Construction of Imidazoles and Pyrimidines via Palladium-catalyzed Decarboxylative Intramolecular Condensation of 1,2,4-Oxadiazol-5(4H)-ones
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1. General. NMR spectra were recorded on JEOL EX-400 spectrometer (400 MHz for \( ^1H \) NMR and 100 MHz for \( ^13C \) NMR) or JEOL AL-300 spectrometer (300 MHz for \( ^1H \) NMR and 75 MHz for \( ^13C \) NMR). Chemical shifts are reported in \( \delta \) ppm referenced to CDCl\(_3\) (\( \delta \) 7.26 for \( ^1H \) NMR and \( \delta \) 77.00 for \( ^13C \) NMR). Melting points (mp) are uncorrected. Elemental analyses were performed at Organic Elemental Analysis Research Center (Kyoto University). High-resolution mass spectra (HRMS) were measured with JEOL JMX-HX110A spectrometer. Toluene, CH\(_2\)Cl\(_2\) and THF were purified by passed through a neutral alumina column under argon atmosphere. 1,4-Dioxane was distilled over sodium and benzophenone under nitrogen. Oxadiazolone 1 [CAS 3201-46-5] was prepared according to the literature procedure.\(^1\) All other materials were purchased and used without further purification.

2. Detection of iminophosphorane.

\[
\begin{align*}
\text{Ph} & \quad \text{N} \quad \text{O} \\
\text{Me} & \quad \text{Pd(PPh}_3\text{)}_4 \quad (25 \text{ mol\%}) \\
& \quad \text{dioxane,} \quad 100 \^\circ \text{C,} \quad 4 \text{ h} \\
\end{align*}
\]

A solution of Pd(PPh\(_3\))\(_4\) (57.8 mg, 50 \( \mu \)mol) and oxadiazolone 1 (35.2 mg, 0.20 mmol) in 1,4-dioxane (1.5 mL) was stirred at 100 \( ^\circ \)C for 4 h. The reaction mixture was concentrated under vacuum. The generation of 2 was detected by \( ^1H\)/\( ^31P \) NMR and mass spectra (FAB, matrix; 3-nitrobenzyl alcohol). Characteristic peak for \( ^1H \) NMR (CDCl\(_3\)): \( \delta \) 2.96 (br s, 3H). \( ^31P \) NMR (CDCl\(_3\)): \( \delta \) 29.4. HRMS (FAB) calcd for C\(_{26}\)H\(_{34}\)N\(_2\)P (M+H\(^+\)) 395.1677, found 395.1674.

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$^1$H NMR spectrum of 1

$^1$H NMR spectrum of the crude mixture
$^{31}$P NMR spectrum of the crude mixture

Mass spectrum of the crude mixture
3. Preparation of Substrates.

The yields have not been optimized.

A typical procedure for the synthesis of oxadiazolone 3a is shown below.

4-(2-Oxo-2-phenylethyl)-3-phenyl-1,2,4-oxadiazol-5(4H)-one (3a)

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

A suspension of phenacyl bromide (597 mg, 3.00 mmol), 3-phenyl-1,2,4-oxadiazol-5(4H)-one (584 mg, 3.60 mmol), K\textsubscript{2}CO\textsubscript{3} (498 mg, 3.60 mmol) in acetone (10 mL) was stirred at 50 °C for 12 h. The reaction mixture was quenched with H\textsubscript{2}O and extracted with EtOAc three times. The combined organic was filtered through Celite, and the filtrate was concentrated under vacuum. The residue was subjected to column chromatography on silica gel (hexane/EtOAc = 3/1 to 1/1) to give 730 mg of 4-(2-oxo-2-phenylethyl)-3-phenyl-1,2,4-oxadiazol-5(4H)-one (3a; 2.60 mmol, 87% yield) as a pale yellow solid (mp 107.5–108.9 °C). \textsuperscript{1}H NMR (CDCl\textsubscript{3}): \(\delta\) 5.06 (s, 2H), 7.44–7.58 (m, 7H), 7.64 (t, \(J = 6.8\) Hz, 1H), 7.89 (d, \(J = 7.8\) Hz, 2H). \textsuperscript{13}C NMR (CDCl\textsubscript{3}): \(\delta\) 48.5, 123.0, 128.0, 128.1, 129.0, 129.4, 132.1, 133.5, 134.6. Elemental analysis calcd for C\textsubscript{16}H\textsubscript{12}N\textsubscript{2}O\textsubscript{3}, C: 68.56%; H: 4.32%, N: 9.99%; found C: 68.61%; H: 4.47%; N: 9.90%.

3-(4-Methoxyphenyl)-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4H)-one (3b)

\[
\begin{align*}
\text{MeO} & \quad \text{N} & \quad \text{O} \\
\text{N} & \quad \text{O} & \quad \text{Ph}
\end{align*}
\]

Oxadiazolone 3b was prepared according to the similar procedure to oxadiazolone 3a, starting from 692 mg of 3-(4-methoxyphenyl)-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 598 mg of phenacyl bromide (3.00 mmol). 913 mg, 2.94 mmol, 98% yield. An pale yellow solid (mp 132.3–133.2 °C). \textsuperscript{1}H NMR (CDCl\textsubscript{3}): \(\delta\) 3.82 (s, 3H), 5.05 (s, 2H), 6.96 (d, \(J = 8.8\) Hz, 2H), 7.45 (d, \(J = 8.8\)Hz, 2H), 7.52 (t, \(J = 7.8\) Hz, 2H), 7.65 (t, \(J = 7.3\) Hz, 1H), 7.91 (d, \(J = 8.3\) Hz, 2H). \textsuperscript{13}C NMR (CDCl\textsubscript{3}): \(\delta\) 48.4, 55.3, 114.8, 127.9, 128.9, 129.6, 133.4, 134.5, 158.9, 159.4, 162.3, 190.5. Elemental analysis calcd for C\textsubscript{17}H\textsubscript{14}N\textsubscript{2}O\textsubscript{4}, C: 65.80%; H: 4.55%, N: 9.03%; found C: 65.86%; H: 4.61%; N: 8.78%.

3-(4-Fluorophenyl)-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4H)-one (3c)
Oxadiazolone 3c was prepared according to the similar procedure to oxadiazolone 3a, starting from 649 mg of 3-(4-fluorophenyl)-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 598 mg of phenacyl bromide (3.00 mmol). 890 mg, 2.98 mmol, 99% yield. An pale yellow solid (mp 102.8–104.0 °C). $^1$H NMR (CDCl$_3$): $\delta$ 5.05 (s, 2H), 7.17 (t, $J$ = 7.3 Hz, 2H), 7.46–7.58 (m, 4H), 7.66 (t, $J$ = 7.3 Hz, 1H), 7.90 (d, $J$ = 7.3 Hz, 2H). $^{13}$C NMR (DMSO-$d_6$): $\delta$ 48.9, 116.6 ($J_{CF}$ = 22.3 Hz), 119.3 ($J_{CF}$ = 3.3 Hz), 128.3, 128.9, 130.9 ($J_{CF}$ = 9.1 Hz), 133.4, 134.6, 158.7, 158.9, 164.1 ($J_{CF}$ = 251 Hz), 192.1. Elemental analysis calcd for C$_{16}$H$_{11}$FN$_2$O$_3$, C: 64.43%; H: 3.72%, N: 9.39%; found C: 64.53%; H: 3.73%; N: 9.35%.

