Supporting Information

Visible-Light-Promoted Direct Trifluoromethylation and Perfluoroalkylation of Imidazopyridines

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1. General Information

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Imidazo[1,2-a]pyridines and liquid trifluoromethylation reagents TMG- CF₃I were prepared according to the literature procedures.¹,² Products were purified by column chromatography on 200-300 mesh silica gel, SiO₂. ¹H NMR, ¹⁹F NMR and ¹³C NMR spectra were measured on a 400 MHz NMR spectrometer using CDCl₃ as the solvent. The chemical shifts are given in δ relative to TMS, and the coupling constants are given in Hertz. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; qui, quintet; sxt, sextet. The HRMS analyses were conducted using a TOF MS instrument with an EI source. Melting points were measured by a melting point instrument and were uncorrected.

2. Experimental section

2.1 General experimental procedure for trifluoromethylation reaction.

Imidazo[1,2-a]pyridine 1 (0.3 mmol, 1.0 eq) was added to a 10 mL Schlenk flask equipped with a high-vacuum PTFE valve-to-glass seal. The flask was evacuated and backfilled with nitrogen for 3 times, and then TMG- CF₃I 2 (0.6 mmol, 2.0 eq), DBU (0.9mmol, 3.0 eq) and CH₃CN (0.75 mL) were added. The mixture was stirred under Blue LED strip irradiation for 16 h. When the reaction was completed, the solvent was removed in vacuum, and the product was purified by silica gel chromatography using petroleum ether/ethyl acetate (20:1 to 8:1, v/v) as eluent to afford the pure product 3.

Larger-scale synthesis of 3aa. 2-phenylimidazo[1,2-a]pyridine 1a (388.5 mg, 2.0mmol) was added to a 25 mL Schlenk flask equipped with a high-vacuum PTFE valve-to-glass seal. The flask was evacuated and backfilled with nitrogen for 3 times, and then TMG- CF₃I 2a (0.8 mL, 4.0
mmol), DBU (913.4 mg, 6.0 mmol) and CH$_3$CN (5.0 mL) were added. The mixture was stirred under blue LED strip irradiation for 16 h. When the reaction was completed, the solvent was removed in vacuum. The residue was purified by silica gel chromatography using petroleum ether/ethyl acetate (10:1, v/v) as eluent to afford the pure product 3aa (411.1 mg, 78% yield).

2.2 Mechanism experiments.

2-phenylimidazo[1,2-a]pyridine 1a (58.3 mg, 0.3 mmol) and TEMPO (187.5 mg, 1.2 mmol) were added to a 10 mL Schlenk flask equipped with a high-vacuum PTFE valve-to-glass seal. The flask was evacuated and backfilled with nitrogen for 3 times, and then TMG-CF$_3$I 2a (0.12 mL, 0.6 mmol), DBU (137.0 mg, 0.9 mmol) and CH$_3$CN (0.75 mL) were added. The mixture was stirred under Blue LED strip irradiation for 16 h. When the reaction was completed, products 3aa and TEMPO-bound adduct could not be detected.

2-phenylimidazo[1,2-a]pyridine 1a (58.3 mg, 0.3 mmol) were added to a 10 mL Schlenk flask equipped with a high-vacuum PTFE valve-to-glass seal. The flask was evacuated and backfilled with nitrogen for 3 times, and then TMG-CF$_3$I 2a (0.12 mL, 0.6 mmol), DBU (137.0 mg, 0.9 mmol) 1,1-diphenylethylene (108.2 mg, 0.6 mmol) and CH$_3$CN (0.75 mL) were added. The mixture was stirred under Blue LED strip irradiation for 16 h. When the reaction was completed, species 5 was detected in the reaction mixture by GC-MS analysis.
2.3 UV/Vis absorption spectra.

