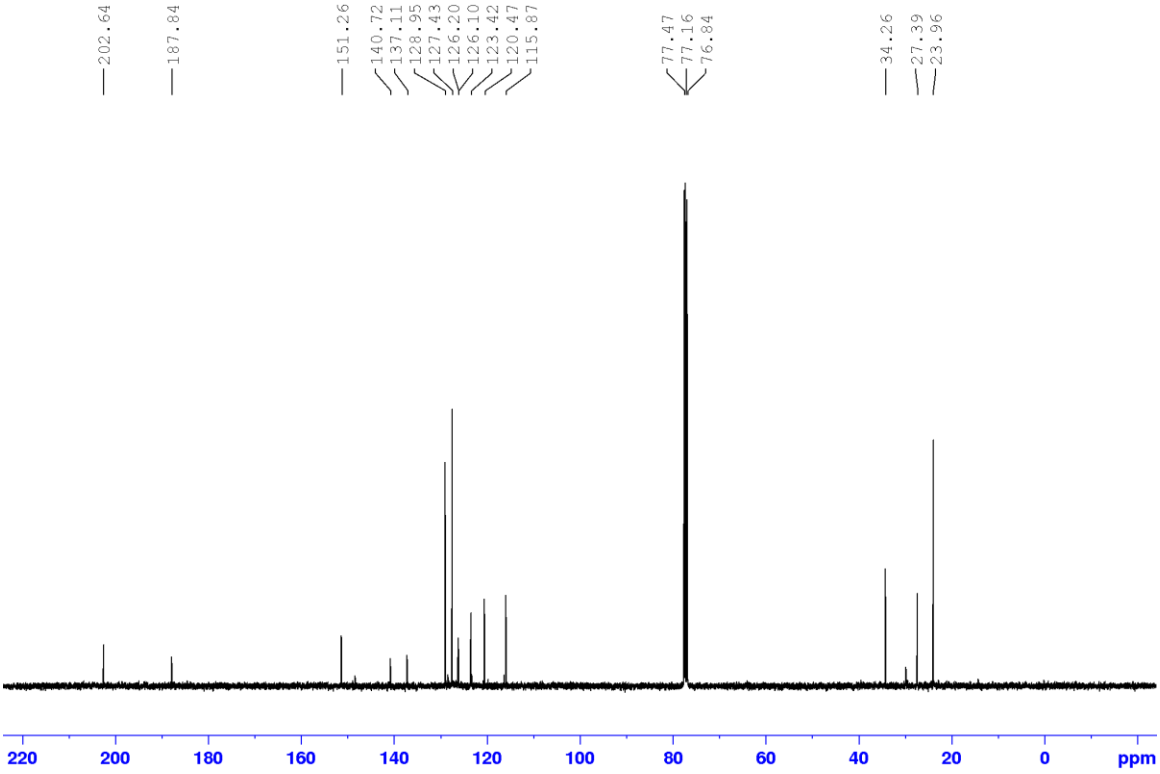


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
309.0858	309.0875	-1.7	-5.5	12.5	1203.4	n/a	n/a	C17 H13 N2 O4

