

**Supporting Information for**

**One-Pot Domino Synthesis of Five and Six-Membered Fused  
Dihydropyridines Promoted by PPh<sub>3</sub>-NBS in Aqueous medium**

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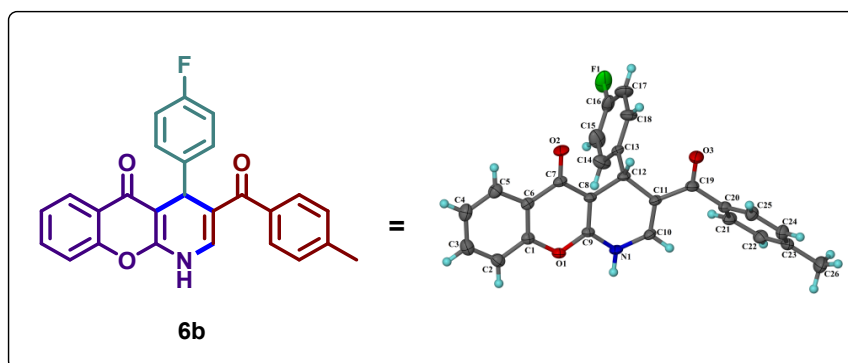
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## 1.1 X-ray crystallography data of compound 6b.



### ORTEP diagram of 6b

Figure caption: ORTEP diagram of KB478 compound with the atom-numbering. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. The CCDC deposition number **2246121** contains the supplementary crystallographic data for this paper which can be obtained free of charge at <https://www.ccdc.cam.ac.uk/structures/>

### Data collection and Structure solution details:

Single crystal X-ray data were collected at room temperature on a Bruker D8 QUEST equipped with a four-circle kappa diffractometer and Photon 100 detector. An I $\mu$ s microfocus Mo source ( $\lambda=0.71073\text{\AA}$ ) supplied the multi-mirror monochromated incident beam. A combination of Phi and Omega scans were used to collect the necessary data. Integration and scaling of intensity data were accomplished using SAINT program.<sup>1</sup> The structures were solved by Direct Methods using SHELXS972 and refinement was carried out by full-matrix least-squares technique using SHELXL-2014/7.2-3 Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms, with C-H distances of 0.93--0.97 Å, and with Uiso(H) = 1.2Ueq (C) or 1.5Ueq for methyl atoms. The CCDC deposition number 2246121 contains the supplementary crystallographic data for this paper which can be obtained free of charge at <https://www.ccdc.cam.ac.uk/structures/>

1. SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.

2. Sheldrick, G. M. SHELXS97 and SHELXL Version 2014/7, <http://shelx.uniuc.gwdg.de/SHELX/index.php>
3. Muller, P, Herbst-Imer, R, Spek, A. L, Schneider, T. R, and Sawaya, M. R. Crystal Structure Refinement: A Crystallographer's Guide to SHELXL. Muller, P. Ed. 2006 Oxford University Press: Oxford, New York, pp. 57–91.

## 1.2 Experimental section

### General

Melting points were measured by CINTEX programmable melting point apparatus and are uncorrected.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  NMR spectra of samples in  $\text{CDCl}_3$  recorded on AVANCE- 300, 400, 500 MHz spectrometers. Chemical shifts ( $\delta$ ) 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.

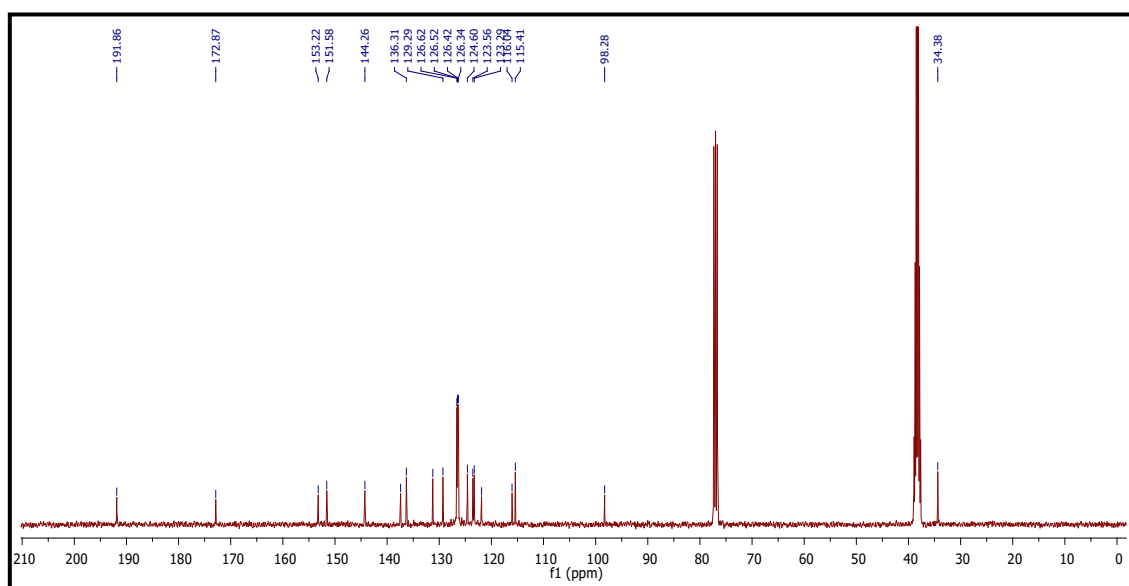
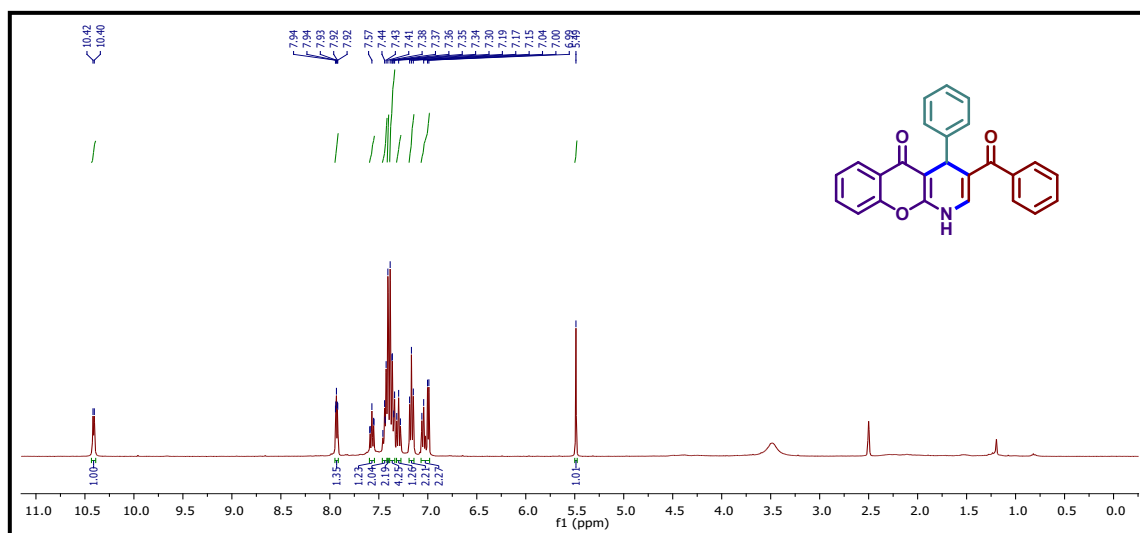
### General Procedure for the Synthesis of chromenodihydropyridines (6a-6s) and pyrazolo/isoxazolodihydropyridines (8a-8i).

A mixture of  $\text{PPh}_3$  (224 mg, 1 equiv) and NBS (152 mg, 1 equiv) were stirred for 30 minutes in water at room temperature. To this reaction mixture added benzaldehyde **3** (90.8 mg, 1 equiv, 0.83 mmol), 2-amino-4*H*-chromenone **1** (165 mg, 1.2 equiv, 1 mmol) and  $\beta$ -enaminone **2** (150 mg, 1 equiv, 0.83 mmol) then stirred at reflux (100 °C) temperature for 3 h. After completion of the reaction monitored by TLC, the resulting mixture was cooled down to room temperature and workup with water (20 mL) and ethyl acetate (30 mL). Further, separated organic layer dried over anhydrous sodium sulphate and evaporated under reduced pressure, crude product was purified by column chromatography, (Silica gel 60-120 mesh, hexane-ethyl acetate) to afford the isolated yield of **6a** is 78% (253 mg) and similar procedure for all the corresponding products **6a-6s** & **8a-8i**.

### 1.3 Spectroscopic data and copies <sup>1</sup>H & <sup>13</sup>C of compounds.

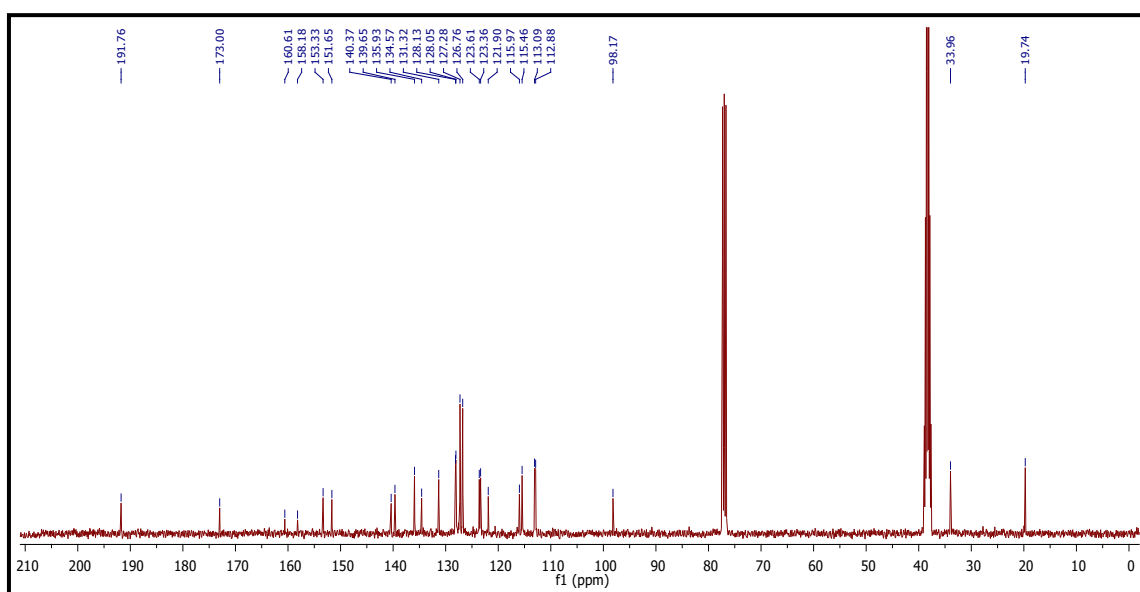
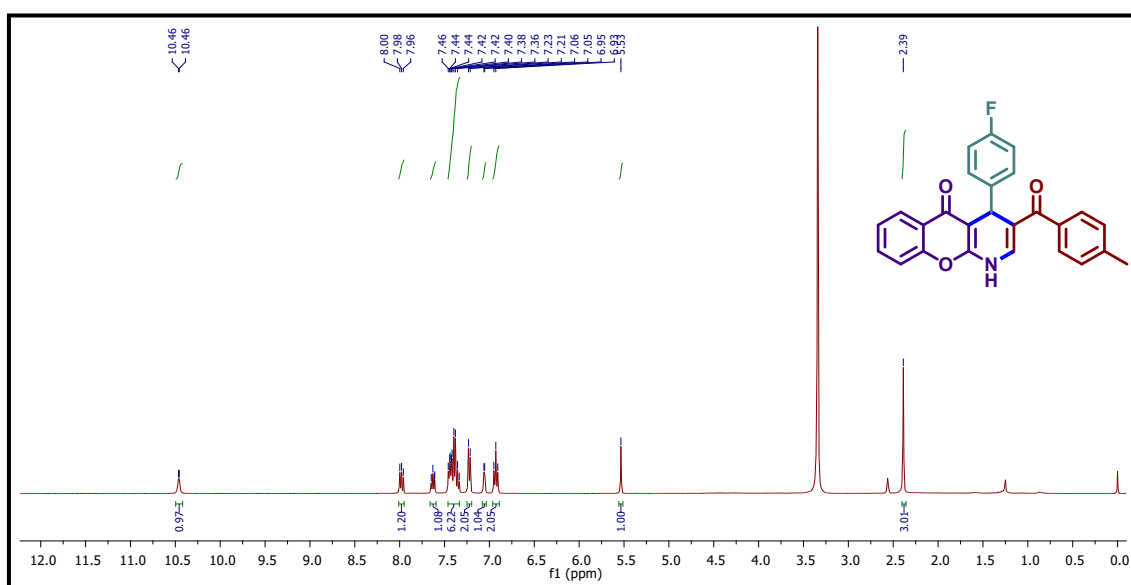
#### 3-benzoyl-4-phenyl-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6a).

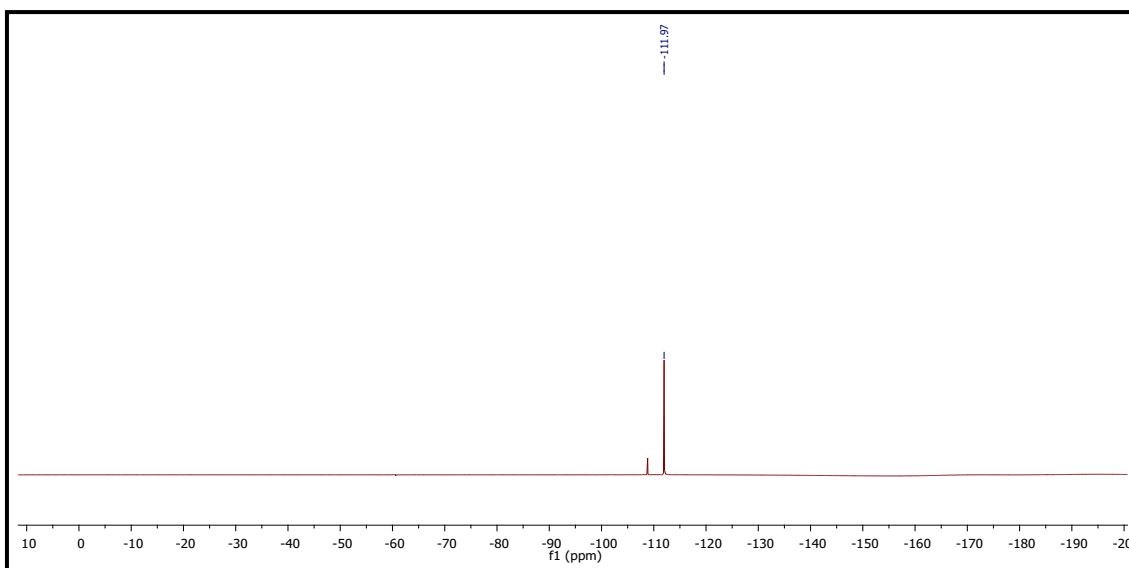
Isolated as a yellow colour solid, yield 78% (253 mg), m.p 228-230 °C, IR (ATR): 3204, 3082, 3010, 1657, 1620, 1572, 1512, 1472, 1363, 1295, 1202, 1132, 942 cm<sup>-1</sup>, <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>) δ 10.41 (br, NH), 7.95 – 7.91 (m, 1H), 7.60 – 7.54 (m, 1H), 7.44 (dd, *J* = 7.8, 5.5 Hz, 2H), 7.41 (s, 2H), 7.39 – 7.34 (m, 4H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 2H), 7.04 – 7.00 (m, 2H), 5.49 (s, 1H) ppm, <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 191.86, 172.87, 153.22, 151.58, 144.26, 137.41, 136.31, 131.24, 129.29, 126.62, 126.52, 126.42, 126.34, 124.60, 123.56, 123.29, 121.88, 116.04, 115.41, 98.28, 34.38 ppm, ESI-MS: *m/z* 380 [M+H]<sup>+</sup>, HRMS (ESI) Anal. calcd. for C<sub>25</sub>H<sub>18</sub>NO<sub>3</sub> *m/z* 380.1281 [M+H]<sup>+</sup>, found 380.1265.



**4-(4-fluorophenyl)-3-(4-methylbenzoyl)-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6b).**

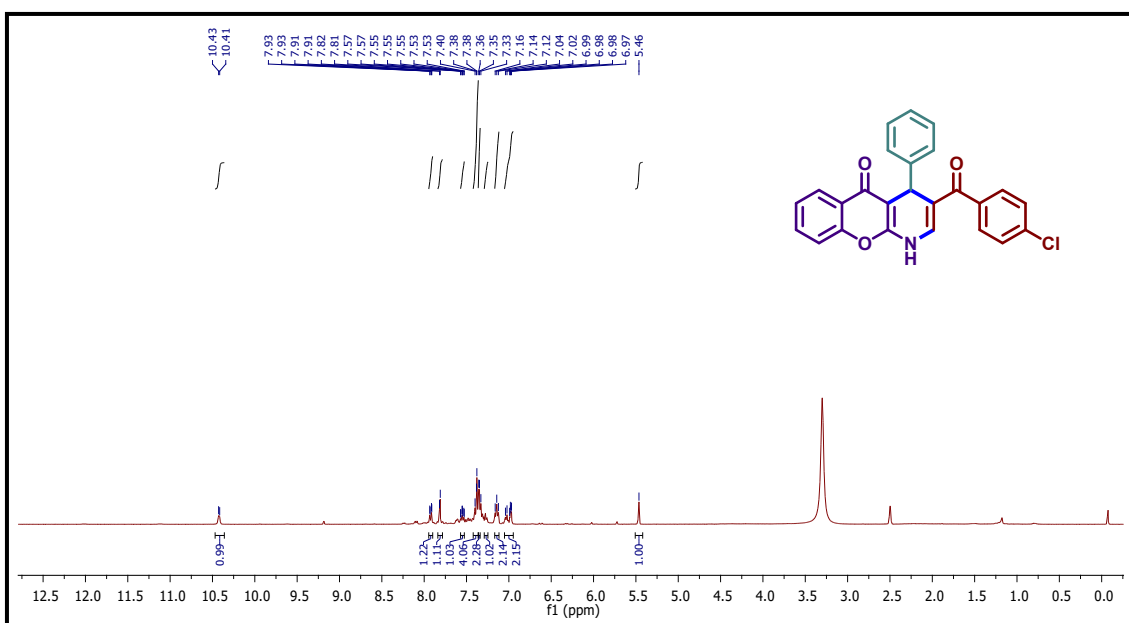
Isolated as a yellow colour solid, yield 80% (240 mg), m.p 245-247 °C, IR (ATR): 3210, 3092, 3026, 1660, 1642, 1582, 1525, 1482, 1380, 1315, 1216, 1142, 950, 780  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  10.46 (br, NH), 8.01 – 7.95 (m, 1H), 7.59 – 7.55 (m, 1H), 7.47 – 7.33 (m, 6H), 7.22 (d,  $J = 7.8$  Hz, 2H), 7.06 (d,  $J = 3.4$  Hz, 1H), 6.93 (t,  $J = 8.7$  Hz, 2H), 5.53 (s, 1H), 2.39 (s, 3H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  191.76, 173.00, 159.39 (d,  $J = 244.0$  Hz), 153.33, 151.65, 140.37, 139.65, 135.93, 134.57, 131.32, 128.13, 128.05, 127.28, 126.76, 123.61, 123.36, 121.90, 115.97, 115.46, 112.98 (d,  $J = 21.0$  Hz), 98.17, 33.96, 19.74,  $^{19}\text{F}$  NMR (376 MHz): -111.97 ppm, ESI-MS:  $m/z$  410  $[\text{M-H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{26}\text{H}_{17}\text{FNO}_3$   $m/z$  410.1187  $[\text{M-H}]^+$ , found 410.1205.

