Supporting Informations

A metal free domino synthesis of 3-arylidiones via two sp$^3$ C-H activation

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General information:

All the reagents were commercial grade and used without purification. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F$^{254}$ (0.25mm). NMR spectra were recorded in CDCl$_3$ with tetramethylsilane as the internal standard for $^1$H NMR (600 MHz), CDCl$_3$ solvent as the internal standard for $^{13}$C NMR (150 MHz). HRMS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat.

Crystallographic Description:

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoK$\alpha$ radiation ($\lambda = 0.71073$ Å) at 298 K. Cell parameters were retrieved using SMART[a] software and refined with SAINT[a] on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS[b]. The structure was solved by direct methods implemented in SHELX-97[c] program and refined by full-matrix
least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. Colourless crystals were isolated in rectangular shape from methanol at room temperature.


Crystallographic description of (2,3-Dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5’g):

C_{19}H_{17}NO, crystal dimensions 0.41 x 0.35 x 0.28 mm, \( M_r = 275.34 \), Triclinic, space group P-1, \( a = 7.5607(4) \) Å, \( b = 9.6755(6) \) Å, \( c = 11.352(1) \) Å, \( \alpha = 107.554(5) \) °, \( \beta = 102.789(5) \) °, \( \gamma = 103.850(4) \) °, \( V = 729.07(10) \) Å³, \( Z = 2 \), \( \rho_{calc} = 1.254 \) mg/m³, \( \mu = 0.077 \) mm⁻¹, \( F(000) = 292.0 \), reflection collected / unique = 3682 / 2529, refinement method = full-matrix least-squares on \( F^2 \), final \( R \) indices \([I > 2\sigma(I)]\): \( R_1 = 0.0487 \), \( wR_2 = 0.1733 \), \( R \) indices (all data): \( R_1 = 0.0634 \), \( wR_2 = 0.1981 \), goodness of fit = 0.932. CCDC-1006843 for (2,3-Dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5’g) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).
General procedure for the synthesis of (1-methyl-1H-indol-3-yl)(phenyl)methanone (1’a): To a solution of N,N-dimethyl-2-(phenylethynyl) aniline (1a) (55.28 mg, 0.25 mmol) in DMSO (1 mL) was added TBAI (18.47 mg, 0.05 mmol), followed by TBHP 70 % wt in water (180 µl, 1.25 mmol ) and the resultant mixture was put into a preheated oil bath (80 °C) for 2 h. The resultant reaction mixture was admixed with water (5 mL) and the product was extracted with ethyl acetate (2 x 20 mL). The organic phase was dried over anhydrous sodium sulphate and concentrated in vacuo. The crude product was purified over a column of silica gel and eluted with (9:1 hexane / ethyl acetate to give (1-methyl-1H-indol-3-yl)(phenyl)methanone (1’a) (43.53 mg, 74 % yield).

Table S1. Screening of Reaction Conditions.a,b

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst (mol%)</th>
<th>Oxidant (equiv)</th>
<th>Solvent</th>
<th>Yield %</th>
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<td>DMSO</td>
<td>49</td>
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<td>TBAI (20)</td>
<td>TBHPc (5)</td>
<td>DMSO</td>
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*aReaction conditions: N,N-dimethyl-2-(phenylethynyl) aniline (1a) (0.25 mmol), time 2 h, temperature 80 °C. bIsolated yield. c70% aqueous solution. dDecane solution (5-6 M). e50% aqueous solution.
**Spectral Data**

(1-Methyl-1H-indol-3-yl)(phenyl)methanone (1'a):

![Chemical structure](image)

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ (ppm) 3.79 (s, 3H), 7.32–7.33 (m, 3H), 7.46 (t, 2H, $J = 7.2$ Hz), 7.48 (s, 1H), 7.52 (t, 1H, $J = 7.2$ Hz), 7.79 (d, 2H, $J = 7.2$ Hz), 8.41–8.43 (m, 1H); $^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ (ppm) 33.7, 109.8, 115.7, 122.8, 122.9, 123.8, 127.4, 128.4, 128.8, 131.2, 137.7, 138.1, 141.1, 191.0; IR (KBr): 2923, 2851, 1621, 1575, 1524, 1465, 1368, 1233, 1155, 1124, 1070, 872, 746, 716 cm$^{-1}$; HRMS (ESI): calcd. for C$_{16}$H$_{13}$NO (MH$^+$) 236.1070; found 236.1077.

