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**Supporting Information** 

# Selective Catalytic synthesis of α-Alkylated Ketones and β-Alkylated Secondary Alcohols via Hydrogen-Borrowing Strategy

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#### **1. General Information:**

All the reagents were purchased commercially and used without further purification. <sup>1</sup>H NMR and <sup>13</sup>C NMR were recorded with Bruker 400 MHz. <sup>1</sup>H NMR (400MHz) and <sup>13</sup>C NMR (100MHz) spectra were recorded in CDCl<sub>3</sub>, CD<sub>3</sub>OD or DMSO-d6 with tetramethylsilane as the internal standard. Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, sep = septet, br = broad resonance. All the NMR spectra were acquired at ambient temperature. Analytical thin layer chromatography (TLC) was performed using Silica Gel 60 Å F254 pre-coated plates (0.25 mm thickness). Visualization of I<sub>2</sub> stained TLC plate was accomplished by a UV lamp and single-crystal data were collected from a Bruker-APEX-II CCD X-ray diffractometer.

#### 2. General experimental procedure for preparation of catalyzed product [7a-7w, 8a-8r and 10aa-10fm] (C):

Ketone or secondary alcohol (1 mmol), alcohol (1.2 mmol), Ir(III) complex (0.005 mmol), 'BuOK (0.2 mmol) and toluene (2 ml) were placed in a 5 ml screw-capped vial and allowed to react at 110°C for 2-10 h. The progress of the reaction was monitored by TLC. After completion of starting material, the reaction mass was evaporated and the residue was purified with column chromatography over silica gel where hexane/ethyl acetate mixture was used as eluent.

#### 3. Characterization data of ligands (3a-3c):

All the reactions were carried out according to the general procedure A. (All reactions were carried out in 4 m.mol scale)

N-(naphthalen-1-yl) picolinamide(3a): Yield 860 mg, 85%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 10.75 (s, 1H), 8.71 (d, J = 4.6 Hz, 1H), 8.40-8.35 (m, 2H), 8.1 (d, J = 8.1 Hz, 1H), 7.95 (t, J = 6.2 Hz, 1H), 7.89 (d, J = 7.9 Hz, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.60-7.52 (m, 4H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) =162.1, 149.9, 148, 137.6, 134, 132.3, 128.7, 126.4, 126.2, 126.1, 125.9, 124.9, 122.3, 120.3, 118.4.

# N-(naphthalen-2-yl) picolinamide (3b): Yield 840 mg, 84%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 10.2 (s, 1H), 8.64 (d, *J* = 7.5 Hz, 1H), 8.5 (s, 1H), 8.33 (d, *J* = 7.7 Hz, 1H), 7.94 (t, *J* = 6.4 Hz, 1H), 7.86 (d, *J* = 5.2 Hz, 2H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.71 (d, *J* = 6.9 Hz, 1H), 7.51-7.45 (m, 2H), 7.43-7.39 (m, 1H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) =162, 149.7, 147.9, 137.6, 135.1, 133.9, 130.6, 128.7, 127.6, 127.5, 126.44, 126.41, 124.9, 122.3, 119.7, 116.3.

N-(2,5-dimethylphenyl)picolinamide (3c): Yield 742 mg, 82%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 10.03 (s, 1H), 8.61 (d, J = 4.4 Hz, 1H), 8.29 (d, J = 7.7 Hz, 1H), 8.11 (s, 1H), 7.9 (t, J = 7.7 Hz, 1H), 7.48-7.45 (m, 1H), 7.09 (d, J = 7.6 Hz, 1H), 6.89 (d, J = 7.4 Hz, 1H), 2.36 (s, 6H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) = 161.6, 150, 147.9, 137.4, 136.4, 135.5, 130, 126.2, 125.1, 124.7, 122.1, 121.7, 21.1, 17.1.

# Characterization data of Ir(III) complexes (4a-Ir-4c-Ir):

All the reaction was carried out according to the general procedure B. (All reactions were carried out in 4 m.mol scale)

# [N-(naphthalen-1-yl) picolinamide] Cp\*Ir(III) chloride (4a-Ir): Yield 2.22 g, 92%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 8.61 (d, *J* = 5.2 Hz, 1H), 8.21 (d, *J* = 7.5 Hz, 1H), 7.96-7.92 (m, 2H), 7.85-7.84 (m, 2H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.52-7.40 (m, 4H), 1.29 (s, 15H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 168.8, 155.1, 149.6, 146, 138.5, 133.6, 130.2, 128.2, 127.5, 127.4, 127.2, 126.6, 126.4, 126.1, 125.8, 125.2, 125.1, 125, 124.1, 122.4, 87.8, 86.7, 86.4, 84.6, 8.7, 8.6, 8.5, 8.

# [N-(naphthalen-2-yl) picolinamide] Cp\*Ir(III) chloride (4b-Ir): Yield 2.1 g, 86%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 8.62 (d, *J* = 5.2 Hz, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 813 (s, 1H), 7.96 (t, *J* = 7.1 Hz, 1H), 7.90-7.87 (m, 1H), 7.84-7.78 (m, 3H), 7.52 (t, *J* = 6.9 Hz, 1H), 7.44-7.37 (m, 2H), 1.40 (s, 15H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) = 168.7, 155.7, 149.7, 145.9, 138.7, 133.8, 131.1, 127.7, 127.5, 127.1, 126.4, 125.6, 124.6, 123.9, 86.7, 8.5.

# [N-(2, 5-dimethylphenyl)picolinamide] Cp\*Ir(III) chloride (4c-Ir): 1.98 g, 85%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 8.57 (d, *J* = 5.2 Hz, 1H), 8.17 (d, *J* = 7.7 Hz, 1H), 8.90 (t, *J* = 6.9 Hz, 1H), 7.49 (s, 1H), 7.46 (t, *J* = 6.7 Hz, 1H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 8.1 Hz, 1H), 2.25-2.21(m, 6H), 1.41 (s, 15H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 167.5, 155.4, 149.1, 146.6, 138.3, 135.3, 131.4, 129, 127, 126.6, 126.5, 125.5, 86.7, 29.5, 29.2, 20.8, 18.5, 8.45, 8.15.

#### 4. Characterization data of Ir catalysed compounds (7a-7w, 8a-8r, 10ab-10fm and 14).

All the reactions were carried out in 1 mmol scale of ketone and according to the general procedure C.

#### 1,3-diphenylpropan-1-one (7a)<sup>, [1]</sup>: Yield 206 mg, 98%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.95 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.31-7.21 (m, 4H), 7.19-7.13 (m, 1H), 3.30 (t, *J* = 7.6 Hz, 2H), 3.06 (t, *J* = 7.6 Hz, 2H).

#### **1-(2-fluorophenyl)-3-phenylpropan-1-one (7b)** <sup>[2]:</sup> Yield 187 mg, 82%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ (ppm) = 7.82-7.77 (m, 1H), 7.60-7.55 (m, 1H), 7.31-7.18 (m, 6H), 7.17-7.13 (m, 1H), 3.27 (m, 2H), 2.99 (t, *J* = 7.5 Hz, 2H).

#### 1-(3-fluorophenyl)-3-phenylpropan-1-one (7c)<sup>[3]</sup>: Yield 184 mg, 85%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD):  $\delta$  (ppm) = 7.79 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 9.6 Hz, 1H), 7.49 (q, *J*<sub>1</sub> = 8.04 Hz, *J*<sub>2 =</sub> 13.8 Hz, 1H), 7.34-7.30 (m, 1H), 7.25-7.23(m, 4H), 7.16-7.12(m, 1H) 3.32 (t, *J* = 7.6 Hz, 2H), 3.00 (t, *J* = 7.2 Hz, 2H).

