Supporting Information for Synthesis of Imidazo[1,2-a]pyridinones via a visible light-photocatalyzed functionalization of alkynes/nitrile insertion/ cyclization tandem sequences using micro-flow technology†

Minghui Wei, Jiankun Chen, Chengkou Liu, Zhao Yang, Hong Qin, Yujing Hu, Jindian Duan, Yuguang Li, Zheng Fang, Kai Guo

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1. General Information

$^1$H/$^{13}$C NMR spectra were recorded on magnet system 400’54 ascend instrument purchased from Bruker Biospin AG. All chemical shifts are given in parts per million and are measured relative to DMSO as an internal standard. ESI-MS spectra were recorded on Agilent Q-TOF 6520. Products were purified by flash chromatography on 200-300 mesh silica gel and visualized using a UV lamp (254 nm or 365 nm). All the solvents were used without further purification, unless otherwise stated. The other commercial chemicals were used without further purification. All reactions were performed under an inert atmosphere of nitrogen.
2. Batch and Microfluidic Reactor Device

Figure 1 Batch reactor device

Figure 2 Microfluidic reactor device

Note: The light source is a simulated solar lamp (10W, 220V, wavelength 420nm-430nm).
3. Select Optimization Results

![Chemical Reaction Diagram]

**Figure 3** Optimization of reaction conditions

3.1 Table 1. Varying the wavelength of light

<table>
<thead>
<tr>
<th>Entry</th>
<th>Wavelength of Light</th>
<th>yield 1(^b) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>360-370 nm</td>
<td>55</td>
</tr>
<tr>
<td>2</td>
<td>380-385 nm</td>
<td>48</td>
</tr>
<tr>
<td>3</td>
<td>390-398 nm</td>
<td>53</td>
</tr>
<tr>
<td>4</td>
<td>420-430 nm</td>
<td>67</td>
</tr>
<tr>
<td>5</td>
<td>435-445 nm</td>
<td>35</td>
</tr>
</tbody>
</table>

[a] Reaction conditions: 1k (1 mmol, 1 equiv), 2a (2 mmol, 2 equiv), PC-C (2 mmol%, 2 equiv%), K\(_3\)PO\(_4\) (1.1 mmol, 1.1 equiv), solvent: DCE (5 mL), N\(_2\), 25°C, 12 h: The models of lamps used are 10 W, 220 V, LED.  
[b] Isolated yield.

3.2 Table 2. Varying the Catalyst

<table>
<thead>
<tr>
<th>Entry</th>
<th>PC</th>
<th>yield 1(^b) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PC-A</td>
<td>58</td>
</tr>
<tr>
<td>2</td>
<td>PC-B</td>
<td>69</td>
</tr>
</tbody>
</table>
3.3 Table 3. Varying the Base\textsuperscript{a}

Table 3 Explore the effect of different Bases on the reaction

<table>
<thead>
<tr>
<th>Entry</th>
<th>Base</th>
<th>yield 1\textsuperscript{b} (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>K\textsubscript{3}PO\textsubscript{4}</td>
<td>69</td>
</tr>
<tr>
<td>2</td>
<td>K\textsubscript{2}CO\textsubscript{3}</td>
<td>53</td>
</tr>
<tr>
<td>3</td>
<td>NaHCO\textsubscript{3}</td>
<td>49</td>
</tr>
<tr>
<td>4</td>
<td>LiOtBu</td>
<td>42</td>
</tr>
<tr>
<td>5</td>
<td>Et\textsubscript{3}N</td>
<td>71</td>
</tr>
<tr>
<td>6</td>
<td>DMAP</td>
<td>48</td>
</tr>
<tr>
<td>7</td>
<td>DBU</td>
<td>36</td>
</tr>
<tr>
<td>8</td>
<td>Pyridine</td>
<td>44</td>
</tr>
<tr>
<td>9</td>
<td>None</td>
<td>37</td>
</tr>
</tbody>
</table>

[a] Reaction conditions: 1k (1 mmol, 1 equiv), 2a (2 mmol, 2 equiv), PC-B (2 mmol\%, 2 equiv\%), Base (1.1 mmol, 1.1 equiv), solvent: DCE (5 mL), N\textsubscript{2}, 25°C, 12 h, bluelight (10 W、220 V、LED、wavelength 420 nm-430 nm). [b] Isolated yield.

3.4 Table 4. Varying the Solvent\textsuperscript{a}

Table 4 Explore the effect of different Solvents on the reaction
<table>
<thead>
<tr>
<th>Entry</th>
<th>solvent</th>
<th>yield $1^b$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>DCE</td>
<td>71</td>
</tr>
<tr>
<td>2</td>
<td>MeCN</td>
<td>82</td>
</tr>
<tr>
<td>3</td>
<td>THF</td>
<td>55</td>
</tr>
<tr>
<td>4</td>
<td>DMA</td>
<td>43</td>
</tr>
<tr>
<td>5</td>
<td>DMF</td>
<td>41</td>
</tr>
<tr>
<td>6</td>
<td>Cyclohexane</td>
<td>50</td>
</tr>
<tr>
<td>7</td>
<td>1,4-Dioxane</td>
<td>78</td>
</tr>
</tbody>
</table>

Table 5 Explore the effect of substrate concentration on the reaction

<table>
<thead>
<tr>
<th>Entry</th>
<th>Concentration</th>
<th>yield $1^b$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1M</td>
<td>80</td>
</tr>
<tr>
<td>2</td>
<td>0.5M</td>
<td>81</td>
</tr>
<tr>
<td>3</td>
<td>0.2M</td>
<td>82</td>
</tr>
<tr>
<td>4</td>
<td>0.1M</td>
<td>64</td>
</tr>
<tr>
<td>5</td>
<td>0.05M</td>
<td>43</td>
</tr>
</tbody>
</table>

3.5 Table 5. Concentration$^a$

[b] Isolated yield.

3.6 Table 6. Catalyst concentration$^a$

[b] Isolated yield.
### 3.7 Table 7. Residence time

**Table 7** Explore the effect of reaction time on the reaction

<table>
<thead>
<tr>
<th>Entry</th>
<th>Time (h)</th>
<th>yield 1b (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>24</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>31</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>57</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>81</td>
</tr>
<tr>
<td>5</td>
<td>6</td>
<td>83</td>
</tr>
<tr>
<td>6</td>
<td>12</td>
<td>82</td>
</tr>
</tbody>
</table>

[a] Reaction conditions: 1k (1 mmol, 1 equiv), 2a (2 mmol, 2 equiv), PC-B (X% mmol, X% equiv), Et3N (1.1 mmol, 1.1 equiv), solvent: MeCN (5 mL), N2, 25°C, 12 h, bluelight (10 W、220 V、LED、wavelenght 420 nm-430 nm). [b] Isolated yield.

### 3.8 Table 8. Reagent Loading

**Table 8** Explore the effect of substrate ratio on the reaction

<table>
<thead>
<tr>
<th>Entry</th>
<th>Phenylacetylene</th>
<th>yield 1b (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>73</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>81</td>
</tr>
</tbody>
</table>

[a] Reaction conditions: 1k (1 mmol, 1 equiv), 2a (2 mmol, 2 equiv), PC-B (2 mmol%, 2 equiv%), Et3N (1.1 mmol, 1.1 equiv), solvent: MeCN (5 mL), N2, 25°C, bluelight (10 W、220 V、LED、wavelenght 420 nm-430 nm). [b] Isolated yield.
3.9 Table 9. Reagent Loadings

Table 9 Optimization of microchannel reaction conditions

<table>
<thead>
<tr>
<th>Entry</th>
<th>PC-B (equiv)</th>
<th>Tube diameter (mm)</th>
<th>Tube length (m)</th>
<th>Residence time (minute)</th>
<th>yield 1 (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2%</td>
<td>1</td>
<td>2</td>
<td>30</td>
<td>85</td>
</tr>
<tr>
<td>2</td>
<td>1%</td>
<td>1</td>
<td>2</td>
<td>30</td>
<td>93</td>
</tr>
<tr>
<td>3</td>
<td>0.5%</td>
<td>1</td>
<td>2</td>
<td>30</td>
<td>53</td>
</tr>
<tr>
<td>4</td>
<td>0.1%</td>
<td>1</td>
<td>2</td>
<td>30</td>
<td>34</td>
</tr>
<tr>
<td>5</td>
<td>1%</td>
<td>1</td>
<td>3</td>
<td>30</td>
<td>84</td>
</tr>
<tr>
<td>6</td>
<td>1%</td>
<td>1</td>
<td>1</td>
<td>30</td>
<td>81</td>
</tr>
<tr>
<td>7</td>
<td>1%</td>
<td>1</td>
<td>0.5</td>
<td>30</td>
<td>68</td>
</tr>
<tr>
<td>8</td>
<td>1%</td>
<td>1</td>
<td>2</td>
<td>5</td>
<td>37</td>
</tr>
<tr>
<td>9</td>
<td>1%</td>
<td>1</td>
<td>2</td>
<td>10</td>
<td>45</td>
</tr>
<tr>
<td>10</td>
<td>1%</td>
<td>1</td>
<td>2</td>
<td>20</td>
<td>91</td>
</tr>
<tr>
<td>11</td>
<td>1%</td>
<td>1</td>
<td>2</td>
<td>40</td>
<td>92</td>
</tr>
</tbody>
</table>

[a] Reaction conditions: **1k** (1.0 mmol, 1.0 equiv), **PC-B** (1.0 mmol%, 1.0 equiv%), **Et,N** (1.1 mmol, 1.1 equiv), 5 mL MeCN (0.2 M) solution, N₂, 25°C; bluelight (10 W, 220 V, LED, wavelength 420 nm-430 nm). [b] Isolated yield.

