Supporting Information
for DOI: 10.1055/s-0036-1588152
© Georg Thieme Verlag KG Stuttgart · New York 2017
Supporting Information

for

Potassium Hydroxide Catalysed Intermolecular Aza-Michael Addition of 3-Cyanoindole to Aromatic Enones

Jingya Yang, a* Tianyuan Li, a Hongyan Zhou, b Nana Li, a Dongtai Xie, a and Zheng Li a

a College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou 730070, P.R. of China
E-mail: yangjy@nwnu.edu.cn

b College of Science, Gansu Agricultural University, Lanzhou 730070, P.R. of China

Table of Contents

1. General information ...........................................................................................................................................S2

2. Characterization data of the products ..............................................................................................................S2

3. NMR spectra of the products .........................................................................................................................S9
1. General information

$^1$H NMR and $^{13}$C NMR spectra were recorded on a Varian Mercury-400 Plus or Agilent Technologies DD2 (600 MHz) spectrometer. High-resolution mass spectra (HRMS) were performed on a Thermo Orbitrap Elite instrument with an ESI source. The X-ray single-crystal diffraction was performed on a Bruker APEX II CCD instrument. Melting points were measured on an XT4A apparatus (uncorrected). Reagents and solvents were commercially available, and were used without further purification. The reaction mixtures were purified by column chromatography over silica gel (PE-EtOAc).

2. Characterization data of the products

1-(3-Oxo-1,3-diphenylpropyl)-1H-indole-3-carbonitrile (2a)

White solid; yield: 71.4 mg (68%); mp 123–125 °C.

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ = 7.93 (d, $J$ = 7.8 Hz, 2H), 7.74 (d, $J$ = 7.8 Hz, 1H), 7.71 (s, 1H), 7.62–7.59 (m, 1H), 7.49–7.47 (m, 3H), 7.36–7.27 (m, 5H), 7.24 (d, $J$ = 7.2 Hz, 2H), 6.42 (t, $J$ = 6.6 Hz, 1H), 3.99 (d, $J$ = 6.6 Hz, 2H).

$^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ = 195.2, 138.4, 136.0, 135.3, 134.0, 132.6, 132.0, 128.6, 128.1, 128.0, 126.4, 124.1, 122.4, 120.0, 115.7, 111.3, 86.8, 56.1, 43.3.

HRMS (ESI): $m/z$ [M+H]$^+$ calcd for C$_{24}$H$_{19}$N$_2$O: 351.1492; found: 351.1494.

1-(3-Oxo-3-phenyl-1-(p-tolyl)propyl)-1H-indole-3-carbonitrile (2b)

White solid; yield: 52.7 mg (48%); mp 148–149 °C.

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ = 7.93 (d, $J$ = 7.8 Hz, 2H), 7.73 (d, $J$ = 7.8 Hz, 1H), 7.69 (s, 1H), 7.61–7.59 (m, 1H), 7.50–7.46 (m, 3H), 7.30–7.28 (m, 2H), 7.16–7.13 (m, 4H), 6.37 (t, $J$ = 6.6 Hz, 1H), 3.96 (d, $J$ = 6.6 Hz, 2H), 2.32 (s, 3H).

$^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ = 195.4, 138.5, 136.0, 135.4, 135.3, 133.9, 132.8, 129.9, 128.9, 128.1, 128.0, 126.4, 124.0, 122.4, 120.0, 115.9, 111.3, 86.6, 55.9, 43.2, 21.1.

HRMS (ESI): $m/z$ [M+H]$^+$ calcd for C$_{25}$H$_{21}$N$_2$O: 365.1648; found: 365.1650.

1-(1-(4-Nitrophenyl)-3-oxo-3-phenylpropyl)-1H-indole-3-carbonitrile (2c)
Light yellow solid; yield: 67.6 mg (57%); mp 146–147 °C.