#### 1-(4-fluorophenyl)-3-phenylpropan-1-one (7d)<sup>[1]</sup>: Yield189 mg, 83%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.98-7.95(m, 2H), 7.31-7.20 (m, 4H), 7.10 (t, *J* = 8.4 Hz, 2H) 3.26 (t, *J* = 7.6 Hz, 2H), 3.05 (t, *J* = 8.4 Hz, 2H).

#### 3-phenyl-1-(o-tolyl)propan-1-one (7e)<sup>[4]</sup>: Yield 188 mg, 84%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ (ppm) = 7.64 (d, *J* = 6.8 Hz, 1H), 7.37-7.31 (m, 1H), 7.26-7.16 (m, 6H), 7.14-7.12 (m, 1H), 3.23 (t, *J* = 7.4 Hz, 2H), 2.97 (t, *J* = 7.4 Hz, 2H), 2.35 (s, 3H).

# 3-phenyl-1-(m-tolyl) propan-1-one (7f) <sup>[4]</sup>: yield197 mg, 88%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.75-7.73 (m, 2H), 7.43-7.13 (m, 7H), 3.28 (t, *J* = 7.6 Hz, 2H), 3.05 (t, *J* = 7.7 Hz, 2H), 2.39 (s, 3H).

<sup>1</sup>H NMR (400 MHz, DMSO-d6):  $\delta$  (ppm) = 7.79-7.76 (m, 2H), 7.45-7.37 (m, 2H), 7.28-7.27 (m, 4H), 7.20-7.15 (m, 1H), 3.37-3.29 (m, 2H), 2.93 (t, J = 7.56 Hz, 2H), 2.36 (s, 3H).

#### 1-(2-methoxyphenyl)-3-phenylpropan-1-one (7g)<sup>[4]</sup>: Yield 207 mg, 86%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ (ppm) = 7.55 (d, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 8.2 Hz, 1H), 7.23-7.09 (m, 6H), 6.98 (t, *J* = 7.4 Hz, 1H), 3.98 (s, 3H), 3.29-3.144 (m, 2H), 2.94 (t, *J* = 7.6 Hz, 2H).

#### 1-(3-methoxyphenyl)-3-phenylpropan-1-one (7h)<sup>[1]</sup>: Yield 214 mg, 89%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.52 (d, *J* = 7.2 Hz, 1H), 7.47 (s, 1H), 7.36-7.19 (m, 6H), 7.13-7.7.08 (m, 1H), 3.83 (s, 3H), 3.28 (t, *J* = 7.6 Hz, 2H), 3.05 (t, *J* = 7.6 Hz, 2H).

#### 1-(4-methoxyphenyl)-3-phenylpropan-1-one (7i)<sup>[1]</sup>: Yield, 216 mg, 90%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.93 (d, *J* = 8.7 Hz, 2H) 7.28-7.19 (m, 5H), 6.91 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H), 3.24 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 7.6 Hz, 2H).

#### 3-phenyl-1-(pyridin-3-yl) propan-1-one (7j)<sup>[5]</sup>: Yield, 159 mg, 75%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD):  $\delta$  (ppm) = 9.07 (s, 1H), 8.69 (d, J = 4.8 Hz, 1H), 8.36-8.33 (m, 1H), 7.55-7.52 (m, 1H), 7.25-7.24(m, 4H), 7.17-7.13 (m, 1H), 3.38 (t, J = 7.4 Hz, 2H), 3.01 (t, J = 7.6 Hz, 2H).

#### 3-phenyl-1-(pyridin-4-yl) propan-1-one (7k)<sup>[5]</sup>: Yield, 163 mg, 77%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ (ppm) = 8.72-8.70 (m, 2H), 7.86-7.84 (m, 2H), 7.26-7.24 (m, 4H), 7.17-7.13 (m, 1H), 3.37 (t, *J* = 7.4 Hz, 2H), 3.02 (t, *J* = 7.4 Hz, 2H).

# 1-(naphthalen-1-yl)-3-phenylpropan-1-one (7l)<sup>[1]</sup>: Yield,242 mg, 93%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.53 (d, *J* = 8 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 6.8 Hz, 1H), 7.81 (d, *J* = 7.2 Hz, 1H), 7.58-7.44 (m, 3H), 7.29-7.13 (m, 6H), 3.44-3.36 (m, 2H), 3.13 (t, *J* = 7.6 Hz, 2H).

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD):  $\delta$  (ppm) = 8.38-8.36 (m, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.91-7.89(m, 2H), 7.53-7.49 (m, 3H), 7.24-7.23(m, 4H), 7.117-7.13 (q, *J*<sub>1</sub> = 4.5 Hz, *J*<sub>2</sub> = 8.6 Hz, 1H), 3.40 (t, *J* = 7.4 Hz, 2H), 3.07 (t, *J* = 7.4 Hz, 2H).

#### 1-(4-(1H-imidazol-1-yl) phenyl)-3-phenylpropan-1-one (7m): Yield 246 mg, 89%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 8.07 (d, *J* = 8.5 Hz, 2H), 7.93 (s, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.33-7.28 (m, 4H), 7.24-7.19 (m, 3H), 3.31 (t, *J* = 7.6 Hz, 2H), 3.08 (t, *J* = 7.8 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) = 197.6, 140.9, 140.5, 135.5, 130.8, 130.0, 128.5, 128.3, 126.2, 120.7, 40.4, 29.9.

#### 2-benzyl-2,3-dihydro-1H-inden-1-one (7n)<sup>[6]</sup>: Yield182 mg, 82%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.77 (d, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 6.8 Hz, 1H), 7.40-7.34 (m, 2H), 7.31-7.27 (m, 2H), 7.24-7.20 (m, 3H), 3.41(m, 1H), 3.19-3.13 (m, 1H), 3.02-2.97 (m, 1H), 2.87-2.82 (m, 1H), 2.65-2.63 (m, 1H).

#### 2-benzyl-3,4-dihydronaphthalen-1(2H)-one (7o) [7]: Yield 201 mg, 85%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 8.06 (d, J = 6.9 Hz, 1H), 7.45 (t, J = 6 Hz, 1H), 7.31-7.21 (m, 7H), 3.51-3.46 (dd,  $J_1$  = 3.6 Hz,  $J_2$  = 13.5 Hz, 1H), 2.93 (m, 2H), 2.76-2.71 (m, 1H), 2.66-2.60 (m, 1H), 2.13-2.08 (m, 1H), 1.88-1.74(m, 1H).

# 1-(3,5-difluorophenyl)-3-phenylpropan-1-one (7p)<sup>[8]</sup>: Yield 224 mg, 91%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.44-7.41 (m, 2H), 7.31-7.27 (m, 2H), 7.25-7.18 (m, 3H), 7.02-6.97 (m, 1H), 3.24 (t, *J* = 7.3 Hz, 2H), 3.05 (t, *J* = 7.7 Hz, 2H).

# 1-(2-bromophenyl)-3-phenylpropan-1-one (7q)<sup>[9]</sup>: Yield 243 mg, 84%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.58 (d, J = 7.8 Hz, 1H), 7.35-7.19 (m, 8H), 3.30-3.22 (m, 2H), 3.05 (t, J = 7.7 Hz, 2H).

#### 1-(3-bromophenyl)-3-phenylpropan-1-one (7r)<sup>[4]</sup>: Yield 254 mg, 88%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 8.06-8.03 (br, 1H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.67 (d, *J* = 8.1 Hz, 1H), 7.34-7.20 (m, 6H), 3.33-3.24 (m, 2H), 3.09-3.03 (m, 2H).

# 1-(4-bromophenyl)-3-phenylpropan-1-one (7s) [7]: Yield 249 mg, 86%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.80 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.30-7.19 (m, 5H), 3.25 (t, *J* = 7.2 Hz, 2H), 3.05 (t, *J* = 7.8 Hz, 2H).

