Supporting Information

Iodine Catalyzed Intramolecular C(Sp3)-H Functionalization: Synthesis of 2, 5-disubstituted Oxazoles from N-arylethylamides

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Experimental Section:

General: All commercially available chemicals and reagents were used without any further purification unless otherwise indicated. Acetonitrile was dried with CaH2, distilled, and stored with molecular sieves. 1H and 13C NMR spectra were recorded at 500 and 125 MHz, respectively. The spectra were recorded in CDCl3 as solvent. Multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); m (multiplet); dd (doublet of doublets), etc. and coupling constants (J) were given in Hz. Chemical shifts are reported in ppm relative to TMS as an internal standard. The peaks around delta values of 1H NMR (7.26), and 13C NMR (77.0) are corresponding to the solvent CDCl3. All products were purified through column chromatography using silica gel 100-200 mesh size using ethyl acetate/hexane as an eluent.

General procedure for the preparation of starting corresponding amides 1a-r and 1v-ae:

1.0 mmol of 2-phenylethylamine, 1.2 mmol of triethylamine and catalytic amount (5 mol%) of DIMAP were dissolved in 5 mL DCM solvent and cooled in ice bath. Then 1.2 mmol of benzoyl chloride was added drop wise and after complete the addition, it was allowed to react at room temperature under stirring for 2 h. After completion of the reaction (monitored by TLC), water was added under stirring for 5 minutes. The DCM layer was separated, dried over anhydrous Na2SO4. Removal of solvent gives white solid N-phenethylbenzamide (1a) 95 % yield. Same procedure has been followed for other starting materials (1b-r and 1v-ae).

General procedure for the preparation of starting corresponding amides 1s-u:

2 mmol of 2-phenylethylamine, 1.0 mmol of picolinamide and chitosan (20 wt. %; 24 mg) was stirred at 150°C temperature for 36 h. After the completion of the reaction (monitored by TLC), cooled to room temperature and the reaction mixture was dissolved with DCM (15 mL). After removal of solvent, the crude reaction mixture left out was purified by column chromatography (eluted with dichloromethane and ethyl acetate) using silica gel (200-400 mesh) to obtain 64% of N-phenethylpicolinamide (1t). Same procedure has been followed for other starting materials (1t-u).

A typical experimental procedure for the synthesis of 2, 5-disubstituted Oxazoles (2a):
In a sealed tube, 45 mg (0.2 mmol) of N-phenethylbenzamide (1a), I2 (0.04 mmol) 10 mg were added in 1 mL of dry acetonitrile and the tube was closed with rubber septum. Initially 120 µL (3 equiv) of TBHP (5 – 6M decane solution) was added through a syringe. Then the sealed tube was heated to 100°C under stirring and the rest of the 80 µL (2 equiv) of TBHP was added to the reaction mixture after 18 h. After complete addition of TBHP the reaction was continued another 18 h. After the completion of the reaction, reaction mixture was cooled to room temperature and added water, extracted the organic portion with DCM (2x10 mL) and dried with anhydrous sodium sulphate. After removing the solvent, the crude product left out was purified by column chromatography on silica gel (100-200 mesh) using ethyl acetate/ hexane mixture as eluent.

2,5-diphenyloxazole (2a)²:

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

Yield (30.0 mg, 68%); \(^1\)H NMR (500 MHz, CDCl\(_3\)): δ 8.12 - 8.10 (m, 2H), 7.72 (d, J = 7.5 Hz, 2H), 7.50 – 7.42 (m, 6H), 7.35 (t, J = 7.5 Hz , 1H); \(^13\)C NMR (125 MHz, CDCl\(_3\)): 155.9, 146.0, 125.1, 123.7, 123.6, 123.2, 122.8, 121.1, 119.0, 118.2.

5-(4-bromophenyl)-2-phenyloxazole (2b)³:

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

Yield (38 mg, 63%); \(^1\)H NMR (500 MHz, CDCl\(_3\)): δ 8.10 - 8.08 (m, 2H), 7.59 - 7.57 (m, 4H), 7.49 - 7.46 (m, 4H); \(^13\)C NMR (125 MHz, CDCl\(_3\)): 161.4, 150.3, 132.5, 130.5,128.8, 127.1, 126.9, 126.3, 125.6, 123.9, 122.3.