The UV/Vis absorption spectra of CH$_3$CN solutions of DBU (0.1 M), TMG-CF$_3$I (0.1 M), and a mixture of TMG-CF$_3$I and DBU are shown in Figure S1. A bathochromic shift can be observed, indicating the formation of an EDA complex.
2.4 Determination of Binding Stoichiometry and Association Constant by $^{19}$F NMR

The $^{19}$F NMR spectra of mixtures of TMG-CF$_3$I (2a) and DBU in CDCl$_3$ were recorded at 298 K by using benzotrifluoride ($\delta = -63.2$ ppm) as internal standard (Fig S2). The total volume of the solution was 0.7 mL. The total amount of 2a and DBU was kept constant at 0.35 mmol (0.5 M). The amount of 2a was varied from 0 to 0.35 mmol, corresponding to 0.0, 0.2, 0.4, 0.5, 0.6, 0.8, 1.0 molar ratio. The chemical shift difference ($\Delta\delta$) between CF$_3$I in the different mixtures was calculated and the binding stoichiometry was then determined using Job’s plot analysis,$^3$ plotting $[2a]/[2a + DBU]$ vs $[2a] \times \Delta\delta$.

![Fig S2, $^{19}$F NMR shift of 2a with DBU](image)

<table>
<thead>
<tr>
<th>Table S1. Experimental data for Job plot analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar Ratio</td>
</tr>
<tr>
<td>----------</td>
</tr>
<tr>
<td>0.0</td>
</tr>
<tr>
<td>0.2</td>
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The Job plot analysis has demonstrated that 2a and DBU are associated in 1:1 ratio complex ratio through halogen bonding.

Then, the association constant (Ka) of the complex has been calculated using Hanna and Ashbaugh's method. 19F NMR spectra of nine mixtures of TMG·CF$_3$I (2a) and DBU were recorded in the CDCl$_3$. Benzotrifluoride was used as the internal standard (25 µL, δ = -63.2 ppm). The total volume of the solution was 0.7 mL. The amount of 2a was kept constant at 0.1 mmol (0.143 M). The amount of DBU was varied from 0 to 3 mmol, corresponding to 0, 1, 1.5, 3, 6, 10, 12, 20, 30 equivalents with respect to 2a. The chemical shift difference

<table>
<thead>
<tr>
<th>0.4</th>
<th>0.2</th>
<th>0.3</th>
<th>2.168</th>
<th>0.4</th>
<th>0.434</th>
</tr>
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<tbody>
<tr>
<td>0.5</td>
<td>0.25</td>
<td>0.25</td>
<td>1.725</td>
<td>0.5</td>
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<tr>
<td>0.6</td>
<td>0.3</td>
<td>0.2</td>
<td>1.468</td>
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<td>0.440</td>
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<tr>
<td>0.8</td>
<td>0.4</td>
<td>0.1</td>
<td>0.714</td>
<td>0.8</td>
<td>0.286</td>
</tr>
<tr>
<td>1.0</td>
<td>0.5</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>
(\(\Delta\delta\)) between CF\(_3\)I in the different mixtures was calculated and the association constant was then determined plotting 1/ [DBU] vs 1/\(\Delta\delta\).

**Table S2. Experimental data for association constant determination.**

<table>
<thead>
<tr>
<th>Entry</th>
<th>[2a]</th>
<th>[DBU]</th>
<th>1/[DBU]</th>
<th>(\Delta\delta)</th>
<th>1/(\Delta\delta)</th>
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<tbody>
<tr>
<td>1</td>
<td>0.143</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0.143</td>
<td>0.14</td>
<td>7</td>
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<tr>
<td>3</td>
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<td>0.21</td>
<td>4.67</td>
<td>2.33</td>
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<tr>
<td>4</td>
<td>0.143</td>
<td>0.43</td>
<td>2.33</td>
<td>4.23</td>
<td>0.24</td>
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<tr>
<td>5</td>
<td>0.143</td>
<td>0.86</td>
<td>1.17</td>
<td>6.72</td>
<td>0.15</td>
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<td>6</td>
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<td>0.70</td>
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<td>0.106</td>
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<tr>
<td>7</td>
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<td>8</td>
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<tr>
<td>9</td>
<td>0.143</td>
<td>4.29</td>
<td>0.23</td>
<td>13.43</td>
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</table>

![Fig S4. Association constant determination](image)

\[
K_a = \frac{\text{intercept}}{\text{gradient}} = \frac{0.0541}{0.0797} = 0.68 \text{ M}^{-1}
\]

The association constant between 2a and DBU was calculated to be 0.68 M\(^{-1}\) in CDCl\(_3\).