3-(4-Methoxycarbonylphenyl)-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4H)-one (3d)

Oxadiazolone 3d was prepared according to the similar procedure to oxadiazolone 3a, starting from 528 mg of 3-(4-methoxycarbonylphenyl)-1,2,4-oxadiazol-5(4H)-one (2.40 mmol) and 398 mg of phenacyl bromide (2.00 mmol). 338 mg, 1.00 mmol, 50% yield. An off-white solid (mp 108.3–109.1 °C). $^1$H NMR (CDCl$_3$): $\delta$ 3.92 (s, 3H), 5.06 (s, 2H), 7.50 (t, $J$ = 7.8 Hz, 2H), 7.62 (d, $J$ = 7.8 Hz, 2H), 7.65 (t, $J$ = 7.3 Hz, 1H), 7.88 (d, $J$ = 7.3 Hz, 2H), 8.13 (d, $J$ = 8.8 Hz, 2H). $^{13}$C NMR (CDCl$_3$): $\delta$ 48.5, 52.5, 127.1, 128.0, 128.2, 129.0, 130.4, 133.3, 133.4, 134.7, 158.4, 159.1, 165.6, 190.2. HRMS (FAB) calcd for C$_{18}$H$_{15}$N$_2$O$_5$ (M+H)$^+$ 339.0981, found 339.0978.

3-(4-Acetylphenyl)-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4H)-one (3e)

Oxadiazolone 3e was prepared according to the similar procedure to oxadiazolone 3a, starting from 449 mg of 3-(4-acetylphenyl)-1,2,4-oxadiazol-5(4H)-one (2.20 mmol) and 398 mg of phenacyl bromide (2.00 mmol). 549 mg, 1.70 mmol, 85% yield. A pale yellow solid (mp 106.1–107.2 °C). $^1$H NMR (DMSO-$d_6$): $\delta$ 2.58 (s, 3H), 5.48 (s, 2H), 7.54 (t, $J$ = 7.8 Hz, 2H), 7.70 (t, $J$ = 7.3 Hz, 1H), 7.79 (d, $J$ = 8.3 Hz, 2H), 7.98 (d, $J$ = 7.8 Hz, 2H), 8.06 (d, $J$ =
8.3 Hz, 2H). $^{13}$C NMR (DMSO-$d_6$): $\delta$ 26.8, 49.0, 126.8, 128.3, 128.5, 128.91, 128.93, 133.3, 134.6, 139.2, 158.86, 158.87, 192.0, 197.3. Elemental analysis calcd for C$_{18}$H$_{14}$N$_2$O$_4$, C: 67.08%; H: 4.38%; N: 8.69%; found C: 67.17%; H: 4.54%; N: 8.60%.

3-(3-Acetylphenyl)-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4$H$)-one (3f)

Oxadiazolone 3f was prepared according to the similar procedure to oxadiazolone 3a, starting from 490 mg of 3-(3-acetylphenyl)-1,2,4-oxadiazol-5(4$H$)-one (2.40 mmol) and 398 mg of phenacyl bromide (2.00 mmol). 561 mg, 1.74 mmol, 87% yield. A pale yellow solid (mp 102.0–103.0 °C). $^1$H NMR (DMSO-$d_6$): $\delta$ 2.55 (s, 3H), 5.44 (s, 2H), 7.54 (t, $J$ = 7.8 Hz, 2H), 7.70 (t, $J$ = 7.8 Hz, 2H), 7.87 (d, $J$ = 7.8 Hz, 1H), 7.97 (d, $J$ = 8.3 Hz, 2H), 8.11 (s, 1H), 8.15 (d, $J$ = 8.3 Hz, 1H). $^{13}$C NMR (DMSO-$d_6$): $\delta$ 26.6, 49.0, 123.3, 127.8, 128.3, 128.9, 129.9, 131.5, 132.4, 133.4, 134.6, 137.4, 158.9, 159.0, 192.2, 196.8. Elemental analysis calcd for C$_{18}$H$_{14}$N$_2$O$_4$, C: 67.08%; H: 4.38%; N: 8.69%; found C: 67.09%; H: 4.51%; N: 8.58%.

3-(2-Methylphenyl)-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4$H$)-one (3g)

Oxadiazolone 3g was prepared according to the similar procedure to oxadiazolone 3a, starting from 352 mg of 3-(2-methylphenyl)-1,2,4-oxadiazol-5(4$H$)-one (2.00 mmol) and 478 mg of phenacyl bromide (2.40 mmol). 582 mg, 1.98 mmol, 99% yield. An off-white solid (mp 114.5–116.0 °C). $^1$H NMR (CDCl$_3$): $\delta$ 2.42 (s, 3H), 4.86 (s, 2H), 7.25 (t, $J$ = 7.8 Hz, 1H), 7.28–7.35 (m, 2H), 7.40 (t, $J$ = 7.3 Hz, 1H), 7.46 (t, $J$ = 7.8 Hz, 2H), 7.61 (t, $J$ = 7.3 Hz, 1H), 7.82 (d, $J$ = 8.1 Hz, 2H). $^{13}$C NMR (CDCl$_3$): $\delta$ 19.3, 47.8, 122.1, 126.3, 127.9, 128.9, 129.3, 131.1, 131.8, 133.4, 134.5, 138.2, 158.7, 159.1, 189.9. Elemental analysis calcd for C$_{17}$H$_{14}$N$_2$O$_3$, C: 69.38%; H: 4.79%; N: 9.52%; found C: 69.55%; H: 4.86%; N: 9.28%.

3-(Naphthalen-2-yl)-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4$H$)-one (3h)
Oxadiazolone 3h was prepared according to the similar procedure to oxadiazolone 3a, starting from 764 mg of 3-(naphthalen-2-yl)-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 598 mg of phenacyl bromide (3.00 mmol). A pale yellow solid (954 mg, 2.89 mmol, 96% yield; mp 125.5–126.7 °C). \( ^1H \) NMR (CDCl\(_3\)): \( \delta \) 5.12 (s, 2H), 7.48 (t, \( J = 7.7 \) Hz, 2H), 7.50–7.66 (m, 4H), 7.88 (t, \( J = 8.0 \) Hz, 4H), 7.93 (d, \( J = 8.5 \) Hz, 1H), 8.07 (s, 1H). \( ^{13}C \) NMR (CDCl\(_3\)): \( \delta \) 48.6, 120.1, 123.5, 127.3, 127.8, 127.9, 128.3, 128.5, 128.9, 129.0, 129.4, 132.4, 133.3, 134.3, 134.5, 159.3, 159.4, 190.5. Elemental analysis calcd for C\(_{20}\)H\(_{14}\)N\(_2\)O\(_3\), C: 72.72%; H: 4.27%; N: 8.48%; found C: 72.78%; H: 4.32%; N: 8.39%.