3.10 A Scale-up Continuous Flow Reaction

![Diagram of a scale-up continuous flow reaction](image)

<table>
<thead>
<tr>
<th>Entry</th>
<th>Structure</th>
<th>yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>![Structure Image]</td>
<td>89</td>
</tr>
</tbody>
</table>
Reaction conditions: 1k (10 mmol), 2a (1 equiv), MeCN (20 mL), Et₃N (1.1 equiv), and PC-B (1 % equiv.) at room temperature for 20 minutes. Isolated yield.
4. Preparation of Substrates

4.1 Method for synthesizing phenazine catalysts

As shown in Figure 4, S1 and S2 are synthesized according to the literature\(^1\).

![Figure 4: Synthetic method of phenazine catalyst](image)

4.2 Method for synthesizing phenethylamine-derived bromide substrates

As shown in Figure 5: 1) To a stirring solution of S3 (12 mmol, 1.0 equiv.) and NaOAc (3.0 equiv.) in MeOH (100 ml, 0.12 M) at 0 °C, BrCN S4 (1.2 equiv.) was added. Then the reaction was warmed to room temperature and stirred for 12 h. Upon completion, the solvent was removed in vacuo. To the residue was added water and extracted with ethyl acetate, and the combined organic layers were washed by brine and dried over Na\(_2\)SO\(_4\), then filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel or recrystallization to give compound S5. 2) To a stirring solution of S5 (12 mmol, 1.0 equiv.) and Et\(_3\)N (2.4 equiv.) in THF (100 ml, 0.12 M) at 0°C, 2-Bromo-2-methylpropionyl bromide S6 (1.2 equiv) was slowly added. Then the reaction was warmed to room temperature and stirred for 12 h. Upon completion, the solvent was removed in vacuo. To the residue was added water and extracted with ethyl acetate, and the combined organic layers were washed by brine and dried over Na\(_2\)SO\(_4\), then filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel or recrystallization to give compound S7.
4.3 Method for synthesizing products (1 as an example)

![Figure 6 Microfluidic reactor device](image)

An oven-dried 10 mL reaction syringe was charged with 2-bromo-N-cyano-N-(2,2-diphenylethyl)-2-methylpropanamide (1 mmol, 1 equiv), phenylacetylene (1 mmol, 1 equiv), PC-B (1 mol %) and Et$_3$N (1.1 mmol, 1.1 equiv). And add 5 mL MeCN (0.2 M) solution. Pass the solutions through a Quartz tubing (id = 1 mm, length =2.0 m) to building the during 20 minutes of residence time under blue light (10 W, 220 V, LED, wavelength 420nm-430nm). The reaction mixture was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexane/ethyl acetate or dichloromethane/methanol to afford the desired product 1 (91% yield).
5. Experiments for Mechanistic Studies

5.1 Free radical capture experiment

![Figure 7 Radical trapping experiment with TEMPO](image)

**Table 10** Variable Control Experiment

<table>
<thead>
<tr>
<th>Entry</th>
<th>Changes to &quot;standard conditions&quot;</th>
<th>yield $1^b$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>No organic photocatalyst</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>No light</td>
<td>0</td>
</tr>
</tbody>
</table>

[a] Reaction conditions: $1k$ (1 mmol, 1 equiv), $2a$ (3 mmol, 3 equiv), $Et_3N$ (1.1 mmol, 1.1 equiv), solvent: MeCN (5 mL), $N_2$, 25°C, 20 minutes, bluelight (10 W, 220 V, LED, wavelength 420 nm–430 nm). [b] Isolated yield.
5.3 Discussion on theoretical reaction mechanism

Figure 9 Reaction mechanism
6. Analytical data for isolated compounds

6.1 Characterization data for phenethylamine-derived bromides substrates

2-bromo-N-cyano-2-methyl-N-phenethylpropanamide: (1a)

Brown oil (3.15 g, 89% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.35 – 7.24 (m, 5H), 3.93 (t, $J = 7.0$ Hz, 2H), 2.94 (t, $J = 7.0$ Hz, 2H), 1.96 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 169.74, 137.32, 129.47, 128.97, 127.28, 110.03, 56.51, 50.48, 33.07, 30.80. HRMS (EI) calcd for C$_{13}$H$_{15}$N$_2$OBr [M+H]: 295.0441; found: 295.0445.

2-bromo-N-cyano-2-methyl-N-(4-methylphenethyl)propanamide: (1b)

Brown oil (3.01 g, 81% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.14 (q, $J = 8.1$ Hz, 4H), 3.89 (t, $J = 7.2$ Hz, 2H), 2.91 (t, $J = 7.1$ Hz, 2H), 2.28 (s, 3H), 1.99 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 169.68, 136.25, 134.12, 129.52, 129.26, 109.97, 56.36, 50.57, 32.74, 30.84, 21.15. HRMS (EI) calcd for C$_{14}$H$_{17}$N$_2$OBr [M+H]: 309.0597; found: 309.0592.

2-bromo-N-cyano-N-(4-fluorophenethyl)-2-methylpropanamide: (1c)

Yellow oil (2.85 g, 76% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.37 – 7.27 (m, 2H), 7.19 – 7.09 (m, 2H), 3.93 (t, $J = 6.9$ Hz, 2H), 2.94 (t, $J = 6.9$ Hz, 2H), 1.97 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 169.74, 161.73, 134.12, 129.52, 129.26, 109.97, 56.44, 50.52, 32.26, 30.80.
19F NMR (376 MHz, DMSO-\textit{d}_6) \delta -116.11. HRMS (EI) calcd for C_{13}H_{14}N_{2}OBrF [M+H]: 313.0346; found: 313.0348.

**2-bromo-N-(4-chlorophenethyl)-N-cyano-2-methylpropanamide:** (1d)

Yellow oil (2.84 g, 72% yield); 1H NMR (400 MHz, DMSO-\textit{d}_6) \delta 7.28 – 7.22 (m, 2H), 7.22 – 7.16 (m, 2H), 3.84 (t, J = 7.0 Hz, 2H), 2.86 (t, J = 6.9 Hz, 2H), 1.89 (s, 6H). 13C NMR (101 MHz, DMSO-\textit{d}_6) \delta 169.69, 136.27, 132.13, 131.27, 128.87, 109.91, 56.26, 50.32, 32.49, 30.84. HRMS (EI) calcd for C_{13}H_{14}N_{2}OBrCl [M+H]: 329.0051; found: 329.0056.

**2-bromo-N-(4-bromophenethyl)-N-cyano-2-methylpropanamide:** (1e)

Yellow oil (3.40 g, 76% yield); 1H NMR (400 MHz, DMSO-\textit{d}_6) \delta 7.41 – 7.32 (m, 2H), 7.24 – 7.15 (m, 2H), 3.98 (t, J = 6.9 Hz, 2H), 2.99 (t, J = 6.9 Hz, 2H), 2.02 (s, 6H). 13C NMR (101 MHz, DMSO-\textit{d}_6) \delta 169.87, 136.45, 132.31, 131.45, 129.05, 110.09, 56.43, 50.49, 32.67, 31.02. HRMS (EI) calcd for C_{13}H_{14}N_{2}OBr [M+H]: 372.9546; found: 372.9546.

**2-bromo-N-cyano-N-(4-methoxyphenethyl)-2-methylpropanamide:** (1f)

Brown oil (3.08 g, 79% yield); 1H NMR (400 MHz, DMSO-\textit{d}_6) \delta 7.35 – 7.08 (m, 2H), 6.95 – 6.81 (m, 2H), 3.88 (t, J = 7.0 Hz, 2H), 3.73 (s, 3H), 2.88 (t, J = 7.0 Hz, 2H), 1.98 (s, 6H). 13C NMR (101 MHz, DMSO-\textit{d}_6) \delta 169.73, 158.64, 130.45, 129.06, 114.34, 110.03, 56.44, 55.43, 50.71, 32.25, 30.82. HRMS (EI) calcd for C_{14}H_{17}N_{2}O_{2}Br [M+H]: 325.0546; found: 325.0548.
2-bromo-N-cyano-2-methyl-N-(4-(trifluoromethyl)phenethyl)propanamide: \(1g\)

Brown oil (2.96 g, 68% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.68 (d, \(J = 8.0\) Hz, 2H), 7.53 (d, \(J = 7.9\) Hz, 2H), 3.99 (t, \(J = 6.9\) Hz, 2H), 3.05 (t, \(J = 6.9\) Hz, 2H), 1.96 (s, 6H). \(^1^3\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 169.73, 142.39, 130.41, 125.74 (q, \(J = 3.8\) Hz), 124.80 (d, \(J = 271.9\) Hz), 109.96, 56.45, 50.07, 46.20, 32.89, 30.77. \(^{19}\)F NMR (376 MHz, DMSO-\(d_6\)) \(\delta\) -60.89. HRMS (EI) calcd for C\(_{14}\)H\(_{14}\)N\(_2\)OBrF\(_3\) [M+H]: 363.0314; found: 363.0318.