**2.5 Light on/off experiments.**

Under an \(N_2\) atmosphere, a mixture of 2-phenylimidazo[1,2-a]pyridine 1a (116.6 mg, 0.6 mmol),
TMG-CF$_3$I 2a (0.24 mL, 1.2 mmol), DBU (274.0 mg, 1.8 mmol) in 1.5 mL CH$_3$CN was stirred at ambient temperature under visible-light irradiation of a 25 W blue LED. The reaction mixture was stirred with the LED irradiation on and off over time. Samples were taken for determining yields of the target product 3aa by GC analysis with 1,3,5-trimethoxybenzene as an internal standard (Table S3).

**Table S3. Light On/Off Experiments**

<table>
<thead>
<tr>
<th>Entry</th>
<th>Time (h)</th>
<th>Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0→2</td>
<td>27</td>
</tr>
<tr>
<td>2</td>
<td>2→4</td>
<td>29</td>
</tr>
<tr>
<td>3</td>
<td>4→6</td>
<td>43</td>
</tr>
<tr>
<td>4</td>
<td>6→8</td>
<td>43</td>
</tr>
<tr>
<td>5</td>
<td>8→10</td>
<td>56</td>
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<tr>
<td>6</td>
<td>10→12</td>
<td>56</td>
</tr>
</tbody>
</table>

$^a$1a (116.6 mg, 0.6 mmol), TMG- CF$_3$I 2a (0.24 mL, 1.2 mmol), DBU (274.0 mg, 1.8 mmol), CH$_3$CN (1.5 mL), 25°C, 25 W blue LED, N$_2$.

$^b$Yields were determined by GC analysis with 1,3,5-trimethoxybenzene as an internal standard.
3. Characterization data of products

![Chemical Structure](image)

**2-phenyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3aa).** White solid, 69 mg, Yield: 88%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.27 (d, $J = 6.9$ Hz, 1H), 7.75 – 7.67 (m, 3H), 7.50 – 7.41 (m, 3H), 7.32 (t, $J = 8.0$ Hz, 1H), 6.91 (t, $J = 7.0$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 147.9 (d, $J = 2.1$ Hz), 146.0, 132.8, 129.5 (d, $J = 1.7$ Hz), 128.8, 128.0, 126.8, 125.3 (q, $J = 3.8$ Hz), 121.8 (q, $J = 265.9$ Hz), 117.9, 113.8 109.4 (q, $J = 39.6$ Hz). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -57.6. The spectral data were in accordance with the literature. 

![Chemical Structure](image)

**2-(o-tolyl)-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ba).** Yellow liquid, 59 mg, Yield: 71%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.32 (d, $J = 7.0$ Hz, 1H), 7.74 (d, $J = 9.1$ Hz, 1H), 7.44 – 7.24 (m, 5H), 7.02 (t, $J = 7.0$ Hz, 1H), 2.29 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 147.5 (d, $J = 2.0$ Hz), 146.0, 136.9, 132.5, 130.1, 129.9, 128.8, 126.8, 125.2, 121.6 (q, $J = 265.7$ Hz), 118.0, 113.8, 110.6 (q, $J = 38.8$ Hz), 19.7. $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -59.4. The spectral data were in accordance with the literature.

![Chemical Structure](image)

**2-(m-tolyl)-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ca)** White solid, 63 mg, Yield: 76%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.30 (d, $J = 6.9$ Hz, 1H), 7.72 (d, $J = 9.2$ Hz, 1H), 7.54 (s, 1H), 7.47 (d, $J = 7.7$ Hz, 1H), 7.40 – 7.30 (m, 2H), 7.25 (d, $J = 8.0$ Hz, 1H), 6.96 (t, $J = 6.9$ Hz, 1H),
2.42 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 148.2 (d, $J = 2.1$ Hz), 146.0, 137.8, 132.7, 130.1 (d, $J = 1.0$ Hz), 129.7, 128.0, 126.8, 126.7 (q, $J = 1.9$ Hz), 125.4 (q, $J = 3.7$ Hz), 122.0 (q, $J = 267.5$ Hz). 118.0, 113.8, 109.4 (q, $J = 39.5$ Hz), 21.3. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.6. The spectral data were in accordance with the literature.  