4-(2-Oxo-2-phenylethyl)-3-(thophen-2-yl)-1,2,4-oxadiazol-5(4H)-one (3i)

Oxadiazolone 3i was prepared according to the similar procedure to oxadiazolone 3a, starting from 605 mg of 3-(2-thienyl)-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 598 mg of phenacyl bromide (3.00 mmol). A pale yellow solid (845 mg, 2.95 mmol, 98% yield; mp 101.0–102.5 °C). \( ^1H \) NMR (CDCl\(_3\)): \( \delta \) 5.21 (s, 2H), 7.13 (dd, \( J = 5.2, 3.9 \) Hz, 1H), 7.39 (d, \( J = 4.6 \) Hz, 1H), 7.54 (t, \( J = 7.7 \) Hz, 2H), 7.56 (d, \( J = 3.8 \) Hz, 1H), 7.69 (t, \( J = 7.4 \) Hz, 1H), 7.97 (d, \( J = 7.3 \) Hz, 2H). \( ^{13}C \) NMR (CDCl\(_3\)): \( \delta \) 48.7, 122.4, 128.0, 128.2, 129.1, 130.3, 130.7, 133.4, 134.7, 154.3, 159.0, 190.3. Elemental analysis calcd for C\(_{14}\)H\(_{10}\)N\(_2\)O\(_3\)S, C: 58.73%; H: 3.52%, N: 9.78%; found C: 58.95%; H: 3.73%; N: 9.80%.

4-(2-(4-Methoxyphenyl)-2-oxoethyl)-3-phenyl-1,2,4-oxadiazol-5(4H)-one (3j)
To a solution of 4’-methoxyacetophenone (300 mg, 2.00 mmol) in CH$_2$Cl$_2$ (4 mL) was added bromine (0.102 mL, 2.00 mmol) dropwise at room temperature, and the mixture was stirred at this temperature for 8 h. Then 3-phenyl-1,2,4-oxadiazol-5(4H)-one (584 mg, 3.60 mmol) and K$_2$CO$_3$ (498 mg, 3.60 mmol), acetone (5 mL) was added to the reaction mixture. After stirring at 50 °C for 12 h, the reaction mixture was quenched with H$_2$O and extracted with EtOAc three times. The combined organic layer was dried over MgSO$_4$, filtered, and concentrated under vacuum. The residue was subjected to column chromatography on silica gel (CH$_2$Cl$_2$/EtOAc = 4/1) to give 578 mg of compound 3j as a pale yellow oil (1.86 mmol, 93% yield). ¹H NMR (CDCl$_3$): δ 3.87 (s, 3H), 5.02 (s, 2H), 6.94 (d, $J = 8.8$ Hz, 2H), 7.46 (t, $J = 7.3$ Hz, 2H), 7.49–7.58 (m, 3H), 7.87 (d, $J = 8.8$ Hz, 2H). ¹³C NMR (CDCl$_3$): δ 47.7, 55.1, 113.8, 122.6, 125.9, 127.6, 128.9, 30.0, 131.6, 158.9, 159.0, 164.2, 188.3. HRMS (FAB) calcd for C$_{17}$H$_{15}$N$_2$O$_4$ (M+H)$^+$ 311.1032, found 311.1035.

4-(2-(4-Chlorophenyl)-2-oxoethyl)-3-phenyl-1,2,4-oxadiazol-5(4H)-one (3k)

Oxadiazolone 3k was prepared according to the similar procedure to oxadiazolone 3j, starting from 357 mg of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (2.20 mmol) and 309 mg of 4’-chloroacetophenone (2.00 mmol). 484 mg, 1.54 mmol, 77% yield. A pale yellow solid (mp 100.1–102.5 °C). ¹H NMR (CDCl$_3$): δ 5.03 (s, 2H), 7.47 (d, $J = 8.3$ Hz, 2H), 7.48–7.60 (m, 5H), 7.83 (d, $J = 8.3$ Hz, 2H). ¹³C NMR (CDCl$_3$): δ 48.4, 122.9, 128.1, 129.37, 129.40, 131.7, 132.1, 141.2, 159.1, 159.2, 189.3. Elemental analysis calcd for C$_{16}$H$_{11}$ClN$_2$O$_3$, C: 61.06%; H: 3.52%, N: 8.90%; found C: 60.84%; H: 3.53%; N: 8.74%.

4-(2-(4-Ethoxycarbonylphenyl)-2-oxoethyl)-3-phenyl-1,2,4-oxadiazol-5(4H)-one (3l)

Oxadiazolone 3l was prepared according to the similar procedure to oxadiazolone 3j, starting from 357 mg of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (2.20 mmol) and 384 mg of 4’-ethoxycarbonylacetophenone (2.00 mmol). 369 mg, 1.05 mmol, 52% yield. An pale
yellow oil. $^1$H NMR (CDCl$_3$): $\delta$ 1.41 (t, $J = 7.3$ Hz, 3H), 4.40 (q, $J = 7.3$ Hz, 2H), 5.13 (s, 2H), 7.26–7.60 (m, 5H), 7.95 (d, $J = 8.7$ Hz, 2H), 8.12 (d, $J = 8.7$ Hz, 2H). $^{13}$C NMR (CDCl$_3$): $\delta$ 14.1, 48.7, 61.6, 122.8, 127.9, 128.0, 129.4, 130.0, 132.1, 135.4, 136.4, 159.0, 159.2, 165.1, 190.2. HRMS (FAB) calcd for C$_{19}$H$_{17}$N$_2$O$_5$ (M+H)$^+$ 353.1137, found 353.1142.

4-(2-(2-Fluorophenyl)-2-oxoethyl)-3-phenyl-1,2,4-oxadiazol-5(4$H$)-one (3m)

Oxadiazolone 3m was prepared according to the similar procedure to oxadiazolone 3j, starting from 357 mg of 3-phenyl-1,2,4-oxadiazol-5(4$H$)-one (2.20 mmol) and 276 mg of 2'-fluoroacetophenone (2.00 mmol). 270 mg, 0.91 mmol, 45% yield. A pale yellow oil. $^1$H NMR (CDCl$_3$): $\delta$ 4.99 (d, $J = 3.4$ Hz, 2H), 7.18 (dd, $J = 11.2$, 8.8 Hz, 1H), 7.28 (t, $J = 7.8$ Hz, 1H), 7.43–7.65 (m, 6H), 7.93 (t, $J = 7.3$ Hz, 1H). $^{13}$C NMR (CDCl$_3$): $\delta$ 52.0 ($J_{CF} = 14.9$ Hz), 116.7 ($J_{CF} = 23.6$ Hz), 121.7 ($J_{CF} = 13.2$ Hz), 123.0, 125.1 ($J_{CF} = 3.3$ Hz), 126.0, 128.1, 129.4, 130.8, 132.1, 136.5 ($J_{CF} = 9.1$ Hz), 159.1 ($J_{CF} = 23.2$ Hz), 162.5 ($J_{CF} = 255$ Hz), 188.6 ($J_{CF} = 5.8$ Hz). HRMS (FAB) calcd for C$_{16}$H$_{12}$F$_2$N$_2$O$_3$ (M+H)$^+$ 299.0832, found 299.0838.

