

Supporting Information for

Fusion of β -Enaminones, 2-Aminopyridines to 3-oxo-Imidazo[1,2-*a*]pyridines Induced by Iodine: A Mechanochemical Approach

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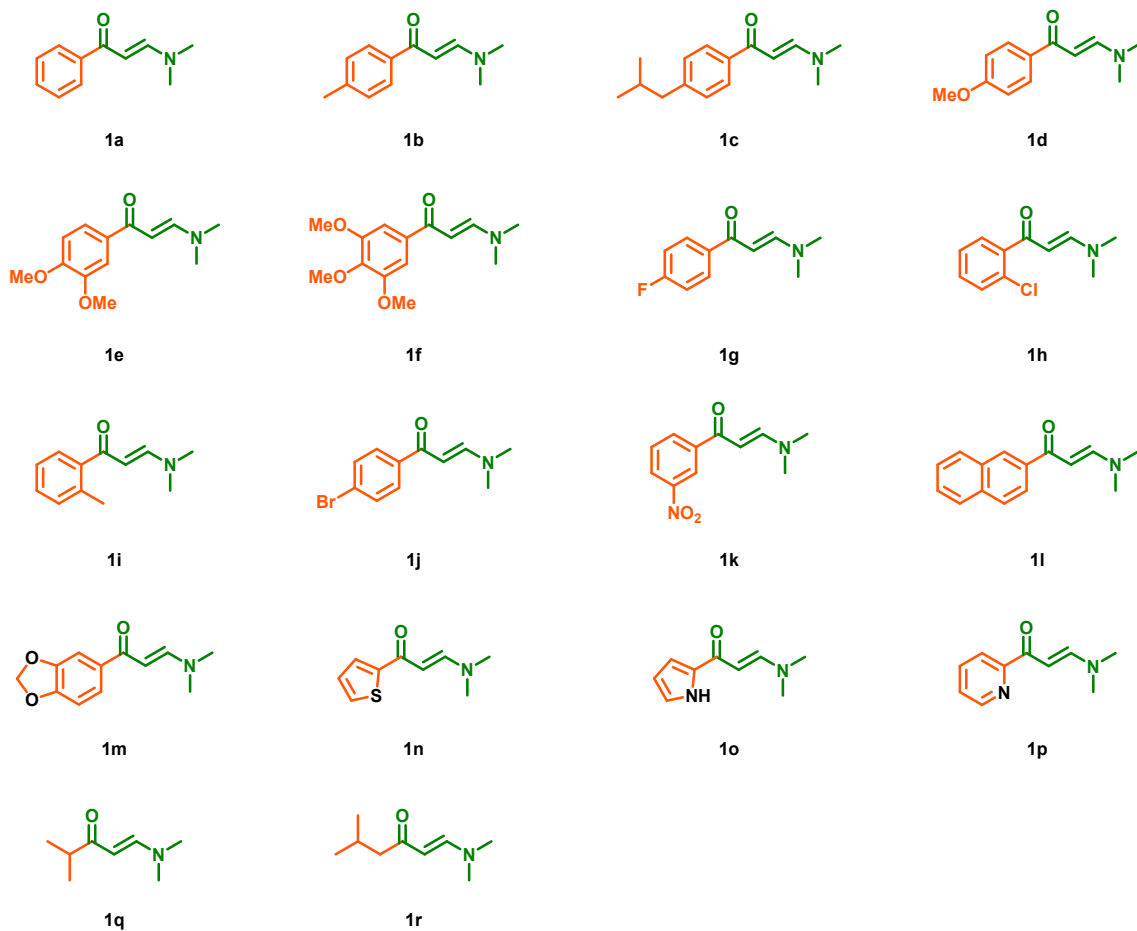
Email: krishnu@iict.res.in

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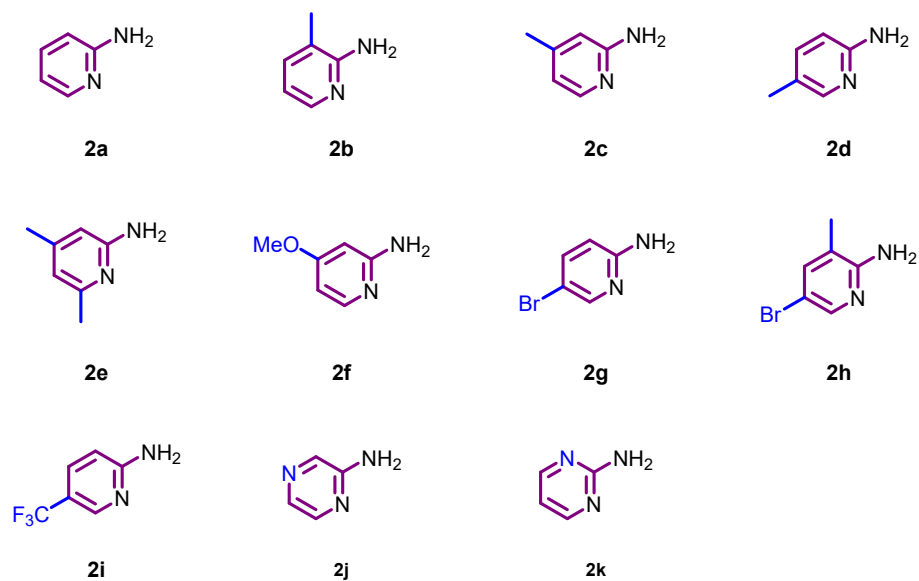
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1.1. Structures of starting materials

1.1.1. Structures of β -Enaminones (1a-r).



1.1.2. Structures of 2-Aminopyridines (2a-i) & heteroaryl amines (2j-k).

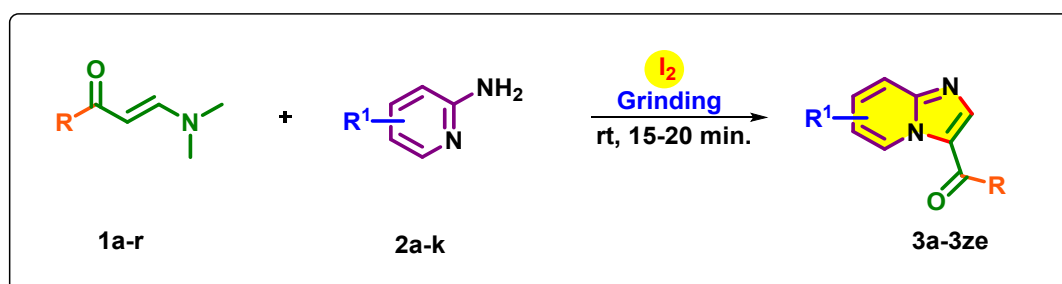


1.2. Experimental section

General

Melting points were measured by CINTEX programmable melting point apparatus and are uncorrected. ^1H , ^{13}C and ^{19}F NMR spectra of samples in CDCl_3 recorded on AVANCE- 300, 400, 500 MHz spectrometers. Chemical shifts (δ) are reported relative to TMS ($\delta = 0.0$) as the internal standard. Mass spectra were recorded in ESI spectrometers. All high-resolution mass spectra were recorded on QSTAR XL hybrid ms/ms system (Applied Bio systems/MDS sciex, foster city, USA), equipped with an ESI source (IICT, Hyderabad). TLC was performed on Merck 60 F-254 silica gel plates. The chemicals used in this work were obtained from commercial channels and were used without purification.

1.2.1. General Procedure for the Synthesis of 3-oyl-imidazo[1,2-*a*]pyridines (**3a-3ze**).

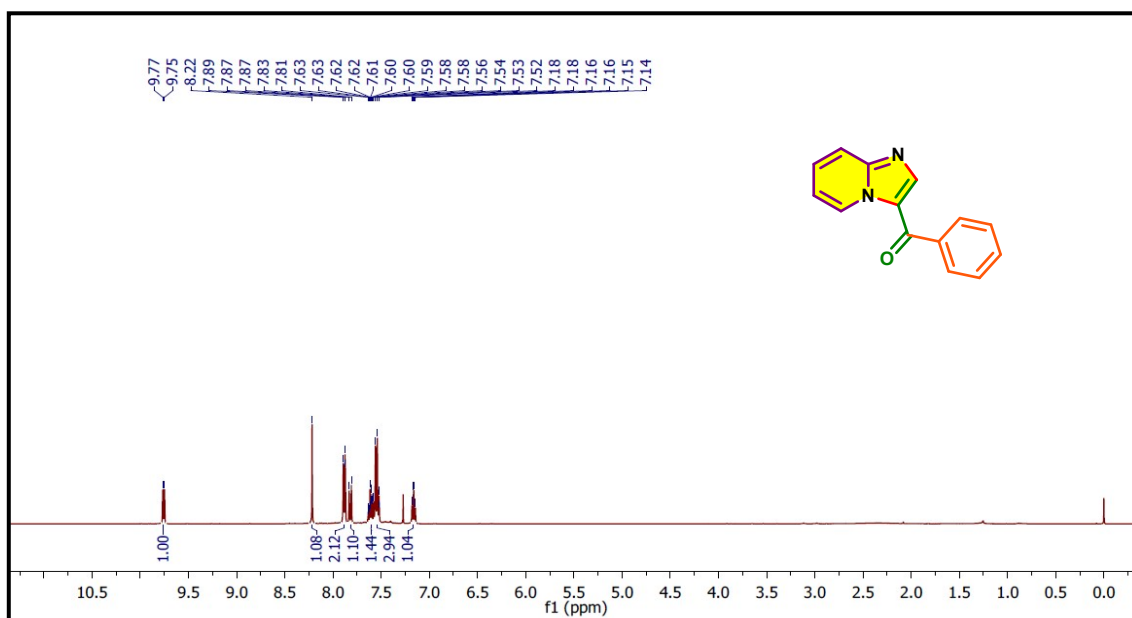


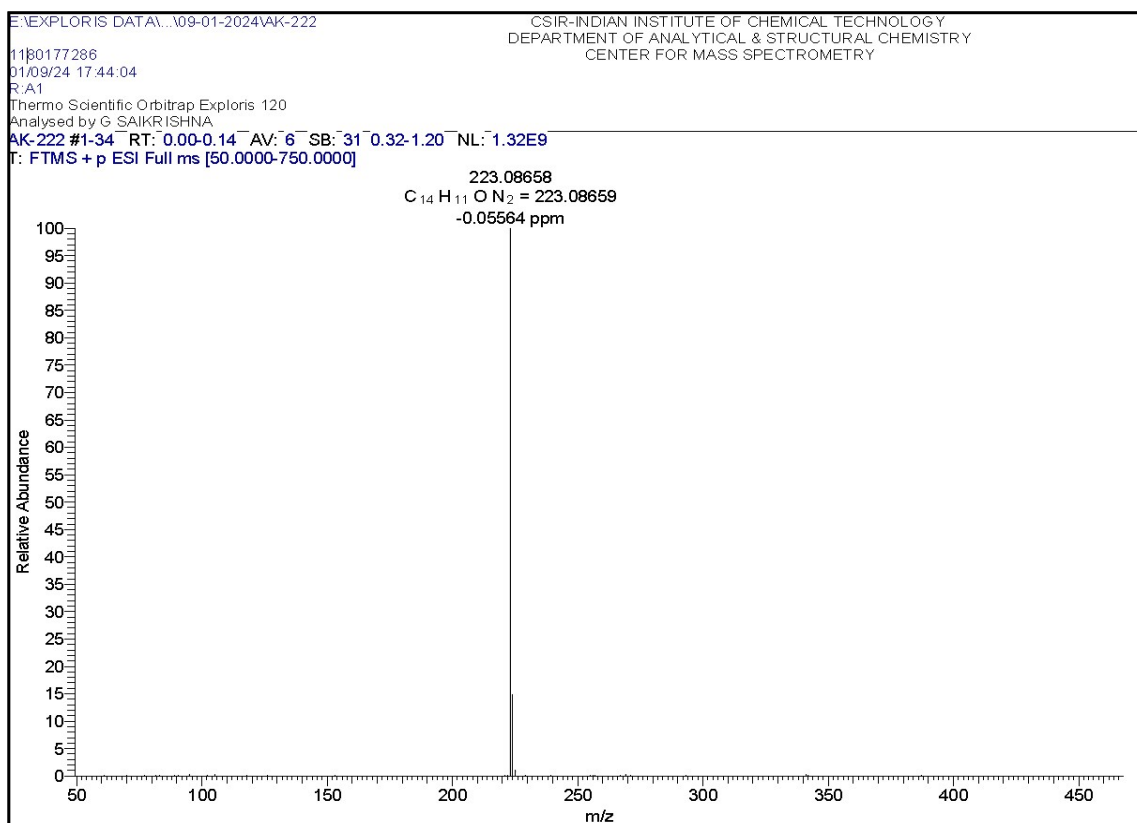
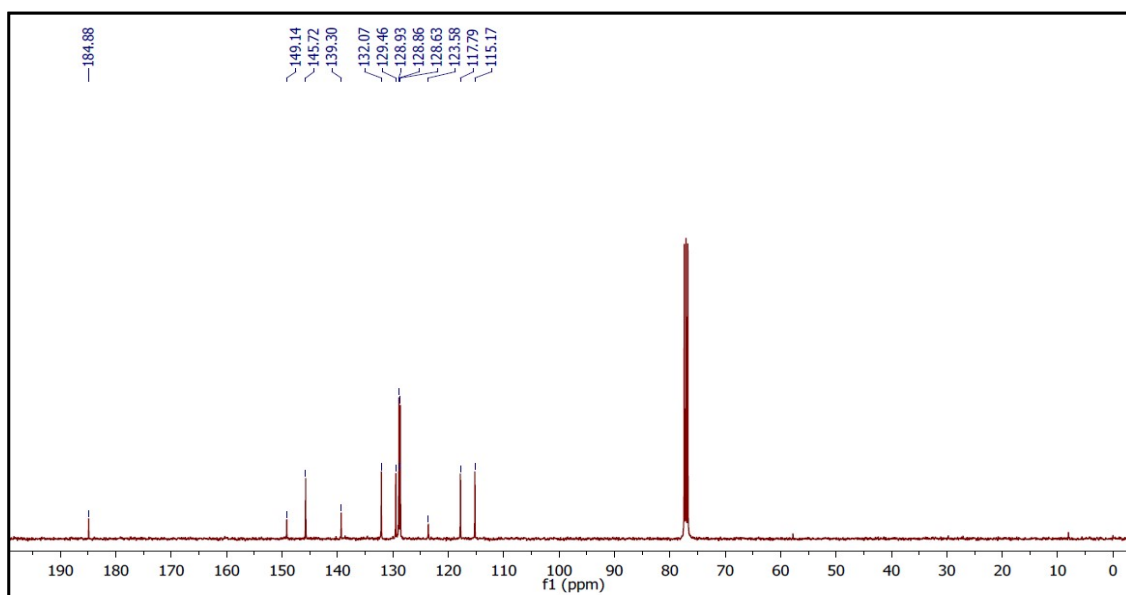
A mixture of β -enaminone (**1a**, 150 mg, 1.0 mmol, 1.0 equiv.), 2-aminopyridine (**2a**, 85 mg, 1.05 mmol, 1.05 equiv.), and molecular iodine (216 mg, 1.0 mmol, 1.0 equiv.) were manually grinded at room temperature for 15-20 minutes. After completion of the reaction as ascertained by TLC, reaction mass dissolved in dichloromethane (DCM) and quenched with sat. sodium thiosulphate ($\text{Na}_2\text{S}_2\text{O}_3$) followed by treated with sat. NaHCO_3 , and separated organic layer dried over sodium sulphate and concentrated under reduced pressure. The leftover mass dissolved in minimum amount of DCM and this was slowly dropped into anti-solvent Pentane/hexane (10 times) in a round bottomed flask and stirred for 15 minutes at room temperature. The obtained solids are filtered and dried in oven at 40-50 $^\circ\text{C}$ for 1 h to afford the desired product **3a** in 92% yield (175 mg) and similar procedure was followed for all the corresponding products **3b-3ze**.

1.3 Spectroscopic data and copies ^1H , ^{19}F & ^{13}C of compounds.

Imidazo[1,2-*a*]pyridin-3-yl(phenyl)methanone (3a)¹

Isolated as a yellow solid, yield 92% (175 mg), m.p 96-98 °C, IR (ATR): 3121, 2920, 2853, 1715 (C=O stretching), 1620, 1474, 1218, 887, 750 cm^{-1} , ^1H NMR (400 MHz, CDCl_3): δ 9.76 (d, J = 6.9 Hz, 1H, Ar), 8.22 (s, 1H, Ar), 7.92 – 7.85 (m, 2H, Ar), 7.82 (d, J = 9.0 Hz, 1H, Ar), 7.64 – 7.57 (m, 1H, Ar), 7.57-7.51 (m, 3H, Ar), 7.16 (t, J = 6.9 Hz, 1H, Ar) ppm, ^{13}C NMR (100 MHz, CDCl_3): δ 184.88 (C=O), 149.14 (Ar), 145.72 (Ar), 139.30 (Ar), 132.07 (Ar), 129.46 (Ar), 128.93 (Ar), 128.86 (Ar), 128.63 (Ar), 123.58 (Ar), 117.79 (Ar), 115.17 (Ar) ppm, ESI-MS: m/z 223 $[\text{M}+\text{H}]^+$, HRMS (ESI) Anal. calcd. for $\text{C}_{14}\text{H}_{11}\text{N}_2\text{O}$ m/z 223.08659 $[\text{M}+\text{H}]^+$, found 223.08658.

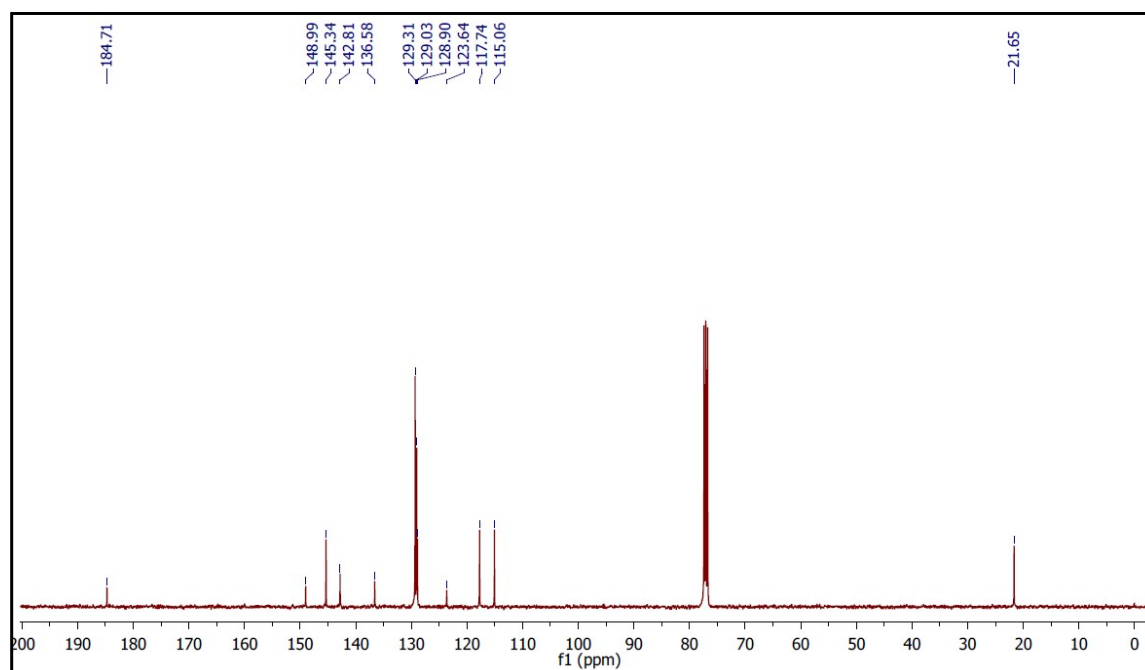
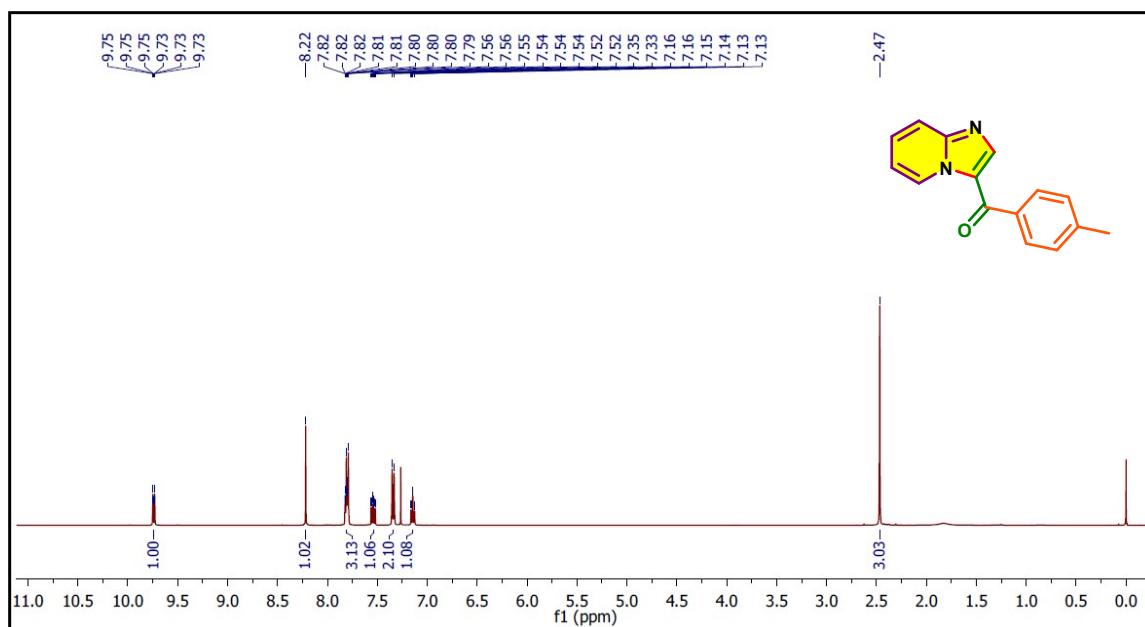


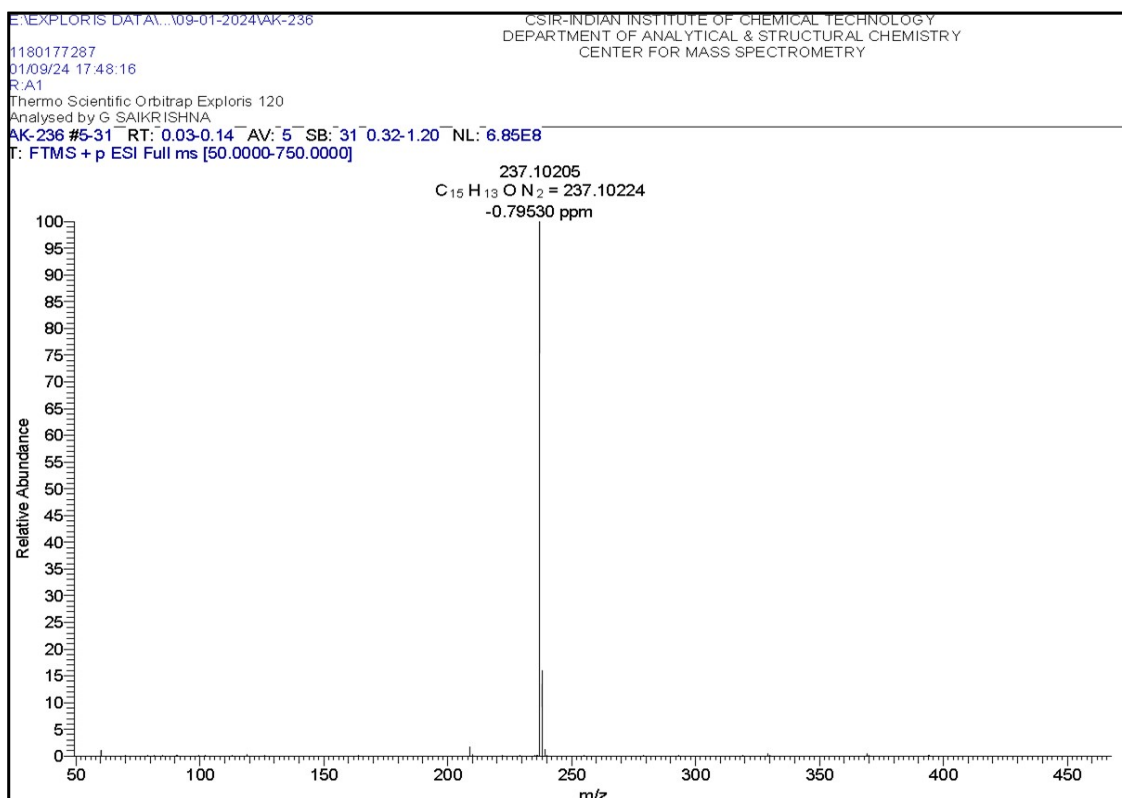


Imidazo[1,2-*a*]pyridin-3-yl(*p*-tolyl)methanone (3b)¹

Isolated as a white solid, yield 85% (159 mg), m.p 117-120 °C, IR (ATR): 3057, 2932, 2829, 1721 (C=O stretching), 1632, 1437, 1225, 893, 749 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.74 (dt, *J* = 6.9 Hz, 1H, Ar), 8.22 (s, 1H, Ar), 7.84 – 7.78 (m, 3H, Ar), 7.57-7.51 (m, 1H, Ar), 7.34 (d, *J* = 7.8 Hz, 2H, Ar), 7.14 (td, *J* = 6.9 Hz, 1H, Ar), 2.47 (s, 3H, -CH₃) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 184.71 (C=O), 148.99 (Ar), 145.34 (Ar), 142.81 (Ar), 136.58 (Ar), 129.31

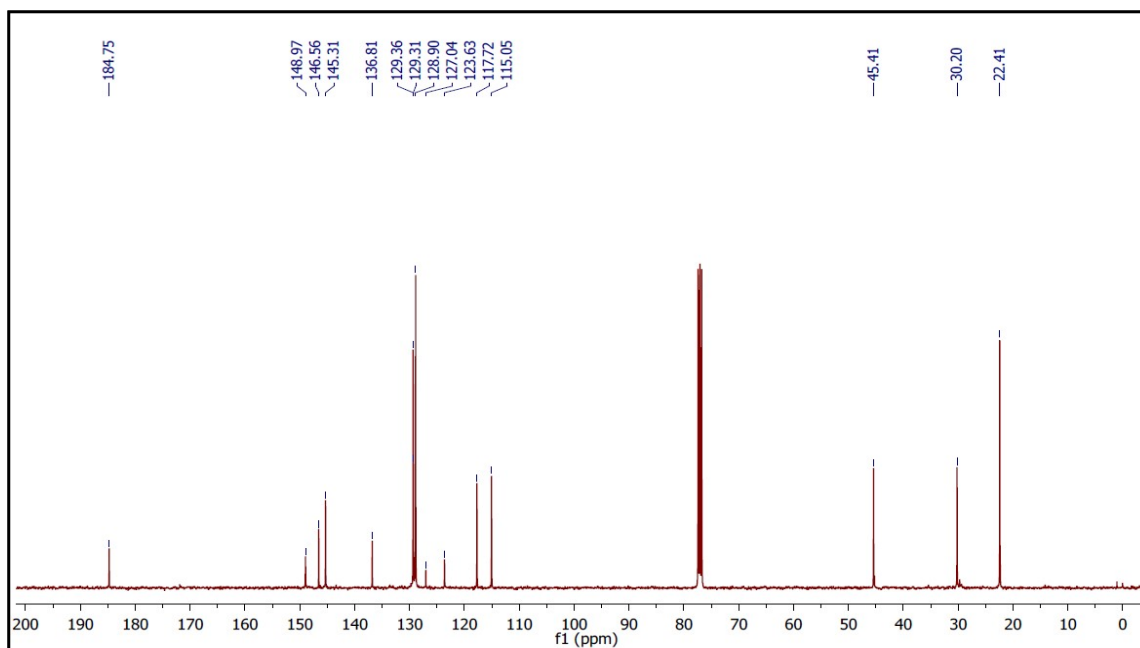
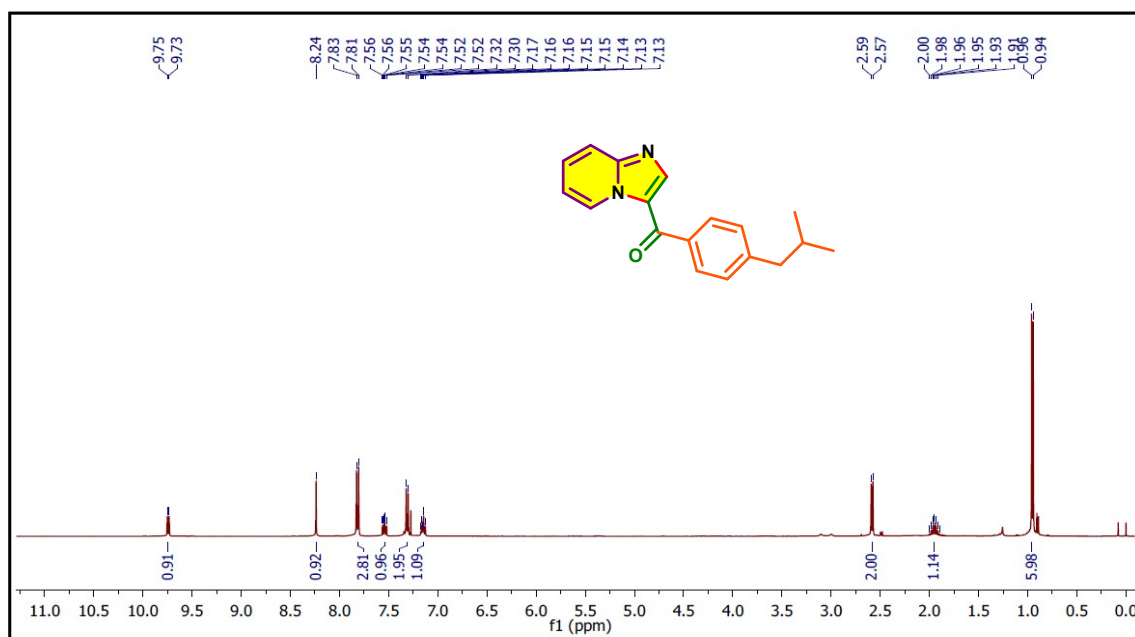
(Ar), 129.03 (Ar), 128.90 (Ar), 123.64 (Ar), 117.74 (Ar), 115.06 (Ar), 21.65 (-CH₃) ppm, ESI-MS: m/z 237 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₅H₁₃N₂O m/z 237.1022 [M+H]⁺, found 237.1020.

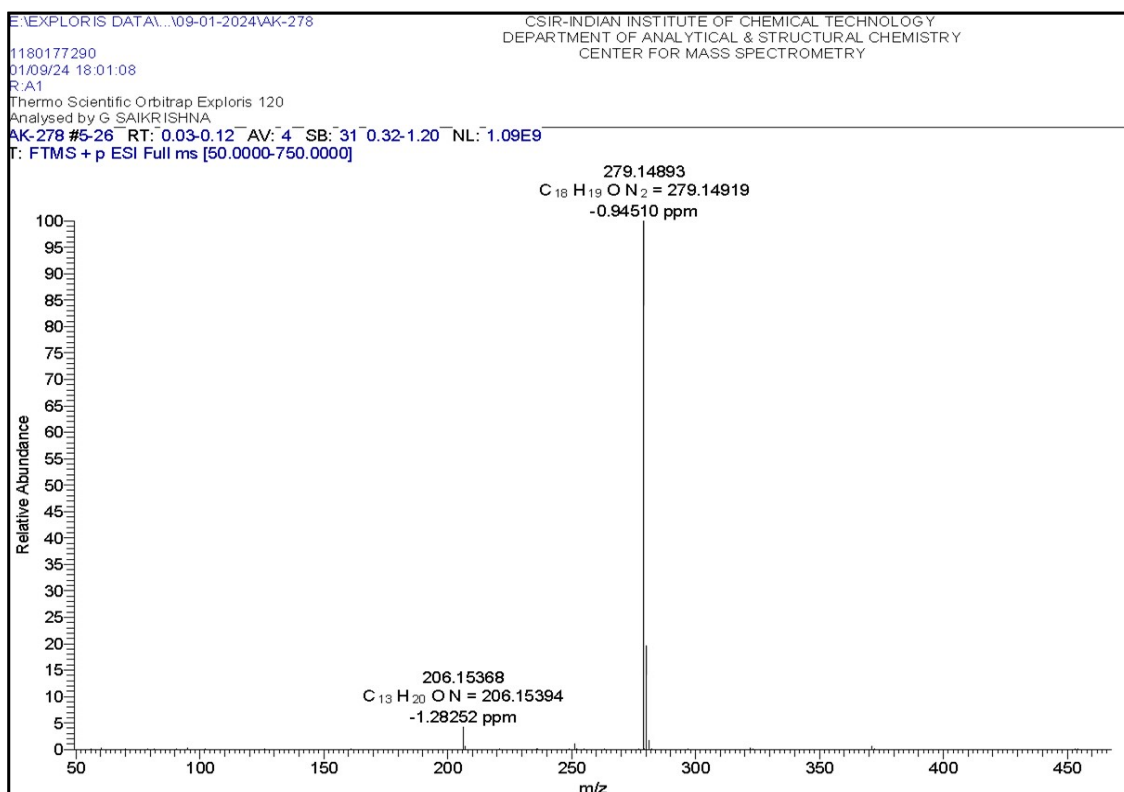




Imidazo[1,2-*a*]pyridin-3-yl(4-isobutylphenyl)methanone (3c)

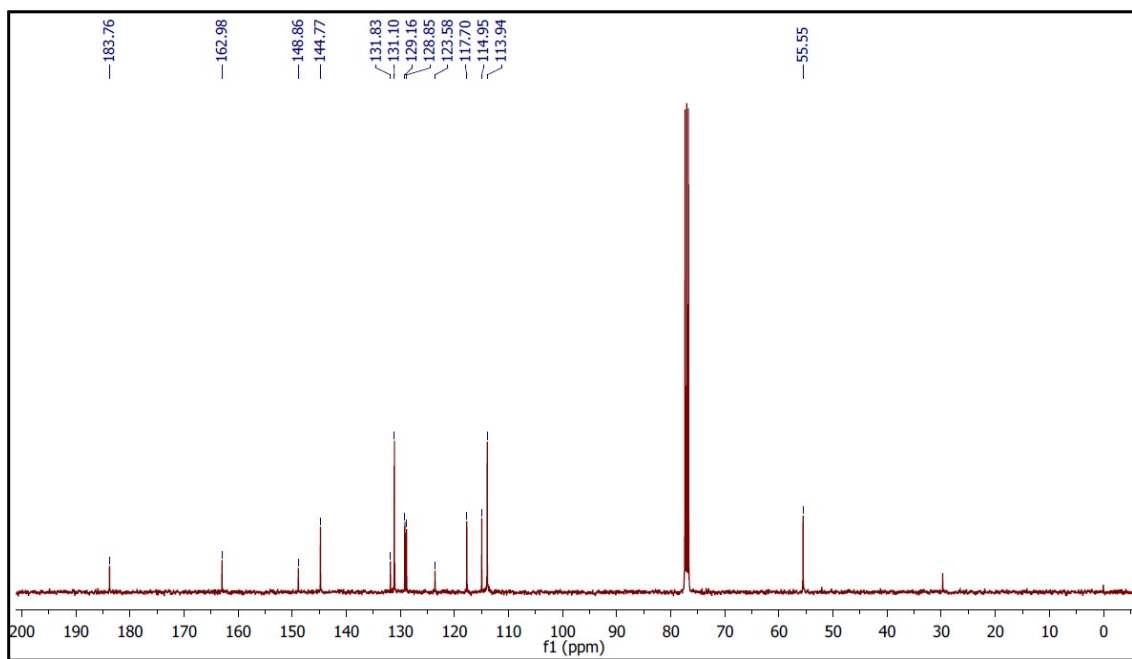
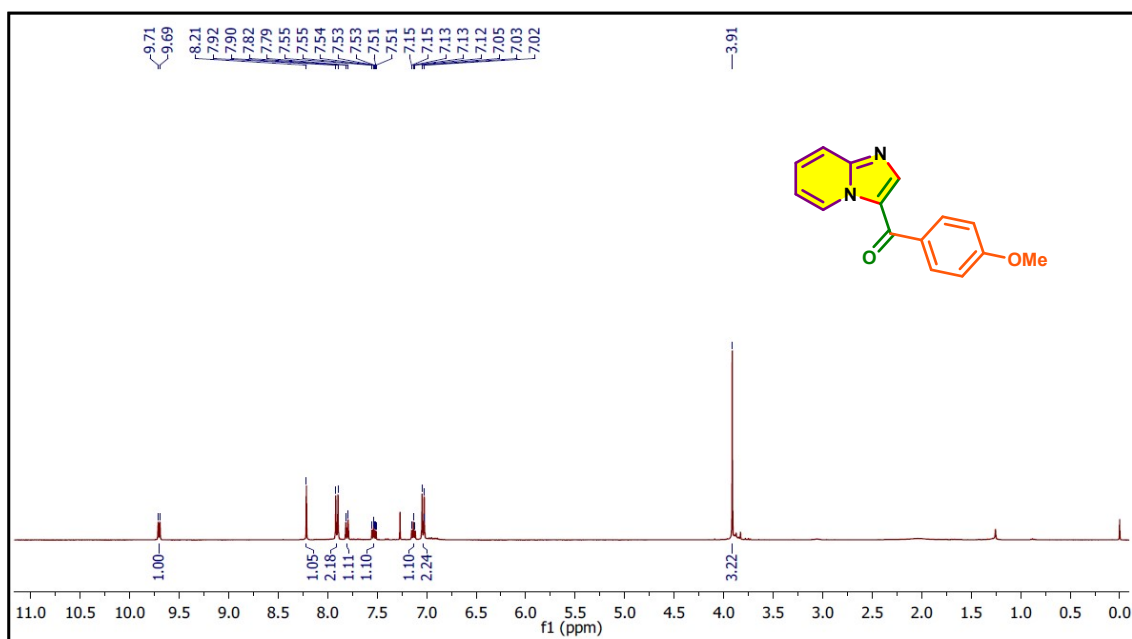
Isolated as a brown solid, yield 83% (150 mg), m.p 89-92 °C, IR (ATR): 3079, 2943, 2832, 1724 (C=O stretching), 1631, 1442, 1226, 887, 752 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.74 (d, *J* = 6.9 Hz, 1H, Ar), 8.24 (s, 1H, Ar), 7.82 (d, *J* = 8.3 Hz, 3H, Ar), 7.57 – 7.51 (m, 1H, Ar), 7.31 (d, *J* = 8.1 Hz, 2H, Ar), 7.18-7.12 (m, 1H, Ar), 2.58 (d, *J* = 7.2 Hz, 2H, (CH₃)₂CHCH₂-), 2.01 – 1.90 (m, 1H, (CH₃)₂CH-), 0.96 (d, *J* = 7.1 Hz, 6H, (CH₃)₂CH-) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 184.75 (C=O), 148.97 (Ar), 146.56 (Ar), 145.31 (Ar), 136.81 (Ar), 129.36 (Ar), 129.31 (Ar), 128.90 (Ar), 127.04 (Ar), 123.63 (Ar), 117.72 (Ar), 115.05 (Ar), 45.41 ((CH₃)₂CHCH₂-), 30.20 ((CH₃)₂CH-), 22.41 ((CH₃)₂CH-) ppm, ESI-MS: *m/z* 279 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₈H₁₉N₂O *m/z* 279.1491 [M+H]⁺, found 279.1489.