#### 3-phenyl-1-(4-(trifluoromethyl) phenyl) propan-1-one (7t) <sup>[5]</sup>: Yield 256 mg, 92%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 8.04 (d, *J* = 8.2 Hz, 2H), 7.7 (d, *J* = 8.4 Hz, 2H), 7.31-7.27 (m, 3H), 7.22-7.20 (m, 2H), 3.31 (t, *J* = 7.4 Hz, 2H), 3.07 (t, *J* = 7.5 Hz, 2H).

# 1-(2-chlorophenyl)-3-phenylpropan-1-one (7u) [10]: Yield 222 mg, 91%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.40-7.34 (m, 3H), 7.27-7.24 (m, 2H), 7.22-7.18 (m, 4H), 3.26 (t, *J* = 7.4 Hz, 2H), 3.04 (t, *J* = 7.8 Hz, 2H).

#### 4-methyl-1-phenylpentan-3-one (7v)<sup>[6]</sup>: Yield 162 mg, 92%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.28-7.24 (m, 2H), 7.17 (d, *J* = 6.8 Hz, 3H), 2.88 (t, *J* = 7.4 Hz, 2H), 2.75 (t, *J* = 7.3 Hz, 2H), 2.59-2.52 (m, 1H), 1.06 (d, *J* = 6.7 Hz, 6H).

4,4-dimethyl-1-phenylpentan-3-one (7w)<sup>[6]</sup>: Yield 165 mg, 87%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.28-7.24 (m, 2H), 7.18-7.16 (m, 3H), 2.84 (d, *J* = 7.1 Hz, 2H), 2.78 (d, *J* = 6.8 Hz, 2H), 1.09 (s, 9H).

# 4-(3-phenylpropanoyl) benzonitrile (7x)<sup>[31]</sup>: Yield 167 mg, 71%

<sup>1</sup>H NMR (400 MHz, DMSO-d6):  $\delta$  (ppm) = 8.12 (d, *J* = 8.24Hz, 2H), 7.99 (d, *J* = 8.16 Hz, 2H), 7.31-7.25 (m, 4H), 7.19-7.16 (m, 1H), 3.43 (t, *J* = 7.4 Hz, 2H), 2.94 (t, *J* = 7.44 Hz, 2H), 1.06 (d, *J* = 6.7 Hz, 6H); IR(ATR): ( $\tilde{v}_{max}$ , cm<sup>-1</sup>) = 3062, 3027, 2925, 2854, **2230**, **1689**, 1605, 1452, 1403, 1290, 1205, 980.

#### 1-(3-nitrophenyl)-3-phenylpropan-1-one (7y) [32]: Yield 107 mg, 42%

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.65 (m, 1H), 8.47-8.45 (m, 1H), 8.42 (d, *J* = 7.72 Hz, 1H), 7.82 (t, *J* = 7.96 Hz, 1H), 7.31-7.26 (m, 4H), 7.26-7.16 (m, 1H), 3.50 (t, *J* = 7.4 Hz, 2H), 2.96 (t, *J* = 7.44 Hz, 2H).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 8.74 (s, 1H), 8.41-8.39 (m, 1H), 8.26 (d, *J* = 7.76 Hz, 1H), 7.65 (t, *J* = 8.04 Hz, 1H), 7.32-7.28 (m, 2H), 7.25-7.24 (m, 2H), 7.21-7.19 (m, 1H), 3.33 (t, *J* = 7.24 Hz, 2H), 3.09 (t, *J* = 7.6 Hz, 2H).

#### 2-methyl-1,3-diphenylpropan-1-one (7z) [33]: Yield 171 mg, 76%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.91 (d, *J* = 7.4 Hz, 2H), 7.56 (t, *J* = 7.48 Hz, 1H), 7.45 (t, *J* = 7.72 Hz, 1H), 7.28-7.16 (m, 4H), 7.13-7.10 (m, 1H), 3.90-3.85 (m, 1H), 3.10-3.04 (m, 1H), 2.71-2.66 (m, 1H), 1.19-1.14 (m, 3H).

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 7.96 (d, *J* = 7.28 Hz, 2H), 7.62 (t, *J* = 7.44 Hz, 1H), 7.51 (t, *J* = 7.36 Hz, 2H), 7.26-7.20 (m, 4H), 7.18-7.13 (m, 1H), 3.94-3.88 (m, 1H), 3.07-2.99 (m, 1H), 2.66-2.63 (m, 1H), 1.10-1.06 (m, 3H).

#### 1-(4-chlorophenyl)-2-methyl-3-phenylpropan-1-one (7za)<sup>[34]</sup>: Yield 209 mg, 81%

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 7.97 (d, *J* = 8.56 Hz, 2H), 7.57 (d, *J* = 8.56 Hz, 2H), 7.26-7.20 (m, 4H), 7.17-7.13 (m, 1H), 3.92-3.88 (m, 1H), 3.02-2.97 (m, 1H), 2.66-2.61 (m, 1H), 1.06 (d, *J* = 6.84 Hz, 3H).

#### 3-(3-chloro-4-methylphenyl)-1-phenylpropan-1-one (8a): Yield 235 mg, 91%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.94 (d, *J* = 7.4 Hz, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.46-7.42 (m, 2H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.03 (d, *J* = 7.5 Hz, 1H), 3.27 (t, *J* = 7.3 Hz, 2H), 3.00 (t, *J* = 7.5 Hz, 2H), 2.32 (s, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 198.7, 140.4, 136.6, 134.1, 133.5, 133, 130, 128.8, 128.5, 128.1, 127.9, 40, 29.2, 19.5;

## 3-(3,4-dimethoxyphenyl)-1-phenylpropan-1-one (8b)<sup>[1]</sup>: Yield 246 mg, 91%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.95 (d, *J* = 7.7 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 6.78- 6.76 (m, 3H), 3.84 (s, 6H), 3.27 (t, *J* = 7.6 Hz, 2H), 3.01 (t, *J* = 7.6 Hz, 2H).

#### 3-(4-methoxyphenyl)-1-phenylpropan-1-one (8c)<sup>[1]</sup>: Yield 216 mg, 90%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.94 (d, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.16 (t, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 8.4 Hz, 2H), 3.78 (s, 3H), 3.26 (t, *J* = 7.6 Hz, 2H), 3.01 (t, *J* = 7.6 Hz, 2H).

## 3-(3,4-dimethoxyphenyl)-1-(p-tolyl) propan-1-one (8d) [11]: Yield 234 mg, 82% to be replaced

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.84 (d, *J* = 8.04 Hz, 1H), 7.24-7.22 (m, 2H), 6.80-6.76 (m, 3H), 3.85-3.84 (m, 6H), 3.24 (t, *J* = 7.32 Hz, 2H), 2.99 (t, *J* = 7.84 Hz, 2H), 2.39 (s, 3H).

#### 1,6-diphenylhexan-1-one (8e)<sup>[1]</sup>: Yield 229 mg, 91%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.94 (d, *J* = 7.4 Hz, 2H), 7.54 (d, *J* = 7.3 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.28-7.25 (m, 2H), 7.17-7.15 (m, 3H), 2.95 (t, *J* = 7.4 Hz, 2H), 2.62 (t, *J* = 7.6 Hz, 2H), 1.80-1.71 (m, 2H), 1.69-1.59 (m, 2H), 1.46-1.42 (m, 2H).

#### 3-(4-bromophenyl)-1-phenylpropan-1-one (8f)<sup>[1]</sup>: Yield 260 mg, 90%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) =7.93 (d, *J* = 7.2 Hz, 2H), 7.55-7.5 (m, 1H), 7.46-7.38 (m, 4H), 7.12 (d, *J* = 7.0 Hz, 2H), 3.27 (t, J = 7.4 Hz, 2H), 3.03-3.02 (m, 2H).

