Supporting Information

One-pot Synthesis of Quinazolines via Hyrdogen-Transfer Catalysis

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Experimental Section

All reactions were carried out under nitrogen. Proton and carbon magnetic resonance spectra (\(^1\)H NMR and \(^{13}\)C NMR) were recorded using tetramethylsilane (TMS) as the internal standard (\(^1\)H NMR: TMS at 0.00 ppm, CHCl\(_3\) at 7.26 ppm; \(^{13}\)C NMR: CDCl\(_3\) at 77.4 ppm) or were recorded using tetramethylsilane (TMS) in the solvent of DMSO-\(d_6\) as the internal standard (\(^1\)H NMR: TMS at 0.00 ppm, DMSO at 2.50 ppm; \(^{13}\)C NMR: DMSO at 39.5 ppm). Melting points are uncorrected. Column chromatographic separations were carried out on ACME silica gel (200 - 300 mesh) using petroleum ether and EtOAc as eluent. All solvents were purified and dried using standard procedures.

General Methods for the Synthesis of Quinazolines between 1 and 2

1 (1 mmol), aldehyde 2 (1 mmol), styrene (4 mmol), [Cp*IrCl\(_2\)]\(_2\) (0.025 mmol) and anhydrous xylene (2 mL) were added to an oven-dried carousel tube. Then the system was degassed and filled with nitrogen. The reaction mixture was stirred and heated to reflux for 24h. After completion of the reaction, the resulting solution was cooled to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 to 5:1) as the eluent to provide the desired products 4.

Optimization of the conditions

![Chemical structure](image)

Table 1

<table>
<thead>
<tr>
<th></th>
<th>Catalyst</th>
<th>Additive</th>
<th>Acceptor</th>
<th>Solvent</th>
<th>Yield(^c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>No</td>
<td>No</td>
<td>xylene</td>
<td>10%</td>
</tr>
<tr>
<td>2</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>No</td>
<td>styrene</td>
<td>xylene</td>
<td>66%(^c)</td>
</tr>
<tr>
<td>3</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>No</td>
<td>E-crotonitrile</td>
<td>xylene</td>
<td>50%(^c)</td>
</tr>
<tr>
<td>4</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>AcOH 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>43%</td>
</tr>
<tr>
<td>5</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>KOH 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>54%</td>
</tr>
<tr>
<td>6</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>r-BuONa 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>60%</td>
</tr>
<tr>
<td>7</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>K(_2)CO(_3) 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>46%</td>
</tr>
<tr>
<td>8</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>No</td>
<td>styrene</td>
<td>toluene</td>
<td>35%</td>
</tr>
<tr>
<td>9</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>No</td>
<td>styrene</td>
<td>DMF</td>
<td>50%</td>
</tr>
<tr>
<td>10</td>
<td>[Cp*IrI(_2)](_2)</td>
<td>No</td>
<td>styrene</td>
<td>xylene</td>
<td>57%</td>
</tr>
<tr>
<td>11</td>
<td>RuCl(_2)(PPh(_3))(_3)</td>
<td>KOH 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>26%</td>
</tr>
<tr>
<td>12</td>
<td>[Ru(p- cymene)Cl(_2)](_2)</td>
<td>KOH 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>52%</td>
</tr>
<tr>
<td>13</td>
<td>[Cp*IrCl(_2)](_2)</td>
<td>4A MS 2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>51%</td>
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</tbody>
</table>
Conditions: 1a (0.5 mmol), 2a (0.5 mmol), catalyst (2.5 mol%), styrene (4.0 eq.) in refluxing temperature of solvent (1 mL) under N₂, 24 h. ² H-NMR yield. ³ Isolated yield. ⁴ 2.5 mol% dppf was added.

