Supporting Information for:

Base-Mediated Regioselective [3 + 2] Annulation of Ketenimines and Isocyanides: Efficient Synthesis of 1,4,5-Trisubstituted Imidazoles

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1. General information
All chemicals which are commercially available were used without further purification unless otherwise noted. Thin-layer chromatography (TLC) was performed on silica gel plates (60F-254) using UV-light (254 and 365 nm). Flash column chromatography was conducted on silica gel (300-400 mesh). ^1H NMR and ^13C NMR spectra were recorded at 25 °C on a Varian 500 MHz and 125 MHz, respectively, and TMS as internal standard. Chemical shifts were reported in parts per million (ppm). High-resolution mass spectra (HRMS) were obtained using a Bruker microTOF II focus spectrometer (ESI). Melting points of all compounds were measured with a micro melting point apparatus. The compound ith dimension 0.21 × 0.19 × 0.16 mm, was glued on a glass fiber. Data were collected at 283 K using graphite-monochromated Mo Kα radiation (λ = 0.71073Å) and Bruker APEX CCD area-detector in the range 3.090<θ<25.00.

2. Synthetic procedures of ketenimines 1
Ketenimines 1 were synthesized by following previously reported procedures.1–5

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\begin{align*}
\text{R}^1\text{N=CPPh}_3 + \text{O=C=N-R}_3 & \xrightarrow{\text{CH}_2\text{Cl}_2} \text{R}^1\text{C=N-R}_3 \\
\text{R}^1\text{N=N-PPh}_3 + \text{ClC} & \xrightarrow{\text{Et}_3\text{N (1.2 eq)}} \text{Et}_2\text{Cl}_2 \\
\text{R}^1\text{N=N-R}_3 & \xrightarrow{t-\text{BuOK (1.0 eq)}} \text{DMF, 40 °C, 0.5 h}
\end{align*}
\]

References:

3. Synthetic procedure and analytical data of compounds 3

\[
\begin{align*}
\text{R}^1\text{N=C-R}_2 & + \text{CN-R}_4 & \xrightarrow{t-\text{BuOK (1.0 eq)}} \text{DMF, 40 °C, 0.5 h}
\end{align*}
\]

Typical synthetic procedure (with 3aa as an example): To a solution of ethyl 3-((4-methoxyphenyl)imino)-2-methylacrylate (1a) (0.3 mmol, 69.9 mg) and ethyl isocyanatoacetate (2a) (0.36 mmol, 0.039 mL) in DMF (2 mL) at 40 °C, t-BuOK (0.3 mmol, 33.7 mg) was added. After stirred for 30 min, substrate 1a was completely consumed as indicated by TLC. The solution was cooled to room temperature, and poured into water (50 mL). The resulting mixture was extracted
by ethyl acetate (3 × 20 mL), the organic layer was combined and washed with brine (3 × 50 mL),
dried over MgSO$_4$ and concentrated. Purification of the crude product with flash column
chromatography (silica gel; petroleum ether: ethyl acetate = 5:1) gave 3aa 89.3 mg, 86% yield as a
yellow solid.

Analytical data of compounds of 3

**Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(4-methoxyphenyl)-1H-imidazole-4-carboxylate**

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 89.3 mg,
86 %, isolated as a yellow solid; $^1$H NMR (600 MHz, CDCl$_3$) δ 1.18 (t, $J = 7.1$
Hz, 3H), 1.40 (t, $J = 7.1$ Hz, 3H), 1.43 (d, $J = 7.2$ Hz, 3H), 3.88 (s, 3H), 4.02 (q, $J = 7.2$
Hz, 1H), 4.09 (q, $J = 7.1$ Hz, 2H), 4.38 (dq, $J = 7.2$, 7.1 Hz, 2H), 7.02 (d, $J = 8.9$ Hz, 2H), 7.23 (d, $J = 8.9$
Hz, 2H), 7.52 (s, 1H); $^{13}$C NMR (151 MHz, CDCl$_3$) δ 13.9, 14.2, 15.7, 35.5, 55.5, 60.3, 60.9,
114.7 (2C), 127.3, 128.0 (2C), 129.2, 137.3, 139.3, 160.3, 162.9, 171.2; HRMS (ESI-TOF) m/z
calculated for C$_{18}$H$_{22}$N$_2$O$_5$Na: 369.1421, Found: 369.1430.

**Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(4-fluorophenyl)-1H-imidazole-4-carboxylate**

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 92.3 mg,
92 %, isolated as a yellow liquid; $^1$H NMR (600 MHz, CDCl$_3$) δ 1.19 (t, $J = 7.1$
Hz, 3H), 1.41 (t, $J = 7.1$ Hz, 3H), 1.43 (d, $J = 7.2$ Hz, 3H), 4.03 (q, $J = 7.2$ Hz, 1H), 4.09 (q, $J = 7.1$
Hz, 2H), 4.39 (dq, $J = 7.2$, 7.1 Hz, 2H), 7.24 (dd, $J = 11.4$, 5.4 Hz, 2H), 7.33 (dd, $J = 8.6$, 4.6 Hz, 2H), 7.54 (s,
1H); $^{13}$C NMR (151 MHz, CDCl$_3$) δ 13.9, 14.2, 15.7, 35.5, 60.5, 61.1, 116.7, 116.8, 128.7, 128.8,
129.6, 130.8 (d, $J = 3.0$ Hz), 137.1, 139.0, 162.1 (d, $J = 250.6$ Hz), 162.9, 171.1; HRMS (ESI-
TOF) m/z calculated for C$_{17}$H$_{19}$F$_2$NaO$_4$ ([M+Na]$^+$): 357.1221, Found: 357.1232.

**Ethyl 1-(4-chlorophenyl)-5-(1-ethoxy-1-oxopropan-2-yl)-1H-imidazole-4-carboxylate**
Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 85.2 mg, 81 %, isolated as a light yellow liquid; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) \(\delta\) 1.19 (t, \(J = 7.1\) Hz, 3H), 1.40 (t, \(J = 7.1\) Hz, 3H), 1.44 (d, \(J = 7.2\) Hz, 3H), 4.03 (q, \(J = 7.2\) Hz, 1H), 4.09 (q, \(J = 7.1\) Hz, 2H), 4.38 (dq, \(J = 7.2, 7.1\) Hz, 2H), 7.29 (d, \(J = 8.5\) Hz, 2H), 7.52 (d, \(J = 8.5\) Hz, 2H), 7.54 (s, 1H); \textsuperscript{13}C NMR (151 MHz, CDCl\textsubscript{3}) \(\delta\) 13.9, 14.3, 15.8, 35.6, 60.5, 61.1, 128.1 (2C), 129.8, 129.9, 133.3, 135.9, 136.9, 138.8, 162.8, 171.1; HRMS (ESI-TOF) m/z calculated for C\textsubscript{17}H\textsubscript{20}ClN\textsubscript{2}O\textsubscript{4}\textsuperscript{+} ([M+H\textsuperscript{+}]): 351.1106, Found: 351.1115.