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



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



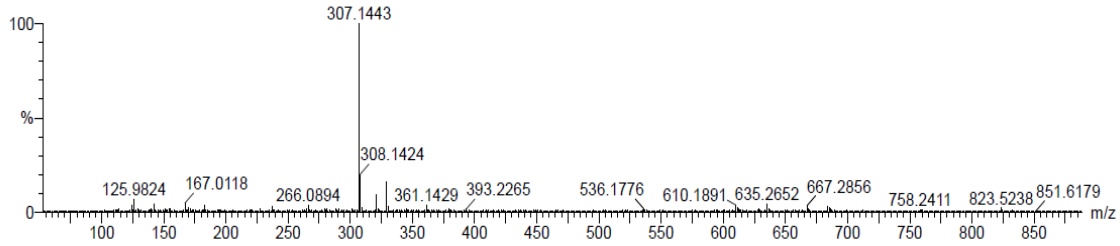
HRMS of 5o

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

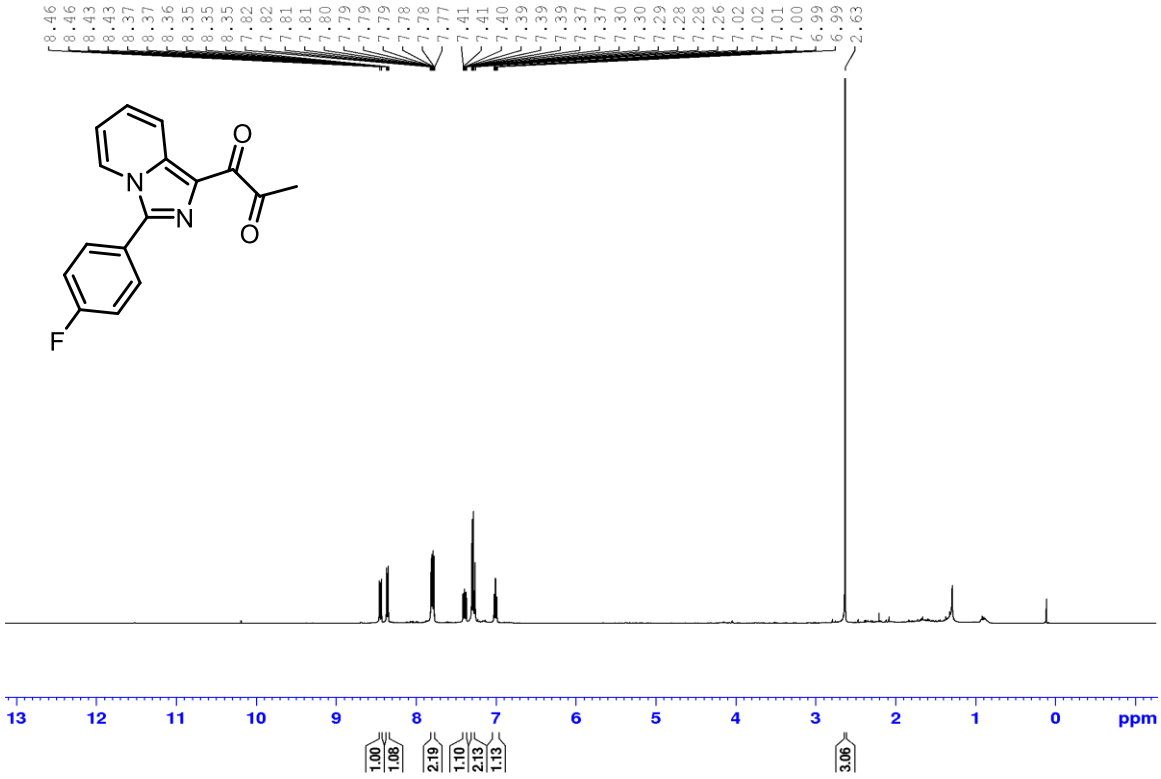
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-2 O: 0-2

SM-428 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024 11:47:43
Xevo G2-XS QTOF YFC2015
300424_05 8 (0.172) Cm (8) 1: TOF MS ES+ 4.36e+006

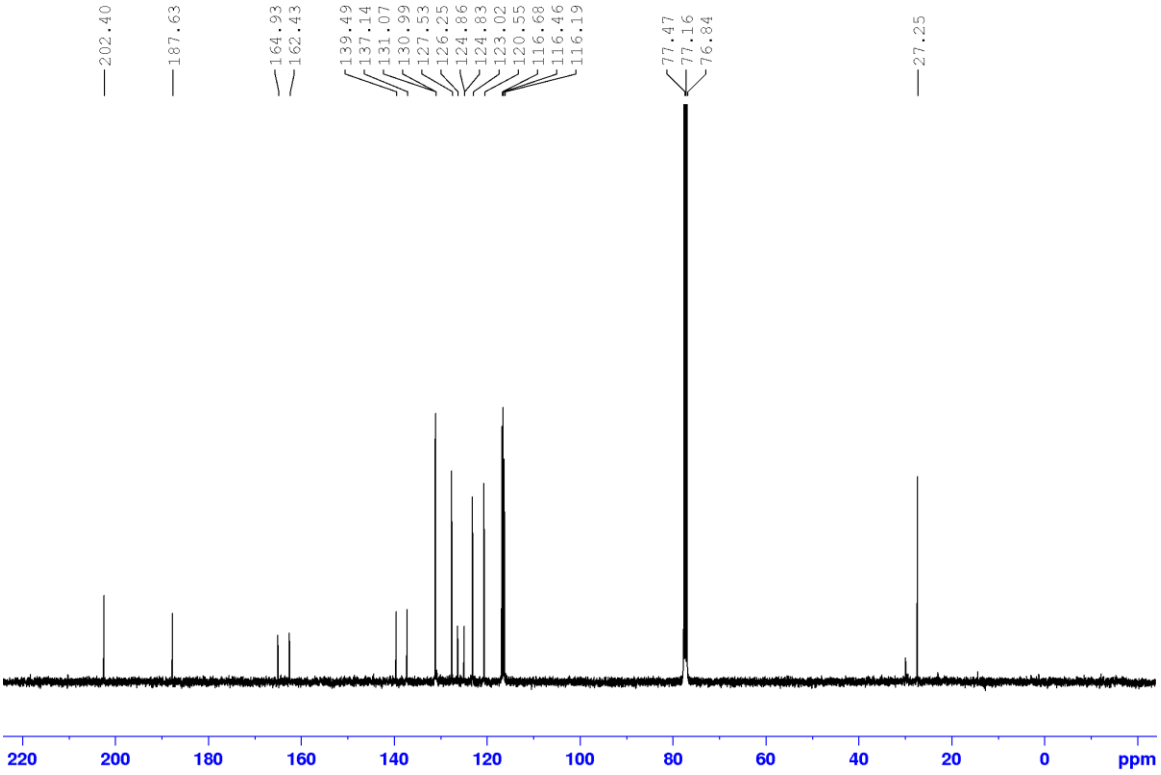


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
307.1443	307.1447	-0.4	-1.3	11.5	35.9	n/a	n/a	C19 H19 N2 O2