4-(2-(Benzofuran-2-yl)-2-oxoethyl)-3-phenyl-1,2,4-oxadiazol-5(4$H$)-one (3n)

Oxadiazolone 3n was prepared according to the similar procedure to oxadiazolone 3a, starting from 324 mg of 3-phenyl-1,2,4-oxadiazol-5(4$H$)-one (2.00 mmol) and 478 mg of 2-bromoacetylbenzofuran (2.00 mmol). 535 mg, 1.62 mmol, 84% yield. An off-white solid (mp 142.5–144.8 °C). $^1$H NMR (CDCl$_3$): $\delta$ 5.08 (s, 2H), 7.35 (t, $J = 7.8$ Hz, 1H), 7.45–7.62 (m, 7H), 7.63 (s, 1H), 7.73 (d, $J = 8.3$ Hz, 1H). $^{13}$C NMR (CDCl$_3$): $\delta$ 48.5, 112.5, 114.47, 114.48, 123.0, 123.7, 124.5, 126.5, 128.2, 129.3, 129.5, 132.2, 149.9, 155.8, 159.0, 181.7. Elemental analysis calcd for C$_{18}$H$_{12}$N$_2$O$_4$: C: 67.50%; H: 3.78%; N: 8.75%; found C: 67.49%; H: 4.02%; N: 8.54%.

4-(2-Oxopropyl)-3-phenyl-1,2,4-oxadiazol-5(4$H$)-one (3o)
Oxadiazolone 3o was prepared according to the similar procedure to oxadiazolone 3a, starting from 584 mg of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 0.252 mL of bromoacetone (3.00 mmol). 460 mg, 2.11 mmol, 70% yield. A white solid (mp 67.3–68.0 °C). 1H NMR (CDCl₃): δ 2.19 (s, 3H), 4.44 (s, 2H), 7.47 (d, J = 8.8 Hz, 2H), 7.52 (t, J = 8.1 Hz, 2H), 7.61 (t, J = 7.6 Hz, 1H). 13C NMR (acetone-d₆): δ 27.0, 52.1, 124.4, 129.0, 130.2, 132.8, 159.9, 160.1, 201.0. Elemental analysis calcd for C₁₁H₁₀N₂O₃, C: 60.55%; H: 4.62%, N: 12.84%; found C: 60.72%; H: 4.67%; N: 12.82%.

4-(2-Cyclohexyl-2-oxoethyl)-3-phenyl-1,2,4-oxadiazol-5(4H)-one (3p)

Oxadiazolone 3p was prepared according to the similar procedure to oxadiazolone 3a, starting from 584 mg of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 1.03 g of bromoacetylcylohexane (5.00 mmol). 368 mg, 1.29 mmol, 36% yield. A pale yellow oil. 1H NMR (CDCl₃): δ 1.15–1.37 (m, 5H), 1.60–1.78 (m, 5H), 2.34–2.39 (m, 1H), 4.46 (s, 2H), 7.46 (d, J = 8.3 Hz, 2H), 7.51 (t, J = 7.8 Hz, 2H), 7.59 (t, J = 7.3 Hz, 1H). 13C NMR (CDCl₃): δ 25.1, 25.3, 27.9, 48.1, 49.1, 123.0, 128.1, 129.3, 132.0, 158.9, 159.2, 204.3. HRMS (FAB) calcd for C₁₆H₁₉N₂O₃ (M+H)+ 287.1396, found 287.1389.

4-(3,3-Dimethyl-2-oxobutyl)-3-phenyl-1,2,4-oxadiazol-5(4H)-one (3q)

Oxadiazolone 3q was prepared according to the similar procedure to oxadiazolone 3a, starting from 584 mg of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 0.404 mL of bromopinacolone (3.00 mmol). 624 mg, 0.160 mmol, 80% yield. A white solid (mp 60.8–61.8 °C). 1H NMR (CDCl₃): δ 1.10 (s, 9H), 4.55 (s, 2H), 7.46 (d, J = 7.3 Hz, 2H), 7.51 (t, J = 7.3 Hz, 2H), 7.58 (t, J = 7.3 Hz, 1H). 13C NMR (CDCl₃): δ 25.8, 43.1, 46.7, 123.1, 128.2, 129.3, 132.1, 159.1, 159.3, 206.3. Elemental analysis calcd for C₁₄H₁₆N₂O₃, C: 64.60%; H: 6.20%, N: 10.76%; found C: 64.77%; H: 6.42%; N: 10.74%.
3-Cyclohexyl-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4H)-one (3r)

Oxadiazolone 3r was prepared according to the similar procedure to oxadiazolone 3a, starting from 605 mg of 3-cyclohexyl-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 597 mg of phenacyl bromide (3.00 mmol). 800 mg, 2.79 mmol, 93% yield. A white solid (mp 94.1–96.2 °C). \(^1\)H NMR (CDCl\(_3\)): \(\delta\) 1.18–1.30 (m, 3H), 1.50–2.00 (m, 7H), 2.27 (tt, \(J = 11.2, 3.4\) Hz, 1H), 5.01 (s, 2H), 7.55 (t, \(J = 6.8\) Hz, 2H), 7.69 (t, \(J = 7.3\) Hz, 1H), 7.99 (d, \(J = 7.3\) Hz, 2H). \(^1^3\)C NMR (CDCl\(_3\)): \(\delta\) 25.3, 25.4, 29.6, 34.9, 47.6, 128.1, 129.2, 133.6, 134.8, 159.4, 162.7, 190.2. Elemental analysis calcd for C\(_{16}\)H\(_{18}\)N\(_2\)O\(_3\), C: 67.12%; H: 6.34%, N: 9.78%; found C: 66.92%; H: 6.28%; N: 9.76%.

3-Isopropyl-4-(2-oxo-2-phenylethyl)-1,2,4-oxadiazol-5(4H)-one (3s)

Oxadiazolone 3s was prepared according to the similar procedure to oxadiazolone 3a, starting from 461 mg of 3-isopropyl-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 597 mg of phenacyl bromide (3.00 mmol). 738 mg, 3.00 mmol, 100% yield. A pale yellow solid (mp 51.3–53.0 °C). \(^1\)H NMR (CDCl\(_3\)): \(\delta\) 1.32 (d, \(J = 6.8\) Hz, 6H), 2.62 (d, \(J = 6.8\) Hz, 1H), 5.03 (s, 2H), 7.55 (t, \(J = 7.8\) Hz, 2H), 7.69 (t, \(J = 7.6\) Hz, 1H), 7.98 (d, \(J = 7.3\) Hz, 2H). \(^1^3\)C NMR (CDCl\(_3\)): \(\delta\) 19.2, 25.7, 47.6, 128.0, 129.1, 133.5, 134.7, 159.5, 163.5, 190.2. Elemental analysis calcd for C\(_{13}\)H\(_{14}\)N\(_2\)O\(_3\), C: 63.40%; H: 5.73%, N: 11.38%; found C: 63.65%; H: 5.78%; N: 11.15%.

