Electronic supplementary information

Metal-free, organocatalytic cascade formation of C–N and C–O bonds through dual sp$^3$ C–H activation: oxidative synthesis of oxazole derivatives

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**General information:** All reactions were carried out under air atmosphere unless otherwise noted. All reagents and solvents were obtained from commercial suppliers and used without further purification. Reactions were monitored by TLC on silica gel plates (GF254). $^1$H NMR and $^{13}$C NMR spectra were recorded on 300 MHz spectrometer at room temperature. Chemical shifts ($\delta$) are reported in ppm downfield from tetramethylsilane. Abbreviations for signal couplings are: s, singlet; d, doublet; t, triplet; m, multiplet.

**Part I. Optimization of the reaction condition**

**Table 1. Optimization of the reaction condition**

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst (20 mol %)</th>
<th>Solvent</th>
<th>T/°C</th>
<th>Additives</th>
<th>Oxidant</th>
<th>Time/h</th>
<th>Yield (%)</th>
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<tr>
<td>1</td>
<td>n-Bu$_4$NI</td>
<td>EtOAc</td>
<td>25</td>
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<td>TBHP</td>
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<td>43</td>
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<tr>
<td>2</td>
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<tr>
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<td>-</td>
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<tr>
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<td>-</td>
<td>H$_2$O$_2$</td>
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<td>O$_2$</td>
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<td>HOAc(20%)</td>
<td>T-HYDRO</td>
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<td>40</td>
<td>TFA (20%)</td>
<td>T-HYDRO</td>
<td>6</td>
<td>ND</td>
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<td>4A MS (80 mg)</td>
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<td>NaOAc</td>
<td>T-HYDRO</td>
<td>8</td>
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</table>
Part II. Control experiment on the reaction mechanism

It was thought that 12 may be the key reaction intermediate derived from 1g and I2. However, when 1g was used as a substrate in the presence of 1.0 equiv n-Bu₄NI and 1.2 equiv T-HYDRO, it did not afford the iodide product 12 at 40 °C. Moreover, from the color of the reaction solution, we supposed that little I₂ was generated until the reaction completed. On the other hand, the reaction of 12 with benzylamine 2a proceeded roughly in the presence of 2.0 equiv. oxidant at 40 °C. As a result, this kind of mechanism pathway could be excluded.
When 3.0 equiv. I₂ was added into the reaction of ethyl acetoacetate 1a with benzylamine 2a, it hardly afforded the desired product. Notably, the reaction proceeded smoothly in the presence of 6.0 equiv. n-Bu₄NOH (25% in water) and 3.0 equiv. I₂, giving the desired product in 43% yield. It was acceptable that hypoiodite [IO] might be generated from I₂ under basic condition, then it disproportioned to iodite anion [IO₂]. In contrast, periodate(−7) was inert under the present conditions. Hence, [IO] (−1) and [IO₂] (−3) species may be the important oxidant in the reaction.

The study of MS (ESI) on mechanism

The reaction of ethyl acetoacetate 1a with benzylamine 2a was performed as the standard reaction condition. After 1 h, the reaction mixture was subjected to MS (ESI) study. In the positive ion mode, we can identify “n-Bu₄N⁺”, the enamine intermediate 6 and product 3a.

MS (ESI, positive) for “n-Bu₄N⁺”, found m/z: 242.15.
MS (ESI, positive) for enamine intermediate 6, found m/z: 222.05 (M+H).
MS (ESI, positive) for product 3a, found m/z: 232.00 (M+H).

Moreover, we can detect [I⁻], [IO⁻] and [IO₂⁻] in the negative ion mode. The details see the following in the MS spectrum.