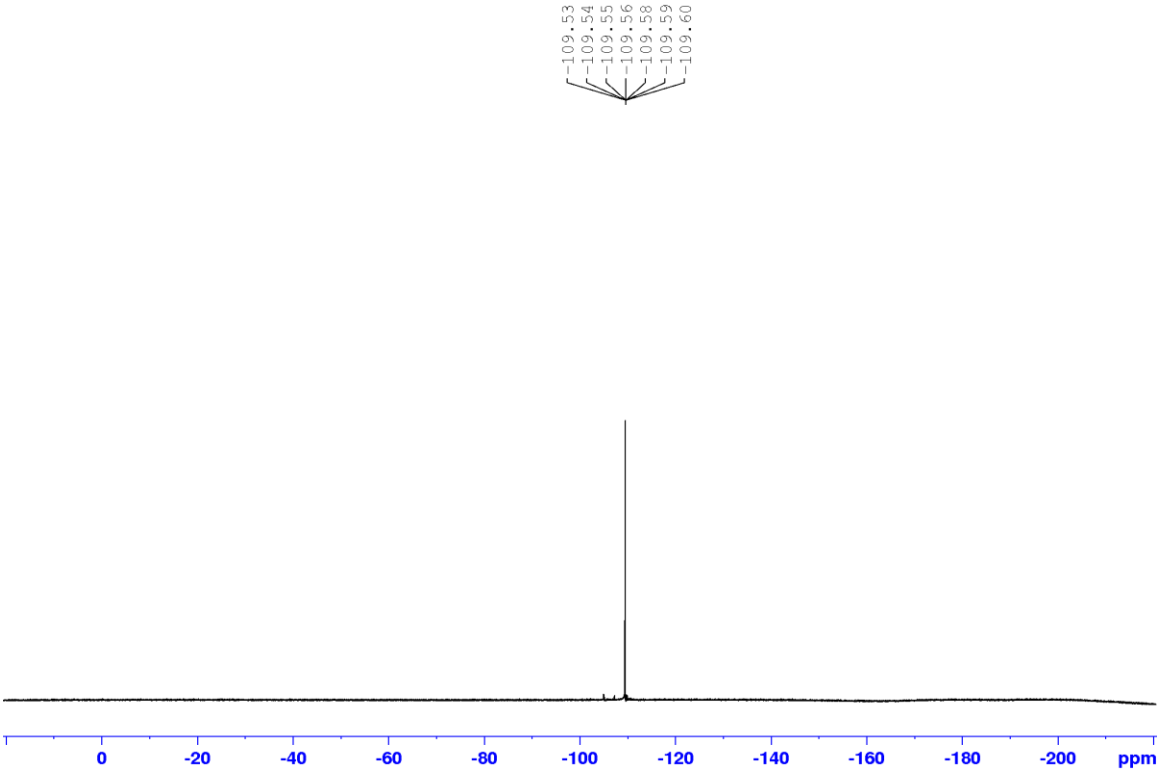
^{1}H NMR (400 MHz, $CDCl_3$) of 5p



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



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



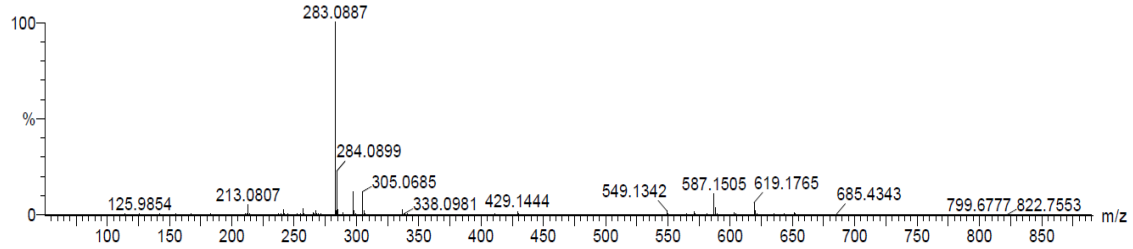
HRMS of 5p

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

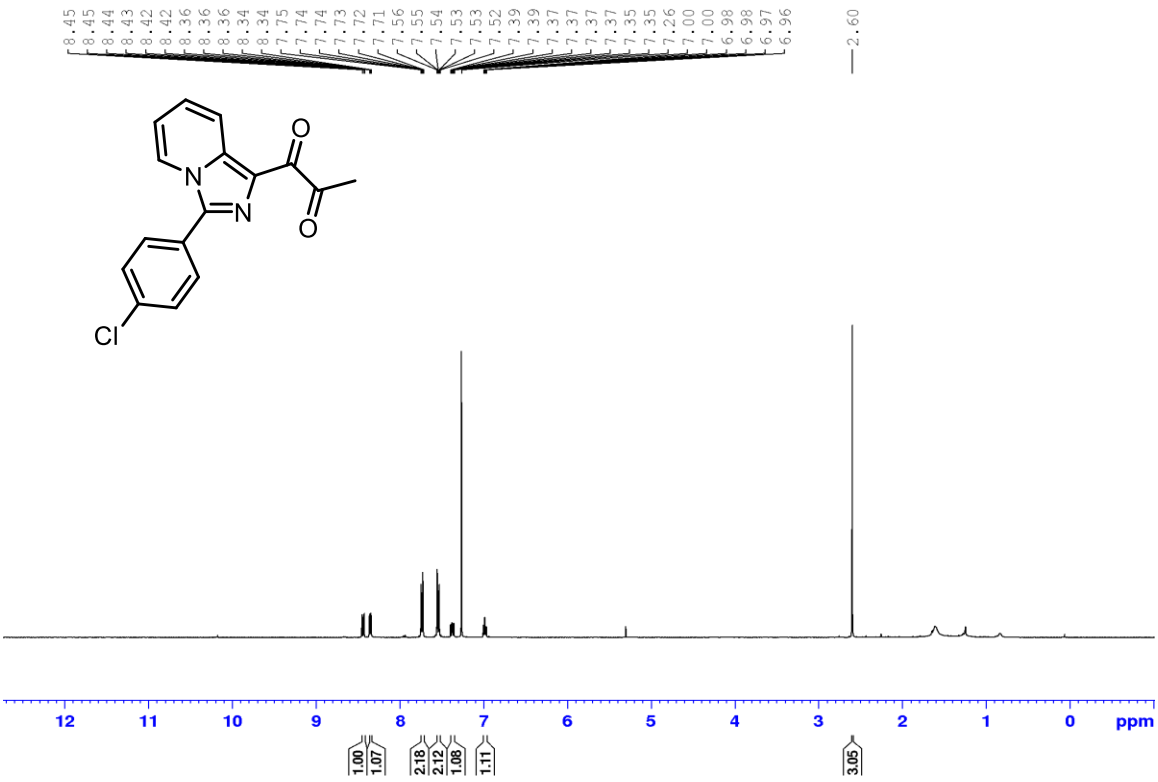
Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-16 H: 0-100 N: 0-2 O: 0-2 F: 0-1