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 8.18 (d, $J$ = 8.4 Hz, 2H), 7.95 (d, $J$ = 7.6 Hz, 2H), 7.80 (s, 1H), 7.77–7.75 (m, 1H), 7.65–7.61 (m, 1H), 7.51–7.48 (m, 2H), 7.41–7.37 (m, 3H), 7.32–7.28 (m, 2H), 6.50 (t, $J$ = 6.8 Hz, 1H), 4.05 (dd, $J$ = 6.8, 10.4 Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 194.7, 148.0, 146.1, 135.4, 134.6, 132.5, 132.4, 129.3, 128.4, 128.2, 127.7, 124.8, 124.6, 123.1, 120.5, 115.6, 111.3, 87.9, 55.7, 43.5.

HRMS (ESI): $m/z$ [M+H]$^+$ calcd for C$_{24}$H$_{18}$N$_3$O$_3$: 396.1343; found: 396.1343.

1-(3-Oxo-3-phenyl-1-(4-(trifluoromethyl)phenyl)propyl)-1H-indole-3-carbonitrile (2d)

White solid; yield: 82.8 mg (66%); mp 163–165 °C.

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ = 7.95–7.93 (m, 2H), 7.77–7.75 (m, 1H), 7.74 (s, 1H), 7.63–7.59 (m, 3H), 7.50–7.48 (m, 2H), 7.42–7.40 (m, 1H), 7.35–7.28 (m, 4H), 6.47 (t, $J$ = 7.2 Hz, 1H), 4.01 (dd, $J$ = 7.2, 13.2 Hz, 2H).

$^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ = 194.7, 142.6, 135.7, 135.2, 134.2, 132.3, 129.0, 128.1, 128.0, 126.8, 126.2 (q, $J$ = 3.8 Hz), 124.4, 122.7, 120.2, 115.5, 111.1, 87.4, 55.6, 43.3.

HRMS (ESI): $m/z$ [M+H]$^+$ calcd for C$_{25}$H$_{18}$F$_3$N$_2$O: 419.1366; found: 419.1365.

1-(1-(4-Chlorophenyl)-3-oxo-3-phenylpropyl)-1H-indole-3-carbonitrile (2e)

White solid; yield: 65.8 mg (57%); mp 138–140 °C.

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 7.93 (d, $J$ = 7.6 Hz, 2H), 7.76–7.73 (m, 1H), 7.71 (s, 1H), 7.63–7.60 (m, 1H), 7.50–7.46 (m, 2H), 7.44–7.42 (m, 1H), 7.32–7.29 (m, 4H), 7.17 (d, $J$ = 8.4 Hz, 2H), 6.38 (t, $J$ = 6.8 Hz, 1H), 3.97 (dd, $J$ = 6.8, 2.0 Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 195.0, 137.0, 135.8, 135.2, 134.5, 134.1, 132.5, 129.4, 128.9, 128.1, 127.9, 127.8, 124.2, 122.6, 120.1, 115.6, 111.2, 87.0, 55.5, 43.2.

HRMS (ESI): $m/z$ [M+H]$^+$ calcd for C$_{24}$H$_{18}$ClN$_2$O: 385.1102; found: 385.1105.
1-(3-Oxo-3-phenyl-1-(m-tolyl)propyl)-1H-indole-3-carbonitrile (2f)

Light yellow oil; yield: 76.5 mg (70%).

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 7.92 (d, $J$ = 7.2 Hz, 2H), 7.73–7.71 (m, 2H), 7.59–7.57 (m, 1H), 7.50–7.44 (m, 3H), 7.31–7.20 (m, 3H), 7.11 (d, $J$ = 7.6 Hz, 1H), 7.05 (s, 2H), 6.36 (t, $J$ = 6.4 Hz, 1H), 3.96 (d, $J$ = 6.8 Hz, 2H), 2.30 (s, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 195.3, 139.0, 138.3, 135.9, 135.3, 133.9, 132.7, 129.4, 129.0, 128.8, 128.0, 127.9, 127.2, 124.0, 123.4, 122.4, 119.9, 115.9, 111.3, 86.5, 56.0, 43.3, 21.5.

HRMS (ESI): m/z [M+H]$^+$ calcd for C$_{25}$H$_{21}$N$_2$O: 365.1648; found: 365.1650.