5-(4-chlorophenyl)-2-phenyloxazole (2c)²:

\[
\begin{align*}
\text{Ph} & \quad \text{O} \\
\text{N} & \quad \text{Cl}
\end{align*}
\]
Yield (34 mg, 67%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.10 - 8.09 (m, 2H), 7.66 (d, $J = 8.0$ Hz, 2H), 7.49 - 7.48 (m, 3H), 7.45 (t, $J = 8.5$ Hz, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$): 162.0, 150.2, 134.2, 130.5, 129.2, 128.8, 127.2, 126.4, 126.3, 125.4, 123.7.

5-(4-fluorophenyl)-2-phenyloxazole ($2d$):

Yield (35 mg, 74%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.10 - 8.09 (m, 2H), 7.71 - 7.69 (m, 2H), 7.49 (d, $J = 7.0$ Hz, 3H), 7.39 (s, 1H), 7.16 (t, $J = 8.5$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$): 163.6, 161.7, 161.1, 150.4, 130.4, 128.8, 127.2, 126.2, 126.1, 126.0, 124.3, 123.0, 116.2, 116.0.

5-(2-methoxyphenyl)-2-phenyloxazole ($2e$):

Yield (21 mg, 42%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.08 (s, 2H), 7.87 (d, $J = 7.5$ Hz, 1H), 7.73 (s, 1H), 7.44 (s, 3H), 7.34 (t, $J = 7.5$ Hz, 1H), 7.09 (t, $J = 7.5$ Hz, 1H), 7.01 (d, $J = 8.0$ Hz, 1H), 3.99 (s, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$): 159.1, 154.7, 146.8, 129.3, 128.2, 127.7, 126.3, 125.5, 124.7, 119.8, 109.9, 54.4.

2-phenyl-5-(pyridin-2-yl)oxazole ($2f$):

Yield (21 mg, 48%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.63 – 8.62 (m, 1H), 8.08 – 8.06 (m, 2H), 7.77 (s, 1H), 7.74 (t, $J = 8.0$ Hz, 1H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.41 – 7.40 (m, 3H), 7.19 – 7.17 (m, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$): 162.0, 150.4, 149.7, 147.0, 137.1, 133.0, 130.7, 129.9, 128.8, 128.3, 127.0, 126.5, 122.9, 119.2.

2-(2-fluorophenyl)-5-phenyloxazole ($2g$):
Yield (34.5 mg, 72%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.12 (t, $J$ = 7.0 Hz, 1H), 7.75 (d, $J$ = 7.5 Hz, 1H), 7.51 (s, 1H), 7.46 (t, $J$ = 8.0 Hz, 2H), 7.38 – 7.34 (m, 1H), 7.30 – 7.21 (m, 4H); $^{13}$C NMR (125 MHz, CDCl$_3$): 161.6, 161.0, 158.9, 157.5, 157.4, 151.4, 131.9, 131.8, 129.8, 129.3, 128.9, 128.6, 128.3, 127.7, 124.3, 123.3, 116.9, 116.8.

2-(3-bromophenyl)-5-phenyloxazole (2h)$^7$:

Yield (37 mg, 62%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.25 (s, 1H), 8.04 (d, $J$ = 8.0 Hz, 1H), 7.73 (d, $J$ = 7.5 Hz, 2H), 7.59 (d, $J$ = 8.0 Hz, 1H), 7.47 – 7.44 (m, 3H), 7.37 – 7.34 (m, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$): 158.6, 150.7, 132.1, 129.3, 128.1, 127.9, 127.6, 126.7, 123.7, 123.2, 122.5, 121.9.

2-(3-chlorophenyl)-5-phenyloxazole (2i)$^3$:

Yield (33 mg, 64%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.11 – 8.09 (m, 1H), 8.00 – 7.99 (m, 1H), 7.73 (d, $J$ = 8.0 Hz, 2H), 7.47 – 7.42 (m, 5H), 7.38 (t, $J$ = 7.5 Hz, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$): 159.7, 151.7, 134.9, 130.3, 130.1, 129.0, 128.7, 126.2, 124.3, 123.5.

2-(3-fluorophenyl)-5-phenyloxazole (2j)$^7$:
Yield (34.5 mg, 72%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.90 (d, $J = 7.5$ Hz, 1H), 7.80 – 7.78 (m, 1H), 7.73 (d, $J = 7.5$ Hz, 2H), 7.47 – 7.44 (m, 4H), 7.37 (t, $J = 7.5$ Hz, 1H), 7.17 – 7.14 (m, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$): 163.9, 161.9, 159.9, 151.6, 130.6, 130.5, 129.0, 128.7, 127.7, 124.2, 123.5, 121.9, 117.3, 117.2, 113.3, 113.1.