(1-Methyl-1H-indol-3-yl)(m-tolyl)methanone (1'b):

![Chemical structure](image)

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ (ppm) 2.42 (s, 3H), 3.83 (s, 3H), 7.32–7.36 (m, 5H), 7.51 (s, 1H), 7.57–7.59 (m, 1H), 7.61 (s, 1H), 8.40–8.41 (m, 1H); $^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ (ppm) 21.6, 33.7, 109.8, 116.0, 122.9, 123.0, 123.8, 126.1, 127.4, 128.2, 129.4, 132.0, 137.8, 138.0, 138.3, 141.2, 191.3; IR (KBr): 2950, 2924, 2857, 1617, 1587, 1521, 1465, 1367, 1268, 1241, 1202, 1120, 1070, 751 cm$^{-1}$; HRMS (ESI): calcd. for C$_{17}$H$_{15}$NO (MH$^+$) 250.1226; found 250.1232.
(4-(tert-Butyl)phenyl)(1-methyl-1H-indol-3-yl)methanone (1′c):

![Chemical Structure Image]

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ (ppm) 1.36 (s, 9H), 3.82 (s, 3H), 7.32–7.35 (m, 3H), 7.48 (d, 2H, $J$ = 8.4 Hz), 7.55 (s, 1H), 7.76 (d, 2H, $J$ = 8.4 Hz), 8.42–8.44 (m, 1H); $^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ (ppm) 31.5, 33.7, 35.2, 109.7, 115.9, 122.8, 123.0, 123.8, 125.4, 127.5, 128.9, 137.7, 137.9, 138.4, 154.8, 190.8; IR (KBr): 2963, 1689, 1612, 1524, 1464, 1367, 1268, 1235, 1185, 1125, 881, 745, 709 cm$^{-1}$; HRMS (ESI): calcd. for C$_{20}$H$_{21}$NO (MH$^+$) 292.1696; found 292.1693.

(4-Methoxyphenyl)(1-methyl-1H-indol-3-yl)methanone (1′d):

![Chemical Structure Image]

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ (ppm) 3.80 (s, 3H), 3.85 (s, 3H), 6.95 (d, 2H, $J$ = 8.4 Hz), 7.29–7.34 (m, 3H), 7.50 (s, 1H), 7.81 (d, 2H, $J$ = 9.0 Hz), 8.35–8.37 (m, 1H); $^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ (ppm) 33.6, 55.6, 109.7, 113.7, 115.8, 122.6, 122.8, 123.6, 127.5, 131.0, 133.6, 137.3, 137.6, 162.3, 189.9; IR (KBr): 3042, 2917, 1614, 1599, 1567, 1528, 1505, 1461, 1371, 1252, 1234, 1169, 1151, 1122, 1023, 878, 845, 748 cm$^{-1}$; HRMS (ESI): calcd. for C$_{17}$H$_{15}$NO$_2$ (MH$^+$) 266.1176; found 266.1172.
(4-Bromophenyl)(1-methyl-1H-indol-3-yl)methanone (1'e):

\[
\text{\( \mathrm{O} \)} \quad \begin{array}{c}
\text{\( \text{Br} \)} \\
\text{\( \text{CH}_3 \)}
\end{array}
\]