1-(1-(3-Bromophenyl)-3-oxo-3-phenylpropyl)-1H-indole-3-carbonitrile (2g)

Colourless oil; yield: 96.6 mg (75%).

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ = 7.94–7.92 (m, 2H), 7.75 (d, $J$ = 7.2 Hz, 1H), 7.72 (s, 1H), 7.62–7.60 (m, 1H), 7.49–7.42 (m, 5H), 7.33–7.27 (m, 2H), 7.22–7.19 (m, 1H), 7.15–7.14 (m, 1H), 6.37 (t, $J$ = 7.2 Hz, 1H), 4.02 (dd, $J$ = 7.2, 17.4, Hz, 1H), 3.93 (dd, $J$ = 18.0, 8.4 Hz, 1H),

$^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ = 194.8, 140.9, 135.8, 135.2, 134.1, 132.3, 131.8, 130.8, 129.5, 128.9, 128.1, 127.9, 125.1, 124.3, 123.3, 122.6, 120.1, 115.6, 111.2, 87.2, 55.5, 43.2.

HRMS (ESI): m/z [M+H]$^+$ calcd for C$_{24}$H$_{18}$BrN$_2$O: 429.0597; found: 429.0596.

1-(1-(2-Chlorophenyl)-3-oxo-3-phenylpropyl)-1H-indole-3-carbonitrile (2h)

White solid; yield: 67.6 mg (58%); mp 77–78 °C.

$^1$H NMR (600 MHz, CDCl$_3$): $\delta$ = 7.95–7.93 (m, 2H), 7.73–7.72 (m, 1H), 7.68 (s, 1H), 7.62–7.59 (m, 1H), 7.49–7.44 (m, 4H), 7.31–7.25 (m, 3H), 7.23–7.20 (m, 1H), 7.06–7.04 (m, 1H), 6.75 (dd, $J$ = 8.4, 5.4 Hz, 1H), 4.01 (dd, $J$ = 18.0, 8.4 Hz, 1H), 3.89 (dd, $J$ = 18.0, 5.4 Hz, 1H).

$^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ = 194.7, 136.1, 135.8, 135.5, 134.0, 133.2, 132.2, 130.5, 129.9, 128.9, 128.1, 127.8, 127.7, 127.0, 124.2, 122.6, 119.9, 115.7, 111.3, 86.9, 53.3, 42.2.

HRMS (ESI): m/z [M+H]$^+$ calcd for C$_{24}$H$_{18}$ClN$_2$O: 385.1102; found: 385.1105.

1-(3-(4-Methoxyphenyl)-3-oxo-1-(p-tolyl)propyl)-1H-indole-3-carbonitrile (2j)
White solid; yield: 56.1 mg (47%); mp 175–177 °C.

\[ ^{1}H\text{ NMR (}600\text{ MHz, CDCl}_{3}\text{): }\delta = 7.91\text{ (d, } J = 8.4\text{ Hz, 2H), 7.73–7.72}\text{ (m, 1H), 7.70 (s, 1H), 7.48}\text{ (d, } J = 8.4\text{ Hz, 1H), 7.30–7.25}\text{ (m, 2H), 7.15–7.12}\text{ (m, 4H), 6.92}\text{ (d, } J = 9.0\text{ Hz, 2H), 6.36}\text{ (t, } J = 7.2\text{ Hz, 1H), 3.90}\text{ (d, } J = 7.2\text{ Hz, 2H), 3.86}\text{ (s, 3H), 2.31}\text{ (s, 3H).} \]

\[ ^{13}C\text{ NMR (}150\text{ MHz, CDCl}_{3}\text{): }\delta = 193.8, 164.1, 138.4, 135.5, 135.3, 132.8, 130.4, 129.8, 129.1, 128.0, 126.4, 124.0, 122.3, 119.9, 115.9, 114.0, 111.4, 86.4, 56.0, 55.6, 42.9, 21.0. \]

HRMS (ESI): \( m/z [\text{M+H}]^{+}\) calcd for \( C_{26}H_{23}N_{2}O_{2} \): 395.1754; found: 395.1754.