2-(4-bromophenyl)-5-phenyloxazole (2k)$^8$:

Yield (36 mg, 60%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.98 (d, $J = 8.5$ Hz, 2H), 7.72 (d, $J = 8.0$ Hz, 2H ), 7.62 (d, $J = 8.5$ Hz, 2H ), 7.46 – 7.43 (m, 3H), 7.37 (t, $J = 7.0$ Hz, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$): 160.2, 151.5, 132.0, 128.9, 128.6, 128.4, 127.8, 127.7, 124.7, 124.2, 123.5.

2-(4-chlorophenyl)-5-phenyloxazole (2l)$^2$:

Yield (33 mg, 64%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.04 (d, $J = 9.0$ Hz, 2H ), 7.71 (d, $J = 7.5$ Hz, 2H ), 7.46 – 7.43 (m, 5H), 7.36 (t, $J = 7.5$ Hz, 1H ); $^{13}$C NMR (125 MHz, CDCl$_3$): 160.2, 151.5, 136.4, 129.1, 128.9, 128.6, 127.7, 127.5, 125.9, 124.2, 123.5.

2-(4-fluorophenyl)-5-phenyloxazole (2m)$^2$:
Yield (36 mg, 76%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.11 – 8.09 (m, 2H), 7.72 (d, $J = 8.0$ Hz, 2H), 7.46 (t, $J = 7.5$ Hz, 3H), 7.36 (t, $J = 7.5$ Hz, 1H), 7.19 (t, $J = 8.5$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$): 165.0, 163.0, 160.3, 151.3, 128.9, 128.5, 128.4, 128.3, 127.8, 124.1, 123.3, 116.1, 115.9.

2-(4-nitrophenyl)-5-phenyloxazole (2n)$^2$:

Yield (39 mg, 74%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.35 (d, $J = 8.0$ Hz, 2H), 8.27 (d, $J = 8.0$ Hz, 2H), 7.75 (d, $J = 7.5$ Hz, 2H), 7.53 (s, 1H), 7.49 (t, $J = 7.5$ Hz, 2H), 7.41 (t, $J = 7.5$ Hz, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$): 158.9, 152.8, 148.5, 132.8, 129.2, 129.1, 127.3, 126.8, 124.5, 124.2.

5-phenyl-2-(4-(trifluoromethyl)phenyl)oxazole (2o)$^2$:

Yield (40 mg, 69%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.22 (d, $J = 8.0$ Hz, 2H), 7.75 – 7.73 (m, 4H), 7.48 – 7.44 (m, 3H), 7.39 – 7.35 (m, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$): 159.7, 152.1, 131.9, 131.7, 130.5, 129.8, 129.0, 128.8, 128.7, 128.5, 127.6, 127.4, 126.4, 125.8, 124.3, 123.7, 122.7.

5-phenyl-2-(p-tolyl)oxazole (2p)$^2$:

Yield (25 mg, 53%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.00 (d, $J = 7.5$ Hz, 2H), 7.72 (d, $J = 7.5$ Hz, 2H), 7.45 – 7.42 (m, 3H), 7.35 (t, $J = 7.5$ Hz, 1H), 7.29 (d, $J = 8.0$ Hz, 2H), 2.41 (s, 3H); $^{13}$C
NMR (125 MHz, CDCl₃): 149.9, 139.6, 128.5, 127.8, 127.2, 127.0, 125.2, 123.7, 123.1, 122.2, 20.4.

2-(4-methoxyphenyl)-5-phenyloxazole (2q):

![Structure of 2q]

Yield (25.5 mg, 51%); ¹H NMR (500 MHz, CDCl₃): δ 8.05 (d, J = 9.0 Hz, 2H), 7.71 (d, J = 7.0 Hz, 2H), 7.45 – 7.41 (m, 3H), 7.34 (t, J = 7.5 Hz, 1H), 7.00 – 6.98 (m, 2H), 3.87 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 160.3, 160.2, 149.7, 127.8, 127.1, 126.9, 123.0, 122.1, 119.2, 113.2, 54.3.