![Chemical Structure](image)

2-(p-tolyl)-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3da) White solid, 69 mg, Yield: 83%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.29 (d, $J = 6.9$ Hz, 1H), 7.71 (d, $J = 9.1$ Hz, 1H), 7.60 (d, $J = 7.7$ Hz, 2H), 7.36 (t, $J = 8.0$ Hz, 1H), 7.27 (d, $J = 7.7$ Hz, 2H), 6.96 (t, $J = 6.9$ Hz, 1H), 2.41 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 148.1 (d, $J = 2.6$ Hz), 146.0, 138.8, 129.9, 129.4 (q, $J = 2.0$ Hz), 128.8, 126.8, 125.4 (q, $J = 4.2$ Hz), 121.9 (q, $J = 267.4$ Hz), 117.9, 113.7, 109.2 (q, $J = 39.5$ Hz), 21.2. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.6. The spectral data were in accordance with the literature.  

![Chemical Structure](image)

8-methyl-2-phenyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ea) Yellow liquid, 67 mg, Yield: 81%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.17 (d, $J = 6.9$ Hz, 1H), 7.69 (d, $J = 6.9$ Hz, 2H), 7.50 – 7.40 (m, 3H), 7.17 (d, $J = 6.9$ Hz, 1H), 6.90 (t, $J = 7.0$ Hz, 1H), 2.68 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 147.5 (d, $J = 2.4$ Hz), 146.5, 133.2, 129.7 (d, $J = 1.7$ Hz), 128.8, 128.2, 128.1, 125.6, 123.2 (q, $J = 4.1$ Hz), 121.0 (q, $J = 266.7$ Hz), 113.9, 109.8, 17.1. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.8. The spectral data were in accordance with the literature.
7-methyl-2-phenyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3fa) Yellow solid, 62 mg, Yield: 74%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.15 (d, $J$ = 7.1 Hz, 1H), 7.68 (d, $J$ = 7.2 Hz, 2H), 7.50 – 7.37 (m, 4H), 6.82 – 6.73 (m, 1H), 2.42 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 147.9 (d, $J$ = 2.3 Hz), 146.5, 138.2, 133.0, 129.5 (q, $J$ = 1.7 Hz), 128.8, 128.1, 124.5 (q, $J$ = 3.6 Hz), 122.0 (q, $J$ = 265.6 Hz), 116.4, 116.3, 108.9 (q, $J$ = 39.1 Hz), 21.2. $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -57.5. The spectral data were in accordance with the literature.$^7$

6-methyl-2-phenyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ga) Yellow solid, 58 mg, Yield: 70%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.07 (s, 1H), 7.68 (d, $J$ = 7.0 Hz, 2H), 7.62 (d, $J$ = 9.2 Hz, 1H), 7.49 – 7.39 (m, 3H), 7.22 (d, $J$ = 9.3 Hz, 1H), 2.38 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 147.7 (d, $J$ = 1.9 Hz), 145.1, 133.1, 130.0, 129.5 (q, $J$ = 1.6 Hz), 128.7, 128.1, 123.8, 123.1 (q, $J$ = 3.6 Hz), 121.9 (q, $J$ = 265.7 Hz), 117.2, 109.1 (q, $J$ = 39.4 Hz), 18.3. $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -57.7. The spectral data were in accordance with the literature.$^6$

5-methyl-2-phenyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ha) White solid; m.p. 69.2-69.9 °C, 47 mg, Yield: 56%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.69 – 7.58 (m, 3H), 7.49 – 7.38 (m,
3H), 7.32 (t, J = 8.0 Hz, 1H), 6.78 (d, J = 6.4 Hz, 1H), 2.80 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 150.8 (d, $J$ = 2.5 Hz), 148.2, 137.4, 134.3, 129.7 (q, $J$ = 1.6 Hz), 128.7, 127.9, 127.5, 121.9 (q, $J$ = 265.5 Hz), 115.7, 109.7 (q, $J$ = 39.8 Hz), 20.5 (q, $J$ = 6.9 Hz). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -46.6; HRMS (EI) m/z: [M]$^+$ calcd for C$_{15}$H$_{11}$F$_3$N$_2$ 276.0869, found 276.0876.