\( 1\)-(3-(4-Methoxyphenyl)-3-oxo-1-(4-(trifluoromethyl)phenyl)propyl)-1\textit{H}-indole-3-carbonitrile (2k) \)

White solid; yield: 80.7 mg (60%); mp 169–170 °C.

\[ ^{1}H\text{ NMR (}600\text{ MHz, CDCl}_{3}\text{): }\delta = 7.94–7.88\text{ (m, 2H), 7.76–7.72}\text{ (m, 2H), 7.58}\text{ (d, } J = 8.4\text{ Hz, 2H), 7.40–7.38}\text{ (m, 1H), 7.34–7.24}\text{ (m, 4H), 6.93}\text{ (d, } J = 9.0\text{ Hz, 2H), 6.45}\text{ (t, } J = 6.6\text{ Hz, 1H), 3.94}\text{ (dd, } J = 6.6, 18.0\text{ Hz, 2H), 3.87}\text{ (s, 3H).} \]

\[ ^{13}C\text{ NMR (}150\text{ MHz, CDCl}_{3}\text{): }\delta = 193.1, 164.3, 142.9, 135.3, 132.5, 130.5, 128.8, 127.9, 126.8, 126.2\text{ (q, } J = 3.6\text{ Hz), 124.3, 122.7, 120.1, 115.6, 114.1, 111.2, 87.2, 55.8, 55.6, 42.9.} \]

HRMS (ESI): \( m/z [\text{M+H}]^{+}\) calcd for \( C_{26}H_{20}F_{3}N_{2}O_{2} \): 449.1471; found: 449.1469.

\( 1\)-(1-(4-Fluorophenyl)-3-(4-methoxyphenyl)-3-oxopropyl)-1\textit{H}-indole-3-carbonitrile (2l) \)

White solid; yield: 83.6 mg (70%); mp 174–175 °C.

\[ ^{1}H\text{ NMR (}600\text{ MHz, CDCl}_{3}\text{): }\delta = 7.91–7.89\text{ (m, 2H), 7.74–7.72}\text{ (m, 1H), 7.69}\text{ (s, 1H), 7.43–7.42}\text{ (m, 1H), 7.30–7.25}\text{ (m, 2H), 7.21–7.19}\text{ (m, 2H), 7.03–7.00}\text{ (m, 2H), 6.93–6.92}\text{ (m, 2H), 6.37}\text{ (t, } J = 7.2\text{ Hz, 1H), 3.89}\text{ (dd, } J = 2.4, 7.2\text{ Hz, 2H), 3.86}\text{ (s, 3H).} \]

\[ ^{13}C\text{ NMR (}150\text{ MHz, CDCl}_{3}\text{): }\delta = 193.5, 164.2, 162.5\text{ (d, } J = 246.9\text{ Hz), 135.2, 134.5}\text{ (d, } J = 3.3\text{ Hz), 132.5, 130.4, 128.9, 128.3\text{ (d, } J = 8.3\text{ Hz), 128.0, 124.1, 122.5, 120.0, 116.1}\text{ (d, } J = 21.6\text{ Hz), 115.7, 114.1, 111.3, 86.8, 55.62, 55.56, 43.0.} \]
HRMS (ESI): m/z [M+Na]⁺ calcd for C_{25}H_{19}FN_{2}NaO_{2}: 421.1323; found: 421.1323.

1-(1-(4-Chlorophenyl)-3-oxo-3-(p-toly1)propyl)-1H-indole-3-carbonitrile (2m)

![Chemical structure of 2m]

White solid; yield: 57.4 mg (48%); mp 198–200 °C.

$^1$H NMR (600 MHz, CDCl₃): $\delta = 7.83$ (d, $J = 7.8$ Hz, 2H), 7.75–7.73 (m, 1H), 7.70 (s, 1H), 7.42 (d, $J = 7.8$ Hz, 1H), 7.31–7.26 (m, 6H), 7.16 (d, $J = 8.4$ Hz, 2H), 6.37 (t, $J = 6.6$ Hz, 1H), 3.93 (t, $J = 6.6$ Hz, 2H), 2.42 (s, 3H).