SM-469 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024 11:57:59
Xevo G2-XS QTOF YFC2015
300424_09 5 (0.121) 1: TOF MS ES+ 2.07e+007

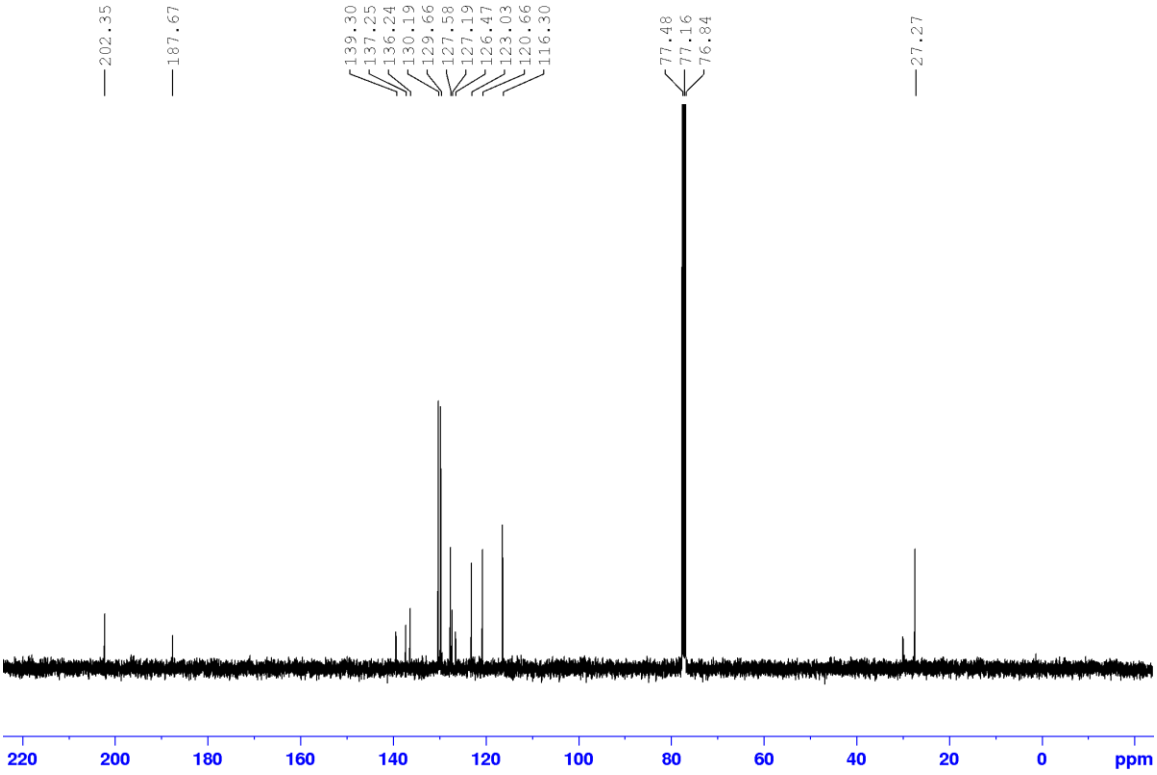


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
283.0887	283.0883	0.4	1.4	11.5	1274.1	n/a	n/a	C16 H12 N2 O2 F