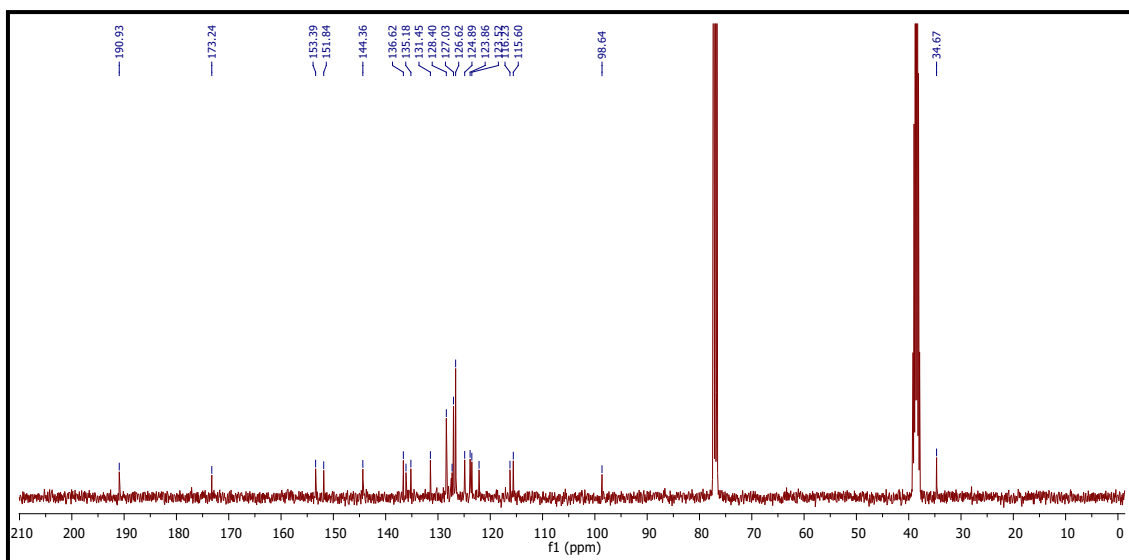




### 3-(4-chlorobenzoyl)-4-phenyl-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6c).

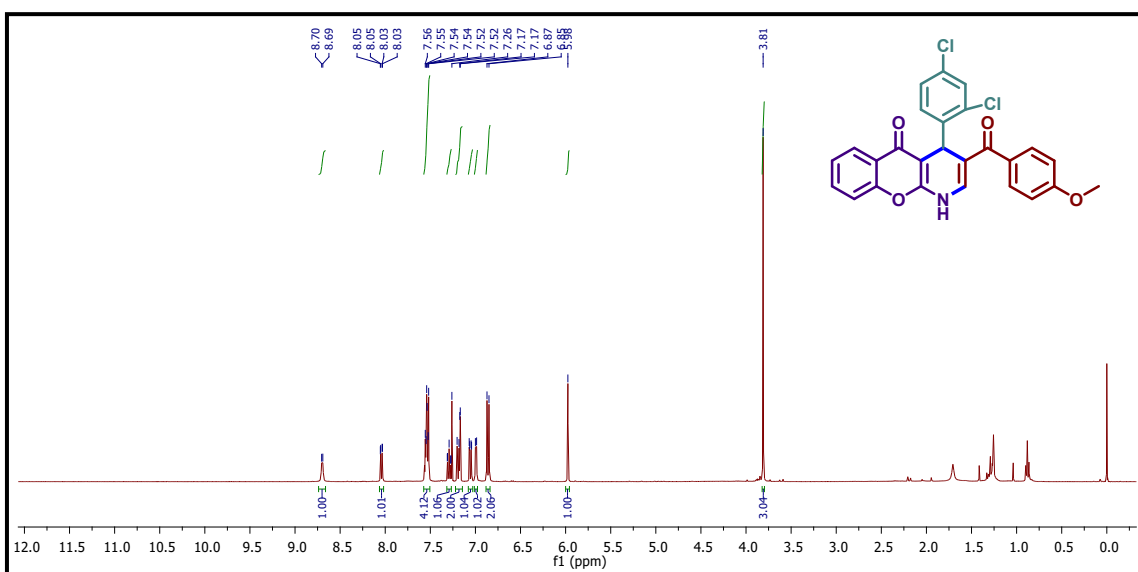
Isolated as a pale yellow colour solid, yield 79% (279 mg), m.p 247-249 °C, IR (ATR): 3201, 3086, 3017, 2924, 2855, 1660, 1614, 1557, 1523, 1490, 1462, 1411, 1351, 1304, 945  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  10.42 (br, NH), 7.92 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.81 – 7.82 (m, 1H), 7.57 – 7.53 (m, 1H), 7.42 – 7.36 (m, 4H), 7.35 – 7.33 (m, 2H), 7.29 – 7.25 (m, 1H), 7.14 (t,  $J = 7.6$  Hz, 2H), 7.05 – 6.95 (m, 2H), 5.46 (s, 1H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3+\text{DMSO-d}_6$ ):  $\delta$  190.93, 173.24, 153.39, 151.84, 144.36, 136.62, 136.11, 135.18, 131.45, 128.4, 127.3, 127.03, 126.62, 124.89, 123.86, 123.52, 122.15, 116.23, 115.6, 98.64, 34.67 ppm, ESI-MS:  $m/z$  412  $[\text{M-H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{25}\text{H}_{15}\text{ClNO}_3$   $m/z$  412.0735  $[\text{M-H}]^+$ , found 412.0750.

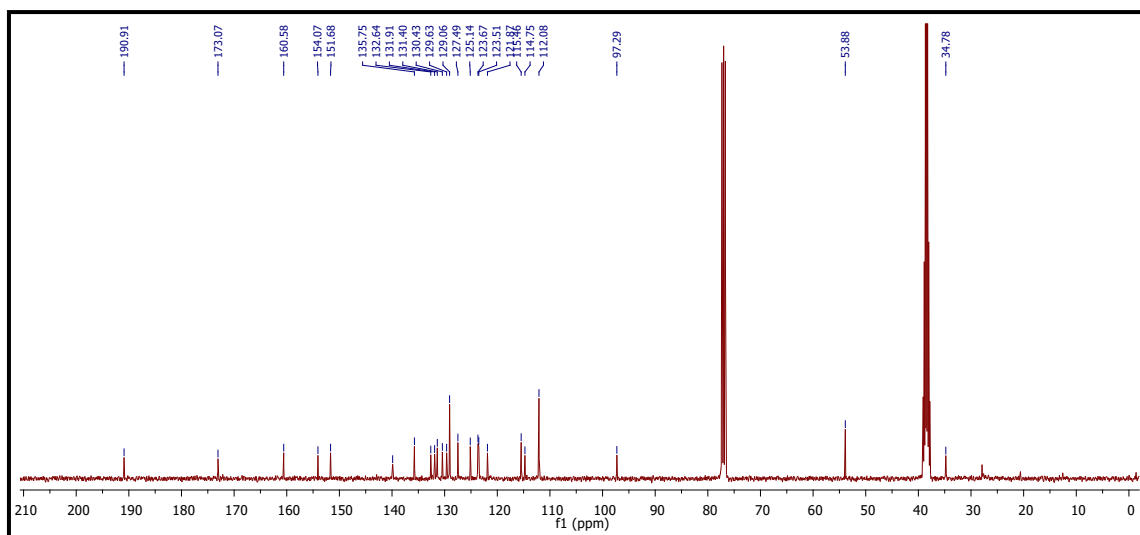




**4-(2,4-dichlorophenyl)-3-(4-methoxybenzoyl)-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6d).**

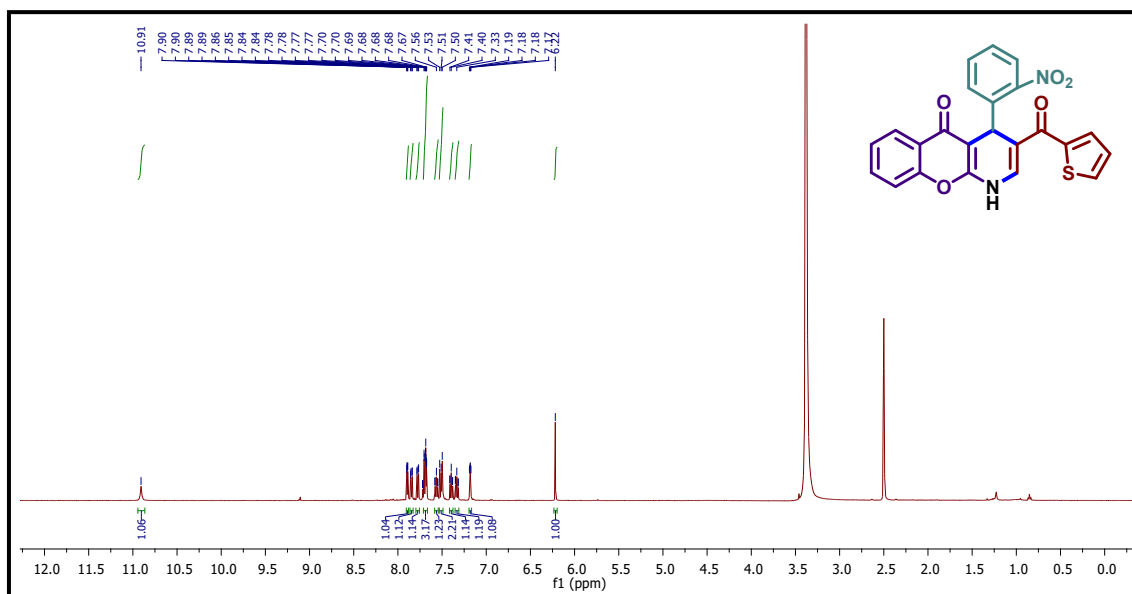
Isolated as a yellow colour solid, yield 87% (215 mg), m.p 158-160 °C, IR (ATR): 3151, 3011, 2925, 2851, 1661, 1598, 1464, 1409, 1369, 1306, 1247, 1167, 970, 906  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ +DMSO- $d_6$ ):  $\delta$  8.70 (br, NH), 8.04 (dd,  $J = 7.9, 1.6$  Hz, 1H), 7.57 – 7.51 (m, 4H), 7.32 – 7.27 (m, 1H), 7.18 (dd,  $J = 8.9, 5.3$  Hz, 2H), 7.06 (dd,  $J = 8.3, 2.2$  Hz, 1H), 6.99 (d,  $J = 5.3$  Hz, 1H), 6.86 (d,  $J = 8.8$  Hz, 2H), 5.98 (s, 1H), 3.81 (s, 3H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ +DMSO- $d_6$ ):  $\delta$  190.91, 173.07, 160.58, 154.07, 151.68, 139.88, 135.75, 132.64, 131.91, 131.4, 130.43, 129.63, 129.06, 127.49, 125.14, 123.67, 123.51, 121.87, 115.46, 114.75, 112.08, 97.29, 53.88, 34.78 ppm, ESI-MS:  $m/z$  476  $[\text{M}-\text{H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{26}\text{H}_{17}\text{Cl}_2\text{NO}_4$   $m/z$  476.0450  $[\text{M}-\text{H}]^+$ , found 476.0475.



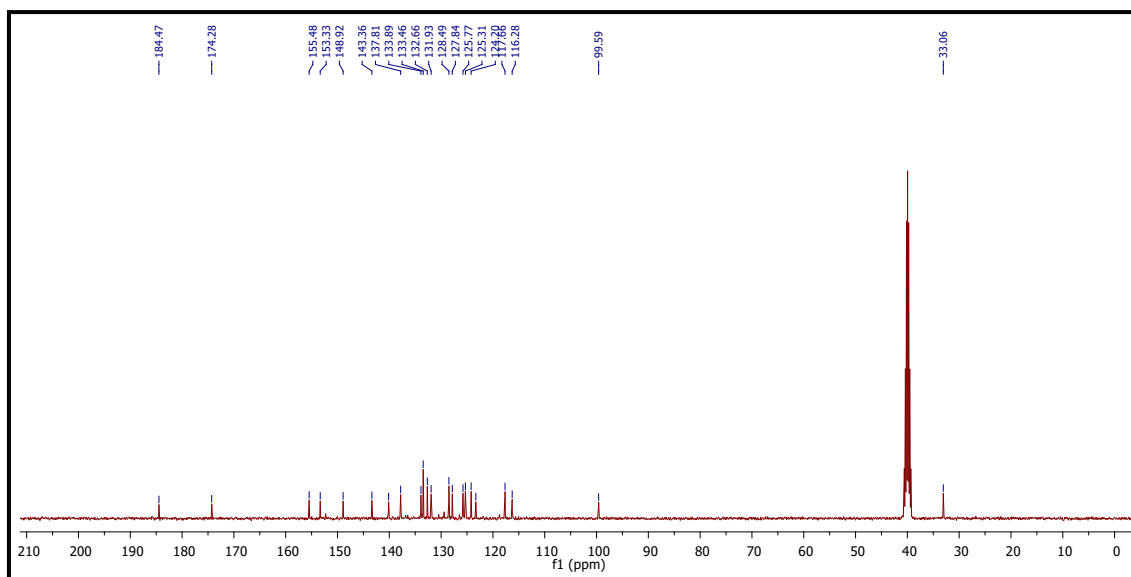


**4-(2-nitrophenyl)-3-(thiophene-3-carbonyl)-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6e).**

Isolated as a pale yellow colour solid, yield 72% (186 mg), m.p 178-180 °C, IR (ATR): 3210, 3019, 2840, 2450, 1721, 1599, 1534, 1254, 1214, 1170, 1026, 970, 850 cm<sup>-1</sup>, <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>): δ 10.91 (br, NH), 7.89 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.85 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.78 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.71 – 7.66 (m, 3H), 7.58 – 7.54 (m, 1H), 7.53 – 7.49 (m, 2H), 7.42 – 7.38 (m, 1H), 7.35 – 7.31 (m, 1H), 7.18 (dd, *J* = 4.9, 3.8 Hz, 1H), 6.22 (s, 1H) ppm, <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>): δ 184.47, 174.28, 155.48, 153.33, 148.92, 143.36, 137.81, 133.89, 133.46, 132.66, 131.93, 128.49, 127.84, 125.31, 124.2, 123.3, 117.66, 116.28, 99.59, 33.06 ppm, ESI-MS: *m/z* 431 [M+H]<sup>+</sup>, HRMS (ESI) Anal. calcd. for C<sub>23</sub>H<sub>15</sub>N<sub>2</sub>O<sub>5</sub>S *m/z* 431.0696 [M+H]<sup>+</sup>, found 431.0677.