![Chemical Structure](image)

**6-methyl-2-(p-tolyl)-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ia)** Pale yellow solid, 66 mg. Yield: 76%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.06 (s, 1H), 7.65 – 7.52 (m, 3H), 7.29 – 7.17 (m, 3H), 2.41 (s, 3H), 2.38 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 147.9, 145.1, 138.7, 130.2, 129.9, 129.4 (q, $J$ = 1.7 Hz), 128.8, 123.6, 123.1 (q, $J$ = 4.3 Hz), 122.0 (q, $J$ = 265.7 Hz), 117.2, 109.0 (q, $J$ = 39.5 Hz), 21.3, 18.3. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.7. The spectral data were in accordance with the literature.$^8$

![Chemical Structure](image)

**2-(4-methoxyphenyl)-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ja)** White solid, 74 mg. Yield: 84%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.26 (d, $J$ = 6.9 Hz, 1H), 7.68 (d, $J$ = 9.1 Hz, 1H), 7.64 (d, $J$ = 8.3 Hz, 2H), 7.32 (t, $J$ = 8.0 Hz, 1H), 7.02 – 6.88 (m, 3H), 3.83 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 160.2, 147.8 (d, $J$ = 2.3 Hz), 146.0, 130.8 (q, $J$ = 1.9 Hz), 126.7, 125.4 (q, $J$ = 3.8 Hz), 125.2, 122.0 (q, $J$ = 265.7 Hz), 117.8, 113.6, 113.6, 108.9 (q, $J$ = 39.5 Hz), 55.2. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.6. The spectral data were in accordance with the literature.$^7$
2-(4-fluorophenyl)-8-methyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ka) White solid, m.p. 90.8 - 91.7, 45 mg, Yield: 76%; 1H NMR (400 MHz, CDCl₃) δ 8.16 (d, J = 6.9 Hz, 1H), 7.72 – 7.62 (m, 2H), 7.21 – 7.08 (m, 3H), 6.89 (t, J = 7.0 Hz, 1H), 2.66 (s, 3H). 13C NMR (100 MHz, CDCl₃) δ 163.2 (d, J = 246.7 Hz), 146.5, 146.4 (d, J = 2.0 Hz), 131.5 (dq, J = 8.5, 1.7 Hz), 129.3 (d, J = 3.2 Hz), 128.2, 125.7, 123.1 (q, J = 3.5 Hz), 121.9 (q, J = 265.7 Hz), 115.2 (d, J = 21.8 Hz), 114.0, 109.9 (q, J = 39.6 Hz), 17.1. 19F NMR (376 MHz, CDCl₃) δ -57.8. HRMS (EI) m/z: [M]+ calcd for C₁₅H₁₀F₄N₂ 294.0775, found 294.0780.

2-(4-chlorophenyl)-7-methyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3la) White solid, m.p. 110.3 - 110.8, 74 mg, Yield: 80%; 1H NMR (400 MHz, CDCl₃) δ 8.17 (d, J = 7.1 Hz, 1H), 7.64 (d, J = 8.1 Hz, 2H), 7.50 – 7.39 (m, 3H), 6.82 (d, J = 6.5 Hz, 1H), 2.45 (s, 3H). 13C NMR (100 MHz, CDCl₃) δ 146.5, 138.5, 134.9, 131.5, 130.8 (q, J = 1.8 Hz), 128.5, 128.3, 124.5 (q, J = 3.7 Hz), 121.8 (q, J = 265.6 Hz), 116.6, 116.3, 109.0 (q, J = 39.5 Hz), 21.2. 19F NMR (376 MHz, CDCl₃) δ -57.5. HRMS (EI) m/z: [M]+ calcd for C₁₅H₁₀ClF₃N₂ 310.0479, found 310.0484.
2-(4-chlorophenyl)-8-methyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3ma) White solid, 74 mg, Yield: 80%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.16 (d, $J = 6.3$ Hz, 1H), 7.64 (d, $J = 7.5$ Hz, 2H), 7.48 – 7.36 (m, 2H), 7.16 (d, $J = 7.0$ Hz, 1H), 6.89 (t, $J = 6.8$ Hz, 1H), 2.66 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 146.5, 146.1 (d, $J = 2.0$ Hz), 134.9, 131.6, 130.9 (q, $J = 1.7$ Hz), 128.3, 128.2, 125.7, 123.1 (q, $J = 3.6$ Hz), 121.8 (q, $J = 265.7$ Hz), 114.0, 109.9 (q, $J = 39.5$ Hz), 17.0. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.8. The spectral data were in accordance with the literature.$^5$

\[
\begin{align*}
\text{\includegraphics[width=0.5\textwidth]{image1.png}}
\end{align*}
\]