Synthesis of quinazolines form alcohol 1a and 7

\[ \text{PhOH} + \text{NH}_2 \rightarrow \text{N} = \text{N} \text{Ph} \]

Table 2

<table>
<thead>
<tr>
<th></th>
<th>Catalyst</th>
<th>Additive</th>
<th>Acceptor</th>
<th>Solvent</th>
<th>Yield ²</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[Cp*IrCl₂]₂</td>
<td>No</td>
<td>styrene</td>
<td>xylene</td>
<td>10%</td>
</tr>
<tr>
<td>2</td>
<td>[Cp*IrCl₂]₂</td>
<td>KOH 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>61% ³</td>
</tr>
<tr>
<td>3</td>
<td>[Cp*IrCl₂]₂</td>
<td>NaOH 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>57%</td>
</tr>
<tr>
<td>4</td>
<td>[Cp*IrCl₂]₂</td>
<td>t-BuONa 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>50%</td>
</tr>
<tr>
<td>5</td>
<td>RuCl₂(PPh₃)₃</td>
<td>KOH 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>46%</td>
</tr>
<tr>
<td>6</td>
<td>[Ru(p-cymene)Cl₂]²d</td>
<td>KOH 0.2 eq.</td>
<td>styrene</td>
<td>xylene</td>
<td>42%</td>
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</table>

² Conditions: 1a (0.5 mmol), 2a (0.5 mmol), catalyst (2.5 mol%), acceptor (4.0 eq.), base (20 mol%) in refluxing temperature of solvent (1 mL) under N₂, 48 h. ³ H-NMR yield. ⁴ Isolated yield. ⁵ 2.5 mol% dppf was added.

2-aminobenzylamines 1a (122 mg, 1 mmol), phenylmethanol 2 (108 mg, 1 mmol), styrene (416 mg, 4 mmol), [Cp*IrCl₂]₂ (20 mg, 0.025 mmol), KOH (11 mg, 0.2 mmol) and anhydrous xylene (2 mL) were added to an oven-dried carousel tube. Then the system was degassed and filled with nitrogen. The reaction mixture was stirred and heated to reflux for 48 h. After completion of the reaction, the resulting solution was cooled to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 to 5:1) as the eluent to provide the desired products 4a (slight yellow solid, 127 mg, 61% yield).

Synthesis of 2-phenyl-4H-benzo[d][1,3]oxazine form aldehyde 2a and 8

Table 3
(2-aminophenyl) methanol 8 (123 mg, 1 mmol), benzaldehyde 2a (106 mg, 1 mmol) and anhydrous xylene (2 mL) were added to an oven-dried carousel tube. Then the system was degassed and filled with nitrogen. The reaction mixture was stirred and heated to reflux for 24 h, the reaction was cooled to room temperature, styrene (416 mg, 4 mmol), [Cp*IrCl₂]₂ (20 mg, 0.025 mmol), KOH (11 mg, 0.2 mmol) were added, the mixture was stirred and heated to reflux for 24 h, the resulting solution was cooled to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 to 5:1) as the eluent to provide the desired products 9 (slight yellow solid, 94 mg, 45% yield).

### Characterization Data of 3, 4, 5, 9 and 10

**2-phenyl-1,2,3,4-tetrahydroquinazoline (3a).** White solid, mp: 102 °C - 103 °C (lit.¹ 102 °C - 105 °C). $^1$H NMR (CDCl₃ - $d_J$, 400 MHz): $\delta$ 7.40 (d, $J = 8.0$ Hz, 2H), 7.25 - 7.31 (m, 3H), 6.95 (t, $J = 8.0$ Hz, 1H), 6.84 (d, $J = 8.0$ Hz, 1H), 6.62 (t, $J = 8.0$ Hz, 1H), 6.47 (d, $J = 8.0$, 1H), 5.11 (s, 1H), 4.13 (d, $J = 16$, 1H), 4.10 (br, 1 H), 3.86 (d, $J = 16$, 1H), 1.81 (br, 1 H). $^{13}$C NMR (CDCl₃ - $d_J$, 100 MHz): $\delta$ 143.7, 141.6, 128.7, 128.5, 126.6, 126.2, 121.3, 118.1, 115.0, 69.6, 46.5. HRMS (ESI): [M + H]$^+$: C₁₄H₁₃N₂ Calcd for 211.1235. Found: 211.1276.