2-bromo-N-cyano-N-(3-fluorophenethyl)-2-methylpropanamide: \(1h\)

Yellow oil (2.93 g, 78% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.35 (td, \(J = 8.1, 6.3\) Hz, 1H), 7.26 – 7.09 (m, 2H), 7.09 – 7.00 (m, 1H), 3.95 (t, \(J = 6.9\) Hz, 2H), 2.97 (t, \(J = 6.9\) Hz, 2H), 1.97 (s, 6H). \(^1^3\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 169.68, 162.68 (d, \(J = 243.5\) Hz), 140.21 (d, \(J = 7.4\) Hz), 130.77 (d, \(J = 8.5\) Hz), 125.63 (d, \(J = 2.5\) Hz), 116.27 (d, \(J = 21.2\) Hz), 114.08 (d, \(J = 20.9\) Hz), 109.94, 56.35, 50.24, 32.78, 30.78. \(^{19}\)F NMR (376 MHz, DMSO-\(d_6\)) \(\delta\) -113.34. HRMS (EI) calcd for C\(_{13}\)H\(_{14}\)N\(_2\)OBrF [M+H]: 313.0346; found: 313.0349.

2-bromo-N-cyano-N-(3,4-dimethoxyphenethyl)-2-methylpropanamide: \(1i\)

Yellow oil (3.66 g, 86% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 6.92 – 6.84 (m, 2H), 6.77 (dd, \(J = 8.2, 2.0\) Hz, 1H), 3.91 (t, \(J = 7.0\) Hz, 2H), 3.75 (s, 3H), 3.73 (s, 3H), 2.88 (t, \(J = 6.9\) Hz, 2H), 1.98 (s, 6H). \(^1^3\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 169.69, 149.18, 148.21, 129.57, 121.41, 113.09, 112.19, 109.99, 56.34, 55.86, 55.84, 50.69, 32.69, 30.76. HRMS (EI) calcd for C\(_{15}\)H\(_{16}\)N\(_2\)O\(_3\)Br [M+H]: 355.0652; found: 355.0655.
2-bromo-N-cyano-2-methyl-N-(3-phenylpropyl)propanamide: (1j)

Yellow oil (3.30 g, 89% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.33 – 7.28 (m, 2H), 7.24 – 7.18 (m, 3H), 3.70 (t, $J = 7.1$ Hz, 2H), 2.69 – 2.63 (m, 2H), 2.05 (s, 6H), 1.99 – 1.93 (m, 2H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 169.85, 141.03, 128.87, 128.71, 126.53, 110.18, 56.79, 48.87, 32.12, 30.86, 28.99. HRMS (EI) calcd for C$_{14}$H$_{17}$N$_2$OBr [M+H]: 309.0597; found: 309.0595.

2-bromo-N-cyano-N-(2,2-diphenylethyl)-2-methylpropanamide: (1k)

White solid (3.16 g, 71% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.33 (ddt, $J = 33.1$, 25.9, 7.4 Hz, 10H), 4.37 (d, $J = 6.8$ Hz, 2H), 3.11 (tt, $J = 7.4$, 3.7 Hz, 1H), 1.86 (d, $J = 6.6$ Hz, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 169.85, 140.99, 129.10, 128.48, 127.58, 109.79, 56.14, 52.65, 48.82, 30.93, 30.66. HRMS (EI) calcd for C$_{19}$H$_{19}$N$_2$OBr [M+H]: 371.0754; found: 371.0757.

N-(2-(1H-indol-3-yl)ethyl)-2-bromo-N-cyano-2-methylpropanamide: (1l)

Yellow oil (3.85 g, 96% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.96 (s, 1H), 7.59 (d, $J = 7.9$ Hz, 1H), 7.39 (d, $J = 8.1$ Hz, 1H), 7.26 (d, $J = 2.4$ Hz, 1H), 7.17 – 7.08 (m, 1H), 7.03 (td, $J = 7.5$, 7.0, 1.1 Hz, 1H), 3.94 (t, $J = 7.3$ Hz, 2H), 3.09 (t, $J = 7.2$ Hz, 2H), 1.99 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 169.85, 136.74, 127.41, 124.18, 121.62, 119.00, 118.48, 112.02, 110.23, 109.50, 56.67, 50.12, 30.82, 23.17. HRMS (EI) calcd for C$_{15}$H$_{16}$N$_3$OBr [M+H]: 334.0551; found: 334.0553.
2-bromo-N-cyano-2-methyl-N-(2-(2-methyl-1H-indol-3-yl)ethyl)propanamide:(1m)

Yellow oil (3.88 g, 93% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.82 (s, 1H), 7.42 (d, $J = 7.6$ Hz, 1H), 7.24 (d, $J = 7.7$ Hz, 1H), 7.03 – 6.90 (m, 2H), 3.84 (t, $J = 7.3$ Hz, 2H), 2.99 (t, $J = 7.3$ Hz, 2H), 2.35 (s, 3H), 1.91 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 169.83, 135.68, 133.49, 128.55, 120.65, 118.81, 117.51, 110.97, 110.31, 105.22, 56.60, 50.08, 30.76, 22.12, 11.71. HRMS (EI) calcd for C$_{18}$H$_{18}$N$_3$OBr [M+H]: 348.0706; found: 348.0709.

2-bromo-N-cyano-N-isobutyl-2-methylpropanamide:(1n)

Yellow oil (2.46 g, 83% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 3.52 (d, $J = 7.3$ Hz, 2H), 2.05 (s, 6H), 1.99 (dd, $J = 13.7$, 7.0 Hz, 1H), 0.94 (d, $J = 6.8$ Hz, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 169.97, 110.58, 56.88, 55.94, 30.89, 27.26, 19.64. HRMS (EI) calcd for C$_9$H$_{13}$N$_2$OBr [M+H]: 247.0441; found: 247.0446

6.2 Product Characterization Data

6,6-dimethyl-2,2,8-triphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(1)
White solid (357.81 mg, 91% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 7.78 (d, $J = 7.5$ Hz, 2H), 7.53 - 7.40 (m, 7H), 7.35 (t, $J = 7.7$ Hz, 4H), 7.26 - 7.22 (m, 2H), 6.75 (s, 1H), 4.50 (s, 2H), 1.39 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 171.60, 152.69, 147.46, 147.34, 135.72, 129.05, 128.92, 128.61, 128.57, 127.34, 126.58, 125.97, 77.82, 56.43, 42.80, 26.93. HRMS (EI) calcd for C$_{27}$H$_{24}$N$_2$O [M+H]: 393.1961; found: 393.1965.

\[ \text{6,6-dimethyl-2,2-diphenyl-8-(p-tolyl)-2,6-dihydropyridazino[1,2-a]pyridin-5(3H)-one: (2)} \]

White solid (358.35 mg, 88% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 7.65 (d, $J = 8.0$ Hz, 2H), 7.45 (d, $J = 7.0$ Hz, 4H), 7.32 (t, $J = 7.7$ Hz, 4H), 7.26 (d, $J = 7.9$ Hz, 2H), 7.21 (t, $J = 7.4$ Hz, 2H), 6.68 (s, 1H), 4.47 (s, 2H), 2.35 (s, 3H), 1.35 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 171.63, 152.77, 147.38, 146.70, 137.95, 132.83, 129.13, 128.91, 127.32, 126.56, 125.82, 77.78, 56.38, 42.73, 26.97, 21.26. HRMS (EI) calcd for C$_{28}$H$_{26}$N$_2$O [M+H]: 407.2118; found: 407.2113.

\[ \text{8-(4-fluorophenyl)-6,6-dimethyl-2,2-diphenyl-2,6-dihydropyridazino[1,2-a]pyridin-5(3H)-one: (3)} \]

Yellow solid (324.84 mg, 79% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 7.90 - 7.74 (m, 2H), 7.45 (dd, $J = 8.4$, 1.3 Hz, 4H), 7.30 (q, $J = 8.9$, 8.2 Hz, 6H), 7.23 - 7.17 (m, 2H), 6.72 (s, 1H), 4.49 (s, 2H), 1.35 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 171.54, 162.52 (d, $J = 245.1$ Hz), 152.70, 147.38, 147.30, 132.03 (d, $J = 3.5$ Hz), 131.10 (d, $J = 8.1$ Hz), 128.89, 127.33, 126.58, 124.95, 115.42 (d, $J = 21.4$ Hz), 77.85, 56.47, 42.82, 26.89. $^{19}$F
NMR (376 MHz, DMSO-\textit{d}_6) \delta -113.77. HRMS (EI) calcd for C_{27}H_{23}N_2OF [M+H]: 411.1867; found: 411.1863.