MS (ESI, negative) for “I⁻”, calculate: 126.90, found 126.85.
MS (ESI, negative) for “IO⁻”, calculate: 142.90, found 142.95.
MS (ESI, negative) for “IO₂⁻”, calculate: 158.89, found 158.95.
Part III. General procedure for the dual sp³ C-H activation reaction

To a solution of 1,3-dicarbonyl compounds (0.15 mmol) in EtOAc (1.0 mL) was added n-Bu₄NI (20 mol%) and benzylamines (0.3 mmol), followed by adding a solution of T-HYDRO (2.5 equiv.) slowly. The resulting mixture was stirred at 40 °C. After 3 hours, the remaining T-HYDRO (1.5 equiv.) was added, and the reaction was still stirred at 40 °C until it completed. When the reaction finished, the reaction mixture was cooled to room temperature and poured into saturated Na₂S₂O₃ solution (3 mL), extracted with EtOAc (3 × 8 mL), then washed with saturated brine. The combined organic layers were dried over anhydrous Na₂SO₄. After removing the solvents in vacuo, the residue was purified by flash column chromatography on silica gel or preparative TLC on GF 254 to afford the desired products 3.

Part IV. Characterization data of compounds

Ethyl 5-methyl-2-phenyloxazole-4-carboxylate 3a[1]

\[
\begin{align*}
\text{Ph} & \quad \text{N} & \quad \text{COOEt} \\
\text{N} & \quad \text{Ph} & \quad \text{Me}
\end{align*}
\]

Known compound. Yield: 70%. Colorless oil. \(^1\)H NMR (300 MHz, CDCl₃): \(\delta\) (ppm) = 8.10-8.02 (m, 2 H), 7.48-7.42 (m, 3 H), 4.41 (q, \(J = 7.2\) Hz, 2 H), 2.69 (s, 3 H), 1.41 (t, \(J = 7.2\) Hz, 3 H). MS (ESI, positive) for C₁₃H₁₃NO₃, found \(m/z: 232.17\) (M+H), 254.17 (M+Na), 485.00 (2M+Na).

Methyl 5-methyl-2-phenyloxazole-4-carboxylate 3b[2]

\[
\begin{align*}
\text{Ph} & \quad \text{N} & \quad \text{COOMe} \\
\text{N} & \quad \text{Ph} & \quad \text{Me}
\end{align*}
\]

Known compound. Yield: 63%. Pale yellow solid, mp 87-88 °C (lit. mp 89-91 °C). \(^1\)H NMR (300 MHz, CDCl₃): \(\delta\) (ppm) = 8.10-8.02 (m, 2 H), 7.50-7.42 (m, 3 H), 3.94 (s, 3 H), 2.70 (s, 3 H); MS (ESI, positive) for C₁₂H₁₁NO₃, found \(m/z: 218.17\) (M+H), 240.17 (M+Na), 456.92 (2M+Na).
tert-Butyl 5-methyl-2-phenyloxazole-4-carboxylate 3c\textsuperscript{[3]}

\begin{center}
\begin{tikzpicture}
  \node[above] at (0,0) \[N] \node[below] at (0,0) \[O] \node[below left] at (0,0) \[Me] \node[below right] at (0,0) \[COO-Bu] \node[below] at (0,0) \[Ph] \end{tikzpicture}
\end{center}

Known compound. Yield: 72%. Pale yellow solid, mp 69-70 °C (lit. mp 72-73 °C). \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) = 8.09-8.02 (m, 2 H), 7.46-7.41 (m, 3 H), 2.65 (s, 3 H), 1.61 (s, 9 H); MS (ESI, positive) for C\textsubscript{15}H\textsubscript{17}NO\textsubscript{3}, found m/z: 260.00 (M+H), 282.08 (M+Na), 541.00 (2M+Na).

Ethyl 2-phenyl-5-propoxyloxazole-4-carboxylate 3d\textsuperscript{[3]}

\begin{center}
\begin{tikzpicture}
  \node[above] at (0,0) \[N] \node[below] at (0,0) \[O] \node[below left] at (0,0) \[COO-nPr] \node[below right] at (0,0) \[Ph] \end{tikzpicture}
\end{center}

Known compound. Yield: 75%. Pale yellow solid, mp 50-52 °C (lit. mp 53-54 °C). \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) = 8.12-8.01 (m, 2 H), 7.48-7.40 (m, 3 H), 4.42 (q, \(J = 7.2\) Hz, 2 H), 3.08 (t, \(J = 7.5\) Hz, 2 H), 1.85-1.72 (m, 2 H), 1.41 (t, \(J = 7.2\) Hz, 3 H), 1.02 (t, \(J = 7.5\) Hz, 3 H); MS (ESI, positive) for C\textsubscript{15}H\textsubscript{17}NO\textsubscript{3}, found m/z: 282.08 (M+Na).