5-phenyl-2-(thiophen-2-yl)oxazole (2r):

![Structure of 2r]

Yield (25 mg, 56%); ¹H NMR (500 MHz, CDCl₃): δ 7.75 – 7.74 (m, 1H), 7.70 (d, J = 8.0 Hz, 2H), 7.45 – 7.42 (m, 3H), 7.39 (s, 1H), 7.35 – 7.32 (m, 1H), 7.15 – 7.13 (m, 1H); ¹³C NMR (125 MHz, CDCl₃): 157.4, 150.8, 130.0, 128.9, 128.6, 128.4, 128.2, 127.9, 127.7, 127.6, 124.1, 123.3.

5-phenyl-2-(pyridin-2-yl)oxazole (2s):

![Structure of 2s]

Yield (17.5 mg, 39%); ¹H NMR (500 MHz, CDCl₃): δ 8.60 – 8.58 (m, 1H), 8.21 (d, J = 7.5 Hz, 1H), 7.88 – 7.81 (m, 3H), 7.53 (d, J = 6.5 Hz, 1H), 7.47 (d, J = 7.0 Hz, 3H), 7.40 (t, J = 6.5 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃): 160.1, 153.1, 149.4, 146.0, 137.3, 128.7, 128.6, 127.3, 126.5, 124.7, 124.6, 122.4.

5-phenyl-2-(pyridin-3-yl)oxazole (2t):
Yield (20.5 mg, 46%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 9.35 (s, 1H), 8.71 – 8.70 (m, 1H), 8.39 (d, $J = 8.0$ Hz, 1H), 8.11 (d, $J = 8.5$ Hz, 1H), 7.74 (d, $J = 8.5$ Hz, 2H) 7.49 – 7.43 (m, 4H); $^{13}$C NMR (125 MHz, CDCl$_3$): 158.6, 152.0, 150.7, 147.3, 133.5, 133.2, 130.0, 129.0, 128.8, 128.7, 128.3, 127.5, 124.3, 123.7, 123.6.

5-phenyl-2-(pyridin-4-yl)oxazole ($2u$)$^9$:

Yield (18 mg, 41%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.73 (d, $J = 6.0$ Hz, 2H), 7.91 (d, $J = 6.0$ Hz, 2H), 7.71 (d, $J = 9.0$ Hz, 2H), 7.49 (s, 1H), 7.43 – 7.41 (m, 2H), 7.36 (t, $J = 7.5$ Hz, 1H) $^{13}$C NMR (125 MHz, CDCl$_3$): 161.4, 154.0, 150.5, 134.2, 132.4, 132.0, 130.8, 129.1, 129.0, 128.82, 128.8,128.7, 128.6, 127.3, 124.5, 124.0, 119.8.

2-cyclohexyl-5-phenyloxazole ($2v$)$^2$:

Yield (23.6 mg, 52%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.58-7.53(m, 2H), 7.35 – 7.33 (m, 2H),7.25 – 7.23 (m, 1H), 7.19 (s, 1H), 2.81 – 2.75 (m,1H), 2.06 – 2.04 (m,2H), 1.79 – 1.76 (m, 2H), 1.58 – 1.52 (m, 3H), 1.36 – 1.30 (m, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$): 168.3, 149.7, 129.2, 128.9, 128.6, 124.1, 121.9, 37.7, 30.7, 25.9, 25.7.

2-(tert-butyl)-5-phenyloxazole ($2w$)$^2$: 

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Yield (26 mg, 64%); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.62 (d, $J = 7.5$ Hz, 2H), 7.41 (t, $J = 7.5$ Hz, 2H), 7.31 (d, $J = 7.5$ Hz, 1H), 7.20 (s, 1H), 1.44 (s, 9H); $^{13}$C NMR (125 MHz, CDCl$_3$): 170.8, 150.6, 128.7, 128.5, 128.4, 128.0, 123.9, 121.4, 33.8, 28.6.

5-(4-chlorophenyl)-2-(2-fluorophenyl)oxazole (2x):

Yield (43 mg, 78%, White solid); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.11 – 8.07 (m, 1H), 7.67 (d, $J = 8.0$ Hz, 1H), 7.50 – 7.47 (m, 1H), 7.43 (d, $J = 8.5$ Hz, 1H), 7.29 – 7.22 (m, 4H), 7.12 – 7.08 (m, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$): 161.7, 161.0, 159.7, 159.0, 157.7, 150.5, 134.0, 133.7, 133.6, 132.2, 131.1, 129.3, 129.2, 128.5, 125.5, 123.7, 117.0, 116.8, 116.2, 116.0. HRMS-calculated for C$_{15}$H$_{10}$NOFCl = 274.0435; found 274.0429.