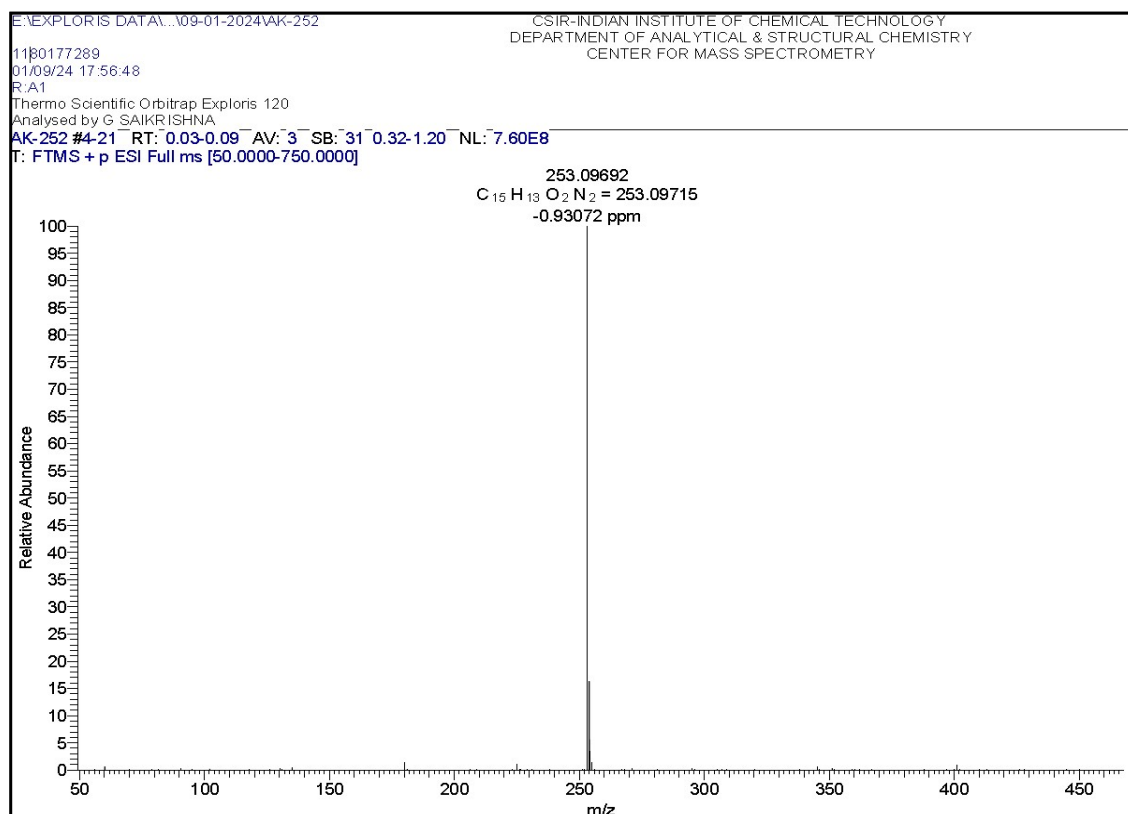




Imidazo[1,2-a]pyridin-3-yl(4-methoxyphenyl)methanone (3d)¹

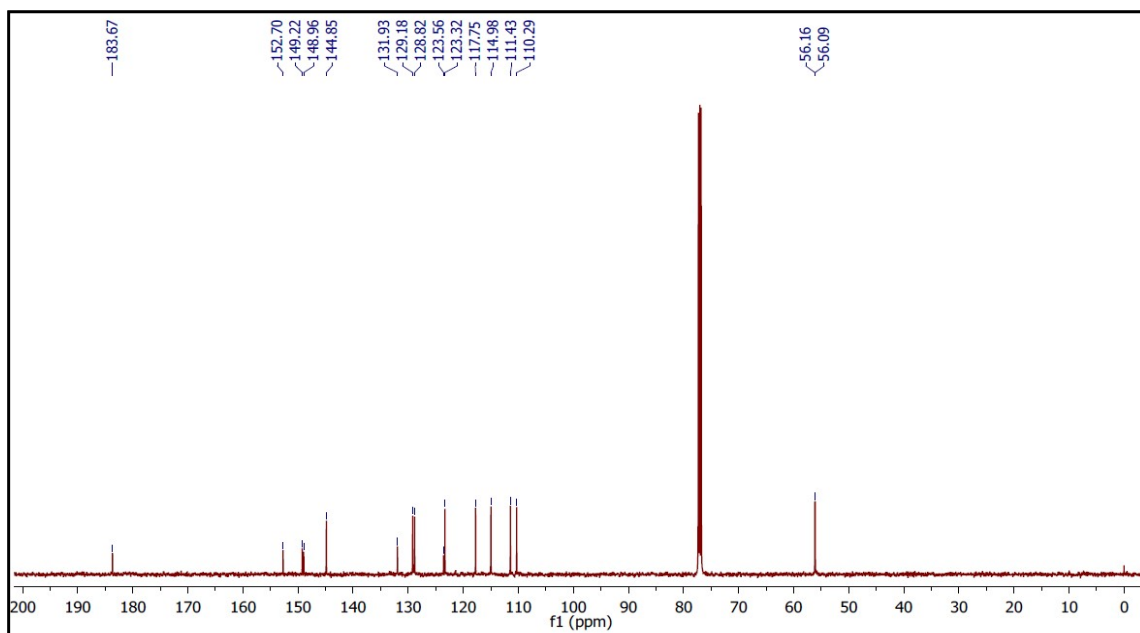
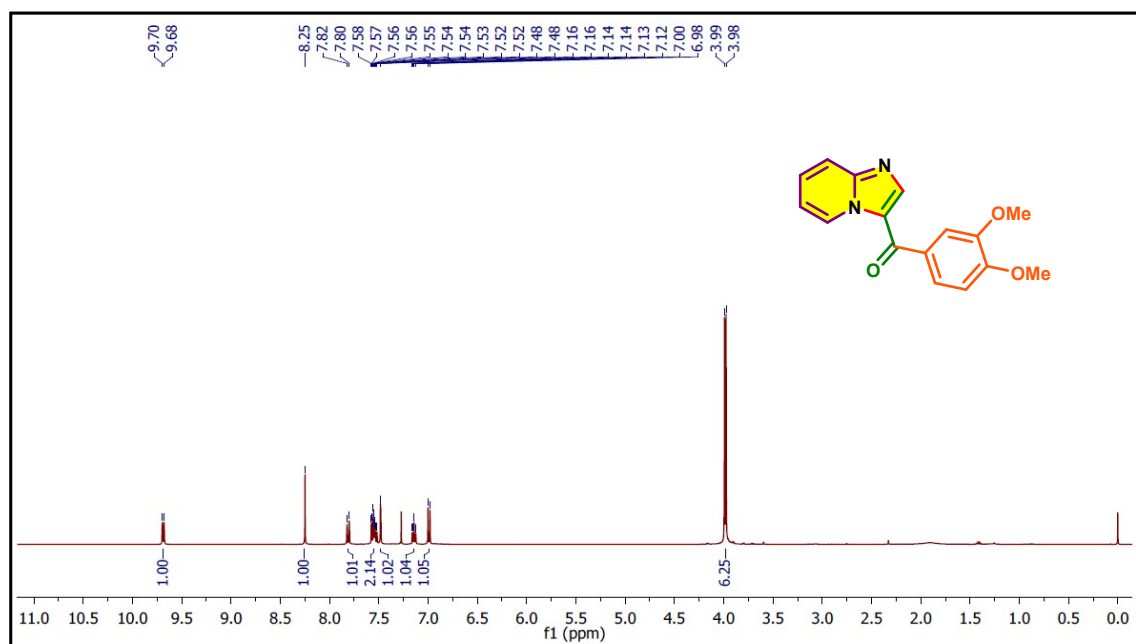
Isolated as a yellow solid, yield 88% (162 mg), m.p 139-141 °C, IR (ATR): 3108, 2918, 2849, 1732 (C=O stretching), 1603, 1505, 1255, 891, 763 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.70 (d, *J* = 6.9 Hz, 1H, Ar), 8.21 (s, 1H, Ar), 7.91 (dd, *J* = 9.2 Hz, 2H, Ar), 7.80 (d, *J* = 9.0 Hz, 1H, Ar), 7.56 – 7.50 (m, 1H, Ar), 7.16 – 7.11 (m, 1H, Ar), 7.06 – 7.01 (m, 2H, Ar), 3.91 (s, 3H, -OCH₃) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 183.76 (C=O), 162.98 (Ar), 148.86 (Ar), 144.77 (Ar), 131.83 (Ar), 131.10 (Ar), 129.16 (Ar), 128.85 (Ar), 123.58 (Ar), 117.70 (Ar), 114.95 (Ar), 113.94 (Ar), 55.55 (-OCH₃) ppm, ESI-MS: *m/z* 253 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₅H₁₃N₂O₂ *m/z* 253.0971 [M+H]⁺, found 253.0969.

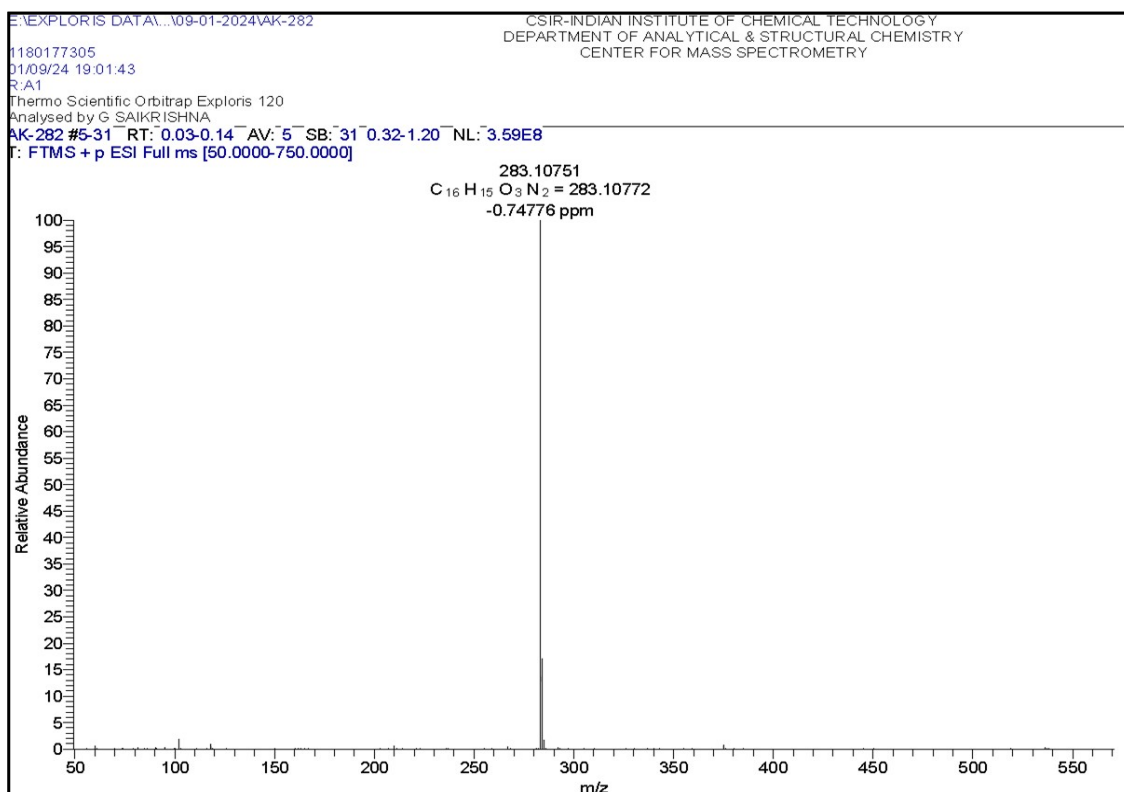




(3,4-dimethoxyphenyl)(imidazo[1,2-*a*]pyridin-3-yl)methanone (3e)²

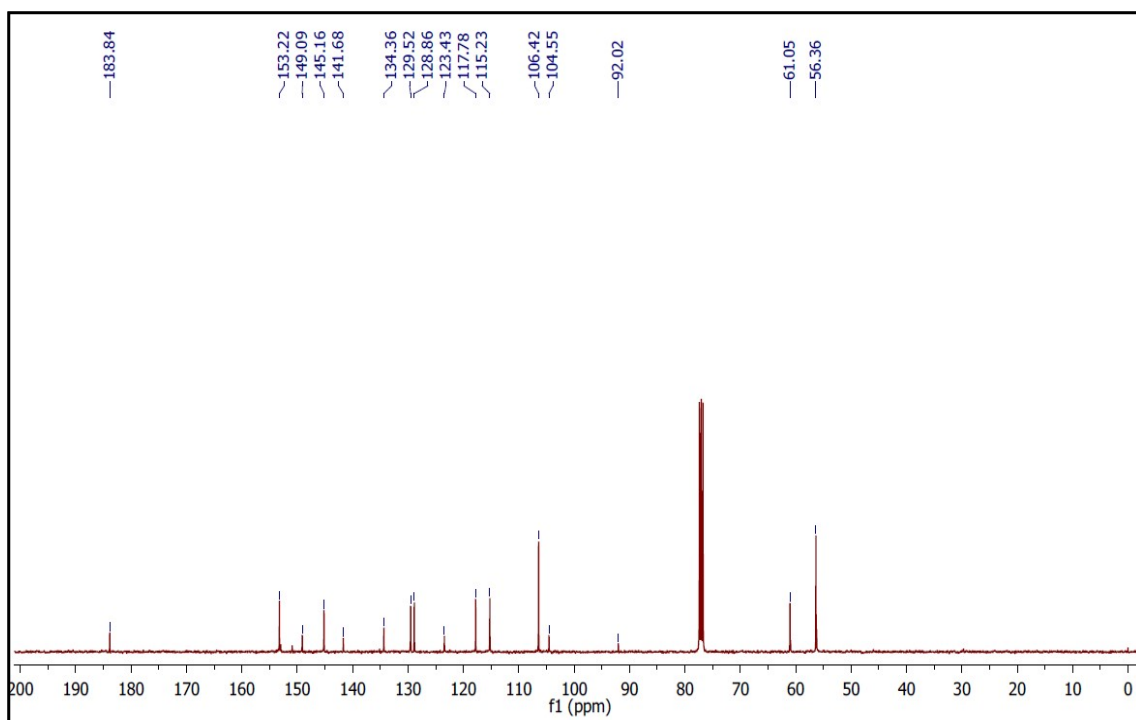
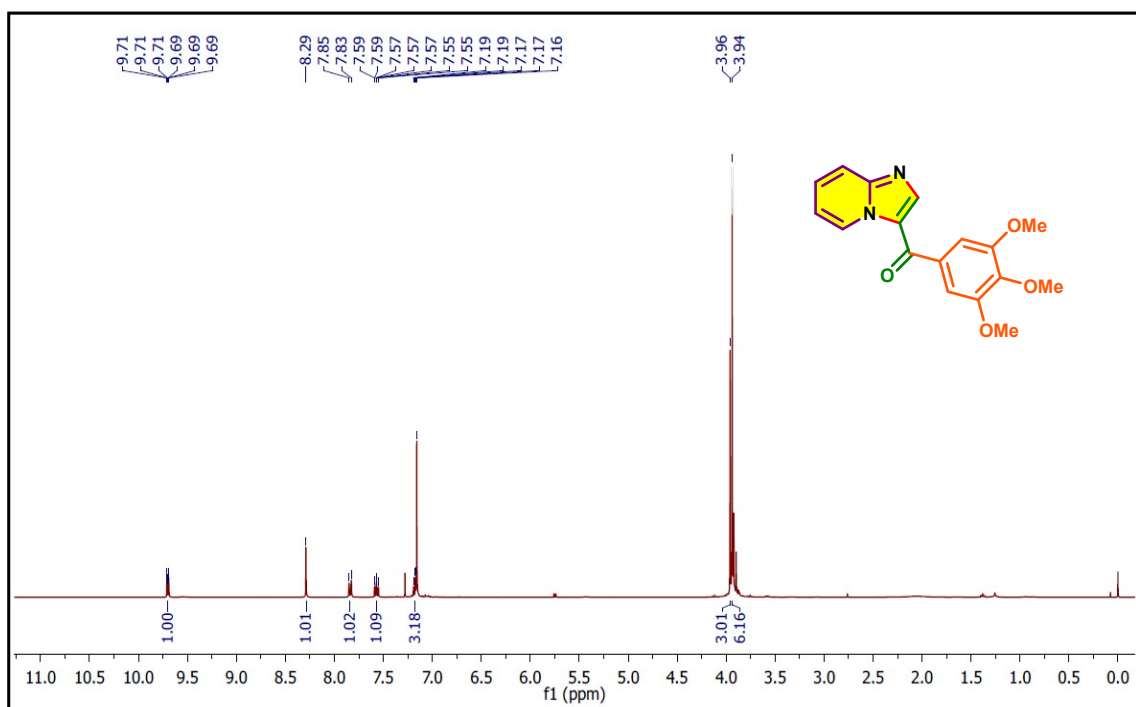
Isolated as a yellow solid, yield 92% (166 mg), m.p 136-140 °C, IR (ATR): 3112, 2920, 2852, 1744 (C=O stretching), 1610, 1525, 1166, 895, 772 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.69 (d, *J* = 6.9 Hz, 1H, Ar), 8.25 (s, 1H, Ar), 7.81 (d, *J* = 9.0 Hz, 1H, Ar), 7.58 – 7.51 (m, 2H, Ar), 7.48 (d, *J* = 1.9 Hz, 1H, Ar), 7.14 (td, *J* = 6.9 Hz, 1H, Ar), 7.01 – 6.97 (m, 1H, Ar), 3.98 (s, *J* = 6.4 Hz, 6H, -OCH₃) ppm, ¹³C NMR (125 MHz, CDCl₃): δ 183.67 (C=O), 152.70 (Ar), 149.22 (Ar), 148.96 (Ar), 144.85 (Ar), 131.93 (Ar), 129.18 (Ar), 128.82 (Ar), 123.56 (Ar), 123.32 (Ar), 117.75 (Ar), 114.98 (Ar), 111.43 (Ar), 110.29 (Ar), 56.16 (-OCH₃), 56.09 (-OCH₃) ppm, ESI-MS: m/z 283 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₆H₁₅N₂O₃ m/z 283.1077 [M+H]⁺, found 283.1075.

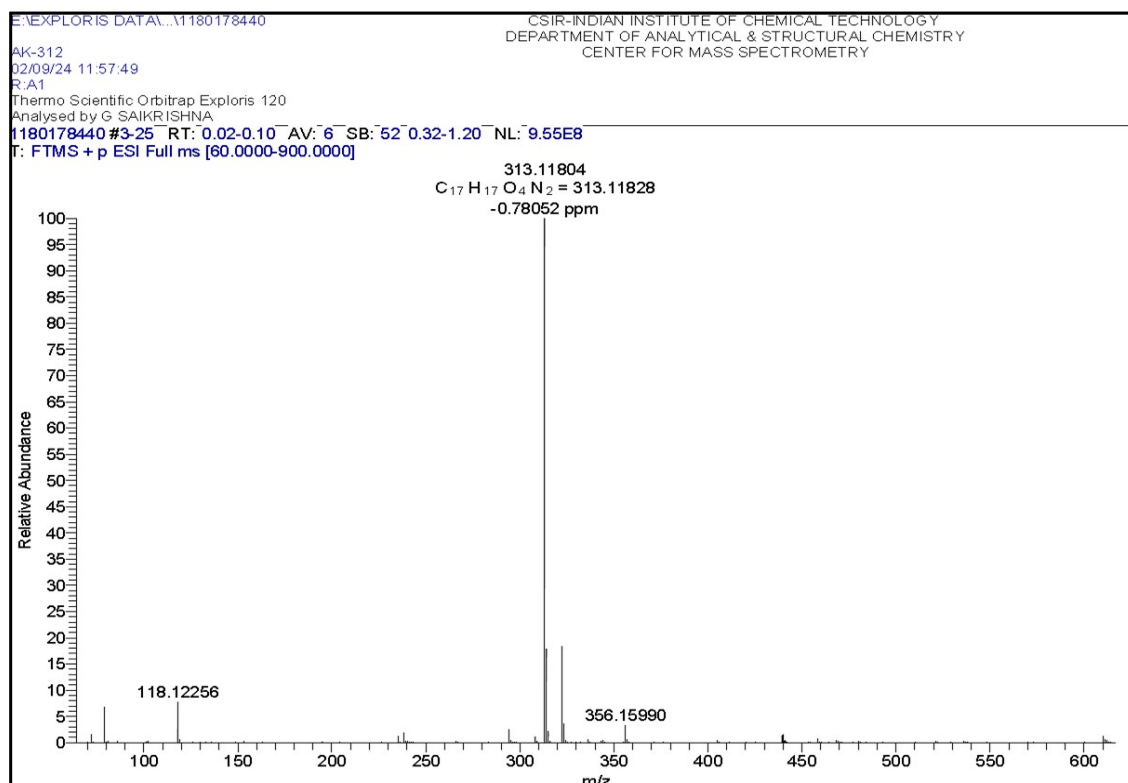




Imidazo[1,2-*a*]pyridin-3-yl(3,4,5-trimethoxyphenyl)methanone (3f)³

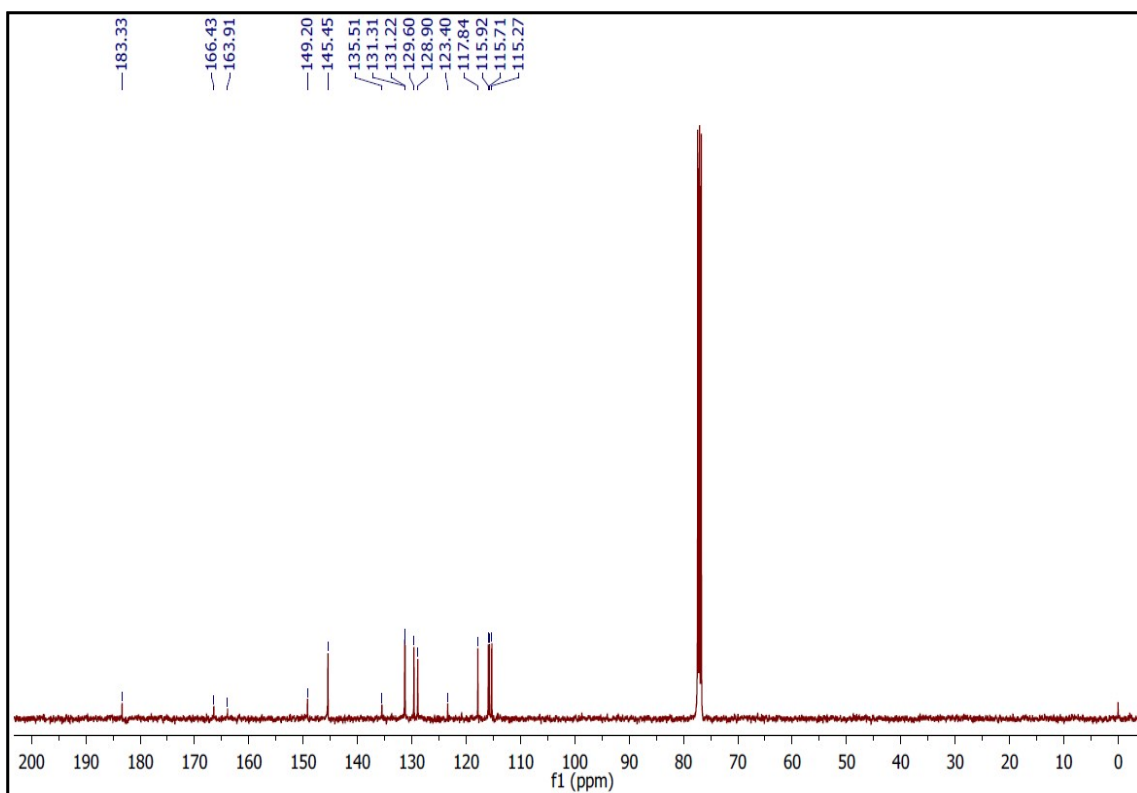
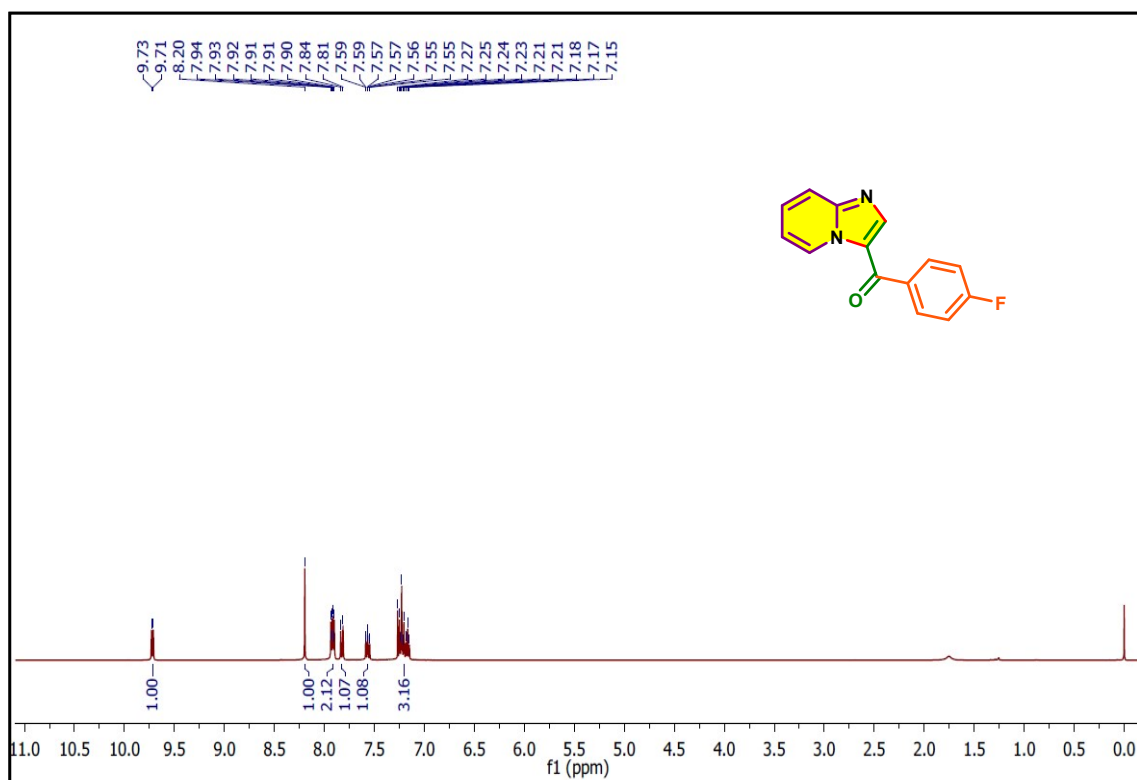
Isolated as a yellow solid, yield 85% (150 mg), m.p 114-116 °C, IR (ATR): 3117, 2932, 2846, 1739 (C=O stretching), 1611, 1492, 1172, 892, 769 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.70 (d, *J* = 6.9 Hz, 1H, Ar), 8.29 (s, 1H, Ar), 7.84 (d, *J* = 9.0 Hz, 1H, Ar), 7.60 – 7.53 (m, 1H, Ar), 7.19 – 7.15 (m, 3H, Ar), 3.96 (s, 3H, p-OCH₃), 3.94 (s, 6H, (m-OCH₃)₂) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 183.84 (C=O), 153.22 (Ar), 149.09 (Ar), 145.16 (Ar), 141.68 (Ar), 134.36 (Ar), 129.52 (Ar), 128.86 (Ar), 123.43 (Ar), 117.78 (Ar), 115.23 (Ar), 106.42 (Ar), 104.55 (Ar), 92.02 (Ar), 61.05 (p-OCH₃), 56.36 (m-OCH₃) ppm, ESI-MS: *m/z* 313 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₇H₁₇N₂O₄ *m/z* 313.1182 [M+H]⁺, found 313.1180.

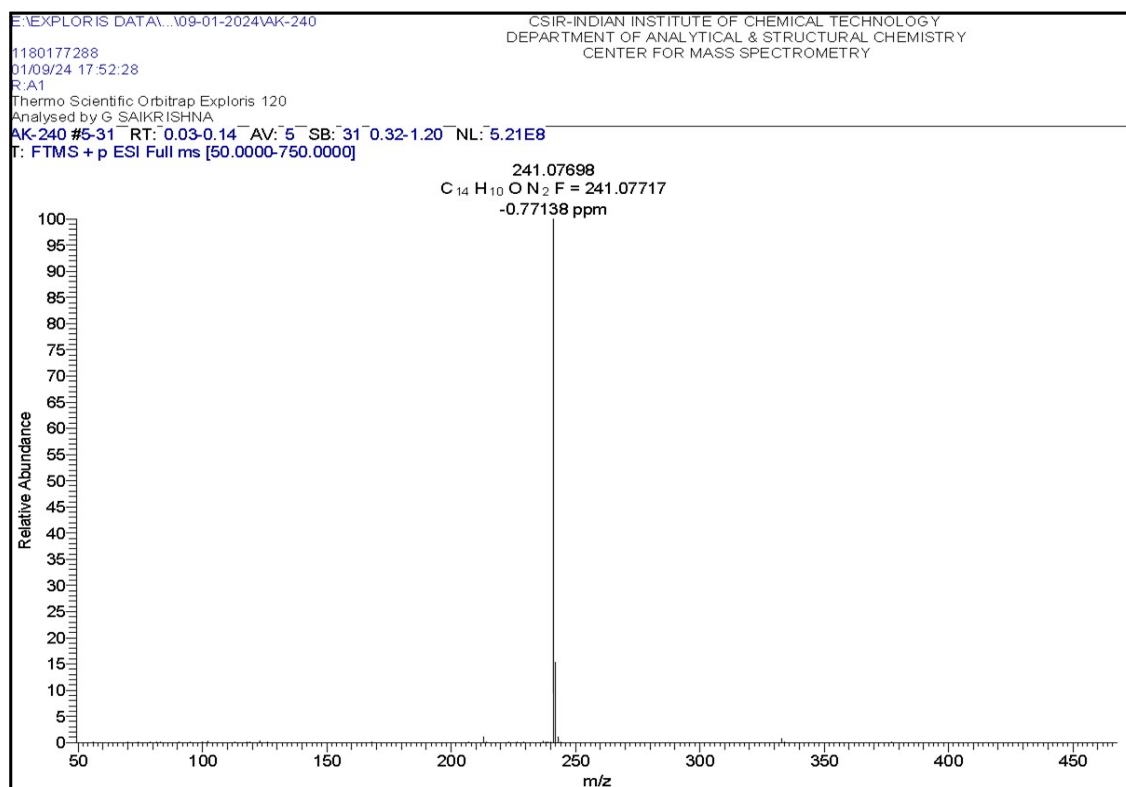




(4-fluorophenyl)(imidazo[1,2-*a*]pyridin-3-yl)methanone (3g)⁴

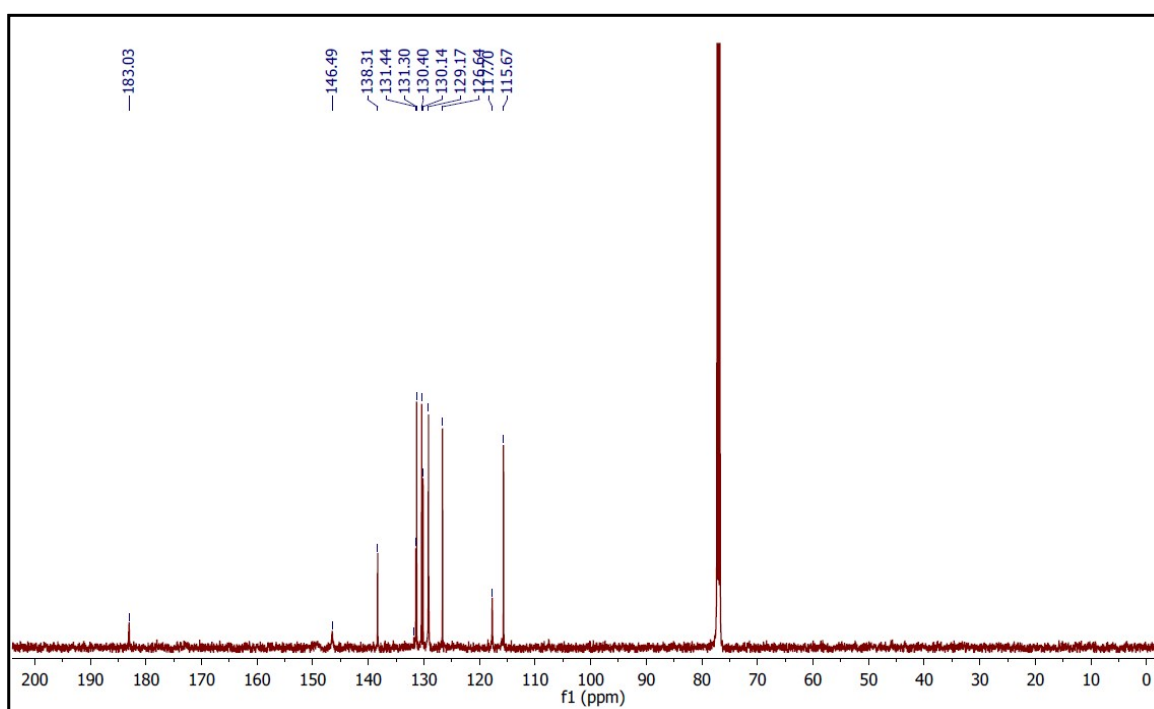
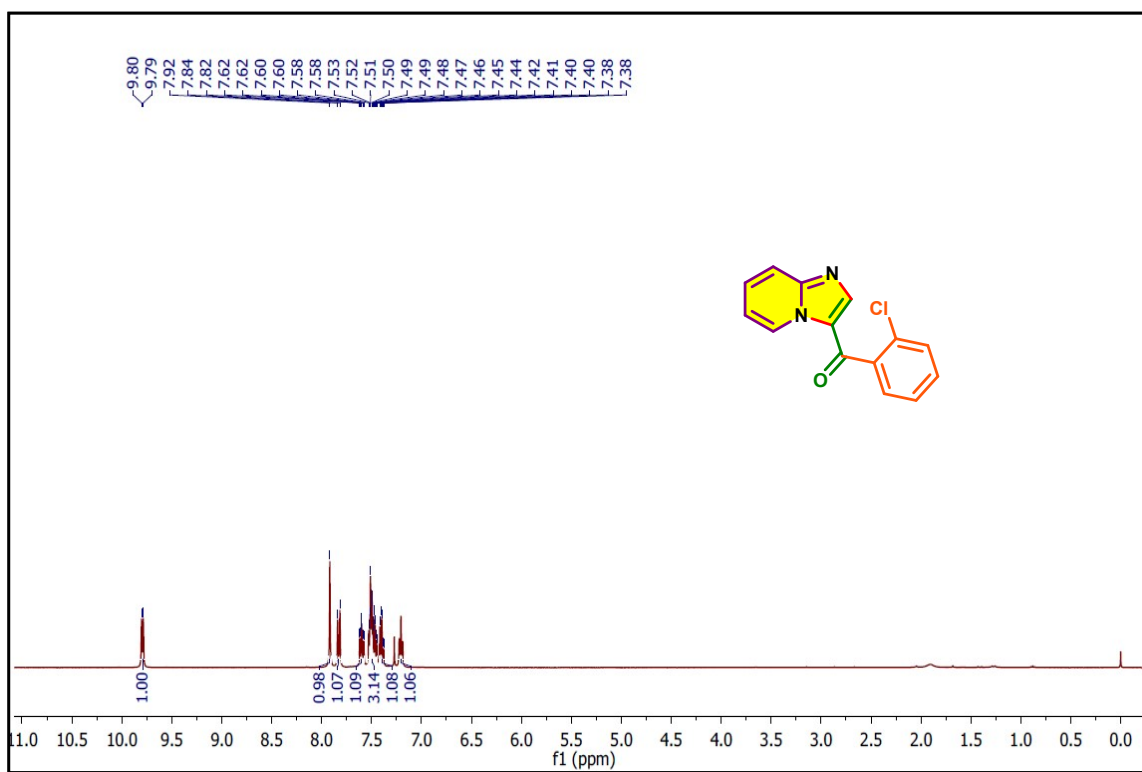
Isolated as a yellow solid, yield 75% (140 mg), m.p 178-182 °C, IR (ATR): 3105, 2916, 2852, 1705 (C=O stretching), 1613, 1506, 1467, 1221, 894, 761 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.72 (d, *J* = 6.9 Hz, 1H, Ar), 8.20 (s, 1H, Ar), 7.95 – 7.88 (m, 2H, Ar), 7.82 (d, *J* = 9.0 Hz, 1H, Ar), 7.60 – 7.53 (m, 1H, Ar), 7.25 – 7.14 (m, 3H, Ar) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 183.33 (C=O), 165.17 (d, *J* = 253.82 Hz, (Ar ¹J_{C-F})), 163.91 (Ar), 149.20 (Ar), 145.45 (Ar), 135.51 (Ar), 131.31 (Ar), 131.22 (Ar), 129.60 (Ar), 128.90 (Ar), 123.40 (Ar), 117.84 (Ar), 115.81 (d, *J* = 21.64 Hz (Ar ²J_{C-F})), 115.27 (Ar) ppm, ESI-MS: m/z 241 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₄H₁₀FN₂O m/z 241.0771 [M+H]⁺, found 241.0769.

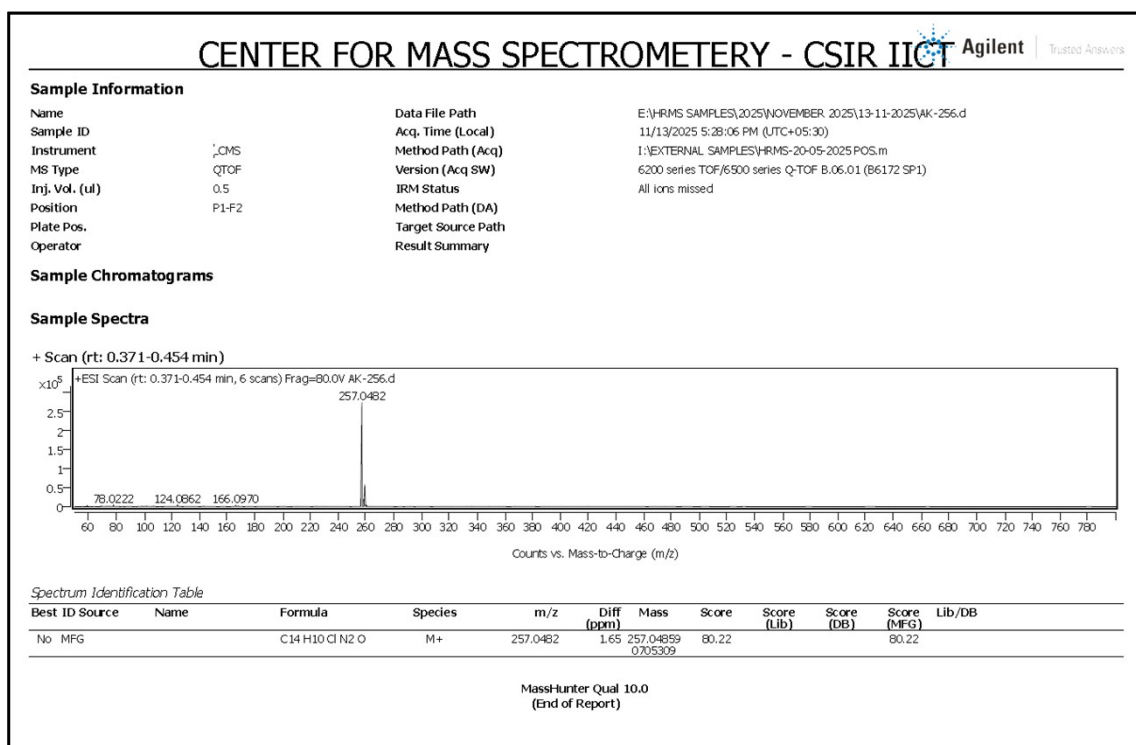




(2-chlorophenyl)(imidazo[1,2-a]pyridin-3-yl)methanone (3h)¹

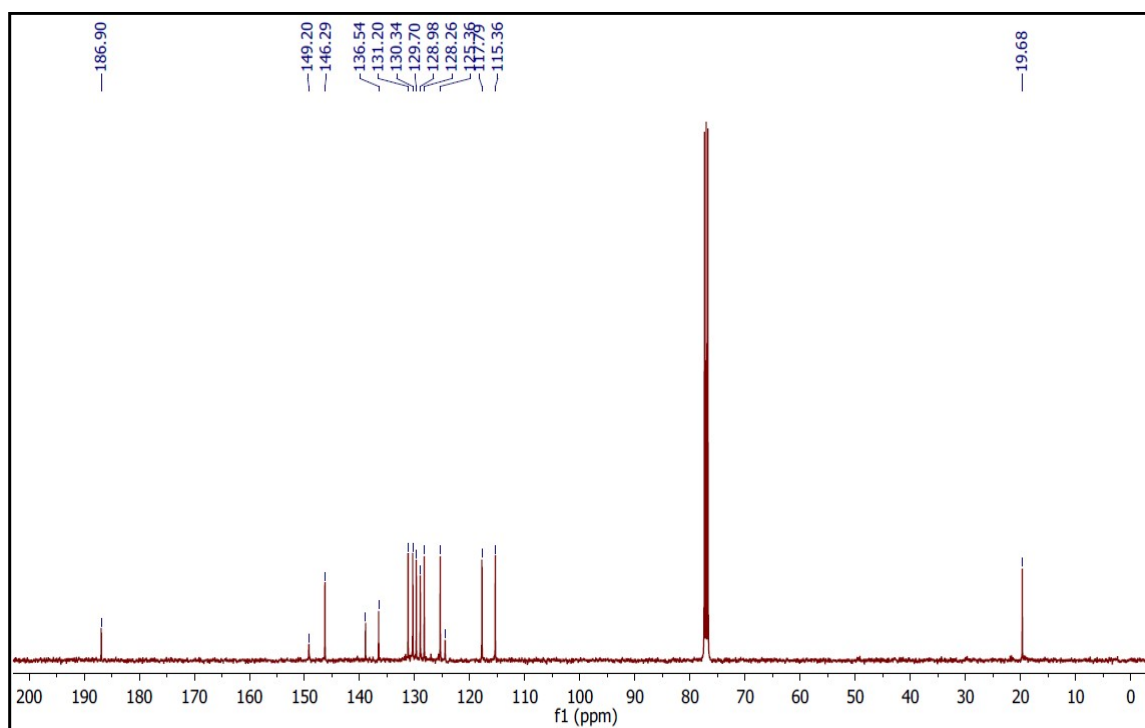
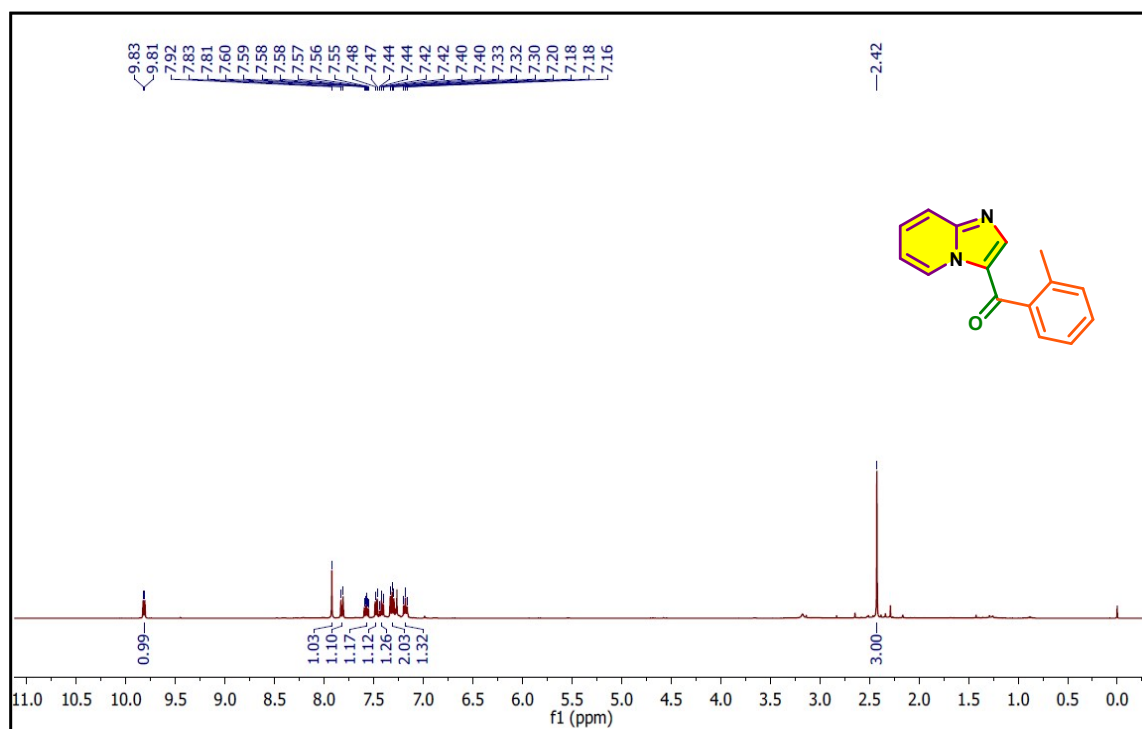
Isolated as pale brown solid, yield 67% (122 mg), m.p 151-153 °C, IR (ATR): 3113, 2923, 2851, 1733 (C=O stretching), 1622, 1592, 1478, 1092, 753, 665 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.79 (d, *J* = 6.8 Hz, 1H, Ar), 7.92 (s, 1H, Ar), 7.83 (d, *J* = 9.0 Hz, 1H, Ar), 7.63 – 7.57 (m, 1H, Ar), 7.55 – 7.43 (m, 3H, Ar), 7.40 (m, 1H, Ar), 7.21 (t, *J* = 6.6 Hz, 1H, Ar) ppm, ¹³C NMR (125 MHz, CDCl₃): δ 183.03 (C=O), 146.49 (Ar), 138.31 (Ar), 131.78 (Ar), 131.44 (Ar), 131.30 (Ar), 130.40 (Ar), 130.14 (Ar), 129.17 (Ar), 126.64 (Ar), 117.70 (Ar), 115.67 (Ar) ppm, ESI-MS: m/z 257 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₄H₁₀ClN₂O m/z 257.0485 [M+H]⁺, found 257.0482.