8-(4-chlorophenyl)-6,6-dimethyl-2,2-diphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(4)

Yellow solid (303.28 mg, 71% yield); \textsuperscript{1}H NMR (400 MHz, DMSO-\textit{d}_6) \delta 7.88 – 7.79 (m, 2H), 7.59 – 7.55 (m, 2H), 7.51 – 7.45 (m, 4H), 7.36 (dd, \textit{J} = 8.4, 7.0 Hz, 4H), 7.28 – 7.22 (m, 2H), 6.83 (s, 1H), 4.51 (s, 2H), 1.40 (s, 6H). \textsuperscript{13}C NMR (101 MHz, DMSO-\textit{d}_6) \delta 171.50, 152.54, 147.87, 147.29, 134.47, 133.38, 130.84, 128.92, 128.61, 127.36, 126.58, 124.81, 77.85, 56.44, 42.88, 26.85. HRMS (EI) calcd for C_{27}H_{23}N_2OCl [M+H]: 427.1572; found: 427.1577.

8-(4-bromophenyl)-6,6-dimethyl-2,2-diphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(5)

Light yellow oily (315.64 mg, 67% yield); \textsuperscript{1}H NMR (400 MHz, DMSO-\textit{d}_6) \delta 7.73 (d, \textit{J} = 8.6 Hz, 2H), 7.65 (d, \textit{J} = 8.6 Hz, 2H), 7.45 (d, \textit{J} = 7.0 Hz, 4H), 7.31 (t, \textit{J} = 7.7 Hz, 4H), 7.20 (t, \textit{J} = 7.3 Hz, 2H), 6.77 (s, 1H), 4.48 (s, 2H), 1.35 (s, 6H). \textsuperscript{13}C NMR (101 MHz, DMSO-\textit{d}_6) \delta 171.47, 152.49, 147.80, 147.28, 134.84, 131.52, 131.15, 128.91, 127.34, 126.58, 124.94, 122.04, 77.87, 56.45, 42.88, 26.84. HRMS (EI) calcd for C_{27}H_{23}N_2OBr [M+H]: 471.1067; found: 471.1065.
8-(4-methoxyphenyl)-6,6-dimethyl-2,2-diphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one (6)

Yellow solid (258.16 mg, 61% yield); \textbf{\textsuperscript{1}H NMR} (400 MHz, DMSO-$d_6$) $\delta$ 7.83 – 7.67 (m, 2H), 7.47 (d, $J$ = 7.8 Hz, 4H), 7.33 (t, $J$ = 7.7 Hz, 4H), 7.24 – 7.20 (m, 2H), 7.06 – 7.02 (m, 2H), 6.66 (s, 1H), 4.48 (s, 2H), 3.81 (s, 3H), 1.36 (s, 6H). \textbf{\textsuperscript{13}C NMR} (101 MHz, DMSO-$d_6$) $\delta$ 171.68, 159.70, 152.88, 147.39, 145.95, 130.23, 128.90, 127.94, 127.32, 126.58, 125.37, 113.97, 77.78, 56.39, 55.62, 42.70, 27.02. \textbf{HRMS} (EI) calcd for C$_{28}$H$_{26}$N$_2$O$_2$ [M+H]: 423.2067; found: 423.2069.

6,6-dimethyl-2,2-diphenyl-8-(4-(trifluoromethyl)phenyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one (7)

Yellow oil (285.93 mg, 62% yield); \textbf{\textsuperscript{1}H NMR} (400 MHz, DMSO-$d_6$) $\delta$ 7.95 – 7.81 (m, 2H), 7.70 (d, $J$ = 8.3 Hz, 2H), 7.39 – 7.29 (m, 4H), 7.19 (t, $J$ = 7.8 Hz, 4H), 7.09 – 7.05 (m, 2H), 6.74 (s, 1H), 4.38 (s, 2H), 1.25 (s, 6H). \textbf{\textsuperscript{13}C NMR} (101 MHz, DMSO-$d_6$) $\delta$ 171.37, 152.40, 148.98, 147.25, 139.73, 129.84, 128.88, 127.32, 126.57, 125.43 (q, $J$ = 3.8 Hz), 124.97, 77.95, 56.47, 42.97, 26.74. \textbf{\textsuperscript{19}F NMR} (376 MHz, DMSO-$d_6$) $\delta$ -61.11. \textbf{HRMS} (EI) calcd for C$_{28}$H$_{23}$N$_2$OF$_3$ [M+H]: 461.1835; found: 461.1837.
8-(4-ethylphenyl)-6,6-dimethyl-2,2-diphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(8)

Yellow solid (341.19 mg, 81% yield); \( ^1H \text{NMR} (400 \text{ MHz, DMSO-}d_6) \delta 7.73 – 7.60 \) (m, 2H), 7.50 – 7.40 (m, 4H), 7.32 (q, \( J = 7.7 \text{ Hz, 6H} \)), 7.26 – 7.18 (m, 2H), 6.70 (s, 1H), 4.46 (s, 2H), 2.66 (q, \( J = 7.5 \text{ Hz, 2H} \)), 1.35 (s, 6H), 1.22 (t, \( J = 7.6 \text{ Hz, 3H} \)). \( ^{13}C \text{NMR} (101 \text{ MHz, DMSO-}d_6) \delta 171.64, 152.76, 147.35, 146.86, 144.24, 133.10, 128.96, 128.92, 127.96, 127.34, 126.58, 125.80, 77.79, 56.38, 42.74, 28.37, 26.98, 15.98. \text{HRMS (EI)} \text{calcd for } C_{29}H_{28}N_2O [M+H]: 421.2274; \text{found: } 421.2278.

4-(6,6-dimethyl-5-oxo-2,2-diphenyl-2,3,5,6-tetrahydroimidazo[1,2-a]pyridin-8-yl)benzaldehyde:(9)

Yellow oil (219.02 mg, 52% yield); \( ^1H \text{NMR} (400 \text{ MHz, DMSO-}d_6) \delta 7.81 – 7.68 \) (m, 2H), 7.35 – 7.27 (m, 6H), 7.17 (t, \( J = 7.7 \text{ Hz, 5H} \)), 7.09 – 7.04 (m, 2H), 6.66 (s, 1H), 4.33 (s, 2H), 1.21 (s, 6H). \( ^{13}C \text{NMR} (101 \text{ MHz, DMSO-}d_6) \delta 171.48, 152.54, 148.63, 148.29, 147.25, 134.90, 130.95, 128.92, 127.36, 126.60, 124.66, 121.08, 77.89, 56.48, 42.89, 26.84. \text{HRMS (EI)} \text{calcd for } C_{28}H_{24}N_2O_2 [M+H]: 421.1911; \text{found: } 421.1913.
methyl 4-(6,6-dimethyl-5-oxo-2,2-diphenyl-2,3,5,6-tetrahydroimidazo[1,2-a]pyridin-8-yl)benzoate:(10)

Yellow oil (212.06 mg, 47% yield); \( ^1H \) NMR (400 MHz, DMSO-\( d_6 \)) \( \delta \) 8.06 (d, \( J = 8.2 \) Hz, 2H), 7.92 (d, \( J = 8.2 \) Hz, 2H), 7.45 (d, \( J = 7.5 \) Hz, 2H), 7.35 – 7.28 (m, 6H), 7.23 – 7.19 (m, 2H), 6.89 (s, 1H), 4.48 (s, 2H), 3.89 (d, \( J = 1.2 \) Hz, 3H), 1.37 (s, 6H). \( ^{13}C \) NMR (101 MHz, DMSO-\( d_6 \)) \( \delta \) 171.41, 166.47, 152.40, 148.85, 147.28, 142.91, 140.34, 129.41, 128.92, 128.82, 128.43, 127.35, 126.58, 77.91, 56.44, 52.67, 42.98, 26.81. HRMS (EI) calcd for C\(_{29}\)H\(_{26}\)N\(_2\)O\(_3\) [M+H]: 451.2016; found: 451.2017.

6,6-dimethyl-2,2-diphenyl-8-(o-tolyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(11)

Yellow solid (346.13 mg, 85% yield); \( ^1H \) NMR (400 MHz, DMSO-\( d_6 \)) \( \delta \) 7.37 – 7.30 (m, 6H), 7.30 – 7.27 (m, 4H), 7.25 (ddd, \( J = 5.4, 3.0, 1.2 \) Hz, 2H), 7.22 – 7.18 (m, 2H), 6.43 (s, 1H), 4.47 (s, 2H), 2.18 (s, 3H), 1.36 (s, 6H). \( ^{13}C \) NMR (101 MHz, DMSO-\( d_6 \)) \( \delta \) 171.78, 153.04, 148.33, 147.20, 136.74, 136.18, 136.03, 130.30, 130.20, 128.82, 128.52, 127.33, 126.77, 126.60, 126.04, 77.66, 56.73, 42.68, 26.89, 20.10. HRMS (EI) calcd for C\(_{28}\)H\(_{26}\)N\(_2\)O [M+H]: 407.2118; found: 407.2112.
8-(2-fluorophenyl)-6,6-dimethyl-2,2-diphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(12)

Yellow oil (320.73 mg, 78% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.31 (td, $J = 7.6, 2.0$ Hz, 1H), 7.28 – 7.23 (m, 1H), 7.21 – 7.19 (m, 3H), 7.09 (t, $J = 7.7$ Hz, 7H), 7.01 – 6.96 (m, 2H), 6.46 (s, 1H), 4.27 (s, 2H), 1.15 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.44, 161.32, 158.87, 152.38, 149.70, 147.30, 132.17, 132.14, 130.88, 130.80, 128.82, 127.30, 126.60, 124.73, 124.69, 123.83, 123.68, 121.60, 116.21, 116.00, 77.73, 56.89, 42.87, 26.82. $^{19}$F NMR (376 MHz, DMSO-$d_6$) $\delta$ -113.32. HRMS (EI) calcd for C$_{27}$H$_{23}$N$_2$OF [M+H]: 411.1867; found: 411.1869.