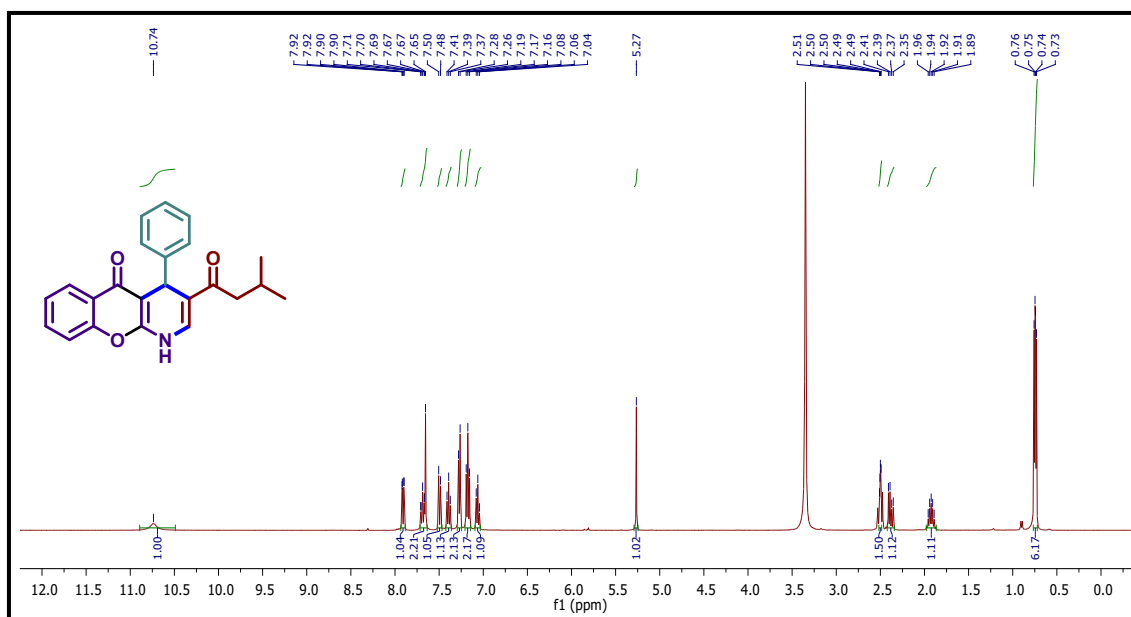


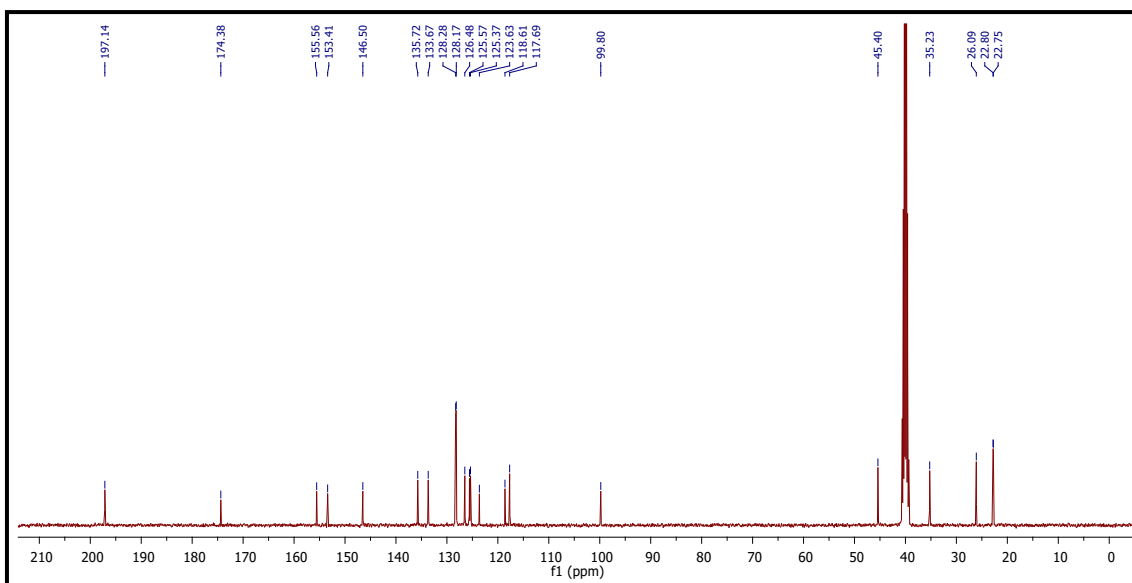




### 3-(3-methylbutanoyl)-4-phenyl-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6f).

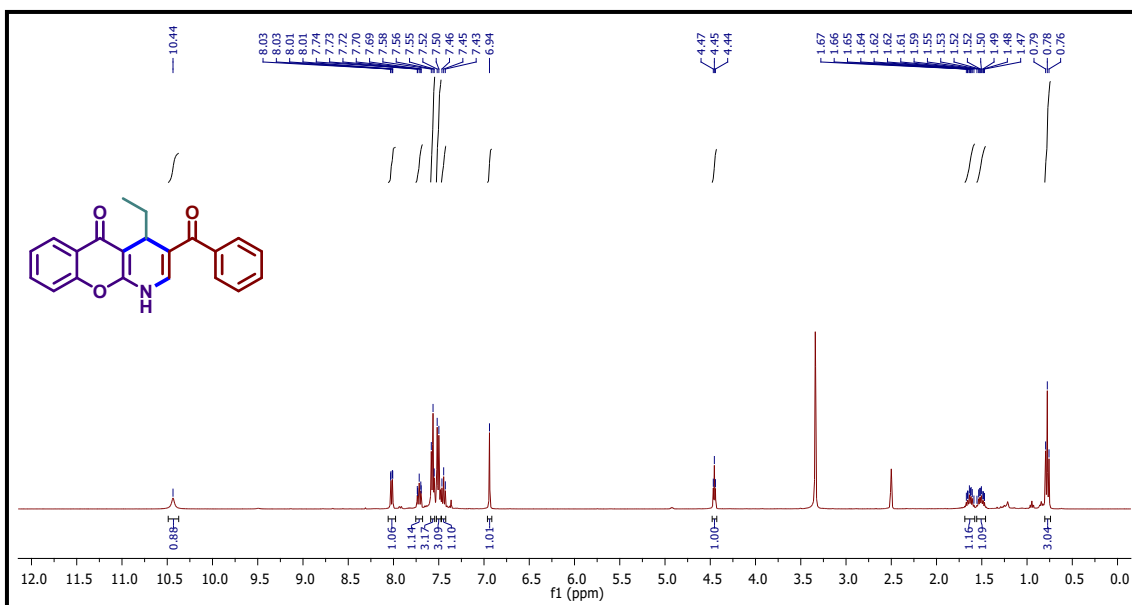
Isolated as a light yellow colour solid, yield 75% (230 mg), m.p 208-210 °C, IR (ATR): 3153, 3018, 2958, 1609, 1539, 1478, 1373, 1271, 1211, 960  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  10.74 (br, NH), 7.91 (dd,  $J = 7.9, 1.6$  Hz, 1H), 7.72 – 7.63 (m, 2H), 7.49 (d,  $J = 8.3$  Hz, 1H), 7.39 (t,  $J = 7.5$  Hz, 1H), 7.27 (d,  $J = 7.3$  Hz, 2H), 7.17 (t,  $J = 7.6$  Hz, 2H), 7.06 (t,  $J = 7.3$  Hz, 1H), 5.27 (s, 1H), 2.52 – 2.49 (m, 1H), 2.38 (dd,  $J = 14.7, 7.3$  Hz, 1H), 1.96 – 1.89 (m, 1H), 0.74 (d,  $J = 6.6$  Hz, 6H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  197.14, 174.38, 155.56, 153.41, 146.5, 135.72, 133.67, 128.28, 128.17, 126.48, 125.57, 125.37, 123.63, 118.61, 117.69, 99.8, 45.4, 35.23, 26.09, 22.8, 22.75 ppm, ESI-MS:  $m/z$  360  $[\text{M}+\text{H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{23}\text{H}_{22}\text{NO}_3$   $m/z$  360.1594  $[\text{M}+\text{H}]^+$ , found 360.1582.





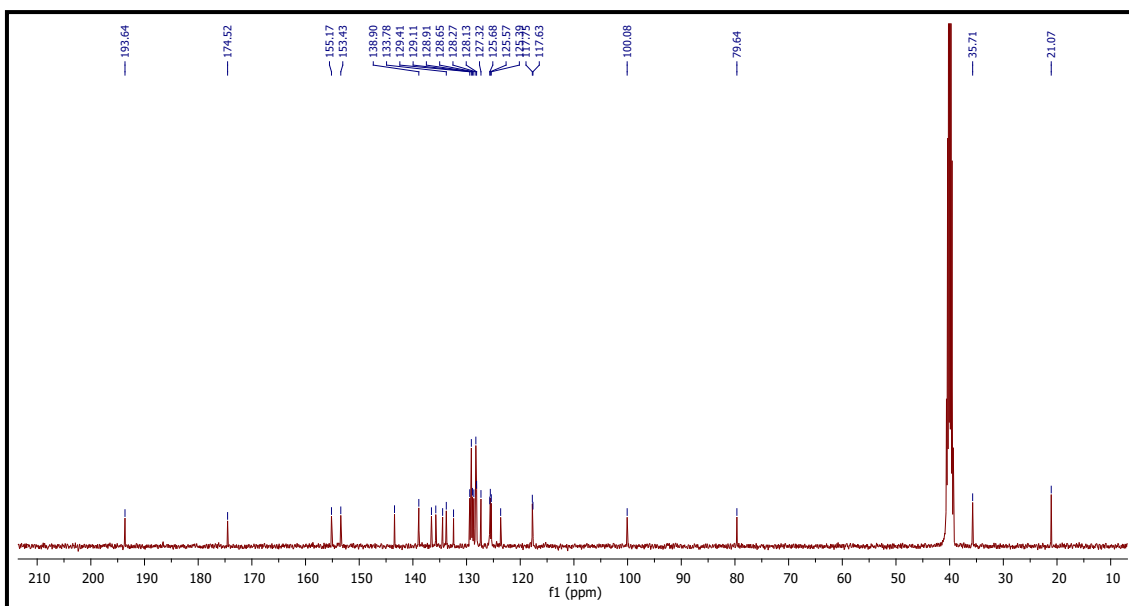
### 3-benzoyl-4-ethyl-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6g).

Isolated as a yellow colour solid, yield 73% (378 mg), m.p 240-242 °C, IR (ATR): 3357, 3017, 2876, 2382, 1659, 1611, 1487, 1310, 1273, 932, 854 cm<sup>-1</sup>, <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ 10.44 (br, NH), 8.02 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.75 – 7.68 (m, 1H), 7.57 (t, *J* = 6.4 Hz, 3H), 7.51 (d, *J* = 7.5 Hz, 3H), 7.45 (t, *J* = 7.5 Hz, 1H), 6.94 (s, 1H), 4.45 (t, *J* = 4.7 Hz, 1H), 1.67 – 1.62 (m, 1H), 1.59 – 1.47 (m, 1H), 0.78 (t, *J* = 7.5 Hz, 3H) ppm, <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>): δ 194.32, 174.84, 156.22, 153.47, 139.96, 139.54, 133.63, 131.44, 128.90, 128.63, 125.63, 125.43, 123.58, 117.72, 116.54, 98.16, 30.92, 27.01, 9.56 ppm, ESI-MS: *m/z* 332 [M+H]<sup>+</sup>, HRMS (ESI) Anal. calcd. for C<sub>21</sub>H<sub>18</sub>NO<sub>3</sub> *m/z* 332.1281 [M+H]<sup>+</sup>, found 332.1269.



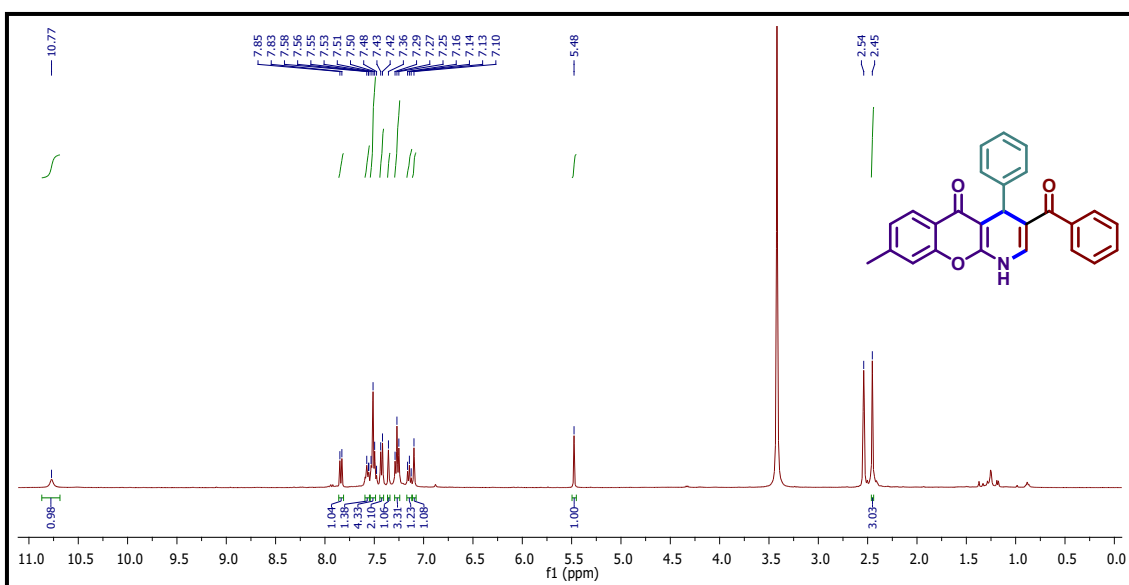


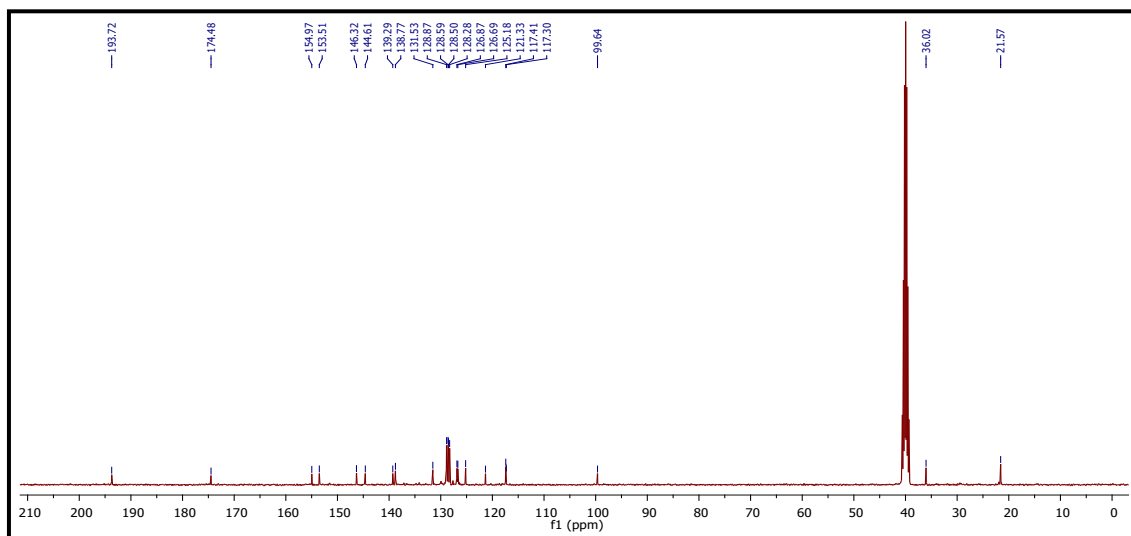




### 3-benzoyl-8-methyl-4-phenyl-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6i).

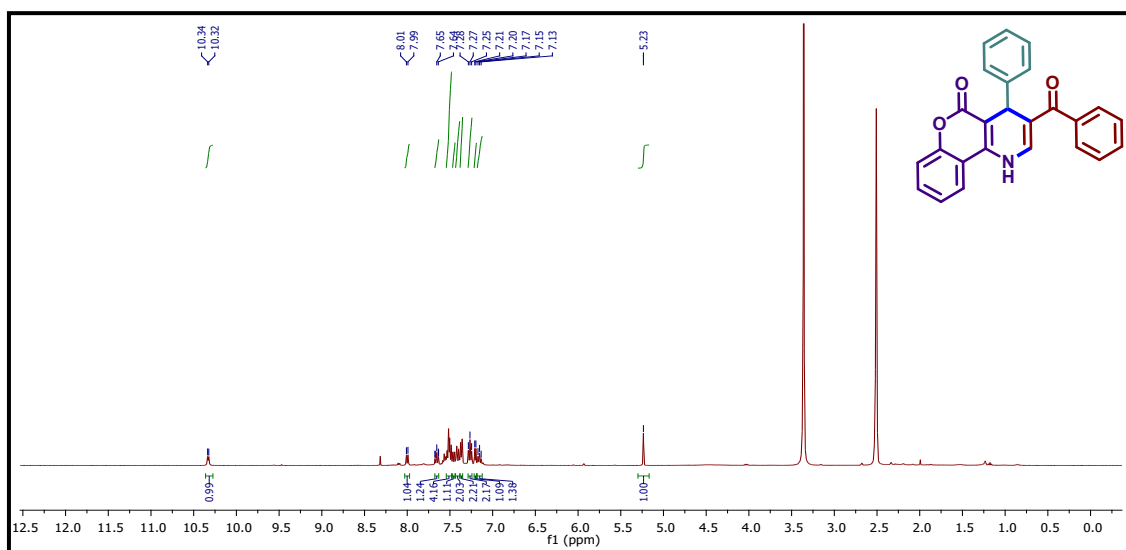
Isolated as a light yellow colour solid, yield 79% (266 mg), m.p 255-257 °C, IR (ATR): 3181, 3061, 2952, 2857, 1613, 1536, 1487, 1374, 1266, 1112, 970  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz, DMSO-  $d_6$ ):  $\delta$  10.73 (br, NH), 7.80 (d,  $J = 8.0$  Hz, 1H), 7.55 – 7.51 (m, 1H), 7.47 (t,  $J = 7.3$  Hz, 4H), 7.39 (d,  $J = 7.3$  Hz, 2H), 7.32 (s, 1H), 7.23 (t,  $J = 7.7$  Hz, 3H), 7.11 (d,  $J = 7.3$  Hz, 1H), 7.06 (s, 1H), 5.44 (s, 1H), 2.41 (s, 3H) ppm,  $^{13}\text{C}$  NMR (101 MHz, DMSO- $d_6$ ):  $\delta$  193.72, 174.48, 154.97, 153.51, 146.32, 144.61, 139.29, 138.77, 131.53, 128.87, 128.59, 128.5, 128.28, 126.87, 126.69, 125.18, 121.33, 117.41, 117.3, 99.64, 36.02, 21.57 ppm, ESI-MS:  $m/z$  392  $[\text{M}-\text{H}]^-$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{26}\text{H}_{18}\text{NO}_3$   $m/z$  392.1281  $[\text{M}-\text{H}]^-$ , found 392.1298.

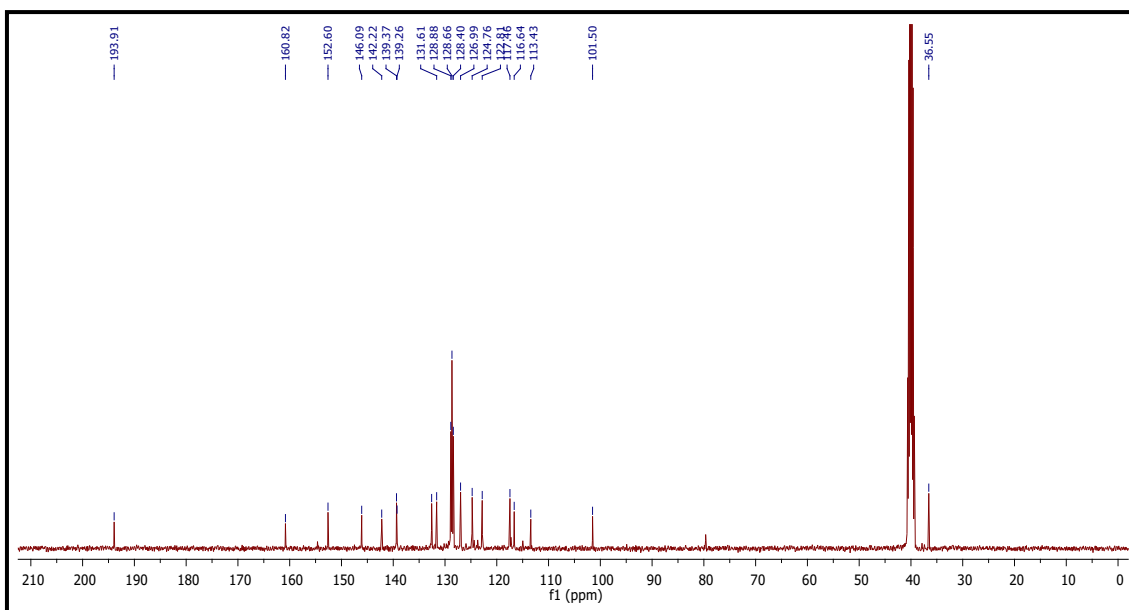




### 3-benzoyl-4-phenyl-1,4-dihydro-5H-chromeno[4,3-b]pyridin-5-one (6j).

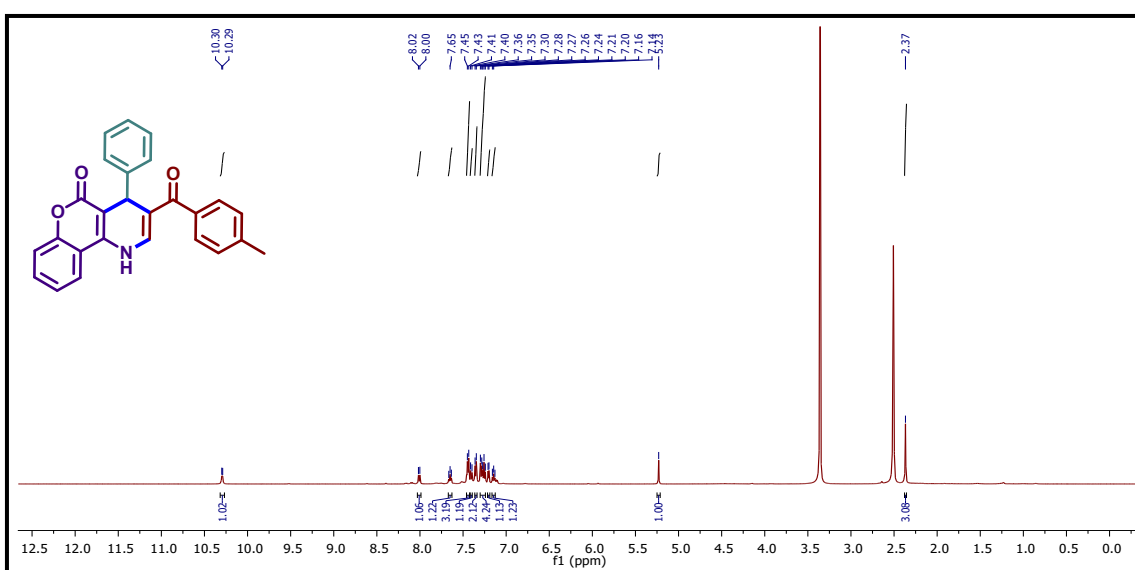
Isolated as a yellow colour solid, yield 80% (259 mg), m.p 210-212 °C, IR (ATR): 3206, 3087, 3023, 1657, 1632, 1571, 1508, 1473, 1369, 1299, 1201, 1131, 940  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  10.33 (br, NH), 8.00 (d,  $J = 7.1$  Hz, 1H), 7.68 – 7.63 (m, 1H), 7.54 – 7.48 (m, 4H), 7.47 – 7.44 (m, 1H), 7.41 (d,  $J = 8.3$  Hz, 2H), 7.37 (d,  $J = 7.2$  Hz, 2H), 7.27 (t,  $J = 7.6$  Hz, 2H), 7.20 (d,  $J = 5.5$  Hz, 1H), 7.15 (t,  $J = 7.3$  Hz, 1H), 5.23 (s, 1H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  193.91, 160.82, 152.6, 146.09, 142.22, 139.37, 139.26, 132.5, 131.61, 128.88, 128.66, 128.4, 126.99, 124.76, 122.81, 117.46, 116.64, 113.43, 101.5, 79.65, 36.55 ppm, ESI-MS:  $m/z$  378  $[\text{M-H}]^-$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{25}\text{H}_{16}\text{NO}_3$   $m/z$  378.1124  $[\text{M-H}]^-$ , found 378.1141.