$^{13}$C NMR (150 MHz, CDCl₃): $\delta = 194.6$, 145.2, 137.2, 135.2, 134.4, 133.4, 132.5, 129.6, 129.4, 128.2, 128.0, 127.8, 124.2, 122.6, 120.1, 115.6, 111.2, 87.0, 55.6, 43.1, 21.7.

HRMS (ESI): m/z [M+H]⁺ calcd for C_{25}H_{20}ClN_{2}O: 399.1259; found: 399.1259.

1-(1-(4-Chlorophenyl)-3-oxo-3-(3-methoxyphenyl)-3-oxopropyl)-1H-indole-3-carbonitrile (2n)

![Chemical structure of 2n]

White solid; yield: 72.2 mg (58%); mp 148–150 °C.

$^1$H NMR (600 MHz, CDCl₃): $\delta = 7.87$ (d, $J = 9.0$ Hz, 2H), 7.73 (s, 1H), 7.60 (d, $J = 7.8$ Hz, 2H), 7.46 (d, $J = 9.0$ Hz, 2H), 7.41–7.39 (m, 4H), 7.38 (t, $J = 6.6$ Hz, 1H), 6.45 (t, $J = 6.6$ Hz, 2H), 3.97 (dd, $J = 6.6$, 13.8 Hz, 2H).

$^{13}$C NMR (150 MHz, CDCl₃): $\delta = 194.9$, 160.0, 137.2, 137.0, 135.2, 134.5, 132.5, 129.9, 129.4, 128.0, 127.8, 124.2, 122.6, 120.5, 120.1, 115.6, 111.2, 87.1, 55.6, 55.5, 43.3.

HRMS (ESI): m/z [M+H]⁺ calcd for C_{25}H_{20}ClN_{2}O: 415.1208; found: 415.1207.

1-(3-(4-Chlorophenyl)-3-oxo-1-(4-(trifluoromethyl)phenyl)propyl)-1H-indole-3-carbonitrile (2o)

![Chemical structure of 2o]

White solid; yield: 74.7 mg (55%); mp 129–130 °C.

$^1$H NMR (600 MHz, CDCl₃): $\delta = 7.88$ (d, $J = 9.0$ Hz, 2H), 7.76–7.75 (m, 1H), 7.73 (s, 1H), 7.60 (d, $J = 7.8$ Hz, 2H), 7.46 (d, $J = 9.0$ Hz, 2H), 7.34–7.29 (m, 4H), 6.45 (t, $J = 6.6$ Hz, 1H), 3.97 (dd, $J = 6.6$, 13.8 Hz, 2H).
$^1$H NMR (600 MHz, CDCl$_3$): \( \delta = 7.91–7.89 \) (m, 2H), 7.73–7.72 (m, 1H), 7.70 (s, 1H), 7.46 (d, \( J = 7.8 \) Hz, 1H), 7.34–7.21 (m, 6H), 6.93–6.91 (m, 2H), 6.40 (t, \( J = 7.2 \) Hz, 1H), 3.91 (t, \( J = 7.2 \) Hz, 2H), 3.86 (s, 3H).

$^{13}$C NMR (150 MHz, CDCl$_3$): \( \delta = 193.7, 164.1, 138.2, 135.3, 134.7, 132.6, 132.2, 129.5, 129.3, 129.25, 128.7, 127.9, 126.4, 124.4, 121.5, 120.0, 115.7, 111.3, 86.8, 56.0, 43.2.$

HRMS (ESI): \([M+H]^+\) calcd for C$_{25}$H$_{21}$N$_2$O: 381.1598; found: 381.1600.

**1-(3-(4-Methoxyphenyl)-3-oxo-1-phenylpropyl)-1H-indole-3-carbonitrile (2p)**

White solid; yield: 72.2 mg (64%); mp 116–118 °C.

$^1$H NMR (600 MHz, CDCl$_3$): \( \delta = 7.86 \) (d, \( J = 8.4 \) Hz, 2H), 7.75–7.73 (m, 1H), 7.70 (s, 1H), 7.47–7.44 (m, 3H), 7.36–7.26 (m, 5H), 7.23 (d, \( J = 7.2 \) Hz, 2H), 6.39 (t, \( J = 6.6 \) Hz, 1H), 3.95 (d, \( J = 6.6 \) Hz, 2H).