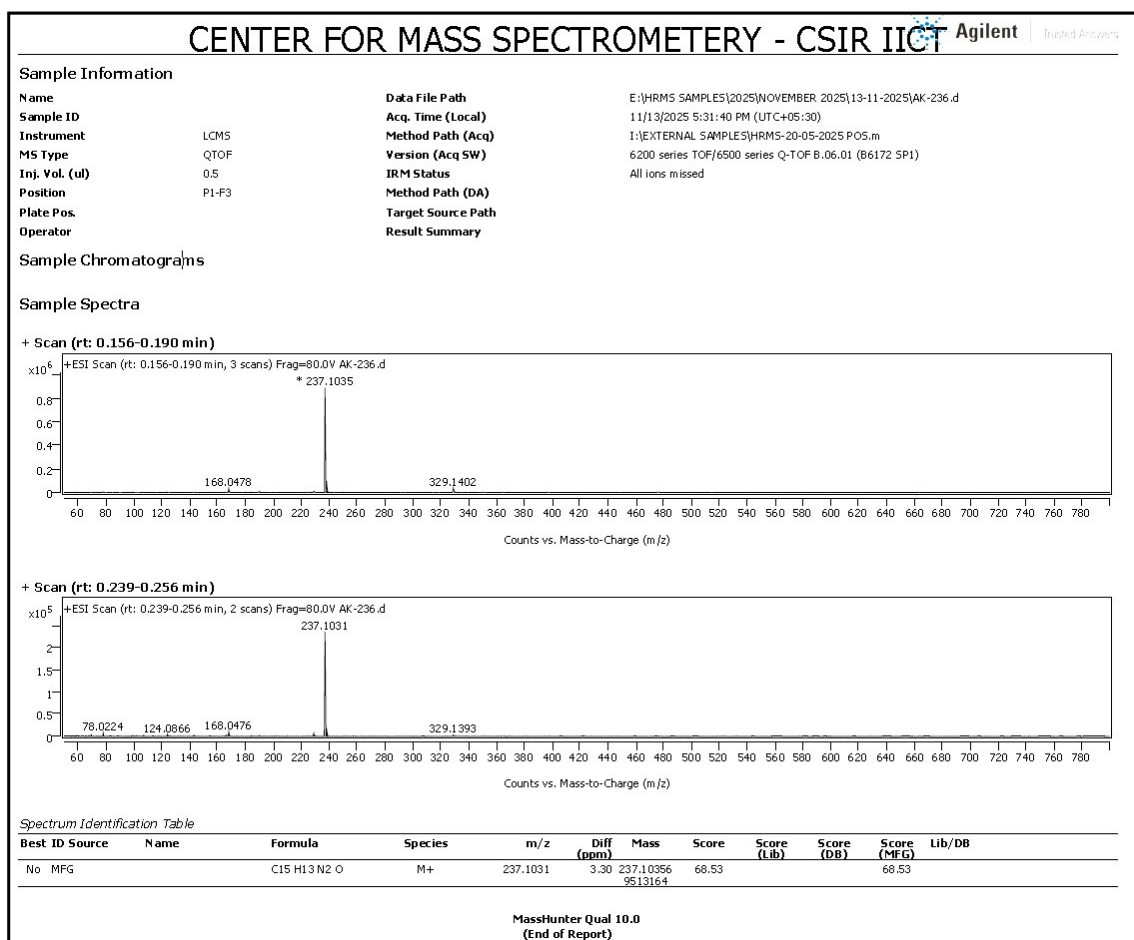




Imidazo[1,2-a]pyridin-3-yl(*o*-tolyl)methanone (**3i**)¹

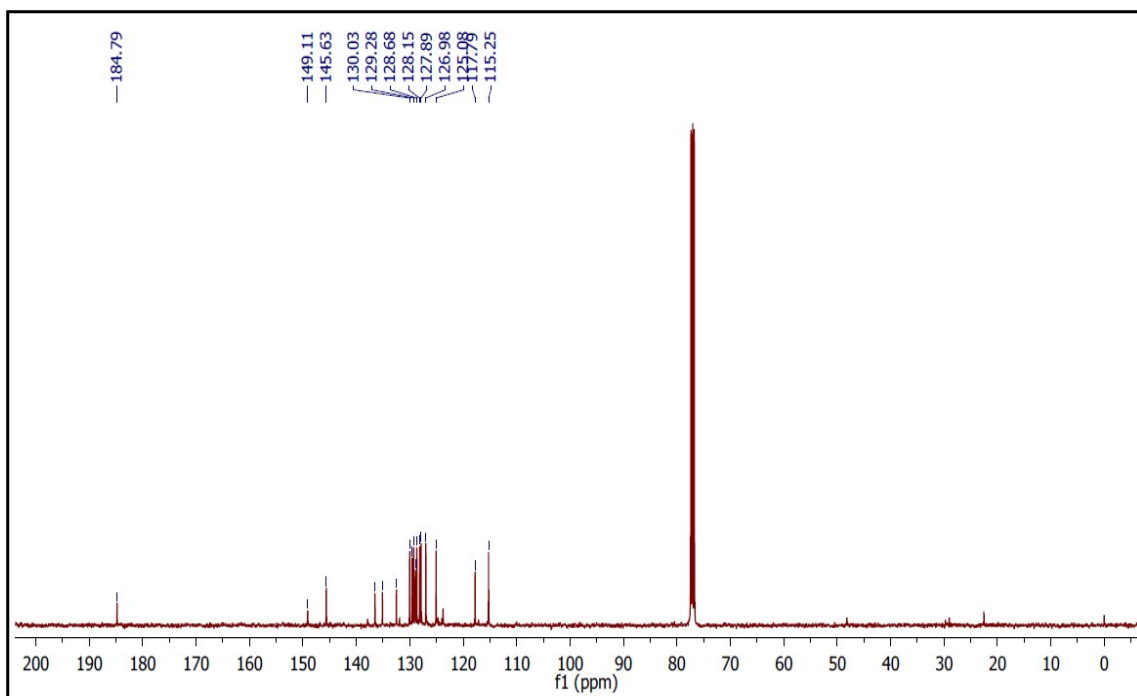
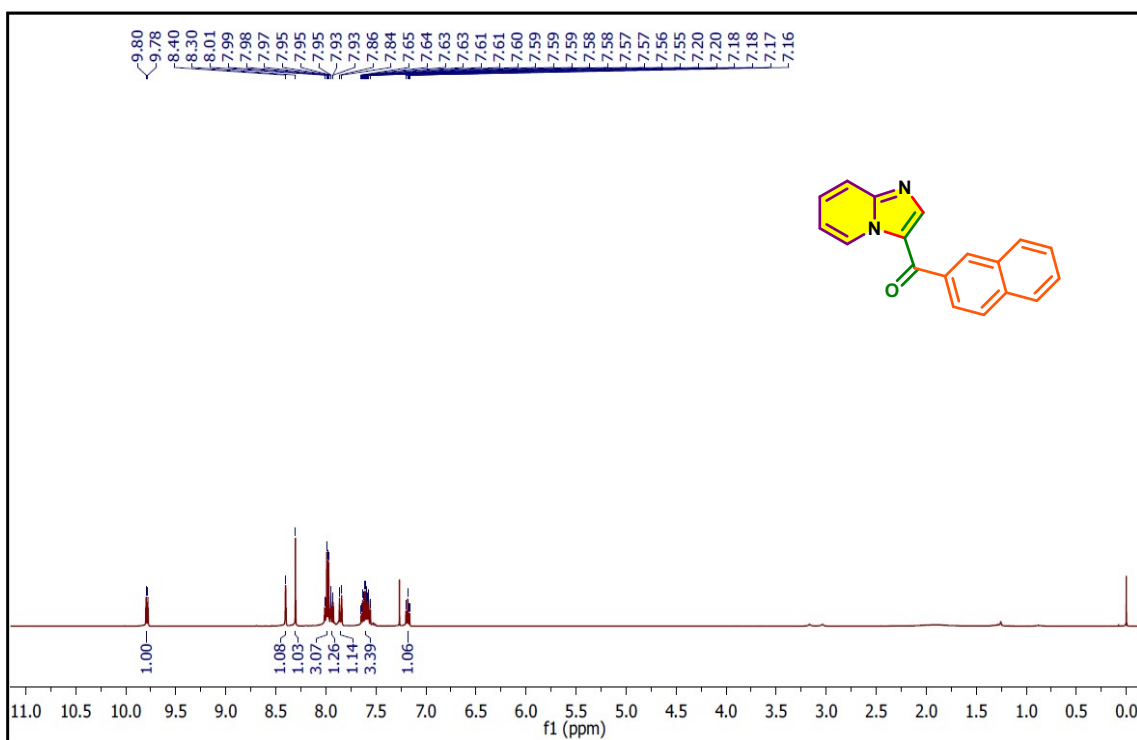
Isolated as pale brown solid, yield 55% (102 mg), m.p 110-111 °C, IR (ATR): 3020, 2924, 2853, 1721 (C=O stretching), 1626, 1509, 1481, 1172, 750, 669 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.82 (d, *J* = 6.9 Hz, 1H, Ar), 7.92 (s, 1H, Ar), 7.82 (d, *J* = 9.0 Hz, 1H, Ar), 7.61 – 7.54 (m, 1H, Ar), 7.44 (m, 2H, Ar), 7.31 (m, 2H, Ar), 7.18 (t, *J* = 6.6 Hz, 1H, Ar), 2.42 (s, 3H, -CH₃) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 186.90 (C=O), 149.20 (Ar), 146.29 (Ar), 138.92 (Ar), 136.54 (Ar), 131.20 (Ar), 130.34 (Ar), 129.70 (Ar), 128.98 (Ar), 128.26 (Ar), 125.36 (Ar), 124.47 (Ar), 117.79 (Ar), 115.36 (Ar), 19.68 ppm, ESI-MS: *m/z* 237 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₅H₁₃N₂O *m/z* 237.1035 [M+H]⁺, found 237.1031.

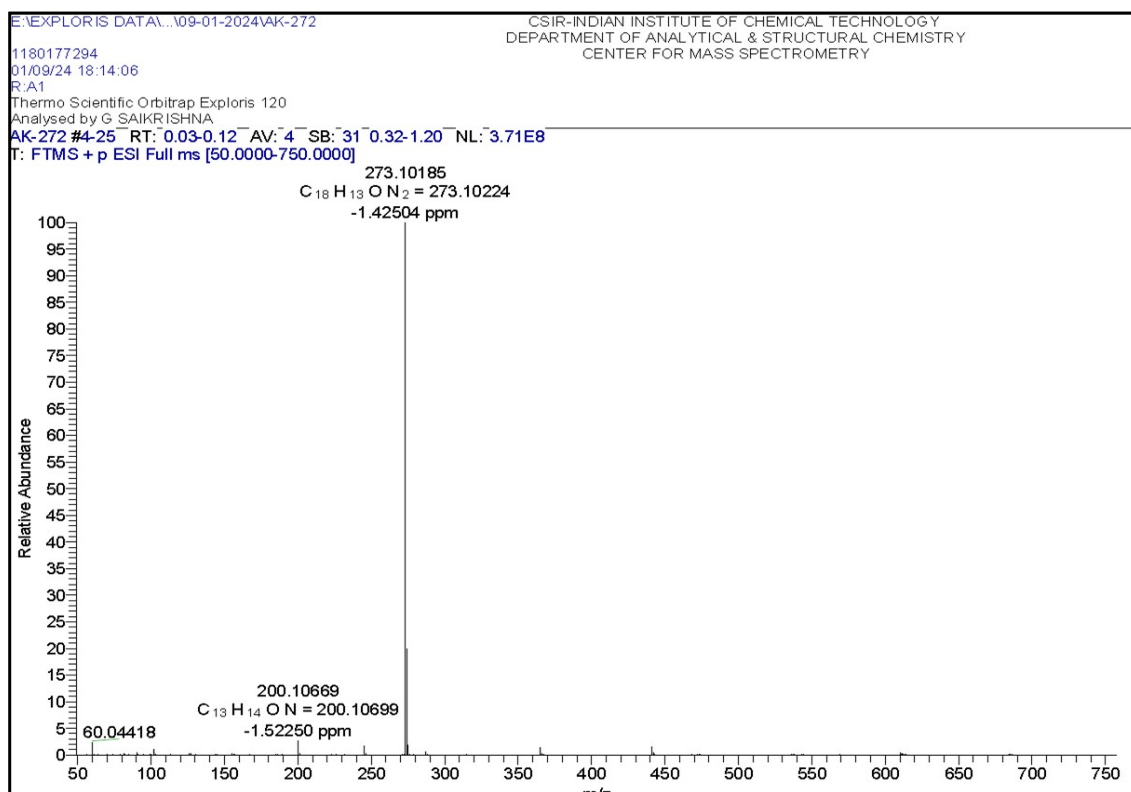




Imidazo[1,2-a]pyridin-3-yl(naphthalen-2-yl)methanone (3j)¹

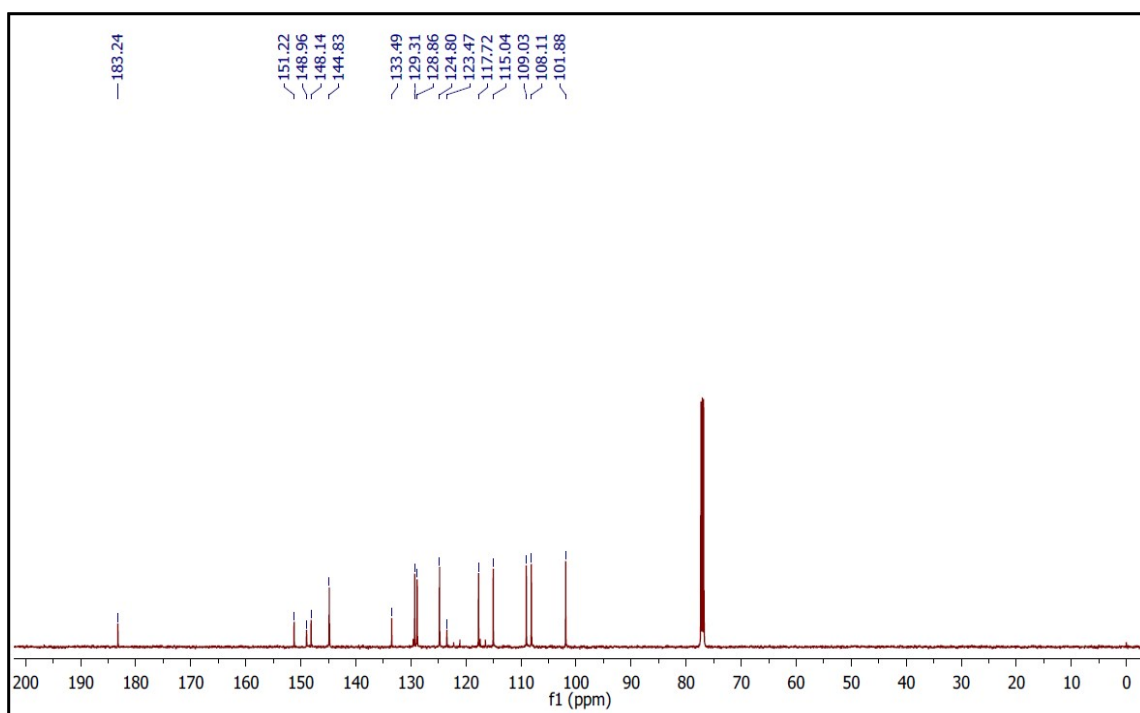
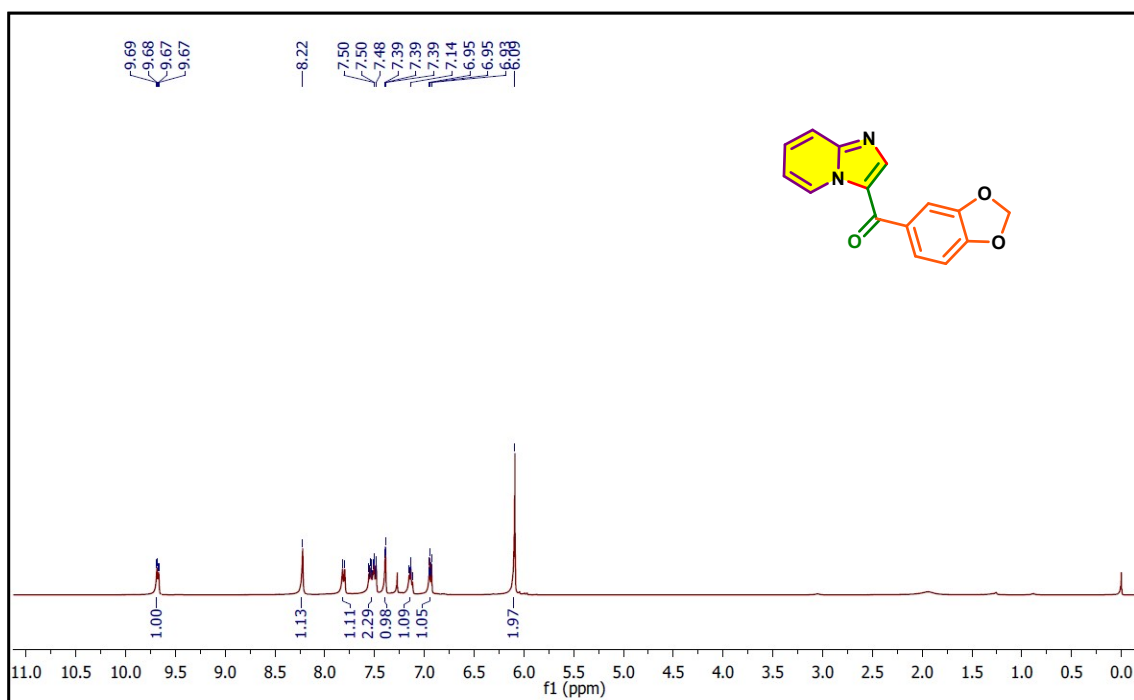
Isolated as a yellow solid, yield 77% (140 mg), m.p 134-137 °C, IR (ATR): 3051, 2918, 2852, 1713 (C=O stretching), 1611, 1472, 1181, 902, 755 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.79 (d, *J* = 6.9 Hz, 1H, Ar), 8.40 (s, 1H, Ar), 8.30 (s, 1H, Ar), 7.99 (dd, *J* = 11.0, 5.0 Hz, 3H, Ar), 7.96 – 7.92 (m, 1H, Ar), 7.88 – 7.82 (m, 1H, Ar), 7.65 – 7.55 (m, 3H, Ar), 7.18 (t, *J* = 6.9 Hz, 1H, Ar) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 184.79 (C=O), 149.11 (Ar), 145.63 (Ar), 136.50 (Ar), 135.12 (Ar), 132.50 (Ar), 130.03 (Ar), 129.56 (Ar), 129.28 (Ar), 128.96 (Ar), 128.68 (Ar), 128.15 (Ar), 127.89 (Ar), 126.98 (Ar), 125.08 (Ar), 117.79 (Ar), 115.25 (Ar) ppm, ESI-MS: m/z 273 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₈H₁₃N₂O m/z 273.1022 [M+H]⁺, found 273.1018.

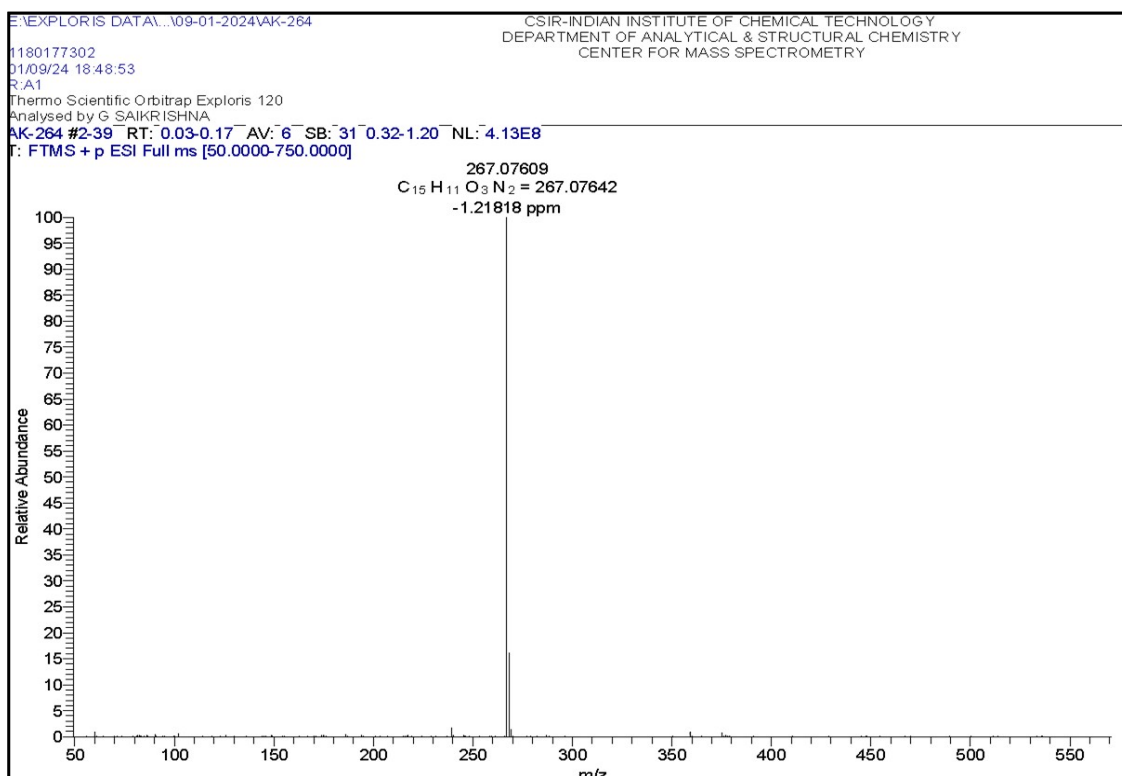




Benzo[d][1,3]dioxol-5-yl(imidazo[1,2-a]pyridin-3-yl)methanone (3k)²

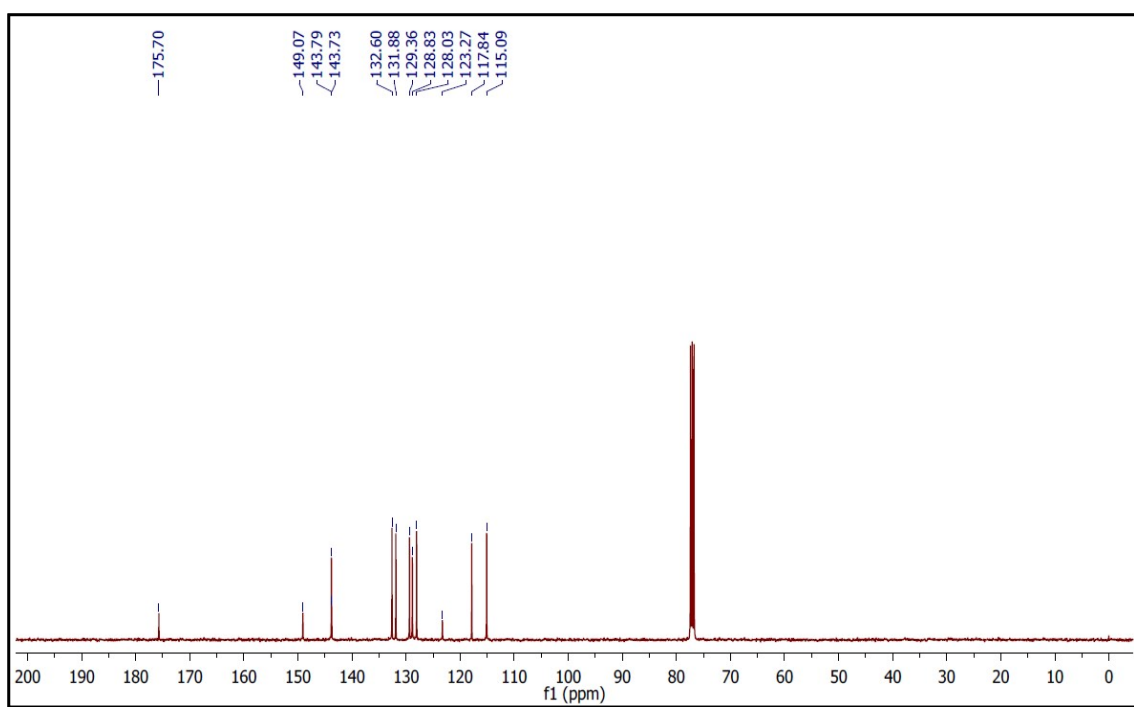
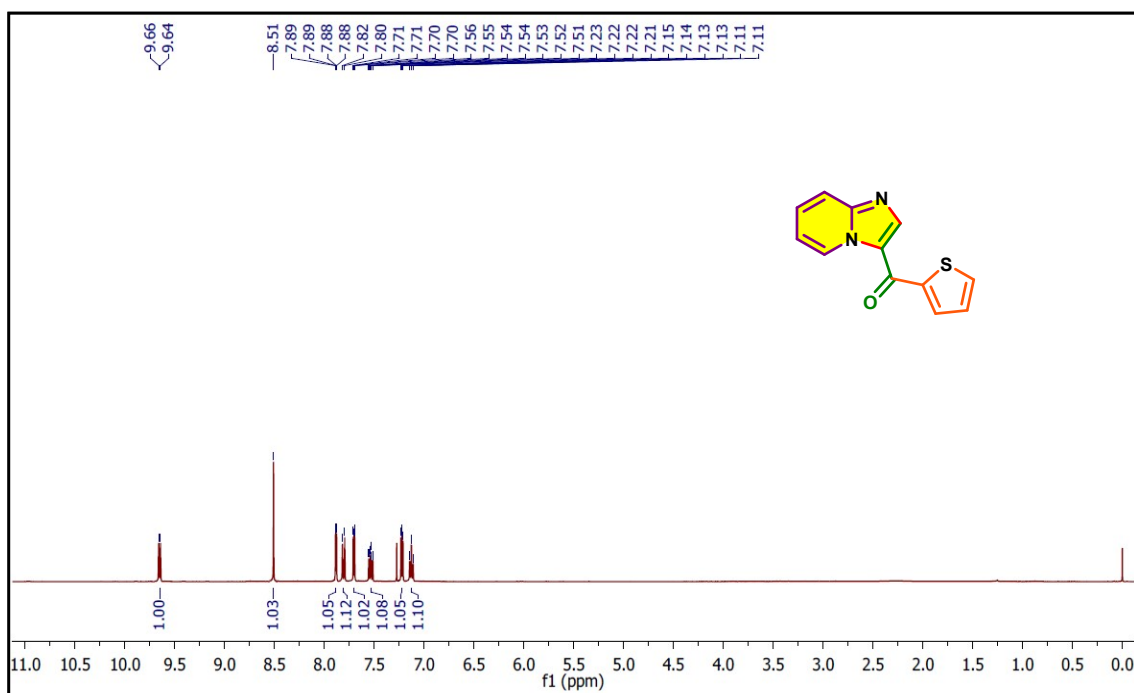
Isolated as a yellow solid, yield 72% (131 mg), m.p 173-175 °C, IR (ATR): 3092, 2915, 2851, 1731 (C=O stretching), 1625, 1455, 1262, 955, 880, 753 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.68 (d, *J* = 6.9 Hz, 1H, Ar), 8.22 (s, 1H, Ar), 7.81 (d, *J* = 8.9 Hz, 1H, Ar), 7.59 – 7.47 (m, 2H, Ar), 7.43 – 7.37 (m, 1H, Ar), 7.19 – 7.11 (m, 1H, Ar), 6.94 (m, 1H, Ar), 6.13 – 6.07 (m, 2H, -CH₂-) ppm, ¹³C NMR (125 MHz, CDCl₃): δ 183.24 (C=O), 151.22 (Ar), 148.96 (Ar), 148.14 (Ar), 144.83 (Ar), 133.49 (Ar), 129.31 (Ar), 128.86 (Ar), 124.80 (Ar), 123.47 (Ar), 117.72 (Ar), 115.04 (Ar), 109.03 (Ar), 108.11 (Ar), 101.88 (-CH₂-) ppm, ESI-MS: *m/z* 267 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₅H₁₁N₂O₃ *m/z* 267.0764 [M+H]⁺, found 267.0760.

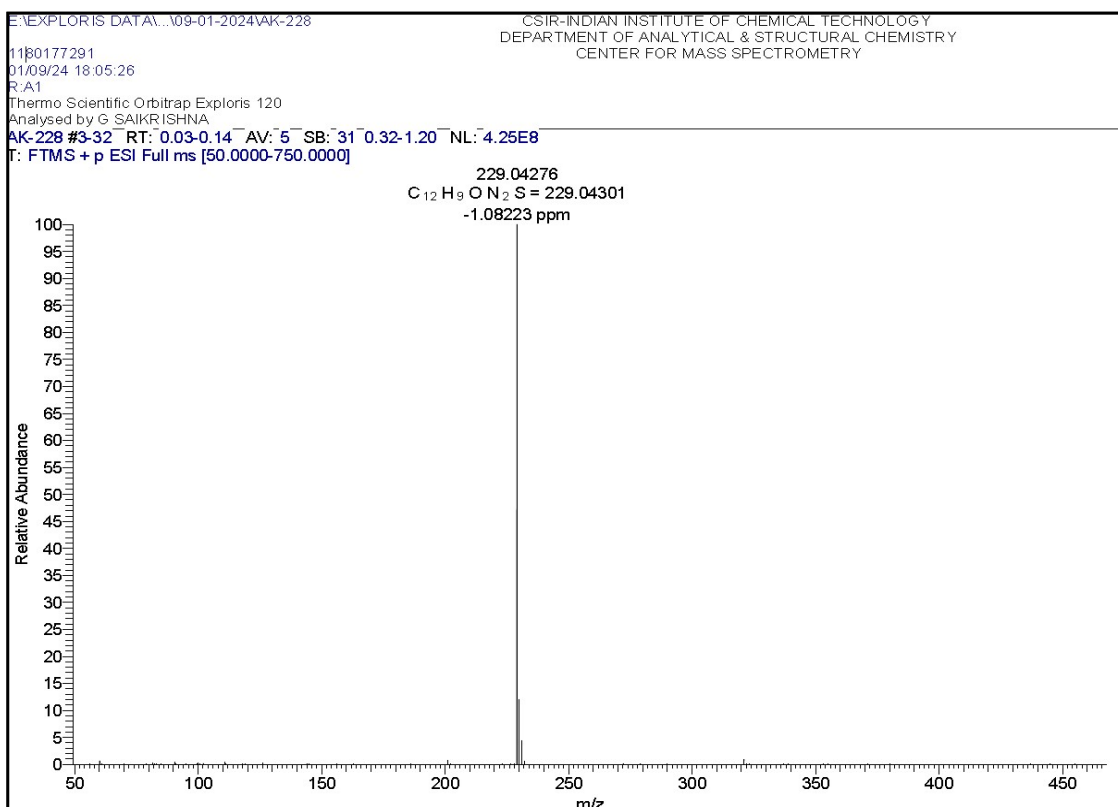




Imidazo[1,2-*a*]pyridin-3-yl(thiophen-2-yl)methanone (3l)¹

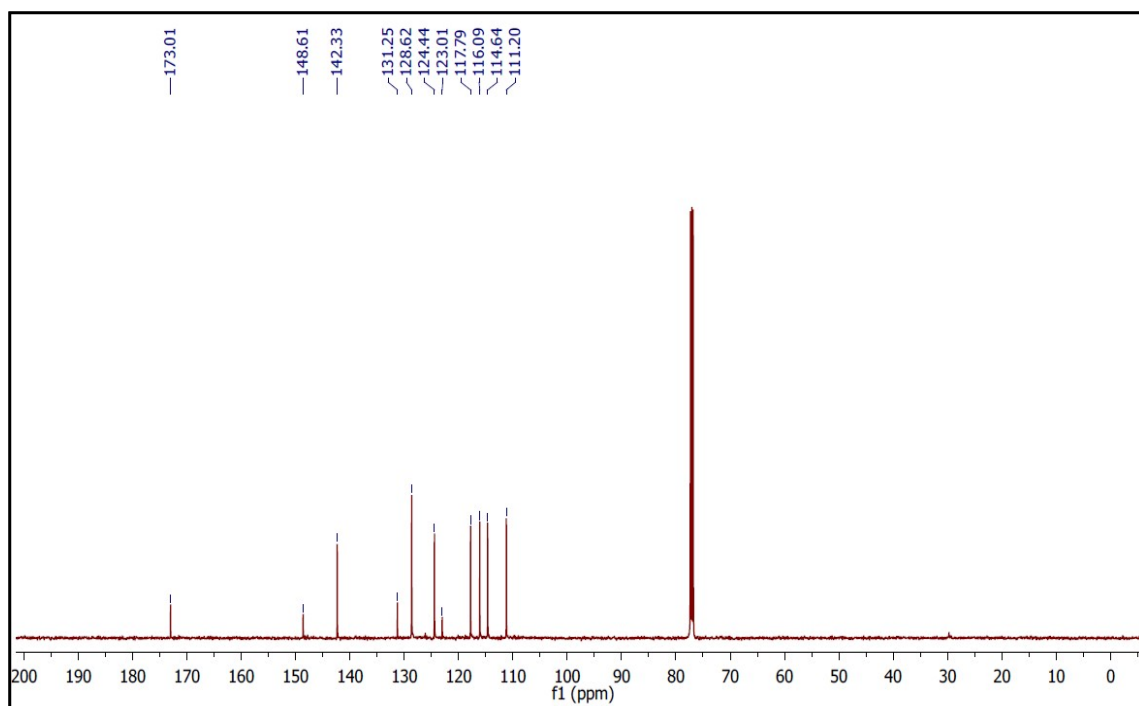
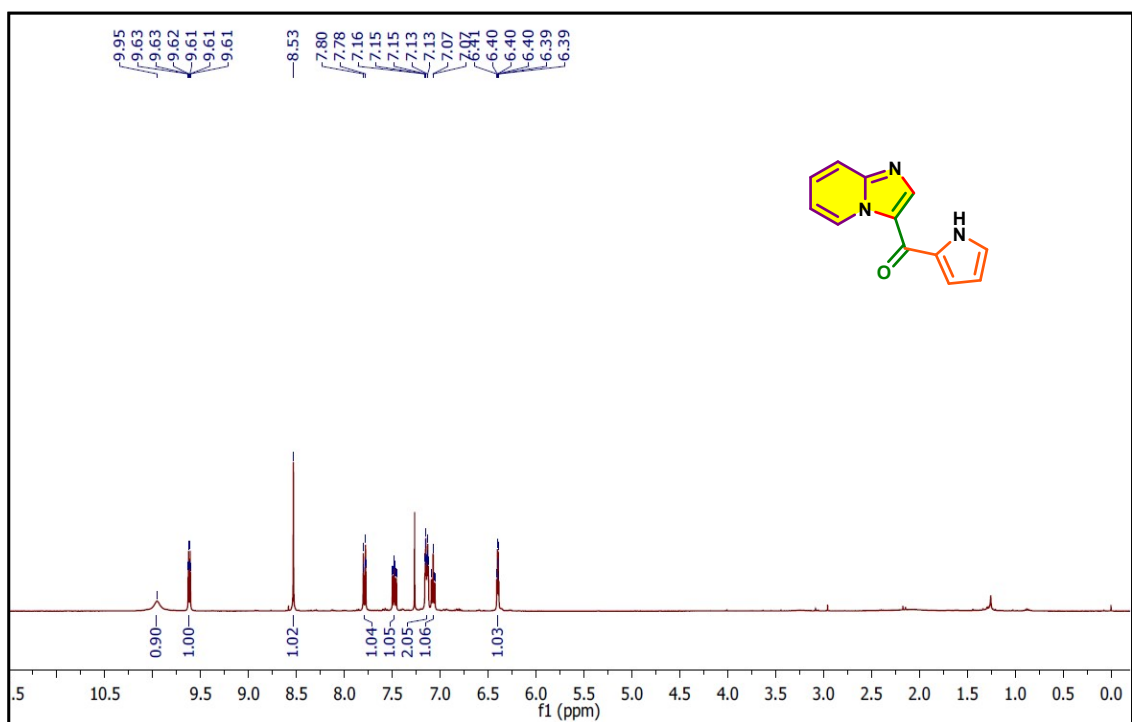
Isolated as a brown solid, yield 82% (155 mg), m.p 114-116 °C, IR (ATR): 3086, 2916, 2852, 1726 (C=O stretching), 1594, 1503, 1414, 1221, 815, 755 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.65 (d, *J* = 6.9 Hz, 1H, Ar), 8.51 (s, 1H, Ar), 7.91 – 7.86 (m, 1H, Ar), 7.81 (d, *J* = 9.0 Hz, 1H, Ar), 7.73 – 7.68 (m, 1H, Ar), 7.57 – 7.50 (m, 1H, Ar), 7.25 – 7.20 (m, 1H, Ar), 7.13 (td, *J* = 6.9 Hz, 1H, Ar) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 175.70 (C=O), 149.07 (Ar), 143.79 (Ar), 143.73 (Ar), 132.60 (Ar), 131.88 (Ar), 129.36 (Ar), 128.83 (Ar), 128.03 (Ar), 123.27 (Ar), 117.84 (Ar), 115.09 (Ar) ppm, ESI-MS: *m/z* 229 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₂H₉N₂OS *m/z* 229.0430 [M+H]⁺, found 229.0427.