\[\text{\( ^1\text{H NMR (600 MHz, CDCl}_{3}\text{): } \delta\text{ (ppm) 3.79 (s, 3H), 7.31–7.33 (m, 3H), 7.45 (s, 1H), 7.57 (d, 2H, } J = 7.8 \text{ Hz), 7.64 (d, 2H, } J = 8.4 \text{ Hz), 8.36–8.38 (m, 1H); } ^{13}\text{C NMR (150 MHz, CDCl}_{3}\text{): } \delta \text{ (ppm) 33.7, 109.9, 115.4, 122.7, 123.0, 123.9, 125.8, 127.2, 130.4, 131.6, 137.7, 137.9, 139.7, 189.6; IR (KBr): 3081, 2925, 1624, 1582, 1520, 1459, 1395, 1370, 1266, 1233, 1155, 1125, 1070, 1034, 1003, 877, 840, 772, 751 \text{ cm}^{-1}; HRMS (ESI): calcd. for } \text{C}_{16}\text{H}_{12}\text{BrNO (MH}^+) \text{ 314.0175; found 314.0184.}\]

(3-Fluorophenyl)(1-methyl-1H-indol-3-yl)methanone (1'f):

\[
\text{\( \mathrm{O} \)} \quad \begin{array}{c}
\text{\( \text{F} \)} \\
\text{\( \text{CH}_3 \)}
\end{array}
\]

\[\text{\( ^1\text{H NMR (600 MHz, CDCl}_{3}\text{): } \delta\text{ (ppm) 3.85 (s, 3H), 7.23–7.26 (m, 1H), 7.34–7.38 (m, 3H), 7.43–7.47 (m, 1H), 7.50 (d, 1H, } J = 9.0 \text{ Hz), 7.52 (s, 1H), 7.59 (d, 1H, } J = 7.2 \text{ Hz), 8.40–8.42 (m, 1H); } ^{13}\text{C NMR (150 MHz, CDCl}_{3}\text{): } \delta \text{ (ppm) 33.8, 109.9, 115.5, 115.7, 115.8, 118.1, 118.2, 122.9, 123.1, 124.1, 124.5, 127.3, 130.1, 130.2, 137.8, 138.1, 143.17, 143.21, 161.9, 163.6, 189.3; IR (KBr): 3050, 2923, 1621, 1578, 1522, 1468, 1426, 1395, 1369, 1266, 1244, 1024, 1152, 1126, 1113, 1080, 833, 828, 769, 753 \text{ cm}^{-1}; HRMS (ESI): calcd. for } \text{C}_{16}\text{H}_{12}\text{FNO (MH}^+) \text{ 254.0976; found 254.0980.}\]
(1,5-Dimethyl-1H-indol-3-yl)(phenyl)methanone (2′a):

\[
\begin{align*}
&\text{H}_3\text{C} \quad \text{O} \\
&\text{N} \quad \text{C} \quad \text{H}_3 \\
&\text{H}_3 \quad \text{N} \quad \text{O} \\
&\text{C} \\
&\text{H}_3
\end{align*}
\]

\(^1\)H NMR (600 MHz, CDCl\(_3\)): \(\delta\) (ppm) 2.50 (s, 3H), 3.77 (s, 3H), 7.16 (d, 1H, \(J = 8.4\) Hz), 7.23 (t, 1H, \(J = 6.6\) Hz), 7.43–7.47 (m, 3H), 7.51 (t, 1H, \(J = 7.8\) Hz), 7.78 (d, 2H, \(J = 7.2\) Hz), 8.26 (s, 1H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)): \(\delta\) (ppm) 21.7, 33.7, 109.4, 115.3, 122.6, 125.3, 127.6, 128.4, 128.8, 131.1, 132.6, 136.1, 138.2, 141.2, 191.0; IR (KBr): 3058, 2918, 1623, 1574, 1484, 1459, 1387, 1364, 1269, 1237, 1146, 1120, 1068, 1021, 907, 837, 795, 758, 718 cm\(^{-1}\); HRMS (ESI): calcd. for C\(_{17}\)H\(_{15}\)NO (MH\(^+\)) 250.1226; found 250.1222.