\textbf{Ethyl 1-(4-bromophenyl)-5-(1-ethoxy-1-oxopropan-2-yl)-1H-imidazole-4-carboxylate}

\begin{center}
\includegraphics[width=0.2\textwidth]{3da}
\end{center}

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 92.5 mg, 78 %, isolated as a yellow liquid; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) \(\delta\) 1.18 (t, \(J = 7.1\) Hz, 3H), 1.40 (t, \(J = 7.1\) Hz, 3H), 1.43 (d, \(J = 7.2\) Hz, 3H), 4.02 (q, \(J = 7.1\) Hz, 1H), 4.09 (q, \(J = 7.1\) Hz, 2H), 4.39 (dq, \(J = 7.2, 7.1\) Hz, 2H), 7.21 (d, \(J = 7.7\) Hz, 2H), 7.53 (s, 1H), 7.67 (d, \(J = 7.7\) Hz, 2H); \textsuperscript{13}C NMR (151 MHz, CDCl\textsubscript{3}) \(\delta\) 14.0, 14.3, 15.8, 35.7, 60.6, 61.2, 124.1, 128.4 (2C), 129.9, 133.0 (2C), 133.9, 136.9, 138.9, 162.9, 171.1; HRMS (ESI-TOF) m/z calculated for C\textsubscript{17}H\textsubscript{19}BrN\textsubscript{2}NaO\textsubscript{4}\textsuperscript{+} ([M+Na\textsuperscript{+}]): 417.0420, Found: 417.0429.

\textbf{Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(p-tolyl)-1H-imidazole-4-carboxylate}

\begin{center}
\includegraphics[width=0.2\textwidth]{3ea}
\end{center}

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 92.2 mg, 93 %, isolated as a light yellow liquid; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) \(\delta\) 1.18 (t, \(J = 7.2\) Hz, 3H), 1.40 (t, \(J = 7.2\) Hz, 3H), 1.44 (d, \(J = 7.2\) Hz, 3H), 2.45 (s, 3H), 4.02 (q, \(J = 7.2\) Hz, 1H), 4.09 (q, \(J = 7.2\) Hz, 2H), 4.39 (dq, \(J = 7.8, 7.2\) Hz, 2H), 7.20 (d, \(J = 7.8\) Hz, 2H), 7.33 (d, \(J = 7.8\) Hz, 2H), 7.53 (s, 1H); \textsuperscript{13}C NMR (151 MHz, CDCl\textsubscript{3}) \(\delta\) 13.9, 14.2, 15.7, 21.0, 35.5, 60.3, 60.9, 126.5 (2C), 129.3, 130.2 (2C), 132.2, 137.0, 139.1, 139.9, 162.9, 171.2; HRMS (ESI-TOF) m/z calculated for C\textsubscript{18}H\textsubscript{23}N\textsubscript{2}O\textsubscript{4}\textsuperscript{+} ([M+H\textsuperscript{+}]): 331.1652, Found: 331.1660.

\textbf{Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(4-(trifluoromethyl)phenyl)-1H-imidazole-4-carboxylate}

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 92.2 mg, 93 %, isolated as a light yellow liquid; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) \(\delta\) 1.18 (t, \(J = 7.2\) Hz, 3H), 1.40 (t, \(J = 7.2\) Hz, 3H), 1.44 (d, \(J = 7.2\) Hz, 3H), 2.45 (s, 3H), 4.02 (q, \(J = 7.2\) Hz, 1H), 4.09 (q, \(J = 7.2\) Hz, 2H), 4.39 (dq, \(J = 7.8, 7.2\) Hz, 2H), 7.20 (d, \(J = 7.8\) Hz, 2H), 7.33 (d, \(J = 7.8\) Hz, 2H), 7.53 (s, 1H); \textsuperscript{13}C NMR (151 MHz, CDCl\textsubscript{3}) \(\delta\) 13.9, 14.2, 15.7, 21.0, 35.5, 60.3, 60.9, 126.5 (2C), 129.3, 130.2 (2C), 132.2, 137.0, 139.1, 139.9, 162.9, 171.2; HRMS (ESI-TOF) m/z calculated for C\textsubscript{18}H\textsubscript{23}N\textsubscript{2}O\textsubscript{4}\textsuperscript{+} ([M+H\textsuperscript{+}]): 331.1652, Found: 331.1660.
Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 86.5 mg, 75 %, isolated as a light yellow liquid; \textbf{1H NMR} (400 MHz, CDCl\textsubscript{3}) \(\delta\) 1.19 (t, \(J = 7.2\) Hz, 3H), 1.41 (t, \(J = 7.2\) Hz, 3H), 1.47 (d, \(J = 7.2\) Hz, 2H), 4.02 (q, \(J = 7.2\) Hz, 1H), 4.10 (q, \(J = 7.2\) Hz, 2H), 4.40 (dq, \(J = 8.4, 7.2\) Hz, 2H), 7.49 (d, \(J = 8.4\) Hz, 2H), 7.57 (s, 1H), 7.83 (d, \(J = 8.4\) Hz, 2H); \textbf{13C NMR} (151 MHz, CDCl\textsubscript{3}) \(\delta\) 14.0, 14.3, 15.8, 35.7, 60.6, 61.2, 123.2 (q, \(J = 270.3\) Hz), 127.0 (q, \(J = 3.5\) Hz), 127.3 (2C), 130.1, 132.0 (q, \(J = 33.0\) Hz), 136.7, 138.0, 138.7, 162.8, 171.0; \textbf{HRMS} (ESI-TOF) m/z calculated for C\textsubscript{18}H\textsubscript{20}F\textsubscript{3}N\textsubscript{2}O\textsubscript{4}+ ([M+H]+): 385.1370, Found: 385.1381.

\textbf{Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(4-(ethoxycarbonyl)phenyl)-1H-imidazole-4-carboxylate}

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 65.3 mg, 56 %, isolated as a yellow liquid; \textbf{1H NMR} (600 MHz, CDCl\textsubscript{3}) \(\delta\) 1.19 (t, \(J = 7.0\) Hz, 3H), 1.42 (dt, \(J = 21.1, 6.8\) Hz, 9H), 4.05 (dd, \(J = 14.4, 7.2\) Hz, 1H), 4.09 (dd, \(J = 13.8, 6.8\) Hz, 2H), 4.33–4.41 (m, 2H), 4.44 (dd, \(J = 14.1, 7.0\) Hz, 2H), 7.42 (d, \(J = 7.9\) Hz, 2H), 7.59 (s, 1H), 8.22 (d, \(J = 7.8\) Hz, 2H); \textbf{13C NMR} (151 MHz, CDCl\textsubscript{3}) \(\delta\) 14.0, 14.3, 15.8, 35.6, 60.6, 61.2, 61.5, 126.7 (2C), 130.0, 131.1 (2C), 131.8, 136.8, 138.5, 138.8, 162.8, 165.0, 171.0; \textbf{HRMS} (ESI-TOF) m/z calculated for C\textsubscript{20}H\textsubscript{25}N\textsubscript{2}O\textsubscript{6}+ ([M+H]+): 389.1707, Found: 389.1717.