5-(4-bromophenyl)-2-(4-(trifluoromethyl)phenyl)oxazole (2y):

Yield (48 mg, 65%, White solid); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.20 (d, $J = 8.5$ Hz, 2H), 7.74 (d, $J = 8.5$ Hz, 2H), 7.58 (s, 4H), 7.48 (s, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$): 154.7, 154.9, 127.2, 127.0, 126.9, 126.6, 125.1, 121.3, 120.7, 120.5, 119.7, 119.0, 117.6, 117.5. HRMS-calculated for C$_{16}$H$_{10}$NOF$_3$Br = 367.9898; found 367.9887.

2,5-bis(4-fluorophenyl)oxazole (2z)$^4$:
Yield (36 mg, 70%); $^1$H NMR (500 MHz, CDCl$_3$): δ 8.10 – 8.07 (m, 2H), 7.70 – 7.67 (m, 2H), 7.37 (s, 1H), 7.19 – 7.13 (m, 4H); $^{13}$C NMR (125 MHz, CDCl$_3$): 165.0, 163.6, 163.0, 161.7, 160.3, 150.5, 128.4, 128.3, 126.1, 126.0, 124.2, 123.6, 123.0, 116.2, 116.1, 116.0, 115.9.

2,5-bis(4-chlorophenyl)oxazole (2aa):  

Yield (39.5 mg, 68%, White solid); $^1$H NMR (500 MHz, CDCl$_3$): δ 8.03 (d, $J = 8.5$ Hz, 2H), 7.64 (d, $J = 8.5$ Hz, 2H), 7.46 – 7.41 (m, 4H), 7.46 – 7.45 (m, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$): 160.4, 150.5, 136.6, 134.4, 129.3, 129.2, 127.5, 126.2, 125.4, 123.8. HRMS - calculated for C$_{15}$H$_{10}$NOCl$_2$ = 290.0139; found 290.0139.

5-(4-bromophenyl)-2-(4-chlorophenyl)oxazole (2ab):  

Yield (43.5 mg, 65%, Yellow solid); $^1$H NMR (500 MHz, CDCl$_3$): δ 8.03 (d, $J = 7.5$ Hz, 2H), 7.61 – 7.57 (m, 4H), 7.46 – 7.45 (m, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$): 160.4, 150.5, 136.6, 132.2, 131.8, 131.6, 129.4, 129.3, 129.2, 127.5, 126.6, 125.6, 123.9, 122.5. HRMS - calculated for C$_{15}$H$_{10}$NOClBr = 333.9634; found 333.9644.

5-(4-bromophenyl)-2-(4-fluorophenyl)oxazole (2ac):
Yield (41 mg, 65%, White solid); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.09 – 8.07 (m, 2H), 7.60 – 7.56 (m, 4H), 7.42 (s, 1H), 7.18 (t, $J = 8.5$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$): 165.1, 163.1, 160.5, 150.3, 132.1, 131.7, 128.5, 128.4, 126.8, 125.6, 123.8, 123.6, 122.3, 116.1, 116.0. HRMS-calculated for C$_{18}$H$_{10}$NOFBr = 317.9930; found 317.9915.

5-(4-chlorophenyl)-2-(4-fluorophenyl)oxazole (2ad):

Yield (37 mg, 67%, White solid); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.10 – 8.07 (m, 2H), 7.64 (d, $J = 8.5$ Hz, 2H), 7.43 – 7.41 (m, 3H), 7.19 (t, $J = 8.5$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$): 165.1, 163.1, 160.5, 150.3, 134.2, 130.5, 129.2, 128.5, 128.4, 126.3, 125.3, 123.7, 116.1. 116.0. HRMS-calculated for C$_{15}$H$_{10}$NOFCl = 274.0435; found 274.0424

5-(4-chlorophenyl)-2-(4-(trifluoromethyl)phenyl)oxazole (2ae):

Yield (41.5 mg, 64%, Yellow solid); $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.21 (d, $J = 8.5$ Hz, 2H), 7.75 (d, $J = 8.0$ Hz, 2H), 7.67 (d, $J = 8.5$ Hz, 2H), 7.48 (s, 1H), 7.44 (d, $J = 8.5$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$): 159.9, 151.1, 134.6, 131.5, 130.3, 129.3, 128.8, 126.5, 126.1, 126.0, 125.9, 125.5, 124.1. HRMS-calculated for C$_{16}$H$_{10}$NOF$_3$Cl = 324.0403; found 324.0406.
5-hexyl-2-phenyloxazole (2af)\(^{11}\):