**2-phenylquinazoline (4a).** Pale yellow solid, mp: 96 °C - 98 °C (lit.² 97 °C - 98 °C). $^1$H NMR (CDCl₃ - $d_J$, 400 MHz): $\delta$ 9.37 (s, 1H), 8.54 (d, $J = 8.0$, 2H), 8.00 (d, $J = 8.0$, 1H), 8.79 - 8.84 (m, 2H), 7.42 - 7.53 (m, 4H). $^{13}$C NMR (CDCl₃ - $d_J$, 100 MHz): $\delta$ 161.0, 160.5, 150.8, 138.0, 134.1, 130.6, 128.6, 127.2, 127.1, 123.6. HRMS (ESI): [M + H]$^+$: C₁₄H₁₁N₂ Calcd for 207.0922. Found: 207.0910.

**2-(3-chlorophenyl)quinazoline (4b).** Pale yellow solid, mp: 148 °C - 149 °C (lit.³ 148 °C - 150 °C). $^1$H NMR (CDCl₃ - $d_J$, 400 MHz): $\delta$ 9.46 (s, 1H), 8.63 (s, 1H), 8.49 - 8.51 (m, 1H), 8.09 (d, $J = 8.0$, 1H), 7.91 - 7.95 (m, 2H), 7.64 (t, $J = 8.0$, 1H), 7.46 - 7.48 (m, 2H). $^{13}$C NMR (CDCl₃ - $d_J$, 100 MHz): $\delta$ 160.5, 159.7, 150.6, 139.8, 134.7, 134.3, 130.5, 129.8, 128.7, 128.6, 127.6, 127.1, 126.6, 123.7. HRMS (ESI): [M + H]$^+$: C₁₄H₁₀N₂Cl Calcd for 241.0533. Found: 241.0522.

**2-(3-bromophenyl)quinazoline (4c).** Yellow solid, mp: 154 °C - 156 °C (lit.³ 153 °C - 155 °C). $^1$H NMR (CDCl₃ - $d_J$, 400 MHz): $\delta$ 9.46 (s, 1H), 8.79 (s, 1H), 8.09 (d, $J = 8.0$, 1H), 7.90 - 7.94 (m, 2H), 7.62 - 7.65 (m, 2H), 7.40 (t, $J = 8.0$, 1H). $^{13}$C NMR (CDCl₃ - $d_J$, 100 MHz): $\delta$ 160.5, 159.5, 150.6.
140.0, 134.3, 133.4, 131.5, 130.1, 128.8, 127.6, 127.1, 127.0, 123.7, 122.9. HRMS (ESI): [M + H]^+\cdot C_{14}H_{10}N_2Br CaIcAl for 285.0027. Found: 241.0007.

2-(3-nitrophenyl)quinazoline (4d). Yellow solid, mp: 160 °C - 162 °C (lit.4 162 °C - 163 °C). ^1H NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 400 MHz): δ 9.51 (s, 1H), 9.50 (s, 1H), 8.98 (d, J = 8.0, 1H), 8.35 (d, J = 8.0, 1H), 8.14 (d, J = 8.0, 1H), 7.96 - 8.00 (m, 2H), 7.67 - 7.73 (m, 2H). ^13C NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 100 MHz): δ 160.7, 158.7, 150.6, 148.5, 139.9, 134.5, 134.2, 129.5, 128.7, 127.2, 125.0, 123.9, 123.6. HRMS (ESI): [M + H]^+\cdot C_{14}H_{10}N_2O2 Calcd for 252.0773. Found: 252.0756.

2-(m-tolyl)quinazoline (4e). Yellow solid , mp: 97 °C - 98 °C. ^1H NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 400 MHz): δ 9.44 (s, 1H), 9.40 - 9.43 (m, 2H), 8.08 (d, J = 8.0, 1H), 7.86 - 7.90 (m, 2H), 7.58 (t, J = 8.0, 1H), 7.43 (t, J = 8.0, 1H), 7.32 (d, J = 8.0, 1H), 2.48 (s, 3H). ^13C NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 100 MHz): δ 161.2, 160.4, 150.7, 138.2, 137.9, 134.0, 131.4, 129.1, 128.6, 128.5, 127.2, 127.1, 125.8, 123.5, 21.5. HRMS (ESI): [M + H]^+\cdot C_{15}H_{13}N_2 Calcd for 221.1079. Found: 221.1057.