6,6-dimethyl-2,2-diphenyl-8-(m-tolyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(13)

Yellow solid (354.27 mg, 87% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.63 (d, $J = 7.9$ Hz, 1H), 7.55 (d, $J = 1.9$ Hz, 1H), 7.49 (dd, $J = 8.3, 1.3$ Hz, 4H), 7.38 (t, $J = 7.9$ Hz, 5H), 7.29 – 7.25 (m, 3H), 6.76 (s, 1H), 4.51 (s, 2H), 2.43 (s, 3H), 1.41 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.61, 152.72, 147.35, 147.25, 137.65, 135.68, 129.55, 129.20, 129.13, 128.92, 128.39, 127.34, 126.57, 126.30, 126.03, 77.79, 56.42, 42.77, 26.96, 21.59. HRMS (EI) calcd for C$_{29}$H$_{26}$N$_2$O [M+H]: 407.2118; found: 407.2113.


8-(3-fluorophenyl)-6,6-dimethyl-2,2-diphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(14)

Yellow oil (312.51 mg, 76% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.68 – 7.59 (m, 2H), 7.54 – 7.48 (m, 1H), 7.44 (d, $J = 8.2$ Hz, 4H), 7.33 (t, $J = 7.6$ Hz, 4H), 7.23 (q, $J =
8-(4-ethynylphenyl)-6,6-dimethyl-2,2-diphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(15)

Yellow solid (2.28 g, 76% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.56 (d, \(J = 8.1\) Hz, 2H), 7.34 (d, \(J = 8.1\) Hz, 2H), 7.21 (d, \(J = 7.5\) Hz, 4H), 7.07 (t, \(J = 7.7\) Hz, 4H), 6.96 (t, \(J = 7.3\) Hz, 2H), 6.55 (s, 1H), 4.45 (s, 2H), 4.03 (s, 1H), 1.11 (s, 6H). \(^{13}\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 171.46, 152.49, 147.37, 145.58, 135.48, 131.08, 128.91, 127.34, 126.58, 125.26, 121.96, 83.75, 82.04, 77.89, 56.42, 42.88, 26.85. HRMS (EI) calcd for C\(_{29}\)H\(_{23}\)N\(_2\)O [M+H]: 417.1961; found: 417.1964.

6,6-dimethyl-2,2-diphenyl-8-(thiophen-3-yl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(16)

Yellow oil (287.39 mg, 72% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 8.44 (d, \(J = 1.6\) Hz, 1H), 7.70 – 7.60 (m, 2H), 7.52 (d, \(J = 7.5\) Hz, 4H), 7.33 (t, \(J = 7.6\) Hz, 4H), 7.22 (t, \(J = 7.4\) Hz, 2H), 7.02 (s, 1H), 4.47 (s, 2H), 1.35 (s, 6H). \(^{13}\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 171.52, 152.53, 147.37, 145.58, 135.48, 131.08, 128.93, 127.32, 126.58, 126.29, 125.16,
6,6-dimethyl-2,2-diphenyl-8-(thiophen-2-yl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one (17)

Yellow oil (243.48 mg, 61% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 7.81 (dd, $J$ = 3.7, 1.2 Hz, 1H), 7.64 (dd, $J$ = 5.1, 1.2 Hz, 1H), 7.56 (dd, $J$ = 8.4, 1.3 Hz, 4H), 7.34 (t, $J$ = 7.8 Hz, 4H), 7.25 – 7.20 (m, 3H), 7.16 (dd, $J$ = 5.2, 3.7 Hz, 1H), 7.05 (s, 1H), 4.50 (s, 2H), 1.35 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 171.41, 151.99, 147.50, 143.96, 136.42, 135.36, 134.42, 128.96, 128.16, 127.42, 127.35, 126.49, 126.37, 119.62, 78.01, 56.54, 42.75, 26.93. HRMS (EI) calcd for C$_{25}$H$_{22}$N$_2$OS [M+H]: 399.1526; found: 399.1529.

6,6-dimethyl-2,8-diphenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one (18)

White solid (225.2 mg, 71% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 7.64 (dd, $J$ = 8.1, 1.6 Hz, 2H), 7.43 – 7.33 (m, 5H), 7.32 – 7.27 (m, 3H), 6.70 (s, 1H), 5.35 (dd, $J$ = 10.3, 7.4 Hz, 1H), 4.28 (dd, $J$ = 11.4, 10.3 Hz, 1H), 3.56 (dd, $J$ = 11.4, 7.5 Hz, 1H), 1.39 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 171.50, 154.20, 146.86, 143.37, 135.81, 129.12, 129.08, 128.47, 128.40, 127.78, 127.20, 126.14, 68.48, 50.96, 42.77, 27.17, 26.84. HRMS (EI) calcd for C$_{21}$H$_{20}$N$_2$O [M]: 317.1648; found: 317.1642.
6,6-dimethyl-2-phenyl-8-(p-tolyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(19)

White solid (215.27 mg, 65% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.57 (d, $J$ = 8.2 Hz, 2H), 7.42 – 7.35 (m, 2H), 7.34 – 7.27 (m, 3H), 7.21 (d, $J$ = 7.9 Hz, 2H), 6.67 (s, 1H), 5.37 (dd, $J$ = 10.3, 7.5 Hz, 1H), 4.30 (dd, $J$ = 11.4, 10.4 Hz, 1H), 3.57 (dd, $J$ = 11.4, 7.5 Hz, 1H), 2.33 (s, 3H), 1.40 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.53, 154.28, 146.13, 143.39, 137.80, 132.92, 129.05, 128.99, 128.94, 127.75, 127.16, 126.00, 68.45, 50.93, 42.70, 27.21, 26.87, 21.23. HRMS (EI) calcd for C$_{22}$H$_{22}$N$_2$O [M+H]: 331.1805; found: 331.1803.

8-(4-fluorophenyl)-6,6-dimethyl-2-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(20)

Yellow solid (191.04 mg, 57% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.74 (ddd, $J$ = 8.9, 5.5, 3.0 Hz, 2H), 7.43 – 7.37 (m, 2H), 7.36 – 7.32 (m, 3H), 7.26 (s, 2H), 6.76 (s, 1H), 5.39 (dd, $J$ = 10.3, 7.5 Hz, 1H), 4.32 (t, $J$ = 10.9 Hz, 1H), 3.64 – 3.56 (m, 1H), 1.42 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.47, 162.40 (d, $J$ = 245.0 Hz), 154.19, 146.84, 143.32, 135.47 (d, $J$ = 8.8 Hz), 131.16 (d, $J$ = 8.2 Hz), 129.07, 127.79, 127.21, 125.06, 115.24 (d, $J$ = 21.3 Hz), 68.49, 50.99, 42.79, 27.14, 26.79. $^{19}$F NMR (376 MHz, DMSO-$d_6$) $\delta$ -114.08. HRMS (EI) calcd for C$_{21}$H$_{19}$N$_2$OF [M+H]: 335.1554; found: 335.1557.

8-(4-chlorophenyl)-6,6-dimethyl-2-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(21)

Yellow solid (191.04 mg, 57% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.74 (ddd, $J$ = 8.9, 5.5, 3.0 Hz, 2H), 7.43 – 7.37 (m, 2H), 7.36 – 7.32 (m, 3H), 7.26 (s, 2H), 6.76 (s, 1H), 5.39 (dd, $J$ = 10.3, 7.5 Hz, 1H), 4.32 (t, $J$ = 10.9 Hz, 1H), 3.64 – 3.56 (m, 1H), 1.42 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.47, 162.40 (d, $J$ = 245.0 Hz), 154.19, 146.84, 143.32, 135.47 (d, $J$ = 8.8 Hz), 131.16 (d, $J$ = 8.2 Hz), 129.07, 127.79, 127.21, 125.06, 115.24 (d, $J$ = 21.3 Hz), 68.49, 50.99, 42.79, 27.14, 26.79. $^{19}$F NMR (376 MHz, DMSO-$d_6$) $\delta$ -114.08. HRMS (EI) calcd for C$_{21}$H$_{19}$N$_2$OF [M+H]: 335.1554; found: 335.1557.
Light yellow oil (175.56 mg, 50% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 7.69 (d, J = 8.5 Hz, 2H), 7.50 – 7.43 (m, 2H), 7.41 – 7.34 (m, 2H), 7.33 – 7.26 (m, 3H), 6.76 (s, 1H), 5.36 (dd, J = 10.4, 7.5 Hz, 1H), 4.29 (t, J = 10.9 Hz, 1H), 3.56 (dd, J = 11.4, 7.5 Hz, 1H), 1.39 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 171.40, 154.03, 147.27, 143.27, 134.56, 133.24, 130.89, 129.07, 128.42, 127.80, 127.22, 124.97, 68.51, 50.97, 42.85, 27.10, 26.74. HRMS (EI) calcd for C$_{21}$H$_{19}$N$_2$OCl [M+H]: 351.1259; found: 351.1253.