\textbf{Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(4-(trifluoromethoxy)phenyl)-1H-imidazole-4-carboxylate}

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 102.1 mg, 85 %, isolated as a yellow liquid; \textbf{1H NMR} (600 MHz, CDCl\textsubscript{3}) \(\delta\) 1.19 (t, \(J = 7.1\) Hz, 3H), 1.41 (t, \(J = 7.1\) Hz, 3H), 1.46 (d, \(J = 7.2\) Hz, 3H), 4.03 (q, \(J = 7.2\) Hz, 1H), 4.10 (q, \(J = 7.1\) Hz, 2H), 4.39 (dq, \(J = 7.2, 7.1\) Hz, 2H), 7.41 (s, 4H), 7.56 (s, 1H); \textbf{13C NMR} (151 MHz, CDCl\textsubscript{3}) \(\delta\) 13.9, 14.2, 15.8, 35.6, 60.5, 61.1, 120.1 (q, \(J = 258.8\) Hz), 122.0 (2C), 128.5 (2C), 129.8, 133.2, 136.9, 138.9,
149.8, 162.8, 171.0; **HRMS** (ESI-TOF) m/z calculated for C_{18}H_{19}F_{3}N_{2}O_{5}^{+}(\text{[M+Na]}^{+}): 423.1138, Found: 423.1154.

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**Ethyl 1-(3-chlorophenyl)-5-(1-ethoxy-1-oxopropan-2-yl)-1H-imidazole-4-carboxylate**

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 76.8 mg, 73 %, isolated as a yellow liquid; **\(^{1}\text{H NMR}** (600 MHz, CDCl\(_3\)) \(\delta\): 1.20 (t, \(J = 7.2\) Hz, 3H), 1.41 (t, \(J = 7.2\) Hz, 3H), 1.45 (d, \(J = 7.2\) Hz, 3H), 4.06 (q, \(J = 7.2\) Hz, 1H), 4.11 (q, \(J = 7.2\) Hz, 2H), 4.39 (dq, \(J = 7.2, 6.6\) Hz, 2H), 7.25 (d, \(J = 7.8\) Hz, 1H), 7.36 (s, 1H), 7.49 (t, \(J = 7.8\) Hz, 1H), 7.53 (s, 1H), 7.55 (s, 1H); **\(^{13}\text{C NMR}** (151 MHz, CDCl\(_3\)) \(\delta\): 14.0, 14.2, 15.8, 35.6, 60.5, 61.1, 125.0, 127.1, 129.8, 130.0, 130.7, 135.4, 135.9, 136.8, 138.8, 162.8, 171.0; **HRMS** (ESI-TOF) m/z calculated for C\(_{17}\)H\(_{20}\)ClN\(_2\)O\(_4\)\(^{+}\) (\text{[M+H]}^{+}): 351.1106, Found: 351.1116.

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**Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(3-methoxyphenyl)-1H-imidazole-4-carboxylate**

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 90.4 mg, 87 %, isolated as a yellow liquid; **\(^{1}\text{H NMR}** (600 MHz, CDCl\(_3\)) \(\delta\): 1.18 (t, \(J = 7.1\) Hz, 3H), 1.40 (t, \(J = 7.1\) Hz, 3H), 1.46 (d, \(J = 7.2\) Hz, 3H), 3.85 (s, 3H), 4.05 (q, \(J = 7.2\) Hz, 1H), 4.10 (q, \(J = 7.0\) Hz, 2H), 4.38 (dq, \(J = 7.2, 7.1\) Hz, 2H), 6.85 (s, 1H), 6.90 (d, \(J = 7.7\) Hz, 1H), 7.06 (d, \(J = 8.3\) Hz, 1H), 7.43 (t, \(J = 8.1\) Hz, 1H), 7.56 (s, 1H); **\(^{13}\text{C NMR}** (151 MHz, CDCl\(_3\)) \(\delta\): 13.9, 14.2, 15.7, 35.5, 55.4, 60.3, 60.9, 112.6, 115.1, 118.6, 129.4, 130.4, 135.8, 136.8, 138.9, 160.3, 162.9, 171.2; **HRMS** (ESI-TOF) m/z calculated for C\(_{18}\)H\(_{23}\)N\(_2\)O\(_5\)\(^{+}\) (\text{[M+H]}^{+}): 347.1601, Found: 347.1608.

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**Ethyl 1-(3-cyanophenyl)-5-(1-ethoxy-1-oxopropan-2-yl)-1H-imidazole-4-carboxylate**

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 73.7 mg, 72 %, isolated as a yellow liquid; **\(^{1}\text{H NMR}** (600 MHz, CDCl\(_3\)) \(\delta\): 1.21 (t, \(J = 7.1\) Hz, 3H), 1.41 (t, \(J = 7.1\) Hz, 3H), 1.44 (d, \(J = 7.2\) Hz, 3H), 4.05 (q, \(J = 7.1\) Hz, 1H), 4.11 (q, \(J = 7.0\) Hz, 2H), 4.39 (dq, \(J = 7.2, 7.1\) Hz, 2H), 7.56 (s, 1H), 7.62 (d, \(J = 8.0\) Hz, 1H), 7.67 (s, 1H), 7.71 (t, \(J = 7.9\) Hz,
1H), 7.86 (d, J = 7.7 Hz, 1H); $^{13}$C NMR (151 MHz, CDCl$_3$) δ 13.9, 14.1, 15.7, 35.5, 60.6, 61.2, 114.1, 116.7, 130.1, 130.2, 130.8, 131.2, 133.3, 135.8, 136.7, 138.5, 162.6, 170.8; HRMS (ESI-TOF) m/z calculated for C$_{18}$H$_{19}$N$_3$NaO$_4$ ([(M+Na)$^+$]): 364.1268, Found: 364.1259.

Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(o-tolyl)-1H-imidazole-4-carboxylate

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 84.2 mg, 85 %, isolated as a light yellow liquid, mixture of diasteroisomers; $^1$H NMR (600 MHz, CDCl$_3$) δ 1.17 (t, J = 7.2 Hz, 3H), 1.40 (d, J = 6.6 Hz, 4H), 1.46 (d, J = 7.2 Hz, 2H), 2.13 (d, J = 10.8 Hz, 3H), 3.58 (q, J = 7.2 Hz, 0.6H), 3.68 (q, J = 7.2 Hz, 0.4H), 4.05–4.14 (m, 2H), 4.33–4.44 (m, 2H), 7.17 (d, J = 7.8 Hz, 0.6H), 7.26 (d, J = 7.2 Hz, 0.4H), 7.34 (t, J = 7.2 Hz, 1H), 7.40 (d, J = 6.6 Hz, 1H), 7.44–7.48 (m, 2H); $^{13}$C NMR (151 MHz, CDCl$_3$) δ 13.9 (d, J = 9.8 Hz), 14.3, 15.6 (d, J = 4.7 Hz), 17.0, 17.2, 35.6 (d, J = 20.1 Hz), 60.4, 60.9, 127.0 (d, J = 5.7 Hz), 127.8, 128.4, 129.0, 129.2, 130.1, 130.3, 131.3 (d, J = 11.5 Hz), 133.6 (d, J = 10.7 Hz), 135.7, 136.4, 136.6, 136.8, 139.1, 139.3, 162.9, 171.0; HRMS (ESI-TOF) m/z calculated for C$_{18}$H$_{23}$N$_2$O$_4$ ([(M+H)$^+$]): 331.1652, Found: 331.1660.