3-Phenyl-4-(2-oxo-1,2-diphenylethyl)-1,2,4-oxadiazol-5(4H)-one (3t)

Oxadiazolone 3t was prepared according to the similar procedure to oxadiazolone 3a, starting from 584 mg of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 825 mg of 2-bromo-1,2-diphenylethanone (3.00 mmol). 237 mg, 0.66 mmol, 22% yield. A white
solid (mp 168.5–169.6 °C).  

\[
\begin{align*}
\text{\( ^1H \) NMR (CDCl}_3): \delta & \ 6.71 \ (s, \ 1H), \ 6.89 \ (d, \ J = 7.4 \ Hz, \ 2H), \ 7.09 \\
& \ (t, \ J = 7.3 \ Hz, \ 2H), \ 7.13–7.40 \ (m, \ 8H), \ 7.53 \ (t, \ J = 7.3 \ Hz, \ 1H), \ 7.79 \ (d, \ J = 8.7 \ Hz, \ 2H). \ \\
\text{\( ^{13}C \) NMR (CDCl}_3): \delta & \ 64.2, \ 123.6, \ 127.3, \ 128.2, \ 128.8, \ 129.1, \ 129.6, \ 129.8, \ 130.9, \ 132.0, \\
& \ 133.8, \ 134.2, \ 159.1, \ 159.7, \ 192.5. \ \\
\text{Elemental analysis calcd for } & \ C_{22}H_{16}N_2O_3, \ C: 74.15%; \ H: 4.53%, \ N: 7.86%; \text{ found } C: 74.37%; \ H: 4.69%; \ N: 7.60%.
\end{align*}
\]

Bis(oxadiazolone) 3u

\[
\text{Oxadiazolone 3u was prepared according to the similar procedure to oxadiazolone 3a, starting from 778 mg of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (4.80 mmol) and 640 mg of 1,1'-(1,4-phenylene)bis(2-bromoethan-1-one) (2.00 mmol). 642 mg, 1.33 mmol, 67% yield.}
\]

A white solid (mp 117.0–118.0 °C).  

\[
\begin{align*}
\text{\( ^1H \) NMR (CDCl}_3): \delta & \ 5.06 \ (s, \ 4H), \ 7.42–7.60 \ (m, \ 10H), \\
& \ 7.98 \ (s, \ 4H). \ \\
\text{\( ^{13}C \) NMR (CDCl}_3): \delta & \ 48.7, \ 122.9, \ 128.1, \ 128.7, \ 129.5, \ 132.3, \ 137.6, \ 158.9, \\
& \ 159.2, \ 189.8. \ \\
\text{HRMS (FAB) calcd for } & \ C_{26}H_{19}N_4O_6 (M+H)^+ 483.1305, \text{ found 483.1304.}
\end{align*}
\]

Bis(oxadiazolone) 3v

\[
\text{Oxadiazolone 3v was prepared according to the similar procedure to oxadiazolone 3a, starting from 584 mg of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (3.60 mmol) and 480 mg of 1,1'-(1,3-phenylene)bis(2-bromoethan-1-one) (1.50 mmol). 304 mg, 0.63 mmol, 42% yield.}
\]

A white solid (mp 135.0 °C (decomp.)).  

\[
\begin{align*}
\text{\( ^1H \) NMR (CDCl}_3): \delta & \ 5.08 \ (s, \ 4H), \ 7.45–7.61 \ (m, \ 10H), \\
& \ 7.66 \ (t, \ J = 7.8 \ Hz, \ 1H), \ 8.14 \ (dd, \ J = 8.2, \ 1.8 \ Hz, \ 2H), \ 7.83 \ (t, \ J = 1.8 \ Hz, \ 1H). \ \\
\text{\( ^{13}C \) NMR (CDCl}_3): \delta & \ 48.7, \ 122.8, \ 127.6, \ 128.1, \ 129.5, \ 130.1, \ 132.3, \ 133.5, \ 134.1, \ 159.1, \ 159.3, \\
& \ 189.7. \ \\
\text{Elemental analysis calcd for } & \ C_{26}H_{18}N_4O_6, \ C: 64.73%; \ H: 3.76%, \ N: 11.61%; \text{ found C: 64.47%; H: 3.76%; N: 11.46%}
\end{align*}
\]

\((E)-4-(3-Oxo-3-phenylprop-1-en-1-yl)-3-phenyl-1,2,4-oxadiazol-5(4H)-one (5)\)
A solution of ethynyl phenyl ketone (130 mg, 1.00 mmol), 3-phenyl-1,2,4-oxadiazol-5(4H)-one (195 mg, 1.20 mmol), Et$_3$N (0.167 mL, 1.20 mmol) in EtOH (5 mL) was stirred at 50 °C for 18 h. The reaction mixture was concentrated under vacuum. The residue was subjected to column chromatography on silica gel (hexane/EtOAc = 6/1) to give 215 mg of compound 5 as a pale yellow solid (0.74 mmol, 74% yield; mp 180.0–181.3 °C). $^1$H NMR (CDCl$_3$): $\delta$ 7.51 (t, $J = 7.8$ Hz, 1H), 7.59 (d, $J = 14.2$ Hz, 1H), 7.61–7.75 (m, 6H), 8.01 (d, $J = 8.3$ Hz, 2H), 8.17 (d, $J = 13.7$ Hz, 1H). $^{13}$C NMR (DMSO-$d_6$): $\delta$ 112.2, 121.8, 128.1, 129.1, 129.3, 129.5, 132.4, 132.6, 133.7, 136.7, 155.5, 157.6, 188.5. HRMS (FAB) calcd for C$_{17}$H$_{13}$N$_2$O$_3$ (M+H)$^+$ 293.0926, found 293.0924.

3. Palladium-catalyzed synthesis of imidazoles and pyrimidines.

A typical procedure for the reaction of oxadiazolone 3a affording imidazole 4a is shown below.

**2,4-Diphenyl-1H-imidazole (4a) [CAS 670-83-7]**

A solution of Pd(PPh$_3$)$_4$ (6.9 mg, 6.0 μmol) and oxadiazolone 3a (56.1 mg, 0.20 mmol) in 1,4-dioxane (1.5 mL) was stirred at 80 °C for 24 h. The reaction mixture was filtered through a pad of Florisil® and the filtrate was concentrated under vacuum. The residue was subjected to column chromatography on Florisil® (hexane/EtOAc = 4/1) to afford 43.8 mg of 4a (0.20 mmol, 99% yield) as a white solid (mp 160.1–160.5 °C). $^1$H NMR (CDCl$_3$): $\delta$ 7.22–7.45 (m, 7H), 7.75 (d, $J = 7.4$ Hz, 2H), 7.87 (d, $J = 7.3$ Hz, 2H). $^{13}$C NMR (acetone-$d_6$): $\delta$ 114.3, 125.4, 125.9, 127.2, 129.0, 129.3, 131.8, 135.6, 142.6, 147.4. HRMS (FAB) calcd for C$_{15}$H$_{13}$N$_2$ (M+H)$^+$ 221.1079, found 221.1069.