2-(3-methoxyphenyl)quinazoline (4f). Pale yellow solid, mp: 89 °C - 90 °C. ^1H NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 400 MHz): δ 9.46 (s, 1H), 8.23 (d, J = 8.0, 1H), 8.17 - 8.19 (m, 1H), 7.88 - 7.93 (m, 2H), 7.61 (t, J = 8.0, 1H), 7.45 (t, J = 8.0, 1H), 7.07 (d, J = 8.0, 1H), 3.95 (s, 3H). ^13C NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 100 MHz): δ 160.8, 160.4, 160.0, 150.7, 139.5, 134.1, 129.6, 128.6, 127.3, 127.1, 123.6, 121.1, 117.2, 113.0. HRMS (ESI): [M + H]^+\cdot C_{15}H_{13}N_2O Calcd for 237.1028. Found: 237.1016.

2-(4-fluorophenyl)quinazoline (4g). White solid, mp: 128 °C - 130 °C (lit.2 129 °C - 130). ^1H NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 400 MHz): δ 9.43 (s, 1H), 8.61 - 8.64 (m, 2H), 8.06 (d, J = 8.0, 1H), 7.88 - 7.92 (m, 2H), 7.59 - 7.62 (m, 1H), 7.18 - 7.22 (m, 2H) . ^13C NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 100 MHz): δ 165.9, 163.4, 160.5, 160.1, 150.7, 134.2, 130.7, 130.6, 128.5, 127.2, 127.1, 123.4, 115.6, 115.4. HRMS (ESI): [M + H]^+\cdot C_{14}H_{10}N_2F Calcd for 225.0828. Found: 225.0887.

2-(4-bromophenyl)quinazoline (4h). White solid, mp: 121 °C - 123 °C (lit.2 120 °C - 121 °C). ^1H NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 400 MHz): δ 9.45 (s, 1H), 8.50 (d, J = 8.0, 2H), 8.07 (d, J = 8.0, 1H), 7.90 - 7.94 (m, 2H), 7.66 (d, J = 8.0, 2H), 7.61 - 7.65 (m, 1H), 7.59 - 7.62 (m, 1H). ^13C NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 100 MHz): δ 160.5, 160.1, 150.7, 136.9, 134.2, 131.8, 130.1, 128.6, 127.5, 127.1, 124.4, 123.6. HRMS (ESI): [M + H]^+\cdot C_{14}H_{10}N_2Br Calcd for 285.0027. Found: 285.0025.

2-(4-nitrophenyl)quinazoline (4i). White solid, mp: 219 °C - 221 °C (lit.2 218 °C - 219°C). ^1H NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 400 MHz): δ 9.52 (s, 1H), 8.82 (d, J = 8.0, 2H), 8.37 (d, J = 8.0, 2H), 8.14 (d, J = 8.0, 1H), 7.96 - 8.00 (m, 2H), 7.69 - 7.73 (m, 1H) . ^13C NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 100 MHz): δ 160.7, 158.8, 150.6, 149.2, 143.8, 134.6, 129.4, 128.8, 128.3, 127.2, 123.8, 123.7. HRMS (ESI): [M + H]^+\cdot C_{14}H_{10}N_2O2 Calcd for 252.0773. Found: 272.0758.

2-(p-tolyl)quinazoline (4j). White solid, mp: 98 °C - 99 °C (lit.2 97 °C - 98). ^1H NMR (CDCl\textsubscript{3} - d\textsubscript{6}, 400 MHz): δ 9.42 (s, 1H), 8.51 (d, J = 8.0, 2H), 8.05 (d, J = 8.0, 1H), 7.84 - 7.88 (m, 2H), 7.55 (t, J = 8.0, 1H).
1H), 7.33 (d, J = 8.0, 2H), 2.43 (s, 3H). 13C NMR (CDCl3 - d3, 100 MHz): δ 161.1, 160.4, 150.8, 140.8, 135.3, 134.0, 129.4, 128.5, 127.0, 123.5, 21.5. HRMS (ESI): [M + H]⁺: C13H13N2 Calcd for 221.1079. Found: 221.1052.