4-(3-(trifluoromethyl)imidazo[1,2-a]pyridin-2-yl)benzonitrile (3na) White solid, 64 mg, Yield: 74%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.31 (d, $J = 7.0$ Hz, 1H), 7.84 – 7.68 (m, 5H), 7.48 – 7.37 (m, 1H), 7.10 – 6.99 (m, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 146.2, 145.7 (d, $J = 1.9$ Hz), 137.4, 131.9, 130.2 (q, $J = 1.8$ Hz), 127.5, 125.5 (q, $J = 3.8$ Hz), 121.5 (q, $J = 265.9$ Hz), 118.5, 118.2, 114.5, 112.6, 110.1 (q, $J = 39.7$ Hz). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.6. The spectral data were in accordance with the literature.$^5$

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\begin{align*}
\text{\includegraphics[width=0.5\textwidth]{image2.png}}
\end{align*}
\]

2-phenyl-3,6-bis(trifluoromethyl)imidazo[1,2-a]pyridine (3oa) White solid, 80 mg, Yield: 81%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.65 (s, 1H), 7.83 (d, $J = 9.3$ Hz, 1H), 7.74 – 7.66 (m, 2H), 7.57 – 7.42 (m, 4H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 149.8 (d, $J = 2.2$ Hz), 145.8, 132.0, 129.5 (q, $J = 1.7$ Hz), 129.4, 128.3, 124.4 (q, $J = 2.1$ Hz), 123.0 (q, $J = 269.8$ Hz), 122.9 (q, $J = 2.6$ Hz), 121.4 (q, $J = 266.3$ Hz).
Hz), 118.9 (d,  J = 34.1 Hz), 118.3 (q,  J = 34.6 Hz), 110.9 (q,  J = 40.0 Hz).  $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.5, -62.4. The spectral data were in accordance with the literature.$^6$

![Diagram of 7-methoxy-2-phenyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3pa)](image)

**7-methoxy-2-phenyl-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3pa)** White solid, 69 mg.

Yield: 78%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.07 (d,  J = 7.5 Hz, 1H), 7.68 (d,  J = 7.0 Hz, 2H), 7.48 – 7.37 (m, 3H), 6.94 (d,  J = 2.6 Hz, 1H), 6.65 (dd,  J = 7.7, 2.5 Hz, 1H), 3.85 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 159.1, 147.9 (d,  J = 1.5 Hz), 132.9, 129.4 (q,  J = 1.7 Hz), 128.7, 128.0, 125.7 (q,  J = 3.6 Hz), 121.9 (d,  J = 265.3 Hz), 108.7, 108.3 (q,  J = 39.6 Hz), 95.0, 55.5. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.2. The spectral data were in accordance with the literature.$^6$

![Diagram of 2-(thiophen-2-yl)-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3qa)](image)

**2-(thiophen-2-yl)-3-(trifluoromethyl)imidazo[1,2-a]pyridine (3qa)** White solid, 48 mg. Yield: 60%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.28 (d,  J = 7.0 Hz, 1H), 7.69 (d,  J = 9.1 Hz, 1H), 7.53 – 7.42 (m, 2H), 7.35 (t,  J = 7.9 Hz, 1H), 7.16 – 7.09 (m, 1H), 6.95 (t,  J = 6.9 Hz, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 145.9, 141.5 (d,  J = 2.0 Hz), 134.8, 128.0 (q,  J = 4.2 Hz), 127.8, 127.7, 127.1, 125.4 (q,  J = 4.2 Hz), 121.9 (q,  J = 265.7 Hz), 117.8, 114.0, 108.3 (q,  J = 40.2 Hz). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.6. The spectral data were in accordance with the literature.$^7$
2-phenyl-3-(trifluoromethyl)benzo[d]imidazo[2,1-b]thiazole (3ra) White solid, 69 mg, Yield: 72%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.93 (d, $J = 8.4$ Hz, 1H), 7.79 – 7.61 (m, 3H), 7.56 – 7.36 (m, 5H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 150.8, 150.0 (q, $J = 2.6$, 0.6 Hz), 132.8, 132.1, 130.1, 129.5 (q, $J = 1.8$ Hz), 128.9, 128.1, 126.8, 125.5, 124.3, 121.4 (q, $J = 267.1$ Hz), 114.7 (q, $J = 4.6$ Hz), 112.5 (q, $J = 40.7$ Hz). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -55.0. The spectral data were in accordance with the literature.