**2-(4-Methoxyphenyl)-4-phenyl-1H-imidazole (4b) [CAS 25206-04-6]**

A white solid (42.4 mg, 0.17 mmol, 85% yield; mp 98.0–99.0 °C). $^1$H NMR (CDCl$_3$): $\delta$ 3.83 (s, 3H), 6.93 (d, $J = 8.8$ Hz, 2H), 7.25 (t, $J = 7.3$ Hz, 1H), 7.33 (s, 1H), 7.38 (t, $J = 7.8$ Hz,
2-(4-Fluorophenyl)-4-phenyl-1H-imidazole (4c)

A white solid (46.0 mg, 0.19 mmol, 97% yield; mp 65.0–66.1 °C). ¹H NMR (CDCl₃): δ 7.08 (dd, Jₕₕ = 8.8 Hz and Jₕᵣ = 8.8 Hz, 2H), 7.27 (t, J = 7.3 Hz, 1H), 7.37 (s, 1H), 7.39 (t, J = 7.3 Hz, 2H), 7.74 (d, J = 7.3 Hz, 2H), 7.82 (dd, Jₕₙ = 8.3 Hz and Jₙᵣ = 4.9 Hz, 2H). ¹³C NMR (CDCl₃): δ 115.7 (d, Jₙᵣ = 21.7 Hz), 117.7, 125.0, 126.4 (d, Jₙᵣ = 3.1 Hz), 127.2, 127.3, 127.5 (d, Jₙᵣ = 8.0 Hz), 128.8, 132.4, 146.7, 163.0 (d, Jₙᵣ = 248 Hz). HRMS (FAB) calcd for C₁₆H₁₅N₂O (M+H)+ 251.1184, found 251.1181.

2-(4-Methoxycarbonylphenyl)-4-phenyl-1H-imidazole (4d)

A white solid (56.5 mg, 0.20 mmol, 98% yield; mp 68.8–69.7 °C). ¹H NMR (CDCl₃): δ 3.94 (s, 3H), 7.26 (t, J = 8.8 Hz, 1H), 7.40–7.60 (m, 4H), 7.78 (br s, 1H), 7.97 (d, J = 8.3 Hz, 2H), 8.08 (d, J = 8.8 Hz, 2H), 9.94 (br s, 1H). ¹³C NMR (acetone-d₆): δ 52.1, 115.6, 125.3, 125.5, 127.2, 128.1, 130.0, 130.4, 132.7, 134.6, 135.5, 146.0, 166.6. HRMS (FAB) calcd for C₁₇H₁₅N₂O₂ (M+H)+ 279.1134, found 279.1125.

2-(4-Acetylphenyl)-4-phenyl-1H-imidazole (4e)

A pale yellow solid (50.0 mg, 0.19 mmol, 95% yield; mp 154.3–155.2 °C). ¹H NMR (CDCl₃): δ 2.61 (s, 3H), 7.29 (t, J = 7.8 Hz, 1H), 7.40 (t, J = 7.8 Hz, 2H), 7.44 (s, 1H), 7.77 (d, J = 7.3 Hz, 2H), 7.97 (s, 4H). ¹³C NMR (CDCl₃): δ 26.6, 118.7, 125.0, 125.3, 127.4, 128.8, 128.9, 132.1, 134.3, 136.4, 139.7, 146.0, 198.1. HRMS (FAB) calcd for C₁₇H₁₅N₂O (M+H)+ 263.1184, found 263.1187.

2-(3-Acetylphenyl)-4-phenyl-1H-imidazole (4f)
A white solid (42.6 mg, 0.16 mmol, 81% yield; mp 182.5–185.0 °C). $^1$H NMR (CDCl$_3$): $\delta$ 2.65 (s, 3H), 7.26 (t, $J = 6.8$ Hz, 1H), 7.41 (t, $J = 7.3$ Hz, 2H), 7.44 (s, 1H), 7.55 (t, $J = 7.3$ Hz, 1H), 7.78 (br d, $J = 7.3$ Hz, 1H), 7.94 (d, $J = 7.3$ Hz, 1H), 8.21 (d, $J = 7.3$ Hz, 1H), 8.47 (s, 1H). $^{13}$C NMR (acetone-$d_6$): $\delta$ 26.6, 125.2, 125.3, 127.1, 128.4, 129.1, 129.7, 130.0, 132.0, 135.5, 138.5, 142.9, 146.3, 197.6. HRMS (FAB) calcd for C$_{17}$H$_{15}$N$_2$O (M+H)$^+$ 263.1184, found 263.1185.

2-(2-Methylphenyl)-4-phenyl-1H-imidazole (4g)

A pale red solid (41.5 mg, 0.18 mmol, 89% yield; mp 74.5–75.5 °C). $^1$H NMR (CDCl$_3$): $\delta$ 2.58 (s, 3H), 7.10–7.17 (m, 5H), 7.37 (s, 1H), 7.39 (t, $J = 7.8$ Hz, 2H), 7.58 (d, $J = 7.3$ Hz, 1H), 7.67 (br d, $J = 5.4$ Hz, 1H), 9.41 (br s, 1H). $^{13}$C NMR (CDCl$_3$): $\delta$ 20.7, 116.1, 124.8, 125.7, 126.8, 128.6, 128.7, 128.9, 130.1, 130.9, 132.9, 136.5, 138.6, 147.3. HRMS (FAB) calcd for C$_{16}$H$_{15}$N$_2$ (M+H)$^+$ 235.1235, found 235.1232.

2-(Naphthalen-2-yl)-4-phenyl-1H-imidazole (4h)

A pale yellow solid (51.6 mg, 0.19 mmol, 95% yield; mp 190.6–193.5 °C). $^1$H NMR (CDCl$_3$): $\delta$ 7.28 (t, $J = 7.3$ Hz, 1H), 7.36–7.52 (m, 5H), 7.74–7.85 (m, 4H), 7.88 (d, $J = 8.3$ Hz, 1H), 8.03 (d, $J = 8.8$ Hz, 1H), 8.31 (s, 1H). $^{13}$C NMR (acetone-$d_6$): $\delta$ 116.7, 124.1, 124.2, 125.3, 126.8, 127.0, 127.2, 128.4, 128.7, 128.95, 129.04, 129.1, 133.9, 134.1, 134.8, 141.2, 147.2. HRMS (FAB) calcd for C$_{19}$H$_{15}$N$_2$ (M+H)$^+$ 271.1235, found 271.1230.

4-Phenyl-2-(thiophen-2-yl)-1H-imidazole (4i)

A white solid (30.1 mg, 0.13 mmol, 67% yield; mp 168.5–171.0 °C). $^1$H NMR (CDCl$_3$): $\delta$ 7.08 (dd, $J = 5.1$, 3.9 Hz, 1H), 7.27 (t, $J = 7.3$ Hz, 1H), 7.34 (d, $J = 5.1$ Hz, 1H), 7.35 (s, 1H), 7.39 (d, $J = 8.1$ Hz, 2H), 7.41 (d, $J = 3.7$ Hz, 1H), 7.72 (br s, 2H). $^{13}$C NMR (acetone-$d_6$): $\delta$ 116.4, 124.1, 125.2, 126.3, 127.0, 128.2, 129.0, 134.4, 135.2, 140.5, 143.1. HRMS (FAB) calcd for C$_{13}$H$_{11}$N$_2$S (M+H)$^+$ 227.0643, found 227.0639.