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



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



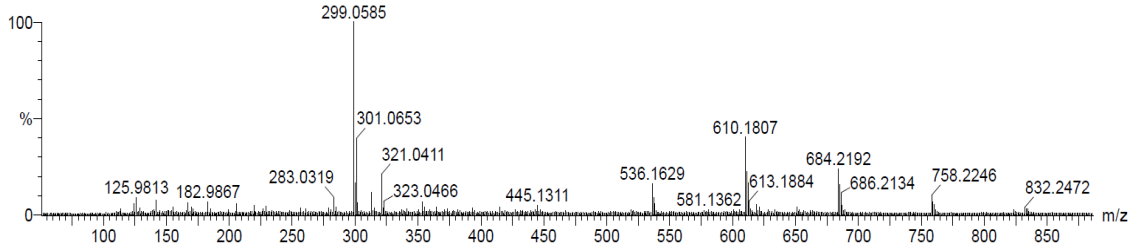
HRMS of 5q

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

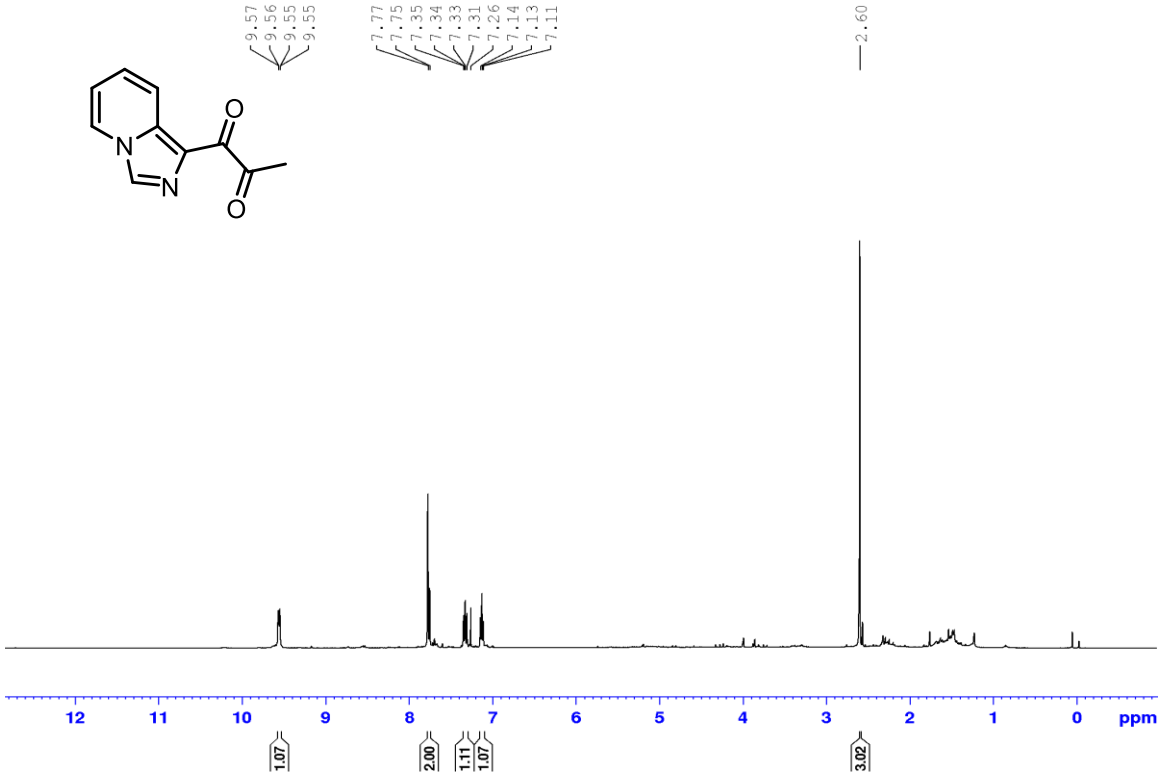
Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-16 H: 0-100 N: 0-2 O: 0-2 Cl: 0-1

SM-385 QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 11:45:10
300424_04 7 (0.155) Cm (7:8) 1: TOF MS ES+
4.69e+006

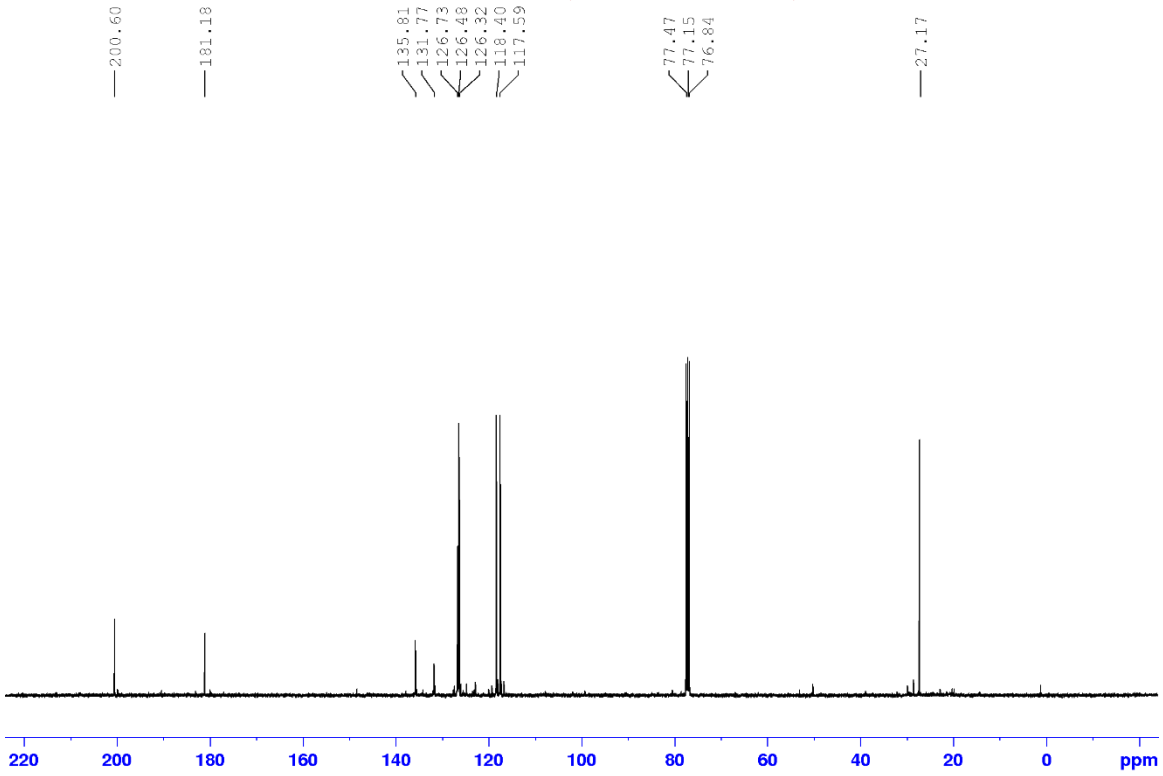


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
299.0585	299.0587	-0.2	-0.7	11.5	54.8	n/a	n/a	C16 H12 N2 O2 Cl