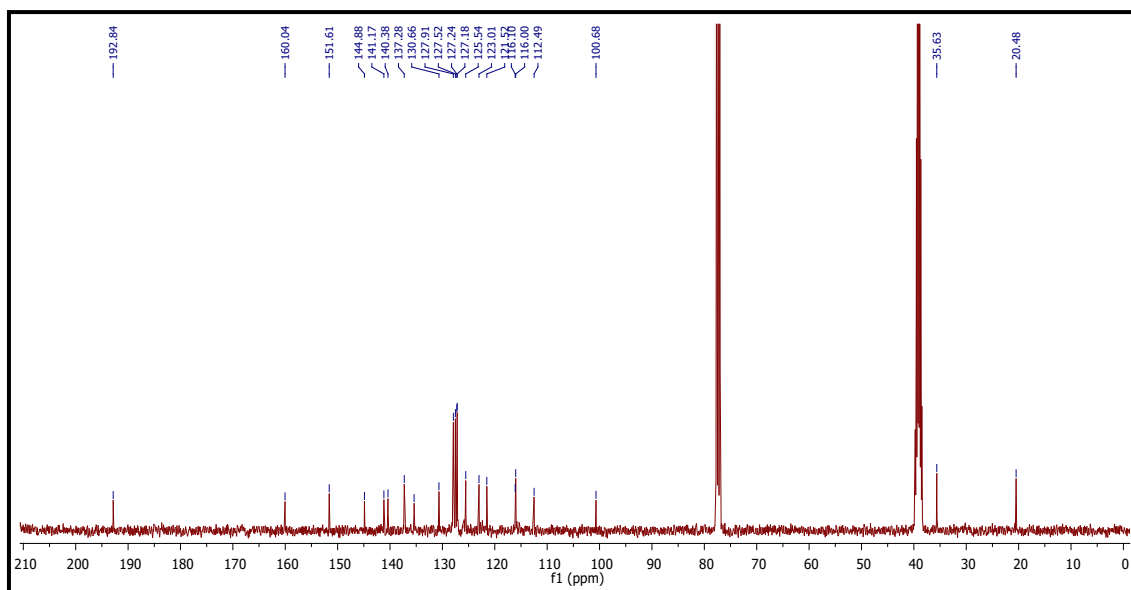




### 3-(4-methylbenzoyl)-4-phenyl-1,4-dihydro-5H-chromeno[4,3-b]pyridin-5-one (6k).

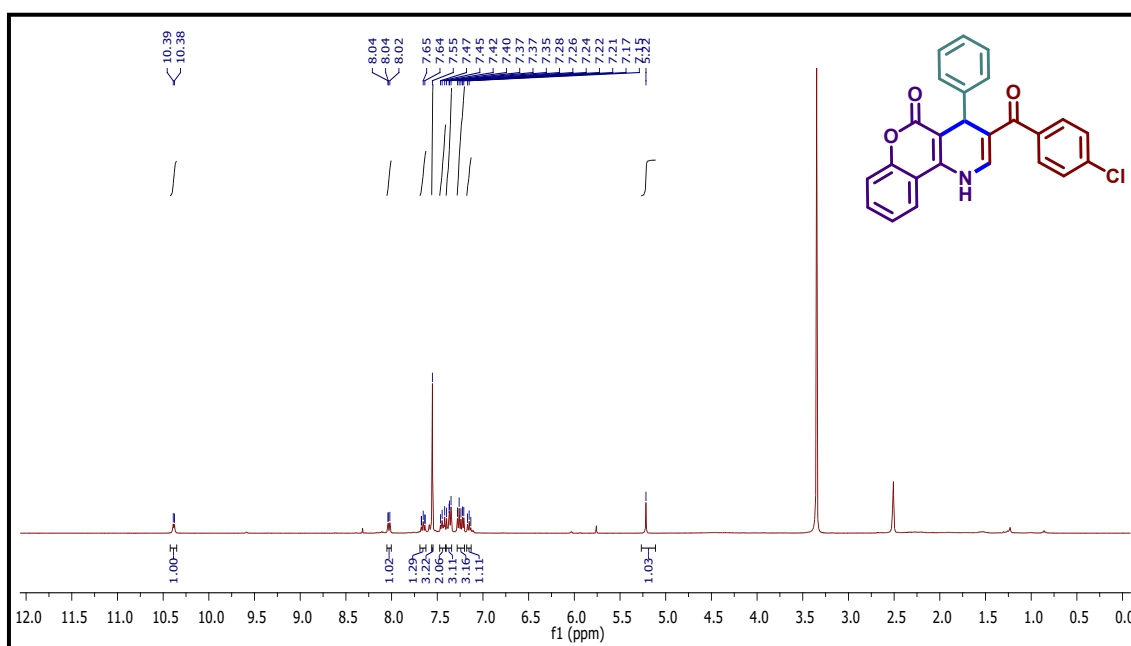
Isolated as a yellow colour solid, yield 80% (269 mg), m.p 210-212 °C, IR (ATR): 3222, 3054, 2956, 1672, 1590, 1485, 1365, 1296, 1191, 1075, 920  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-d}_6+\text{CDCl}_3$ ):  $\delta$  10.29 (br, NH), 8.01 (d,  $J = 8.0$  Hz, 1H), 7.65 (t,  $J = 7.4$  Hz, 1H), 7.44 (d,  $J = 7.9$  Hz, 3H), 7.40 (d,  $J = 8.3$  Hz, 1H), 7.35 (d,  $J = 7.2$  Hz, 2H), 7.30 – 7.24 (m, 4H), 7.20 (d,  $J = 5.4$  Hz, 1H), 7.14 (t,  $J = 7.3$  Hz, 1H), 5.23 (s, 1H), 2.37 (s, 3H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-d}_6+\text{CDCl}_3$ ):  $\delta$  192.84, 160.04, 151.61, 144.88, 141.17, 140.38, 137.28, 135.4, 130.66, 127.91, 127.52, 127.24, 127.18, 125.54, 123.01, 121.52, 116.1, 116.0, 112.49, 100.68, 35.63, 20.48 ppm, ESI-MS:  $m/z$  392  $[\text{M-H}]^-$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{26}\text{H}_{18}\text{NO}_3$   $m/z$  392.1281  $[\text{M-H}]^-$ , found 392.1298.



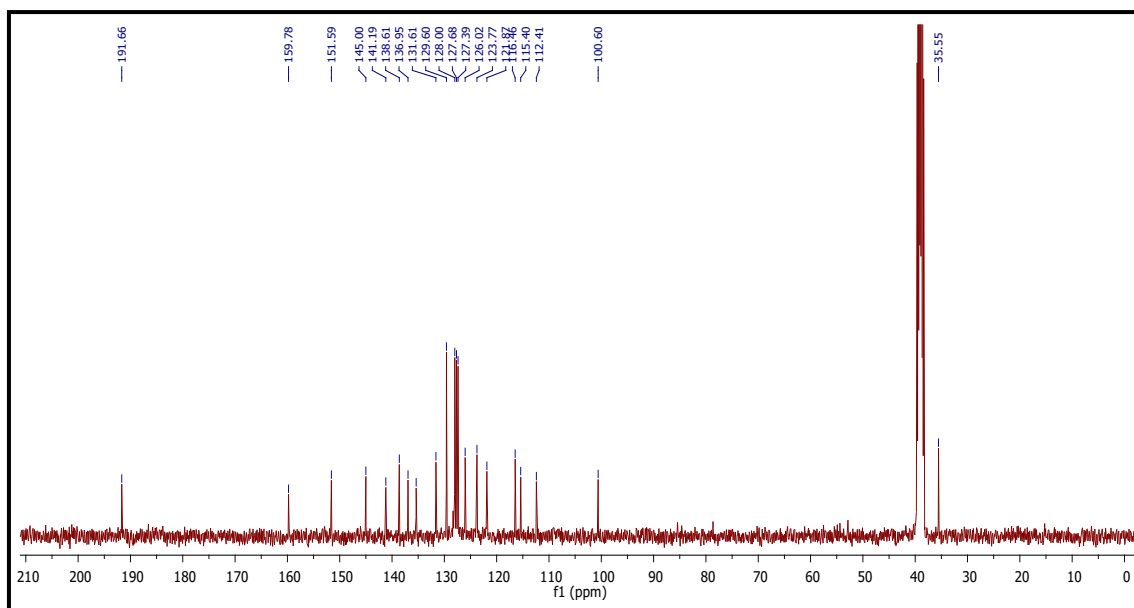


### 3-(4-chlorobenzoyl)-4-phenyl-1,4-dihydro-5H-chromeno[4,3-b]pyridin-5-one (6l).

Isolated as a yellow colour solid, yield 78% (276 mg), m.p 263-265 °C, IR (ATR): 3202, 3084, 3012, 2955, 2861, 1672, 1615, 1560, 1525, 1492, 1472, 1412, 1353, 1306, 952  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  10.38 (br, NH), 8.05 – 8.00 (m, 1H), 7.69 – 7.62 (m, 1H), 7.55 (s, 3H), 7.47 – 7.41 (m, 2H), 7.37 (dd,  $J = 10.3, 9.1$  Hz, 3H), 7.28 – 7.20 (m, 3H), 7.15 (t,  $J = 7.3$  Hz, 1H), 5.22 (s, 1H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  191.66, 159.78, 151.59, 145.0, 141.19, 138.61, 136.95, 135.39, 131.61, 129.6, 128.0, 127.68, 127.39, 126.02, 123.77, 121.87, 116.46, 115.4, 112.41, 100.6, 35.55 ppm, ESI-MS:  $m/z$  412  $[\text{M-H}]^-$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{25}\text{H}_{15}\text{ClNO}_3$   $m/z$  412.0735  $[\text{M-H}]^-$ , found 412.0747.

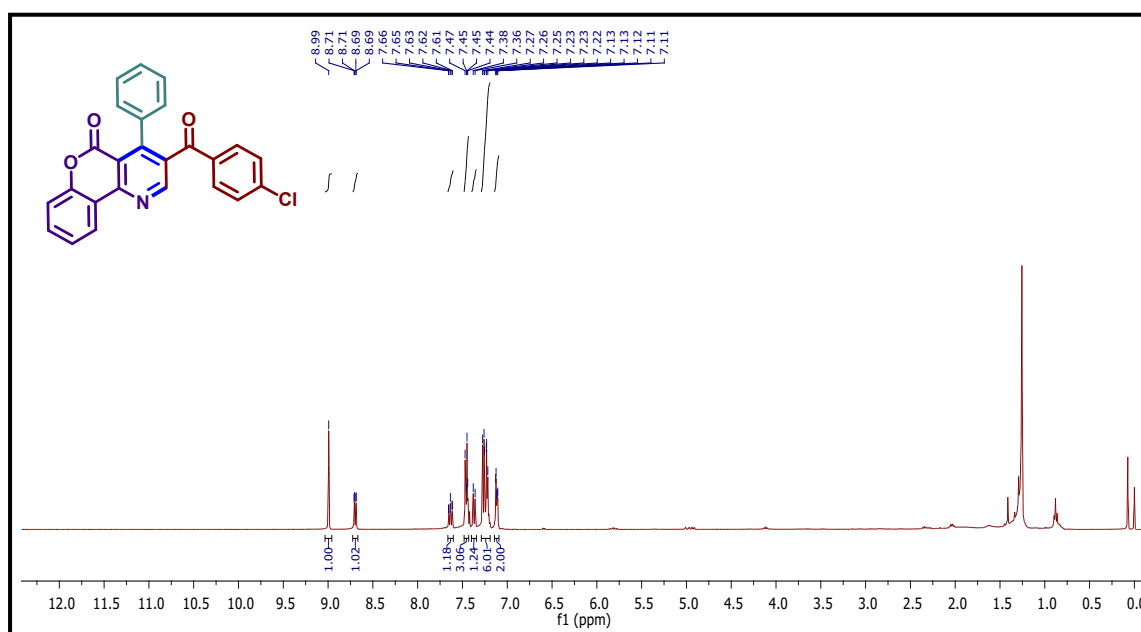


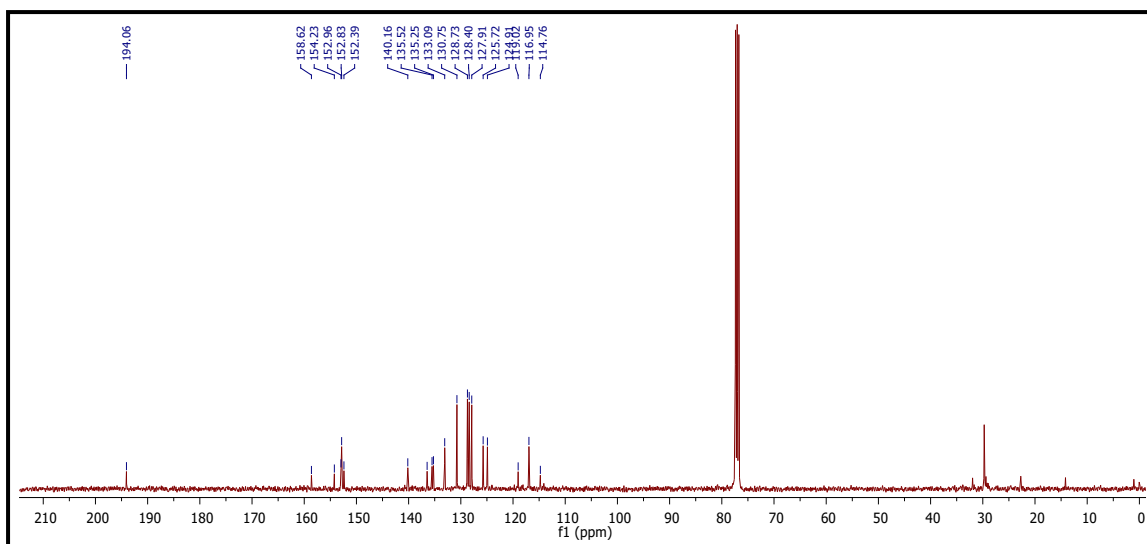




### 3-benzoyl-4-phenyl-5H-chromeno[2,3-b]pyridin-5-one (6II).

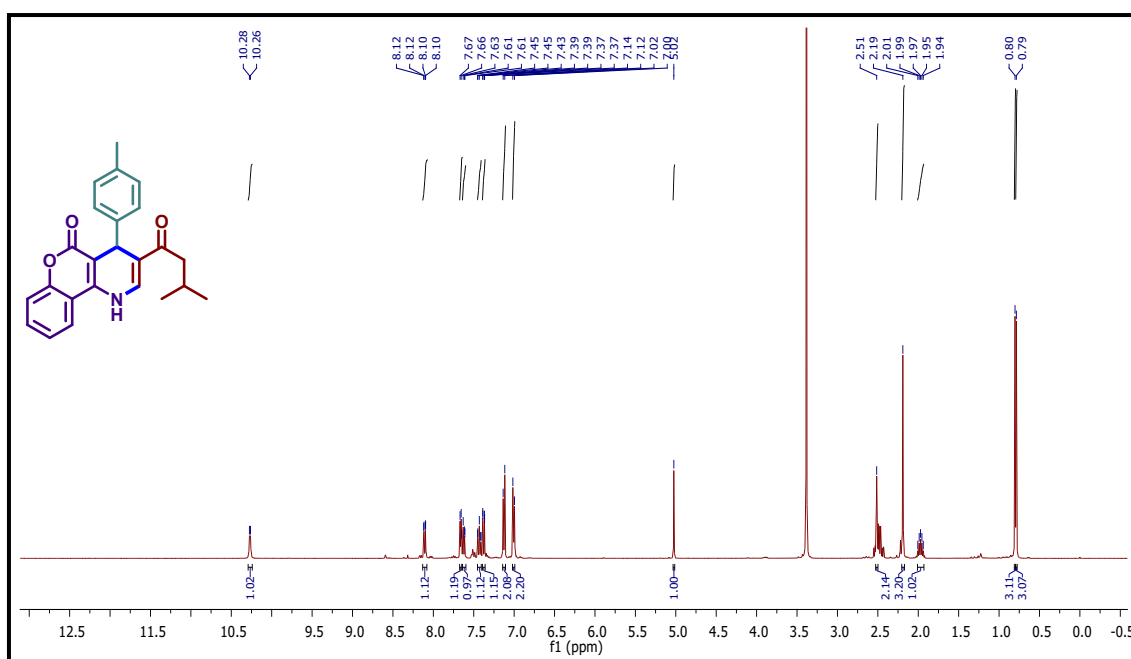
Isolated as a yellow colour solid, yield 72% (253 mg), m.p 178-180 °C, IR (ATR): 3082, 3012, 1707, 1650, 1567, 1512, 1450, 1363, 1273, 1210, 1120, 957  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.99 (s, 1H), 8.70 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.66 – 7.60 (m, 1H), 7.45 (dd,  $J = 6.8, 5.0$  Hz, 3H), 7.37 (d,  $J = 8.3$  Hz, 1H), 7.29 – 7.19 (m, 6H), 7.14 – 7.09 (m, 2H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  194.06, 158.62, 154.23, 152.96, 152.83, 152.39, 140.16, 136.46, 135.52, 135.25, 133.09, 130.75, 128.73, 128.4, 127.91, 125.72, 124.91, 119.02, 116.95, 114.76 ppm, ESI-MS:  $m/z$  412  $[\text{M}+\text{H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{25}\text{H}_{14}\text{ClNO}_3$   $m/z$  412.07350  $[\text{M}+\text{H}]^+$ , found 412.07234.