(1,5-Dimethyl-1H-indol-3-yl)(4-methoxyphenyl)methanone (2′d):

\[
\begin{align*}
&\text{H}_3\text{C} \quad \text{O} \\
&\text{N} \quad \text{C} \quad \text{H}_3 \\
&\text{O} \\
&\text{C} \\
&\text{H}_3
\end{align*}
\]

\(^1\)H NMR (600 MHz, CDCl\(_3\)): \(\delta\) (ppm) 2.50 (s, 3H), 3.83 (s, 3H), 3.89 (s, 3H), 6.98 (d, 2H, \(J = 8.4\) Hz), 7.17 (d, 1H, \(J = 7.8\) Hz), 7.25–7.26 (m, 1H), 7.49 (s, 1H), 7.83 (d, 2H, \(J = 8.4\) Hz), 8.21 (s, 1H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)): \(\delta\) (ppm) 21.8, 33.7, 55.6, 109.4, 113.7, 115.5, 122.6, 125.3, 127.8, 131.0, 132.4, 133.9, 136.1, 137.4, 162.3, 190.0; IR (KBr): 2956, 2923, 1614, 1596, 1523, 1508, 1451, 1363, 1304, 1254, 1163, 1116, 1060, 1021, 910, 844, 775 cm\(^{-1}\); HRMS (ESI): calcd. for C\(_{18}\)H\(_{17}\)NO\(_2\) (MH\(^+\)) 280.1332; found 280.1335.
(1,5-Dimethyl-1H-indol-3-yl)(3-fluorophenyl)methanone (2′f):

![Chemical structure](image1.png)

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ (ppm) 2.52 (s, 3H), 3.82 (s, 3H), 7.19 (d, 1H, $J = 9.0$ Hz), 7.22–7.25 (m, 1H), 7.26 (d, 1H, $J = 8.4$ Hz), 7.43–7.46 (m, 1H), 7.47 (s, 1H), 7.48–7.50 (m, 1H), 7.58 (d, 1H, $J = 7.8$ Hz), 8.25 (s, 1H); $^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ (ppm) 21.7, 33.8, 109.6, 115.0, 115.6, 115.8, 118.0, 118.1, 122.6, 124.5, 125.6, 127.5, 130.09, 130.14, 132.9, 136.2, 138.2, 143.3, 143.4, 161.9, 163.6, 189.3; IR (KBr): 2922, 1624, 1581, 1523, 1482, 1452, 1428, 1364, 1269, 1244, 1206, 1149, 1116, 1065, 1032, 941, 893, 809, 792, 765, 739 cm$^{-1}$; HRMS (ESI): calcd. for C$_{17}$H$_{14}$FNO (MH$^+$) 268.1132; found 268.1137.

(5-Chloro-1-methyl-1H-indol-3-yl)(phenyl)methanone (3′a):

![Chemical structure](image2.png)

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ (ppm) 3.82 (s, 3H), 7.24–7.28 (m, 2H), 7.48 (t, 2H, $J = 7.8$ Hz), 7.51 (s, 1H), 7.56 (t, 1H, $J = 7.2$ Hz), 7.78 (d, 2H, $J = 7.2$ Hz), 8.43 (s, 1H); $^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ (ppm) 33.9, 110.9, 115.3, 122.4, 124.2, 128.4, 128.5, 128.8, 128.9, 131.5, 136.1, 138.8, 140.7, 190.7; IR (KBr): 3050, 2928, 1610, 1598, 1575, 1528, 1470, 1449, 1362, 1235, 1179, 1082, 1023, 891, 812, 717, 698 cm$^{-1}$; HRMS (ESI): calcd. for C$_{16}$H$_{12}$ClNO (MH$^+$) 270.0680; found 270.0678.
(5-Chloro-1-methyl-1H-indol-3-yl)(p-tolyl)methanone (3’g):

\[
\begin{align*}
\text{O} & \quad \text{Cl} \\
\text{CH}_3 & \quad \text{CH}_3 \\
\end{align*}
\]