Ethyl 5-isopropyl-2-phenyloxazole-4-carboxylate 3e

\begin{center}
\begin{tikzpicture}
  \node[above] at (0,0) \[N] \node[below] at (0,0) \[O] \node[below left] at (0,0) \[COO-iPr] \node[below right] at (0,0) \[Ph] \end{tikzpicture}
\end{center}

New compound. Yield: 76%. Pale yellow solid, mp 57-58 °C. \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) = 8.12-8.05 (m, 2 H), 7.50-7.42 (m, 3 H), 4.42 (q, \(J = 7.2\) Hz, 3 H), 3.90-3.76 (m, 1 H), 1.41 (t, \(J = 7.2\) Hz, 3 H), 1.36 (d, \(J = 7.2\) Hz, 6 H); \textsuperscript{13}C NMR (75 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) = 164.0, 162.3, 159.3, 130.6, 128.6, 126.8, 126.7, 126.5, 60.9, 26.2, 20.6, 14.3. HRMS (ESI) m/z [M+Na]\textsuperscript{+} calcd for C\textsubscript{15}H\textsubscript{17}NNaO\textsubscript{3} : 282.1101, found :282.1108.

Methyl 5-isopropyl-2-phenyloxazole-4-carboxylate 3f\textsuperscript{[4]}

\begin{center}
\begin{tikzpicture}
  \node[above] at (0,0) \[N] \node[below] at (0,0) \[O] \node[below left] at (0,0) \[COOCMe] \node[below right] at (0,0) \[Ph\] \end{tikzpicture}
\end{center}

Known compound. Yield: 69%. Yellow solid, mp 68-69 °C (lit. mp 67-68 °C). \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) = 8.10-8.03 (m, 2 H), 7.51-7.41 (m, 3 H), 3.94 (s, 3 H), 3.90-3.77 (m, 1 H), 1.36 (d, \(J = 6.9\) Hz, 6 H); MS (ESI, positive) for C\textsubscript{16}H\textsubscript{15}NO\textsubscript{3}, found m/z: 246.17 (M+H), 268.17 (M+Na), 513.00 (2M+Na).

Ethyl 2,5-diphenyloxazole-4-carboxylate 3g\textsuperscript{[4]}

\begin{center}
\begin{tikzpicture}
  \node[above] at (0,0) \[N] \node[below] at (0,0) \[O] \node[below left] at (0,0) \[COOEt] \node[below right] at (0,0) \[Ph] \end{tikzpicture}
\end{center}

Known compound. Yield: 67%. Light yellow solid, mp 47-48 °C (lit. mp 86-87 °C). \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) = 8.20-8.06 (m, 4 H), 7.55-7.45 (m, 6 H), 4.46 (q, \(J = 7.2\) Hz, 2 H), 1.43 (t, \(J = 7.2\) Hz, 3 H); MS (ESI, positive) for C\textsubscript{18}H\textsubscript{15}NO\textsubscript{3}, found m/z: 294.17 (M+H), 316.17 (M+Na), 609.00 (2M+Na).

1-(5-methyl-2-phenyloxazol-4-yl)ethanone 3h\textsuperscript{[3]}

\begin{center}
\begin{tikzpicture}
  \node[above] at (0,0) \[N] \node[below] at (0,0) \[O] \node[below left] at (0,0) \[Me] \node[below right] at (0,0) \[Me] \node[below] at (0,0) \[Ph\] \end{tikzpicture}
\end{center}

Known compound. Yield: 61%. Pale yellow solid, mp 77-78 °C (lit. mp 78-79 °C). \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) = 8.05-7.99 (m, 2 H), 7.50-7.42 (m, 3 H), 2.69 (s, 3 H), 2.60 (s, 3 H); MS (ESI, positive) for C\textsubscript{12}H\textsubscript{11}NO\textsubscript{2}, found m/z: 202.17 (M+H), 224.08 (M+Na).