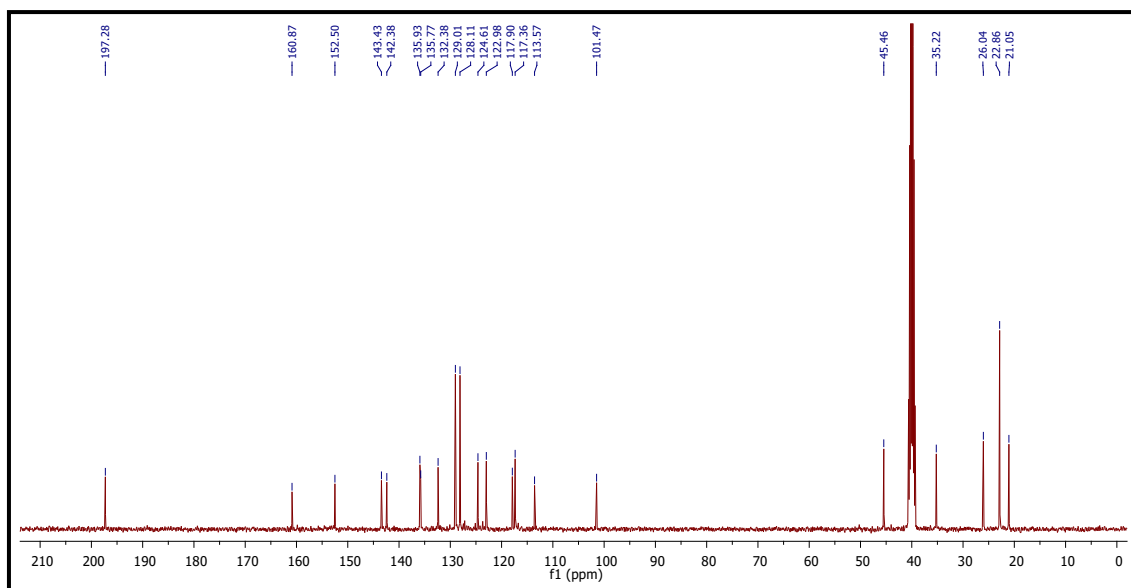




### 3-(3-methylbutanoyl)-4-(*p*-tolyl)-1,4-dihydro-5*H*-chromeno[4,3-*b*]pyridin-5-one (6m).

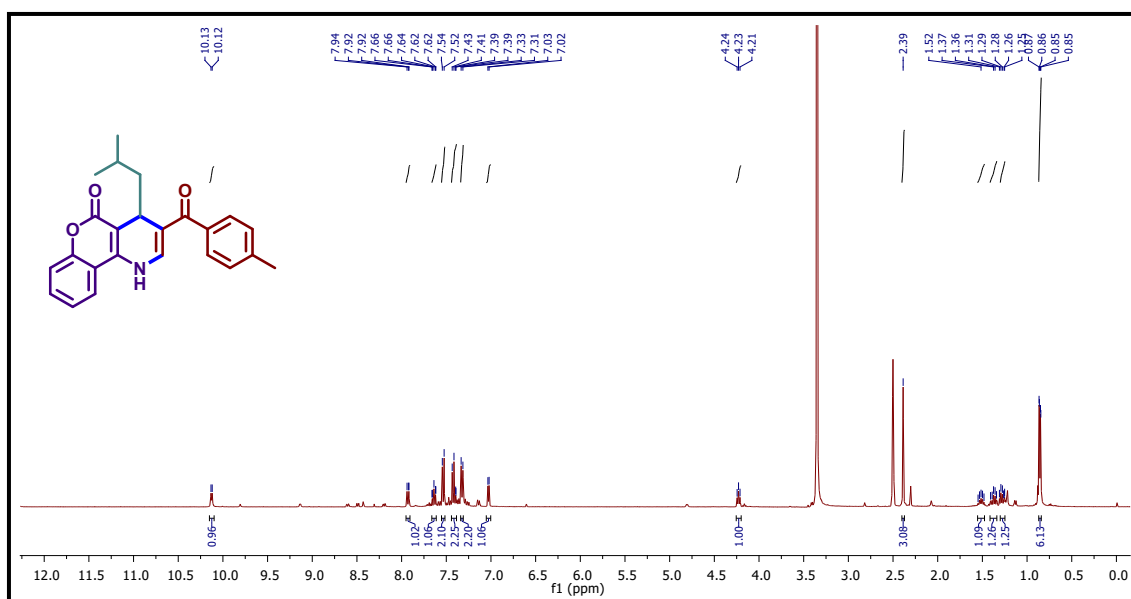
Isolated as a yellow colour solid, yield 75% (211 mg), m.p 254-256 °C, IR (ATR): 3152, 3021, 2959, 1612, 1542, 1482, 1373, 1273, 1213, 960 cm<sup>-1</sup>, <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ 10.27 (br, NH), 8.11 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.67 – 7.65 (m, 1H), 7.64 – 7.60 (m, 1H), 7.45 – 7.41 (m, 1H), 7.38 (dd, *J* = 8.3, 0.8 Hz, 1H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.01 (d, *J* = 7.9 Hz, 2H), 5.02 (s, 1H), 2.51 (d, *J* = 1.9 Hz, 2H), 2.19 (s, 3H), 1.97 – 1.94 (m, 1H), 0.80 (s, 3H), 0.79 (s, 3H) ppm, <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>): δ 197.28, 160.87, 152.5, 143.43, 142.38, 135.93, 135.77, 132.38, 129.01, 128.11, 124.61, 122.98, 117.9, 117.36, 113.57, 101.47, 45.46, 35.22, 26.04, 22.86, 21.05 ppm, ESI-MS: *m/z* 372 [M-H]<sup>-</sup>, HRMS (ESI) Anal. calcd. for C<sub>24</sub>H<sub>22</sub>NO<sub>3</sub> *m/z* 372.1594 [M-H]<sup>-</sup>, found 372.1606.

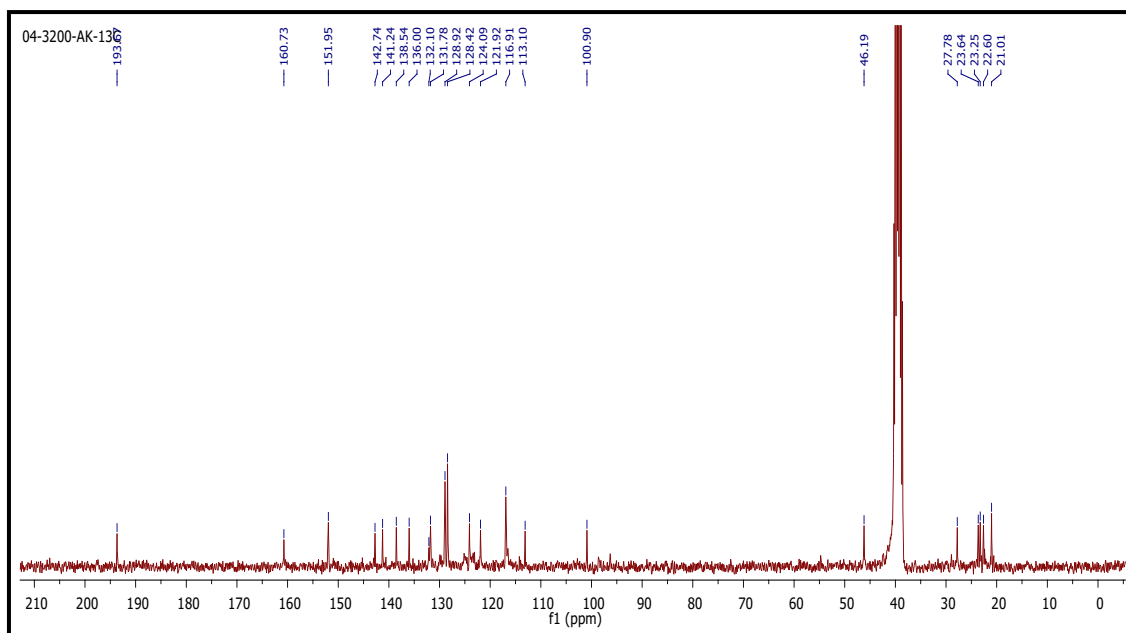




#### 4-isobutyl-3-(4-methylbenzoyl)-1,4-dihydro-5H-chromeno[4,3-b]pyridin-5-one (6n).

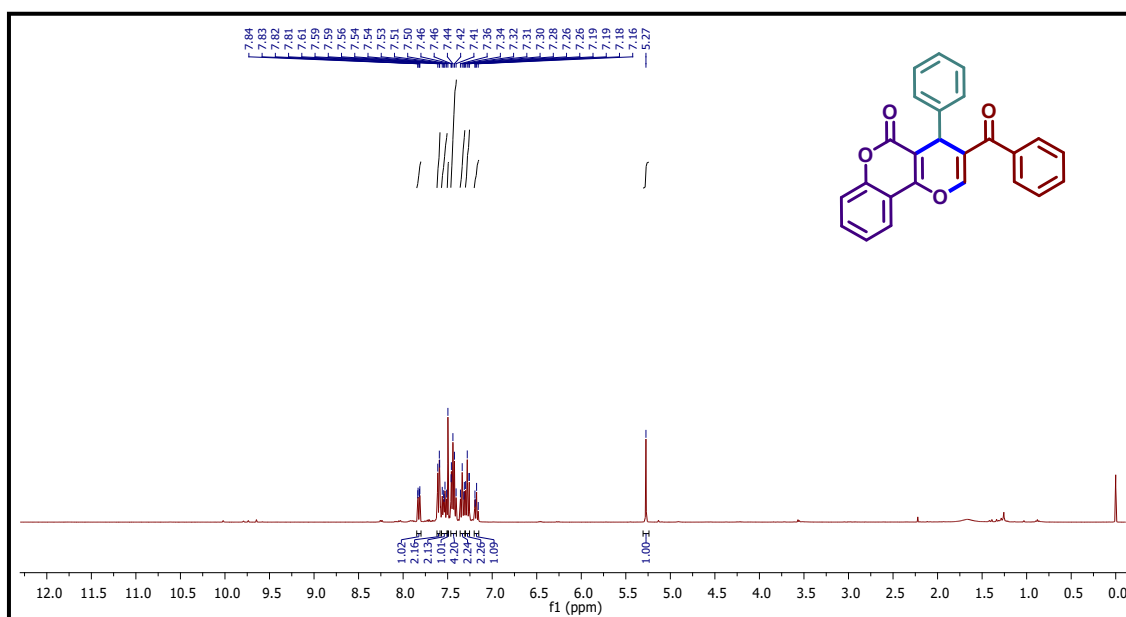
Isolated as a yellow colour solid, yield 73% (284 mg), m.p 252-254 °C, IR (ATR): 3257, 3016, 2861, 2381, 1662, 1605, 1483, 1312, 1272, 933  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  10.13 (br, NH), 7.95 – 7.91 (m, 1H), 7.66 – 7.61 (m, 1H), 7.53 (d,  $J$  = 8.1 Hz, 2H), 7.41 (dd,  $J$  = 12.2, 4.5 Hz, 2H), 7.32 (d,  $J$  = 7.9 Hz, 2H), 7.03 (d,  $J$  = 5.4 Hz, 1H), 4.23 (t,  $J$  = 6.5 Hz, 1H), 2.39 (s, 3H), 1.52 – 1.49 (m, 1H), 1.41 – 1.34 (m, 1H), 1.30 – 1.25 (m, 1H), 0.86 (dd,  $J$  = 6.5, 1.5 Hz, 6H) ppm,  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta$  193.67, 160.73, 151.95, 142.74, 141.24, 138.54, 136.0, 132.1, 131.78, 128.92, 128.42, 124.09, 121.92, 116.91, 113.10, 100.9, 46.19, 27.78, 23.64, 23.25, 22.6, 21.01 ppm, ESI-MS:  $m/z$  372  $[\text{M}-\text{H}]^-$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{24}\text{H}_{22}\text{NO}_3$   $m/z$  372.1678  $[\text{M}-\text{H}]^-$ , found 372.1680.

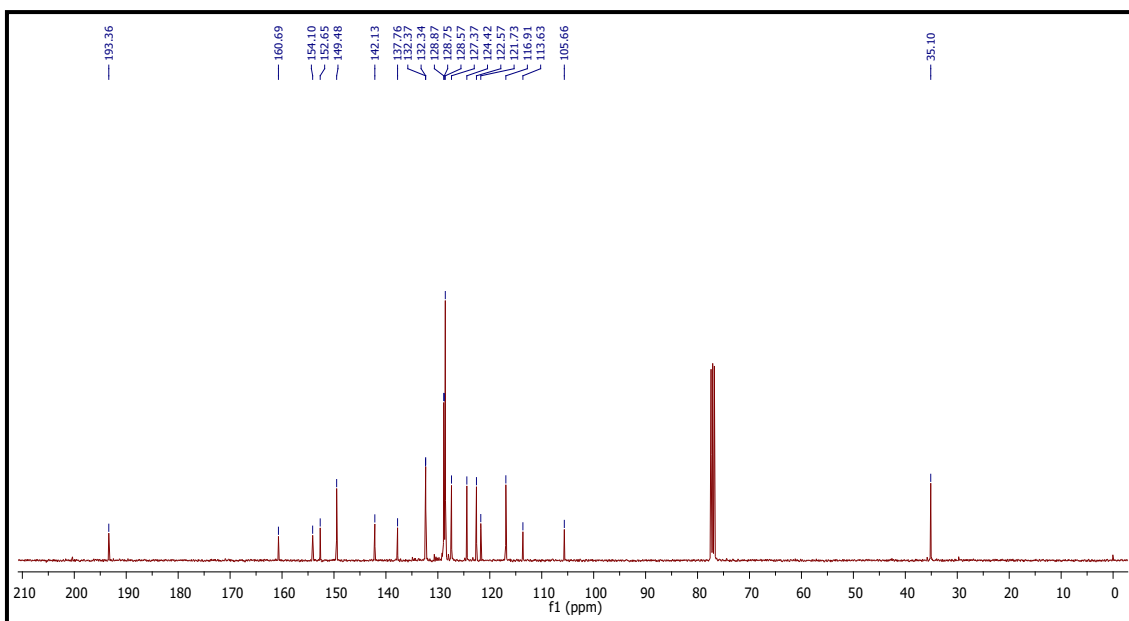




### 3-benzoyl-4-phenyl-4*H*,5*H*-pyrano[3,2-*c*]chromen-5-one (6o).

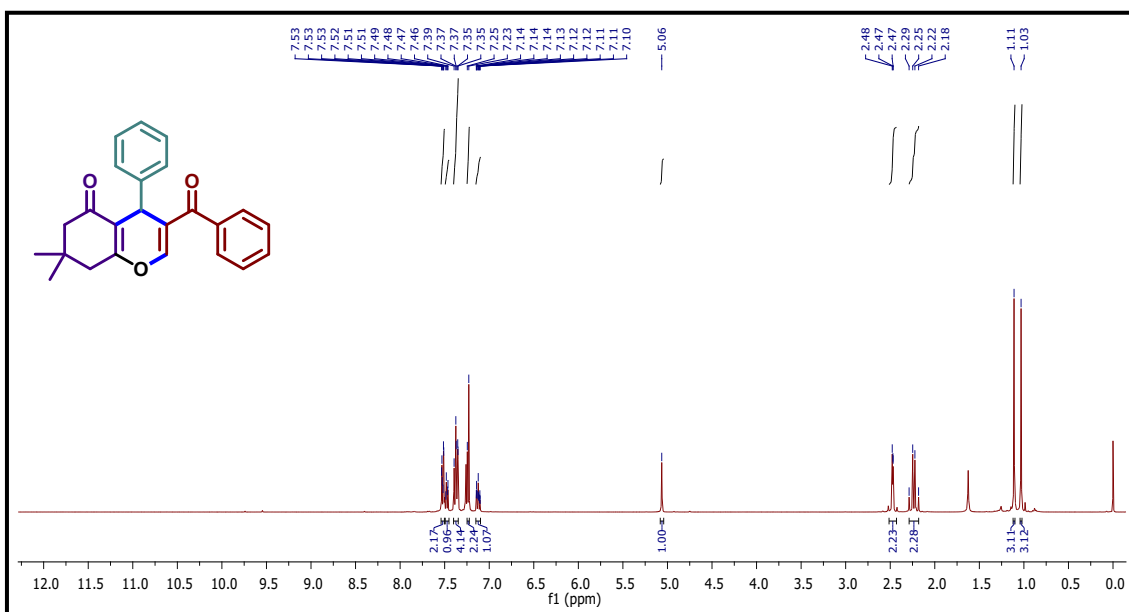
Isolated as a light yellow colour solid, yield 80% (260 mg), m.p 196-198 °C, IR (ATR): 3021, 2972, 2850, 1718, 1657, 1606, 1492, 1374, 1293, 1213, 1169, 1075, 942, 835  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.82 (dd,  $J = 7.9, 1.3$  Hz, 1H), 7.62 – 7.59 (m, 2H), 7.54 – 7.51 (m, 2H), 7.50 (s, 1H), 7.46 – 7.41 (m, 4H), 7.36 – 7.31 (m, 2H), 7.30 – 7.26 (m, 2H), 7.18 (dd,  $J = 10.5, 4.3$  Hz, 1H), 5.27 (s, 1H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  193.36, 160.69, 154.1, 152.65, 149.48, 142.13, 137.76, 132.37, 132.34, 128.87, 128.75, 128.57, 127.37, 124.42, 122.57, 121.73, 116.91, 113.63, 105.66, 35.1 ppm, ESI-MS:  $m/z$  381  $[\text{M}+\text{H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{25}\text{H}_{17}\text{O}_4$   $m/z$  381.1121  $[\text{M}+\text{H}]^+$ , found 381.1112.

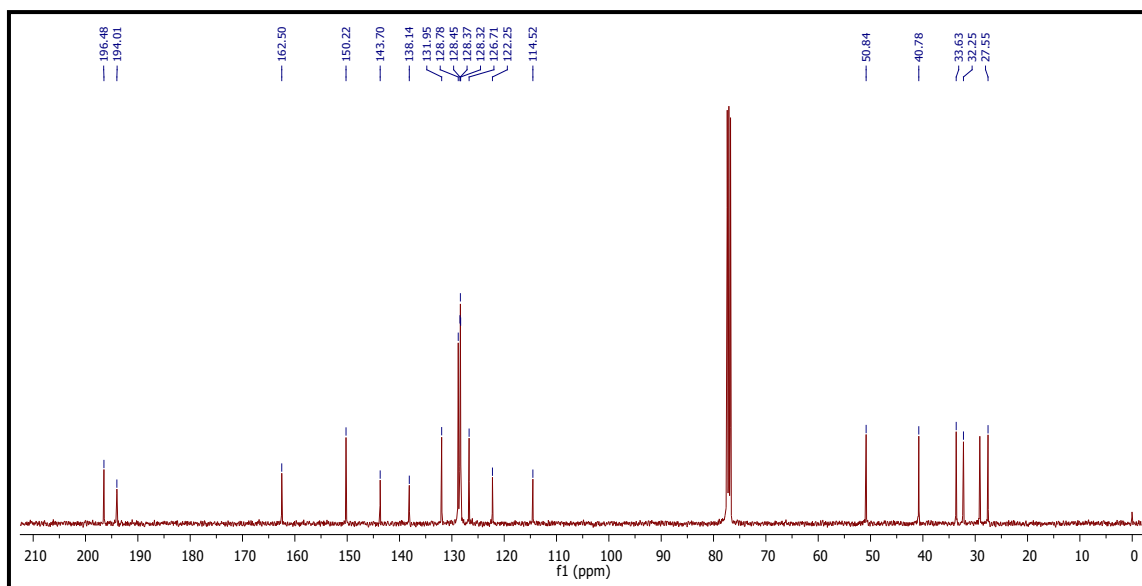




### 3-benzoyl-7,7-dimethyl-4-phenyl-4,6,7,8-tetrahydro-5H-chromen-5-one (6p).

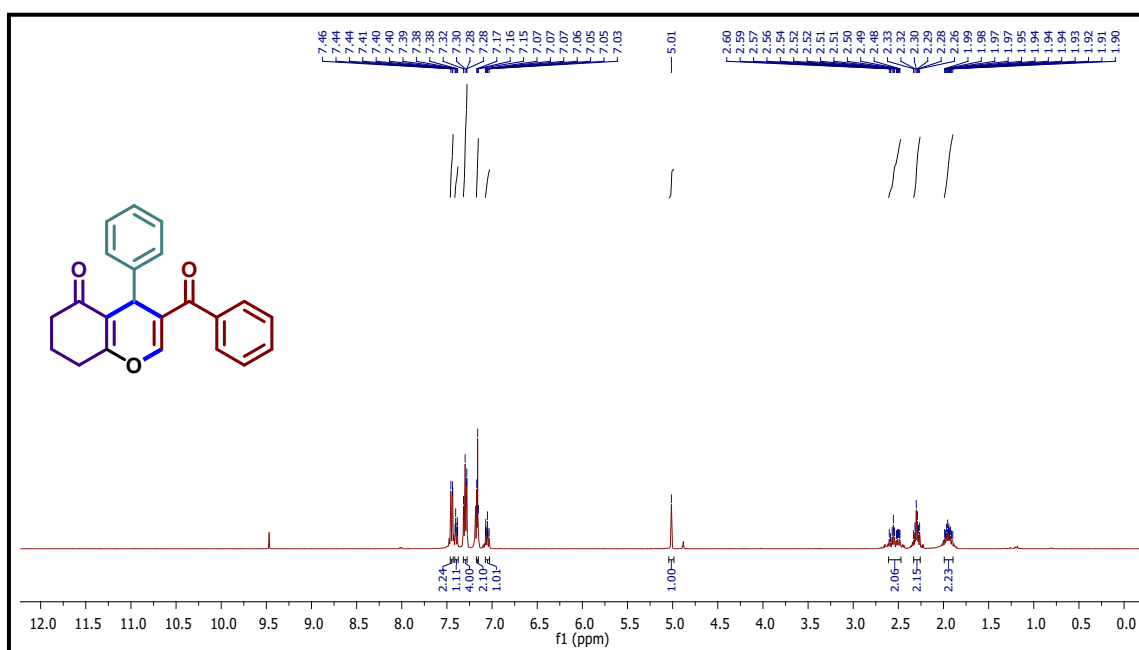
Isolated as a white colour solid, yield 76% (233 mg), m.p 126-128 °C, IR (ATR): 3019, 2962, 1665, 1610, 1491, 1452, 1368, 1305, 1290, 1214, 1140, 1075, 933, 839  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.53 – 7.51 (m, 2H), 7.49 – 7.46 (m, 1H), 7.39 – 7.35 (m, 4H), 7.24 (d,  $J = 6.8$  Hz, 2H), 7.15 – 7.10 (m, 1H), 5.06 (s, 1H), 2.51 – 2.43 (m, 2H), 2.29 – 2.18 (m, 2H), 1.11 (s, 3H), 1.03 (s, 3H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  196.48, 194.01, 162.5, 150.22, 143.7, 138.14, 131.95, 128.78, 128.45, 128.37, 128.32, 126.71, 122.25, 114.52, 50.84, 40.78, 33.63, 32.25, 29.12, 27.55 ppm, ESI-MS:  $m/z$  359  $[\text{M}+\text{H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{24}\text{H}_{23}\text{O}_3$   $m/z$  359.1641  $[\text{M}+\text{H}]^+$ , found 359.1636.