#### 1-phenyl-3-(pyridin-2-yl) propan-1-one (8g)<sup>[12]</sup>: Yield 175 mg, 83%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 8.51-8.50 (m, 1H), 7.98 (d, *J* = 7.2 Hz, 2H), 7.61-7.52 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.21-7.20 (m, 1H), 7.12-7.09 (m, 1H), 3.51 (t, *J* = 7.2 Hz, 2H), 3.23 (t, *J* = 7.2 Hz, 2H).

#### 3-(6-(dimethylamino) pyridin-3-yl)-1-phenylpropan-1-one (8h): Yield 206 mg, 81%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 8.05 (s, 1H), 7.93 (d, J = 7.2 Hz, 2H), 7.54 (t, J = 7.2 Hz, 1H), 7.43 (t, J = 7.6 Hz, 2H), 7.37-7.35 (m, 1H), 6.46 (d, J = 8.4 Hz, 1H), 3.22 (t, J = 7.4 Hz, 2H), 3.04 (s, 6H), 2.92 (t, J = 7.6 Hz, 2H). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 198.6, 158.1, 147, 137.6, 136.7, 133.1, 128.6, 128.5, 127.4, 123.6, 105.7, 40.4, 38.2, 26.7;

#### 3-(3-bromophenyl)-1-phenylpropan-1-one (8i) <sup>[13]</sup>: Yield 263 mg 91%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.95-7.93 (m, 2H), 7.55 (t, *J* = 6.8 Hz, 1H), 7.47-7.40 (m, 3H), 7.33-7.31 (m, 1H), 7.18-7.12 (m, 2H), 3.28 (t, *J* = 7.4 Hz, 2H), 3.03 (t, *J* = 7.4 Hz, 2H).

#### 3-(4-methoxy-3-(trifluoromethyl) phenyl)-1-phenylpropan-1-one (8j): Yield 290 mg, 94%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) =7.94 (d, *J* = 7.4 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.46-7.42 (m, 3H), 7.38-7.36 (m, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 3.86 (s, 3H), 3.32 (t, *J* = 4.5 Hz, 2H), 3.03 (t, *J* = 7.2 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) = 198.8, 155.8, 136.7, 133.18, 133.13, 132.9, 128.6, 127.9, 126.9, 126.8, 125, 122.3, 118.7, 118.4, 112.1, 55.9, 40.2, 29.6, 28.9.

#### 1-phenyl-3-(5-phenylthiophen-2-yl) propan-1-one (8k): Yield 269 mg, 92%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.97 (d, *J* = 7.3 Hz, 2H), 7.59-7.53 (m, 4H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.11 (d, *J* = 3.5 Hz, 1H), 6.82 (d, *J* = 3.5 Hz, 1H), 3.39 (t, *J* = 6.5 Hz, 2H), 3.28 (t, *J* = 6.8 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) = 198.4, 145, 143.6, 142.7, 139.9, 136.6, 134.6, 134.3, 133.1, 129.1, 128.8, 128.7, 128.5, 127.9, 127.7, 127, 125.7, 125.5, 122.7, 122.5, 40.31, 24.4

#### 3-(2-chlorophenyl)-1-phenylpropan-1-one (81)<sup>[14]</sup>: Yield 201 mg, 82%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ (ppm) = 7.98-7.96 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.36-7.32 (m, 2H), 7.22-7.15 (m, 2H), 3.35-3.29 (m, 2H), 3.13 (t, *J* = 7.4 Hz, 2H).

### 3-(2-(3-chlorophenyl) thiazol-4-yl)-1-phenylpropan-1-one (8m): yield 258 mg, 79%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.99 (d, *J* = 7.3 Hz, 2H), 7.92 (s, 1H), 7.76-7.74 (m, 1H), 7.55-7.53 (m, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.35-7.31 (m, 2H), 7.01 (s, 1H), 3.48 (t, *J* = 7.2 Hz, 2H), 3.26 (t, *J* = 7.3 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) =199, 165, 157.2, 136.8, 135.3, 134.8, 133, 130.8, 130.3, 130, 129.6, 128.5, 128, 127.2, 126.7, 126.3, 124.9, 114.4, 37.8, 25.9

#### **Propiophenone (8n)**<sup>[15]</sup>: Yield 114 mg, 85%,

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.95 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 3.0 (q, *J*<sub>1</sub> = 7.2 Hz, *J*<sub>2</sub> = 14.4 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H);

#### 1-phenylbutan-1-one (80)<sup>[16]</sup>: Yield 132 mg, 89%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.95 (d, *J* = 7.1 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 2.94 (t, *J* = 7.3 Hz, 2H), 1.79-1.73 (m, 2H), 0.99 (t, *J* = 7.5 Hz, 3H);

#### 4-methyl-1-phenylpentan-1-one (8p)<sup>[1]</sup>: Yield 149 mg, 84%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.95 (d, *J* = 7.1 Hz, 2H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 2.97-2.89 (m, 2H), 1.62 (t, *J* = 6.7 Hz, 3H), 0.94 (d, *J* = 6.1 Hz, 6H);

#### 1-phenylhexan-1-one (8q)<sup>[1]</sup>: Yield 148 mg, 84%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.95 (d, *J* = 7.4 Hz, 2H), 7.56-7.52 (m, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 2.95 (t, *J* = 7.4 Hz, 2H), 1.73-1.71 (m, 2H), 1.36-1.35 (m, 4H), 0.90-0.83 (m, 3H);

#### 1-phenylheptan-1-one (8r)<sup>[14]</sup>: Yield 167 mg, 88%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.94 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 2.95 (t, *J* = 7.3 Hz, 2H), 1.74-1.68 (m, 2H), 1.37-1.30 (m, 6H), 0.88(s, 3H);

#### Ethyl 2-(3-oxo-3-phenylpropyl) thiazole-4-carboxylate(8s): Yield 148 mg, 51%

<sup>1</sup>H NMR (400 MHz, MeOD):  $\delta$  (ppm) = 8.23 (s, 1H), 8.01 (d, *J* = 7.44 Hz, 2H), 7.60 (t, *J* = 7.44 Hz, 1H), 7.49 (t, *J* = 7.68 Hz, 2H), 4.36-4-32 (m, 2H), 3.62 (t, *J* = 6.88 Hz, 2H), 3.43 (t, *J* = 6.76 Hz, 2H), 1.38-1.27 (m, 3H), 2.32 (s, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 197.76, 170.36, 161.31, 153.34, 146.71, 136.29, 133.30, 128.58, 128.54, 127.99, 127.24, 127.09, 61.29, 3792, 27.41, 14.27.

#### 2-(3-oxo-3-phenylpropyl) thiazole-4-carboxylic acid(8s'): Yield 65 mg, 25%z

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 12.93 (br, 1H), 8.27 (m, 1H), 8.01-7.99 (m, 1H), 7.65-7.63 (m, 1H), 7.55-7.53 (m, 2H), 3.59 (br, 2H), 3.31 (br, 2H).