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



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



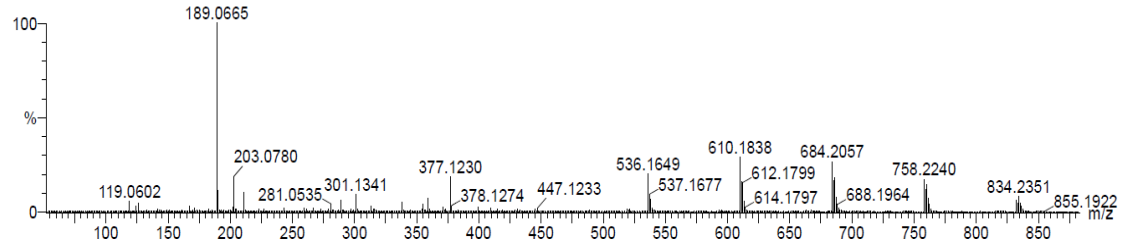
HRMS of 5r

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

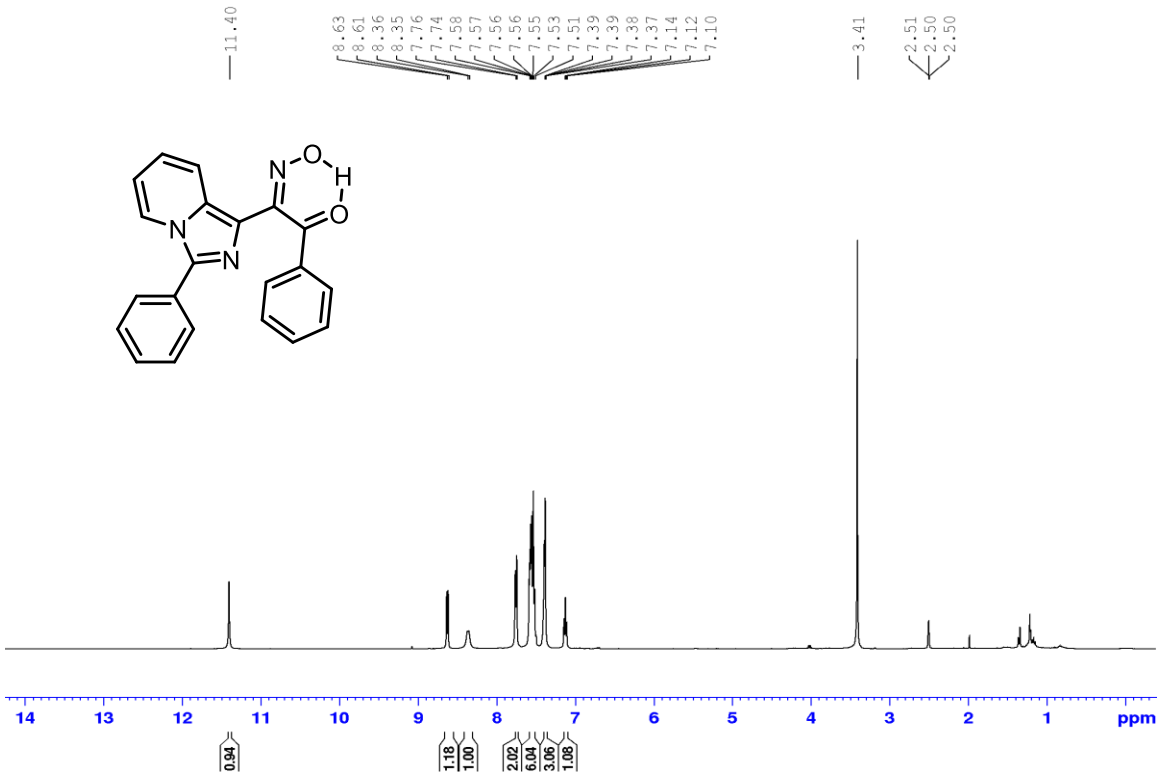
Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-10 H: 0-100 N: 0-2 O: 0-2

SM-521 QMI DIVISION, CSIR-IIIM JAMMU 07-May-2024
Xevo G2-XS QTOF YFC2015 14:41:43
070524_40 6 (0.138) Cm (5:7) 1: TOF MS ES+
6.87e+006