$^{13}$C NMR (150 MHz, CDCl$_3$): \( \delta = 194.4, 138.2, 135.3, 134.7, 132.6, 132.2, 129.5, 129.3, 129.25, 128.7, 127.9, 126.4, 124.1, 122.5, 120.0, 115.7, 111.3, 86.8, 56.0, 43.2.$

HRMS (ESI): \([M+H]^+\) calcd for C$_{24}$H$_{18}$BrN$_2$O: 429.0597; found: 429.0596.

**1-(3-(4-Bromophenyl)-3-oxo-1-phenylpropyl)-1H-indole-3-carbonitrile (2q)**

White solid; yield: 68.2 mg (53%); mp 199–202 °C.

$^1$H NMR (600 MHz, CDCl$_3$): \( \delta = 7.86 \) (d, \( J = 8.4 \) Hz, 2H), 7.75–7.73 (m, 1H), 7.70 (s, 1H), 7.47–7.44 (m, 3H), 7.36–7.26 (m, 5H), 7.23 (d, \( J = 7.2 \) Hz, 2H), 6.39 (t, \( J = 6.6 \) Hz, 1H), 3.95 (d, \( J = 6.6 \) Hz, 2H).

$^{13}$C NMR (150 MHz, CDCl$_3$): \( \delta = 194.4, 138.2, 135.3, 134.7, 132.6, 132.2, 129.5, 129.3, 129.25, 128.7, 127.9, 126.4, 124.1, 122.5, 120.0, 115.7, 111.3, 86.8, 56.0, 43.2.$

HRMS (ESI): \([M+H]^+\) calcd for C$_{24}$H$_{18}$BrN$_2$O: 429.0597; found: 429.0596.

**1-(3-(4-Chlorophenyl)-3-oxo-1-phenylpropyl)-1H-indole-3-carbonitrile (2r)**

White solid; yield: 75.0 mg (65%); mp 201–203 °C.

$^1$H NMR (600 MHz, CDCl$_3$): \( \delta = 7.86 \) (d, \( J = 8.4 \) Hz, 2H), 7.75–7.73 (m, 1H), 7.70 (s, 1H), 7.47–7.44 (m, 3H), 7.36–7.26 (m, 5H), 7.23 (d, \( J = 7.2 \) Hz, 2H), 6.39 (t, \( J = 6.6 \) Hz, 1H), 3.95 (d, \( J = 6.6 \) Hz, 2H).
\[^{13}\text{C}\] NMR (150 MHz, CDCl\(_3\)): \(\delta = 194.1, 140.6, 138.2, 135.3, 134.3, 132.6, 129.5, 129.3, 129.2, 128.7, 128.0, 126.4, 124.1, 122.5, 120.0, 115.7, 111.2, 86.8, 56.0, 43.2\).

HRMS (ESI): \(m/z\) [M+H]\(^+\) calcd for C\(_{24}\)H\(_{18}\)ClN\(_2\)O: 385.1102; found: 385.1105.

1-(3-(4-Nitrophenyl)-3-oxo-1-phenylpropyl)-1H-indole-3-carbonitrile (2s)

White solid; yield: 65.2 mg (55%); mp 175–178 °C.

\(^1\text{H}\) NMR (600 MHz, CDCl\(_3\)): \(\delta = 8.30\) (d, \(J = 9.0\) Hz, 2H), 8.07 (d, \(J = 9.0\) Hz, 2H), 7.74 (d, \(J = 7.8\) Hz, 1H), 7.72 (s, 1H), 7.48 (d, \(J = 7.8\) Hz, 1H), 7.38–7.25 (m, 7H), 6.40 (t, \(J = 7.2\) Hz, 1H), 4.04 (d, \(J = 7.2\) Hz, 2H).

\[^{13}\text{C}\] NMR (150 MHz, CDCl\(_3\)): \(\delta = 194.0, 150.7, 140.2, 137.8, 135.2, 132.6, 129.4, 129.2, 128.9, 127.9, 126.4, 124.3, 124.1, 122.6, 120.1, 115.6, 111.2, 87.0, 55.9, 43.7.