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

Yield (13 mg, 28\%); \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.99 (d, \(J = 6.5\) Hz, 2H), 7.45 – 4.41 (m, 3H), 6.83 (s, 1H), 2.71 (t, \(J = 7.5\) Hz, 2H), 1.71 – 1.66 (m, 2H), 1.41 – 1.37 (m, 2H), 1.33 – 1.32 (m, 4H), 0.89 (t, \(J = 7.0\) Hz, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)): 160.5, 153.2, 129.8, 128.6, 127.8, 125.9, 123.5, 31.4, 28.7, 27.5, 25.6, 22.5, 14.0.

5-octyl-2-phenyloxazole (2ag)\(^{2}\):

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

Yield (13 mg, 25\%); \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.98 (d, \(J = 6.5\) Hz, 2H), 7.43 – 4.39 (m, 3H), 6.82 (s, 1H), 2.69 (t, \(J = 7.5\) Hz, 2H), 1.71 – 1.65 (m, 2H), 1.39 – 1.35 (m, 2H), 1.32 – 1.28 (m, 8H), 0.88 (t, \(J = 7.0\) Hz, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)): 160.5, 153.2, 129.8, 128.6, 127.8, 125.9, 123.5, 31.4, 29.2, 29.1, 29.0, 27.6, 25.6, 22.6, 14.0.

References:


Copies of $^1$H & $^{13}$C- NMR

$^1$H NMR of 2a

$^{13}$C NMR of 2a
$^1$H NMR of 2c

$^{13}$C NMR of 2c
\(^1\)H NMR of 2d

\(^{13}\)C NMR of 2d
$^1$H NMR of 2e

$^{13}$C NMR of 2e
$^1$H NMR of 2f

$^{13}$C NMR of 2f
$^1$H NMR of 2g

$^{13}$C NMR of 2g
$^1$H NMR of 2h

$^{13}$C NMR of 2h
$^1$H NMR of 2i

$^{13}$C NMR of 2i
$^1$H NMR of 2j

$^{13}$C NMR of 2j
$^{1}H$ NMR of 2k

$^{13}C$ NMR of 2k
$^1$H NMR of 2l

$^{13}$C NMR of 2l
$^{1}H$ NMR of 2m

$^{13}C$ NMR of 2m
**H NMR of 2n**

Supravat
SS-779
H1 in CDCl3
500 MHz

**13C NMR of 2n**

Supravat
SS-779
13C in CDCl3
500 MHz
$^{1}H$ NMR of 2o

$^{13}C$ NMR of 2o
$^1$H NMR of 2p

$^{13}$C NMR of 2p

S30
$^{1}H$ NMR of 2q

$^{13}C$ NMR of 2q

S31
$^1$H NMR of 2t

$^{13}$C NMR of 2t
$^1$H NMR of 2u

$^{13}$C NMR of 2u
$^1$H NMR of 2v

$^{13}$C NMR of 2v
\(^1\text{H NMR of 2w}\)

\(^{13}\text{C NMR of 2w}\)
$^1$H NMR of 2x

$^{13}$C NMR of 2x
$^1$H NMR of 2y

$^{13}$C NMR of 2y
$^{13}$C NMR of 2z

$^1$H NMR of 2z
\textbf{H NMR of 2aa}

\textbf{\textsuperscript{13}C NMR of 2aa}
H NMR of 2ab

Supravat
SS-771
H1m CDCl3
600 MHz

1H NMR of 2ab

Supravat
SS-771
13C in CDCl3
500 MHz

13C NMR of 2ab
$^1$H NMR of 2ac

$^{13}$C NMR of 2ac
$^1$H NMR of 2ad

$^{13}$C NMR of 2ad
1H NMR of 2ae

13C NMR of 2ae
$^1$H NMR of 2af

$^{13}$C NMR of 2af
HRMS of 2x

HRMS of 2y
**HRMS of 2aa**

**Elemental Composition Report**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monosotopic Mass, Even Electron ions
12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used
C: 0-18  H: 0-10  N: 0-1  O: 0-1  Cl: 0-1

**HRMS of 2ab**

**Elemental Composition Report**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monosotopic Mass, Even Electron ions
12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used
C: 0-18  H: 0-10  N: 0-1  O: 0-1  Br: 0-1
HRMS of 2ac

HRMS of 2ad
HRMS of 2ae

HRMS of the reaction mixture using TEMPO (3):