Ethyl 1-(2-chlorophenyl)-5-(1-ethoxy-1-oxopropan-2-yl)-1H-imidazole-4-carboxylate

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 80.0 mg, 76 %, isolated as a light yellow liquid, mixture of diasteroisomers; $^1$H NMR (600 MHz, CDCl$_3$) δ 1.18 (t, J = 6.6 Hz, 3H), 1.35 (d, J = 7.2 Hz, 1.5H), 1.41 (s, 3H), 1.51 (d, J = 6.6 Hz, 1.5H), 3.58 (q, J = 7.2, 6.6 Hz, 0.5H), 4.04 (q, J = 7.2, 6.6 Hz, 0.5H), 4.09 (q, J = 6.6, 6.0 Hz, 2H), 4.38–4.44 (m, 2H), 7.35 (d, J = 7.8 Hz, 0.5H), 7.40 (d, J = 7.8 Hz, 0.5H), 7.42–7.52 (m, 3H), 7.61 (t, J = 7.2 Hz, 1H); $^{13}$C NMR (151 MHz, CDCl$_3$) δ 14.0 (d, J = 12.4 Hz), 14.3, 15.3 (d, J = 13.0 Hz), 35.7 (d, J = 15.9 Hz), 60.5, 61.0 (d, J = 7.2 Hz), 127.7, 127.9, 129.2, 129.5, 129.6, 130.0, 130.7 (d, J = 9.4 Hz), 131.5, 132.4, 132.6, 132.7, 132.9, 136.9, 137.3, 138.9, 139.2, 162.8, 163.0, 170.9, 171.2; HRMS (ESI-TOF) m/z calculated for C$_{17}$H$_{21}$ClN$_2$O$_4$ ([(M+H)$^+$]): 351.1106, Found: 351.1114.

Ethyl 1-(3,4-dichlorophenyl)-5-(1-ethoxy-1-oxopropan-2-yl)-1H-imidazole-4-carboxylate

Ethyl 1-(3,4-dichlorophenyl)-5-(1-ethoxy-1-oxopropan-2-yl)-1H-imidazole-4-carboxylate
Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 95.9 mg, 83 %, isolated as a yellow liquid; **¹H NMR** (600 MHz, CDCl₃) δ 1.20 (t, J = 7.1 Hz, 3H), 1.40 (t, J = 7.1 Hz, 3H), 1.44 (d, J = 7.2 Hz, 3H), 4.07 (dd, J = 14.1, 6.7 Hz, 1H), 4.11 (dd, J = 14.0, 6.9 Hz, 2H), 4.38 (dq, J = 7.2, 7.1 Hz, 2H), 7.22 (d, J = 8.5 Hz, 1H), 7.48 (s, 1H), 7.53 (s, 1H), 7.63 (d, J = 8.4 Hz, 1H); **¹³C NMR** (151 MHz, CDCl₃) δ 14.0, 14.2, 15.8, 35.6, 60.6, 61.3, 126.1, 128.8, 130.1, 131.4, 133.9, 134.1, 134.6, 136.8, 138.7, 162.8, 170.9; **HRMS** (ESI-TOF) m/z calculated for C₁₇H₁₉Cl₂N₂O₄⁺ ([M+H]⁺): 385.0716, Found: 385.0724.

**Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(naphthalen-1-yl)-1H-imidazole-4-carboxylate**

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 83.5 mg, 76 %, isolated as a yellow liquid, mixture of diastereoisomers; **¹H NMR** (600 MHz, CDCl₃) δ 1.12 (t, J = 7.2 Hz, 1.2H), 1.18 (t, J = 7.2 Hz, 1.8H), 1.37 (d, J = 7.2 Hz, 1.8H), 1.40 (d, J = 7.2 Hz, 1.2H), 1.42–1.45 (m, 3H), 3.61 (q, J = 7.2 Hz, 0.6H), 3.72 (q, J = 7.2 Hz, 0.4H), 3.83–3.89 (m, 0.4H), 3.95–3.98 (m, 0.4H), 4.06–4.09 (m, 1.2H), 4.37–4.48 (m, 2H), 7.29 (d, J = 8.4 Hz, 0.4H), 7.45 (q, J = 8.4 Hz, 1.2H), 7.51–7.55 (m, 1.4H), 7.59–7.64 (m, 3H), 7.98 (q, J = 7.8 Hz, 1H), 8.06 (d, J = 8.4 Hz, 1H); **¹³C NMR** (151 MHz, CDCl₃) δ 13.8 (d, J = 6.3 Hz), 14.2, 15.8 (d, J = 8.6 Hz), 35.6 (d, J = 23.2 Hz), 60.4, 60.8, 121.6, 122.3, 124.9 (d, J = 11.8 Hz), 125.6, 126.1, 127.1 (d, J = 13.6 Hz), 127.8 (d, J = 14.5 Hz), 128.0, 128.2, 129.1 (d, J = 13.4 Hz), 130.3, 130.4, 130.5, 130.6, 130.7, 130.8, 133.9, 137.7 (d, J = 5.9 Hz), 140.2, 140.3, 162.8, 170.8 (d, J = 16.2 Hz); **HRMS** (ESI-TOF) m/z calculated for C₂₁H₂₂N₂NaO₄⁺ ([M+Na]⁺): 389.1472, Found: 389.1467.

**Ethyl 1-cyclohexyl-5-(1-ethoxy-1-oxopropan-2-yl)-1H-imidazole-4-carboxylate**

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 79.3 mg, 82 %, isolated as a light yellow liquid; **¹H NMR** (400 MHz, CDCl₃) δ 1.21 (t, J = 7.1 Hz, 3H), 1.24–1.29 (m, 1H), 1.29–1.46 (m, 5H), 1.51 (d, J = 7.3 Hz, 3H), 1.66 (qd, J = 12.4, 3.3 Hz, 2H), 1.77 (d, J = 12.7 Hz, 1H), 1.93 (d, J = 14.0 Hz, 2H), 1.99 (d, J = 12.6 Hz, 1H), 2.06 (d, J = 12.7 Hz, 3H).
Hz, 1H), 3.75 (tt, J = 12.0, 3.5 Hz, 1H), 4.15 (qq, J = 10.8, 7.1 Hz, 2H), 4.36 (dq, J = 7.3, 7.1 Hz, 2H), 4.85 (q, J = 7.2 Hz, 1H), 7.54 (s, 1H); 13C NMR (151 MHz, CDCl3) δ 13.9, 14.2, 16.0, 24.9, 25.6, 34.1, 34.8, 35.0, 55.4, 60.2, 61.2, 128.4, 134.4, 136.8, 163.4, 172.1; HRMS (ESI-TOF) m/z calculated for C17H26N2NaO4+ ([M+Na]+): 345.1785, Found: 345.1790.

Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-ethyl-1H-imidazole-4-carboxylate

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 69.2 mg, 86 %, isolated as a light yellow liquid; 1H NMR (600 MHz, CDCl3) δ 1.19 (t, J = 7.1 Hz, 3H), 1.39 (t, J = 7.1 Hz, 3H), 1.45 (t, J = 7.3 Hz, 3H), 1.53 (d, J = 7.3 Hz, 3H), 3.95 (q, J = 7.3 Hz, 2H), 4.15 (q, J = 7.1 Hz, 2H), 4.35 (dq, J = 7.3, 7.1 Hz, 2H), 4.60 (q, J = 7.3 Hz, 1H), 7.49 (s, 1H); 13C NMR (151 MHz, CDCl3) δ 13.9, 14.2, 15.7, 16.0, 40.1, 60.2, 61.1, 129.2, 136.1, 137.3, 163.2, 171.7; HRMS (ESI-TOF) m/z calculated for C13H20N2NaO4+ ([M+Na]+): 291.1315, Found: 291.1317.

Ethyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-isopropyl-1H-imidazole-4-carboxylate

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 64.4 mg, 76 %, isolated as a light yellow liquid; 1H NMR (400 MHz, CDCl3) δ 1.21 (t, J = 7.1 Hz, 3H), 1.39 (t, J = 7.1 Hz, 3H), 1.48 (d, J = 6.7 Hz, 3H), 1.51 (d, J = 4.8 Hz, 3H), 1.52 (d, J = 5.4 Hz, 3H), 4.08-4.21 (m, 2H), 4.25 (dd, J = 13.4, 6.7 Hz, 1H), 4.35 (dq, J = 7.1, 6.7 Hz, 2H), 4.84 (q, J = 7.2 Hz, 1H), 7.58 (s, 1H); 13C NMR (151 MHz, CDCl3) δ 14.0, 14.3, 15.9, 23.4, 24.0, 34.5, 47.6, 60.2, 61.2, 128.5, 133.9, 136.8, 163.4, 172.0; HRMS (ESI-TOF) m/z calculated for C14H22N2NaO4+ ([M+Na]+): 305.1472 , Found: 305.1450.

Ethyl 5-benzhydryl-1-phenyl-1H-imidazole-4-carboxylate

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 86.1 mg, 75 %, isolated as a yellow liquid; 1H NMR (600 MHz, CDCl3) δ 1.24 (t, J = 7.1 Hz, 3H), 4.20 (q,
\[ J = 7.1 \text{ Hz, 2H}, 6.29 \text{ (d, } J = 7.9 \text{ Hz, 2H)}, 6.95–7.06 \text{ (m, 4H), 7.11–7.19 \text{ (m, 6H), 7.22 \text{ (t, } J = 7.7 \text{ Hz, 2H})}, 7.33 \text{ (s, 1H), 6.94–7.06 \text{ (m, 4H), 7.11–7.19 \text{ (m, 6H), 7.22 \text{ (t, } J = 7.7 \text{ Hz, 2H})}, 7.33 \text{ (s, 1H)}; \]

**13C NMR (151 MHz, CDCl}_3 \text{) } \delta 14.1, 46.2, 60.3, 126.4 \text{ (2C), 127.3 \text{ (2C), 127.9 \text{ (4C), 128.9, 129.0 \text{ (4C), 129.1, 130.7, 135.4, 138.0, 140.0, 140.2, 162.9}}; \text{ HRMS (ESI-TOF) m/z calculated for C}_{25}H_{22}N_2NaO_2^- ([M+Na]^+: 405.1573, Found: 405.1587.}

**Ethyl 1-phenyl-5-(9H-xanthen-9-yl)-1H-imidazole-4-carboxylate**

![Image of 3a]

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 76.1 mg, 64 %, isolated as a yellow solid; m.p. 144-146 °C; \(^1H\text{ NMR (600 MHz, CDCl}_3 \text{) } \delta 1.49 \text{ (t, } J = 6.0 \text{ Hz, 3H), 4.51 \text{ (q, } J = 6.0 \text{ Hz, 2H), 6.25 \text{ (s, 2H), 6.67 \text{ (d, } J = 7.8 \text{ Hz, 2H), 6.85 \text{ (s, 1H)), 6.94 \text{ (t, } J = 7.2 \text{ Hz, 2H), 6.99 \text{ (t, } J = 7.2 \text{ Hz, 2H), 7.05–7.13 \text{ (m, 4H), 7.23 \text{ (t, } J = 7.2 \text{ Hz, 1H), 7.34 \text{ (s, 1H); \text{ 13C NMR (151 MHz, CDCl}_3 \text{) } \delta 14.4, 32.3, 60.7, 116.0 \text{ (2C), 127.0 \text{ (2C), 128.3 \text{ (2C), 128.4, 128.8, 129.4, 130.0, 134.6, 138.4, 142.5, 150.2, 163.8; \text{ HRMS (ESI-TOF) m/z calculated for C}_{25}H_{20}N_2NaO_3^+ ([M+Na]^+: 419.1366, Found: 419.1374.}

**Ethyl 5-(1-ethoxy-1-oxobutan-2-yl)-1-(4-methoxyphenyl)-1H-imidazole-4-carboxylate**

![Image of 3ua]

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 85.4 mg, 79 %, isolated as a light yellow liquid; \(^1H\text{ NMR (600 MHz, CDCl}_3 \text{) } \delta 0.68 \text{ (t, } J = 7.5 \text{ Hz, 3H), 1.20 \text{ (t, } J = 7.1 \text{ Hz, 3H), 1.40 \text{ (t, } J = 7.1 \text{ Hz, 3H), 1.67–1.97 \text{ (m, 1H), 2.04–2.25 \text{ (m, 1H), 3.88 \text{ (d, } J = 6.1 \text{ Hz, 3H), 3.90 \text{ (dd, } J = 9.8, 5.5 \text{ Hz, 1H), 4.08 \text{ (dq, } J = 7.2, 6.6 \text{ Hz, 2H), 4.39 \text{ (dq, } J = 8.4, 7.2 \text{ Hz, 2H), 7.00 \text{ (d, } J = 8.7 \text{ Hz, 2H), 7.21 \text{ (d, } J = 8.7 \text{ Hz, 2H), 7.53 \text{ (s, 1H); \text{ 13C NMR (151 MHz, CDCl}_3 \text{) } \delta 12.0, 14.0, 14.2, 23.1, 42.6, 55.5, 60.3, 60.8, 114.6 \text{ (2C), 127.5, 128.3 \text{ (2C), 129.7, 137.5, 137.9, 160.3, 163.0, 170.9; \text{ HRMS (ESI-TOF) m/z calculated for C}_{19}H_{28}N_2NaO_5^+ ([M+Na]^+: 383.1577, Found: 383.1586.}

**5-benzhydryl-1-phenyl-4-tosyl-1H-imidazole**
Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 90.6 mg, 65 %, isolated as a yellow solid; m.p. 194-195 °C; $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 2.37 (s, 3H), 6.71 (d, $J = 8.0$ Hz, 2H), 6.78 (s, 1H), 6.88 (d, $J = 7.5$ Hz, 4H), 7.05–7.13 (m, 6H), 7.15 (t, $J = 7.6$ Hz, 4H), 7.25 (t, $J = 7.5$ Hz, 1H), 7.47 (s, 1H), 7.60 (d, $J = 8.0$ Hz, 2H); $^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 21.4, 45.3, 126.5 (2C), 127.3 (2C), 127.7 (2C), 128.0 (4C), 128.8 (2C), 129.1, 129.2 (4C), 129.3, 135.2, 137.1, 138.3, 138.5, 139.1, 139.2, 143.6; HRMS (ESI-TOF) m/z calculated for C$_{29}$H$_{24}$N$_2$NaO$_2$S$^+$ ([M+Na]$^+$): 487.1451, Found: 487.1461.