3-(perfluoropropyl)-2-phenylimidazo[1,2-a]pyridine (3ab) White solid, 94 mg, Yield: 86%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.29 (d, $J = 7.0$ Hz, 1H), 7.72 (d, $J = 9.0$ Hz, 1H), 7.65 – 7.57 (m, 2H), 7.47 – 7.31 (m, 4H), 6.93 (t, $J = 6.9$ Hz, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 150.7, 146.9, 133.3, 129.5, 128.7, 127.8, 127.1, 126.1 – 125.8 (m), 119.7 – 118.7 (m), 118.1, 117.1 – 115.8 (m), 113.8, 110.6 – 109.0 (m), 107.6 (t, $J = 31.8$ Hz). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -80.2 (t, $J = 10.6$ Hz, 3F), -106.5 – -107.2 (m, 2F), -125.0 – -125.4 (m, 2F). The spectral data were in accordance with the literature.

3-(perfluorobutyl)-2-phenylimidazo[1,2-a]pyridine (3ac) White solid, 108 mg, Yield: 87%;
$^1$H NMR (400 MHz, CDCl$_3$) δ 8.31 (d, $J = 7.0$ Hz, 1H), 7.73 (d, $J = 9.1$ Hz, 1H), 7.66 – 7.57 (m, 2H), 7.49 – 7.34 (m, 4H), 6.97 (t, $J = 7.0$ Hz, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 150.9, 146.9, 133.3, 129.5, 128.8, 127.9, 127.1, 126.0, 119.2 – 118.4 (m), 118.2, 116.8 – 115.5 (m), 115.4 – 114.4 (m), 113.9, 108.3 – 107.3 (m). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -80.8 – -81.1 (m, 3F), -105.9 – -106.2 (m, 2F), -121.5 – -121.9 (m, 2F), -125.7 – -126.1 (m, 2F). The spectral data were in accordance with the literature.$^{11}$

![](image)

3-(perfluorohexyl)-2-phenylimidazo[1,2-a]pyridine (3ad) Pale yellow solid, 117 mg, Yield: 76%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.30 (d, $J = 7.1$ Hz, 1H), 7.73 (d, $J = 9.1$ Hz, 1H), 7.65 – 7.57 (m, 2H), 7.47 – 7.32 (m, 4H), 6.94 (t, $J = 7.0$ Hz, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 150.8 (d, $J = 1.9$ Hz), 146.9, 133.3, 129.5, 128.8, 127.9, 127.1, 126.1 – 125.8 (m), 119.0 – 117.0 (m), 118.1, 116.1 – 115.2 (m), 115.3 – 114.3 (m), 113.9, 108.4 – 107.1 (m). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -80.7 – -81.3 (m, 3F), -105.5 – -106.5 (m, 2F), -120.4 – -121.1 (m, 2F), -121.5 – -122.2 (m, 2F), -122.5 – -123.3 (m, 2F), -126.0 – -126.5 (m, 2F). The spectral data were in accordance with the literature.$^{11}$

![](image)

3-(perfluorooctyl)-2-phenylimidazo[1,2-a]pyridine (3ae) White solid, 132 mg, Yield: 72%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.30 (d, $J = 7.0$ Hz, 1H), 7.73 (d, $J = 7.8$ Hz, 1H), 7.65 – 7.57 (m, 2H), 7.48 – 7.31 (m, 4H), 6.92 (t, $J = 6.9$ Hz, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 150.9, 146.9, 133.3,
129.5, 128.8, 127.9, 127.1, 126.2 – 125.7 (m), 118.2, 119.2 – 116.7 (m), 116.0 – 114.4 (m), 113.9, 113.0 – 112.0 (m), 111.7 – 109.8 (m), 108.4 – 107.3 (m). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -80.4 – -81.7 (m, 3F), -105.6 – -106.3 (m, 2F), -120.4 – -121.1 (m, 2F), -121.3 – -122.4 (m, 4F), -122.6 – -123.4 (m, 2F), -125.9 – -126.6 (m, 2F). The spectral data were in accordance with the literature.$^{11}$

![Chemical Structure](image)