8-(4-bromophenyl)-6,6-dimethyl-2-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(22)

Light yellow oil (168.54 mg, 48% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 7.45 – 7.33 (m, 4H), 7.10 (dq, J = 16.3, 8.7, 8.1 Hz, 5H), 6.53 (s, 1H), 5.13 (dd, J = 10.3, 7.5 Hz, 1H), 4.06 (t, J = 10.9 Hz, 1H), 3.34 (dd, J = 11.4, 7.6 Hz, 1H), 1.16 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 171.36, 153.98, 147.23, 143.27, 134.92, 131.34, 131.20, 129.05, 127.78, 127.21, 125.08, 121.90, 68.53, 50.98, 42.86, 27.10, 26.74. HRMS (EI) calcd for C$_{21}$H$_{19}$N$_2$OBr [M+H]: 395.0754; found: 395.0758.

8-(4-methoxyphenyl)-6,6-dimethyl-2-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(23)

Yellow solid (177.06 mg, 51% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 7.70 – 7.55 (m, 2H), 7.44 – 7.33 (m, 2H), 7.33 – 7.23 (m, 3H), 7.01 – 6.88 (m, 2H), 6.70 – 6.56 (m, 1H), 5.35 (dd, J = 10.3, 7.5 Hz, 1H), 4.28 (dd, J = 11.4, 10.4 Hz, 1H), 3.76 (s, 3H), 3.56 (dd, J = 11.4, 7.5 Hz, 1H), 1.38 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 171.58, 159.60,
154.39, 145.41, 143.41, 130.30, 129.05, 128.06, 127.75, 127.18, 125.55, 113.79, 68.45, 55.59, 50.93, 42.67, 27.26, 26.92. HRMS (EI) calcd for C$_{22}$H$_{22}$N$_2$O$_2$ [M+H]: 347.1754; found: 347.1755.

8-(4-ethylphenyl)-6,6-dimethyl-2-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(24)

Yellow solid (214.02 mg, 62% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.56 (d, $J$ = 7.8 Hz, 2H), 7.41 – 7.33 (m, 2H), 7.33 – 7.26 (m, 3H), 7.22 (d, $J$ = 7.9 Hz, 2H), 6.65 (s, 1H), 5.35 (dd, $J$ = 10.4, 7.5 Hz, 1H), 4.28 (t, $J$ = 10.9 Hz, 1H), 3.56 (dd, $J$ = 11.4, 7.5 Hz, 1H), 2.60 (q, $J$ = 7.5 Hz, 2H), 1.38 (s, 6H), 1.18 (t, $J$ = 7.6 Hz, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.53, 154.29, 146.21, 144.13, 143.38, 133.20, 129.06, 127.77, 127.18, 126.03, 68.46, 50.94, 42.71, 28.38, 27.22, 26.88, 16.08. HRMS (EI) calcd for C$_{23}$H$_{24}$N$_2$O [M+H]: 345.1961; found: 345.1961.

6,6-dimethyl-2-phenyl-8-(o-tolyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(25)

White solid (228.51 mg, 69% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.34 (ddd, $J$ = 7.4, 6.3, 1.3 Hz, 2H), 7.27 – 7.21 (m, 5H), 7.19 (dd, $J$ = 4.7, 1.3 Hz, 2H), 6.47 – 6.39 (m, 1H), 5.25 (dd, $J$ = 10.3, 7.4 Hz, 1H), 4.28 (dd, $J$ = 11.4, 10.3 Hz, 1H), 3.57 (dd, $J$ = 11.4, 7.5 Hz, 1H), 2.23 (s, 3H), 1.39 (d, $J$ = 2.1 Hz, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.66, 154.46, 147.69, 143.33, 136.65, 136.22, 130.24, 130.17, 129.01, 128.39, 127.77,
6,6-dimethyl-2-phenyl-8-(m-tolyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(26)

White solid (225.21 mg, 68% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.52 – 7.44 (m, 2H), 7.42 – 7.36 (m, 2H), 7.33 – 7.26 (m, 4H), 7.18 (d, \(J = 7.5\) Hz, 1H), 6.69 (s, 1H), 5.38 (dd, \(J = 10.3, 7.4\) Hz, 1H), 4.30 (dd, \(J = 11.4, 10.4\) Hz, 1H), 3.58 (dd, \(J = 11.4, 7.4\) Hz, 1H), 2.35 (s, 3H), 1.41 (s, 6H). \(^{13}\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 171.52, 154.25, 146.70, 143.39, 137.47, 135.80, 129.55, 129.06, 128.24, 127.77, 127.16, 126.43, 126.27, 68.45, 50.98, 42.73, 27.17, 26.86, 21.52. HRMS (EI) calcd for C\(_{22}\)H\(_{22}\)N\(_2\)O [M+H]: 331.1805; found: 331.1807.

8-(3-fluorophenyl)-6,6-dimethyl-2-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(27)

Yellow oil (194.39 mg, 58% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.58 – 7.50 (m, 2H), 7.43 (td, \(J = 8.2, 6.2\) Hz, 1H), 7.40 – 7.34 (m, 2H), 7.33 – 7.28 (m, 3H), 7.19 (td, \(J = 6.6, 1.1\) Hz, 1H), 6.82 (s, 1H), 5.37 (dd, \(J = 10.3, 7.5\) Hz, 1H), 4.29 (dd, \(J = 11.4, 10.4\) Hz, 1H), 3.57 (dd, \(J = 11.4, 7.5\) Hz, 1H), 1.40 (s, 6H). \(^{13}\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 171.39, 162.15 (d, \(J = 242.6\) Hz), 153.94, 147.72, 143.25, 137.98 (d, \(J = 8.6\) Hz), 130.33 (d, \(J = 8.4\) Hz), 129.07, 127.80, 127.18, 125.10 (d, \(J = 2.7\) Hz), 124.87 (d, \(J = 2.8\) Hz), 115.97 (d, \(J = 22.7\) Hz), 115.24 (d, \(J = 20.9\) Hz), 68.52, 50.95, 42.84, 27.04, 26.69. \(^{19}\)F
NMR (376 MHz, DMSO-$d_6$) $\delta$ -113.64. HRMS (EI) calcd for C$_{21}$H$_{19}$N$_2$OF [M+H]: 335.1554; found: 335.1559.

6,6-dimethyl-8-phenyl-2-(p-tolyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(28)

Yellow oil (228.51 mg, 69% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.69 – 7.59 (m, 2H), 7.42 – 7.33 (m, 3H), 7.21 – 7.12 (m, 4H), 6.69 (s, 1H), 5.30 (dd, $J$ = 10.3, 7.4 Hz, 1H), 4.25 (dd, $J$ = 11.4, 10.4 Hz, 1H), 3.54 (dd, $J$ = 11.4, 7.5 Hz, 1H), 2.28 (s, 3H), 1.39 (s, 6H).

$^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.49, 154.02, 146.74, 140.41, 136.89, 135.82, 129.60, 129.12, 128.46, 128.38, 127.10, 126.18, 68.29, 50.98, 42.74, 27.18, 26.84, 21.17. HRMS (EI) calcd for C$_{22}$H$_{22}$N$_2$O [M+H]: 331.1805; found: 331.1808.

2-(4-fluorophenyl)-6,6-dimethyl-8-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(29)

Yellow oil (204.44 mg, 61% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.55 (dd, $J$ = 8.1, 1.6 Hz, 2H), 7.33 – 7.22 (m, 5H), 7.09 (t, $J$ = 8.9 Hz, 2H), 6.60 (s, 1H), 5.27 (dd, $J$ = 10.4, 7.6 Hz, 1H), 4.19 (dd, $J$ = 11.4, 10.4 Hz, 1H), 3.45 (dd, $J$ = 11.5, 7.7 Hz, 1H), 1.30 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.53, 161.88 (d, $J$ = 242.8 Hz), 154.36, 146.92, 139.56 (d, $J$ = 3.2 Hz), 135.81, 129.22 (d, $J$ = 8.1 Hz), 129.13, 128.47, 128.39, 126.17, 115.77 (d, $J$ = 21.1 Hz), 67.78, 50.96, 42.77, 27.17, 26.77. $^{19}$F NMR (376 MHz, DMSO-$d_6$) $\delta$ -115.37. HRMS (EI) calcd for C$_{21}$H$_{19}$N$_2$OF [M+H]: 335.1554; found: 335.1557.
2-(4-chlorophenyl)-6,6-dimethyl-8-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one: (30)

Yellow oil (193.12 mg, 55% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.70 (d, \(J = 8.5\) Hz, 2H), 7.47 (d, \(J = 8.6\) Hz, 2H), 7.40 – 7.35 (m, 2H), 7.34 – 7.28 (m, 3H), 6.77 (s, 1H), 5.36 (dd, \(J = 10.4, 7.5\) Hz, 1H), 4.30 (t, \(J = 10.9\) Hz, 1H), 3.57 (dd, \(J = 11.4, 7.5\) Hz, 1H), 1.40 (s, 6H). \(^{13}\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 171.37, 154.00, 147.24, 143.24, 134.53, 133.21, 130.86, 129.04, 128.39, 127.77, 127.19, 124.94, 68.48, 50.94, 42.81, 27.07, 26.71.