#### 1,3-diphenylpropan-1-one(10aa)<sup>[1]</sup>: Yield 195 mg, 93%

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 7.98 (d, *J* = 7.6 Hz, 2H), 7.64-7.61 (m, 1H), 7.53-7.49 (m, 2H), 7.28-7.27 (m, 4H), 7.18-7.17 (m, 1H), 3.39 (m, 2H), 2.94 (t, *J* = 7.4, 2H);

#### 3-(2,4-dimethoxyphenyl)-1-phenylpropan-1-one (10ab)<sup>[17]</sup>. Yield 238 mg, 88%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ (ppm) = 7.95-7.94 (m, 2H), 7.57 (m, 1H), 7.48-7.46 (m, 2H), 7.02 (d, *J* = 7.8 Hz, 1H), 6.47 (s, 1H), 6.41-6.39 (m, 1H), 3.77-3.74 (m, 6H), 3.21-3.18 (m, 2H), 2.91-2.89 (m, 2H);

#### 3-(2-bromo-4-fluorophenyl)-1-phenylpropan-1-one(10ac): Yield 255 mg, 83%

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ (ppm) = 7.95 (d, *J* = 7.2 Hz, 2H), 7.58-7.56 (m, 1H), 7.49-7.46 (m, 2H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.03 (t, *J* = 8.0 Hz, 1H), 3.32-3.29 (m, 2H), 3.12 (t, *J* = 7.2 Hz, 2H ); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>):δ (ppm) =198.7, 162.2, 159.7, 136.6, 136.3, 133, 131.5, 131.4, 128.6, 120, 119.7, 114.7, 114.5, 38.4, 29.8;

#### 3-(5-fluoro-2-methoxyphenyl)-1-phenylpropan-1-one (10ad): Yield 221 mg, 86%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.96 (d, *J* = 7.2 Hz, 2H), 7.59-7.56 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 6.95-6.92 (m, 1H), 6.88-6.86 (m, 2H), 3.81 (s, 3H), 3.29 (m, 2H), 2.96 (t, *J* = 7.6 Hz, 2H);

<sup>1</sup>H NMR (400 MHz, CDCl3):  $\delta$  (ppm) = 7.96 (d, *J* = 7.4 Hz, 2H), 7.54-7.52 (m, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 6.93-6.90 (m, 1H), 6.86-6.83 (m, 1H), 6.76-6.73 (m, 1H), 3.79 (s, 3H), 3.24 (t, *J* = 7.2 Hz, 2H), 3.01 (t, *J* = 7.8 Hz, 2H);<sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) = 199.4, 157.96, 155.6, 153.5, 136.7, 132.9, 131.2, 131.1, 128.4, 128, 116.9, 116.7, 113.1, 113, 110.8, 110.7, 56.1, 55.6, 38.4, 25.4

1-phenyl-3-(2-(trifluoromethoxy)phenyl)propan-1-one (10ae): Yield 232 mg, 79%

<sup>1</sup>H NMR (400 MHz, MeOD):  $\delta$  (ppm) = 7.98-7.96 (m, 2H), 7.60-7.57 (m, 1H), 7.49-7.46 (m, 2H), 7.41-7.39 (m, 1H), 7.29-7.24 (m, 3H), 3.34-3.29 (m, 2H), 3.08 (t, *J* = 7.6 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) =198.8, 147.7, 147.6,136.6, 133.1, 131, 128.6, 127.6,126.8, 121.9, 120.4, 119, 38.7, 24.7

#### 3-(4-methoxy-3-(trifluoromethyl)phenyl)-1-phenylpropan-1-one(10af): Yield 241 mg, 78%

<sup>1</sup>H NMR (400 MHz, DMSO-d6):  $\delta$  (ppm) =7.98 (d, *J* = 7.4 Hz, 2H), 7.64-7.61 (m, 1H), 7.53-7.49 (m, 4H), 7.16 (d, *J* = 8.4 Hz, 1H), 3.84 (s, 3H), 3.40-3.30 (m, 2H), 3.03 (t, *J* = 7.2 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) = 198.8, 155.8, 136.7, 133.18, 133.1, 132.9, 128.6, 127.9, 126.9,126.8, 124.9, 122.2, 118.7, 118.4, 112.1, 55.9, 40.2, 28.9;

#### 3-(4-chloro-2-fluorophenyl)-1-phenylpropan-1-one (10ag): Yield 213 mg, 81%

<sup>1</sup>H NMR (400 MHz, MeOD):  $\delta$  (ppm) = 7.96 (d, *J* = 7.4 Hz, 2H), 7.60-7.56 (m, 1H), 7.49-7.45 (m, 2H), 7.29 (t, *J* = 8.6 Hz, 1H), 7.11 (t, *J* = 7.8Hz, 2H), 3.35-3.29 (m, 2H), 3.02 (t, *J* = 7.4 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) =198.64 162.1, 159.6, 136.5, 133.1, 132.8, 132.5, 131.6, 131.5, 128.5, 128.3, 128.1, 128, 126.7, 124.3, 116.1, 115.8, 38.4, 23.3, 23.2;

#### 3-(3-bromo-5-methylphenyl)-1-phenylpropan-1-one (10ah): Yield 252 mg, 83%

<sup>1</sup>H NMR (400 MHz, MeOD):  $\delta$  (ppm) = 7.96 (d, J = 7.4 Hz, 2H), 7.58 (t, J = 7.4Hz, 1H), 7.47 (t, J = 7.6Hz, 2H), 7.21 (s, 1H), 7.15 (s, 1H), 7.04 (s, 1H), 3.34-3.30 (m, 2H), 2.95 (t, J = 7.4 Hz, 2H), 2.27 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) =198.6, 143.3, 140.1, 136.6, 133.1, 129.8, 128.5, 128.3, 128.0, 127.9, 122.2, 40.0, 29.5, 21.0;

#### 3-(5-chloro-2-fluorophenyl)-1-phenylpropan-1-one (10ai): Yield 245 mg, 92%

<sup>1</sup>H NMR (400 MHz, DMSO-d6):  $\delta$  (ppm) = 7.99 (d, *J* = 7.4 Hz, 2H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.54-7.48 (m, 3H), 7.32-7.28 (m, 1H), 7.20 (t, *J* = 9.2 Hz, 1H), 3.40 (t, *J* = 7.4 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) =198.3160.9, 158.5, 136.5, 133.1, 130.69, 130.64, 129.9, 129.8, 128.96, 128.93, 128.6, 127.9, 127.0, 116.6, 116.4, 38.3, 23.6;

#### **1-phenylhexan-1-one (10aj)**<sup>[1]</sup>: Yield 148 mg,84%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.97-7.95 (m, 2H), 7.60-7.56 (m, 1H), 7.48 (t, *J* = 7.8Hz, 2H), 3.0 (t, *J* = 7.4 Hz, 2H), 1.73-1.66 (m, 2H), 1.39-1.32 (m, 4H), 0.94-0.90 (m, 3H);

# 1-phenyl-3-(pyridin-2-yl)propan-1-one (10ak) [12]: Yield 170 mg,80%

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.44-8.43 (m, 1H), 7.98 (d, *J* = 7.4Hz, 2H), 7.70-7.68 (m, 1H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.19-7.16 (m, 1H) 3.49 (t, *J* = 7.08 Hz, 2H), 3.11 (t, *J* = 7.08 Hz, 2H)

3-(6-methoxypyridin-3-yl)-1-phenylpropan-1-one (10al): Yield 209 mg, 87%

<sup>1</sup>H NMR (400 MHz, MeOD):  $\delta$  (ppm) = 7.99-7.95 (m, 3H), 7.62-7.56 (m, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 6.71 (d, *J* = 8.4 Hz, 1H), 3.85 (s, 3H), 3.35-3.29 (m, 2H), 2.96 (t, *J* = 7.2 Hz, 2H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): $\delta$  (ppm) =198.7, 162.7, 146, 139, 136.6, 133.1, 129.1, 128.5, 128.3, 128, 127.9, 127.3, 125, 110, 53.2, 40, 26.1;

### 3-phenyl-1-(p-tolyl)propan-1-one (10ba)<sup>[14]</sup>: Yield 201 mg,89%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.86 (d, *J* = 8.0 Hz, 2H), 7.29-7.23 (m, 6H), 7.16-7.14 (m, 1H), 3.29-3.27 (m, 2H), 2.99 (t, *J* = 7.6 Hz, 2H), 2.38 (s, 3H);