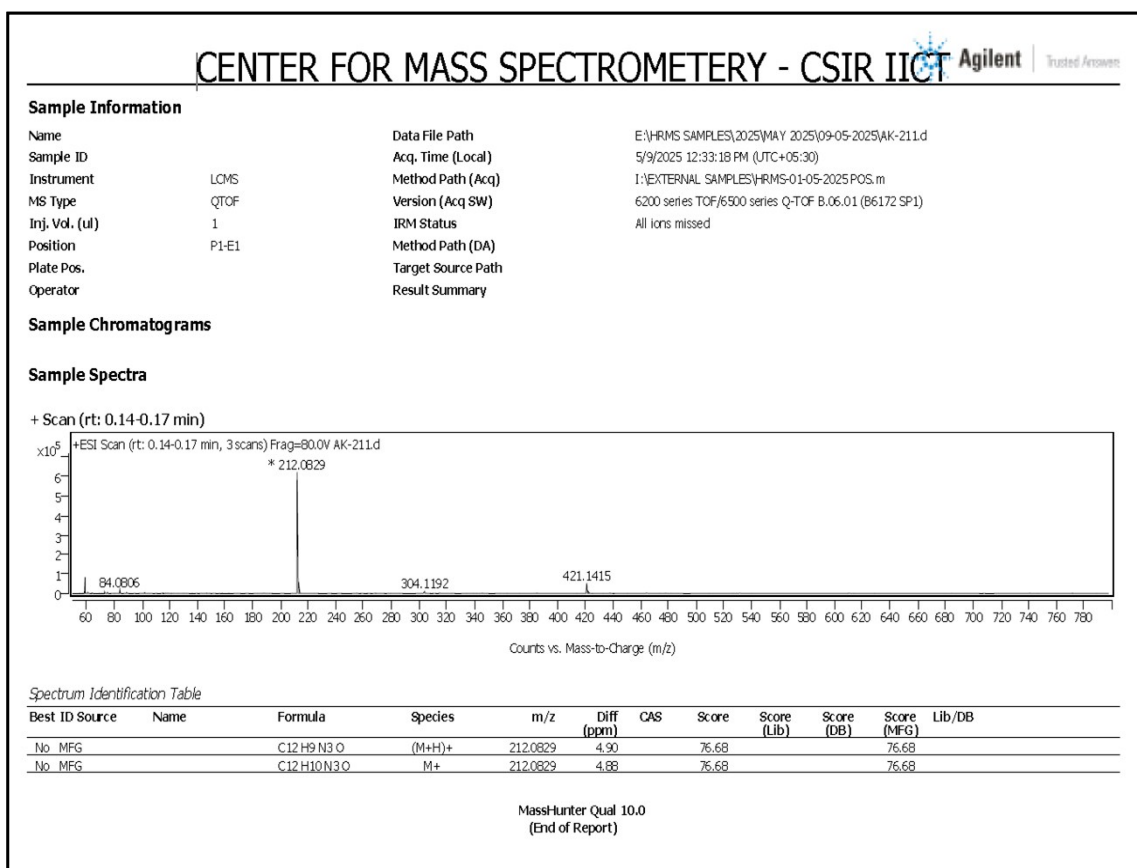




Imidazo[1,2-a]pyridin-3-yl(1H-pyrrol-2-yl)methanone (3m)

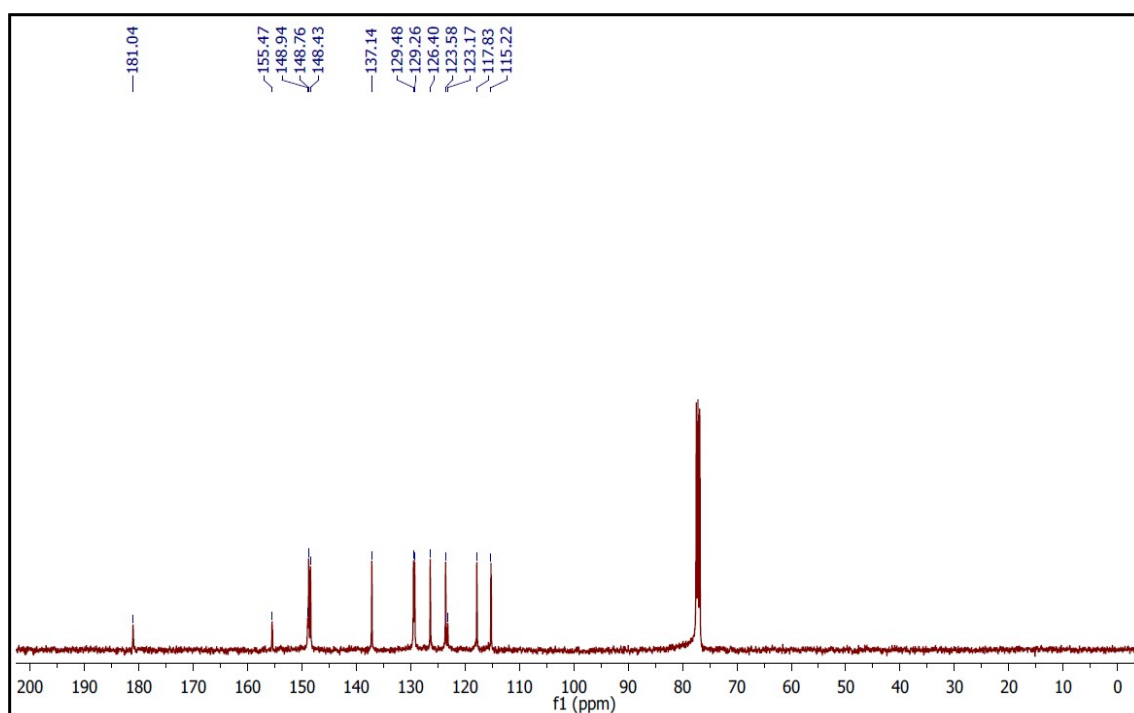
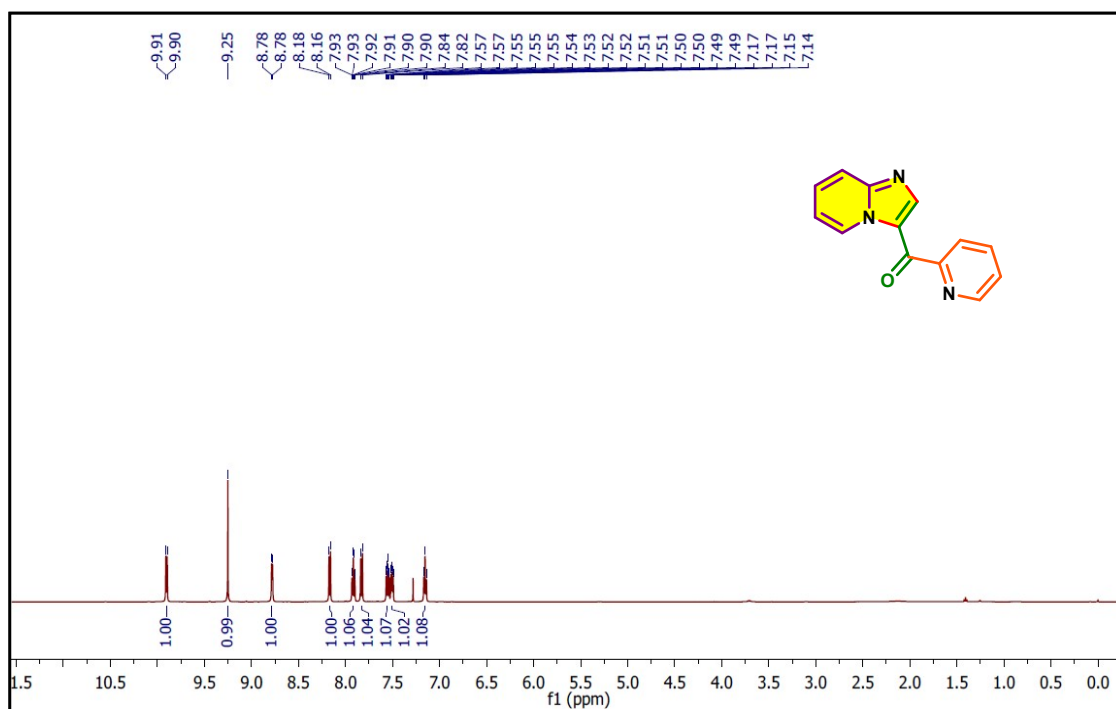
Isolated as a yellow solid, yield 79% (152 mg), m.p 206-209 °C, IR (ATR): 3329 (N-H stretching), 3124, 2917, 2862, 1735 (C=O stretching), 1592, 1510, 1425, 1025, 815, 755 cm^{-1} , ^1H NMR (400 MHz, CDCl_3): δ 9.95 (s, 1H, -NH-), 9.62 (dt, $J = 7.0$ Hz, 1H, Ar), 8.53 (s, 1H, Ar), 7.79 (dt, $J = 9.0$ Hz, 1H, Ar), 7.52-7.44 (m, 1H, Ar), 7.17 – 7.11 (m, 2H, Ar), 7.07 (td, $J = 6.9$ Hz, 1H, Ar), 6.43-6.36 (m, 1H, Ar) ppm, ^{13}C NMR (125 MHz, CDCl_3): δ 173.01 (C=O), 148.61 (Ar), 142.33 (Ar), 131.25 (Ar), 128.62 (Ar), 124.44 (Ar), 123.01 (Ar), 117.79 (Ar), 116.09 (Ar), 114.64 (Ar), 111.20 (Ar) ppm, ESI-MS: m/z 212 $[\text{M}+\text{H}]^+$, HRMS (ESI) Anal. calcd. for $C_{12}H_{10}N_3O$ m/z 212.0823 $[\text{M}+\text{H}]^+$, found 212.0829.

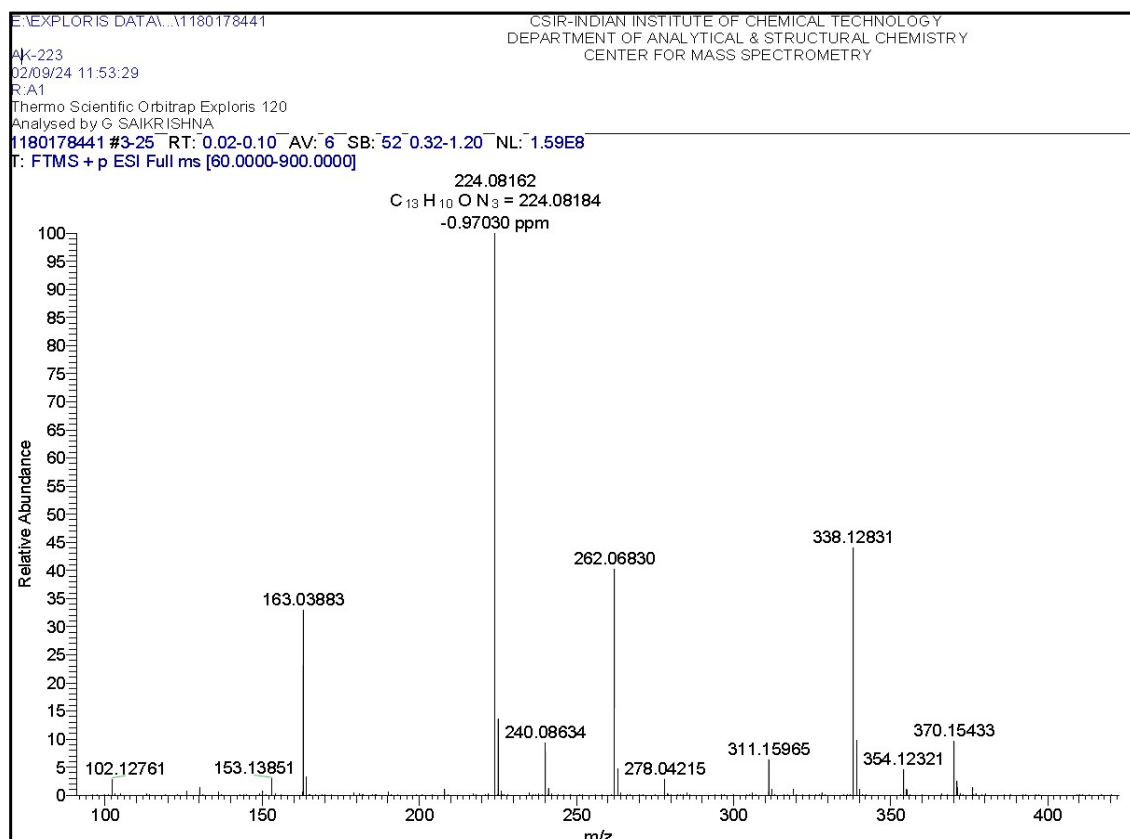




Imidazo[1,2-*a*]pyridin-3-yl(pyridin-2-yl)methanone (3n)⁵

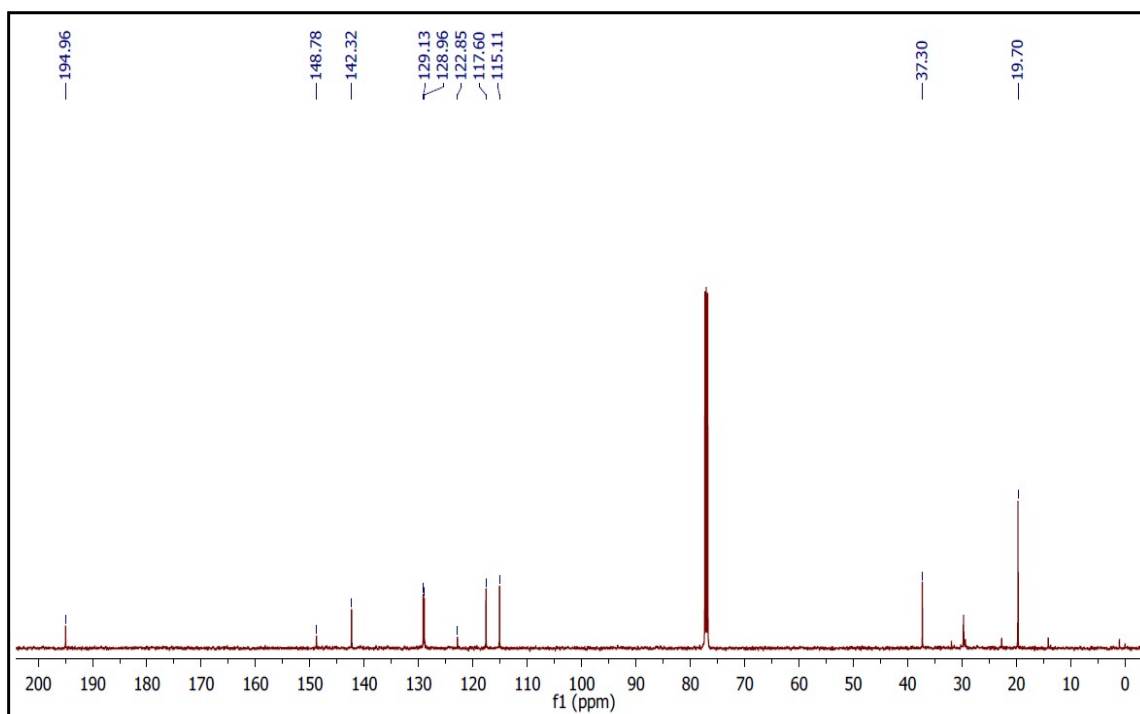
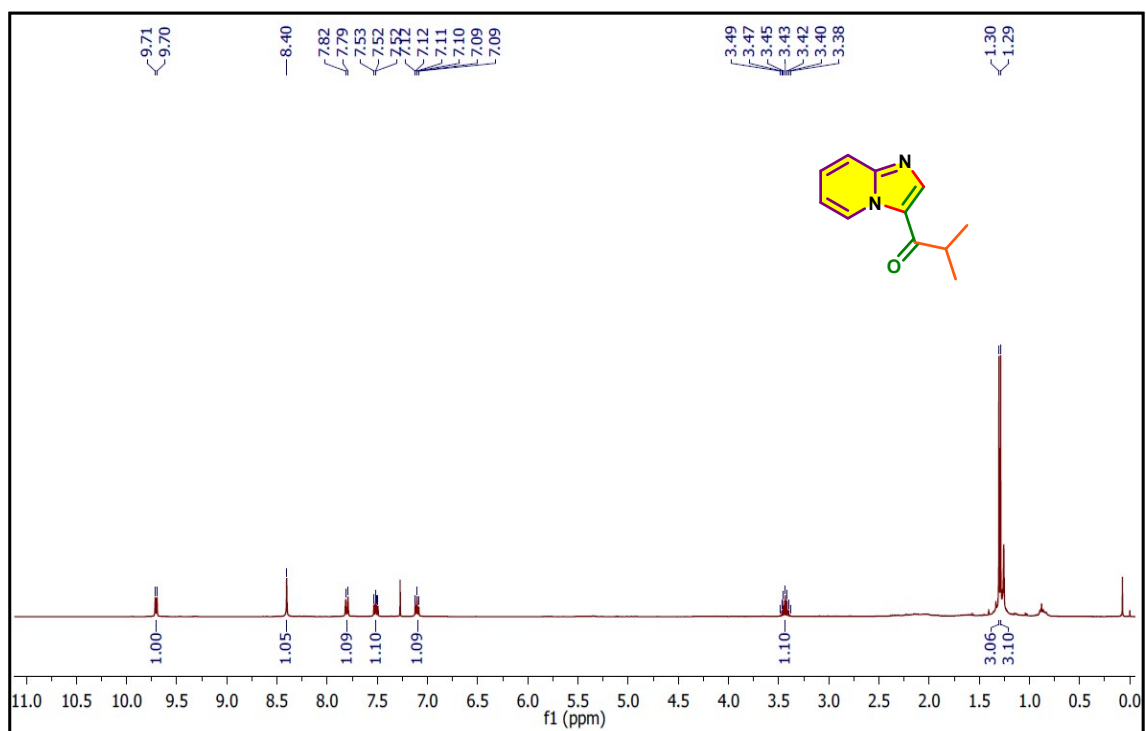
Isolated as a white solid, yield 69% (131 mg), m.p 115-118 °C, IR (ATR): 3020, 2917, 2812, 1716 (C=O stretching), 1626, 1491, 1221, 892, 757 cm⁻¹, ¹H NMR (500 MHz, CDCl₃): δ 9.90 (d, *J* = 6.9 Hz, 1H, Ar), 9.25 (s, 1H, Ar), 8.78 (d, *J* = 4.2 Hz, 1H, Ar), 8.17 (d, *J* = 7.9 Hz, 1H, Ar), 7.92 (td, *J* = 7.7 Hz, 1H, Ar), 7.83 (d, *J* = 8.9 Hz, 1H, Ar), 7.58 – 7.53 (m, 1H, Ar), 7.52-7.48 (m, 1H, Ar), 7.16 (dd, *J* = 10.0, 3.8 Hz, 1H, Ar) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 181.04 (C=O), 155.47 (Ar), 148.94 (Ar), 148.76 (Ar), 148.43 (Ar), 137.14 (Ar), 129.48 (Ar), 129.26 (Ar), 126.40 (Ar), 123.58 (Ar), 123.17 (Ar), 117.83 (Ar), 115.22 (Ar) ppm, ESI-MS: m/z 224 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₃H₁₀N₃O m/z 224.0818 [M+H]⁺, found 224.0816.

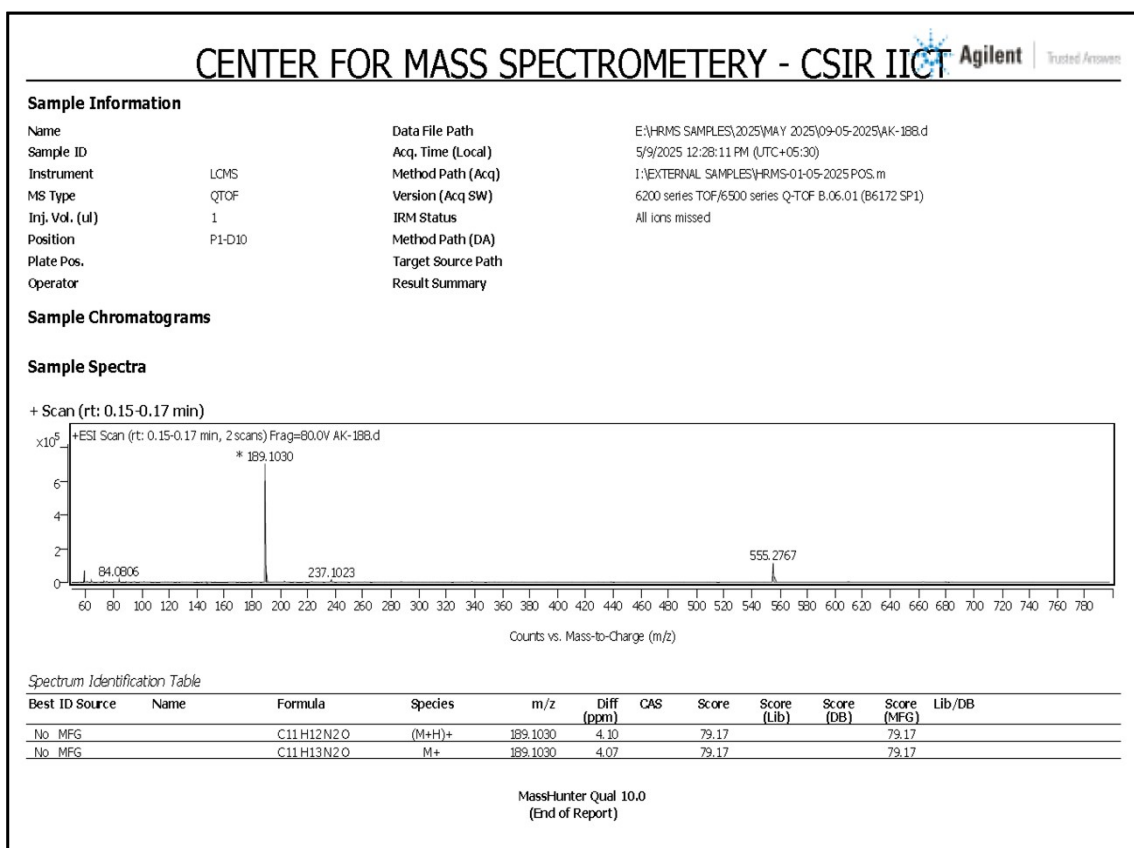




1-(imidazo[1,2-a]pyridin-3-yl)-2-methylpropan-1-one (3o)

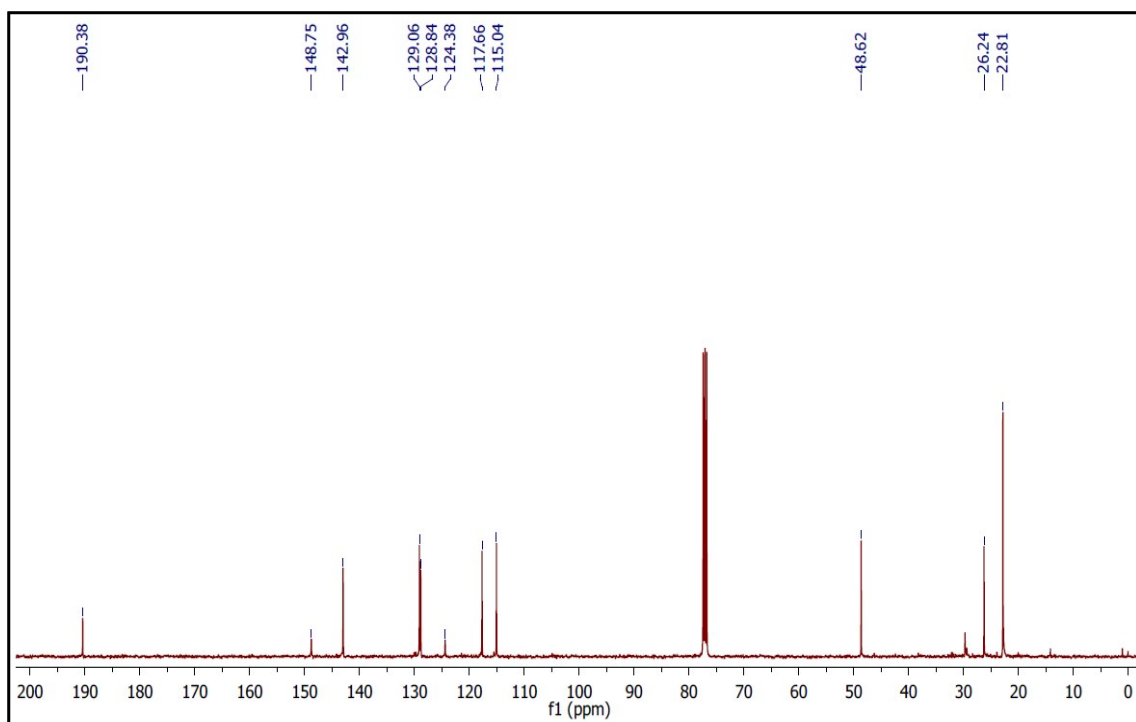
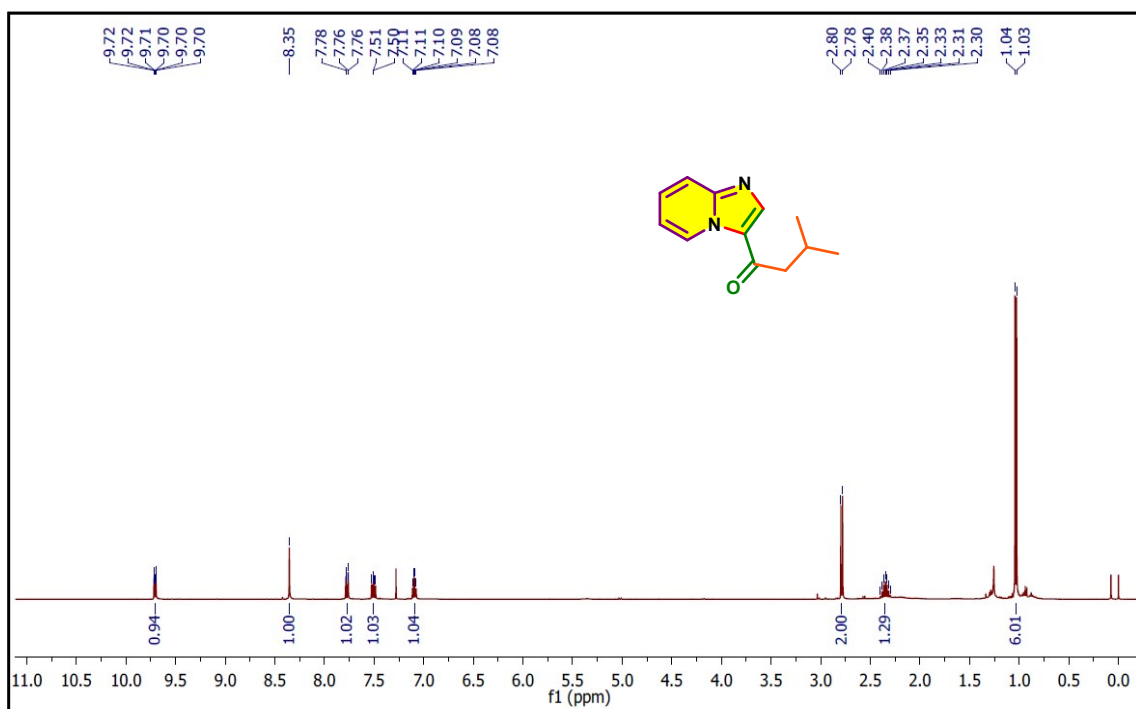
Isolated as a yellow liquid, yield 65% (130 mg), IR (ATR): 3109, 2919, 2855, 1722 (C=O stretching), 1640, 1472, 1190, 940, 855, 760 cm^{-1} , ^1H NMR (400 MHz, CDCl_3): δ 9.71 (d, J = 6.9 Hz, 1H, Ar), 8.40 (s, 1H, Ar), 7.80 (d, J = 9.0 Hz, 1H, Ar), 7.55 – 7.48 (m, 1H, Ar), 7.10 (td, J = 6.9, 0.8 Hz, 1H, Ar), 3.43 (hept, J = 6.8 Hz, 1H, $(\text{CH}_3)_2\text{CH-}$), 1.30 (s, 3H, $-\text{CH}_3$), 1.29 (s, 3H, $-\text{CH}_3$) ppm, ^{13}C NMR (125 MHz, CDCl_3): δ 194.96 (C=O), 148.78 (Ar), 142.32 (Ar), 129.13 (Ar), 128.96 (Ar), 122.85 (Ar), 117.60 (Ar), 115.11 (Ar), 37.30 ($(\text{CH}_3)_2\text{CH-}$), 19.70 ($(\text{CH}_3)_2\text{CH-}$) ppm, ESI-MS: m/z 189 $[\text{M}+\text{H}]^+$, HRMS (ESI) Anal. calcd. for $\text{C}_{11}\text{H}_{13}\text{N}_2\text{O}$ m/z 189.1027 $[\text{M}+\text{H}]^+$, found 189.1030.

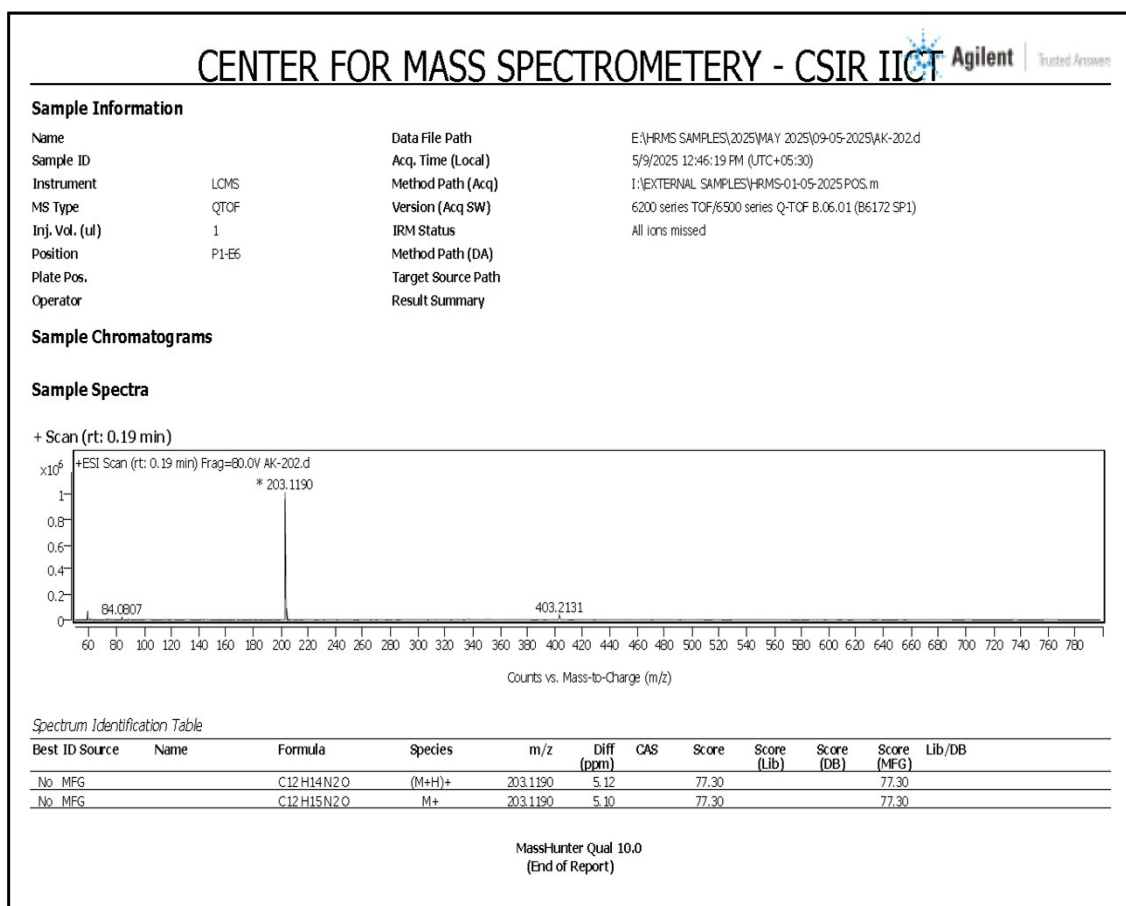




1-(imidazo[1,2-a]pyridin-3-yl)-3-methylbutan-1-one (3p)

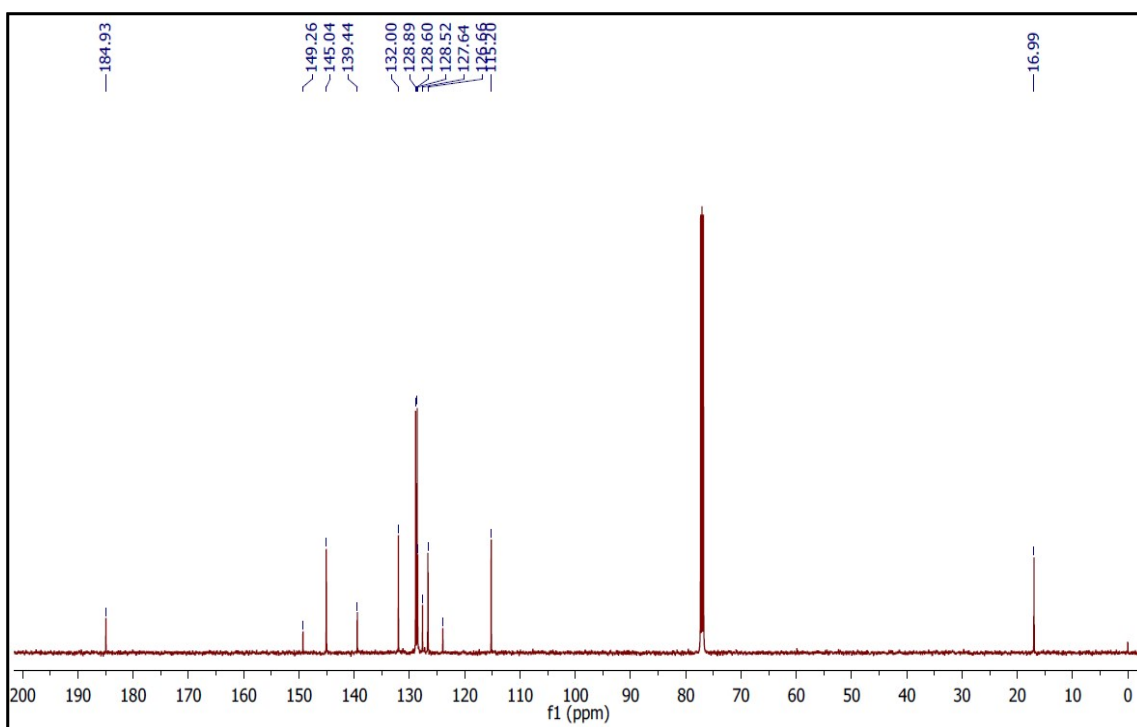
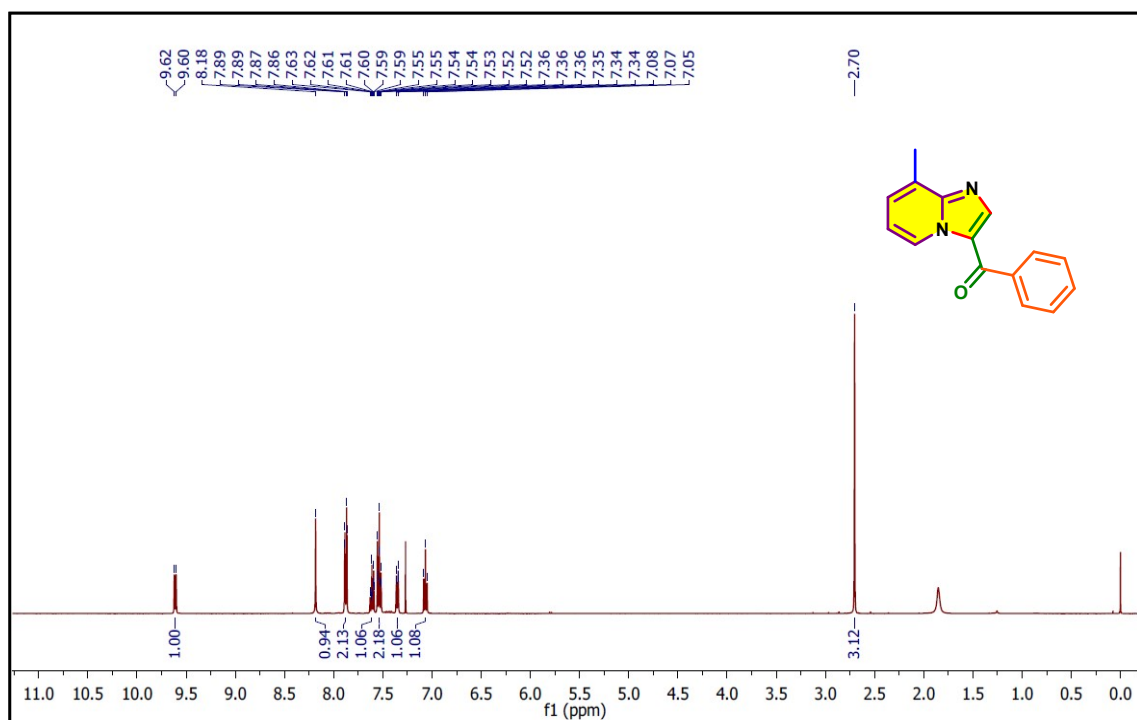
Isolated as a brown liquid, yield 63% (123 mg), IR (ATR): 3110, 2951, 2862, 1716 (C=O stretching), 1636, 1511, 1475, 1180, 976, 757 cm^{-1} , ^1H NMR (400 MHz, CDCl_3): δ 9.71 (dt, J = 6.9 Hz, 1H, Ar), 8.35 (s, 1H, Ar), 7.77 (dt, J = 9.0 Hz, 1H, Ar), 7.53 – 7.48 (m, 1H, Ar), 7.09 (td, J = 6.9 Hz, 1H, Ar), 2.79 (d, J = 7.09 Hz, 2H, $(\text{CH}_3)_2\text{CHCH}_2-$), 2.39-2.31 (m, 1H, $(\text{CH}_3)_2\text{CH}-$), 1.03 (d, J = 6.6 Hz, 6H, $(\text{CH}_3)_2\text{CH}-$) ppm, ^{13}C NMR (100 MHz, CDCl_3): δ 190.38 (C=O), 148.75 (Ar), 142.96 (Ar), 129.06 (Ar), 128.84 (Ar), 124.38 (Ar), 117.66 (Ar), 115.04 (Ar), 48.62 ($(\text{CH}_3)_2\text{CHCH}_2-$), 26.24 ($(\text{CH}_3)_2\text{CH}-$), 22.81 ($(\text{CH}_3)_2\text{CH}-$) ppm, ESI-MS: m/z 203 $[\text{M}+\text{H}]^+$, HRMS (ESI) Anal. calcd. for $\text{C}_{12}\text{H}_{15}\text{N}_2\text{O}$ m/z 203.1184 $[\text{M}+\text{H}]^+$, found 203.1190.