\(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) (ppm) 2.44 (s, 3H), 3.82 (s, 3H), 7.25-7.28 (m, 4H), 7.52 (s, 1H), 7.70 (d, 2H, \(J = 6.6\) Hz), 8.41 (s, 1H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)): \(\delta\) (ppm) 21.7, 33.9, 110.8, 115.4, 122.4, 124.1, 128.4, 128.8, 128.9, 129.2, 136.0, 137.9, 138.5, 142.0, 190.4; IR (KBr): 3056, 2917, 1614, 1601, 1566, 1525, 1471, 1448, 1368, 1236, 1182, 1144, 1131, 1082, 1034, 892, 873, 838, 787, 763, 740, 702 cm\(^{-1}\); HRMS (ESI): calcd. for C\(_{17}\)H\(_{14}\)ClNO (MH\(^+\)) 284.0837; found 284.0841.

(4-Bromophenyl)(5-chloro-1-methyl-1H-indol-3-yl)methanone (3’e):

\[
\begin{align*}
\text{O} & \quad \text{Cl} \\
\text{Br} & \quad \text{CH}_3 \\
\end{align*}
\]

\(^1\)H NMR (600 MHz, CDCl\(_3\)): \(\delta\) (ppm) 3.84 (s, 3H), 7.26–7.30 (m, 2H), 7.49 (s, 1H), 7.61 (d, 2H, \(J = 9.0\) Hz), 7.66 (d, 2H, \(J = 8.4\) Hz), 8.39 (s, 1H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)): \(\delta\) (ppm) 34.0, 110.9, 115.1, 122.4, 124.4, 126.2, 128.3, 129.2, 130.4, 131.8, 136.2, 138.5, 139.4, 189.3; IR (KBr): 3056, 2924, 1605, 1586, 1525, 1470, 1364, 1234, 1085, 1033, 1010, 892, 842, 811, 765, 741 cm\(^{-1}\); HRMS (ESI): calcd. for C\(_{16}\)H\(_{13}\)BrClNO (MH\(^+\)) 347.9785; found 347.9782.
Phenyl(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4'a):

\[
\text{O} \quad \text{C} \\
\text{N} \quad \text{H}
\]

\(^1\)H NMR (600 MHz, CDCl\(_3\)): \(\delta\) (ppm) 1.87–1.92 (m, 2H), 2.09–2.13 (m, 2H), 3.15 (t, 2H, \(J = 6.6\) Hz), 4.11 (t, 2H, \(J = 6.6\) Hz), 7.07 (t, 1H, \(J = 6.6\) Hz), 7.18 (t, 1H, \(J = 7.2\) Hz), 7.28–7.30 (m, 2H), 7.43 (t, 2H, \(J = 7.8\) Hz), 7.51 (t, 1H, \(J = 7.8\) Hz), 7.71 (d, 2H, \(J = 7.2\) Hz); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)): \(\delta\) (ppm) 20.4, 22.7, 25.4, 42.8, 109.2, 112.3, 121.1, 121.9, 122.1, 127.2, 128.4, 128.8, 131.2, 136.3, 142.1, 146.5, 192.6; IR (KBr): 3055, 2928, 1617, 1511, 1487, 1472, 1456, 1437, 1419, 1374, 1315, 1225, 1160, 1057, 929, 880, 740, 731 cm\(^{-1}\); HRMS (ESI): calcd. for C\(_{19}\)H\(_{17}\)NO (MH\(^+\)) 276.1383; found 276.1385.