#### 1-(p-tolyl)hexan-1-one (10bj) [18]: Yield 165 mg,86%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.86 (d, *J* = 7.8 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 2H), 2.96 (t, *J* = 7.2 Hz, 2H), 2.39 (s, 3H), 1.68-1.66 (m, 2H), 1.44-1.21 (m, 4H), 0.97-0.90 (m, 3H);

#### **1-(4-methoxyphenyl)-3-phenylpropan-1-one (10ca)** [14]: Yield 195 mg,81%

<sup>1</sup>H NMR (400 MHz, MeOD):  $\delta$  (ppm) = 7.95 (d, J = 8.8 Hz, 2H), 7.24-7.23 (m, 4H), 7.15-7.14 (m, 1H), 6.96 (d, J = 7.8 Hz, 1H), 3.85 (s, 2H), 3.29-3.25 (m, 2H), 2.98 (t, J = 7.4 Hz, 2H);

#### 1-(4-methoxyphenyl) hexan-1-one (10cj)<sup>[19]</sup>: Yield 178 mg,86%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.95 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H), 2.94 (t, *J* = 7.4 Hz, 2H), 1.70-1.66 (m, 2H), 1.37-1.33 (m, 4H), 0.93-0.89 (m, 3H);

**3-phenyl-1-(pyridin-3-yl) propan-1-one (10da)**<sup>[5]</sup>: Yield 181 mg,85%

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 9.13 (s, 1H), 8.87-8.77 (m, 1H), 8.31 (d, *J* = 8.0 Hz, 1H), 7.56-7.53 (m, 1H), 7.29-7.28 (m, 4H), 7.18-7.17 (m, 1H), 3.43 (t, *J* = 7.4 Hz, 2H), 2.94 (t, *J* = 7.4 Hz, 2H);

#### 3-phenyl-1-(pyridin-4-yl) propan-1-one (10ea) [5]: Yield 191 mg,90%

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.79 (d, *J* = 4.4 Hz, 2H), 7.83 (d, *J* = 4.4 Hz, 2H), 7.33-7.27 (m, 4H), 7.19-7.18 (m, 1H), 3.42 (t, *J* = 7.2 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H);

#### **1-(naphthalen-1-yl)-3-phenylpropan-1-one (10fa)**<sup>[1]</sup>: Yield 224 mg,86%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 8.53 (d, *J* = 8.2 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.81(d, *J* = 7.08 Hz, 1H), 7.60-7.50 (m, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.31-7.24 (m, 4H), 7.21-7.18 (m, 4H), 3.42 (t, *J* = 8.4 Hz, 2H), 3.13 (t, *J* = 7.8 Hz, 2H);

#### 3-(3,4-dimethoxyphenyl)-1-(naphthalen-1-yl)propan-1-one (10fm)<sup>[20]</sup>: Yield 259 mg,81%

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.39 (d, *J* = 7.6 Hz, 1H), 8.12 (d, *J* = 9.2 Hz, 1H), 8.07 (d, *J* = 6.8 Hz, 1H), 8.0(s, 1H), 7.61-7.57 (m, 3H), 6.87 (s, 1H), 3.69 (s, 6H), 3.42 (t, *J* = 7.2 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H);

3-phenyl-1-(pyridin-3-yl)propan-1-ol (10da')<sup>[10]</sup>: Yield 90 mg, 42%, 2h

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.52 (s, 1H), 8.44 (d, *J* = 3.6 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.36-7.33 (m, 1H), 7.28-7.24 (m, 2H), 7.19-7.14 (m, 3H), 5.44 (d, *J* = 3.6 Hz, 1H), 4.60-4.57(m, 1H), 2.67-2.63 (m, 1H), 2.61-2.56(m, 1H), 1.92-1.90 (m, 2H);

3-phenyl-1-(pyridin-4-yl)propan-1-ol (10ea') <sup>[21]</sup>: Yield 75 mg, 35%, 2h

<sup>1</sup>H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.49 (d, *J* = 5.6 Hz, 2H), 7.34-7.33 (m, 2H), 7.28-7.24 (m, 2H), 7.19-7.14 (m, 3H), 5.51(d, J = 4.8 Hz, 1H), 4.56-4.53 (m, 1H), 2.66-2.60 (m, 2H), 1.91-1.82 (m, 2H);

2,5-dibenzylcyclopentan-1-one (12aa)<sup>[22]</sup>: Yield 246 mg 93%

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.27-7.23 (m, 2H), 7.19-7.15 (m, 2H), 7.14-7.12 (m, 6H), 3.18-3.14 (dd,  $J_1 = 4.2$  Hz,  $J_2 = 13.8$  Hz, 2H), 2.62-2.56 (m, 2H), 2.31-2.24 (m, 2H), 2.0-1.94 (m, 2H), 1.41-1.36 (m, 2H);

<sup>1</sup>H NMR (400 MHz, MeOD):  $\delta$  (ppm) = 7.26-7.22 (m, 4H), 7.18-7.11 (m, 6H), 2.95-2.90 (dd,  $J_1 = 3.6 \text{ Hz}, J_2 = 13.6 \text{ Hz}, 2H$ ), 2.54 (m, 2H), 2.47-2.42 (m, 2H), 1.89-1.79 (m, 2H), 1.56-1.53 (m, 2H);

2,6-dibenzylcyclohexan-1-one (12ab)<sup>[9]</sup>: Yield 253 mg, 91%

<sup>1</sup>H NMR (400 MHz, MeOD):  $\delta$  (ppm) = 7.38-7.24 (m, 4H), 7.22-7.13 (m, 6H), 3.15-3.10 (dd,  $J_1 = 4.8Hz$ ,  $J_2 = 13.8$  Hz, 2H), 2.73-2.76 (m, 2H), 2.40-2.34 (m, 2H), 2.02-2.00 (m, 2H), 1.77-1.73 (m, 1H), 1.62-1.56(m, 1H), 1.32-1.28(m, 2H);

2,7-dibenzylcycloheptan-1-one (12ac)<sup>[23]</sup>: Yield 213 mg, 73%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.22-7.18 (m, 4H), 7.14 (d, *J* = 7.2 Hz, 2H), 7.01-6.99 (m, 4H), 2.80-2.76 (m, 2H), 2.68-2.63(m, 2H), 4.50-2.45 (m, 2H), 1.83-1.76 (m, 4H), 1.34-1.25 (m, 2H), 1.23-1.8(m, 2H);

2-benzylcycloheptan-1-one (12ac')<sup>[24]</sup>: Yield 27 mg, 15%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.25-7.21 (m, 2H), 7.15-7.13 (m, 3H), 3.0-2.95 (m, 1H), 2.91-2.85 (m, 1H), 2.57-2.52(m, 1H), 2.44-2.41 (m, 2H), 1.85-1.78 (m, 4H), 1.68-1.59 (m, 1H), 1.37-1.26 (m, 3H);

2,8-dibenzylcyclooctan-1-one (12ad)<sup>[22]</sup>: Yield 220 mg, 72%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.17-7.15 (m, 4H), 7.12.7-10 (m, 2H), 7.05-7.03 (m, 4H), 3.07-3.02 (m, 2H), 2.95-2.92(m, 2H), 2.48-2.43 (m, 2H), 1.79 (m, 2H), 1.60 (m, 3H), 1.46 (m, 2H), 1.40-1.28 (m, 3H);

2-benzylcyclooctan-1-one (12ad')<sup>[25]</sup>: Yield 54 mg, 25%

<sup>1</sup>H NMR (400 MHz, MeOD): δ (ppm) = 7.24-7.20 (m, 2H), 7.15-7.11 (m, 3H), 3.03-3.01 (m, 1H), 2.91-2.86 (m, 1H), 2.64-2.59(m, 1H), 2.31-2.24 (m, 1H), 2.14-2.11(m, 1H), 2.09-2.01 (m, 1H), 1.89-1.84(m, 1H), 1.76-1.74 (m,, 1H), 1.71-1.58(m, 4H), 1.51-1.45 (m, 1H), 1.44-1.39 (m, 1H), 1.20-1.18(m, 1H);

#### H-indole (14): Yield: 2.45 g, 96% (22 mmol scale reaction).

<sup>1</sup>H NMR (400 MHz, DMSO): δ (ppm) =11.05 (s, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.32-7.31 (m, 1H), 7.06 (t, *J* = 7.2 Hz, 1H), 6-97 (t, *J* = 7.5 Hz, 1H), 6.41 (br, 1H).