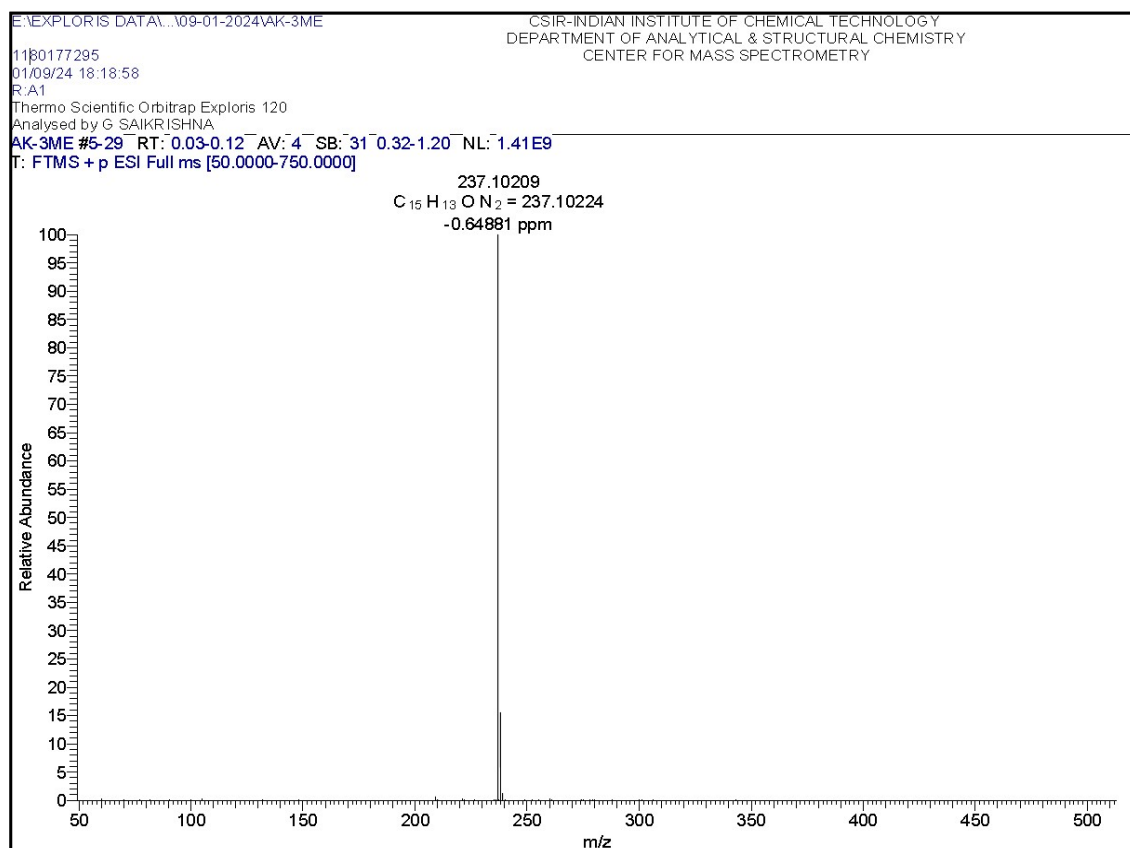




(8-methylimidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (3q)¹

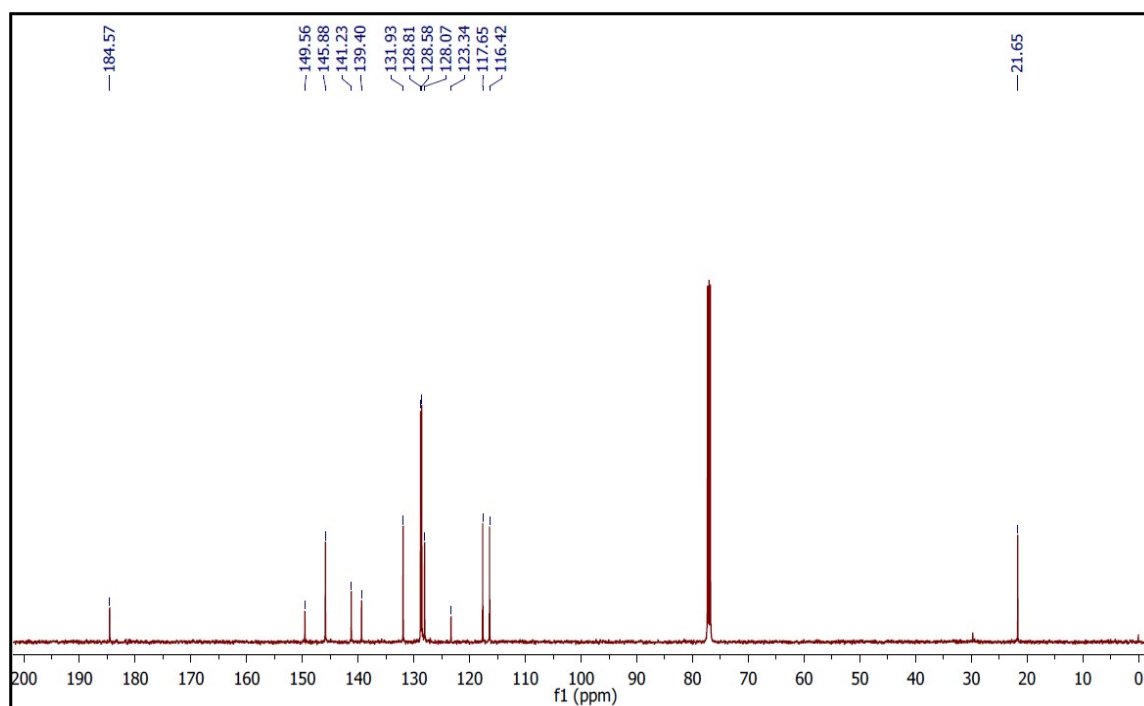
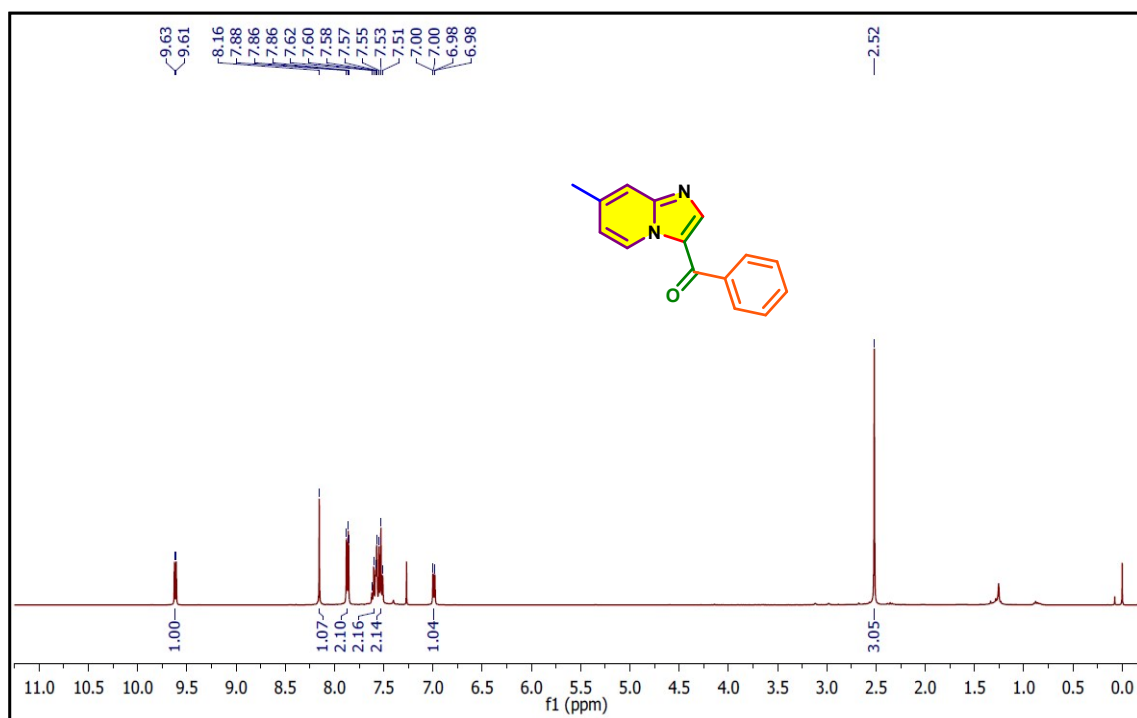
Isolated as a yellow solid, yield 76% (154 mg), m.p 96-98 °C, IR (ATR): 3115, 2918, 2852, 1721 (C=O stretching), 1619, 1505, 1470, 1247, 895, 767 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.61 (d, *J* = 6.7 Hz, 1H, Ar), 8.18 (s, 1H, Ar), 7.90 – 7.86 (m, 2H, Ar), 7.64 – 7.59 (m, 1H, Ar), 7.56-7.51 (m, 2H, Ar), 7.37 – 7.33 (m, 1H, Ar), 7.07 (t, *J* = 7.0 Hz, 1H, Ar), 2.70 (s, 3H, -CH₃) ppm, ¹³C NMR (125 MHz, CDCl₃): δ 184.93 (C=O), 149.26 (Ar), 145.04 (Ar), 139.44 (Ar), 132.00 (Ar), 128.89 (Ar), 128.60 (Ar), 128.52 (Ar), 127.64 (Ar), 126.66 (Ar), 123.96 (Ar), 115.20 (Ar), 16.99 (-CH₃) ppm, ESI-MS: m/z 237 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₅H₁₃N₂O m/z 237.1022 [M+H]⁺, found 237.1020.

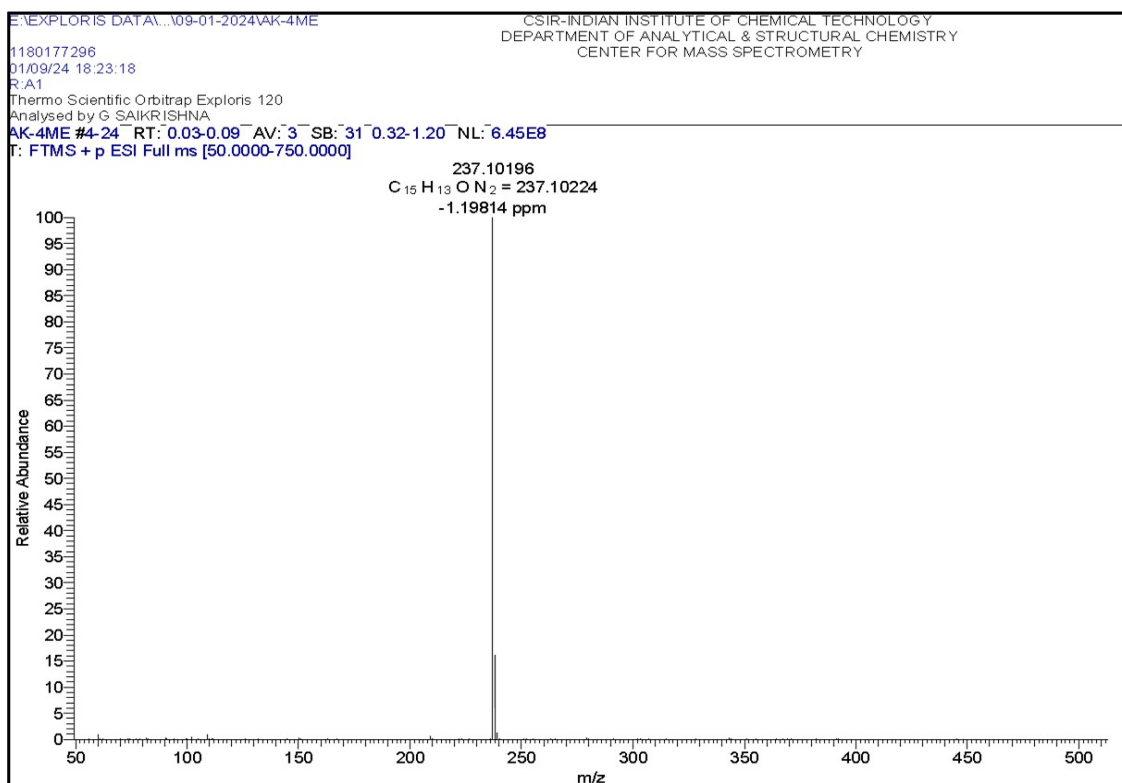




(7-methylimidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (3r)¹

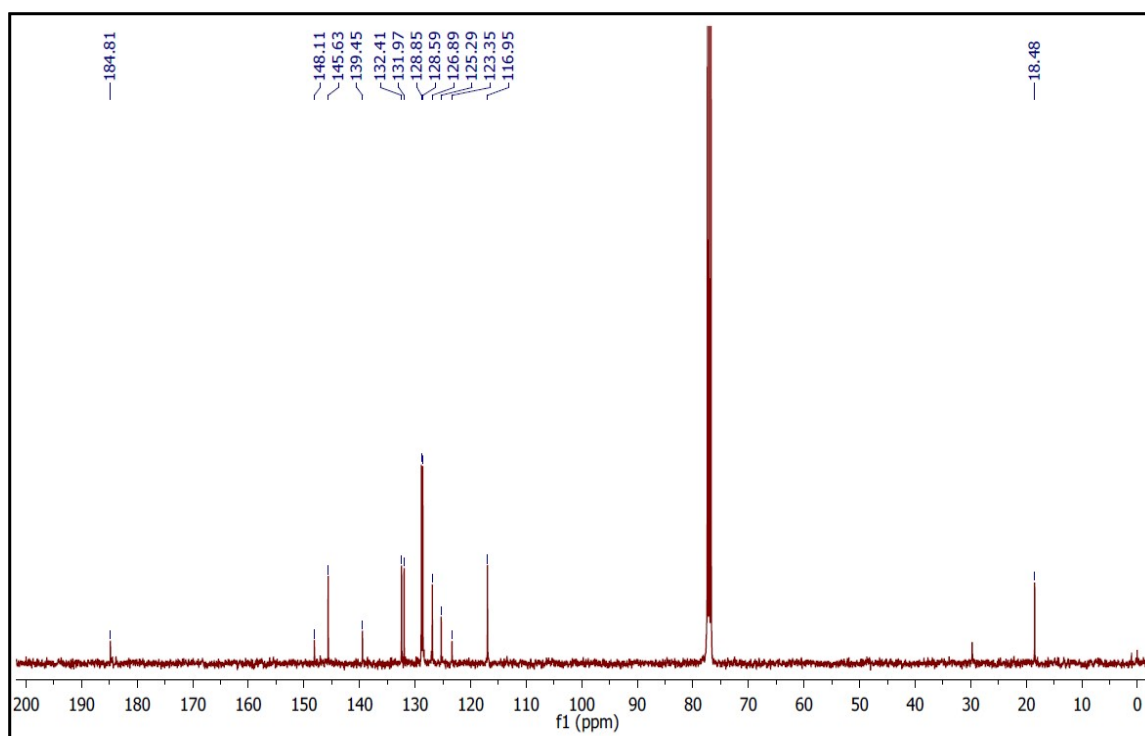
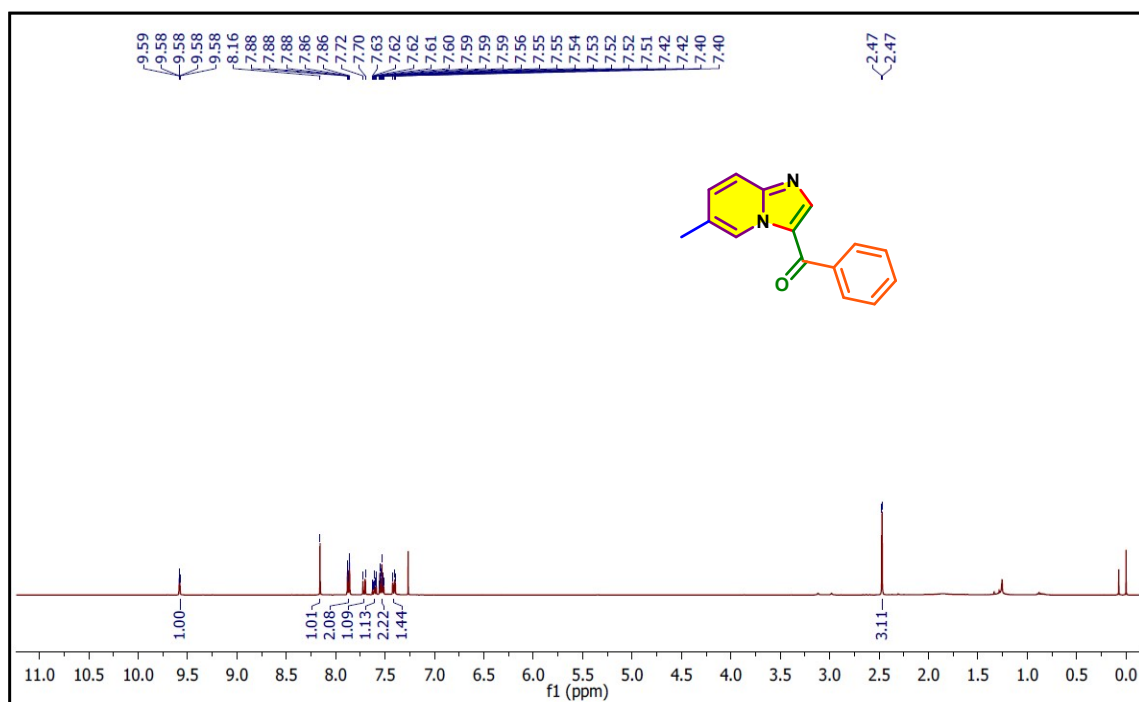
Isolated as a yellow solid, yield 80% (162 mg), m.p 127-130 °C, IR (ATR): 3117, 2914, 2863, 1736 (C=O stretching), 1622, 1521, 1436, 1254, 894, 762 cm^{-1} , ^1H NMR (400 MHz, CDCl_3): δ 9.62 (d, $J = 7.0$ Hz, 1H, Ar), 8.16 (s, 1H, Ar), 7.90 – 7.84 (m, 2H, Ar), 7.60 (m, 2H, Ar), 7.53 (t, $J = 7.4$ Hz, 2H, Ar), 6.99 (dd, $J = 7.0$ Hz, 1H, Ar), 2.52 (s, 3H, $-\text{CH}_3$) ppm, ^{13}C NMR (125 MHz, CDCl_3): δ 184.57 (C=O), 149.56 (Ar), 145.88 (Ar), 141.23 (Ar), 139.40 (Ar), 131.93 (Ar), 128.81 (Ar), 128.58 (Ar), 128.07 (Ar), 123.34 (Ar), 117.65 (Ar), 116.42 (Ar), 21.65 ($-\text{CH}_3$) ppm, ESI-MS: m/z 237 $[\text{M}+\text{H}]^+$, HRMS (ESI) Anal. calcd. for $C_{15}H_{13}N_2O$ m/z 237.1022 $[\text{M}+\text{H}]^+$, found 237.1019.

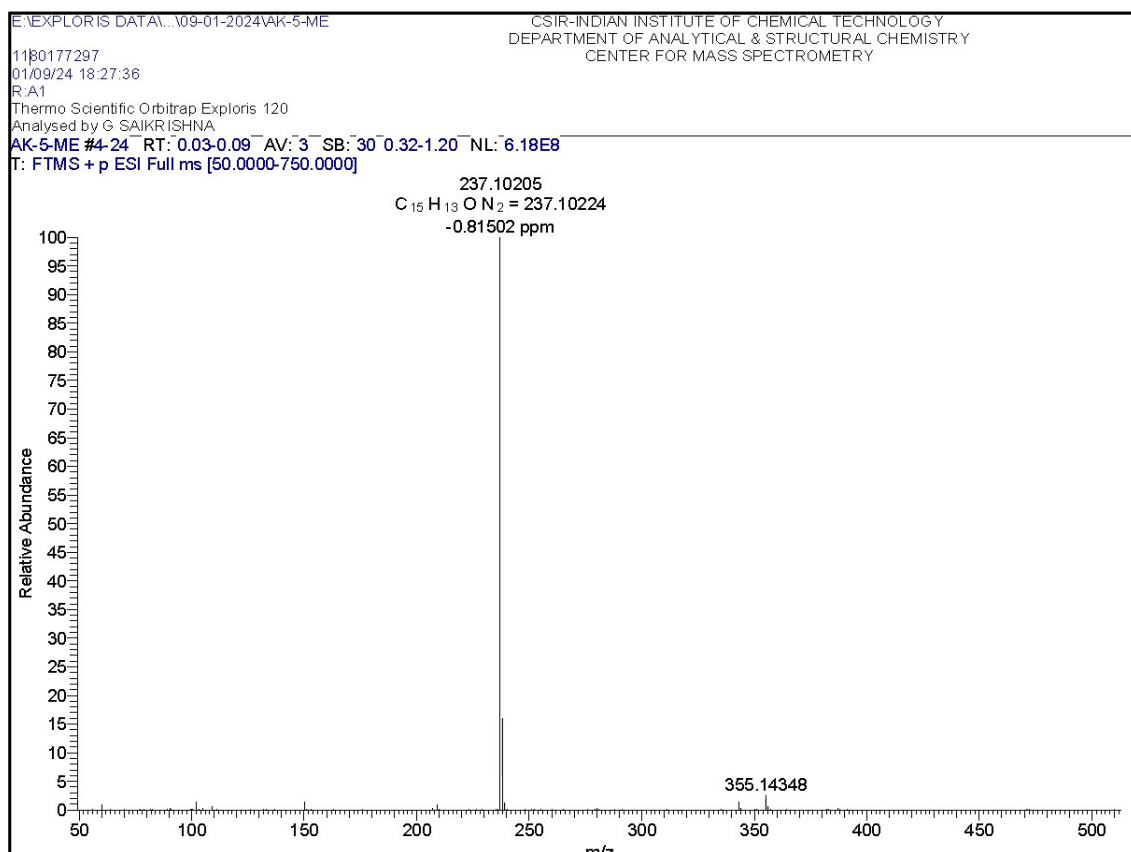




(6-methylimidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (**3s**)¹

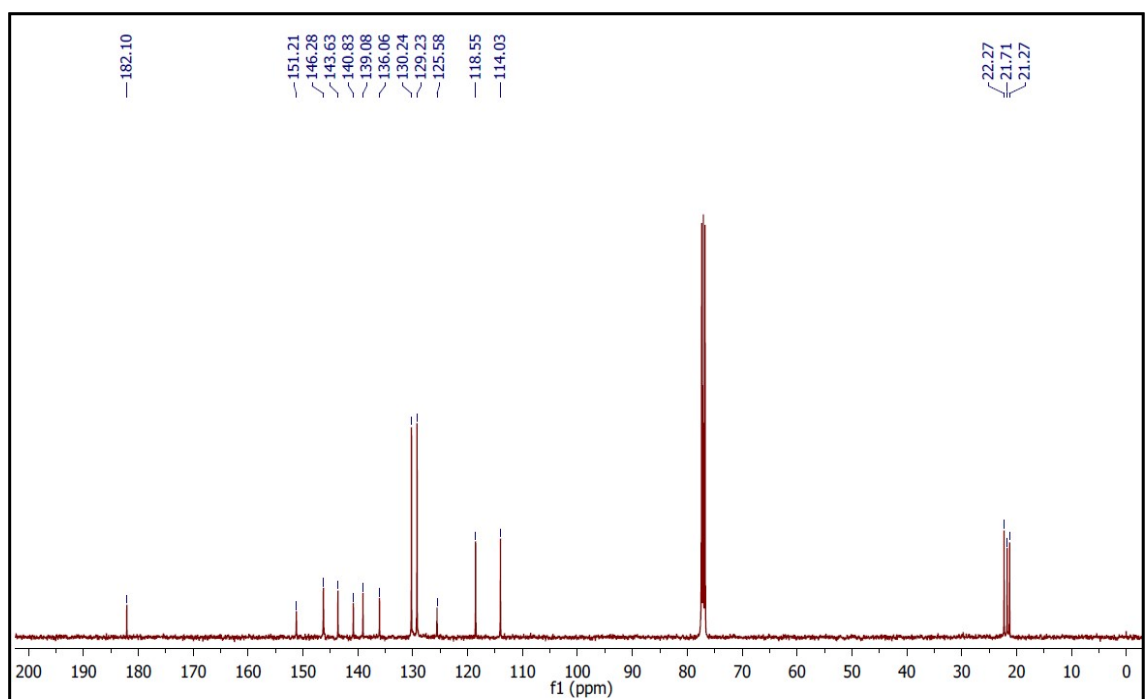
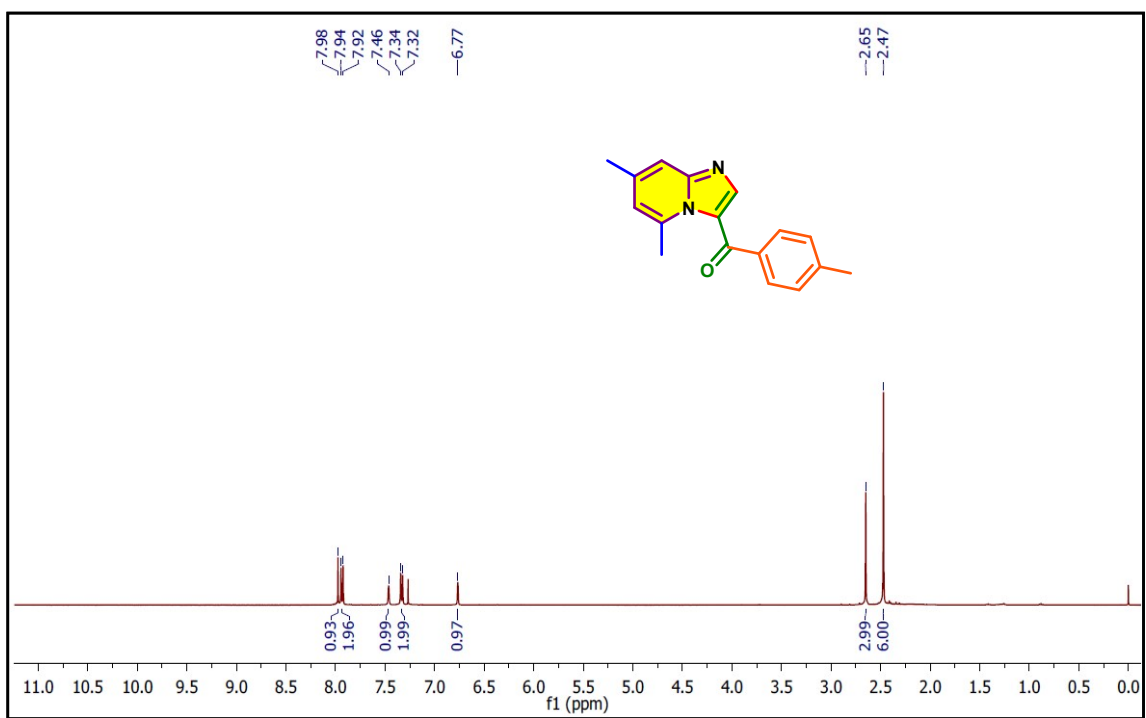
Isolated as a pale brown solid, yield 78% (158 mg), m.p 78-82 °C, IR (ATR): 3112, 2921, 2844, 1711 (C=O stretching), 1602, 1511, 1432, 1244, 912, 772 cm^{-1} , ^1H NMR (400 MHz, CDCl_3): δ 9.60-9.56 (m, 1H, Ar), 8.16 (s, 1H, Ar), 7.89 – 7.85 (m, 2H, Ar), 7.71 (d, $J = 9.1$ Hz, 1H, Ar), 7.64 – 7.58 (m, 1H, Ar), 7.56 – 7.51 (m, 2H, Ar), 7.44 – 7.39 (m, 1H, Ar), 2.47 (s, 3H, $-\text{CH}_3$) ppm, ^{13}C NMR (100 MHz, CDCl_3): δ 184.81 (C=O), 148.11 (Ar), 145.63 (Ar), 139.45 (Ar), 132.41 (Ar), 131.97 (Ar), 128.85 (Ar), 128.59 (Ar), 126.89 (Ar), 125.29 (Ar), 123.35 (Ar), 116.95 (Ar), 18.48 ($-\text{CH}_3$) ppm, ESI-MS: m/z 237 $[\text{M}+\text{H}]^+$, HRMS (ESI) Anal. calcd. for $C_{15}H_{13}N_2O$ m/z 237.1022 $[\text{M}+\text{H}]^+$, found 237.1020.

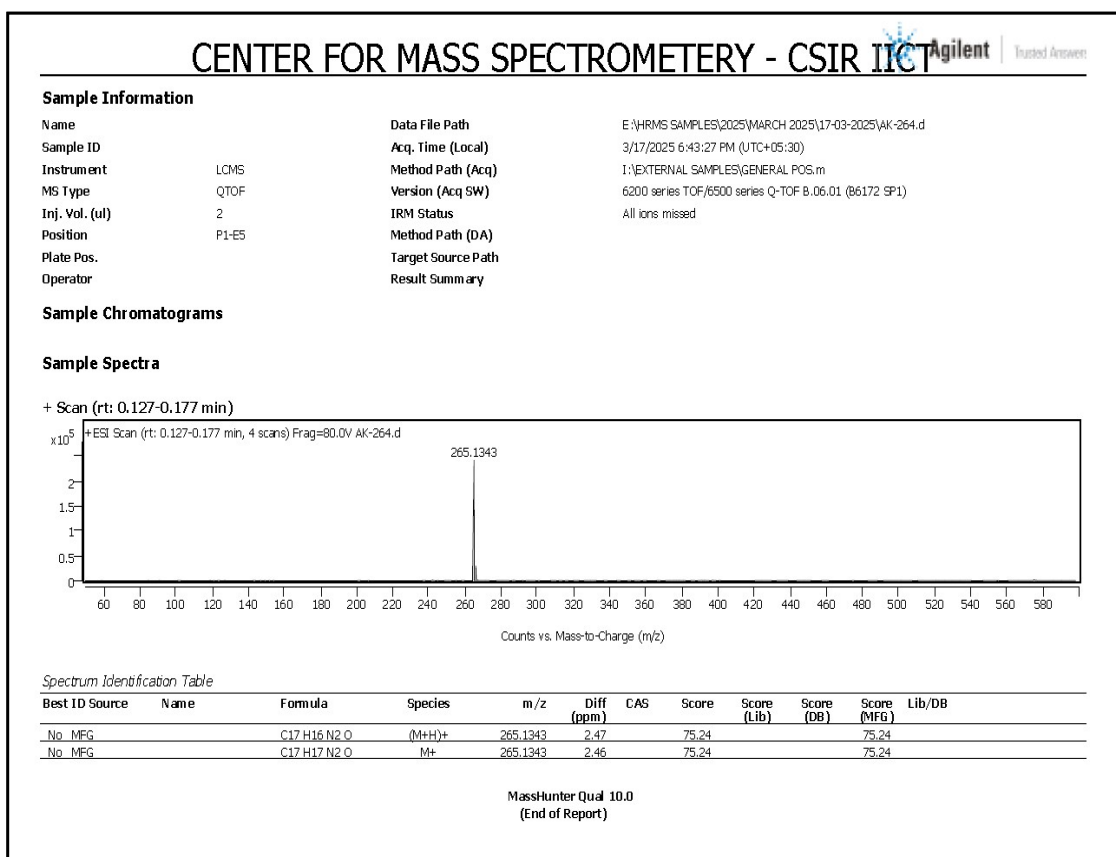




(5,7-dimethylimidazo[1,2-*a*]pyridin-3-yl)(*p*-tolyl)methanone (3t)

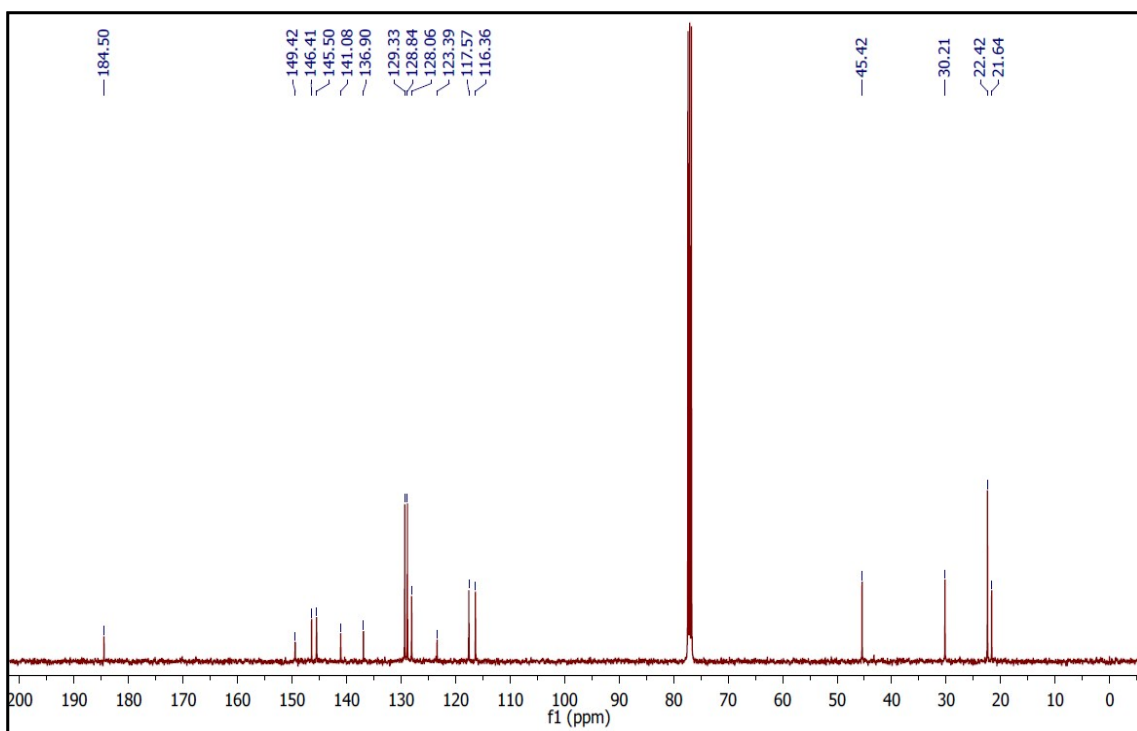
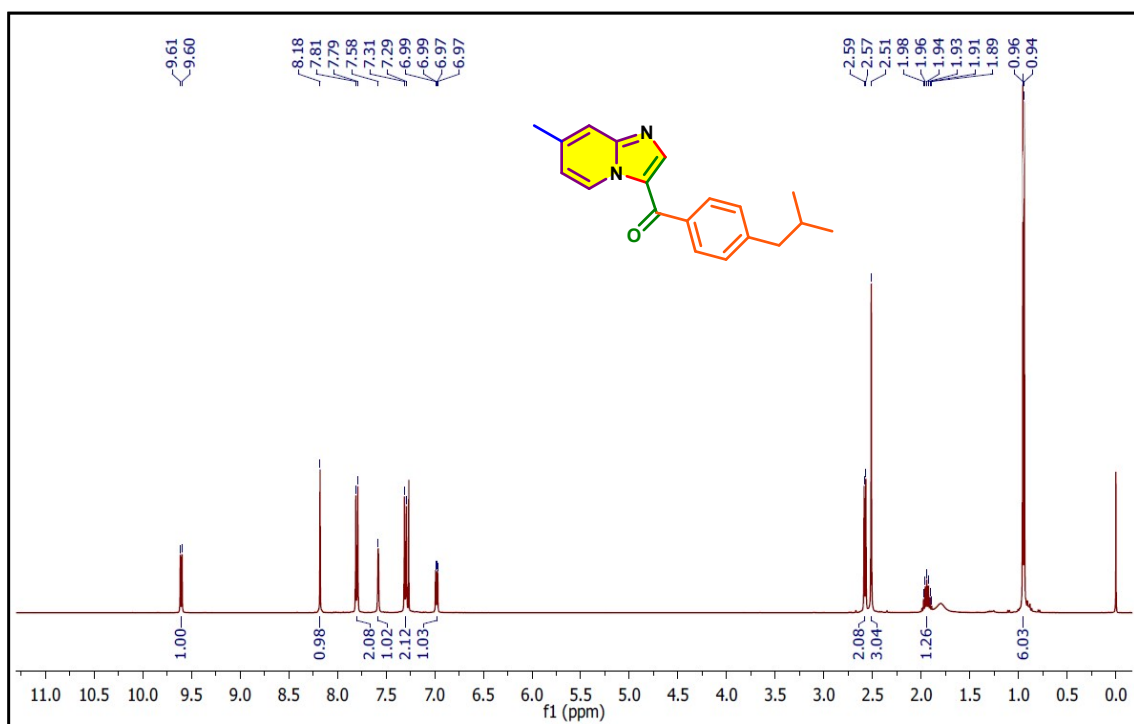
Isolated as a yellow solid, yield 82% (172 mg), m.p 125-127 °C, IR (ATR): 3123, 2911, 2831, 1701 (C=O stretching), 1619, 1521, 1432, 1253, 877, 766 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 7.98 (s, 1H, Ar), 7.93 (d, *J* = 8.2 Hz, 2H, Ar), 7.46 (s, 1H, Ar), 7.33 (d, *J* = 7.9 Hz, 2H, Ar), 6.77 (s, 1H, Ar), 2.65 (s, 3H, -CH₃Ar), 2.47 (s, 6H, -CH₃) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 182.10 (C=O), 151.21 (Ar), 146.28 (Ar), 143.63 (Ar), 140.83 (Ar), 139.08 (Ar), 136.06 (Ar), 130.24 (Ar), 129.23 (Ar), 125.58 (Ar), 118.55 (Ar), 114.03 (Ar), 22.27 (-CH₃), 21.71 (-CH₃), 21.27 (-CH₃) ppm, ESI-MS: *m/z* 265 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₇H₁₇N₂O *m/z* 265.1340 [M+H]⁺, found 265.1343.

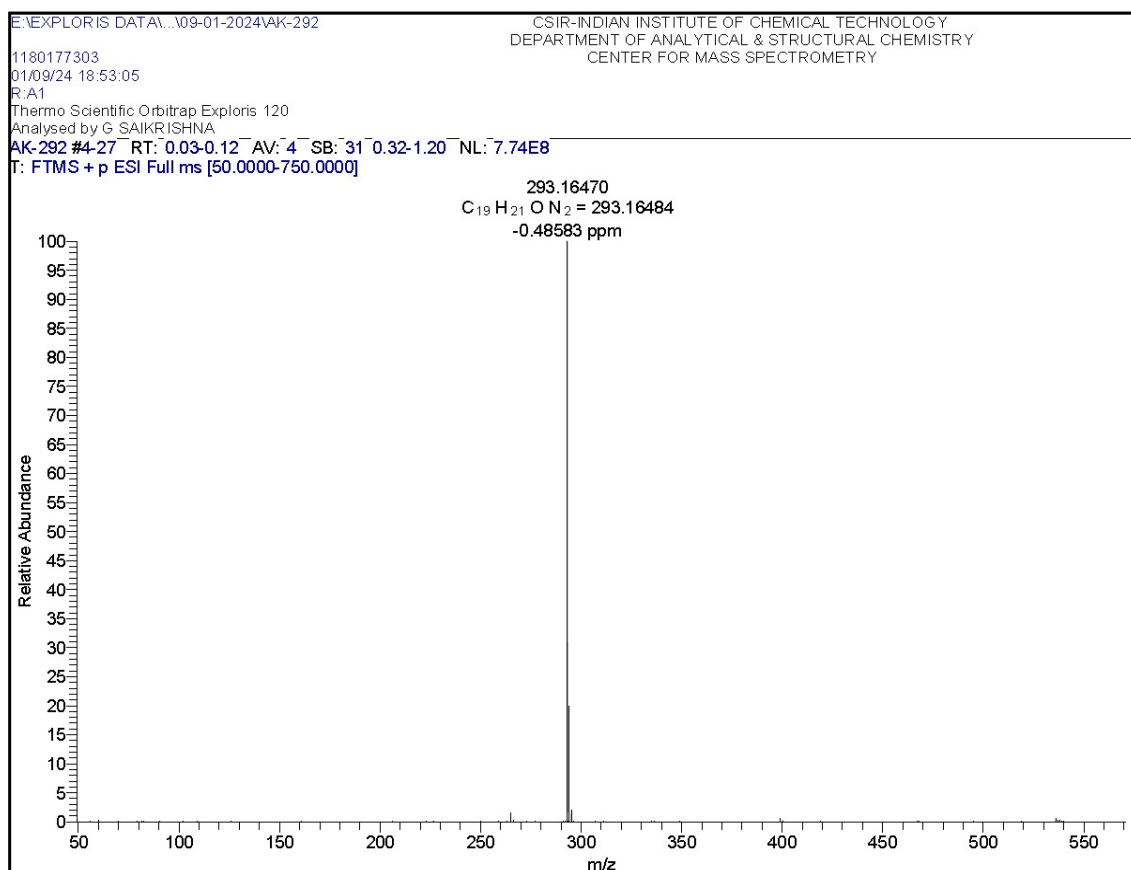




(4-isobutylphenyl)(7-methylimidazo[1,2-a]pyridin-3-yl)methanone (**3u**)

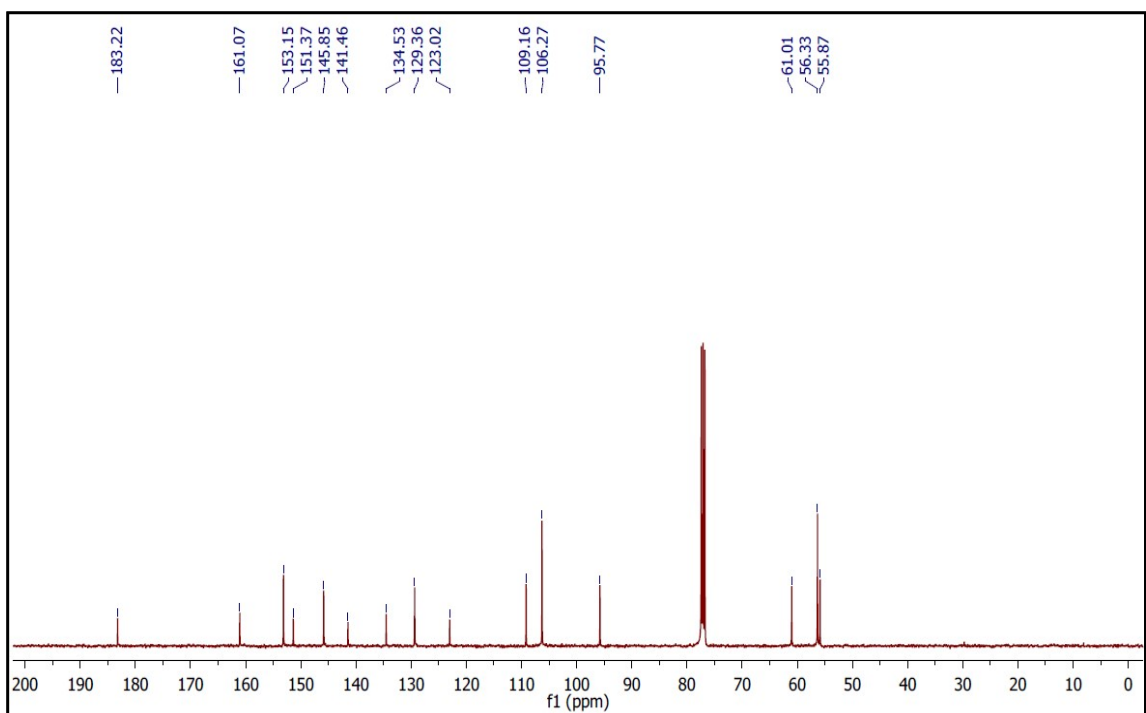
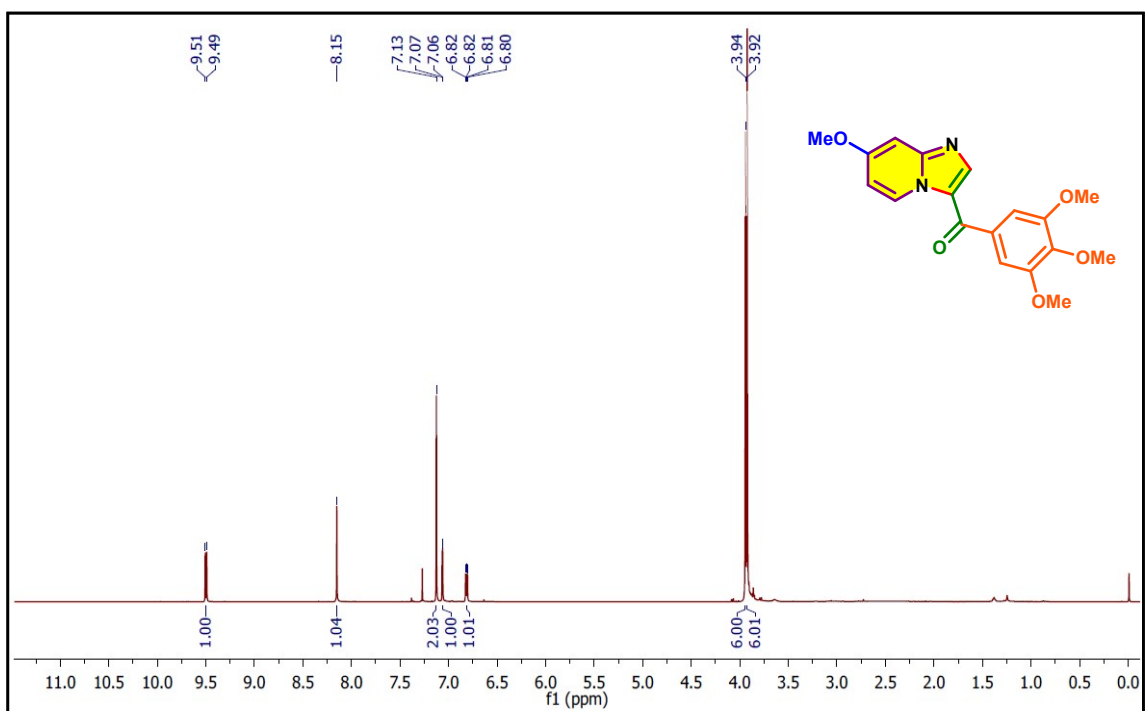
Isolated as a yellow solid, yield 87% (165 mg), m.p 118-122 °C, IR (ATR): 3127, 2943, 2837, 1720 (C=O stretching), 1629, 1513, 1473, 1218, 882, 764 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.60 (d, *J* = 7.0 Hz, 1H, Ar), 8.18 (s, 1H, Ar), 7.80 (d, *J* = 8.2 Hz, 2H, Ar), 7.58 (s, 1H, Ar), 7.30 (d, *J* = 8.1 Hz, 2H, Ar), 6.98 (dd, *J* = 7.1 Hz, 1H, Ar), 2.58 (d, *J* = 7.2 Hz, 2H, (CH₃)₂CHCH₂-), 2.51 (s, 3H, -CH₃), 2.00 – 1.89 (m, 1H, (CH₃)₂CH-), 0.95 (d, *J* = 6.6 Hz, 6H, (CH₃)₂CH-) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 184.50 (C=O), 149.42 (Ar), 146.41 (Ar), 145.50 (Ar), 141.08 (Ar), 136.90 (Ar), 129.33 (Ar), 128.84 (Ar), 128.06 (Ar), 123.39 (Ar), 117.57 (Ar), 116.36 (Ar), 45.42 ((CH₃)₂CHCH₂-), 30.21 ((CH₃)₂CH-), 22.42 ((CH₃)₂CH-), 21.64 (-CH₃) ppm, ESI-MS: m/z 293 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₉H₂₁N₂O m/z 293.1648 [M+H]⁺, found 293.1647.