6-benzhydryl-1-(p-tolyl)-4-tosyl-1H-imidazole

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 111.9 mg, 78 %, isolated as a white solid; m.p. 204-206 °C; $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 2.28 (s, 3H), 2.36 (s, 3H), 6.59 (d, $J = 8.2$ Hz, 2H), 6.72 (s, 1H), 6.89 (t, $J = 7.7$ Hz, 6H), 7.05–7.21 (m, 8H), 7.45 (s, 1H), 7.58 (d, $J = 8.2$ Hz, 2H); $^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 20.9, 21.4, 45.3, 126.5 (2C), 127.1 (2C), 127.8 (2C), 127.9 (4C), 129.2, 129.3 (4C), 129.4 (2C), 132.6, 137.2, 138.3, 138.4, 139.2, 139.3, 143.6; HRMS (ESI-TOF) m/z calculated for C$_{30}$H$_{26}$N$_2$NaO$_2$S$^+$ ([M+Na]$^+$): 501.1607, Found: 501.1614.

5-benzhydryl-1-(4-(tert-butyl)phenyl)-4-tosyl-1H-imidazole

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 118.7 mg, 76 %, isolated as a white solid; m.p. 228-229 °C; $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 1.24 (s, 9H), 2.36 (s, 3H), 6.63 (d, $J = 8.5$ Hz, 2H), 6.82 (s, 1H), 6.87 (d, $J = 7.4$ Hz, 4H), 7.06 (d, $J = 8.6$ Hz, 2H), 7.09 (t, $J = 7.5$ Hz, 4H), 7.14 (dd, $J = 11.9$, 4.5 Hz, 4H), 7.46 (s, 1H), 7.58 (d, $J = 8.2$ Hz, 2H); $^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 21.4, 31.0, 34.5, 45.3, 125.7 (2C), 126.4 (2C), 126.8 (2C), 127.7 (2C), 127.9 (4C), 129.2 (4C), 129.3, 132.5, 137.2, 138.3, 138.4, 139.2, 139.3, 143.6, 152.4; HRMS (ESI-TOF) m/z calculated for C$_{33}$H$_{32}$N$_2$NaO$_2$S$^+$ ([M+Na]$^+$): 543.2077, Found: 543.2090.
1-([1,1′-biphenyl]-4-yl)-5-benzhydryl-4-tosyl-1H-imidazole

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 111.9 mg, 69 %, isolated as a yellow liquid; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 2.29 (s, 3H), 6.68 (d, \(J = 8.4\) Hz, 2H), 6.78 (s, 1H), 6.83 (d, \(J = 7.5\) Hz, 4H), 7.03 (t, \(J = 7.5\) Hz, 4H), 7.08 (dd, \(J = 12.4, 7.5\) Hz, 4H), 7.18 (d, \(J = 8.5\) Hz, 2H), 7.29 (t, \(J = 7.1\) Hz, 1H), 7.35 (t, \(J = 7.6\) Hz, 2H), 7.38 (d, \(J = 7.2\) Hz, 2H), 7.43 (s, 1H), 7.53 (d, \(J = 8.2\) Hz, 2H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \(\delta\) 21.5, 45.3, 126.6 (2C), 127.0 (2C), 127.4 (2C), 127.7 (2C), 127.8 (2C), 128.0 (4C), 128.9 (2C), 129.3 (4C), 129.4, 134.3, 137.3, 138.3, 138.6, 139.2, 139.3, 139.4, 142.1, 143.7; HRMS (ESI-TOF) m/z calculated for C\(_{35}\)H\(_{28}\)N\(_2\)O\(_2\)S\(^+\) ([M+Na]\(^+\)): 563.1764, Found: 563.1781.

6-benzhydryl-1-(4-nitrophenyl)-4-tosyl-1H-imidazole

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 71.9 mg, 47 %, isolated as a brown liquid; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 2.38 (s, 3H), 6.85 (d, \(J = 7.6\) Hz, 4H), 6.89 (d, \(J = 8.8\) Hz, 2H), 6.98 (s, 1H), 7.11 (t, \(J = 7.6\) Hz, 4H), 7.17 (dd, \(J = 16.8, 8.0\) Hz, 4H), 7.48 (s, 1H), 7.62 (d, \(J = 8.1\) Hz, 2H), 7.89 (d, \(J = 8.8\) Hz, 2H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \(\delta\) 21.5, 45.0, 123.9 (2C), 126.9 (2C), 127.7 (2C), 128.3 (4C), 128.5 (2C), 129.1 (4C), 129.4, 137.2, 137.9, 138.7, 138.7, 139.4, 140.6, 144.1, 147.5; HRMS (ESI-TOF) m/z calculated for C\(_{29}\)H\(_{23}\)N\(_3\)NaO\(_4\)S\(^+\) ([M+Na]\(^+\)): 532.1301, Found: 532.1306.

5-benzhydryl-1-(4-iodophenyl)-4-tosyl-1H-imidazole

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 139.9 mg, 79 %, isolated as a light brown solid; m.p. 212-213 ºC; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 2.37 (s, 3H), 6.42 (d, \(J = 8.5\) Hz, 2H), 6.85 (d, \(J = 7.7\) Hz, 4H), 6.87 (s, 1H), 7.13 (dd, \(J = 14.6, 7.3\) Hz, 6H), 7.18 (t, \(J = 7.3\) Hz, 2H), 7.38 (d, \(J = 8.5\) Hz, 2H), 7.43 (s, 1H), 7.60 (d, \(J = 8.1\) Hz, 2H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \(\delta\) 21.4, 45.1, 94.8, 126.6 (2C), 127.7 (2C), 128.1 (4C), 129.0 (2C),
129.1 (4C), 129.3 (2C), 134.9, 137.1, 137.9, 138.1, 138.7, 138.9, 138.9, 143.8; **HRMS (ESI-TOF)** m/z calculated for C_{29}H_{23}IN_{2}NaO_{2}S"([M+Na]^{+}): 613.0417, Found: 613.0423.

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**5-benzhydryl-1-(3,4-dimethoxyphenyl)-4-tosyl-1H-imidazole**

![Image](image_1.png)

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 91.3 mg, 58 %, isolated as a brown solid; m.p. 155-157 °C; **1H NMR** (600 MHz, CDCl_{3}) δ 2.39 (s, 3H), 3.41 (s, 3H), 3.84 (s, 3H), 6.05 (d, J = 2.1 Hz, 1H), 6.42 (dd, J = 8.6, 2.1 Hz, 1H), 6.59 (d, J = 8.5 Hz, 1H), 6.81 (s, 1H), 7.16 (dt, J = 14.5, 3.7 Hz, 6H), 7.19 (d, J = 4.5 Hz, 2H), 7.49 (s, 1H), 7.66 (d, J = 8.0 Hz, 2H); **13C NMR** (151 MHz, CDCl_{3}) δ 21.4, 45.1, 55.3, 56.0, 110.2, 110.6, 119.5, 126.4, 127.7 (2C), 127.8 (4C), 127.9 (4C), 129.2 (2C), 129.3, 137.2, 138.3, 138.4, 139.1, 139.3, 143.6, 149.5; **HRMS (ESI-TOF)** m/z calculated for C_{31}H_{28}N_{2}NaO_{4}S"([M+Na]^{+}): 547.1662, Found: 547.1662.