HRMS (EI) calcd for C\(_{21}\)H\(_{19}\)N\(_2\)OCl [M+H]: 351.1259; found: 351.1259.

2-(4-bromophenyl)-6,6-dimethyl-8-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one: (31)

Yellow oil (213.34 mg, 54% yield); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 7.44 – 7.32 (m, 4H), 7.10 (dq, \(J = 16.3, 8.7, 8.1\) Hz, 5H), 6.53 (s, 1H), 5.13 (dd, \(J = 10.3, 7.5\) Hz, 1H), 4.06 (t, \(J = 10.9\) Hz, 1H), 3.34 (dd, \(J = 11.4, 7.6\) Hz, 1H), 1.16 (s, 6H). \(^{13}\)C NMR (101 MHz, DMSO-\(d_6\)) \(\delta\) 171.38, 154.00, 147.26, 143.24, 134.95, 131.37, 131.22, 129.08, 127.81, 127.23, 125.11, 121.92, 68.55, 51.00, 42.88, 27.13, 26.76. HRMS (EI) calcd for C\(_{21}\)H\(_{19}\)N\(_2\)OBr [M+H]: 395.0754; found: 395.0759.

2-(4-methoxyphenyl)-6,6-dimethyl-8-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-
5(3H)-one:(32)

Light yellow oily (177.06 mg, 51% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.66 (dd, $J = 8.1, 1.6$ Hz, 2H), 7.41 – 7.31 (m, 3H), 7.26 – 7.20 (m, 2H), 6.94 – 6.87 (m, 2H), 6.68 (s, 1H), 5.30 (dd, $J = 10.2, 7.4$ Hz, 1H), 4.25 (dd, $J = 11.4, 10.3$ Hz, 1H), 3.72 (s, 3H), 3.56 (dd, $J = 11.4, 7.5$ Hz, 1H), 1.40 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.47, 158.98, 153.90, 146.66, 135.85, 135.38, 129.13, 128.45, 128.36, 128.34, 126.26, 114.41, 68.06, 55.50, 51.05, 42.74, 27.18, 26.85. HRMS (EI) calcd for C$_{22}$H$_{22}$N$_2$O$_2$ [M+H]: 347.1754; found: 347.1757.

6,6-dimethyl-8-phenyl-2-(4-(trifluoromethyl)phenyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(33)

Yellow oil (215.69 mg, 56% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.73 (d, $J = 7.7$ Hz, 2H), 7.66 – 7.63 (m, 2H), 7.56 (d, $J = 8.1$ Hz, 2H), 7.42 – 7.36 (m, 3H), 6.72 (d, $J = 0.6$ Hz, 1H), 5.47 (dd, $J = 10.4, 7.6$ Hz, 1H), 4.33 (dd, $J = 11.4, 10.5$ Hz, 1H), 3.58 (dd, $J = 11.5, 7.7$ Hz, 1H), 1.39 (d, $J = 3.0$ Hz, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.55, 154.85, 147.94, 147.17, 135.75, 129.13, 128.51, 128.42, 128.14, 126.17 – 125.88 (m), 67.96, 50.69, 42.82, 27.17, 26.75. $^{19}$F NMR (376 MHz, DMSO-$d_6$) $\delta$ -60.85. HRMS (EI) calcd for C$_{22}$H$_{19}$N$_2$OF$_3$ [M+H]: 385.1522; found: 385.1525.

2-(3-fluorophenyl)-6,6-dimethyl-8-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(34)

Yellow oil (194.39 mg, 58% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.51 – 7.38 (m, 2H), 7.23 – 7.13 (m, 4H), 7.01 – 6.96 (m, 2H), 6.92 (td, $J = 7.5, 2.1$ Hz, 1H), 6.51 (s, 1H),
5.18 (dd, $J = 10.4$, 7.7 Hz, 1H), 4.10 (dd, $J = 11.4$, 10.4 Hz, 1H), 3.36 (dd, $J = 11.4$, 7.7 Hz, 1H), 1.19 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.53, 162.76 (d, $J = 243.5$ Hz), 154.66, 147.04, 146.20 (d, $J = 7.3$ Hz), 135.79, 131.04 (d, $J = 8.1$ Hz), 129.12, 128.48, 128.40, 126.11, 123.32 (d, $J = 2.8$ Hz), 114.57 (d, $J = 21.0$ Hz), 114.10 (d, $J = 21.7$ Hz), 67.92, 50.78, 42.78, 27.21, 26.71. $^{19}$F NMR (376 MHz, DMSO-$d_6$) $\delta$ -112.84. HRMS (EI) calcd for C$_{21}$H$_{16}$N$_2$OF [M+H]: 335.1554; found: 335.1558.

2-(1H-indol-3-yl)-6,6-dimethyl-8-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(35)

White solid (227.95 mg, 64% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 11.03 (s, 1H), 7.62 (dd, $J = 7.9$, 1.7 Hz, 2H), 7.44 – 7.31 (m, 6H), 7.14 – 7.06 (m, 1H), 7.02 – 6.95 (m, 1H), 6.70 (s, 1H), 5.59 (dd, $J = 10.2$, 7.2 Hz, 1H), 4.42 – 4.22 (m, 1H), 3.79 (dd, $J = 11.3$, 7.2 Hz, 1H), 1.43 (d, $J = 4.9$ Hz, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.53, 153.17, 146.41, 137.24, 135.87, 129.09, 128.44, 128.35, 126.32, 126.32, 121.75, 119.23, 118.83, 116.21, 112.30, 62.49, 49.52, 42.70, 27.23, 27.11. HRMS (EI) calcd for C$_{23}$H$_{21}$N$_3$O [M+H]: 356.1757; found: 356.1753.

6,6-dimethyl-2-(2-methyl-1H-indol-3-yl)-8-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(36)

White solid (229.52 mg, 62% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 11.02 (s, 1H), 7.51 (d, $J = 8.1$ Hz, 2H), 7.39 (d, $J = 8.1$ Hz, 2H), 7.32 (d, $J = 2.4$ Hz, 1H), 7.15 (d, $J = 8.0$ Hz, 2H), 7.12 – 7.06 (m, 1H), 7.00 – 6.94 (m, 1H), 6.65 (s, 1H), 5.57 (dd, $J = 10.2$, 7.2 Hz, 1H), 4.32 – 4.18 (m, 1H), 3.77 (dd, $J = 11.3$, 7.2 Hz, 1H), 2.28 (s, 3H), 1.41 (d, $J = 4.5$ Hz,
6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.57, 153.24, 145.70, 137.75, 137.23, 132.97, 128.95, 128.90, 126.13, 125.92, 123.26, 121.74, 119.21, 118.85, 116.24, 112.28, 62.46, 49.47, 42.64, 27.25, 27.15, 21.21. HRMS (EI) calcd for C$_{24}$H$_{23}$N$_3$O [M+H]: 370.1914; found: 370.1918.

![Structural formula of the compound](image)

2-(3,4-dimethoxyphenyl)-6,6-dimethyl-8-phenyl-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(37)

Light yellow oily (203.68 mg, 54% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.71 – 7.61 (m, 2H), 7.42 – 7.34 (m, 3H), 6.95 – 6.90 (m, 2H), 6.82 (dd, $J = 8.3$, 2.0 Hz, 1H), 6.68 (s, 1H), 5.29 (dd, $J = 10.2$, 7.5 Hz, 1H), 4.25 (t, $J = 10.8$ Hz, 1H), 3.75 (d, $J = 9.4$ Hz, 6H), 3.59 (dd, $J = 11.4$, 7.6 Hz, 1H), 1.39 (d, $J = 2.1$ Hz, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.50, 153.93, 149.27, 148.56, 146.67, 135.87, 135.82, 129.12, 128.46, 128.38, 126.27, 119.10, 112.40, 111.22, 68.28, 56.01, 55.95, 50.96, 42.74, 27.18, 26.85. HRMS (EI) calcd for C$_{23}$H$_{24}$N$_2$O$_3$ [M+H]: 377.1860; found: 377.1866.

![Structural formula of the compound](image)

2-(3-fluorophenyl)-6,6-dimethyl-8-(p-tolyl)-2,6-dihydroimidazo[1,2-a]pyridin-5(3H)-one:(38)

Yellow oil (195.54 mg, 56% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.51 – 7.42 (m, 2H), 7.34 (td, $J = 7.9$, 6.0 Hz, 1H), 7.15 – 7.00 (m, 6H), 6.58 (s, 1H), 5.30 (dd, $J = 10.4$, 7.7 Hz, 1H), 4.21 (dd, $J = 11.4$, 10.4 Hz, 1H), 3.47 (dd, $J = 11.4$, 7.7 Hz, 1H), 2.24 (s, 3H), 1.30 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 171.59, 162.77 (d, $J = 243.4$ Hz), 154.74, 146.36, 146.24 (d, $J = 6.7$ Hz), 137.83, 132.91, 131.05 (d, $J = 8.1$ Hz), 128.98, 125.94,
123.30 (d, $J = 2.8$ Hz), 114.55 (d, $J = 21.0$ Hz), 114.07 (d, $J = 21.8$ Hz), 67.88, 50.73, 42.72, 27.24, 26.75, 21.22. $^{19}$F NMR (376 MHz, DMSO-$d_6$) $\delta$ -112.87. HRMS (EI) calcd for C$_{22}$H$_{21}$N$_2$OF [M+H]: 349.1711; found: 349.1718.