(4-Methoxyphenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4'd):

\[
\text{O} \quad \text{CH}_3
\]

\(^1\)H NMR (600 MHz, CDCl\(_3\)): \(\delta\) (ppm) 1.87–1.91 (m, 2H), 2.09–2.13 (m, 2H), 3.16 (t, 2H, \(J = 6.6\) Hz), 3.87 (s, 3H), 4.10 (t, 2H, \(J = 6.6\) Hz), 6.92 (d, 2H, \(J = 9.0\) Hz), 7.08 (t, 1H, \(J = 7.8\) Hz), 7.17 (t, 1H, \(J = 7.8\) Hz), 7.28 (d, 1H, \(J = 7.8\) Hz), 7.36 (d, 1H, \(J = 8.4\) Hz), 7.75 (d, 2H, \(J = 8.4\) Hz); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)): \(\delta\) (ppm) 20.5, 22.8, 25.3, 42.7, 55.6, 109.2, 112.4, 113.5, 121.1, 121.7, 121.8, 127.3, 131.4, 134.4, 136.2, 145.7, 162.5, 191.5; IR (KBr): 2926, 1601, 1510, 1557, 1422, 1373, 1318, 1252, 1230, 1161, 1059, 933, 928, 884, 840, 779, 746 cm\(^{-1}\); HRMS (ESI): calcd. for C\(_{20}\)H\(_{19}\)NO\(_2\) (MH\(^+\)) 306.1489; found 306.1493.
(4-Bromophenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′e):

\[
\begin{align*}
\text{H NMR (600 MHz, CDCl}_3\text{): } & \delta \text{ (ppm) } 1.91–1.95 \text{ (m, 2H), } 2.12–2.16 \text{ (m, 2H), } 3.18 \text{ (t, 2H, } J = 6.6 \text{ Hz), } 4.13 \text{ (t, 2H, } J = 6.0 \text{ Hz), } 7.10 \text{ (t, 1H, } J = 7.8 \text{ Hz), } 7.20 \text{ (t, 1H, } J = 7.2 \text{ Hz), } 7.26 \text{ (d, 1H, } J = 4.2 \text{ Hz), } 7.31 \text{ (d, 1H, } J = 7.8 \text{ Hz), } 7.60 \text{ (q, 4H, } J = 8.4 \text{ Hz); } ^{13}\text{C NMR (150 MHz, CDCl}_3\text{): } \delta \text{ (ppm) 20.3, 22.7, 25.5, 42.8, 109.3, 112.0, 121.0, 122.1, 122.3, 125.9, 127.0, 130.6, 131.7, 136.4, 140.8, 146.9, 191.2; IR (KBr): 2934, 1614, 1587, 1505, 1491, 1455, 1413, 1392, 1361, 1320, 1273, 1221, 1162, 1069, 1011, 929, 884, 836, 769, 746, 735 \text{ cm}^{-1}; HRMS (ESI): calcd. for C}_{19}\text{H}_{16}\text{BrNO (MH}^+\text{) 354.0488; found 354.0485.}
\end{align*}
\]

(2,3-Dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(phenyl)methanone (5′a):

\[
\begin{align*}
\text{H NMR (600 MHz, CDCl}_3\text{): } & \delta \text{ (ppm) 2.56 (quin, 2H, } J = 7.2 \text{ Hz), } 2.87 \text{ (t, 2H, } J = 7.2 \text{ Hz), } 4.12 \text{ (t, 2H, } J = 7.2 \text{ Hz), } 7.21–7.25 \text{ (m, 2H), } 7.26–7.28 \text{ (m, 1H), } 7.44–7.47 \text{ (m, 2H), } 7.50–7.53 \text{ (m, 1H), } 7.68–7.69 \text{ (m, 2H), } 8.03–8.05 \text{ (m, 1H); } ^{13}\text{C NMR (150 MHz, CDCl}_3\text{): } \delta \text{ (ppm) 26.9, 27.1, 44.6, 109.5, 109.9, 122.4, 122.5, 128.1, 128.3, 130.8, 131.5, 133.3, 142.0, 153.6, 191.9; IR (KBr): 3049, 2928, 1608, 1570, 1508, 1451, 1420, 1384, 1345, 1043, 1009, 960, 927, 841, 746 \text{ cm}^{-1}; HRMS (ESI): calcd. for C}_{18}\text{H}_{15}\text{NO (MH}^+\text{) 262.1226; found 262.1221.}
\end{align*}
\]
(2,3-Dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5g):