2-(furan-2-yl)quinazoline (4k). Brown liquid. 1H NMR (CDCl3 - d3, 400 MHz): δ 9.36 (s, 1H), 8.09 (d, J = 8.0, 1H), 7.86 - 7.90 (m, 2H), 7.69 (s, 1H), 7.57 (t, J = 4.0, 1H), 7.46 (d, J = 4.0, 1H). 13C NMR (CDCl3 - d3, 100 MHz): δ 160.6, 154.0, 152.4, 150.3, 145.3, 134.4, 128.3, 127.2, 123.3, 114.0, 111.2. HRMS (ESI): [M + H]⁺: C13H13N2O Calcd for 197.0715. Found: 197.0695.

2-benzylquinazoline (4l). Slight yellow solid, mp: 68 °C - 69 °C (lit. 6 70 -71 °C). 1H NMR (CDCl3 - d3, 400 MHz): δ 9.33 (s, 1H), 8.01 (d, J = 8.0, 1H), 7.87 - 7.89 (m, 2H), 7.58 (t, J = 8.0, 1H), 7.43 (d, J = 8.0, 2H), 7.30 (t, J = 8.0, 2H), 7.19 - 7.22 (m, 1H), 4.46 (s, 2H). 13C NMR (CDCl3 - d3, 100 MHz): δ 166.1, 160.8, 150.4, 138.5, 134.1, 129.2, 128.5, 128.1, 127.2, 127.0, 126.5, 123.1. HRMS (ESI): [M + H]⁺: C13H13N2 Calcd for 221.1079. Found: 221.1019.

2-pentyquinazoline (4m). Pale yellow liquid. 1H NMR (CDCl3 - d3, 400 MHz): δ 9.35 (s, 1H), 7.98 (d, J = 8.0, 1H), 7.85 - 7.89 (m, 2H), 7.58 (t, J = 8.0, 1H), 3.12 (t, J = 8.0, 2H), 1.89 - 1.97 (m, 2H), 1.36 - 1.45 (m, 4H), 0.91 (t, J = 8.0, 3H). 13C NMR (CDCl3 - d3, 100 MHz): δ 167.9, 160.3, 150.0, 133.9, 127.8, 127.0, 126.8, 123.0, 39.9, 31.7, 28.7, 22.5, 14.0. HRMS (ESI): [M + H]⁺: C10H17N2 Calcd for 201.1392. Found: 201.1387.

5-fluoro-2-phenylquinazoline (4n). Pale yellow solid, mp: 100 °C - 102 °C (lit. 2 101 - 102 °C). 1H NMR (CDCl3 - d3, 400 MHz): δ 9.73 (s, 1H), 8.61 - 8.63 (m, 2H), 7.79 - 7.89 (m, 2H), 7.52 - 7.57 (m, 3H), 7.20 - 7.25 (m, 1H). 13C NMR (CDCl3 - d3, 100 MHz): δ 161.7, 158.2 (d, J = 250, 1C), 154.8, 151.5, 137.5, 134.1, 131.0, 128.6, 124.6, 114.4, 110.0. HRMS (ESI): [M + H]⁺: C14H10FN2 Calcd for 225.0828. Found: 225.0815.

2-(4-bromophenyl)-5-fluoroquinazoline (4o). Pale yellow solid, mp: 176 °C - 177 °C. 1H NMR (CDCl3 - d3, 400 MHz): δ 9.70 (s, 1H), 8.49 (d, J = 8.0, 2H), 7.82 - 7.87 (m, 2H), 7.65 (d, J = 8.0, 2H), 7.22 - 7.26 (m, 1H). 13C NMR (CDCl3 - d3, 100 MHz): δ 160.7, 158.0 (d, J = 260, 1C), 154.9, 151.2, 136.5, 134.2, 131.8, 130.2, 125.8, 124.5, 114.4, 111.3. HRMS (ESI): [M + H]⁺: C16H13FBrN2 Calcd for 302.9933. Found: 302.9927.

5-fluoro-2-(p-toly)quinazoline (4p). Pale yellow solid, mp: 132 °C - 133 °C. 1H NMR (CDCl3 - d3, 400 MHz): δ 9.71 (s, 1H), 8.51 (d, J = 8.0, 2H), 7.81 - 7.87 (m, 2H), 7.34 (d, J = 8.0, 2H), 7.19 - 7.21 (m, 1H), 2.45 (s, 3H). 13C NMR (CDCl3 - d3, 100 MHz): δ 161.8, 160.7, 158.2 (d, J = 250, 1C), 154.7, 151.5, 141.3, 134.9, 134.0, 129.4, 128.7, 124.5, 114.3, 110.7, 21.5. HRMS (ESI): [M + H]⁺: C13H12FN2 Calcd for 239.0985. Found: 239.0989.