#### 5. Characterization data of controlled experiments (10, 10a, 10b & 7bd):

# Benzaldehyde (10):

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 10.01 (s, 1H), 7.87 (d, *J* = 6.9 Hz, 2H), 7.54-7.44 (m, 3H);

# 2-fluorobenzaldehyde (10b):

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 10.36 (s, 1H), 7.86 (t, *J* = 7.2 Hz, 1H), 7.62-7.57 (m, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.16 (t, *J* = 8.9 Hz, 1H);

# 2-hydroxybenzaldehyde (10c):

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 11.0 (s, 1H), 9.89 (s, 1H), 7.56-7.50 (m, 2H), 7.03-6.97 (m, 2H).

## chalcone (7bd):

<sup>1</sup>H NMR (400 MHz, DMSO-d6):  $\delta$  (ppm) = 7.88 (d, *J* = 7.7 Hz, 1H), 7.71 (s, 1H), 7.53-7.41 (m, 3H), 7.30-7.14 (m, 7H).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.79 (m, 2H), 7.55-7.53 (m, 1H), 7.47-7.42 (m, 1H), 7.39-7.30 (m, 5H), 7.21-7.12 (m, 4H).

## 6. Crystallographic data and refinement details of 4a-Ir

A Bruker SMART APEX-II area detector single crystal X-ray diffractometer was used to collect the X-ray diffraction data of suitable crystal of **picolinamidato complex 4a-Ir** using monochromatic Cu K\ $\alpha$ , ( $\lambda$ = 1.54178 Å) with the  $\omega$  and  $\varphi$  scan technique. The data collection of **4a-Ir** was done by using Bruker SAINT system and the data were corrected for absorption using Bruker SADABS <sup>[26]</sup> software. The structure of **4a-Ir** was solved using olex2.solve 1.5 <sup>[27]</sup> and was refined by full matrix least squares based on  $F^2$  using SHELXL-2018/3 <sup>[28]</sup>. All non-hydrogen

atoms were refined anisotropically and the H atoms bonded to carbon atoms were included at calculated positions as riding atoms with C(sp<sup>2</sup>)–H distances of 0.95 Å and C(sp<sup>3</sup>)–H distances of 0.98 Å whereas the hydrogen atoms of water molecule were located from respective Q-peaks. ORTEP-plot and packing diagram were generated with ORTEP-3 for Windows <sup>[28d]</sup>. WinGX <sup>[28d]</sup> was used to prepare the material for publication. CCDC reference number **2165585** contains supplementary crystallographic data for this paper. Crystal data, data collection and structure refinement details of the complex have been summarized in **table S1**.

To prepare suitable single crystal of picolinamidato complex 4a-Ir, slow evaporation of the methanolic solution was followed. The Complex crystallizes in monoclinic space group  $P2_1/n$ . The selected bond lengths and bond angles are presented in table S2 while the intermolecular hydrogen bonding interactions are presented in table S3 & figure S2. FigureS1 represents the ORTEP view of asymmetric unit of 4a-Ir. Crystal packing diagram of 4a-Ir has been shown in figure S3 in the supplementary section. X-ray crystallography showed that the asymmetric unit possesses half-sandwich pseudo-octahedral "three-legged piano-stool" structures, with Cp\* as the seat and three coordination positions are occupied by neutral N,N-chelating picolinamide ligand and a terminal chloride. Each asymmetric unit experiences one intermolecular classical O-H---Cl type hydrogen bonding between uncoordinated water molecule and Cl atom bonded to the central metal ion with a bond distance 3.335(3) Å while two other intermolecular nonclassical C-H···O type hydrogen bonding interactions with the distances 3.228(4) Å, 3.488(4) Å are shown in figure S2 & table S3. Here in, the picolinamide ligand bind to the metal center through the amine nitrogen and the pyridine N forming a five member chelate ring with an angle of N1-Ir1-N2 76.40°, indicating a distortion from the regular octahedron, in analogy with similar Cp\*Ir(III) Complexes bearing a picolinamide ligand and Ru-arenethiosemicarbazone complexes. <sup>[29]</sup>. The dihedral angle between the naphthalene ring plane and the picoline moiety is around -176.9°. Notably, this type of ligand adopts a flat conformation <sup>[30]</sup> but owing to exceptional metal coordination sites, it's coplanarity is lost. The T-shaped edge-to-face stacking orientation of the complex is developed through intramolecular C-H--- $\pi$  interactions between two hydrogen atoms (H24B and H25B) of the Cp\* ring and the  $\pi$  electron density from the naphthalene ring Cg3 and Cg4 of the picolinamide ligand (distances from 2.74 to 2.82 Å).

Figure S1. The ORTEP diagram of 4a-Ir with ellipsoid of 50% probability.



**Figure S2.** Intermolecular hydrogen bonding interactions in **4a-Ir** along *b* axis.



Figure S3. Molecular packing diagram of 4a-Ir in *bc* plane.



# <u>Tables</u>

# Table S1: Crystal data collection and structure refinement for 4a-Ir

Crystal data

CCDC reference number	2165585	
Empirical formula	$C_{26}H_{22}ClIrN_2O_2$	
Moiety formula	C <sub>26</sub> H <sub>26</sub> ClIrN <sub>2</sub> O, H <sub>2</sub> O	
Formula weight	622.10	
Crystal system	Monoclinic	
Space group	P 2 <sub>1</sub> /n	
Colour, habit	Orange red, block	
Size, mm	$0.2 \times 0.12 \times 0.1$	
Unit cell dimensions		
	a = 9.4305(7) Å	
	b = 11.9858(9) Å	
	c = 20.8802(17)Å	
	$\alpha = 90^{\circ}$	

	$\beta = 100.870(2)^{\circ}$
	$\gamma=90^\circ$
Volume Å <sup>3</sup>	2317.8(3)
Z	4
Density (calculated), Mg/m <sup>3</sup>	1.783
Absorption coefficient, mm <sup>-1</sup>	12.417
F(000)	1232.0
Data collection	
Temperature, K	101.00
Theta range for data collection	8.544° to 136.492°
Index ranges	$-11 \le h \le 11$
	$-14 \le k \le 14$
	$-25 \le 1 \le 23$
Reflections collected	39503
Unique reflections	4246
Observed reflections (> $2\sigma(I)$ )	4099
R <sub>int</sub>	0.0486

Completeness to $\theta$ , %	68.246, 97.7%
Absorption correction	SADABS-2016/2 (Bruker,2016/2)
	$T_{\rm min} = 0.209, \ T_{\rm max} = 0.289$

Refinement

Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	4146 / 0 / 298
Goodness-of-fit on $F^2$	1.198
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0303, wR_2 = 0.0837$
R indices (all data)	$R_1 = 0.0306, wR_2 = 0.0839$
Largest diff. peak and hole	1.07 and -1.54 e.Å <sup>-3</sup>