\[
\begin{align*}
\text{\textsuperscript{1}H NMR (600 MHz, CDCl} & \text{\textsubscript{3}): } \delta \text{ (ppm) 2.44 (s, 3H), 2.54 (quin, 2H, } J = 7.2 \text{ Hz), 2.90 (t, 2H, } J \\
& = 7.2 \text{ Hz), 4.10 (t, 2H, } J = 7.2 \text{ Hz), 7.20–7.23 (m, 2H), 7.24–7.26 (m, 3H), 7.61 (d, 2H, } J = \\
& 7.8 \text{ Hz), 8.03–8.04 (m, 1H); } \text{\textsuperscript{13}C NMR (150 MHz, CDCl} & \text{\textsubscript{3}): } \delta \text{ (ppm) 21.7, 27.0, 27.2, 44.6,} \\
& 109.6, 109.9, 122.2, 122.35, 122.42, 128.5, 129.0, 131.5, 133.2, 139.1, 141.3, 153.3, 191.8;} \\
\text{IR (KBr): 3049, 2983, 1614, 1602, 1570, 1520, 1464, 1448, 1437, 1419, 1382, 1305, 1220,} \\
& 1205, 1137, 1043, 1010, 962, 828, 771, 745 \text{ cm}^{-1}; \text{HRMS (ESI): calcd. for } C_{19}H_{17}NO (MH} & + \text{) } \\
& 276.1383 \text{; found 276.1389.}
\end{align*}
\]
SPECTRA

(1-Methyl-1H-indol-3-yl)(phenyl)methanone (1'a): $^1$H NMR (600 MHz, CDCl$_3$)
(1-Methyl-1H-indol-3-yl)(phenyl)methanone (1'a): $^{13}$C NMR (150 MHz, CDCl$_3$)
(1-Methyl-1H-indol-3-yl)(m-tolyl)methanone (1'b): $^1$H NMR (600 MHz, CDCl$_3$)
(1-Methyl-1H-indol-3-yl)(m-tolyl)methanone (1b): $^{13}$C NMR (150 MHz, CDCl$_3$)
(4-(tert-Butyl)phenyl)(1-methyl-1H-indol-3-yl)methanone (1'c): \(^1\)H NMR (600 MHz, CDCl\(_3\))
(4-(tert-Butyl)phenyl)(1-methyl-1H-indol-3-yl)methanone (1'c): $^{13}$C NMR (150 MHz, CDCl$_3$)
(4-Methoxyphenyl)(1-methyl-1H-indol-3-yl)methanone (1'd): $^1$H NMR (600 MHz, CDCl$_3$)
(4-Methoxyphenyl)(1-methyl-1H-indol-3-yl)methanone (1'd): $^{13}$C NMR (150 MHz, CDCl$_3$)
(4-Bromophenyl)(1-methyl-1H-indol-3-yl)methanone (1'e): $^1$H NMR (600 MHz, CDCl$_3$)
(4-Bromophenyl)(1-methyl-1H-indol-3-yl)methanone (1'c): $^{13}$C NMR (150 MHz, CDCl$_3$)
(3-Fluorophenyl)(1-methyl-1H-indol-3-yl)methanone (1f): $^1$H NMR (600 MHz, CDCl$_3$)
(3-Fluorophenyl)(1-methyl-1H-indol-3-yl)methanone (1f): $^{13}$C NMR (150 MHz, CDCl$_3$)
(1,5-Dimethyl-1\textit{H}-indol-3-yl)(phenyl)methanone (2'a): $^1$H NMR (600 MHz, CDCl$_3$)
(1,5-Dimethyl-1H-indol-3-yl)(phenyl)methanone (2’a): $^{13}$C NMR (150 MHz, CDCl$_3$)

![NMR Spectrum](image-url)