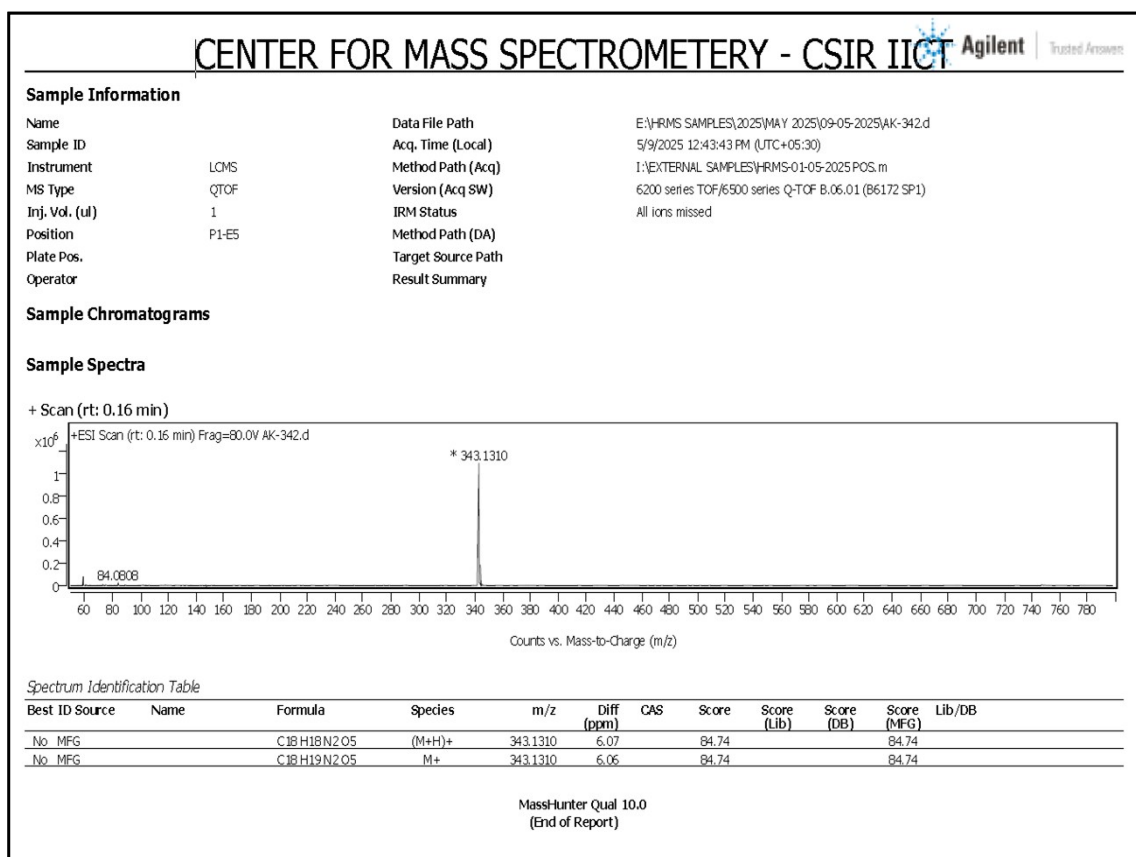




(7-methoxyimidazo[1,2-*a*]pyridin-3-yl)(3,4,5-trimethoxyphenyl)methanone (3v)¹

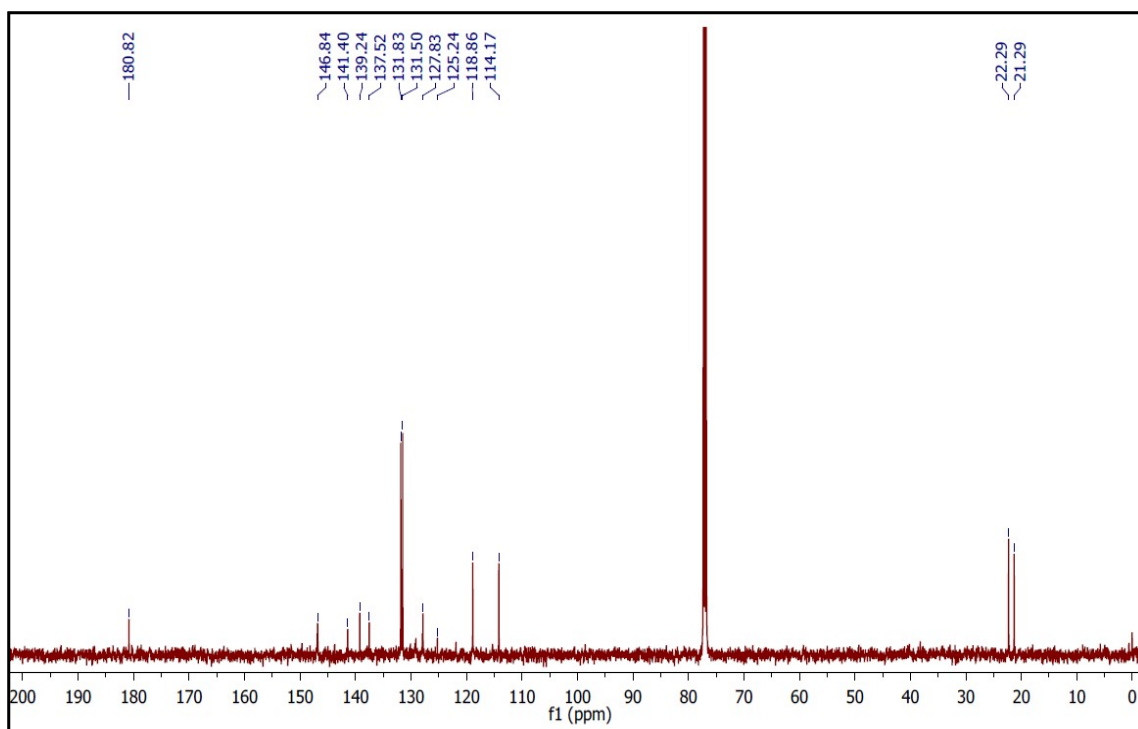
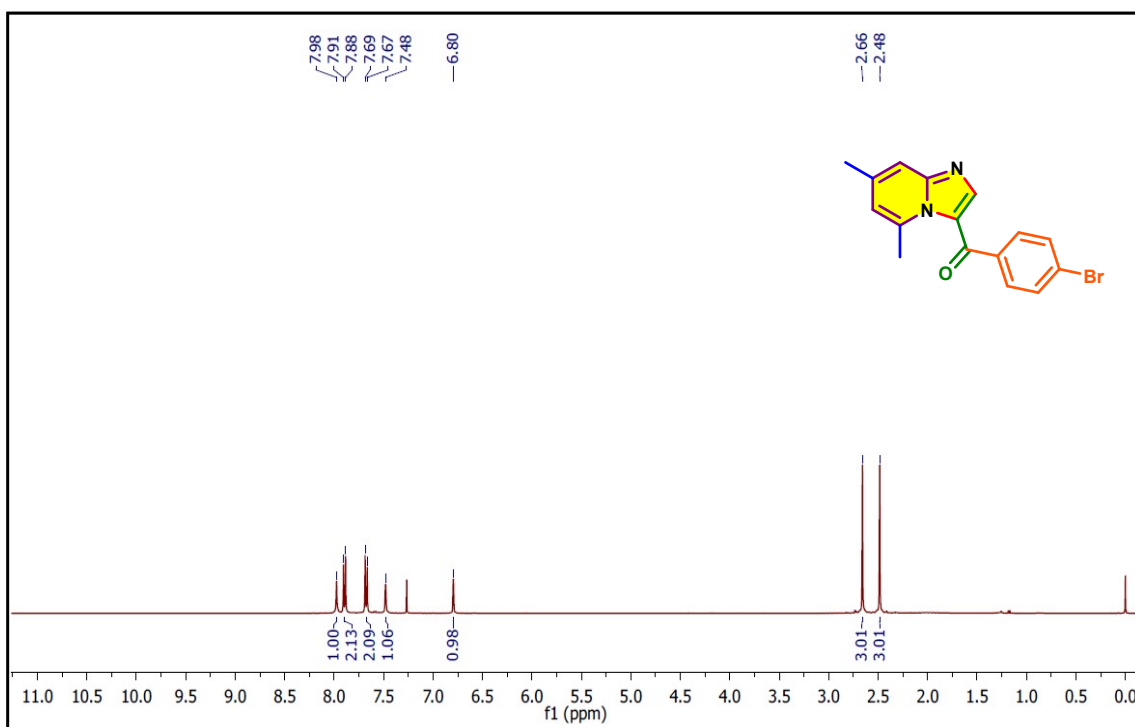
Isolated as a pale brown solid, yield 83% (160 mg), m.p 190-193 °C, IR (ATR): 3117, 2973, 2840, 1727 (C=O stretching), 1614, 1499, 1144, 863, 770 cm⁻¹, ¹H NMR (500 MHz, CDCl₃): δ 9.50 (d, *J* = 7.6 Hz, 1H, Ar), 8.15 (s, 1H, Ar), 7.13 (s, 2H, Ar), 7.06 (d, *J* = 2.4 Hz, 1H, Ar), 6.81 (dd, *J* = 7.6 Hz, 1H, Ar), 3.94 (s, 6H, -OCH₃), 3.92 (s, 6H, -OCH₃) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 183.22 (C=O), 161.07 (Ar), 153.15 (Ar), 151.37 (Ar), 145.85 (Ar), 141.46 (Ar), 134.53 (Ar), 129.36 (Ar), 123.02 (Ar), 109.16 (Ar), 106.27 (Ar), 95.77 (Ar), 61.01 (p-OCH₃), 56.33 (m-OCH₃), 55.87 (-OCH₃) ppm, ESI-MS: m/z 343 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₈H₁₉N₂O₅ m/z 343.1293 [M+H]⁺, found 343.1310.

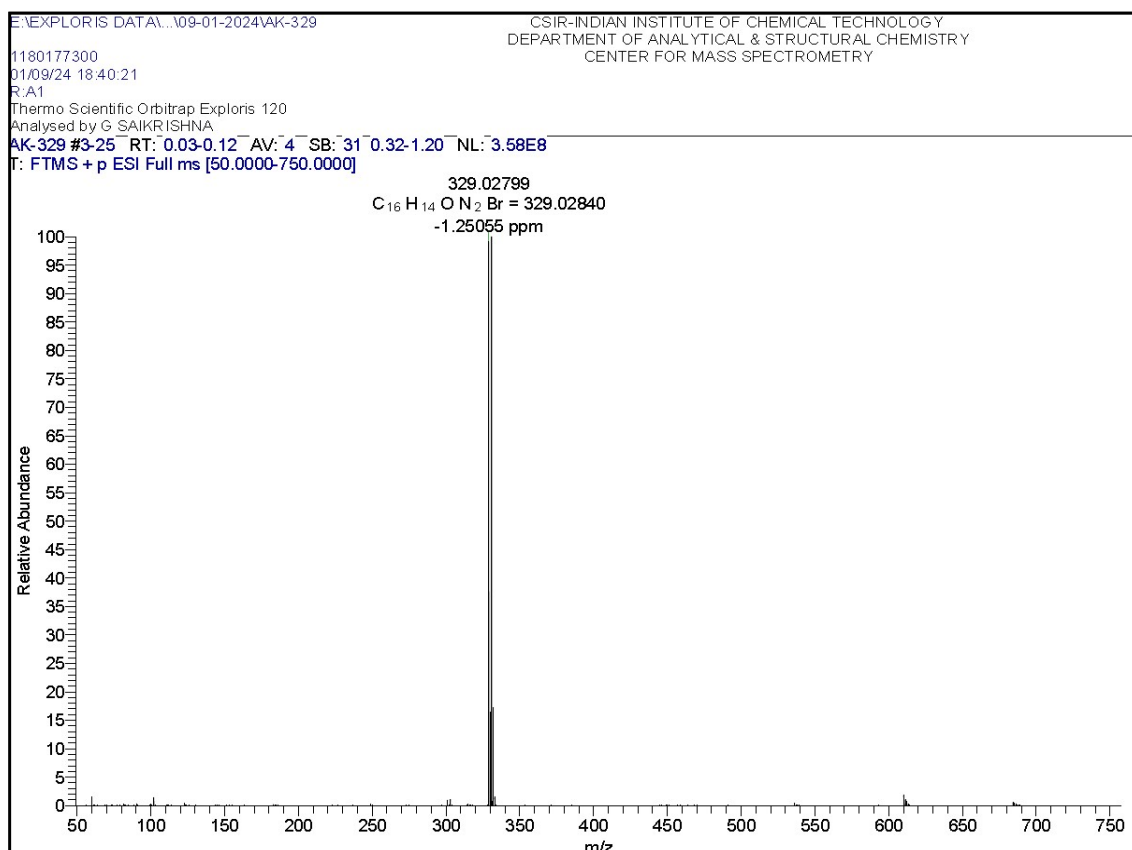




(4-bromophenyl)(5,7-dimethylimidazo[1,2-a]pyridin-3-yl)methanone (3w)

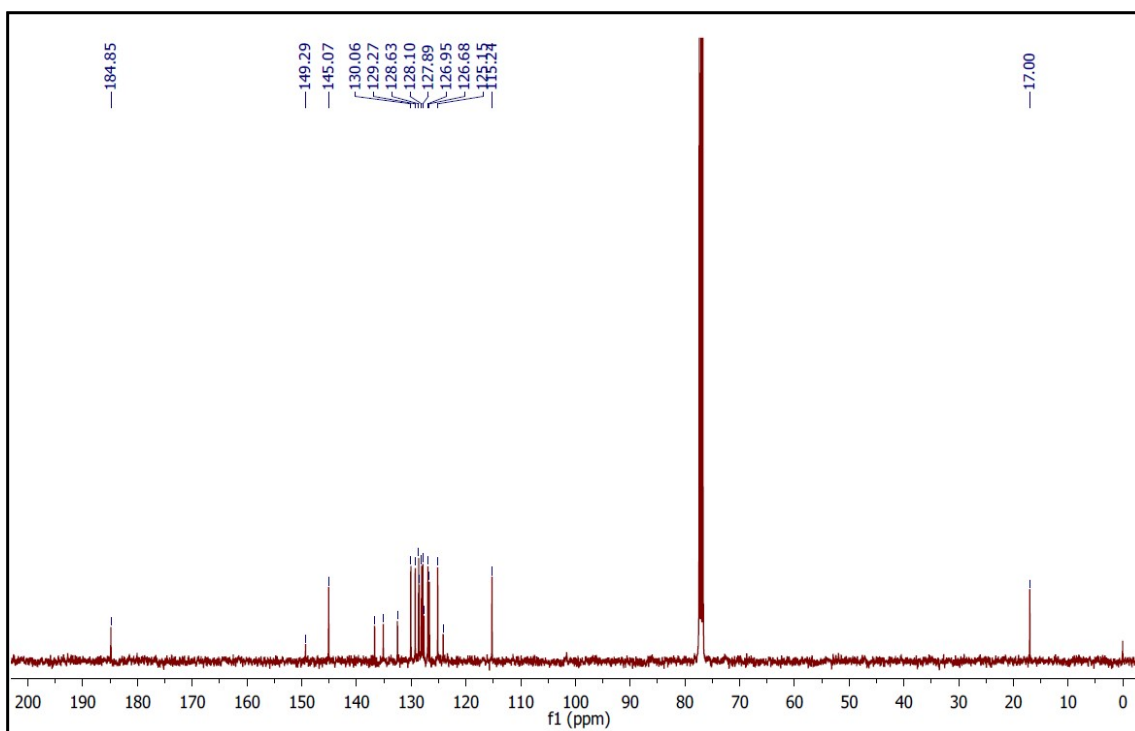
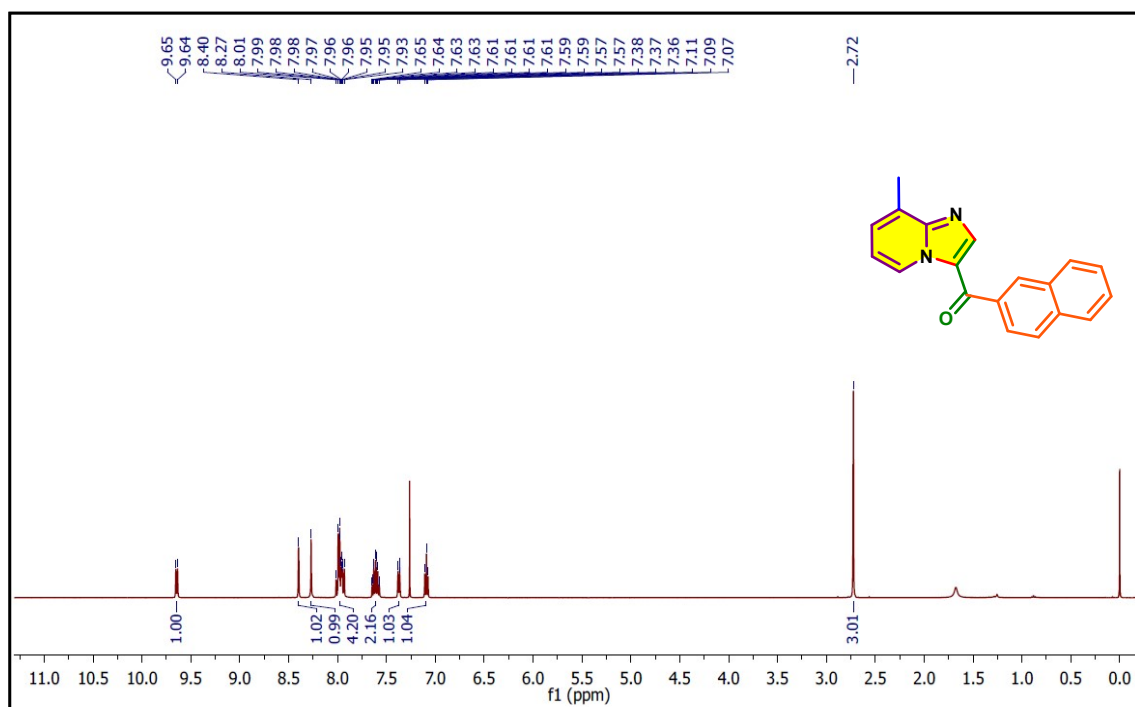
Isolated as a yellow solid, yield 73% (143 mg), m.p 137-140 °C, IR (ATR): 3086, 2938, 2796, 1727 (C=O stretching), 1620, 1511, 1421, 1271, 882, 767 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 7.98 (s, 1H, Ar), 7.89 (d, *J* = 8.5 Hz, 2H, Ar), 7.68 (d, *J* = 8.5 Hz, 2H, Ar), 7.48 (s, 1H, Ar), 6.80 (s, 1H, Ar), 2.66 (s, 3H, -CH₃), 2.48 (s, 3H, -CH₃) ppm, ¹³C NMR (125 MHz, CDCl₃): δ 180.82 (C=O), 146.84 (Ar), 141.40 (Ar), 139.24 (Ar), 137.52 (Ar), 131.83 (Ar), 131.50 (Ar), 127.83 (Ar), 125.24 (Ar), 118.86 (Ar), 114.17 (Ar), 22.29, 21.29 ppm, ESI-MS: m/z 329 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₆H₁₄BrN₂O m/z 329.0284 [M+H]⁺, found 329.0279.

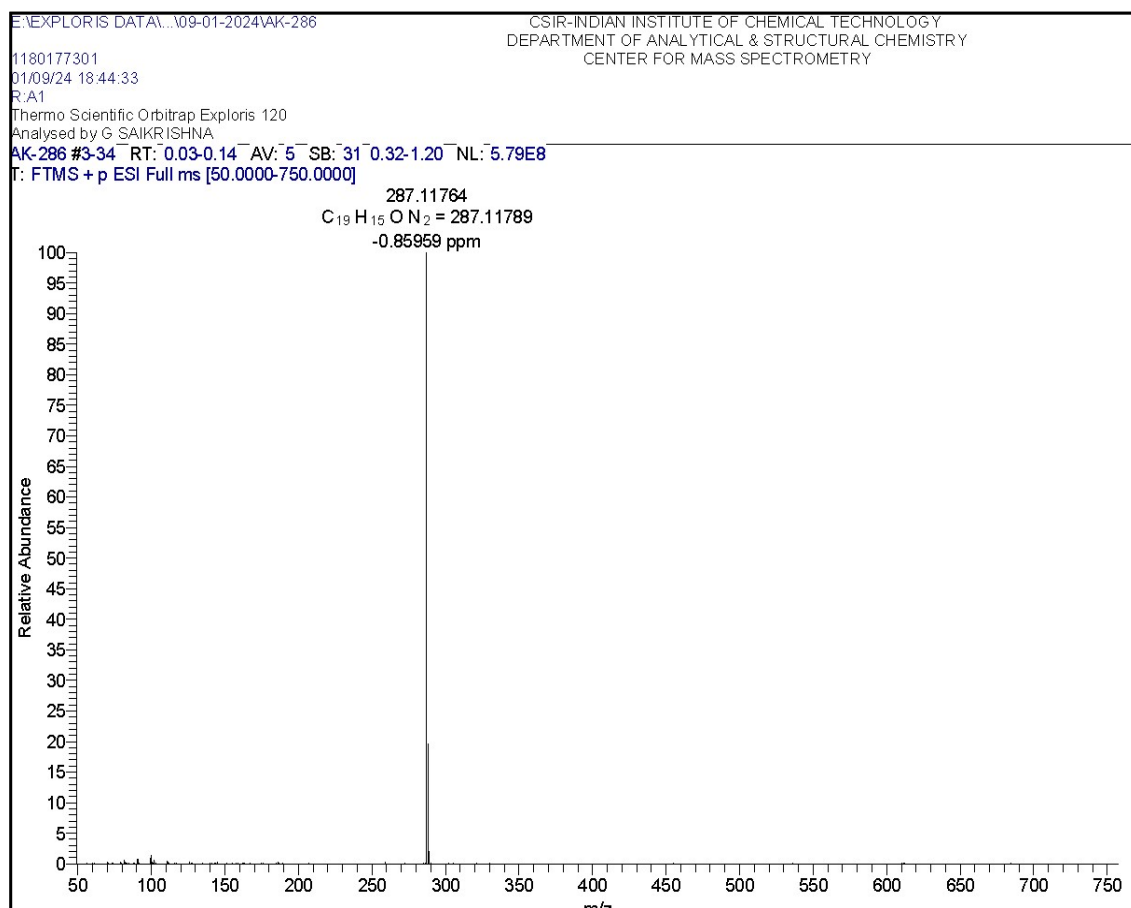




(8-methylimidazo[1,2-*a*]pyridin-3-yl)(naphthalen-2-yl)methanone (3x)

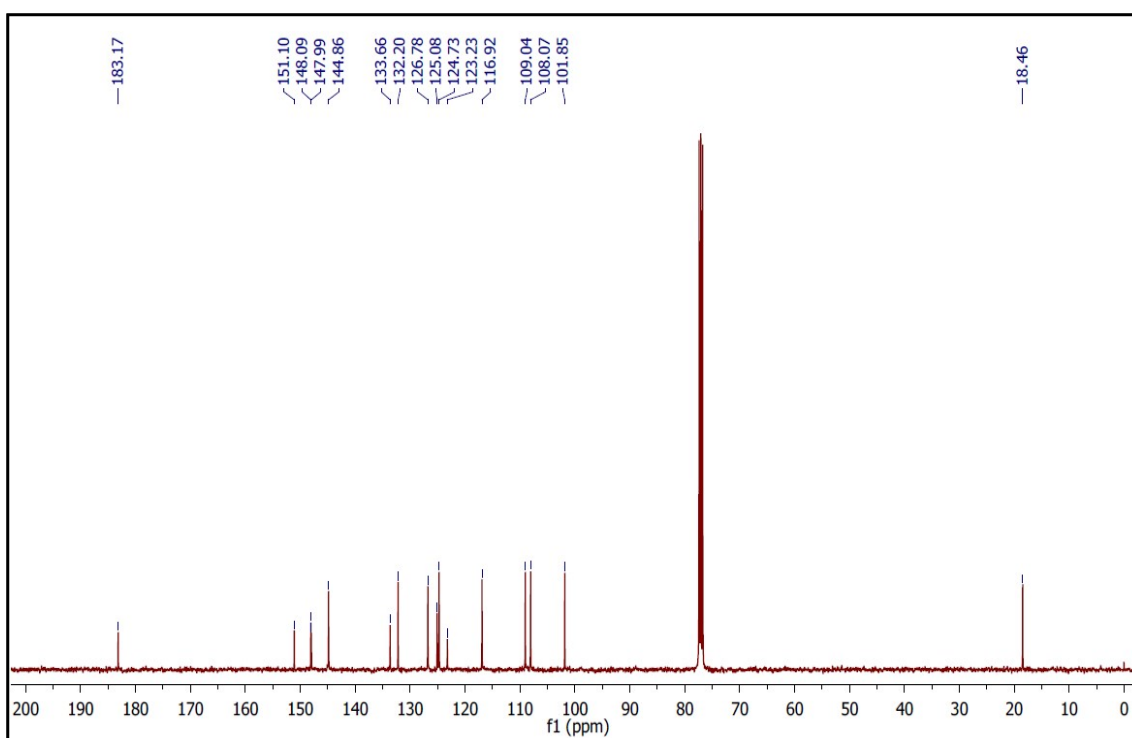
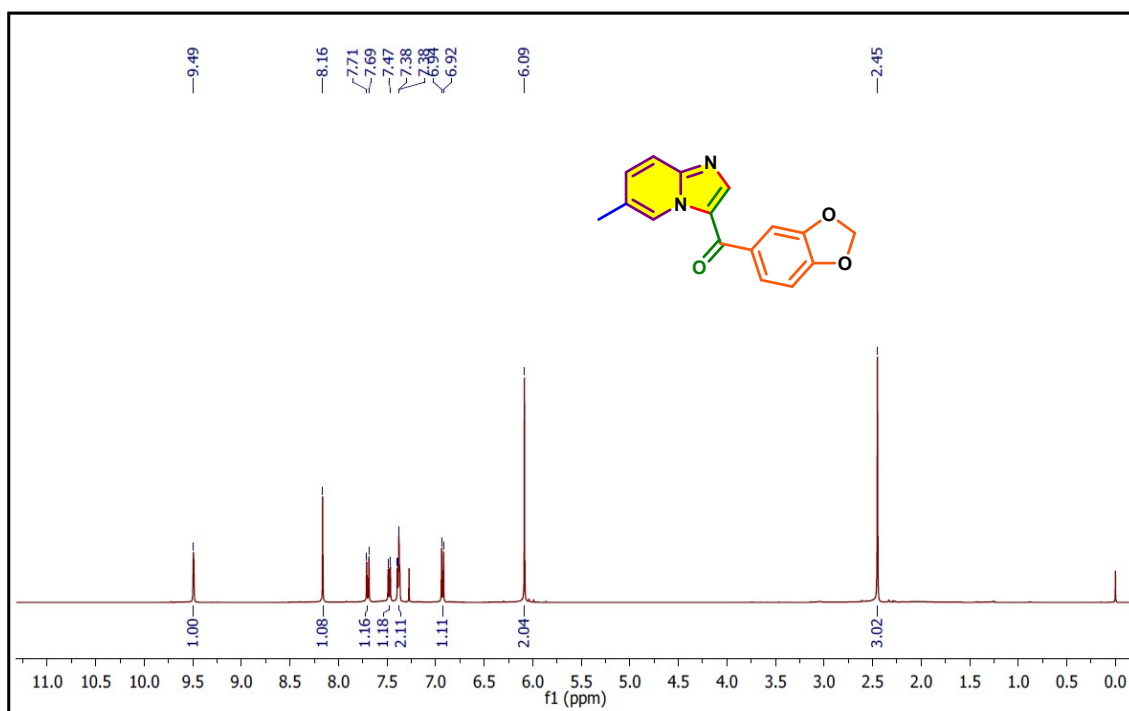
Isolated as a white solid, yield 84% (160 mg), m.p 142-144 °C, IR (ATR): 3021, 2933, 2846, 1721 (C=O stretching), 1601, 1517, 1187, 923, 761 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.64 (d, *J* = 6.8 Hz, 1H, Ar), 8.40 (s, 1H, Ar), 8.27 (s, 1H, Ar), 8.02 – 7.93 (m, 4H, Ar), 7.66 – 7.56 (m, 2H, Ar), 7.40 – 7.35 (m, 1H, Ar), 7.09 (t, *J* = 6.9 Hz, 1H, Ar), 2.72 (s, 3H, -CH₃) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 184.85 (C=O), 149.29 (Ar), 145.07 (Ar), 136.68 (Ar), 135.10 (Ar), 132.51 (Ar), 130.06 (Ar), 129.27 (Ar), 128.63 (Ar), 128.54 (Ar), 128.10 (Ar), 127.89 (Ar), 127.67 (Ar), 126.95 (Ar), 126.68 (Ar), 125.15 (Ar), 124.17 (Ar), 115.24 (Ar), 17.00 ppm, ESI-MS: m/z 287 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₉H₁₅N₂O m/z 287.1178 [M+H]⁺, found 287.1176.

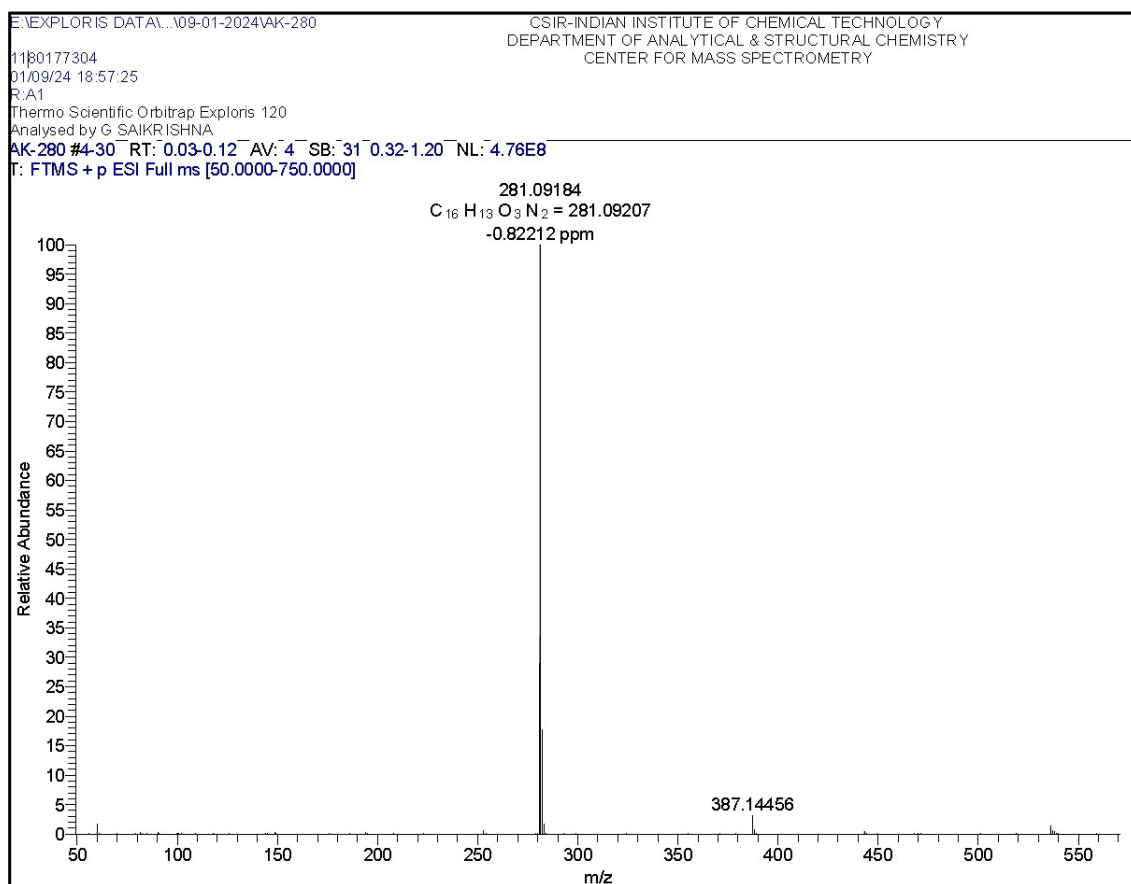




Benzo[d][1,3]dioxol-5-yl(6-methylimidazo[1,2-a]pyridin-3-yl)methanone (3y)

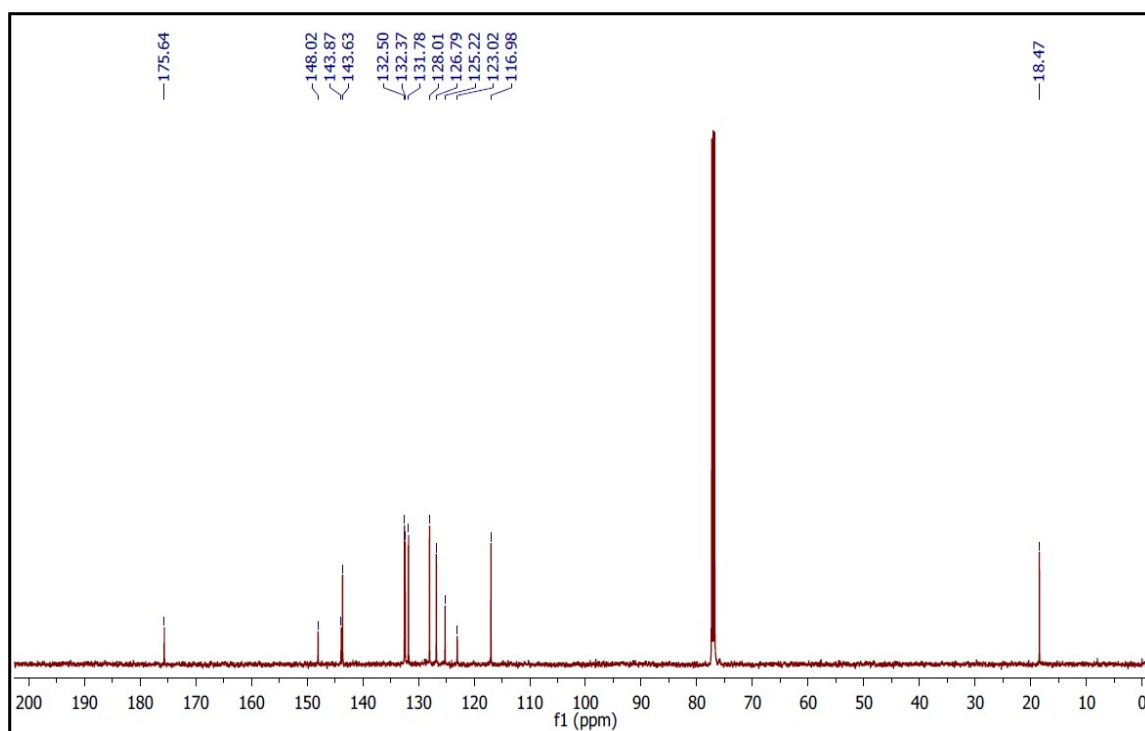
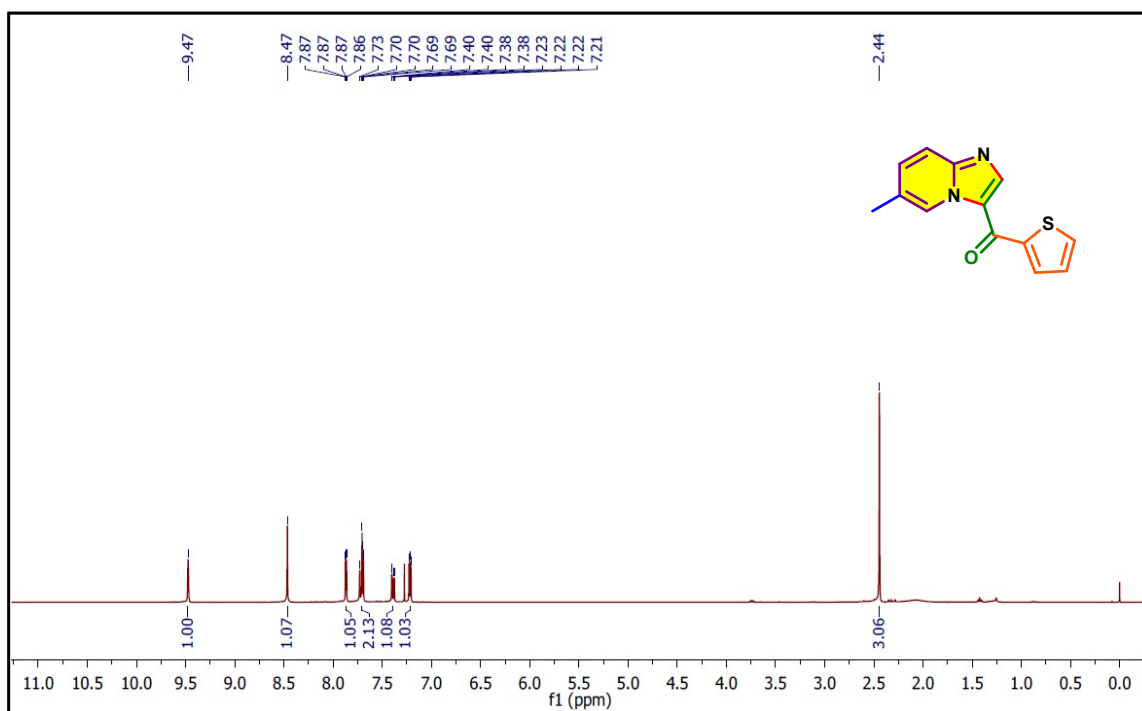
Isolated as a yellow solid, yield 80% (153 mg), m.p 170-173 °C, IR (ATR): 3106, 2930, 2877, 1703 (C=O stretching), 1617, 1457, 1263, 955, 892, 765 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.49 (s, 1H, Ar), 8.16 (s, 1H, Ar), 7.70 (d, *J* = 9.1 Hz, 1H, Ar), 7.50 – 7.45 (m, 1H, Ar), 7.41 – 7.35 (m, 2H, Ar), 6.95 – 6.90 (m, 1H, Ar), 6.09 (s, 2H, -CH₂-), 2.45 (s, 3H, -CH₃) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 183.17 (C=O), 151.10 (Ar), 148.09 (Ar), 147.99 (Ar), 144.86 (Ar), 133.66 (Ar), 132.20 (Ar), 126.78 (Ar), 125.08 (Ar), 124.73 (Ar), 123.23 (Ar), 116.92 (Ar), 109.04 (Ar), 108.07 (Ar), 101.85, 18.46 ppm, ESI-MS: *m/z* 281 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₆H₁₃N₂O₃ *m/z* 281.0920 [M+H]⁺, found 281.0918.