4-(4-Methoxyphenyl)-2-phenyl-1H-imidazole (4j)

S15
A pale yellow solid (35.0 mg, 0.14 mmol, 70% yield; mp 124.3–126.2 °C).  $^1$H NMR (CDCl$_3$): δ 3.84 (s, 3H), 6.93 (d, $J = 8.8$ Hz, 2H), 7.27 (d, $J = 8.5$ Hz, 2H), 7.35 (t, $J = 7.6$ Hz, 1H), 7.42 (t, $J = 7.8$ Hz, 2H), 7.67 (d, $J = 8.5$ Hz, 2H), 7.87 (d, $J = 7.1$ Hz, 2H).  $^{13}$C NMR (acetone-$d_6$): δ 55.3, 114.6, 125.7, 125.8, 126.6, 128.7, 129.3, 129.9, 131.1, 131.8, 146.9, 159.4.  HRMS (FAB) calcd for C$_{16}$H$_{15}$N$_2$O (M+H)$^+$ 251.1184, found 251.1181.

4-(4-Chlorophenyl)-2-phenyl-1H-imidazole (4k)

A pale yellow solid (46.0 mg, 0.18 mmol, 90% yield; mp 69.1–69.9 °C).  $^1$H NMR (CDCl$_3$): δ 7.32–7.40 (m, 4H), 7.43 (t, $J = 7.8$ Hz, 2H), 7.72 (br d, $J = 8.3$ Hz, 2H), 7.86 (d, $J = 8.3$ Hz, 2H).  $^{13}$C NMR (acetone-$d_6$): δ 116.3, 125.9, 127.0, 129.1, 129.3, 129.5, 131.6, 132.1, 134.2, 140.6, 147.5.  HRMS (FAB) calcd for C$_{15}$H$_{12}$ClN$_2$ (M+H)$^+$ 255.0689, found 255.0680.

4-(4-Ethoxycarbonylphenyl)-2-phenyl-1H-imidazole (4l)

37.4 mg of 3l (0.106 mmol) was reacted under the downscaled conditions.  A white solid (29.6 mg, 0.101 mmol, 95% yield; 199.5–201.0 °C).  $^1$H NMR (acetone-$d_6$): δ 1.36 (t, $J = 7.3$ Hz, 3H), 4.34 (q, $J = 7.3$ Hz, 2H), 7.38 (t, $J = 7.8$ Hz, 1H), 7.48 (t, $J = 7.3$ Hz, 2H), 7.82 (br s, 1H), 7.90–8.05 (m, 4H), 8.08 (d, $J = 8.3$ Hz, 2H), 12.0 (br s, 1H).  $^{13}$C NMR (acetone-$d_6$): δ 14.6, 61.2, 116.1, 125.2, 126.0, 129.0, 129.3, 129.5, 130.5, 131.5, 140.4, 141.8, 147.8, 166.7.  HRMS (FAB) calcd for C$_{18}$H$_{17}$N$_2$O$_2$ (M+H)$^+$ 293.1290, found 293.1284.

4-(2-Fluorophenyl)-2-phenyl-1H-imidazole (4m)

S16
A pale yellow solid (54.7 mg, 0.18 mmol, 92% yield; mp 122.2–124.0 °C).  \(^1\)H NMR (CDCl\(_3\)): \(\delta \) 7.08–7.25 (m, 3H), 7.32–7.42 (m, 3H), 7.54 (dd, \(J \) = 7.3, 2.7 Hz, 1H), 7.74 (td, \(J \) = 6.1, 2.4 Hz, 2H), 8.08 (br s, 1H).  \(^{13}\)C NMR (acetone-\(d_6\)): \(\delta \) 115.9 (d, \(J \) = 21.4 Hz), 124.9 (d, \(J \) = 3.3 Hz), 125.8, 128.1 (d, \(J \) = 8.2 Hz), 128.2, 129.0, 129.3, 131.4, 132.5 (d, \(J \) = 9.9 Hz), 146.8, 159.0, 161.5.  HRMS (FAB) calcd for C\(_{15}\)H\(_{12}\)F\(_2\)N (M+H)\(^+\) 239.0985, found 239.0981.

4-(Benzofuran-2-yl)-2-phenyl-1\(H\)-imidazole (4n)

A yellow solid (42.6 mg, 0.16 mmol, 82% yield; mp 198.1–199.0 °C).  \(^1\)H NMR (CDCl\(_3\)): \(\delta \) 7.10 (s, 1H), 7.21 (t, \(J \) = 7.4 Hz, 1H), 7.26 (t, \(J \) = 7.3 Hz, 1H), 7.38 (t, \(J \) = 7.4 Hz, 1H), 7.42–7.51 (m, 3H), 7.60 (d, \(J \) = 7.3 Hz, 1H), 7.69 (s, 1H), 8.08 (d, \(J \) = 7.3 Hz, 2H).  \(^{13}\)C NMR (CDCl\(_3\)): \(\delta \) 100.8, 111.4, 118.0, 121.5, 123.7, 124.5, 126.2, 129.5, 129.6, 130.2, 131.3, 133.6, 148.2, 153.2, 155.2.  HRMS (FAB) calcd for C\(_{17}\)H\(_{12}\)N\(_2\)O (M+) 260.0951, found 260.0949.

4-Methyl-2-phenyl-1\(H\)-imidazole (4o)

A white solid (29.7 mg, 0.19 mmol, 94% yield; mp 180.5–181.6 °C).  \(^1\)H NMR (CDCl\(_3\)): \(\delta \) 2.29 (s, 3H), 6.82 (s, 1H), 7.31 (t, \(J \) = 6.4 Hz, 1H), 7.37 (t, \(J \) = 6.8 Hz, 2H), 7.81 (d, \(J \) = 7.8 Hz, 2H).  \(^{13}\)C NMR (CDCl\(_3\)): \(\delta \) 12.0, 119.4, 125.0, 128.2, 128.8, 130.4, 132.1, 146.0.  HRMS (FAB) calcd for C\(_{10}\)H\(_{11}\)N\(_2\) (M+H)\(^+\) 159.0922, found 159.0923.

4-Cyclohexyl-2-phenyl-1\(H\)-imidazole (4p)

A colorless oil (38.1 mg, 0.17 mmol, 84% yield).  \(^1\)H NMR (CDCl\(_3\)): \(\delta \) 1.15–1.45 (m, 5H), 1.64–1.81 (m, 3H), 1.95–2.08 (m, 2H), 2.55–2.62 (m, 1H), 7.28 (t, \(J \) = 7.3 Hz, 1H), 7.34 (t, \(J \) = 6.8 Hz, 2H), 7.81 (d, \(J \) = 6.8 Hz, 2H), 10.10 (br s, 1H).  \(^{13}\)C NMR (CDCl\(_3\)): \(\delta \) 26.0, 26.2, 33.0, 36.0, 118.5, 125.3, 128.1, 128.6, 130.5, 142.8, 145.8.  HRMS (FAB) calcd for C\(_{16}\)H\(_{19}\)N\(_2\) (M+H)\(^+\) 227.1548, found 227.1542.