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**3-(5-benzhydryl-4-tosyl-1H-imidazol-1-yl)pyridine**

![Image](image_2.png)

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 90.8 mg, 65 %, isolated as a white solid; m.p. 188-190 °C; **1H NMR** (600 MHz, CDCl_{3}) δ 2.38 (s, 3H), 6.85 (d, J = 7.4 Hz, 4H), 6.89–6.94 (m, 1H), 6.94–6.98 (m, 1H), 6.99 (s, 1H), 7.12 (t, J = 7.6 Hz, 4H), 7.14–7.20 (m, 4H), 7.45 (s, 1H), 7.63 (d, J = 7.6 Hz, 2H), 8.05 (s, 1H), 8.39–8.49 (m, 1H); **13C NMR** (151 MHz, CDCl_{3}) δ 21.5, 45.0, 123.2, 126.8, 127.7 (2C), 128.2 (4C), 129.0 (4C), 129.4 (2C), 132.4, 134.5, 137.4, 137.9, 138.8, 139.1, 139.2, 143.9, 147.8, 149.9; **HRMS (ESI-TOF)** m/z calculated for C_{28}H_{23}N_{3}NaO_{4}S"([M+Na]^{+}): 488.1403, Found: 488.1419.

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**1-phenyl-5-(1-phenylethyl)-4-tosyl-1H-imidazole**

![Image](image_3.png)

Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 88.1 mg, 73 %, isolated as a light yellow liquid; **1H NMR** (600 MHz, CDCl_{3}) δ 1.55 (d, J = 7.4 Hz, 3H), 2.43 (s, 3H), 5.29 (q, J = 7.3 Hz, 1H), 6.74 (d, J = 7.6 Hz, 2H), 6.89 (d, J = 7.1 Hz, 2H), 7.07–7.16
(m, 3H), 7.22 (t, \( J = 7.8 \) Hz, 2H), 7.32 (d, \( J = 8.2 \) Hz, 2H), 7.36 (t, \( J = 7.6 \) Hz, 1H), 7.38 (s, 1H), 7.89 (d, \( J = 8.2 \) Hz, 2H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \( \delta \) 17.5, 21.5, 32.9, 126.2, 127.3 (2C), 127.4 (2C), 127.7 (2C), 128.0 (2C), 128.9 (2C), 129.4, 129.5 (2C), 135.0, 137.3, 138.5, 138.8, 140.5, 140.8, 143.8; HRMS (ESI-TOF) m/z calculated for C\(_{24}\)H\(_{22}\)N\(_2\)NaO\(_2\)S\(^+\) ([M+Na]\(^+\) ): 425.1294, Found: 425.1305.

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1-phenyl-5-(1-(p-tolyl)ethyl)-4-tosyl-1H-imidazole

\( \text{Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 77.5 mg, 62 %, isolated as a light yellow liquid; }^1\)H NMR (600 MHz, CDCl\(_3\)) \( \delta \) 1.52 (d, \( J = 7.4 \) Hz, 3H), 2.29 (s, 3H), 2.43 (s, 3H), 5.22 (q, \( J = 7.2 \) Hz, 1H), 6.77 (d, \( J = 7.9 \) Hz, 4H), 6.88–6.97 (m, 2H), 7.23 (t, \( J = 7.8 \) Hz, 2H), 7.31 (d, \( J = 8.2 \) Hz, 2H), 7.36 (d, \( J = 7.6 \) Hz, 1H), 7.38 (s, 1H), 7.88 (d, \( J = 8.2 \) Hz, 2H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \( \delta \) 17.6, 20.8, 21.5, 32.7, 127.2 (2C), 127.5 (2C), 127.8 (2C), 128.6 (2C), 128.8 (2C), 129.4, 129.5 (2C), 135.1, 135.8, 137.3, 137.9, 138.5, 138.9, 140.7, 143.8; HRMS (ESI-TOF) m/z calculated for C\(_{25}\)H\(_{24}\)N\(_2\)NaO\(_2\)S\(^+\) ([M+Na]\(^+\) ): 439.1451, Found: 439.1462.

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Ethyl 2-(1-(4-methoxyphenyl)-4-tosyl-1H-imidazol-5-yl)-2-phenylacetate

\( \text{Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 115 mg, 78%, isolated as a white solid; m.p. 168-169 °C; }^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 1.24 (t, \( J = 6.8 \) Hz, 3H), 2.42 (s, 3H), 3.79 (s, 3H), 4.19 (dq, \( J = 7.2, 6.8 \) Hz, 2H), 6.24 (s, 1H), 6.71 (d, \( J = 8.8 \) Hz, 2H), 6.80 (d, \( J = 8.8 \) Hz, 2H), 6.86 (d, \( J = 7.2 \) Hz, 2H), 7.03–7.19 (m, 3H), 7.32 (d, \( J = 8.0 \) Hz, 2H), 7.42 (s, 1H), 7.94 (d, \( J = 8.0 \) Hz, 2H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \( \delta \) 13.9, 21.5, 46.2, 55.4, 61.6, 113.9 (2C), 126.9, 127.2, 127.7 (2C), 128.0 (2C), 128.7 (2C), 129.5 (2C), 133.7, 134.7, 138.1, 138.4, 139.4, 144.0, 160.2, 169.4; HRMS (ESI-TOF) m/z calculated for C\(_{27}\)H\(_{26}\)N\(_2\)O\(_2\)S\(^+\) ([M+Na]\(^+\) ): 513.6012, Found: 513.6018.

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methyl 5-((1-ethoxy-1-oxopropan-2-yl)-1-(4-methoxyphenyl)-1H-imidazole-4-carboxylate

\( \text{Conditions: 40 °C for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 115 mg, 78%, isolated as a white solid; m.p. 168-169 °C; }^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 1.24 (t, \( J = 6.8 \) Hz, 3H), 2.42 (s, 3H), 3.79 (s, 3H), 4.19 (dq, \( J = 7.2, 6.8 \) Hz, 2H), 6.24 (s, 1H), 6.71 (d, \( J = 8.8 \) Hz, 2H), 6.80 (d, \( J = 8.8 \) Hz, 2H), 6.86 (d, \( J = 7.2 \) Hz, 2H), 7.03–7.19 (m, 3H), 7.32 (d, \( J = 8.0 \) Hz, 2H), 7.42 (s, 1H), 7.94 (d, \( J = 8.0 \) Hz, 2H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \( \delta \) 13.9, 21.5, 46.2, 55.4, 61.6, 113.9 (2C), 126.9, 127.2, 127.7 (2C), 128.0 (2C), 128.7 (2C), 129.5 (2C), 133.7, 134.7, 138.1, 138.4, 139.4, 144.0, 160.2, 169.4; HRMS (ESI-TOF) m/z calculated for C\(_{27}\)H\(_{26}\)N\(_2\)O\(_2\)S\(^+\) ([M+Na]\(^+\) ): 513.6012, Found: 513.6018.
Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 67.8 mg, 68 %, isolated as a light yellow liquid; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 1.18 (t, \(J = 7.1\) Hz, 3H), 1.42 (d, \(J = 7.0\) Hz, 3H), 3.88 (s, 3H), 3.90 (s, 3H), 4.03 (q, \(J = 7.3\) Hz, 1H), 4.09 (q, \(J = 7.1\) Hz, 2H), 7.01 (d, \(J = 8.7\) Hz, 2H), 7.23 (d, \(J = 8.7\) Hz, 2H), 7.51 (s, 1H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \(\delta\) 14.0, 15.8, 35.6, 51.5, 55.6, 61.1, 114.8 (2C), 127.4, 128.1 (2C), 129.0, 137.4, 139.6, 160.4, 163.5, 171.3; HRMS (ESI-TOF) m/z calculated for C\(_{17}\)H\(_{20}\)N\(_2\)NaO\(_5\)^+ ([M+Na]^+): 355.1264, Found: 355.1266.