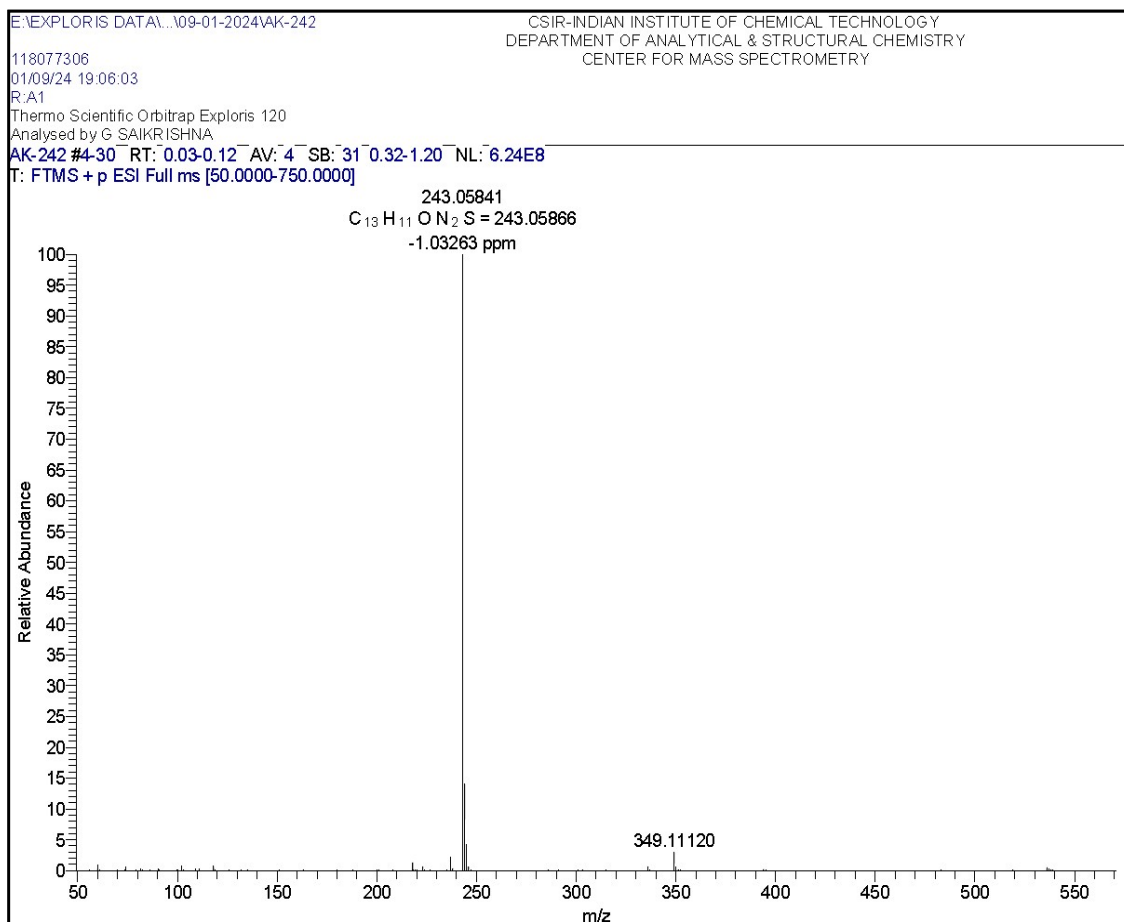




(6-methylimidazo[1,2-*a*]pyridin-3-yl)(thiophen-2-yl)methanone (3z)

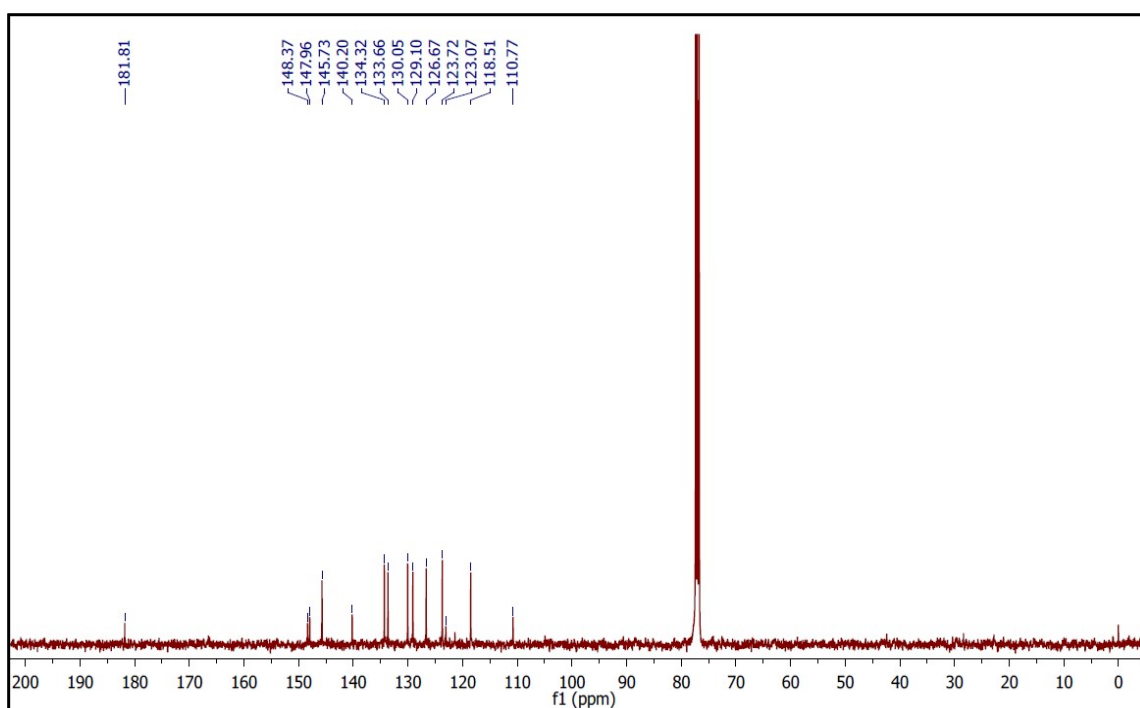
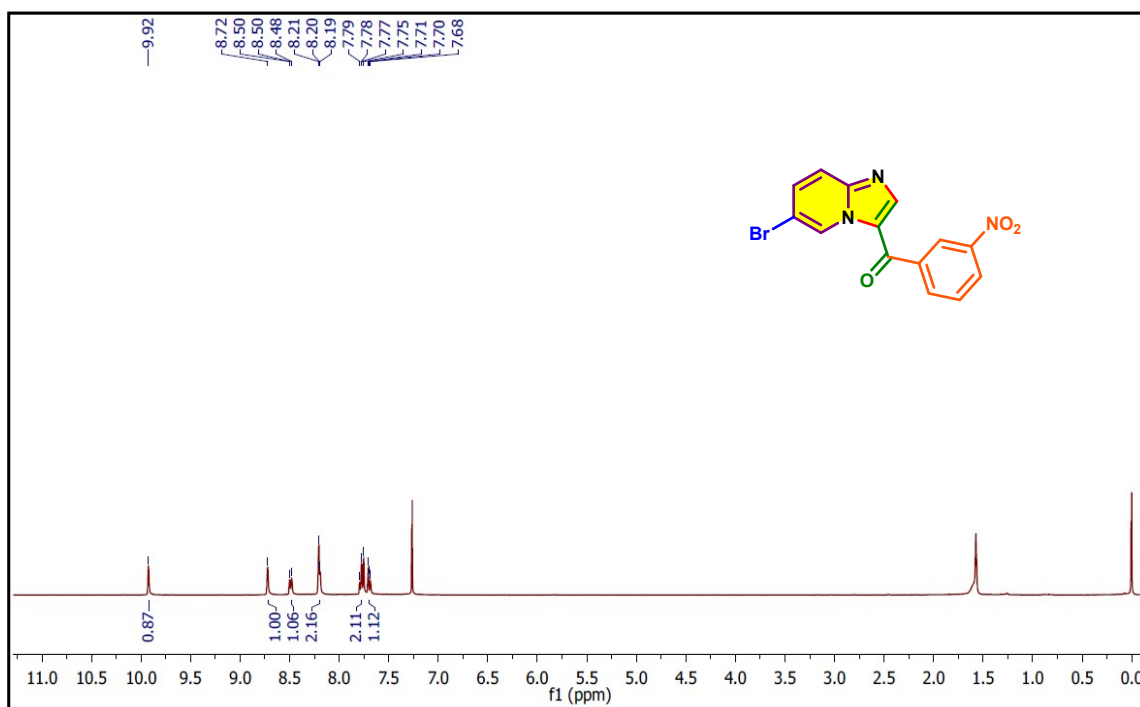
Isolated as a brown solid, yield 77% (154 mg), m.p 76-78 °C, IR (ATR): 3084, 2947, 2814, 1714 (C=O stretching), 1645, 1508, 1412, 1263, 892, 821, 776 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.47 (s, 1H, Ar), 8.47 (s, 1H, Ar), 7.88 – 7.85 (m, 1H, Ar), 7.74 – 7.68 (m, 2H, Ar), 7.39 (dd, *J* = 9.1, Hz, 1H, Ar), 7.24 – 7.19 (m, 1H, Ar), 2.44 (s, 3H, -CH₃) ppm, ¹³C NMR (125 MHz, CDCl₃): δ 175.64 (C=O), 148.02 (Ar), 143.87 (Ar), 143.63 (Ar), 132.50 (Ar), 132.37 (Ar), 131.78 (Ar), 128.01 (Ar), 126.79 (Ar), 125.22 (Ar), 123.02 (Ar), 116.98 (Ar), 18.47 ppm, ESI-MS: m/z 243 [M+H]⁺, HRMS (ESI) Anal. Calcd. for C₁₃H₁₁N₂OS m/z 243.0586 [M+H]⁺, found 243.0584.

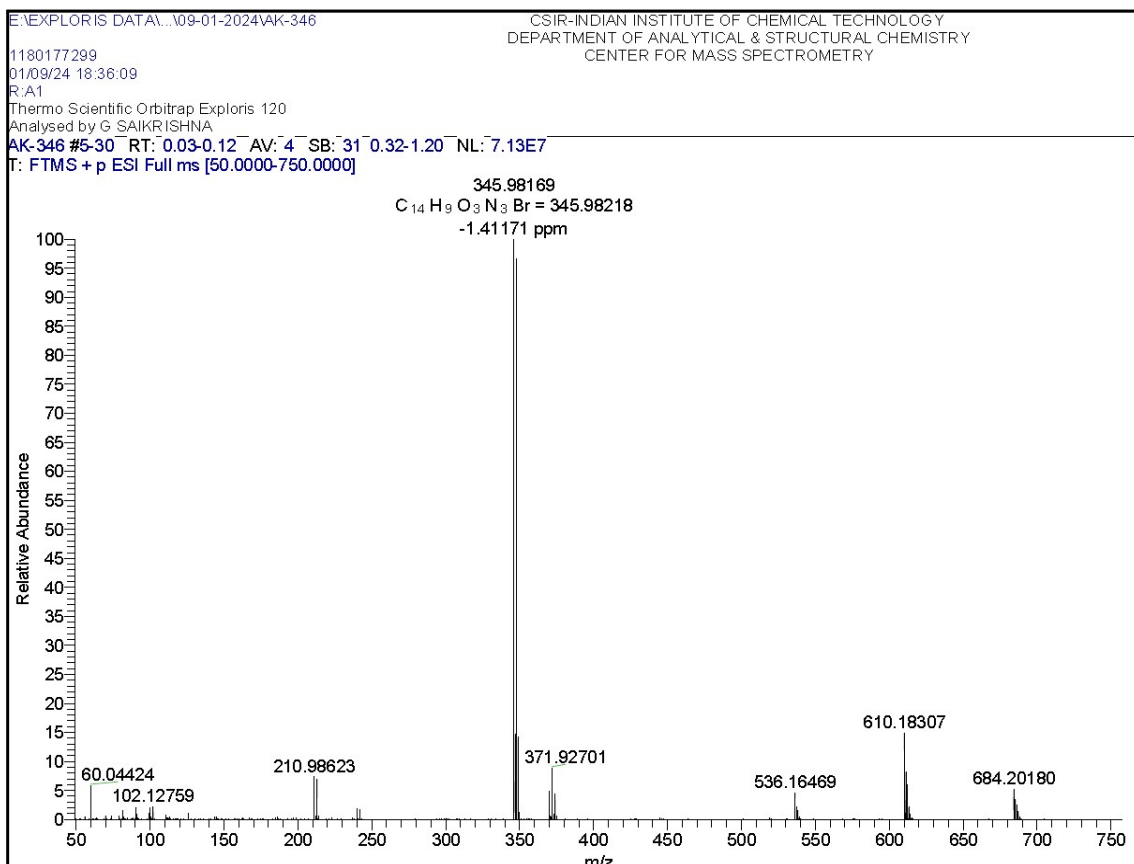




(6-bromoimidazo[1,2-a]pyridin-3-yl)(3-nitrophenyl)methanone (3za)

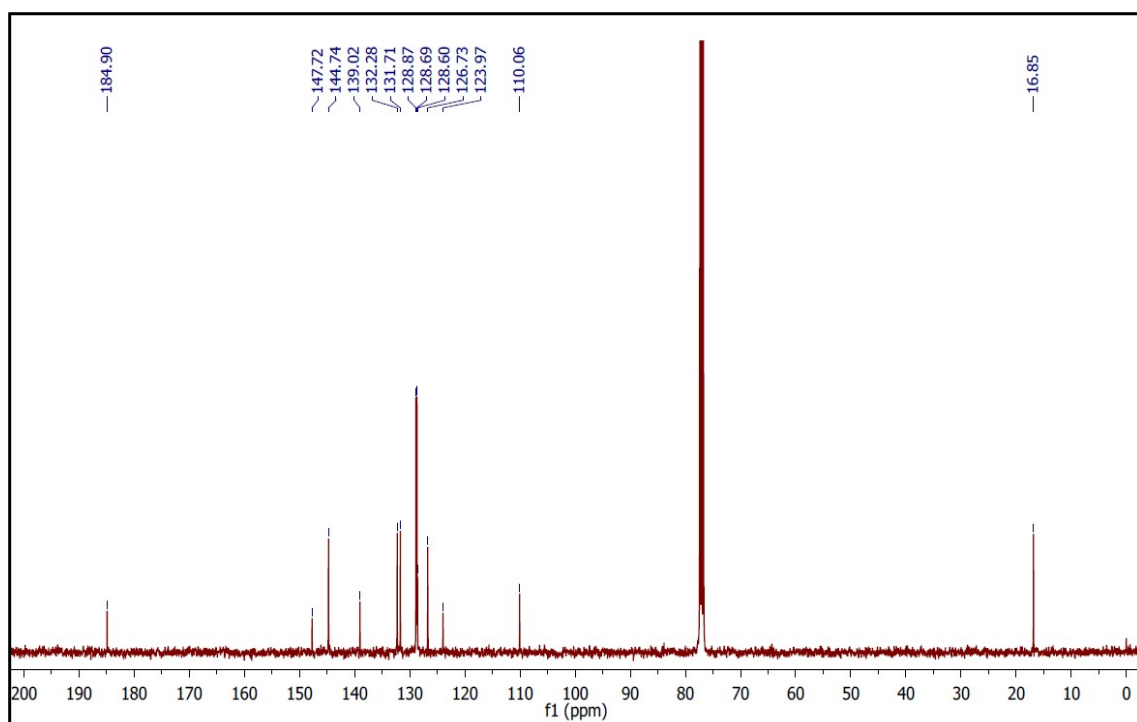
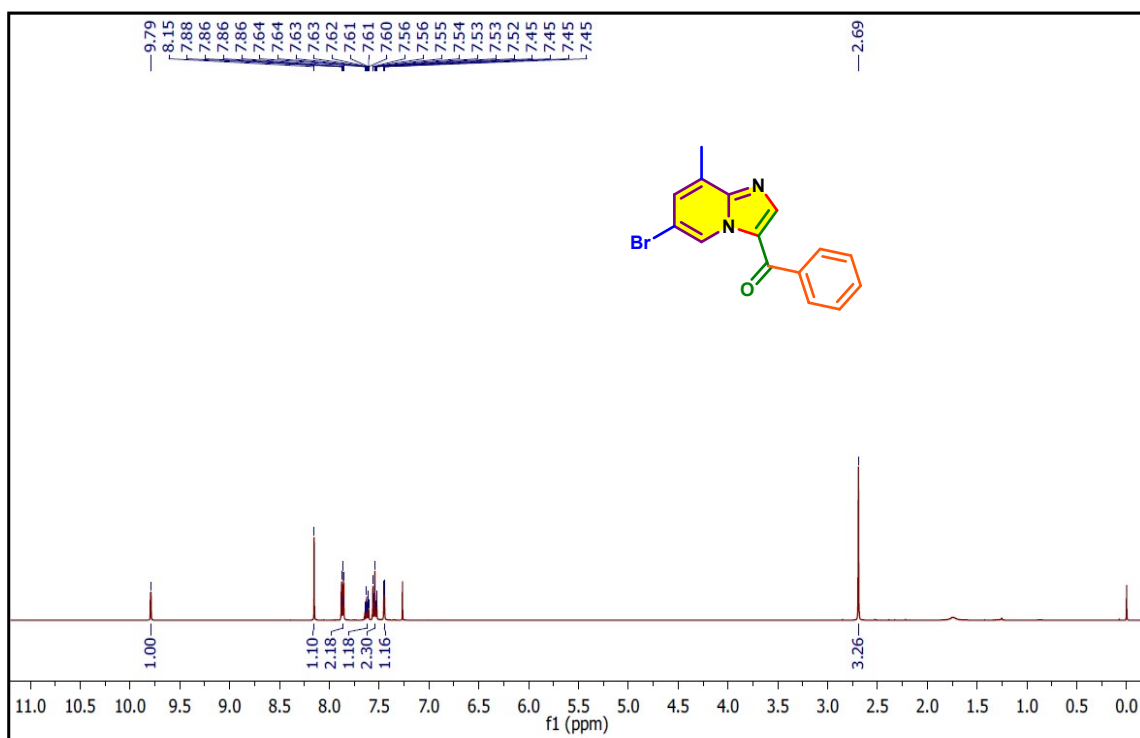
Isolated as a brown solid, yield 67% (158 mg), m.p 218-222 °C, IR (ATR): 3085, 2917, 2852, 1707 (C=O stretching), 1620, 1524, 1461, 1348, 1225, 904, 724 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.92 (s, 1H, Ar), 8.72 (s, 1H, Ar), 8.52 – 8.45 (m, 1H, Ar), 8.23 – 8.17 (m, 2H, Ar), 7.77 (dd, *J* = 8.4 Hz, 2H, Ar), 7.72 – 7.67 (m, 1H, Ar) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 181.81 (C=O), 148.37 (Ar), 147.96 (Ar), 145.73 (Ar), 140.20 (Ar), 134.32 (Ar), 133.66 (Ar), 130.05 (Ar), 129.10 (Ar), 126.67 (Ar), 123.72 (Ar), 123.07 (Ar), 118.51 (Ar), 110.77 (Ar) ppm, ESI-MS: *m/z* 346 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₄H₉BrN₃O₃ *m/z* 345.9821 [M+H]⁺, found 345.9816.

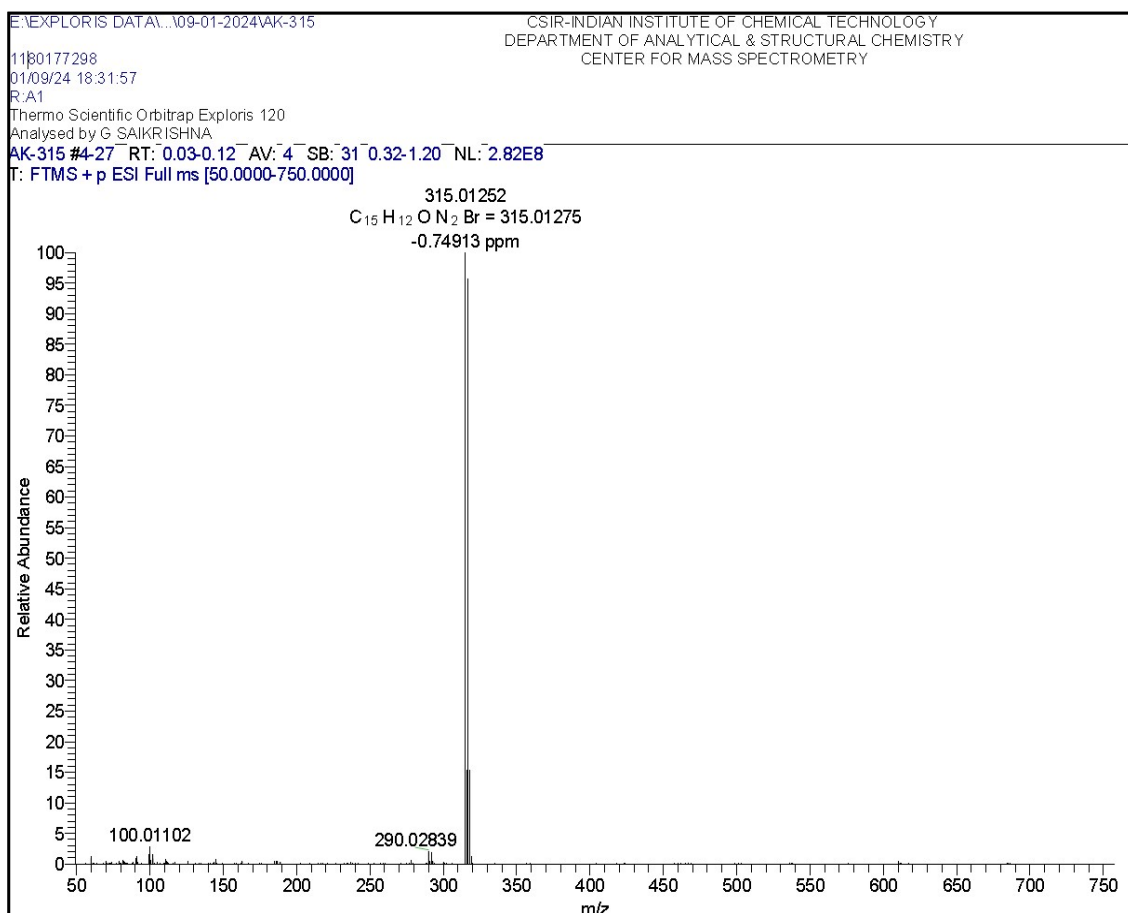




(6-bromo-8-methylimidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (3b)

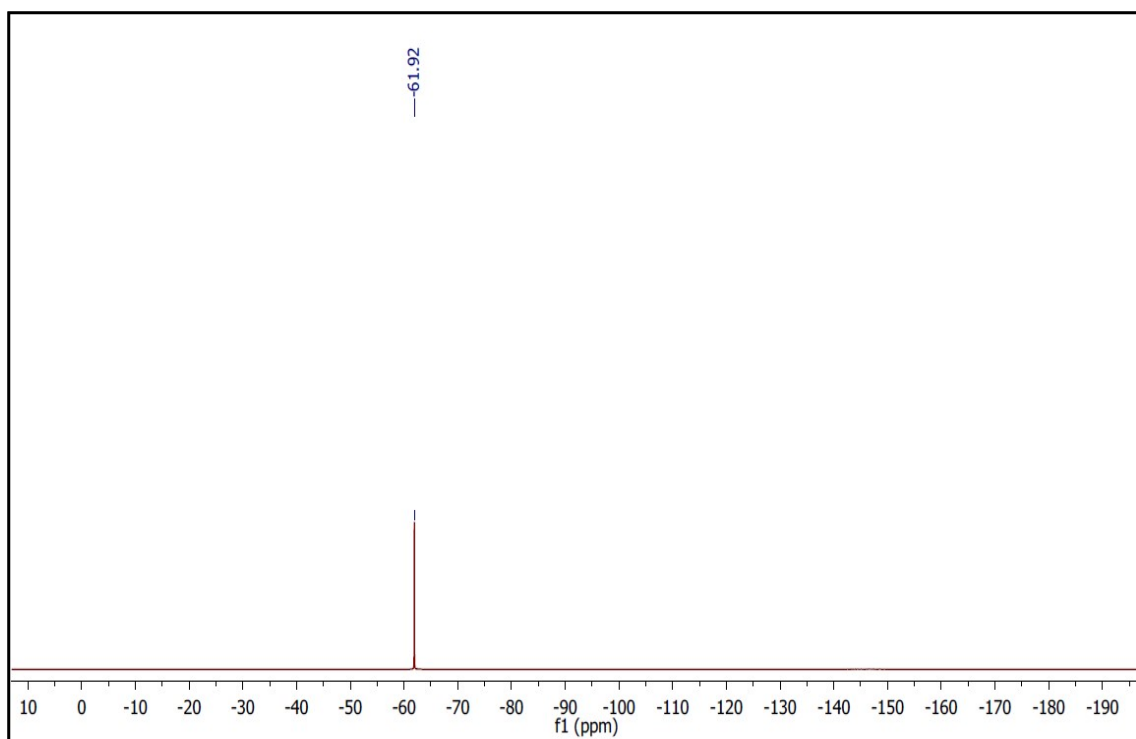
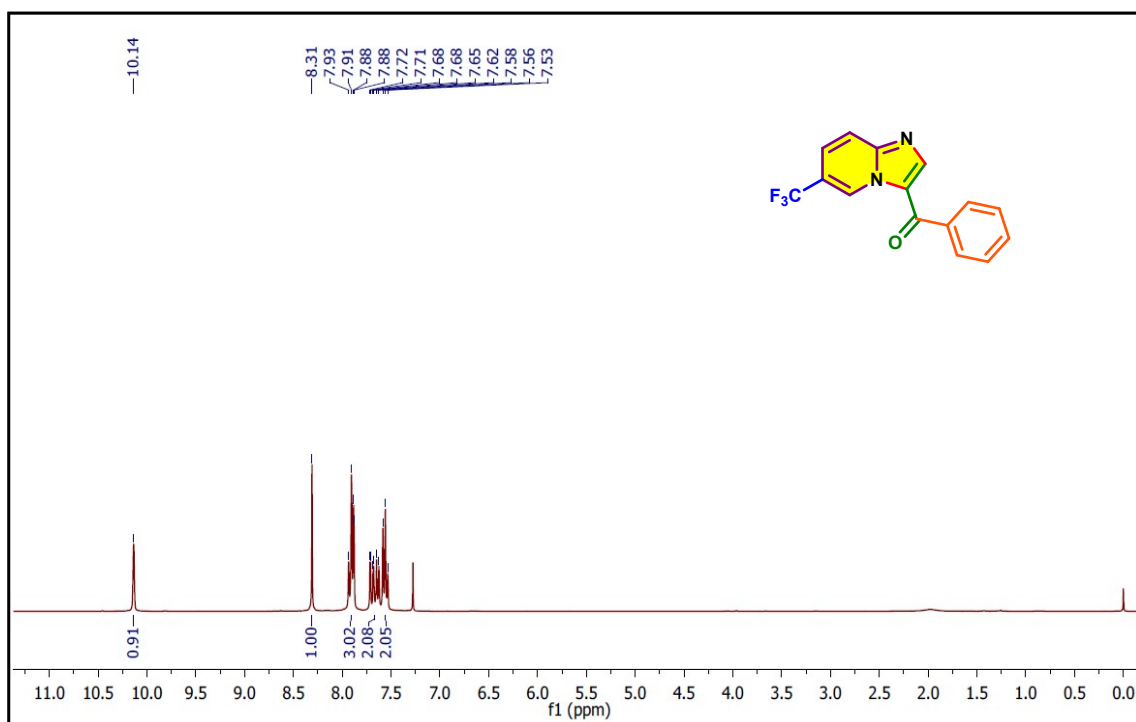
Isolated as a yellow solid, yield 78% (211 mg), m.p 202-205 °C, IR (ATR): 3117, 2917, 2852, 1728 (C=O stretching), 1621, 1460, 1247, 891, 715 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.79 (s, 1H, Ar), 8.15 (s, 1H, Ar), 7.88 – 7.84 (m, 2H, Ar), 7.65 – 7.60 (m, 1H, Ar), 7.57 – 7.52 (m, 2H, Ar), 7.47 – 7.43 (m, 1H, Ar), 2.69 (s, 3H, -CH₃) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 184.90 (C=O), 147.72 (Ar), 144.74 (Ar), 139.02 (Ar), 132.28 (Ar), 131.71 (Ar), 128.87 (Ar), 128.69 (Ar), 128.60 (Ar), 126.73 (Ar), 123.97 (Ar), 110.06 (Ar), 16.85 ppm, ESI-MS: m/z 315 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₅H₁₂BrN₂O m/z 315.0127 [M+H]⁺, found 315.0125.

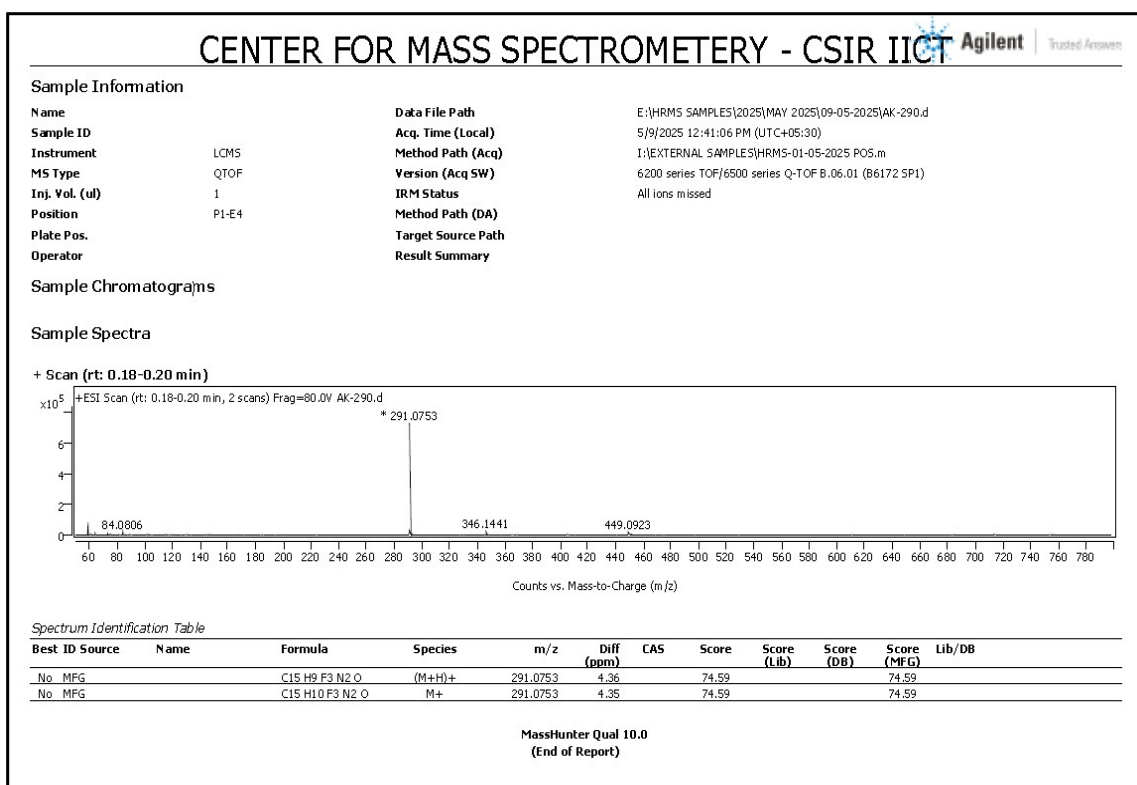
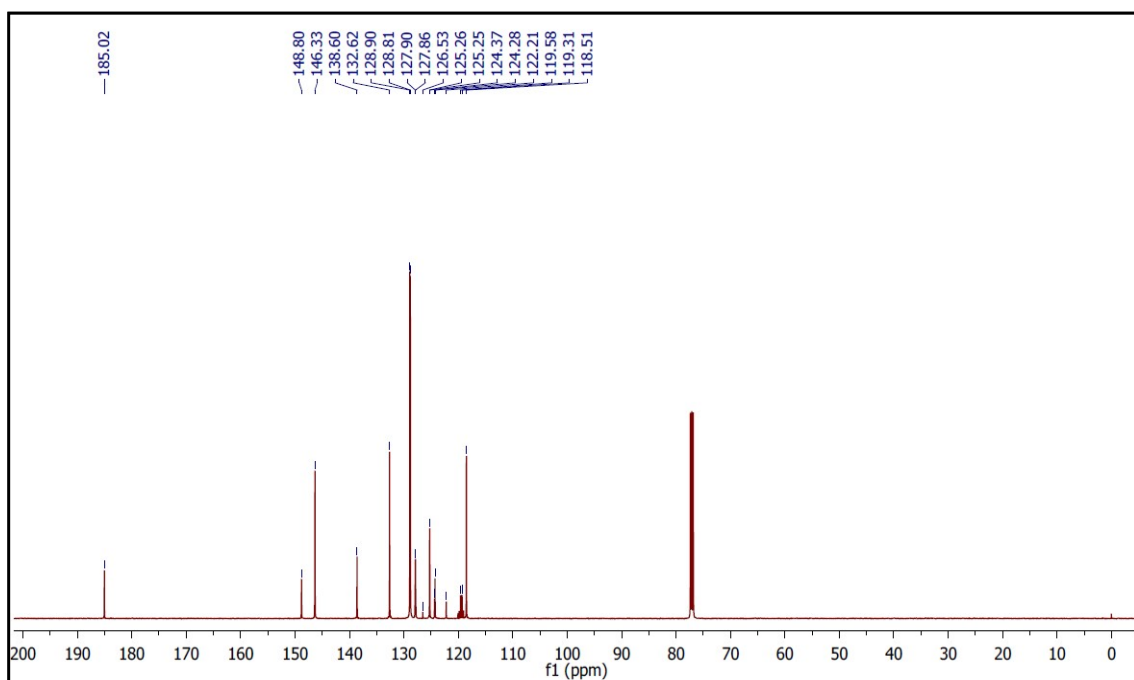




Phenyl(6-(trifluoromethyl)imidazo[1,2-*a*]pyridin-3-yl)methanone (3zc)¹

Isolated as a yellow solid, yield 75% (186 mg), m.p 146-148 °C, IR (ATR): 3102, 2917, 2852, 1726 (C=O stretching), 1611, 1456, 1213, 1050, 752, 668 cm⁻¹, ¹H NMR (300 MHz, CDCl₃): δ 10.14 (s, 1H, Ar), 8.31 (s, 1H, Ar), 7.95 – 7.86 (m, 3H, Ar), 7.73 – 7.61 (m, 2H, Ar), 7.56 (t, *J* = 7.3 Hz, 2H, Ar) ppm, ¹⁹F NMR (375 MHz, CDCl₃): δ -61.92 ppm, ¹³C NMR (125 MHz, CDCl₃): δ 185.02 (C=O), 148.80 (Ar), 146.33 (Ar), 138.60 (Ar), 132.62 (Ar), 128.90 (Ar), 128.81 (Ar), 127.90 (Ar), 127.86 (Ar), 125.26 (Ar), 125.25 (Ar), 123.17 (q, *J* = 271.62 Hz, (Ar C-CF₃)), 124.28 (Ar), 122.21 (Ar), 119.34 (d, *J* = 34.74 Hz, (Ar C-CF₃)), 118.51 (Ar) ppm, ESI-MS: m/z 291 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₅H₁₀F₃N₂O m/z 291.0745 [M+H]⁺, found 291.0753.

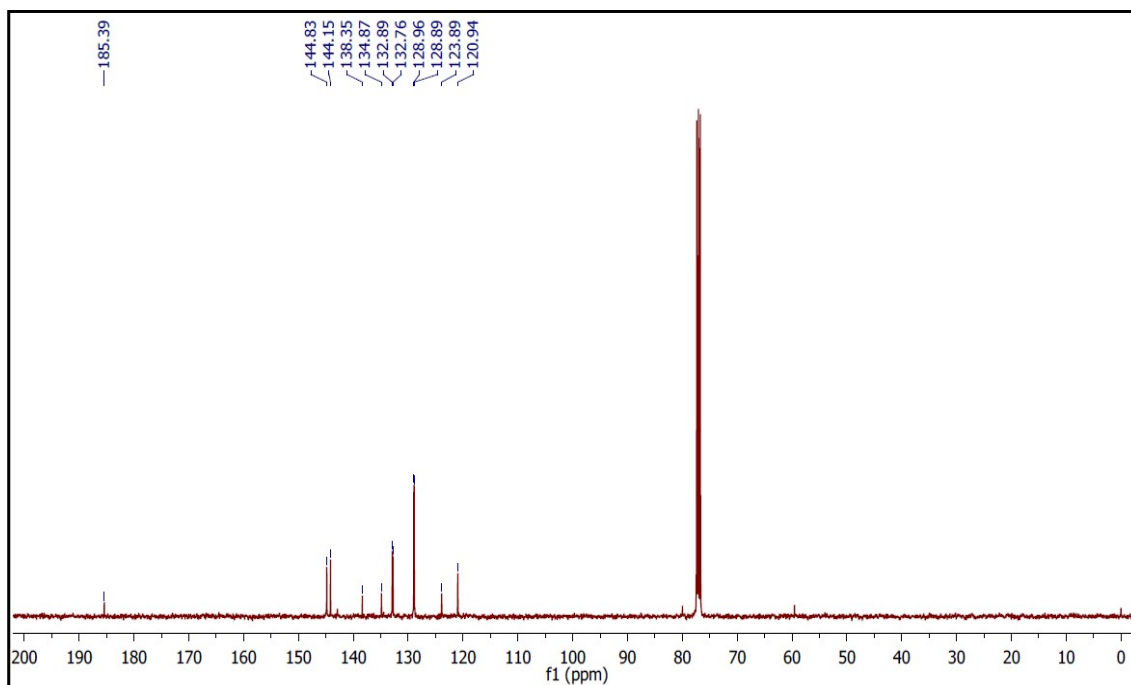
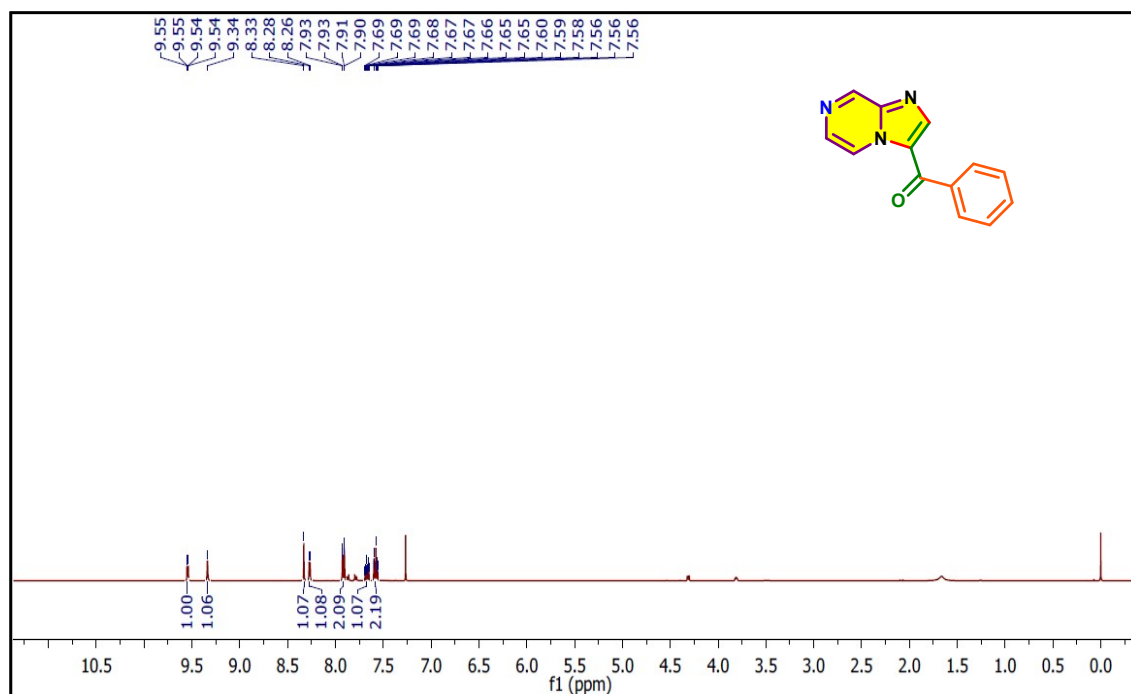


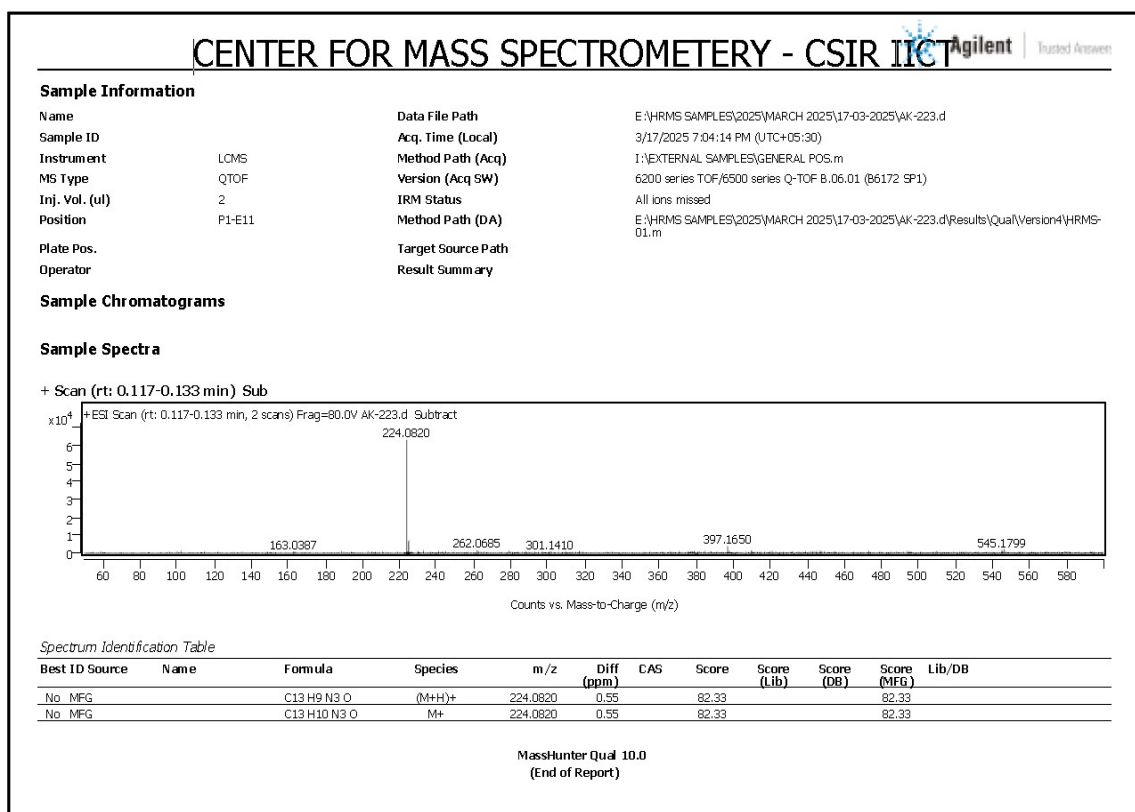


Imidazo[1,2-a]pyrazin-3-yl(phenyl)methanone (3zd)⁶

Isolated as a yellow solid, yield 71% (136 mg), m.p 210-214 °C, IR (ATR): 3057, 2921, 2828, 1732 (C=O stretching), 1657, 1545, 1461, 1023, 766, 691 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 9.54 (dd, *J* = 4.6 Hz, 1H, Ar), 9.34 (s, 1H, Ar), 8.33 (s, 1H, Ar), 8.27 (d, *J* = 4.6 Hz, 1H, Ar), 7.94 – 7.89 (m, 2H, Ar), 7.71 – 7.64 (m, 1H, Ar), 7.61 – 7.55 (m, 2H, Ar) ppm, ¹³C NMR (100

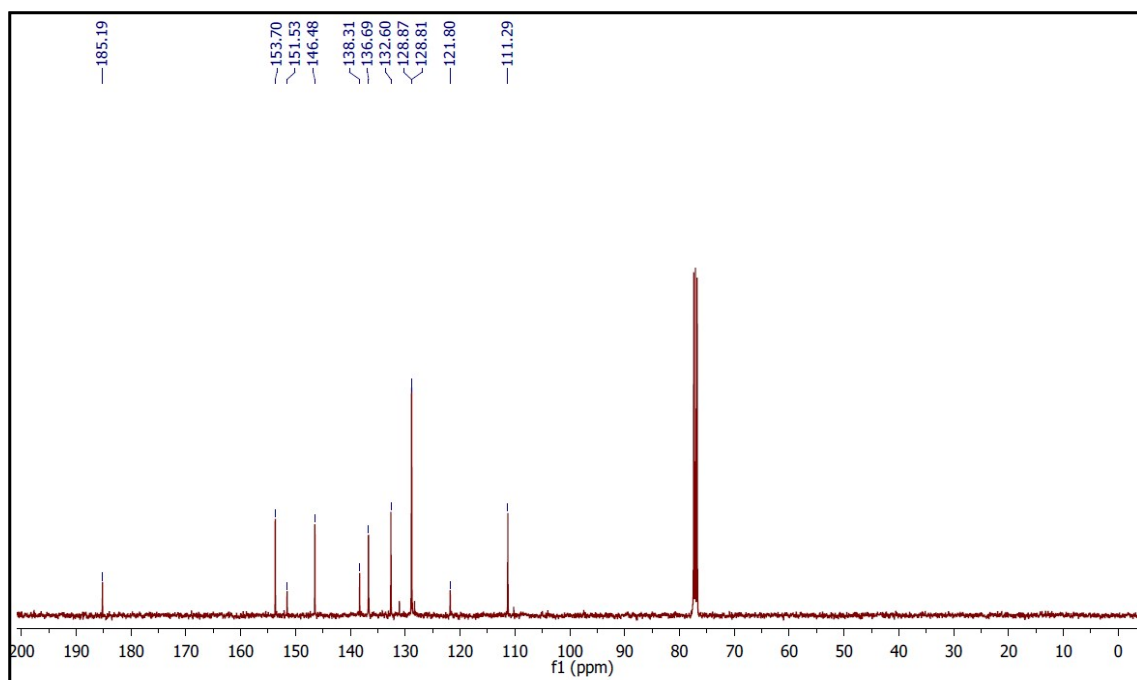
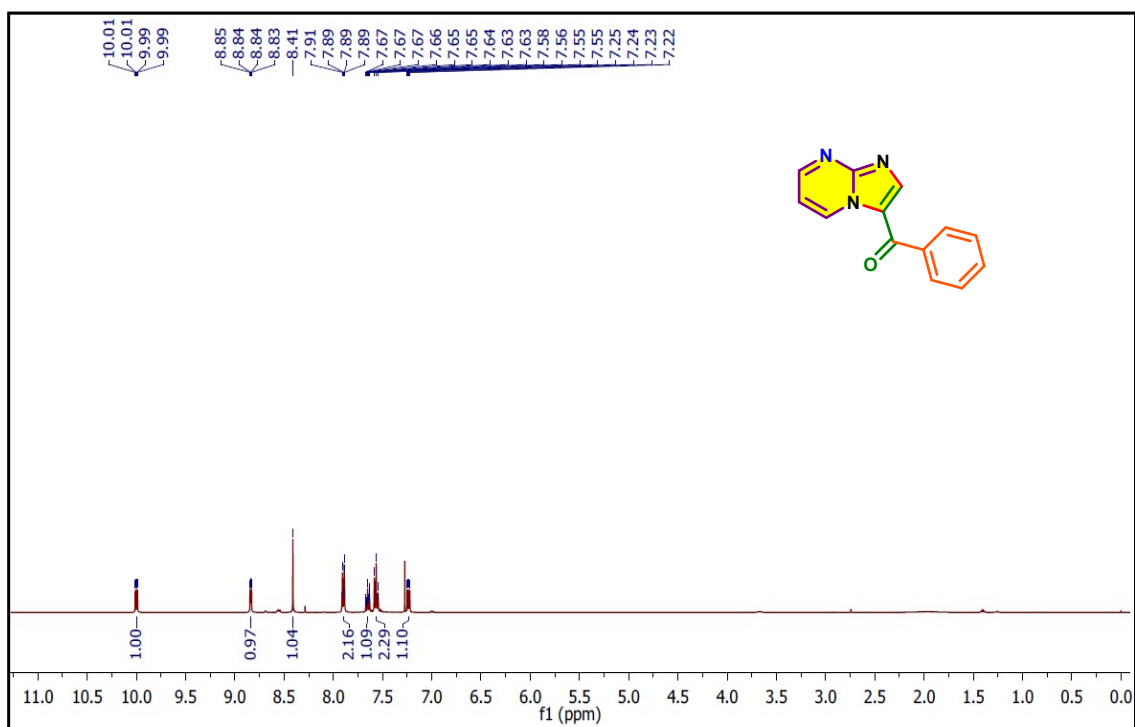
MHz, CDCl₃): δ 185.39 (C=O), 144.83 (Ar), 144.15 (Ar), 138.35 (Ar), 134.87 (Ar), 132.89 (Ar), 132.76 (Ar), 128.96 (Ar), 128.89 (Ar), 123.89 (Ar), 120.94 (Ar) ppm, ESI-MS: m/z 224 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₃H₁₀N₃O m/z 224.0823 [M+H]⁺, found 224.0820.