(2,5-diphenyloxazol-4-yl)(phenyl)methanone 3i\textsuperscript{[5]}

\begin{center}
\begin{tikzpicture}
  \node[above] at (0,0) \[N] \node[below] at (0,0) \[O] \node[below left] at (0,0) \[COOEt] \node[below right] at (0,0) \[Ph] \end{tikzpicture}
\end{center}

Known compound. Yield: 40%. Pale yellow solid, mp 84-85 °C (lit. mp 80-81 °C). \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) = 8.22-8.16 (m, 3 H), 8.15-8.05 (m, 2 H), 8.00-7.95 (m, 1 H), 7.65-7.39 (m, 9 H); MS (ESI, positive) for C\textsubscript{22}H\textsubscript{15}NO\textsubscript{2}, found m/z: 326.25 (M+H), 348.17 (M+Na), 672.92 (2M+Na).
(5-methyl-2-phenyloxazol-4-yl)(phenyl)methanone 3j

New compound. Yield: 56%. Light yellow solid, mp 58-59 °C. 1H NMR (300 MHz, CDCl3): δ (ppm) = 8.39-8.32 (m, 2 H), 8.12-8.06 (m, 2 H), 7.63-7.58 (m, 1 H), 7.57-7.45 (m, 5 H), 2.77 (s, 3 H); 13C NMR (75 MHz, CDCl3): δ (ppm) = 187.9, 158.4, 157.2, 137.4, 132.7, 130.5, 130.4, 129.8, 128.8, 128.7, 128.1, 128.6, 126.4, 12.7. MS (ESI, positive) for C11H14NO4, found m/z: 263.85 (M+H+); HRMS (ESI) m/z [M+Na]+ calcld for C11H13NNO4 : 286.0838, found: 238.0836.

Ethyl 2-(4-chlorophenyl)-5-methylloxazole-4-carboxylate 3k [5]

Known compound. Yield: 64%. Yellow solid, mp 68-69 °C (lit. mp 81-83 °C). 1H NMR (300 MHz, CDCl3): δ (ppm) = 8.03-7.96 (m, 2 H), 7.45-7.38 (m, 2 H), 2.69 (s, 3 H), 1.41 (t, J = 7.2 Hz, 2 H), 2.72 (s, 3 H), 1.41 (t, J = 7.2 Hz); MS (ESI, positive) for C13H12CINO3, found m/z: 266.08 (M+H+), 288.17 (M+Na), 552.92 (2M+Na).

Ethyl 2-(2-chlorophenyl)-5-methylloxazole-4-carboxylate 3l [5]

Known compound. Yield: 73%. Yellow solid, mp 62-64 °C (lit. mp 65-66 °C). 1H NMR (300 MHz, CDCl3): δ (ppm) = 8.02-7.96 (m, 1 H), 7.50-7.45 (m, 1 H), 7.43-7.30 (m, 2 H), 4.42 (q, J = 7.2 Hz, 2 H), 2.72 (s, 3 H), 1.41 (t, J = 7.2 Hz); MS (ESI, positive) for C13H12CINO3, found m/z: 288.08 (M+H+), 552.92 (2M+Na).

Ethyl 2-(4-fluorophenyl)-5-methylloxazole-4-carboxylate 3m [5]

Known compound. Yield: 65%. Yellow solid, mp 71-72 °C (lit. mp 72-73 °C). 1H NMR (300 MHz, CDCl3): δ (ppm) = 7.95 (d, J = 7.5 Hz, 2 H), 7.28-7.22 (m, 2 H), 4.43 (q, J = 7.2 Hz, 2 H), 2.69 (s, 3 H), 2.39 (s, 3 H), 1.41 (t, J = 7.2 Hz, 3 H); MS (ESI, positive) for C13H12FNO3, found m/z: 250.17 (M+H+), 272.17 (M+Na), 520.92 (2M+Na).