5-fluoro-2-pentylquinazoline (4q). Slight yellow liquid. 1H NMR (CDCl3 - d3, 400 MHz): δ 9.52 (s, 1H), 7.67 - 7.75 (m, 2H), 7.10 - 7.14 (m, 1H), 3.04 (t, J = 8.0, 2H), 1.80 - 1.88 (m, 2H), 1.28 - 1.35 (m,
4H), 0.82 (t, J = 8.0, 3H). $^{13}$C NMR (CDCl$_3$ - d$_3$, 100 MHz): $\delta$ 168.8, 158.1 (d, J = 250, 1C), 154.6, 151.0, 134.0, 123.8, 113.9, 110.6, 39.9, 31.6, 28.5, 22.5, 13.9. HRMS (ESI): [M + H]$^+$: C$_{13}$H$_{16}$FN$_2$

2-((benzylamino)methyl)aniline (5). Slight yellow liquid. $^1$H NMR (CDCl$_3$ - d$_3$, 400 MHz): $\delta$ 7.27 - 7.39 (m, 5H), 7.13 (t, J = 8.0 Hz, 1H), 7.06 (d, J = 8.0 Hz, 1H), 6.69 - 6.73 (m, 2H), 4.74 (br, 2), 3.86 (s, 2H), 3.82 (s, 2H), 1.52 (br, 1 H). $^{13}$C NMR (CDCl$_3$ - d$_3$, 100 MHz): $\delta$ 146.9, 140.2, 129.9, 128.5, 128.4, 128.1, 127.0, 123.8, 117.7, 115.7, 53.2, 52.4. HRMS (ESI): [M + H]$^+$: C$_{13}$H$_{17}$N$_2$ Calcd for 213.1392. Found: 213.1377.

2-phenyl-4H-benzo[d][1,3]oxazine (9). White solid, mp: 91 °C - 92 °C (lit.$^2$ 92 °C - 93 °C). $^1$H NMR (CDCl$_3$ - d$_3$, 400 MHz): $\delta$ 8.13 (d, J = 8.0, 2H), 7.41 - 7.51 (m, 3H), 7.25 - 7.34 (m, 2H), 7.16 - 7.20 (m, 1H), 7.01 (d, J = 8.0, 2H). $^{13}$C NMR (CDCl$_3$ - d$_3$, 100 MHz): $\delta$ 157.6, 139.7, 132.3, 131.4, 128.9, 128.2, 128.0, 126.4, 124.6, 123.7, 122.3, 66.4. HRMS (ESI): [M + H]$^+$: C$_{12}$H$_{17}$N$_2$ Calcd for 213.1392. Found: 213.1377.

2-phenyl-2,4-dihydro-1H-benzo[d][1,3]oxazine (10). White solid, mp: 117 °C - 118 °C (lit.$^3$ 116 °C - 117 °C). $^1$H NMR (CDCl$_3$ - d$_3$, 400 MHz): $\delta$ 7.57 (d, J = 8.0, 2H), 7.40 - 7.44 (m, 3H), 7.11 (t, J = 8, 1H), 6.98 (d, J = 8.0, 1H), 6.85 (t, J = 8, 1H), 6.72 (d, J = 8.0, 1H), 5.59 (d, J = 4.0, 1H), 5.13 (d, J = 16.0, 1H), 4.95 (d, J = 16.0, 1H), 4.12 (br, 1H). $^{13}$C NMR (CDCl$_3$ - d$_3$, 100 MHz): $\delta$ 141.6, 139.1, 129.1, 128.6, 127.4, 126.5, 125.0, 122.2, 119.8, 117.1, 85.2, 67.6. HRMS (ESI): [M + H]$^+$: C$_{14}$H$_{15}$NO Calcd for 212.1075. Found: 212.1077.

Reference


$^1$H and $^{13}$C NMR Spectra of 3, 4, 5, 9 and 10

3a
4a
4b

[Chemical structure image]

Electronic Supplementary Material (ESI) for RSC Advances
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4k
4m