Compound		Bond lengths (Å)	)		
	Ir(1)-N(1)	2.096(4)	Ir(1)-N(2)	2.090(3)	
4 - T.	Ir(1)-C(17)	2.180(3)	Ir(1)-C(18)	2.177(3)	
4a-1r	Ir(1)-C(19)	2.170(4)	Ir(1)-C(20)	2.169(3)	
	Ir(1)-C(21)	2.156(3)	Ir(1)- $Cl(1)$	2.4368(8)	
Bond angles (°)					
	N(1)-Ir(1)-N(2)	76.40(12)	N(1)-Ir(1)-C(17)	103.57(12)	
	N(2)-Ir(1)-C(17)	156.90(11)	N(1)-Ir(1)-C(18)	130.71(14)	
	N(2)-Ir(1)-C(18)	152.24(12)	N(1)-Ir(1)-C(19)	168.64(15)	
	N(2)-Ir(1)-C(19)	114.43(14)	N(1)-Ir(1)-C(20)	139.58(11)	
4a-Ir	N(2)-Ir(1)-C(20)	99.91(11)	N(1)-Ir(1)-C(21)	106.78(11)	
	N(2)-Ir(1)-C(21)	118.15(11)	N(1)-Ir(1)-Cl(1)	87.17(7)	
	N(2)-Ir(1)-Cl(1)	82.65(7)	C(17)-Ir(1)-Cl(1)	120.43(9)	
	C(18)-Ir(1)-Cl(1)	91.93(10)	C(19)-Ir(1)-Cl(1)	97.35(9)	
	C(20)-Ir(1)-Cl(1)	132.82(9)	C(21)-Ir(1)-Cl(1)	156.82(9)	

Table S2: Selected bond lengths (Å), bond angles (°) and torsion angles (°) for 4a-Ir

# Table S3: Hydrogen bonded geometries in 4a-Ir

Compound	Bond	D–H(Å)	H…A(Å)	D…A(Å)	$D-H\cdots A(^{\circ})$
	$O(2)-H(2B)\cdots Cl(1)$	0.87	2.48	3.335(3)	169
4a-Ir	$C(1)-H(1)\cdots O(2)^{i}$	0.95	2.55	3.228(4)	129
	C(24)–H(24A)····O(1) <sup>ii</sup>	0.98	2.54	3.488(4)	163

*Symmetry codes: (i)* 2-*x*, 1--*y*, 1-*z; (ii)* 1+*x*, *y*, *z* 

# 7. Copies of 1H NMR of <sup>1</sup>H NMR, <sup>13</sup>C NMR Spectra





3a IN CDC13-13C



3a IN CDC13-APT



3b IN CDCI3



3b IN CDCI3-13C



3b IN CDCI3-APT



3c IN CDCI3



3c IN CDCI3-13C





4a-Ir IN CDC13

130.2515 127.291 127.24389 127.24785 127.24785 125.2478 126.6819 126.6819 126.1429 126.1429 125.8245 125.2595 125.2595 125.2595 125.25980 122.4989 155.1428 149.6590 146.0133 138.5572 133.6383 Current Data Parameters NAME 4a-Ir EXPNO 60 PROCNO 1 PROCNO 1
P2 - Acquisito Parameters
Date. 20211127
Time 17.13 h
INSTRUM spect
PROBHD 218738\_0162 (
PTL-PROBH\_021768
P300
SOLVENT COCI3
NS 424
SOLVENT COCI3
NS 424
SON 422 528 H4
SPIRES 1.541222 H4
AO 0.648564 sec
DH 1.5400486
DH 1.5400480
DH 1.5400480
DH 1.2.0000000 sec
T1 0.3228888 MHz
NO1 2.5000000 sec
P1 0.3228888 MHz
NO1 2.5000000 sec
P1 8.00 usec
P1 9.00 usec
P1 
 F2
 Processing parameters

 SI
 16364

 SF
 100.6226359 MHz

 WDW
 EM

 SSB
 0

 LB
 1.00 Hz

 GB
 0

 PC
 1.40
 155 150 145 140 135 130 125 ppm 

 155.1428

 149.6590

 1449.6590

 133.65572

 133.65572

 133.65572

 133.65572

 133.65690

 128.2762

 133.65762

 133.65715

 133.65572

 133.65572

 133.65572

 128.2762

 127.2478

 127.2478

 126.6819

 127.2478

 127.2478

 125.2595

 125.1428

 125.1428

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 127.488

 < 168.8518 87.8150 86.7800 86.4248 84.6526 77.3279 77.0083 76.6892 8.7226 8.6798 8.5840 8.0815 NVIII – CI--Ir-N Ò 4a-Ir ...... ..... ..... ..... ..... \*\*\*\*\*\*\* 190 180 170 160 150 140 130 120 110 100 90 80 70 50 20 60 40 30 10 ppm

4a-Ir IN CDCI3-13C


4a-Ir IN CDCI3-APT



4b-Ir IN CDCI3



4b-Ir IN CDCI3-13C



4b-Ir IN CDCI3-APT



4c-Ir IN CDC13



4c-Ir IN CDC13-13C



4c-Ir IN CDC13-APT



7a IN CDCI3



7b IN MeOD



7c IN MeOD



7d IN CDC13



7e IN MeOD



7f IN CDC13



7f IN DMSO



7g IN MeOD



7h IN CDC13



7i IN CDC13



7j IN MeOD



7k IN MeOD



71 IN MeOD





7m IN CDC13-13C



7m IN CDC13-APT



7n IN CDC13



7º IN CDC13



7p IN CDC13



7q IN CDC13



7r IN CDC13





7t IN CDCI3



7u IN CDC13



7v IN CDC13



7W IN CDC13



7x IN DMSO








7z IN DMSO









8a IN CDC13-13C



8a IN CDC13-APT



8b IN CDCI3



8c IN CDCI3



8d IN CDC13



8e IN CDCI3



8f IN CDC13



8g IN CDC13



8h IN CDC13



8h IN CDCl3-13C



8i IN CDC13



8j IN CDC13



8j IN CDCI3-13C



8j IN CDCI3-APT



8k IN CDC13



8k IN CDC13-13C



8k IN CDCL3-APT



81 IN MeOD



8m IN CDC13



8m IN CDCI3-13C



8m IN CDCI3-APT



8n IN CDCI3



80 IN CDCI3



8p IN CDC13



8q IN CDC13



8r IN CDC13



8s IN MeOD



8s IN CDC13-13C



8s IN CDC13-APT



8s' IN DMSO



10aa IN DMSO


10ab IN MeOD



10ac IN MeOD

10ac IN CDCI3-13C





10ac IN CDCI3-APT



10ad IN CDC13



10ad IN MeOD







10ae IN MeOD



10ae IN CDCl3-13C



10ae IN CDCl3-APT



10af IN DMSO



10af IN CDCl3-13C



10af IN CDCl3-APT



10ag IN MeOD



10ag IN CDC13-13C



10ag IN CDC13-APT



10ah IN MeOD



10ah IN CDCl3-13C



10ah IN CDC13-APT



10ai IN DMSO





10ai IN CDCl3-13C

10ai IN CDCl3-APT





10aj IN MeOD



10ak IN DMSO



10al IN MEOD



10al IN CDC13-13C



10al IN CDC13-APT



10ba IN MeOD



10bj IN MeOD



10ca IN MeOD



10cj IN MeOD



10da IN DMSO



10ea IN DMSO



10fa IN CDC13



10fm IN DMSO


10da' IN DMSO



10ea' IN DMSO



12aa IN MeOD



12aa IN CDC13



12ab IN MeOD



12ac IN MeOD



12ac' IN MeOD



12ad IN MeOD



12ad' IN MeOD

12da' IN DMSO AT 100 DEG C



12da' IN DMSO AT 100 DEG C



12da' IN DMSO AT 100 DEG C





14 IN DMSO



10 IN CDC13





10c IN CDCI3



7bd IN DMSO



7bd IN CDC13

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