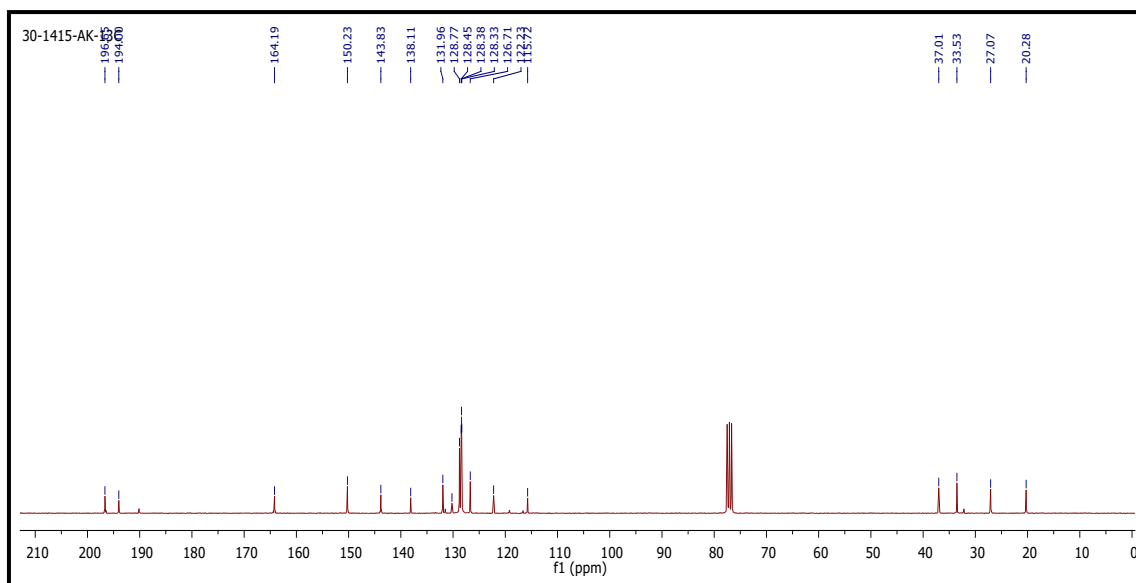




### 3-benzoyl-4-phenyl-4,6,7,8-tetrahydro-5H-chromen-5-one (6q).

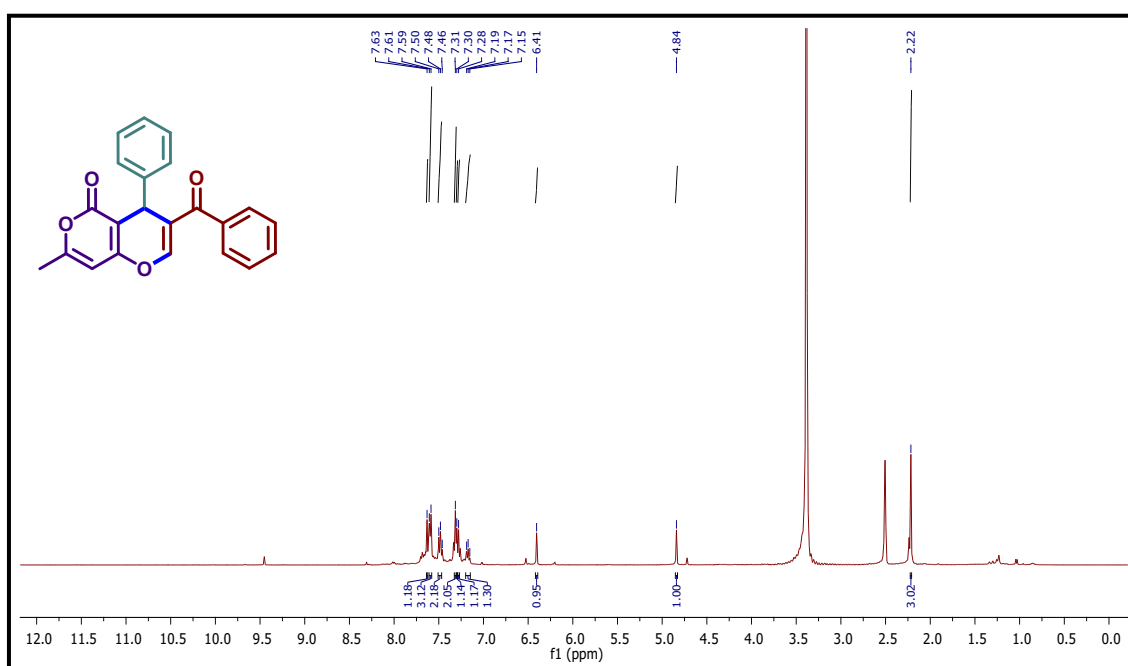
Isolated as a white colour solid, yield 78% (220 mg), m.p 204-206 °C, IR (ATR): 3022, 2860, 1661, 1606, 1492, 1450, 1367, 1247, 1212, 1125, 1076, 1005, 930, 835  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.46 – 7.43 (m, 2H), 7.39 – 7.30 (m, 1H), 7.29 – 7.28 (m, 4H), 7.17 – 7.15 (m, 2H), 7.07 – 7.03 (m, 1H), 5.01 (s, 1H), 2.61 – 2.47 (m, 2H), 2.33 – 2.26 (m, 2H), 1.99 – 1.90 (m, 2H) ppm,  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  196.66, 194.0, 190.12, 164.19, 150.23, 143.83, 138.11, 131.96, 130.21, 128.77, 128.45, 128.38, 126.71, 122.23, 115.72, 37.01, 33.53, 27.07, 20.28 ppm, ESI-MS: m/z 331  $[\text{M}+\text{H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{22}\text{H}_{19}\text{O}_3$  m/z 331.1328  $[\text{M}+\text{H}]^+$ , found 331.1324.

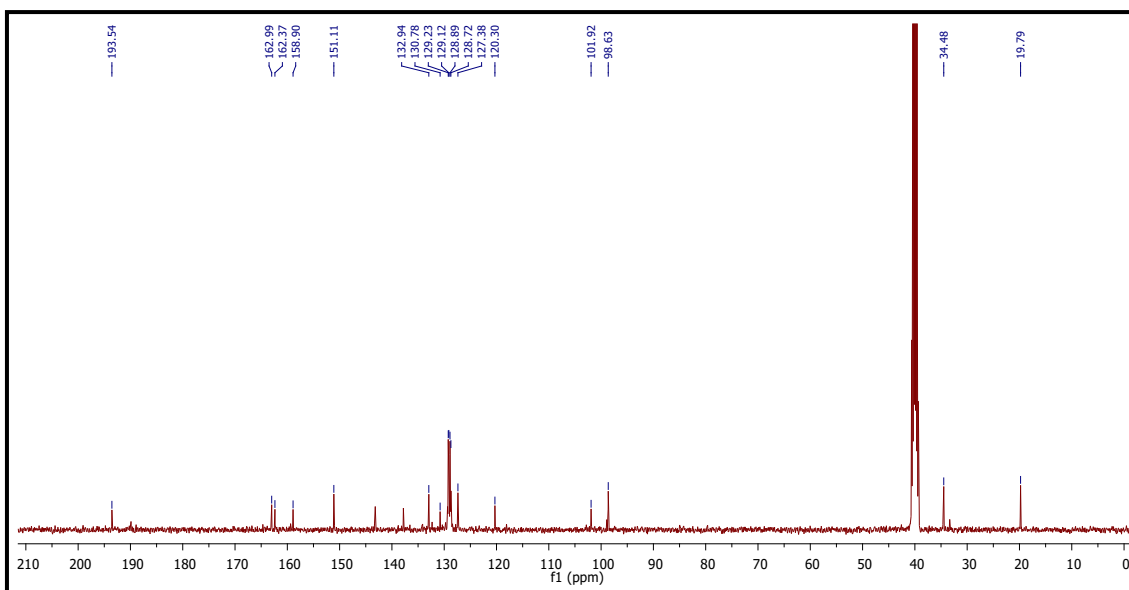




### 3-benzoyl-7-methyl-4-phenyl-4*H*,5*H*-pyrano[4,3-*b*]pyran-5-one (6r).

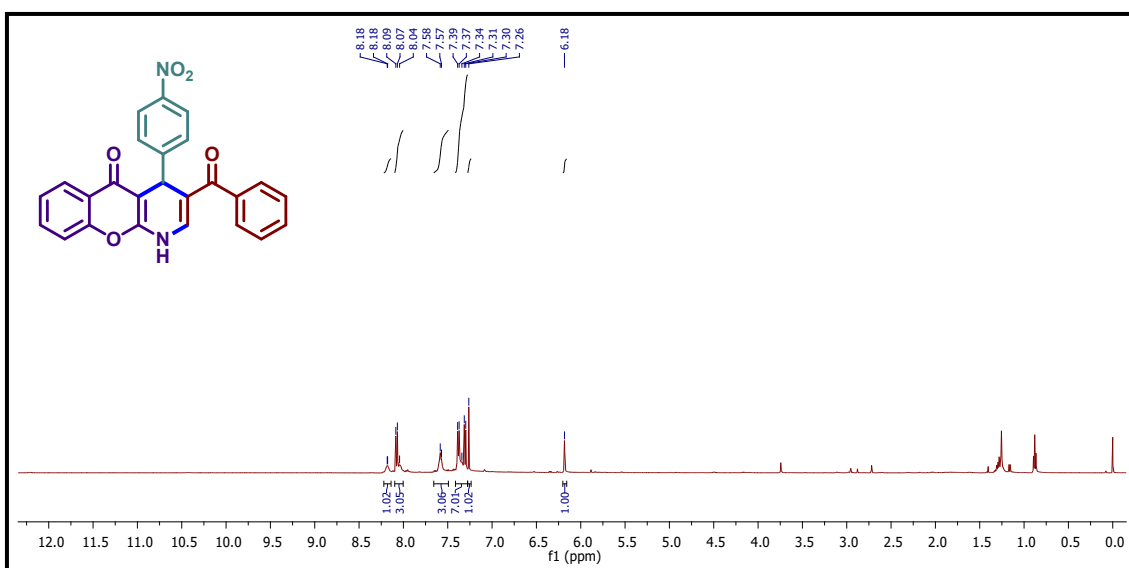
Isolated as a light brown colour solid, yield 75% (221 mg), m.p 135-137 °C, IR (ATR): 3429, 3063, 1719, 1625, 1591, 1491, 1446, 1301, 1198, 1149, 1086, 976, 837, 808  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  7.63 (s, 1H), 7.60 (d,  $J = 7.6$  Hz, 3H), 7.49 (d,  $J = 7.3$  Hz, 2H), 7.31 (s, 2H), 7.30 (s, 1H), 7.28 (s, 1H), 7.17 (t,  $J = 7.1$  Hz, 1H), 6.41 (s, 1H), 4.84 (s, 1H), 2.22 (s, 3H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  193.54, 162.99, 162.37, 158.9, 151.11, 132.94, 130.78, 129.23, 129.12, 128.89, 128.72, 127.38, 120.3, 101.92, 98.63, 34.48, 19.79 ppm, ESI-MS:  $m/z$  345  $[\text{M}+\text{H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{22}\text{H}_{17}\text{O}_4$   $m/z$  345.1121  $[\text{M}+\text{H}]^+$ , found 345.1114.



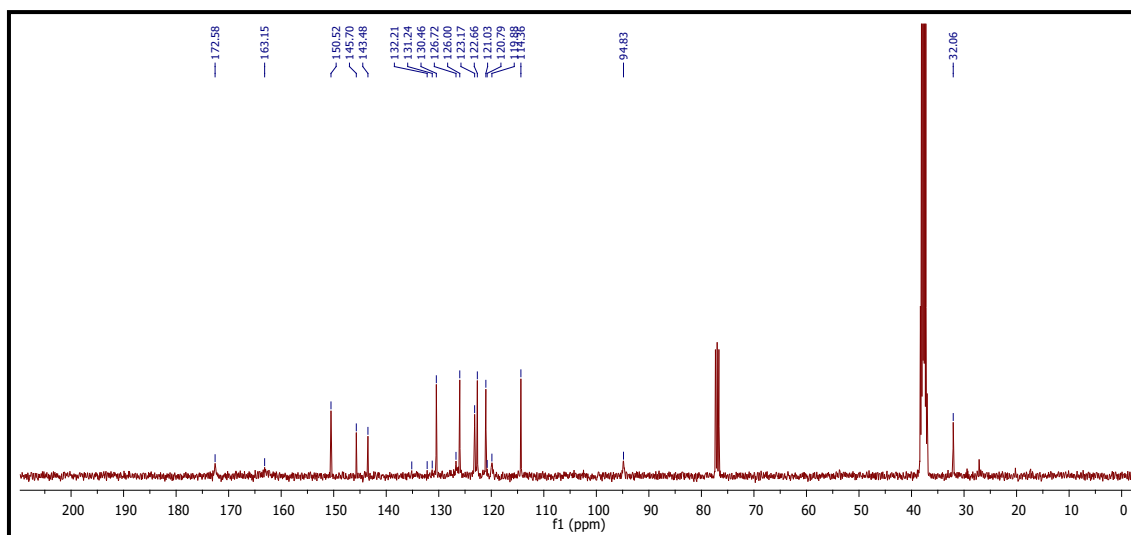


### 3-benzoyl-4-(4-nitrophenyl)-1,4-dihydro-5H-chromeno[2,3-b]pyridin-5-one (6s)

Isolated as a yellow colour solid, yield 72% (184 mg), m.p 182-184 °C, IR (ATR): 3210, 3019, 2840, 2450, 1721, 1645, 1572, 1512, 1472, 1354, 1285, 1205, 1170, 1083, 970 cm<sup>-1</sup>, <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.18 (br, NH), 8.07 (t, *J* = 10.6 Hz, 3H), 7.58 (d, *J* = 7.0 Hz, 3H), 7.41 – 7.28 (m, 7H), 7.26 (s, 1H), 6.18 (s, 1H) ppm, <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 172.58, 163.15, 150.52, 145.70, 143.48, 135.14, 132.21, 131.24, 130.46, 126.72, 126.0, 123.17, 122.66, 121.03, 120.79, 119.88, 114.36, 94.83, 32.06 ppm, ESI-MS: *m/z* 425 [M+H]<sup>+</sup>, HRMS (ESI) Anal. calcd. for C<sub>26</sub>H<sub>20</sub>N<sub>2</sub>O<sub>6</sub> *m/z* 456.1315 [M+MeOH]<sup>+</sup>, found 456.1326.