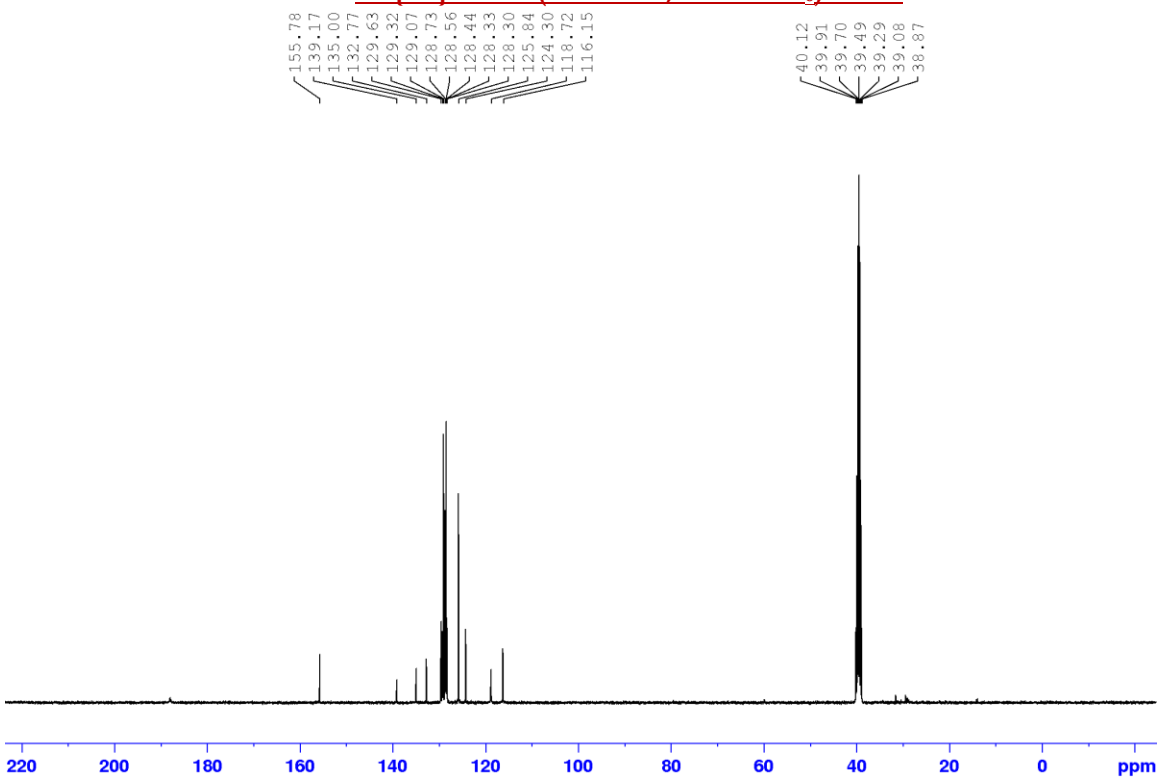


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
189.0665	189.0664	0.1	0.5	7.5	27.7	n/a	n/a	C10 H9 N2 O2

^{1}H NMR (400 MHz, DMSO-d_6) of 6a



$^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO-d_6) of 6a



HRMS of 6a

Elemental Composition Report **Page 1**

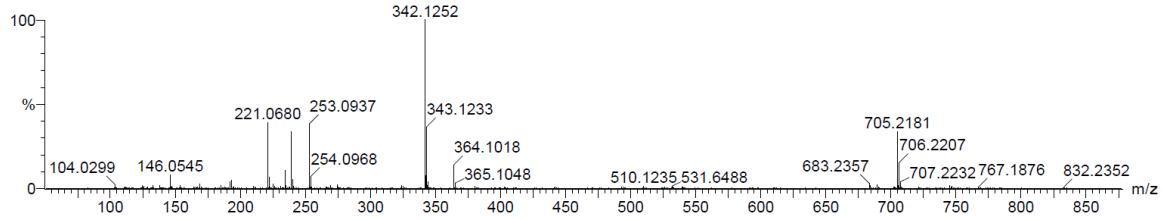
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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
190324_17 8 (0.172)

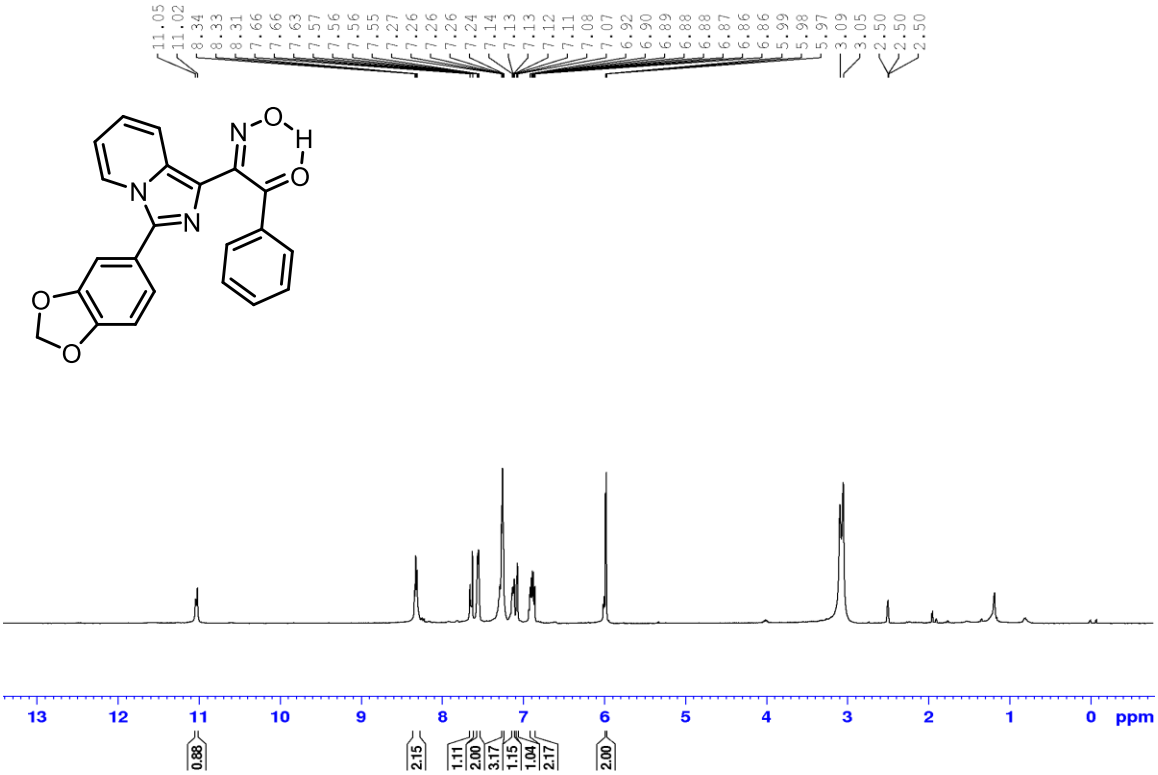
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