7,7-dimethyl-2,9-diphenyl-2,3,4,7-tetrahydro-6H-pyrido[1,2-a]pyrimidin-6-one:(39)

Light yellow oily (135.78 mg, 41% yield); $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.47 – 7.41 (m, 2H), 7.35 – 7.25 (m, 7H), 7.23 – 7.17 (m, 1H), 6.39 (s, 1H), 4.60 (dd, $J = 9.4$, 4.1 Hz, 1H), 3.93 (dt, $J = 13.2$, 4.5 Hz, 1H), 3.58 (ddd, $J = 13.2$, 11.1, 4.3 Hz, 1H), 2.26 (dq, $J = 13.0$, 4.3 Hz, 1H), 1.63 (ddd, $J = 13.8$, 11.0, 9.4, 4.7 Hz, 1H), 1.37 (d, $J = 2.9$ Hz, 6H).

$^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ 174.12, 147.07, 144.88, 141.89, 138.15, 132.27, 130.10, 128.59, 127.81, 127.68, 126.89, 56.97, 40.58, 39.67, 29.13, 27.77, 27.58. HRMS (EI) calcd for C$_{22}$H$_{22}$N$_2$O [M+H]: 331.1805; found: 331.1809.

7. Crystal Data and Structure Refinements
Figure 9 Structure of 3a by X-Ray crystallographic (CCDC = 2263771)
Single crystal suitable for X-ray diffraction was obtained by slow evaporation of a saturated solution of compound 3a (cyclohexane/CH₂Cl₂) in a loosely capped vial.

Table 11 Crystal data and structure refinement for 3a

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<td>Empirical formula</td>
<td>C₂₀H₁₉NO</td>
</tr>
<tr>
<td>Formula weight</td>
<td>406.51</td>
</tr>
<tr>
<td>Temperature/K</td>
<td>193</td>
</tr>
<tr>
<td>Crystal system</td>
<td>monoclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>P2₁/c</td>
</tr>
<tr>
<td>a/Å</td>
<td>11.9263(8)</td>
</tr>
<tr>
<td>b/Å</td>
<td>17.9508(11)</td>
</tr>
<tr>
<td>c/Å</td>
<td>10.8524(8)</td>
</tr>
<tr>
<td>α/°</td>
<td>90</td>
</tr>
<tr>
<td>β/°</td>
<td>106.642(2)</td>
</tr>
<tr>
<td>γ/°</td>
<td>90</td>
</tr>
<tr>
<td>Volume/Å³</td>
<td>2226.0(3)</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>ρcalcg/cm³</td>
<td>1.213</td>
</tr>
<tr>
<td>μ/mm⁻¹</td>
<td>0.074</td>
</tr>
<tr>
<td>F(000)</td>
<td>864.0</td>
</tr>
<tr>
<td>Crystal size/mm³</td>
<td>0.13 × 0.12 × 0.1</td>
</tr>
<tr>
<td>Radiation</td>
<td>MoKα (λ = 0.71073)</td>
</tr>
<tr>
<td>2Θ range for data</td>
<td>4.528 to 55.03</td>
</tr>
<tr>
<td>collection/°</td>
<td></td>
</tr>
<tr>
<td>Index ranges</td>
<td>-15 ≤ h ≤ 13, -23 ≤ k ≤ 23, -13 ≤ 1 ≤ 14</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------------------</td>
<td>---------------</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>21000</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>5107 [Rint = 0.0597, Rsigma = 0.0564]</td>
</tr>
<tr>
<td>Data/restraints/parameters</td>
<td>5107/0/283</td>
</tr>
<tr>
<td>Final R indexes [I&gt;=2σ(I)]</td>
<td>R1 = 0.0573, wR2 = 0.1164</td>
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<tr>
<td>Final R indexes [all data]</td>
<td>R1 = 0.0998, wR2 = 0.1354</td>
</tr>
<tr>
<td>Largest diff. peak/hole / e Å⁻³</td>
<td>0.23/-0.20</td>
</tr>
</tbody>
</table>
8. $^1$H NMR and $^{13}$C NMR spectra

$^1$H NMR Spectrum of Compound 1a

$^{13}$C NMR Spectrum of Compound 1a
$\text{H NMR Spectrum of Compound 1b}$

$\text{C NMR Spectrum of Compound 1b}$
$^{13}$C NMR Spectrum of Compound 1d

$^1$H NMR Spectrum of Compound 1e
$^{13}$C NMR Spectrum of Compound 1e

$^1$H NMR Spectrum of Compound 1f
H NMR Spectrum of Compound 1h

\[\begin{align*}
\text{\textsuperscript{13}C NMR Spectrum of Compound 1h}
\end{align*}\]
$^{19}$F NMR Spectrum of Compound 1h

$^1$H NMR Spectrum of Compound 1i
$^{13}$C NMR Spectrum of Compound 1i

$^1$H NMR Spectrum of Compound 1j
$^{13}$C NMR Spectrum of Compound 1j

$^1$H NMR Spectrum of Compound 1k
$^{13}$C NMR Spectrum of Compound 1k

$^1$H NMR Spectrum of Compound 1l
$^{13}$C NMR Spectrum of Compound 1l

$^1$H NMR Spectrum of Compound 1m
\[ \text{\textsuperscript{13}C NMR Spectrum of Compound 1m} \]

\[ \text{\textsuperscript{1}H NMR Spectrum of Compound 1n} \]
C NMR Spectrum of Compound 1n

1H NMR Spectrum of Compound 1
$^{13}$C NMR Spectrum of Compound 1

$^1$H NMR Spectrum of Compound 2
$^{13}$C NMR Spectrum of Compound 2

$^1$H NMR Spectrum of Compound 3
13C NMR Spectrum of Compound 3

19F NMR Spectrum of Compound 3
$^1$H NMR Spectrum of Compound 4

$^{13}$C NMR Spectrum of Compound 4
$^{1}$H NMR Spectrum of Compound 7

$^{13}$C NMR Spectrum of Compound 7
C NMR Spectrum of Compound 8

H NMR Spectrum of Compound 9
$^{13}$C NMR Spectrum of Compound 9

$^1$H NMR Spectrum of Compound 10
$^{13}$C NMR Spectrum of Compound 10

$^1$H NMR Spectrum of Compound 11
$^{13}$C NMR Spectrum of Compound 11

$^1$H NMR Spectrum of Compound 12
$^{13}$C NMR Spectrum of Compound 12

$^{19}$F NMR Spectrum of Compound 12
$^1$H NMR Spectrum of Compound 13

$^{13}$C NMR Spectrum of Compound 13
19F NMR Spectrum of Compound 14

1H NMR Spectrum of Compound 15
13C NMR Spectrum of Compound 16

1H NMR Spectrum of Compound 17
$^1^3$C NMR Spectrum of Compound 18

$^1$H NMR Spectrum of Compound 19
C NMR Spectrum of Compound 20

F NMR Spectrum of Compound 20
$^{1}H$ NMR Spectrum of Compound 21

$^{13}C$ NMR Spectrum of Compound 21
H NMR Spectrum of Compound 22

\[ \text{1H NMR Spectrum of Compound 22} \]

\[ \text{13C NMR Spectrum of Compound 22} \]
$^1\text{H NMR Spectrum of Compound 27}$

$^{13}\text{C NMR Spectrum of Compound 27}$
$^{19}$F NMR Spectrum of Compound 27

$^1$H NMR Spectrum of Compound 28
$^{13}\text{C} \text{ NMR Spectrum of Compound 28}$

$^{1}\text{H} \text{ NMR Spectrum of Compound 29}$
$^{13}$C NMR Spectrum of Compound 29

$^{19}$F NMR Spectrum of Compound 29
H NMR Spectrum of Compound 30

\[ \text{\textsuperscript{1}H NMR Spectrum of Compound 30} \]

\[ \text{\textsuperscript{13}C NMR Spectrum of Compound 30} \]

87
H NMR Spectrum of Compound 31

\(^1\text{H} \text{NMR Spectrum of Compound 31}\)

\(^13\text{C} \text{NMR Spectrum of Compound 31}\)
H NMR Spectrum of Compound 32

\[
\begin{align*}
\text{H NMR Spectrum of Compound 32} & \\
\text{C NMR Spectrum of Compound 32} & \\
\end{align*}
\]
$^1$H NMR Spectrum of Compound 33

$^{13}$C NMR Spectrum of Compound 33
$^{19}$F NMR Spectrum of Compound 33

$^1$H NMR Spectrum of Compound 34
13C NMR Spectrum of Compound 34

19F NMR Spectrum of Compound 34
$^1$H NMR Spectrum of Compound 35

$^{13}$C NMR Spectrum of Compound 35
H NMR Spectrum of Compound 37

\[ \text{13C NMR Spectrum of Compound 37} \]
H NMR Spectrum of Compound 38

\[ \text{1H NMR Spectrum of Compound 38} \]

C NMR Spectrum of Compound 38

\[ \text{13C NMR Spectrum of Compound 38} \]
$^{19}$F NMR Spectrum of Compound 38

$^1$H NMR Spectrum of Compound 39
$^{13}$C NMR Spectrum of Compound 39
9. References