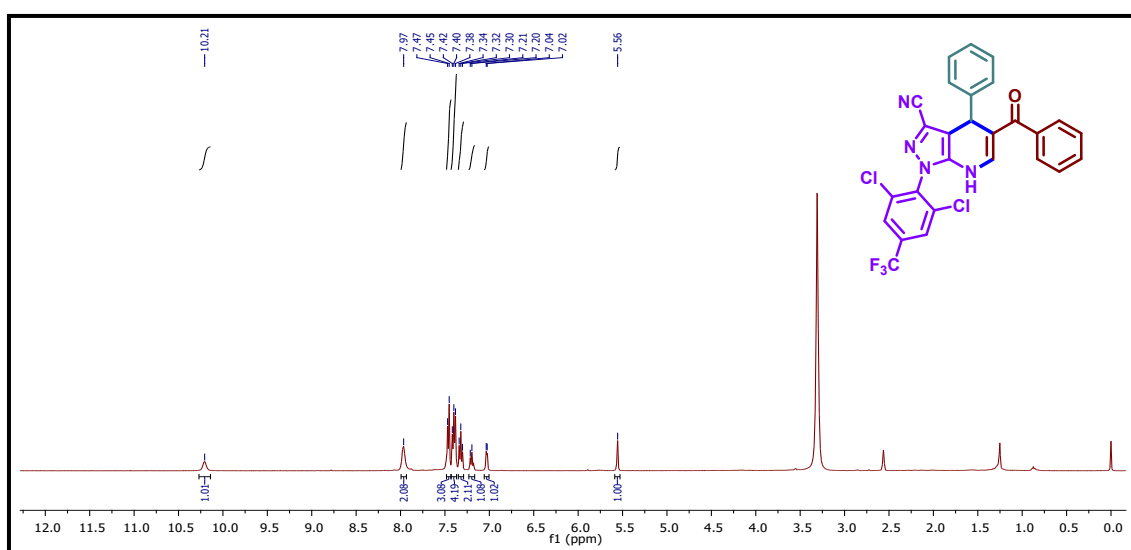


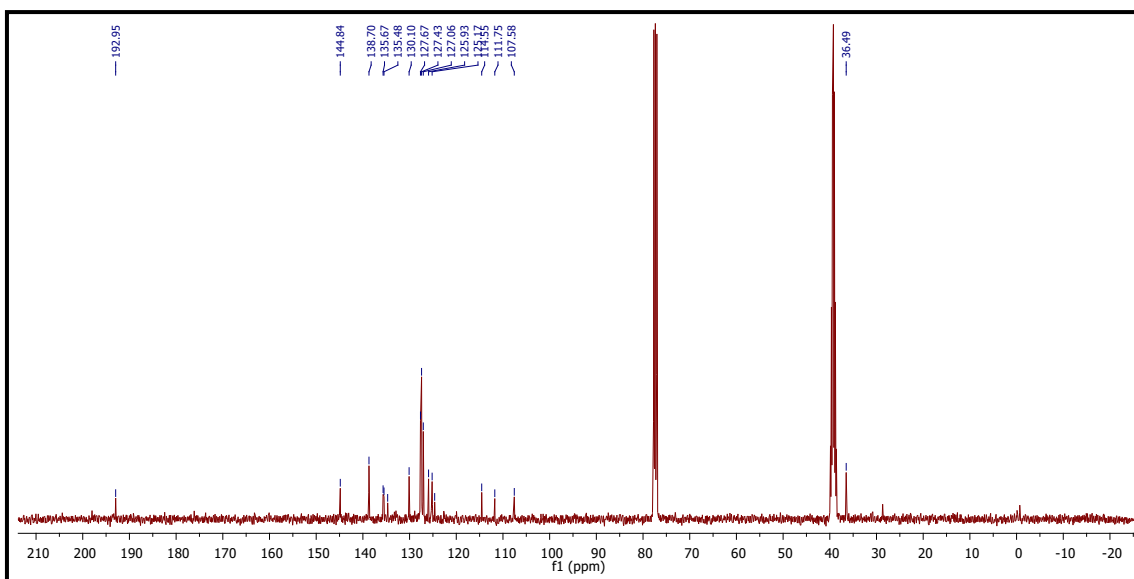




**5-benzoyl-1-(2,6-dichloro-4-(trifluoromethyl)phenyl)-4-phenyl-4,7-dihydro-1H-pyrazolo[3,4-*b*]pyridine-3-carbonitrile (8a).**

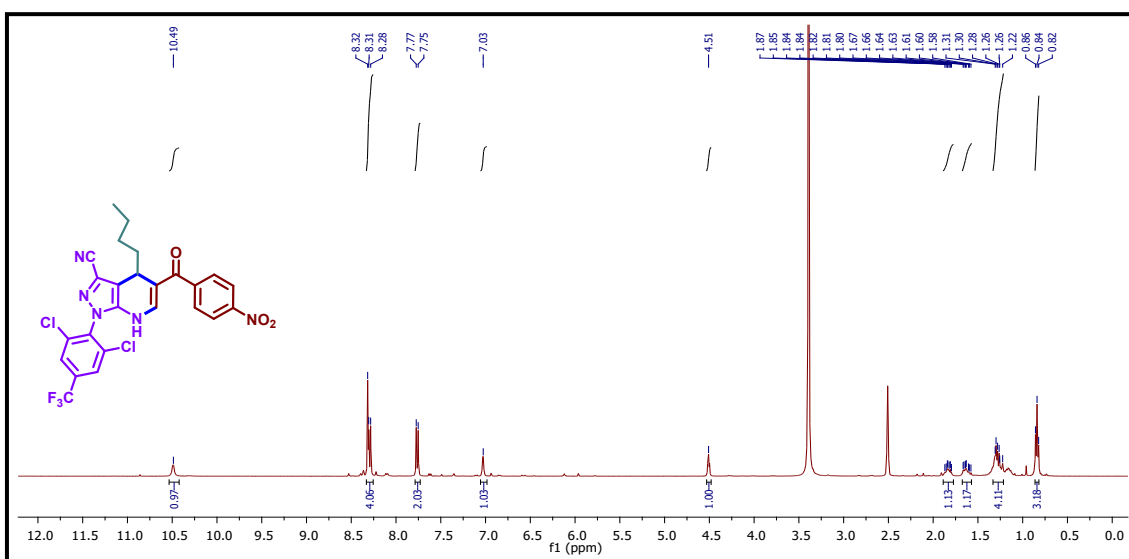
Isolated as a yellow colour solid, yield 85% (391 mg), m.p 271-273 °C, IR (ATR): 3223, 3020, 2922, 2853, 2359, 2245, 1663, 1568, 1451, 1393, 1268, 1175, 1099, 881 cm<sup>-1</sup>, <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>+CDCl<sub>3</sub>): δ 10.21 (br, NH), 7.97 (s, 2H), 7.46 (d, *J* = 7.3 Hz, 3H), 7.43 – 7.37 (m, 4H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.03 (d, *J* = 4.3 Hz, 1H), 5.56 (s, 1H) ppm, <sup>13</sup>C NMR (101 MHz DMSO-d<sub>6</sub>+CDCl<sub>3</sub>): δ 192.95, 144.84, 138.70, 135.22 (d, *J* = 19.6 Hz), 134.69, 130.10, 127.67, 127.43, 127.06, 125.93, 125.17, 124.63, 120.97 (q, *J* = 274.35 Hz) 114.55, 111.75, 107.58, 36.49 ppm, ESI-MS: *m/z* 539 [M+H]<sup>+</sup>, HRMS (ESI) Anal. calcd. for C<sub>27</sub>H<sub>16</sub>Cl<sub>2</sub>F<sub>3</sub>N<sub>4</sub>O *m/z* 539.0647 [M+H]<sup>+</sup>, found 539.0622.



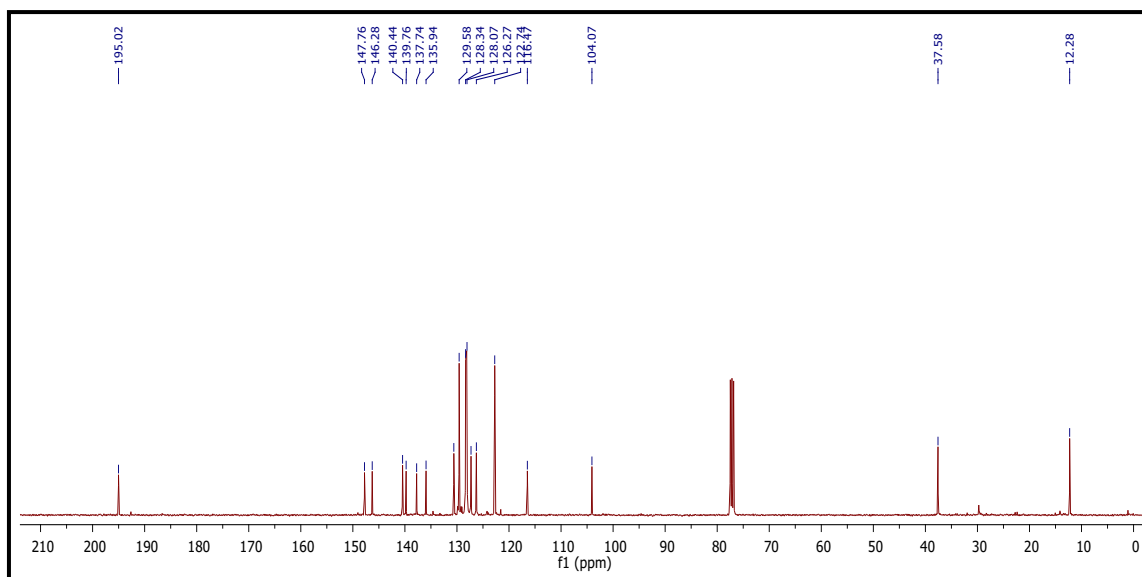


**4-butyl-1-(2,6-dichloro-4-(trifluoromethyl)phenyl)-5-(4-nitrobenzoyl)-4,7-dihydro-1*H*-pyrazolo[3,4-*b*]pyridine-3-carbonitrile (8b).**

Isolated as a yellow colour solid, yield 78% (464 mg), m.p 120-122 °C, IR (ATR): 3225, 3023, 2895, 2843, 2350, 2241, 1570, 1452, 1394, 1282, 1212, 1160, 1080, 952, 820 cm<sup>-1</sup>, <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ 10.49 (br, NH), 8.33 – 8.26 (m, 4H), 7.76 (d, *J* = 8.7 Hz, 2H), 7.03 (s, 1H), 4.51 (s, 1H), 1.87 – 1.80 (m, 1H), 1.67 – 1.57 (m, 1H), 1.33 – 1.21 (m, 4H), 0.84 (t, *J* = 7.0 Hz, 3H) ppm, <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>): δ <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ 192.45, 148.91, 145.88, 143.23, 140.85, 136.08, 135.89, 133.76 (d, *J* = 33.8 Hz), 129.86, 127.21, 127.09, 124.54, 124.08, 119.34 (q, *J* = 273.26 Hz), 113.91, 113.50, 108.07, 35.23, 30.79, 27.28, 22.60, 14.42 ppm, ESI-MS: *m/z* 564 [M-H]<sup>-</sup>, HRMS (ESI) Anal. calcd. for C<sub>25</sub>H<sub>17</sub>Cl<sub>2</sub>F<sub>3</sub>N<sub>5</sub>O<sub>3</sub> *m/z* 562.0655 [M-H]<sup>-</sup>, found 562.0675.

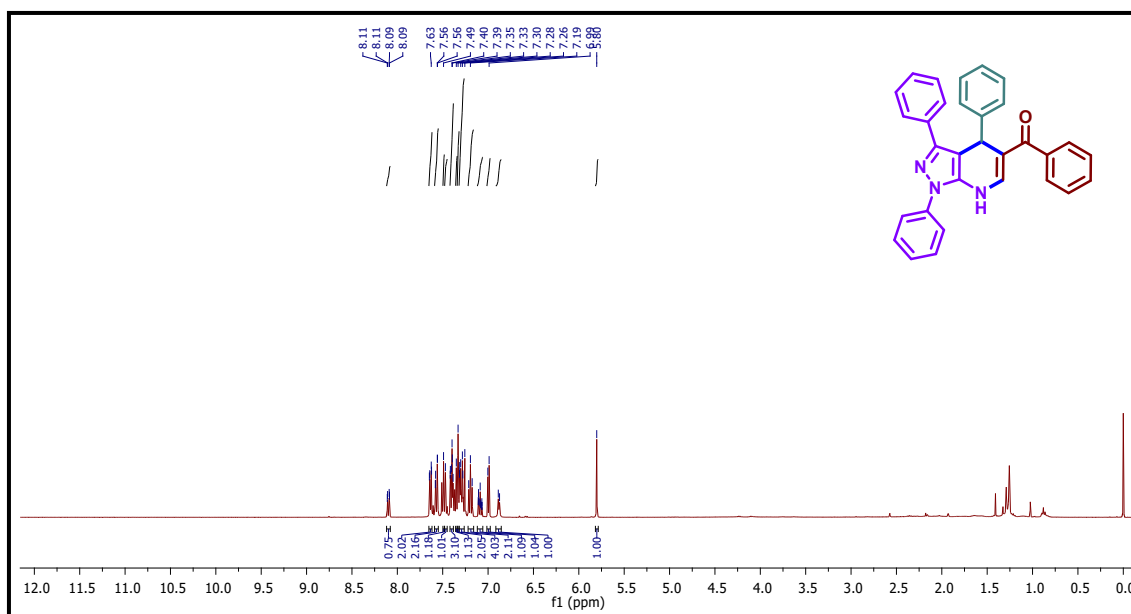


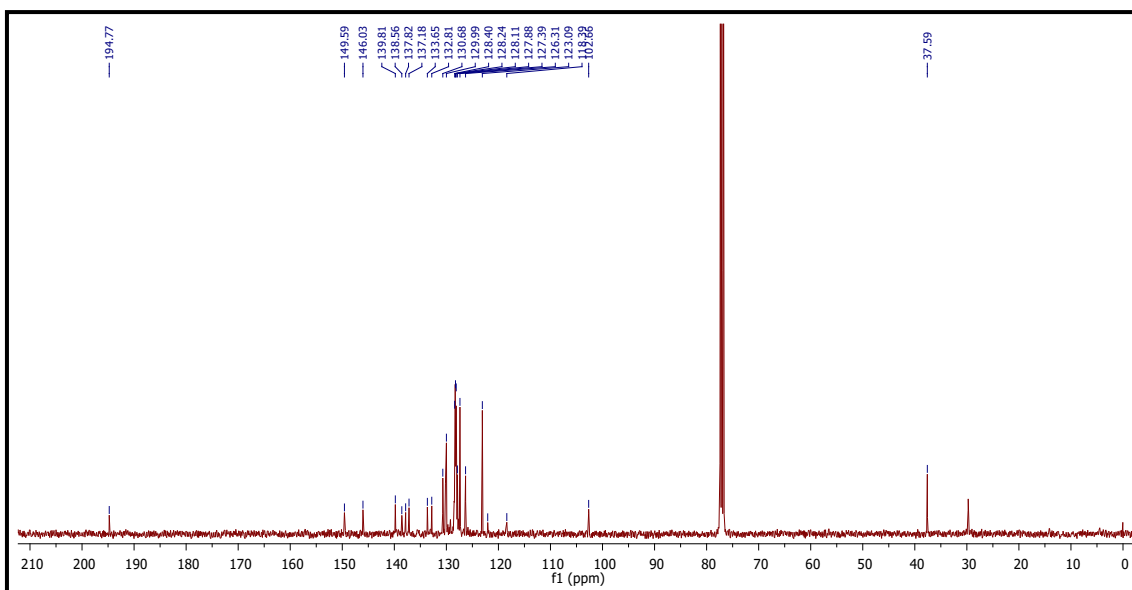




**phenyl(1,3,4-triphenyl-4,7-dihydro-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (8d).**

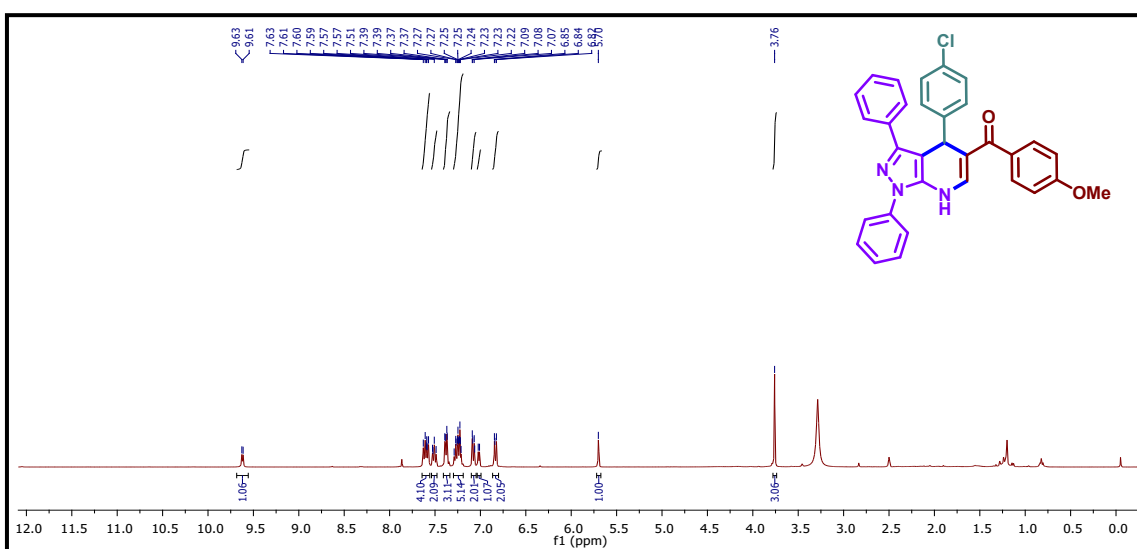
Isolated as a light brown colour solid, yield 82% (318 mg), m.p 105-107 °C, IR (ATR): 3250, 3120, 2910, 2860, 1712, 1620, 1452, 1398, 1275, 1183, 1083, 962  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.10 (br, NH), 7.63 (dd,  $J = 8.1, 1.6$  Hz, 2H), 7.57 (dd,  $J = 8.5, 1.2$  Hz, 2H), 7.49 (s, 1H), 7.47 (s, 1H), 7.42 – 7.38 (m, 3H), 7.35 (s, 1H), 7.33 (s, 2H), 7.32 – 7.26 (m, 4H), 7.19 (t,  $J = 7.6$  Hz, 2H), 7.12 – 7.06 (m, 1H), 7.00 (d,  $J = 5.6$  Hz, 1H), 6.88 (d,  $J = 5.6$  Hz, 1H), 5.80 (s, 1H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  194.77, 149.59, 146.03, 139.81, 138.56, 137.82, 137.18, 133.65, 132.81, 130.68, 129.99, 128.40, 128.24, 128.11, 127.88, 127.39, 126.31, 123.09, 122.06, 118.39, 102.66, 37.59 ppm, ESI-MS:  $m/z$  452  $[\text{M}-\text{H}]^-$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{31}\text{H}_{22}\text{N}_3\text{O}$   $m/z$  452.1757  $[\text{M}-\text{H}]^-$ , found 452.1757.