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tert-butyl 5-(1-ethoxy-1-oxopropan-2-yl)-1-(4-methoxyphenyl)-1H-imidazole-4-carboxylate

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 84.2 mg, 75 %, isolated as a light yellow liquid; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 1.18 (t, \(J = 7.1\) Hz, 3H), 1.43 (d, \(J = 7.2\) Hz, 3H), 1.61 (s, 9H), 3.87 (s, 3H), 4.02 (q, \(J = 7.2\) Hz, 1H), 4.04–4.10 (m, 2H), 7.00 (d, \(J = 8.7\) Hz, 2H), 7.21 (d, \(J = 8.7\) Hz, 2H), 7.49 (s, 1H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \(\delta\) 13.9, 15.7, 28.2, 35.4, 55.4, 60.9, 80.9, 114.6, 126.5 (2C), 128.0, 130.2 (2C), 137.1, 138.4, 160.3, 162.4, 171.4; HRMS (ESI-TOF) m/z calculated for C\(_{20}\)H\(_{26}\)N\(_2\)NaO\(_5\)^+ ([M+Na]^+): 397.1734, Found: 397.1743.

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ethyl 2-(1-(4-methoxyphenyl)-4-phenyl-1H-imidazol-5-yl)propanoate

Conditions: 40 ºC for 0.5 h. Purification: Flash chromatography (PE/EtOAc, 5:1). Yield: 65.2 mg, 62 %, isolated as a yellow solid; m.p. 87-89 ºC; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 1.18 (t, \(J = 7.2\) Hz, 3H), 1.40 (d, \(J = 7.2\) Hz, 3H), 1.42 (t, \(J = 7.2\) Hz, 3H), 3.88 (s, 3H), 4.02 (q, \(J = 7.3\) Hz, 1H), 4.08 (q, \(J = 7.2\) Hz, 2H), 4.37 (dq, \(J = 7.3, 7.2\) Hz, 2H), 7.02 (d, \(J = 8.4\) Hz, 2H), 7.23 (d, \(J = 9.0\) Hz, 2H), 7.52 (s, 1H); \(^{13}\)C NMR (151 MHz, CDCl\(_3\)) \(\delta\) 14.1 (d, \(J = 43.3\) Hz), 15.7, 35.5, 60.5, 61.1, 116.7 (d, \(J = 23.1\) Hz), 128.7, 128.8, 129.6, 130.8, 130.9, 137.1, 139.0, 162.1, 162.9, 163.8, 171.1; HRMS (ESI-TOF) m/z calculated for C\(_{21}\)H\(_{23}\)N\(_2\)O\(_3\)^+ ([M+H]^+): 351.1703, Found: 351.1712.
1. Copies of $^1$H NMR and $^{13}$C NMR spectra of compounds 3

$^1$H NMR (600 MHz, CDCl$_3$) for 3aa

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3aa
$^1$H NMR (600 MHz, CDCl$_3$) for 3ba

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ba
$^1$H NMR (600 MHz, CDCl$_3$) for 3ca

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ca
$^1$H NMR (600 MHz, CDCl$_3$) for 3da

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3da
$^1$H NMR (600 MHz, CDCl$_3$) for 3ea

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ea
$^1$H NMR (600 MHz, CDCl$_3$) for 3fa

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3fa
$^1$H NMR (600 MHz, CDCl$_3$) for 3ga

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ga
$^1$H NMR (600 MHz, CDCl$_3$) for 3ha

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ha
$^1$H NMR (600 MHz, CDCl$_3$) for 3ia

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ia
$^1$H NMR (600 MHz, CDCl$_3$) for 3ja

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ja
$^1$H NMR (600 MHz, CDCl$_3$) for 3ka

13C NMR (151 MHz, CDCl$_3$) for 3ka
$^1$H NMR (600 MHz, CDCl$_3$) for 3la

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3la
$^1$H NMR (600 MHz, CDCl$_3$) for 3ma

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ma
$^1$H NMR (600 MHz, CDCl$_3$) for 3na

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3na
\(^1\)H NMR (600 MHz, CDCl\(_3\)) for 3oa

\(^{13}\)C NMR (151 MHz, CDCl\(_3\)) for 3oa
$^1$H NMR (600 MHz, CDCl$_3$) for 3pa

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3pa
$^1$H NMR (600 MHz, CDCl$_3$) for 3qa

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3qa
$^1$H NMR (400 MHz, CDCl$_3$) for 3ra

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ra
$^1$H NMR (600 MHz, CDCl$_3$) for 3sa

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3sa
$^1$H NMR (600 MHz, CDCl$_3$) for 3ta

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ta
$^1$H NMR (600 MHz, CDCl$_3$) for 3ua

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ua
$^1$H NMR (600 MHz, CDCl$_3$) for 3ab

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ab
$\text{H NMR (600 MHz, CDCl}_3\text{) for 3bb}$

$\text{C NMR (151 MHz, CDCl}_3\text{) for 3bb}$
\(^1\)H NMR (600 MHz, CDCl\(_3\)) for 3cb

13C NMR (151 MHz, CDCl\(_3\)) for 3cb
$^1$H NMR (600 MHz, CDCl$_3$) for 3db

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3db
$^1$H NMR (600 MHz, CDCl$_3$) for 3eb

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3eb
$^1$H NMR (600 MHz, CDCl$_3$) for 3fb

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3fb
$^1$H NMR (600 MHz, CDCl$_3$) for 3gb

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3gb
$^1$H NMR (600 MHz, CDCl$_3$) for 3hb

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3hb
$^1$H NMR (600 MHz, CDCl$_3$) for 3ib

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ib
**$^1$H NMR (600 MHz, CDCl$_3$) for 3jb**

![1H NMR spectrum for 3jb](image)

**$^{13}$C NMR (151 MHz, CDCl$_3$) for 3jb**

![$^{13}$C NMR spectrum for 3jb](image)
$^1$H NMR (400 MHz, CDCl$_3$) for 3kb

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3kb
$^1$H NMR (600 MHz, CDCl$_3$) for 3ac

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ac
$^1$H NMR (600 MHz, CDCl$_3$) for 3ad

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ad
$^1$H NMR (600 MHz, CDCl$_3$) for 3ae

$^{13}$C NMR (151 MHz, CDCl$_3$) for 3ae
5. X-ray Crystallographic Data of compounds 3fb

![Chemical Structure Image]

**Table 1. Crystal data and structure refinement for liujun181221_1_0m_a.**

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<th>liujun181221_1_0m_a</th>
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<td>Value</td>
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<td>--------------------------------------------</td>
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<td>Absorption correction</td>
<td>Semi-empirical from equivalents</td>
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<td>Max. and min. transmission</td>
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<td>Refinement method</td>
<td>Full-matrix least-squares on $F^2$</td>
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<tr>
<td>Data / restraints / parameters</td>
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