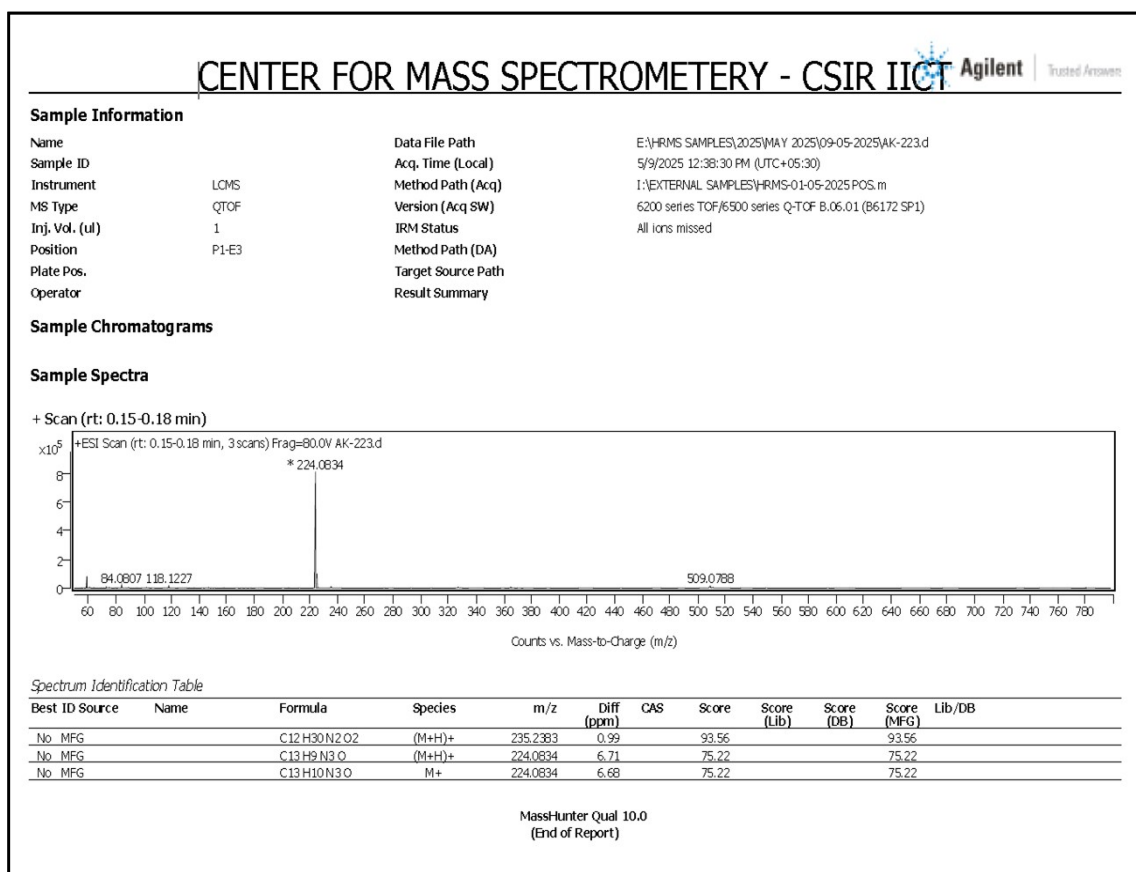




Imidazo[1,2-a]pyrimidin-3-yl(phenyl)methanone (3ze)¹

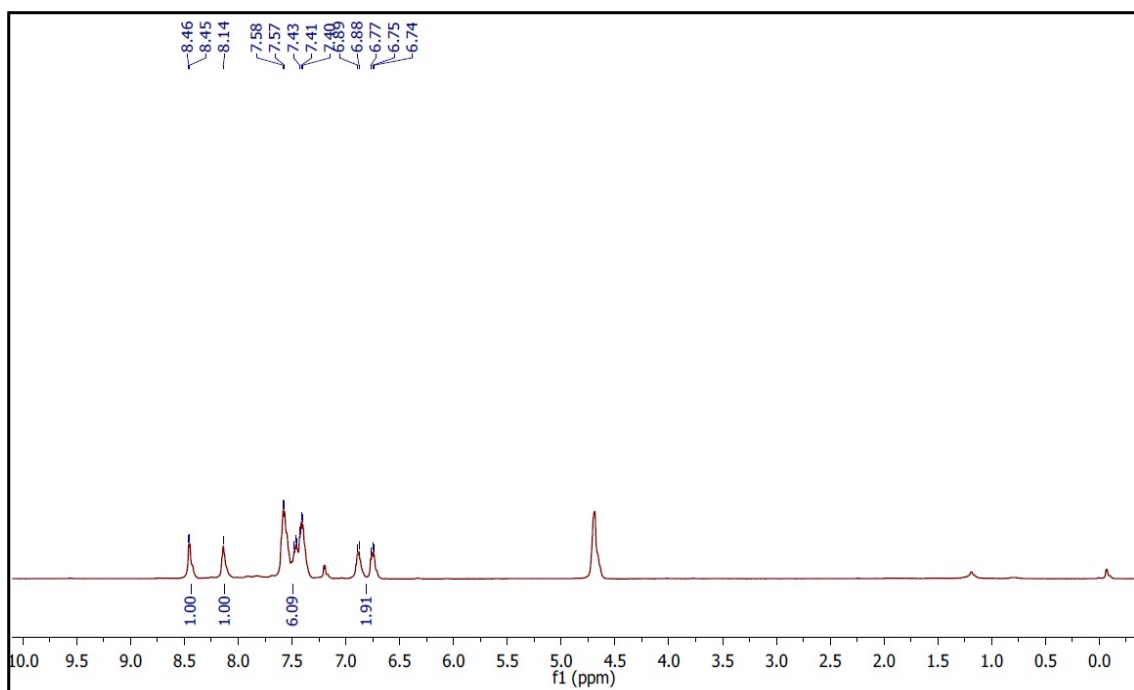
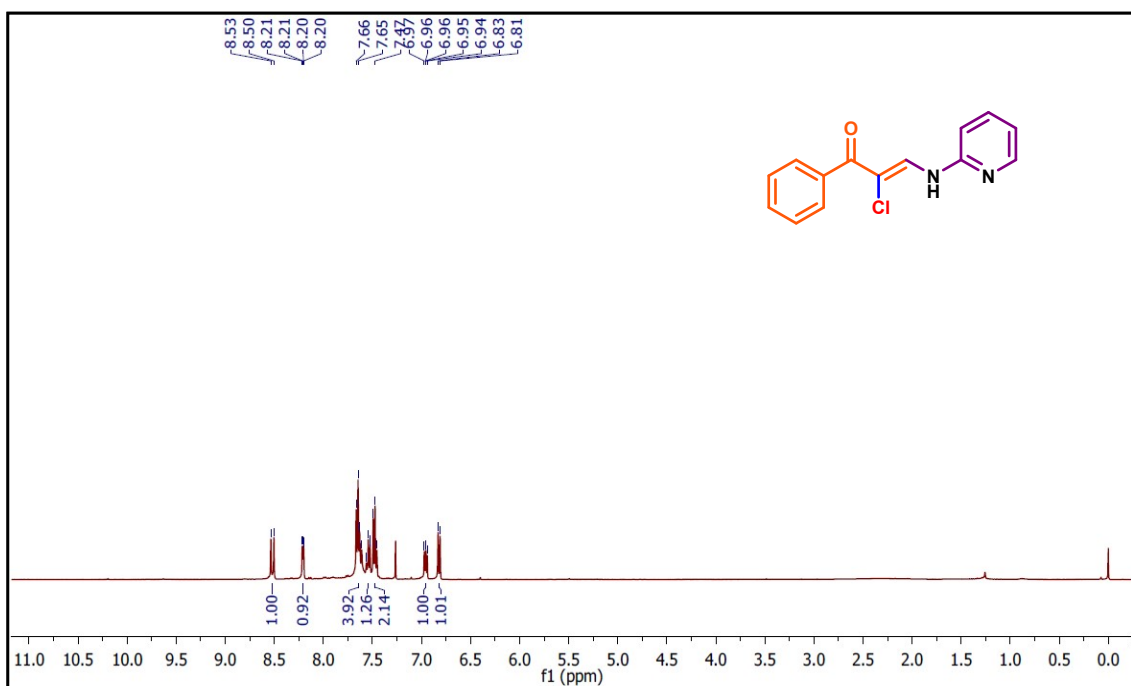
Isolated as a yellow solid, yield 68% (130 mg), m.p 147-151 °C, IR (ATR): 3105, 2927, 2821, 1736 (C=O stretching), 1603, 1534, 1428, 1046, 777, 689 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 10.00 (dd, *J* = 6.9 Hz, 1H, Ar), 8.84 (dd, *J* = 4.2 Hz, 1H, Ar), 8.41 (s, 1H, Ar), 7.93 – 7.87 (m, 2H, Ar), 7.68 – 7.62 (m, 1H, Ar), 7.59 – 7.54 (m, 2H, Ar), 7.24 (dd, *J* = 6.9 Hz, 1H, Ar) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 185.19 (C=O), 153.70 (Ar), 151.53 (Ar), 146.48 (Ar), 138.31 (Ar), 136.69 (Ar), 132.60 (Ar), 128.87 (Ar), 128.81 (Ar), 121.80 (Ar), 111.29 (Ar) ppm, ESI-MS: m/z 224 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₃H₁₀N₃O m/z 224.0823 [M+H]⁺, found 224.0834.

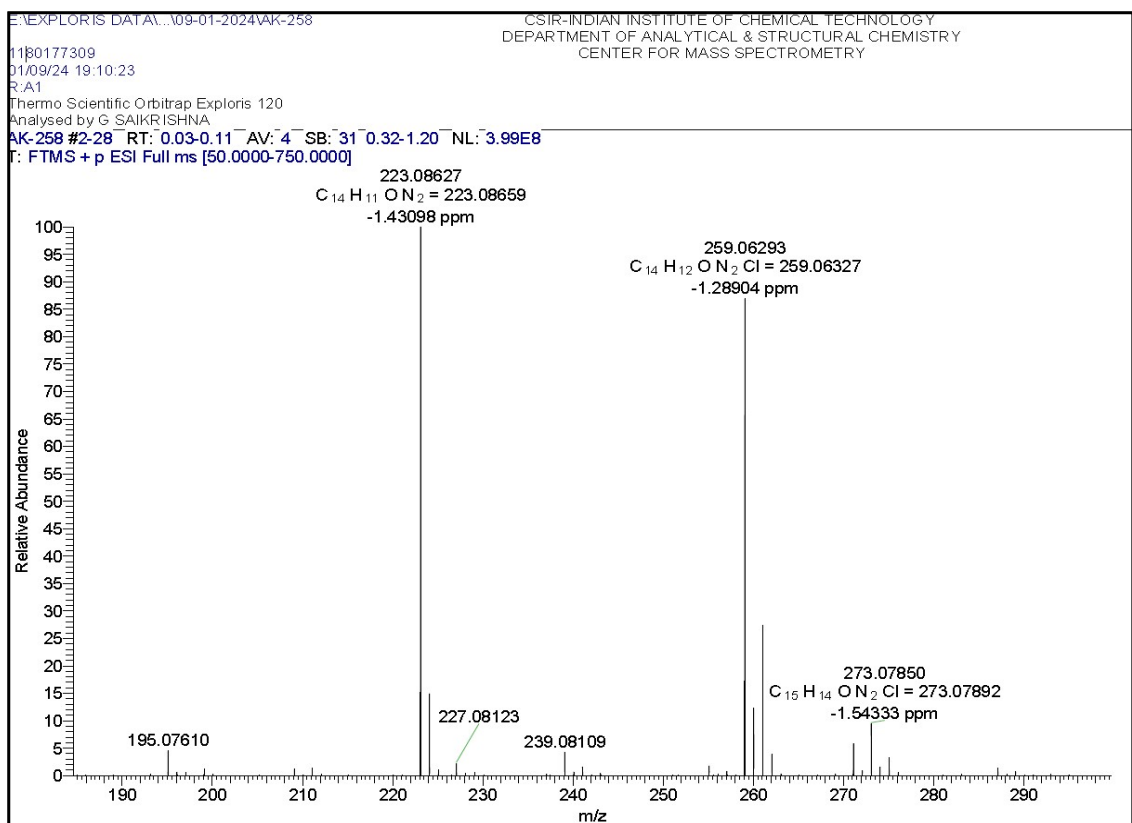
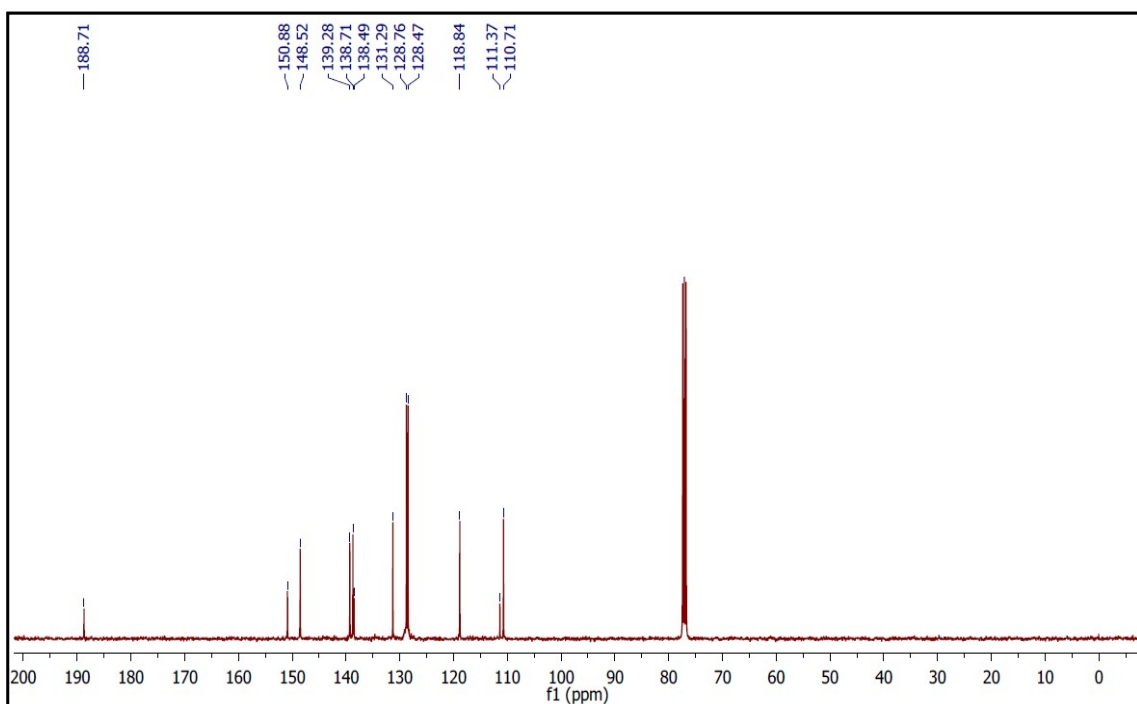




2-chloro-1-phenyl-3-(pyridin-2-ylamino)prop-2-en-1-one (4a)²

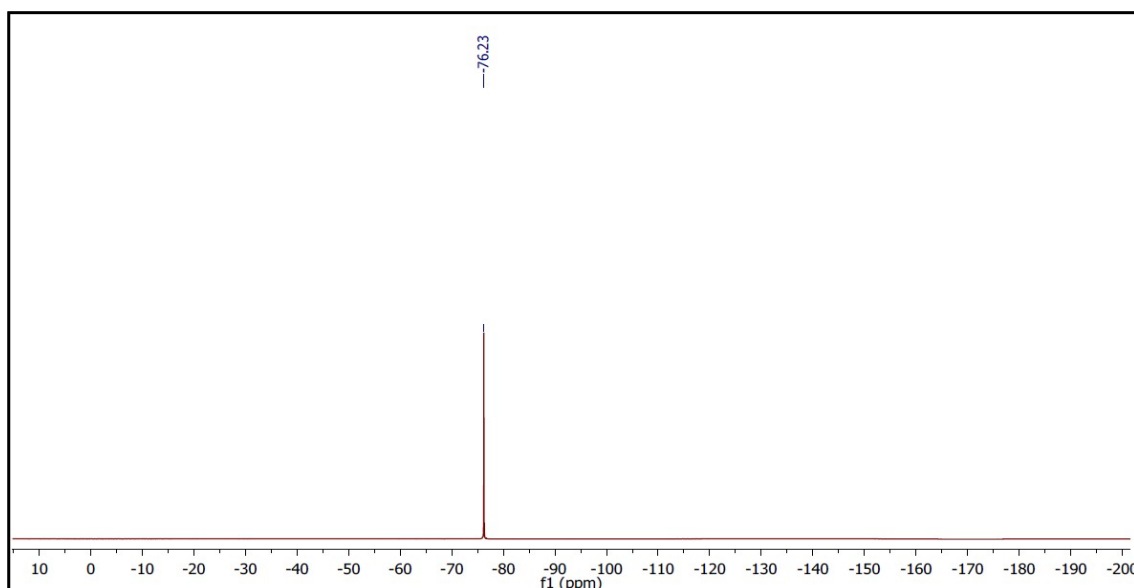
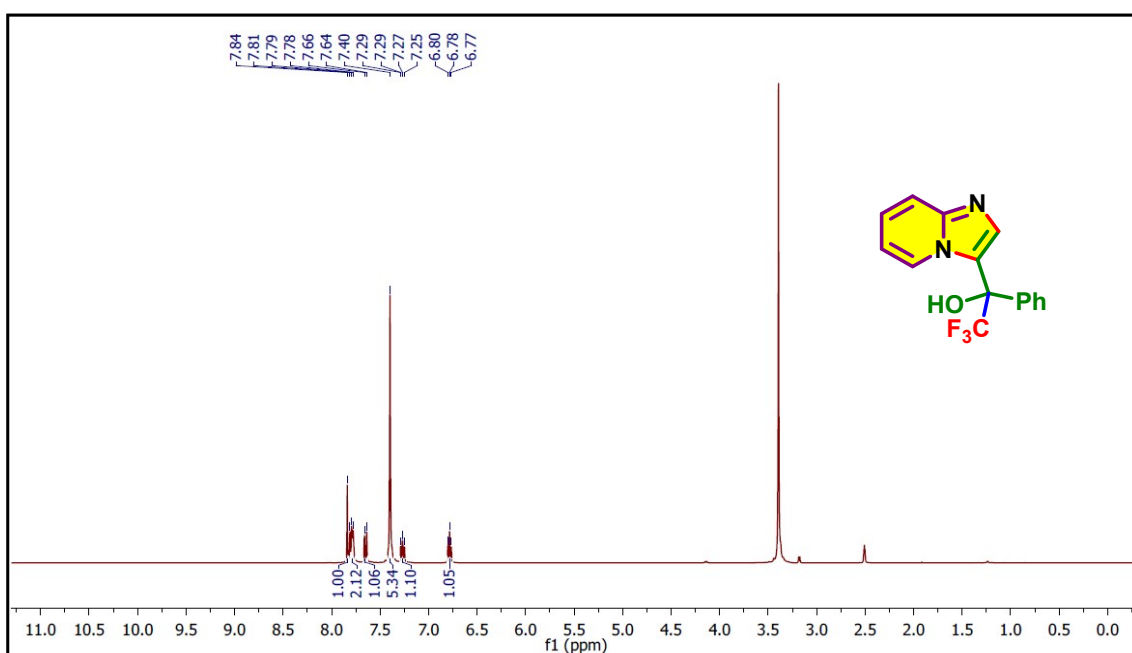
Isolated as yellow solid, yield 62% (137 mg), m.p 198-200 °C, IR (ATR): 3354 (NH stretching), 3098, 3016, 2927, 1727 (C=O stretching), 1533, 1428, 1213, 928, 721 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 8.52 (d, *J* = 12.3 Hz, 1H, C=CH), 8.21 (dd, *J* = 4.9 Hz, 1H, Ar), 7.63 (ddd, *J* = 8.2 Hz, 4H, Ar), 7.57 – 7.52 (d, *J* = 12.5 Hz, 1H, -NH), 7.48 (dd, *J* = 11.2 Hz, 2H, Ar), 6.99 – 6.93 (m, 1H, Ar), 6.82 (d, *J* = 8.2 Hz, 1H, Ar) ppm, ¹H NMR (400 MHz, D₂O): δ 8.45 (d, *J* = 3.8 Hz, 1H), 8.14 (s, 1H), 7.62 – 7.37 (m, 6H), 6.94 – 6.67 (m, 2H) ppm, ¹³C NMR (100 MHz, CDCl₃): δ 188.71 (C=O), 150.88 (Ar), 148.52 (Ar), 139.28 (ClC=CH), 138.71 (Ar), 138.49 (Ar), 131.29 (Ar), 128.76 (Ar), 128.47 (Ar), 118.84 (Ar), 111.37 (ClC=CH), 110.71 (Ar) ppm, ESI-MS: *m/z* 259 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₄H₁₂ClN₂O *m/z* 259.0632 [M+H]⁺, found 259.0629.

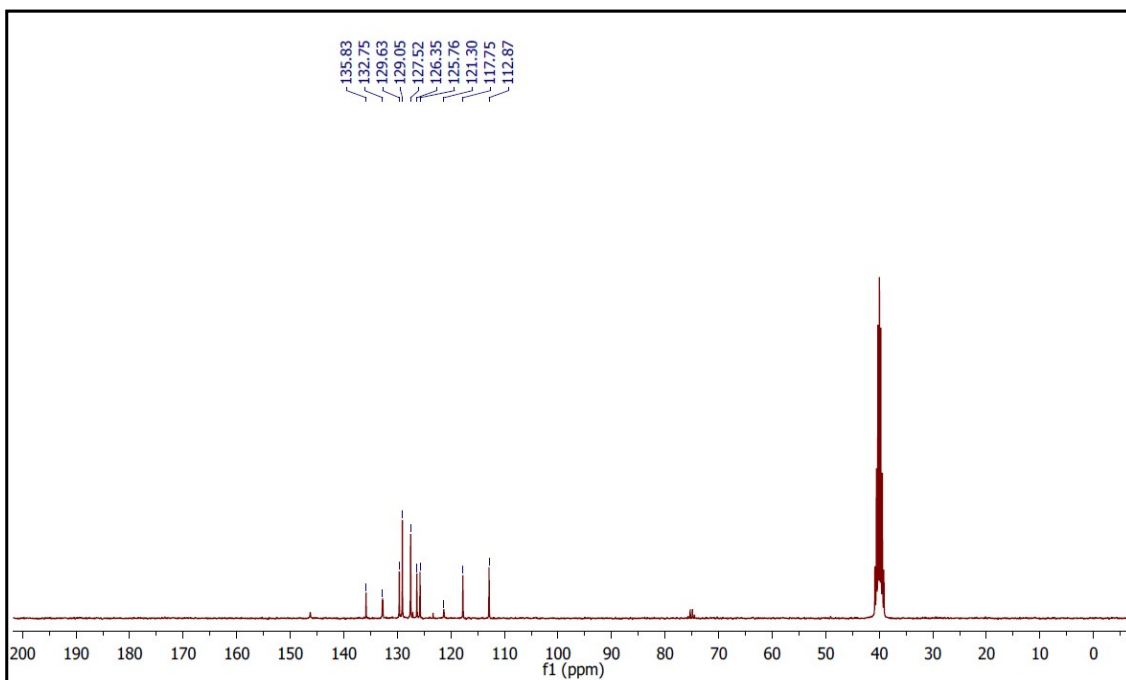




2,2,2-Trifluoro-1-(imidazo[1,2-*a*]pyridin-3-yl)-1-phenylethan-1-ol (5a)

Isolated as a white solid, yield 76% (150 mg), m.p 259-262 °C, IR (ATR): 3432 (O-H stretching), 3113, 2942, 1592, 1513, 1422, 1039, 725, 676 cm⁻¹, ¹H NMR (400 MHz, DMSO): δ 7.84 (s, 1H, -OH), 7.82 – 7.76 (m, 2H, Ar), 7.65 (d, J = 9.1 Hz, 1H, Ar), 7.43 – 7.36 (m, 5H, Ar), 7.27 (dd, J = 11.4 Hz, 1H, Ar), 6.78 (t, J = 6.6 Hz, 1H, Ar) ppm, ¹⁹F NMR (375 MHz, CDCl₃): δ -76.23 ppm, ¹³C NMR (75 MHz, DMSO): δ 135.83 (Ar), 132.75 (Ar), 129.63 (C-CF₃), 129.05 (Ar), 127.52 (Ar), 126.35 (Ar), 125.76 (Ar), 124.07 (q, J = 286.91 Hz, C-F), 121.30 (Ar), 117.75 (Ar), 112.87 (Ar) ppm, ESI-MS: m/z 293 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₁₅H₁₂F₃N₂O m/z 293.0901 [M+H]⁺, found 293.0906.





CENTER FOR MASS SPECTROMETRY - CSIR IIC Agilent | Trusted Answers

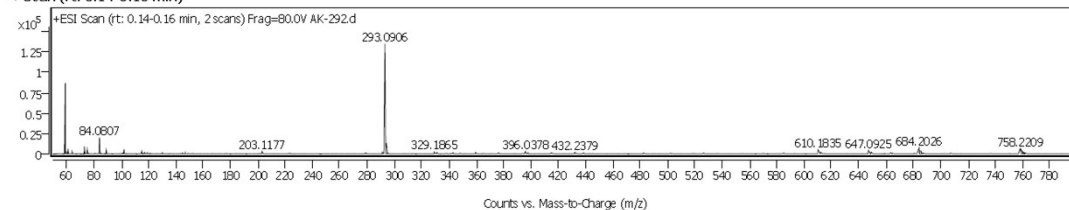
Sample Information

Name		Data File Path	E:\HRMS SAMPLES\2025\MAY_2025\09-05-2025\AK-292.d
Sample ID		Acq. Time (Local)	5/9/2025 12:48:56 PM (UTC+05:30)
Instrument	LCMS	Method Path (Acq)	I:\EXTERNAL SAMPLES\HRMS-01-05-2025 POS.m
MS Type	QTOF	Version (Acq SW)	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)
Inj. Vol. (ul)	1	IRM Status	All ions missed
Position	P1-E7	Method Path (DA)	
Plate Pos.		Target Source Path	
Operator		Result Summary	

Sample Chromatograms

Sample Spectra

+ Scan (rt: 0.14-0.16 min)



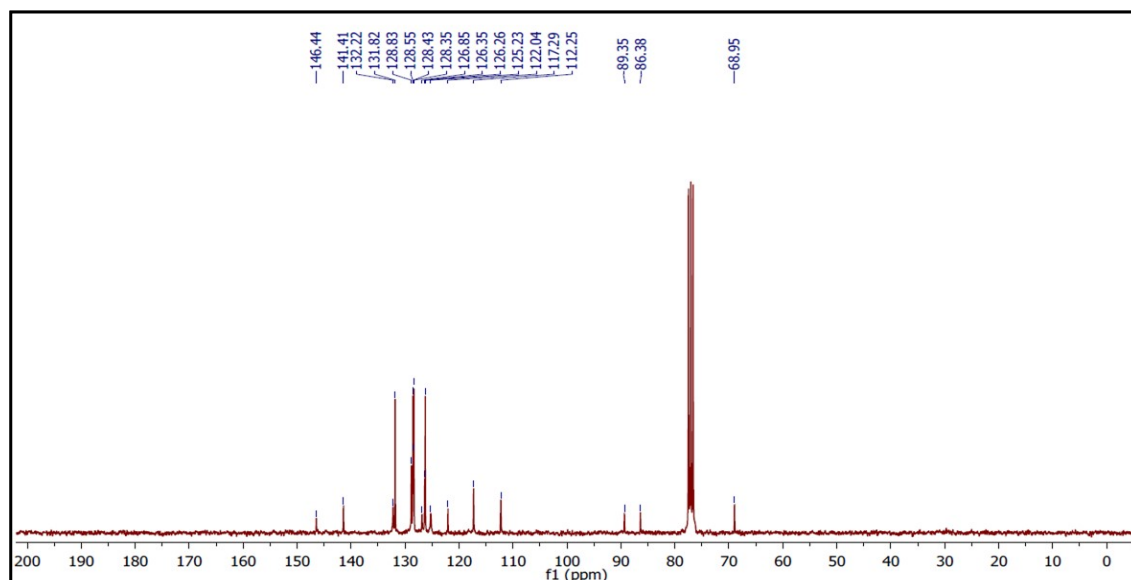
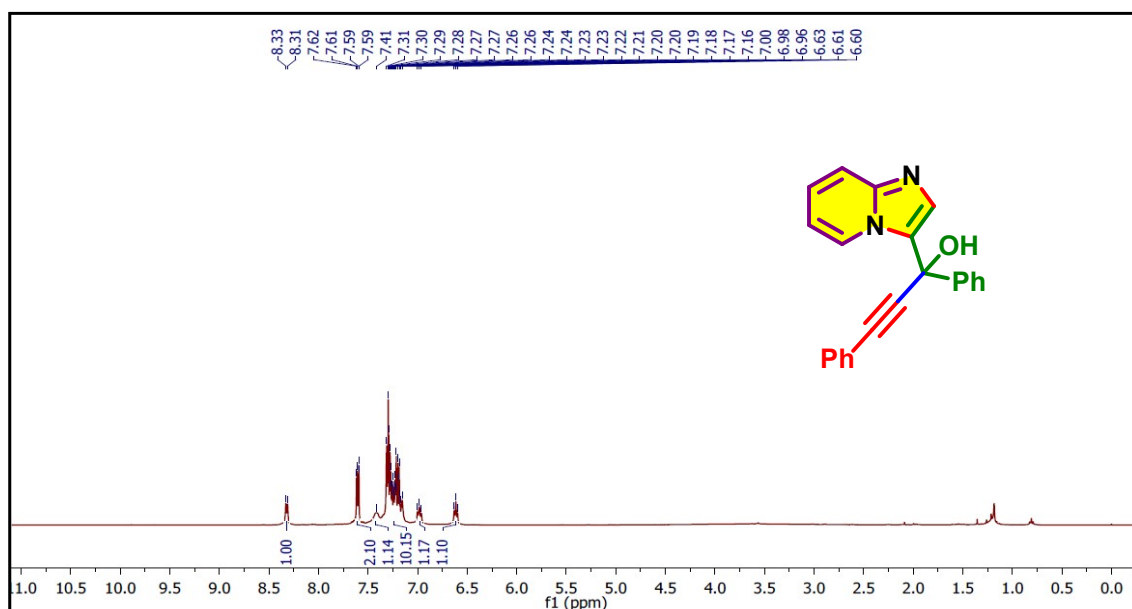
Spectrum Identification Table

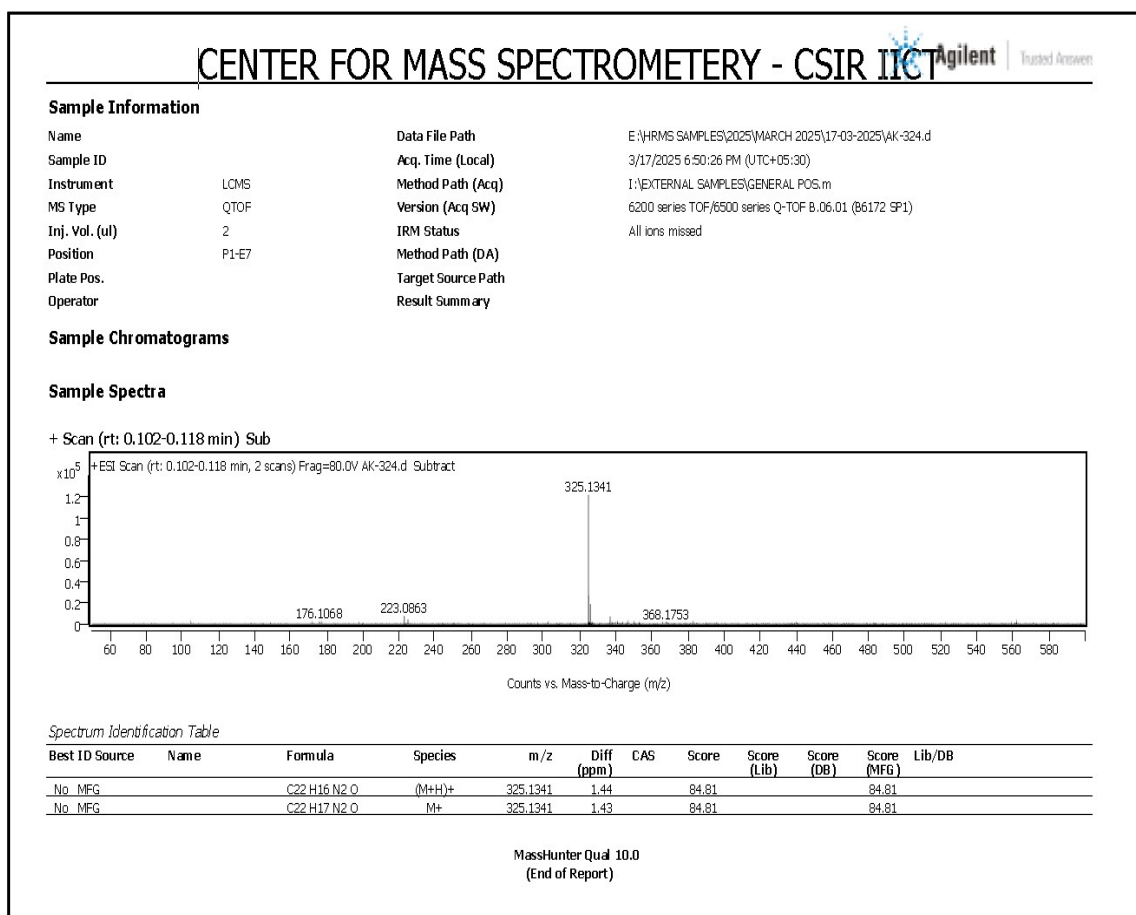
Best ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
No. MFG		C15H9F3N2O	(M+H)+	291.0735	-1.43		84.77			84.77	
No. MFG		C15H10F3N2O	M+	291.0735	-1.43		84.77			84.77	
No. MFG		C15H10N5O2	(M+H)+	293.0906	-0.58		73.25			73.25	
No. MFG		C15H11N5O2	M+	293.0906	-0.57		73.25			73.25	

MassHunter Qual 10.0
(End of Report)

1-(imidazo[1,2-*a*]pyridin-3-yl)-1,3-diphenylprop-2-yn-1-ol (6a)

Isolated as pale yellow solid, yield 83% (181 mg), m.p 212-214 °C, IR (ATR): 3421 (O-H stretching), 3142, 2961, 2127, 1596, 1524, 1462, 1044, 786, 721 cm⁻¹, ¹H NMR (400 MHz, CDCl₃): δ 8.32 (d, *J* = 6.8 Hz, 1H, Ar), 7.60 (dd, *J* = 8.0 Hz, 2H, Ar), 7.41 (s, 1H, -OH), 7.32 – 7.16 (m, 10H, Ar), 7.02 – 6.94 (m, 1H, Ar), 6.61 (t, *J* = 6.7 Hz, 1H, Ar) ppm, ¹³C NMR (75 MHz, CDCl₃): δ 146.44 (Ar), 141.41 (Ar), 132.22 (Ar), 131.82 (Ar), 128.83 (Ar), 128.55 (Ar), 128.43 (Ar), 128.35 (Ar), 126.85 (Ar), 126.35 (Ar), 126.26 (Ar), 125.23 (Ar), 122.04 (Ar), 117.29 (Ar), 112.25 (Ar), 89.35 (-C≡C-Ph), 86.38 (-C≡C-Ph), 68.95 (4°-Carbon) ppm, ESI-MS: *m/z* 325 [M+H]⁺, HRMS (ESI) Anal. calcd. for C₂₂H₁₇N₂O *m/z* 325.1340 [M+H]⁺, found 325.1341.





References:

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