4-\(\text{tert}\)-Butyl-2-phenyl-1\(H\)-imidazole (4q)
A white solid (32.0 mg, 0.16 mmol, 80% yield; mp 57.5–58.8 °C). $^1$H NMR (CDCl$_3$): $\delta$ 1.35 (s, 9H), 6.83 (s, 1H), 7.32 (t, $J$ = 7.3 Hz, 1H), 7.39 (t, $J$ = 7.6 Hz, 2H), 7.79 (d, $J$ = 7.6 Hz, 2H). $^{13}$C NMR (acetone-$d_6$): $\delta$ 30.3, 31.7, 115.8, 125.5, 128.3, 129.1, 131.9, 145.9, 149.0. HRMS (FAB) calcd for C$_{13}$H$_{17}$N$_2$ (M+H)$^+$ 201.1392, found 201.1395.

2-Cyclohexyl-4-phenyl-1H-imidazole (4r)

A pale yellow oil (27.4 mg, 0.12 mmol, 61% yield). $^1$H NMR (CDCl$_3$): $\delta$ 1.20–1.60 (m, 5H), 1.66–1.89 (m, 3H), 2.10 (br d, $J$ = 11.2 Hz, 2H), 2.80 (tt, $J$ = 11.7, 3.4 Hz, 1H), 7.19 (s, 1H), 7.22 (t, $J$ = 7.3 Hz, 1H), 7.35 (t, $J$ = 7.8 Hz, 2H), 7.66 (br s, 2H). $^{13}$C NMR (CDCl$_3$): $\delta$ 25.8, 26.0, 32.0, 38.0, 115.3, 124.7, 126.6, 128.6, 133.1, 137.3, 153.6. HRMS (FAB) calcd for C$_{15}$H$_{19}$N$_2$ (M+H)$^+$ 227.1548, found 227.1542.

2-Isopropyl-4-phenyl-1H-imidazole (4s)

A pale red solid (27.7 mg, 0.15 mmol, 75% yield; mp 169.8–172.5 °C). $^1$H NMR (CDCl$_3$): $\delta$ 1.38 (d, $J$ = 7.1 Hz, 6H), 3.14 (sept, $J$ = 6.8 Hz, 1H), 7.20 (s, 1H), 7.22 (t, $J$ = 7.3 Hz, 1H), 7.36 (t, $J$ = 7.6 Hz, 2H), 7.67 (br d, $J$ = 6.8 Hz, 2H). $^{13}$C NMR (acetone-$d_6$): $\delta$ 21.8, 28.9, 114.1, 125.0, 126.4, 128.6, 128.9, 135.4, 154.3. HRMS (FAB) calcd for C$_{12}$H$_{15}$N$_2$ (M+H)$^+$ 187.1235, found 187.1237.

2,4,5-Triphenyl-1H-imidazole (4t)

37.4 mg of 3l (0.106 mmol) was reacted under the downscaled conditions. A white solid (55.0 mg, 0.19 mmol, 93% yield; mp 272.3–273.5 °C). $^1$H NMR (DMSO-$d_6$): $\delta$ 7.21 (t, $J$ = 6.8 Hz, 1H), 7.30 (t, $J$ = 7.8 Hz, 2H), 7.37 (t, $J$ = 6.8 Hz, 2H), 7.40–7.49 (m, 6H), 7.53 (t, $J$ = 8.8 Hz, 2H), 8.07 (d, $J$ = 8.3 Hz, 2H), 12.68 (br s, 1H). $^{13}$C NMR (DMSO-$d_6$): $\delta$ 125.2, 126.5, 126.8, 127.1, 127.5, 127.7, 128.2, 128.3, 128.5, 128.6, 130.3, 131.1, 135.2, 137.1, 145.5. HRMS (FAB) calcd for C$_{21}$H$_{17}$N$_2$ (M+H)$^+$ 297.1392, found 297.1393.

Bisimidazole 4u
A solution of CpPd(η³-C₃H₅) (1.3 mg, 6.1 μmol), tppms (88.9 mg, 0.244 mmol), and oxadiazolone 3u (48.2 mg, 0.10 mmol) in 1,4-dioxane (1.5 mL) was stirred at 80 °C for 90 h. The reaction mixture was filtered through a pad of Florisil® and the filtrate was concentrated under vacuum. The residue was subjected to column chromatography on Florisil® (CH₂Cl₂/acetone = 4/1) to afford 29.3 mg of 4u (80.8 mmol, 81% yield) as a white solid (mp >300 °C). ¹H NMR (DMSO-d₆): δ 7.36 (t, J = 7.3 Hz, 2H), 7.47 (t, J = 7.9 Hz, 4H), 7.74 (br s, 2H), 7.87 (s, 4H), 8.03 (d, J = 8.0 Hz, 4H), 12.64 (br s, 2H). ¹³C NMR (DMSO-d₆): δ 114.3, 124.5, 124.9, 128.0, 128.7, 130.6, 132.5, 141.0, 146.0. HRMS (FAB) calcd for C₂₄H₁₉N₄ (M+H)+ 363.1610, found 363.1601.

**Bisimidazole 4v**

Imidazole 4v was prepared according to the similar procedure to 4u. A yellow solid (34.7 mg, 95.7 μmol, 96% yield; mp 157.2–158.8 °C). ¹H NMR (DMSO-d₆): δ 7.32–7.42 (m, 4H), 7.48 (t, J = 6.8 Hz, 4H), 7.70 (br d, J = 6.8 Hz, 2H), 7.78 (br s, 1H), 8.04 (d, J = 7.8 Hz, 4H), 8.31 (s, 1H), 12.68 (br s, 2H). ¹³C NMR (DMSO-d₆): δ 114.4, 120.4, 122.6, 125.0, 125.2, 128.1, 128.2, 128.7, 130.6, 134.7, 146.0. HRMS (FAB) calcd for C₂₄H₁₉N₄ (M+H)+ 363.1610, found 363.1611.

**1,3-Diphenylpyrimidine (6)**

A pale yellow oil (34.2 mg, 0.14 mmol, 70% yield). ¹H NMR (CDCl₃): δ 7.44–7.58 (m, 6H), 7.61 (d, J = 5.1 Hz, 1H), 8.20–8.28 (m, 2H), 8.55–8.62 (m, 2H), 8.85 (d, J = 5.1 Hz, 1H). ¹³C NMR (CDCl₃): δ 114.5, 127.2, 128.3, 128.5, 128.9, 130.7, 130.9, 136.9, 137.8, 157.8, 163.8, 164.6. HRMS (FAB) calcd for C₁₆H₁₃N₂ (M+H)+ 233.1079, found 233.1073.