19-Mar-2024
14:10:43
1: TOF MS ES+
2.68e+007

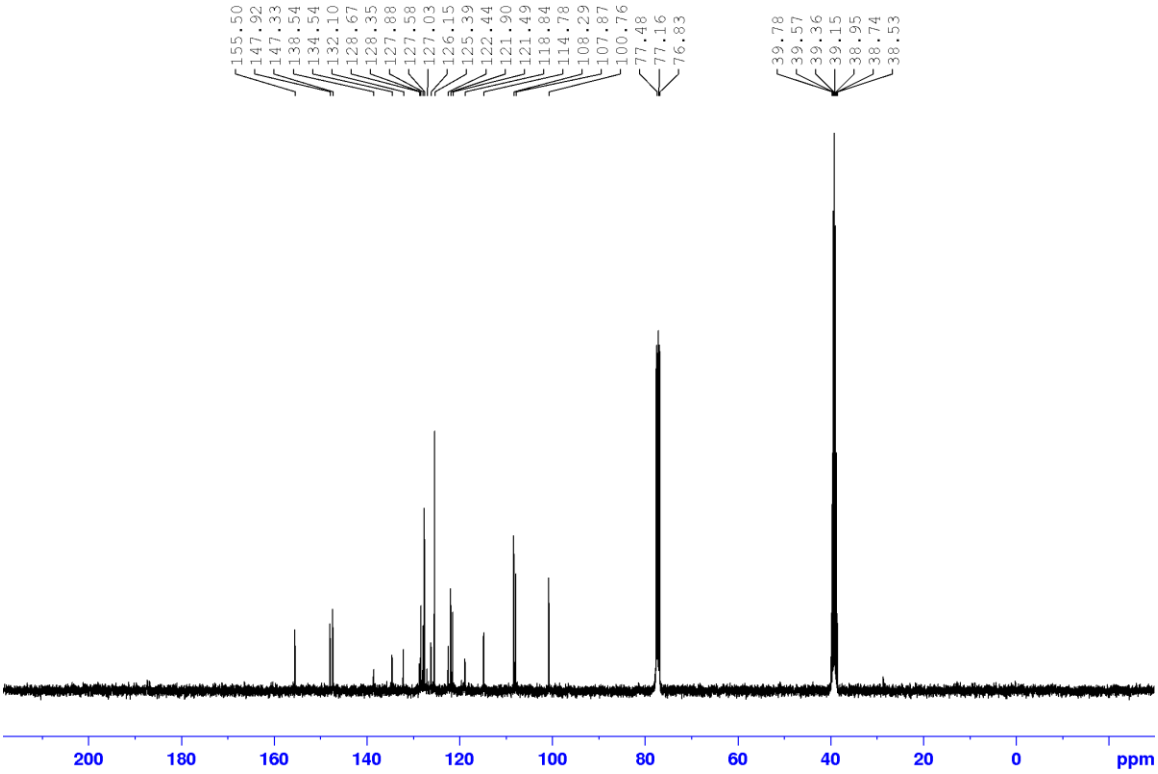


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
342.1252	342.1243	0.9	2.6	15.5	1205.1	n/a	n/a	C21 H16 N3 O2

^{1}H NMR (400 MHz, DMSO-d_6) of 6b



^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of 6b



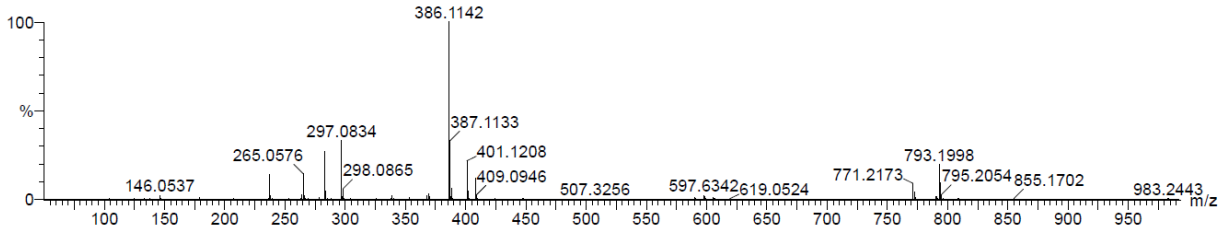
HRMS of 6b

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
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 17-May-2024
Xevo G2-XS QTOF YFC2015 13:41:34
170524_02 6 (0.138) 1: TOF MS ES+
4.08e+007



Minimum:				-1.5				
Maximum:		2.0	50.0	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