Ethyl 5-methyl-2-p-tolylloxazole-4-carboxylate 3n [5]

Known compound. Yield: 62%. Yellow solid, mp 65-66 °C (lit. mp 67-68 °C). 1H NMR (300 MHz, CDCl3): δ (ppm) = 7.95 (d, J = 7.5 Hz, 2 H), 7.28-7.22 (m, 2 H), 4.43 (q, J = 7.2 Hz, 2 H), 2.69 (s, 3 H), 2.39 (s, 3 H), 1.41 (t, J = 7.2 Hz, 3 H); MS (ESI, positive) for C14H15NO3, found m/z: 246.17 (M+H+), 268.17 (M+Na), 513.00 (2M+Na).

Ethyl 2-(furan-2-yl)-5-methyloxazole-4-carboxylate 3o [5]

Known compound. Yield: 50%. Pale yellow solid, mp 76-78 °C (lit. mp 75-76 °C). 1H NMR (300 MHz, CDCl3): δ (ppm) = 7.57-7.54 (m, 1 H), 7.10-7.06 (m, 1 H), 6.56-6.50 (m, 1 H), 4.40 (q, J = 7.2 Hz, 2 H), 2.68 (s, 3 H), 1.40 (t, J = 7.2 Hz, 3 H); MS (ESI, positive) for C11H11NO3, found m/z: 222.17 (M+H+), 244.17 (M+Na), 464.92 (2M+Na).
Ethyl 2-(furan-2-yl)-5-propyloxazole-4-carboxylate $3p$ \(^{(3)}\)

Known compound. Yield: 56%. Yellow solid, mp 75-76 °C (lit. mp 77-78 °C). $^1$H NMR (300 MHz, CDCl$_3$): $\delta$ (ppm) = 7.58-7.52 (m, 1 H), 7.12-7.06 (m, 1 H), 6.56-6.50 (m, 1 H), 4.41 (q, $J = 7.2$ Hz, 2 H), 3.07 (t, $J = 7.5$ Hz, 2 H), 1.84-1.70 (m, 2 H), 1.40 (t, $J = 7.2$ Hz, 3 H), 1.00 (t, $J = 7.5$ Hz, 3 H);

MS (ESI, positive) for $C_{13}H_{15}NO_4$ found m/z: 250.17 (M+H), 272.17 (M+Na), 521.00 (2M+Na).

(Z)-ethyl 3-(benzylamino)but-2-enoate (intermediate 6) \(^{(7)}\)

Known compound. Oil. $^1$H NMR (300 MHz, CDCl$_3$): $\delta$ (ppm) = 8.96 (brs, 1 H, NH), 7.40-7.21 (m, 5 H), 4.54 (s, 1 H), 4.43 (d, $J = 6.3$ Hz, 2 H), 4.10 (q, $J = 7.2$ Hz, 2 H), 1.91 (s, 3 H), 1.26 (t, $J = 7.2$ Hz, 3 H);

$^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ (ppm) = 170.5, 161.7, 138.7, 128.7, 127.2, 126.6, 83.1, 58.3, 46.7, 19.3, 14.5; MS (ESI, positive) for $C_{13}H_{17}NO_2$, found m/z: 220.17 (M+H), 242.17 (M+Na).

References:

Part V. Copies of $^1$H NMR, $^{13}$C NMR and MS

$^1$H NMR of ethyl 5-isopropyl-2-phenyloxazole-4-carboxylate 3e
$^{13}$C NMR of ethyl 5-isopropyl-2-phenoxazole-4-carboxylate 3e
$^1$H NMR of (5-methyl-2-phenyloxazol-4-yl)(phenyl)methanone 3j

Electronic Supplementary Material (ESI) for Chemical Communications
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$^{13}$C NMR of (5-methyl-2-phenyloxazol-4-yl)(phenyl)methanone 3j
$^1$H NMR of ethyl 2-(4-chlorophenyl)-5-methyl-oxazole-4-carboxylate 3k
MS (ESI) of ethyl 2-(4-chlorophenyl)-5-methyl-4-carboxylate 3k
$^1$H NMR of intermediate 6
$^{13}\text{C}$ NMR of intermediate 6