HRMS (ESI): \(m/z\) [M+H]\(^+\) calcd for C\(_{24}\)H\(_{18}\)N\(_3\)O: 396.1343; found: 396.1343.

1-(1-(Furan-2-yl)-3-oxo-1-phenylpropyl)-1H-indole-3-carbonitrile (2t)

Light yellow solid; yield: 26.8 mg (26%); mp 132–134 °C.

\(^1\text{H}\) NMR (600 MHz, CDCl\(_3\)): \(\delta = 7.93–7.92\) (m, 2H), 7.75–7.74 (m, 2H), 7.61–7.59 (m, 1H), 7.56 (d, \(J = 7.8\) Hz, 1H), 7.48–7.46 (m, 2H), 7.35–7.27 (m, 3H), 6.99–6.96 (m, 2H), 6.64 (t, \(J = 6.6\) Hz, 1H), 4.05 (dd, \(J = 6.6, 17.4\) Hz, 1H), 3.98 (dd, \(J = 6.6, 17.4\) Hz, 1H).

\[^{13}\text{C}\] NMR (150 MHz, CDCl\(_3\)): \(\delta = 194.9, 141.6, 135.8, 134.9, 134.0, 132.9, 128.9, 128.1, 127.9, 127.2, 126.0, 125.9, 124.2, 122.5, 120.1, 115.6, 111.1, 87.1, 52.1, 44.2.

HRMS (ESI): \(m/z\) [M+K]\(^+\) calcd for C\(_{22}\)H\(_{16}\)N\(_2\)O\(_2\): 379.0843; found: 379.0880.
3. NMR spectra of the products

Figure S1. $^1$H NMR spectrum of 2a

Figure S2. $^{13}$C NMR spectrum of 2a
Figure S3. $^1$H NMR spectrum of 2b

Figure S4. $^{13}$C NMR spectrum of 2b
Figure S5. $^1$H NMR spectrum of 2c

Figure S6. $^{13}$C NMR spectrum of 2c
Figure S7. $^1$H NMR spectrum of 2d

Figure S8. $^{13}$C NMR spectrum of 2d
Figure S9. $^1$H NMR spectrum of 2e

Figure S10. $^{13}$C NMR spectrum of 2e
Figure S11. $^1$H NMR spectrum of 2f

Figure S12. $^{13}$C NMR spectrum of 2f
Figure S13. $^1$H NMR spectrum of 2g

Figure S14. $^{13}$C NMR spectrum of 2g
Figure S15. $^1$H NMR spectrum of 2h

Figure S16. $^{13}$C NMR spectrum of 2h
Figure S17. $^1$H NMR spectrum of 2j

Figure S18. $^{13}$C NMR spectrum of 2j
Figure S19. $^1$H NMR spectrum of 2k

Figure S20. $^{13}$C NMR spectrum of 2k
Figure S21. $^1$H NMR spectrum of 2l

Figure S22. $^{13}$C NMR spectrum of 2l
Figure S23. $^1$H NMR spectrum of 2m

Figure S24. $^{13}$C NMR spectrum of 2m
Figure S25. $^1$H NMR spectrum of 2n

Figure S26. $^{13}$C NMR spectrum of 2n
Figure S27. $^1$H NMR spectrum of 2o

Figure S28. $^{13}$C NMR spectrum of 2o
Figure S29. $^1$H NMR spectrum of 2p

Figure S30. $^{13}$C NMR spectrum of 2p
Figure S31. $^1$H NMR spectrum of 2q

Figure S32. $^{13}$C NMR spectrum of 2q
Figure S33. $^1$H NMR spectrum of 2r

Figure S34. $^{13}$C NMR spectrum of 2r
Figure S35. $^1$H NMR spectrum of 2s

Figure S36. $^{13}$C NMR spectrum of 2s
Figure S37. $^1$H NMR spectrum of 2t

Figure S38. $^{13}$C NMR spectrum of 2t