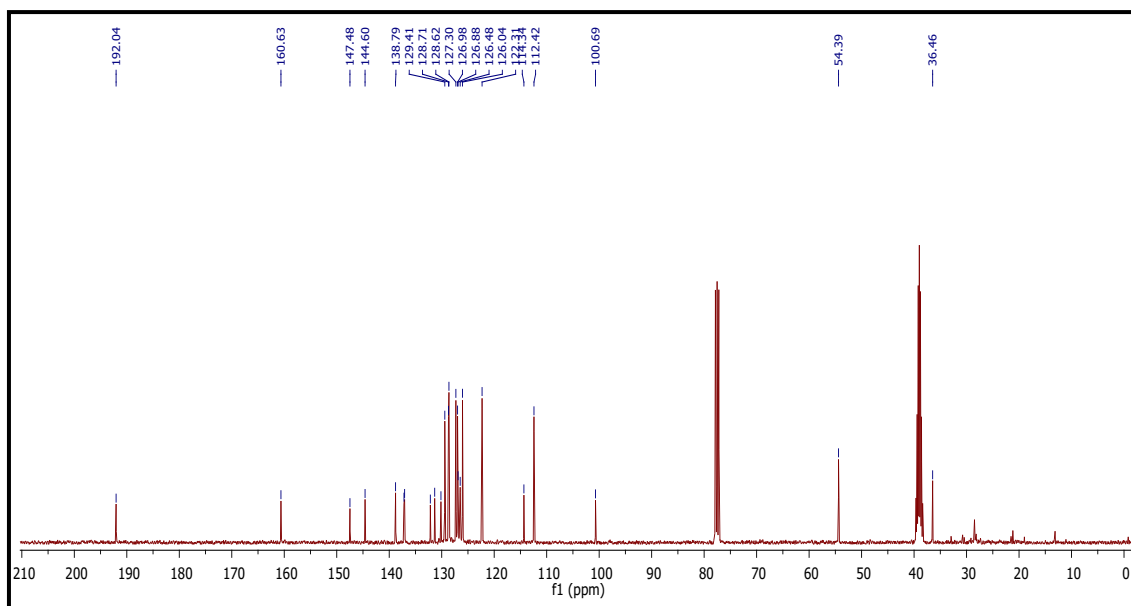




**(4-(4-chlorophenyl)-1,3-diphenyl-4,7-dihydro-1H-pyrazolo[3,4-b]pyridin-5-yl)(4-methoxyphenyl)methanone (8e).**

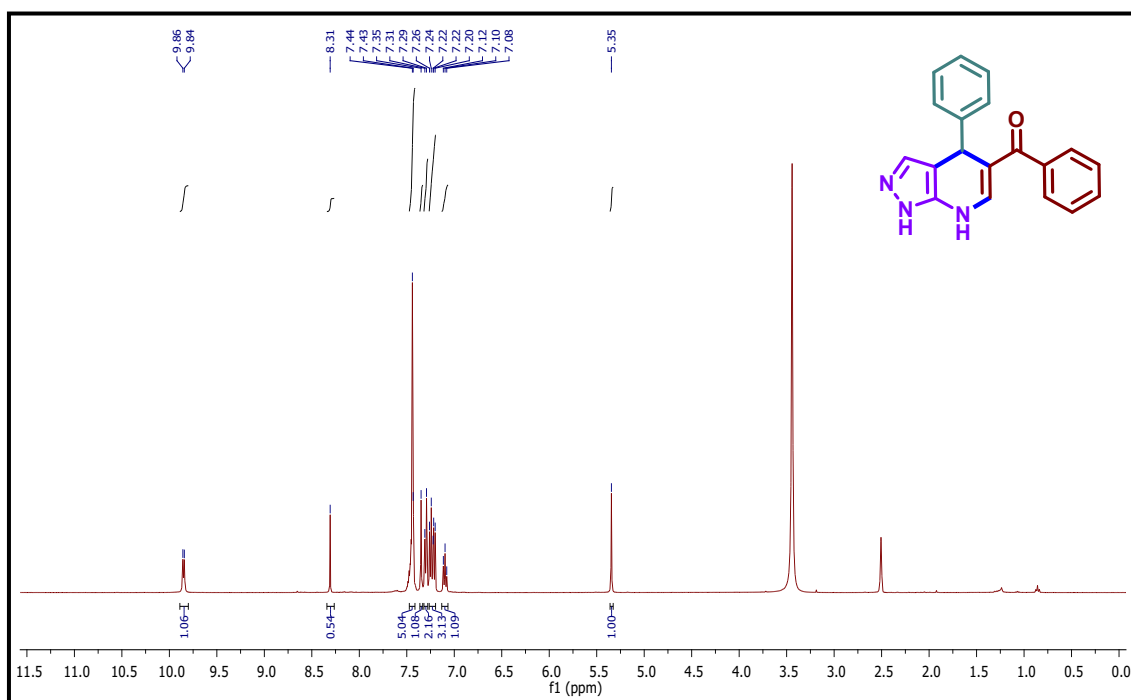
Isolated as a light brown colour solid, yield 88% (295 mg), m.p 106-108 °C, IR (ATR): 3250, 3126, 2954, 2643, 1709, 1609, 1493, 1350, 1265, 1183, 1084, 952, 813 cm<sup>-1</sup>, <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 9.62 (br, NH), 7.64 – 7.56 (m, 4H), 7.51 (dd, *J* = 10.8, 5.0 Hz, 2H), 7.38 (dd, *J* = 8.5, 1.9 Hz, 3H), 7.30 – 7.19 (m, 5H), 7.08 (dd, *J* = 8.5, 2.0 Hz, 2H), 7.02 (d, *J* = 5.7 Hz, 1H), 6.87 – 6.80 (m, 2H), 5.70 (s, 1H), 3.76 (s, 3H) ppm, <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>+DMSO-d<sub>6</sub>): δ 192.04, 160.63, 147.48, 144.60, 138.79, 137.19, 137.07, 132.17, 131.34, 130.15, 129.41, 128.71, 128.62, 127.3, 126.98, 126.88, 126.48, 126.04, 122.31, 114.34, 112.42, 100.69, 54.39, 36.46 ppm, ESI-MS: *m/z* 516 [M-H]<sup>-</sup>, HRMS (ESI) Anal. calcd. for C<sub>32</sub>H<sub>23</sub>ClN<sub>3</sub>O<sub>2</sub> *m/z* 516.1473 [M-H]<sup>-</sup>, found 516.1491.

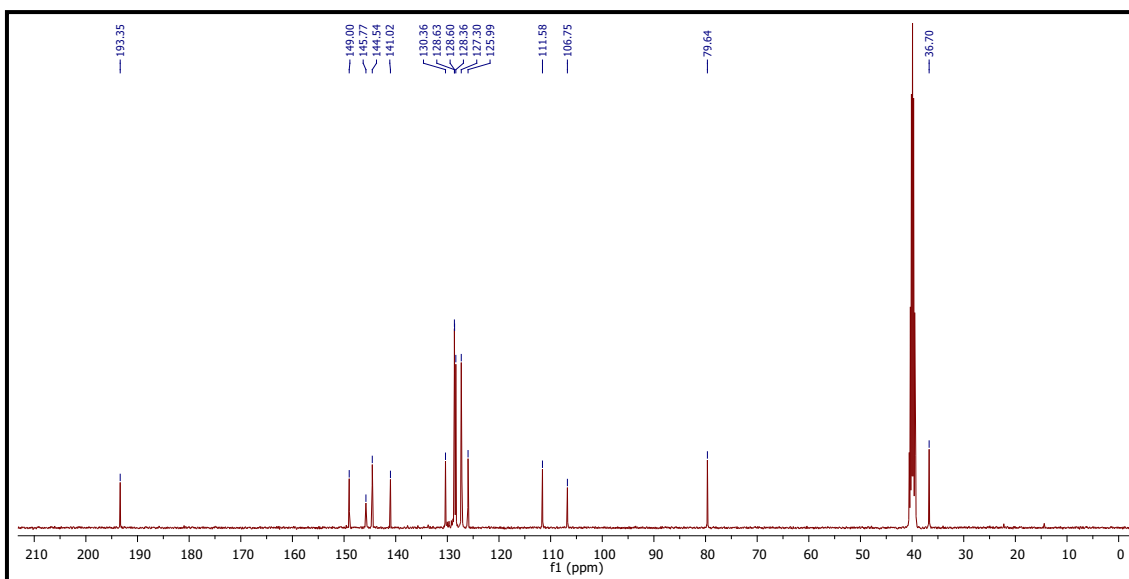




**phenyl(4-phenyl-4,7-dihydro-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (8f).**

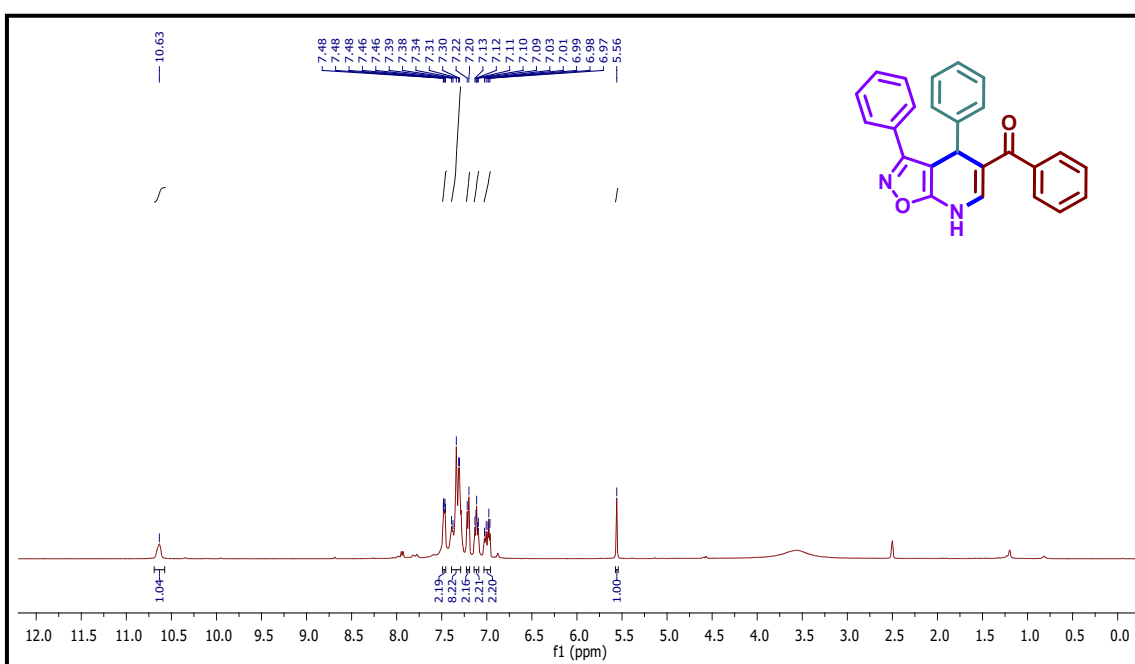
Isolated as a white colour solid, yield 84% (216 mg), m.p 175-177 °C, IR (ATR): 3283, 3121, 2987, 2842, 1661, 1572, 1453, 1396, 1251, 1176, 1103, 875 cm<sup>-1</sup>, <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ 9.85 (br, NH), 8.31 (br, NH), 7.44 (d, *J* = 3.3 Hz, 5H), 7.35 (s, 1H), 7.30 (d, *J* = 7.1 Hz, 2H), 7.26 – 7.20 (m, 3H), 7.10 (t, *J* = 7.2 Hz, 1H), 5.35 (s, 1H) ppm, <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>): δ 193.35, 149.0, 145.77, 144.54, 141.02, 130.36, 128.63, 128.6, 128.36, 127.3, 125.99, 111.58, 106.75, 79.64, 36.7 ppm, ESI-MS: *m/z* 302 [M+H]<sup>+</sup>, HRMS (ESI) Anal. calcd. for C<sub>19</sub>H<sub>16</sub>N<sub>3</sub>O *m/z* 302.1287 [M+H]<sup>+</sup>, found 302.1278.

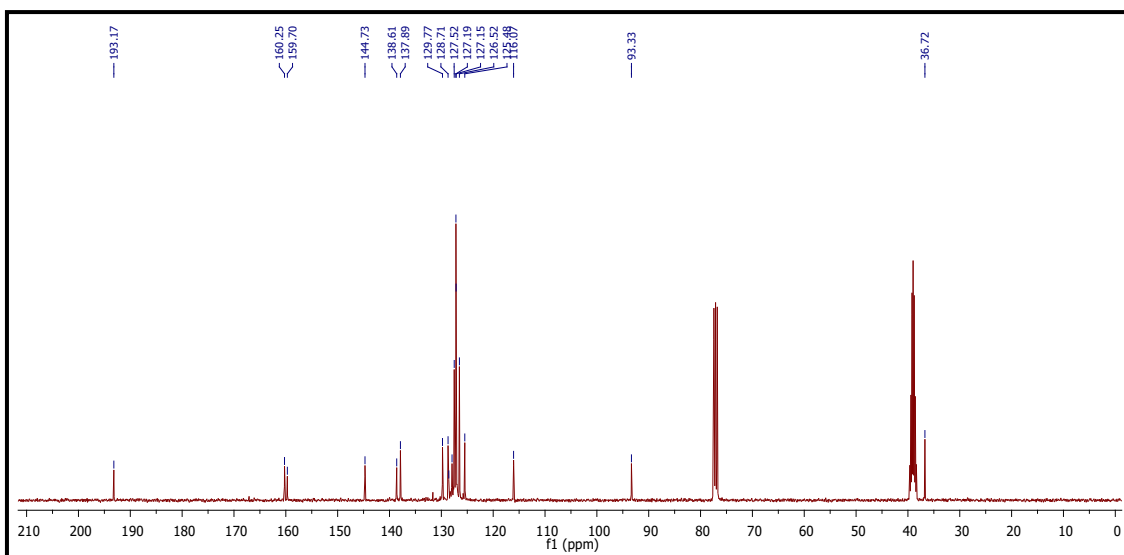




**(3,4-diphenyl-4,7-dihydroisoxazolo[5,4-*b*]pyridin-5-yl)(phenyl)methanone (8g).**

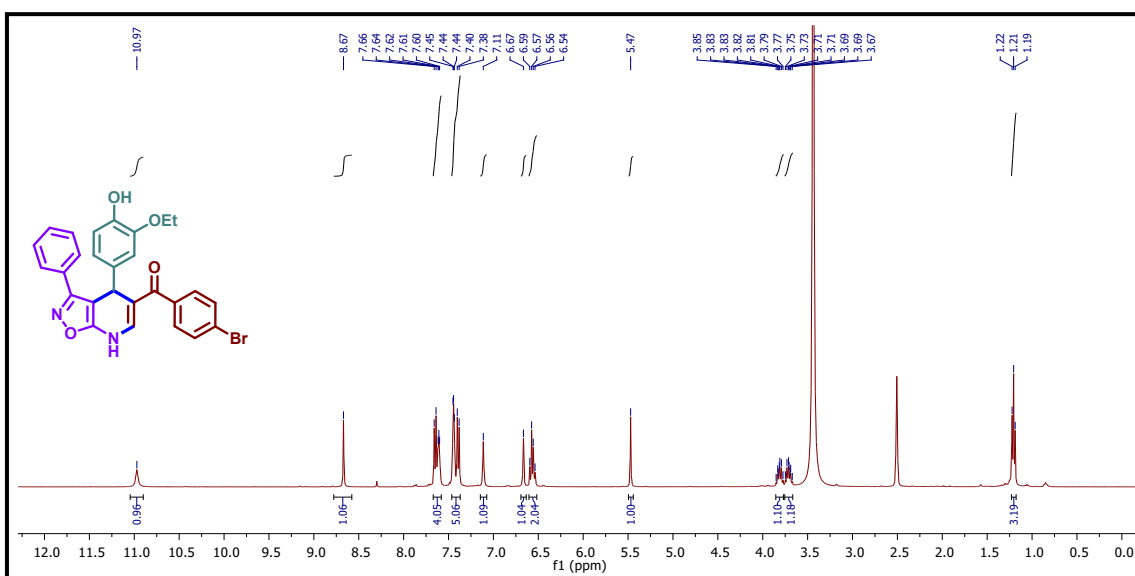
Isolated as a light yellow colour solid, yield 80% (259 mg), m.p 192-194 °C, IR (ATR): 3212, 3062, 3025, 2926, 1664, 1621, 1509, 1447, 1362, 1317, 1272, 1191, 860  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ + $\text{DMSO-d}_6$ ):  $\delta$  10.63 (br, NH), 7.49 – 7.45 (m, 2H), 7.34 (dd,  $J = 22.7, 12.3$  Hz, 8H), 7.21 (d,  $J = 7.6$  Hz, 2H), 7.11 (dd,  $J = 8.8, 6.2$  Hz, 2H), 7.04 – 6.96 (m, 2H), 5.56 (s, 1H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ + $\text{DMSO-d}_6$ ):  $\delta$  193.17, 160.25, 159.7, 144.73, 138.61, 137.89, 129.77, 128.71, 128.56, 127.94, 127.52, 127.19, 127.15, 126.52, 125.48, 116.07, 93.33, 36.72 ppm, ESI-MS:  $m/z$  379  $[\text{M}+\text{H}]^+$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{25}\text{H}_{19}\text{N}_2\text{O}_2$   $m/z$  379.14410  $[\text{M}+\text{H}]^+$ , found 379.1429.



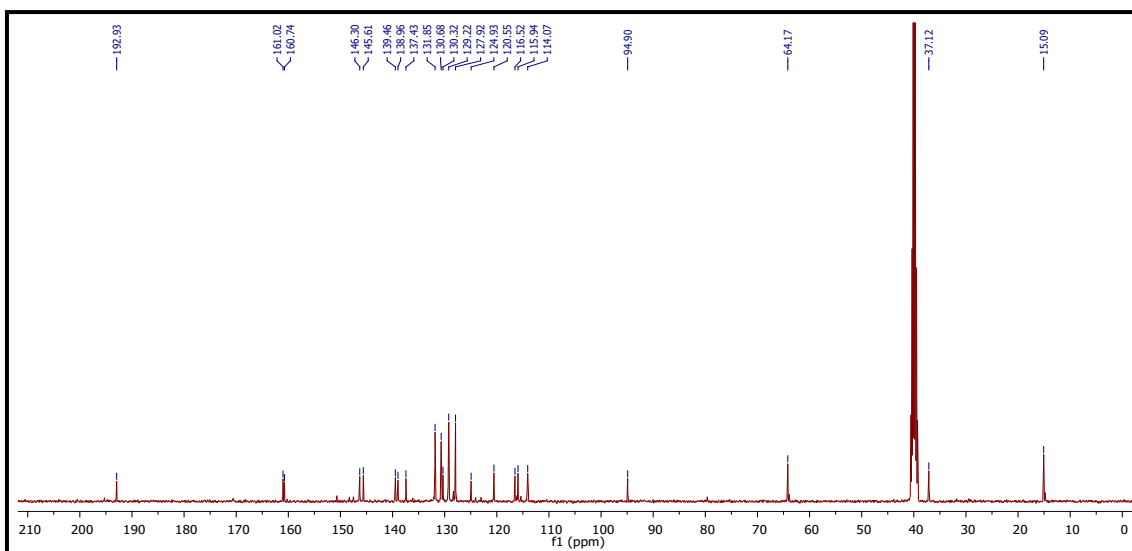


**(4-bromophenyl)(4-(3-ethoxy-4-hydroxyphenyl)-3-phenyl-4,7-dihydroisoxazolo[5,4-*b*]pyridin-5-yl)methanone (8h).**

Isolated as a yellow colour solid, yield 84% (237 mg), m.p 190-192 °C, IR (ATR): 3242, 3020, 2912, 1660, 1612, 1583, 1510, 1437, 1364, 1270, 1213, 1114, 1044, 908  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  10.97 (br, NH), 8.67 (s, 1H), 7.67 – 7.58 (m, 4H), 7.46 – 7.37 (m, 5H), 7.11 (s, 1H), 6.67 (s, 1H), 6.59 – 6.54 (m, 2H), 5.47 (s, 1H), 3.85 – 3.81 (m, 1H), 3.79 – 3.67 (m, 1H), 1.21 (t,  $J = 6.9$  Hz, 3H) ppm,  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  192.93, 161.02, 160.74, 146.3, 145.61, 139.46, 138.96, 137.43, 131.85, 130.68, 130.32, 129.22, 127.92, 124.93, 120.55, 116.52, 115.94, 114.07, 94.9, 64.17, 37.12, 15.09 ppm, ESI-MS:  $m/z$  515  $[\text{M-H}]^-$ , HRMS (ESI) Anal. calcd. for  $\text{C}_{27}\text{H}_{20}\text{O}_4\text{N}_2\text{Br}$   $m/z$  515.0601  $[\text{M-H}]^-$ , found 515.0620.







**(3-isobutyl-4-phenyl-4,7-dihydroisoxazolo[5,4-b]pyridin-5-yl)(phenyl)methanone (8i).**

Isolated as a yellow colour solid, yield 79% (242 mg), m.p 158-160 °C, IR (ATR): 3210, 3050, 3010, 2915, 1665, 1615, 1514, 1320, 1214, 1180, 875 cm<sup>-1</sup>, <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.31 (br, NH), 7.45 (d, *J* = 7.4 Hz, 3H), 7.34 (dd, *J* = 14.7, 7.4 Hz, 4H), 7.25 (t, *J* = 7.4 Hz, 2H), 7.15 (t, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 3.7 Hz, 1H), 5.37 (s, 1H), 2.17 (dd, *J* = 14.0, 8.3 Hz, 1H), 2.06 (dd, *J* = 14.0, 6.2 Hz, 1H), 1.83 – 1.70 (m, 1H), 0.88 (d, *J* = 6.6 Hz, 3H), 0.79 (d, *J* = 6.6 Hz, 3H) ppm, <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 194.94, 162.55, 158.7, 145.05, 139.23, 138.2, 131.12, 129.85, 128.92, 128.5, 128.3, 126.8, 117.95, 95.99, 37.91, 34.12, 26.74, 22.66, 21.99 ppm, ESI-MS: *m/z* 357 [M-H]<sup>-</sup>, HRMS (ESI) Anal. calcd. for C<sub>23</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub> *m/z* 357.1597 [M-H]<sup>-</sup>, found 357.1611.