**Current Data Parameters**
- NAME: AG-761-R1_13C
- EXPNO: 1
- PROCNO: 1

**F2 - Acquisition Parameters**
- Time: 16.04
- INSTRUM: spect
- PROBND: 5 mm PASCO BR
- PULPROG: zpg30
- TD: 32x68
- SOLVENT: CDCl$_3$
- NS: 164
- ES: 2
- SNR: 36057.691 Hz
- FTRES: 1.102393 Hz
- AQ: 0.454829 sec
- BW: 65.24
- DW: 18.867 usec
- DE: 6.50 usec
- TE: 300.7 K
- DL: 2.000000000 sec
- D11: 0.030000000 sec
- TDR: 1

**--- CHANNEL f1 ---**
- SFO1: 150.979571 MHz
- MFC1: 13C
- P1: 10.50 usec
- PLW1: 95.000000000 W

**--- CHANNEL f2 ---**
- SFO2: 600.1724007 MHz
- MFC2: 128
- CPDPFG[2]: 16
- CPD5: 70.00 usec
- PLW2: 21.000000000 W
- PLW12: 0.617140000 W
- PLW13: 0.302399999 W

**F2 - Processing parameters**
- SI: 16384
- SF: 150.9128459 MHz
- WOW: EN
- SSB: 0
- LB: 1.00 Hz
- GB: 0
- FC: 1.40
(1,5-Dimethyl-1H-indol-3-yl)(4-methoxyphenyl)methanone (2'd): $^1$H NMR (600 MHz, CDCl$_3$)
(1,5-Dimethyl-1H-indol-3-yl)(4-methoxyphenyl)methanone (2':d): $^{13}$C NMR (150 MHz, CDCl$_3$)
(1,5-Dimethyl-1H-indol-3-yl)(3-fluorophenyl)methanone (2'f): $^1$H NMR (600 MHz, CDCl$_3$)
(1,5-Dimethyl-1H-indol-3-yl)(3-fluorophenyl)methanone (2f): $^{13}$C NMR (150 MHz, CDCl$_3$)
(5-Chloro-1-methyl-1H-indol-3-yl)(phenyl)methanone (3'a): $^1$H NMR (600 MHz, CDCl$_3$)
(5-Chloro-1-methyl-1H-indol-3-yl)(phenyl)methanone (3'a): $^{13}$C NMR (150 MHz, CDCl$_3$)
(5-Chloro-1-methyl-1H-indol-3-yl)(p-tolyl)methanone (3'g): $^1$H NMR (600 MHz, CDCl$_3$)
(5-Chloro-1-methyl-1H-indol-3-yl)(p-tolyl)methanone (3′g): $^{13}$C NMR (150 MHz, CDCl$_3$)
(4-Bromophenyl)(5-Chloro-1-methyl-1H-indol-3-yl)methanone (3'e): $^1$H NMR (600 MHz, CDCl$_3$)
(4-Bromophenyl)(5-Chloro-1-methyl-1H-indol-3-yl)methanone (3'e): $^{13}$C NMR (150 MHz, CDCl$_3$)
Phenyl(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4'a): ^1^H NMR (600 MHz, CDCl$_3$)
(Phenyl(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4'a): $^{13}$C NMR (150 MHz, CDCl$_3$)
(4-Methoxyphenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4'd): $^1$H NMR (600 MHz, CDCl$_3$)
(4-Methoxyphenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4'd): $^{13}$C NMR (150 MHz, CDCl$_3$)
(4-Bromophenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′c): $^1$H NMR (600 MHz, CDCl$_3$)
(4-Bromophenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4':c): $^{13}$C NMR (150 MHz, CDCl$_3$)
(2,3-Dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(phenyl)methanone (5'a): $^1$H NMR (600 MHz, CDCl$_3$)
(2,3-Dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(phenyl)methanone (5'a): $^{13}$C NMR (150 MHz, CDCl$_3$)
(2,3-Dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5g): 'H NMR (600 MHz, CDCl₃)
(2,3-Dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5g): $^{13}$C NMR (150 MHz, CDCl$_3$)