3-(perfluorobutyl)-2-(m-tolyl)imidazo[1,2-a]pyridine (3bc) Yellow liquid, 105 mg, Yield: 82%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.31 (d, $J = 7.0$ Hz, 1H), 7.73 (d, $J = 8.9$ Hz, 1H), 7.53 – 7.18 (m, 5H), 6.99 – 6.90 (m, 1H), 2.41 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 151.0, 146.8, 137.5, 133.2, 130.2, 129.5, 127.7, 127.1, 126.5, 126.1 – 125.7 (m), 119.5 – 118.3 (m), 118.1, 117.8 – 116.9 (m), 116.4 – 115.4 (m), 115.3 – 114.0 (m), 113.8, 108.2 – 107.0 (m), 21.2. $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -80.3 – -82.0 (m, 3F), -105.5 – -106.9 (m, 2F), -120.9 – -122.3 (m, 2F), -125.3 – -126.8 (m, 2F). HRMS (EI) m/z: [M]$^+$ calcd for C$_{18}$H$_{11}$F$_9$N$_2$ 426.0773, found 426.0776.

![Chemical Structure](image)

3-(perfluorobutyl)-2-(p-tolyl)imidazo[1,2-a]pyridine (3cc) White solid, 101 mg, Yield: 79%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.30 (d, $J = 7.0$ Hz, 1H), 7.72 (d, $J = 9.0$ Hz, 1H), 7.50 (d, $J = 7.7$ Hz, 2H), 7.42 – 7.33 (m, 1H), 7.29 – 7.20 (m, 2H), 6.95 (t, $J = 7.2$ Hz, 1H), 2.41 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 151.0, 146.9, 138.6, 130.4, 129.4, 128.6, 127.0, 126.1 – 125.7 (m), 119.2 – 118.3 (m), 118.1, 116.5 – 115.5 (m), 115.3 – 114.2 (m), 113.7, 108.2 – 107.0 (m), 21.2. $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$
-79.4 – 83.0 (m, 3F), -104.6 – 107.6 (m, 2F), -120.4 – 122.8 (m, 2F), -124.4 – 127.5 (m, 2F). The spectral data were in accordance with the literature.\(^{11}\)

![Chemical structure](image)

**8-methyl-3-(perfluorobutyl)-2-phenylimidazo[1,2-a]pyridine (3dc)** White solid, 100 mg, Yield: 78%; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.18 (d, \(J = 7.1\) Hz, 1H), 7.62 – 7.57 (m, 2H), 7.48 – 7.36 (m, 3H), 7.17 (d, \(J = 6.9\) Hz, 1H), 6.87 (t, \(J = 7.0\) Hz, 1H), 2.67 (s, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 150.3, 147.3, 133.6, 129.7, 128.6, 128.2, 127.9, 125.8, 123.9 – 123.5 (m), 119.3 – 118.1 (m), 116.5 – 115.5 (m), 115.3 – 114.4 (m), 113.9, 113.2 – 111.1 (m), 108.7 – 107.7 (m), 17.1. \(^{19}\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -80.0 – -82.1 (m, 3F), -105.1 – -106.9 (m, 2F), -120.8 – -122.7 (m, 2F), -125.3 – -127.3 (m, 2F)). The spectral data were in accordance with the literature.\(^{11}\)

![Chemical structure](image)

**7-methyl-3-(perfluorobutyl)-2-phenylimidazo[1,2-a]pyridine (3ec)** White solid, m.p. 65.6-66.8 °C, 112 mg, Yield: 88%; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.16 (d, \(J = 7.2\) Hz, 1H), 7.64 – 7.57 (m, 2H), 7.49 – 7.36 (m, 4H), 6.76 (d, \(J = 7.2\) Hz, 1H), 2.42 (s, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 150.7, 147.3, 133.5, 133.4, 129.5, 128.6, 127.8, 125.3 – 124.8 (m), 119.3 – 118.2 (m), 118.0 – 116.7 (m), 116.4 (d, \(J = 3.4\) Hz), 116.0 – 114.0 (m), 107.8 – 106.6 (m), 21.1. \(^{19}\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -80.6 – -81.6 (m, 3F), -105.6 – -106.6 (m, 2F), -121.3 – -122.4 (m, 2F), -125.7 – -126.7 (m, 2F). HRMS (EI) \(m/z\): [M\(^+\)] calcd for C\(_{18}\)H\(_{11}\)F\(_3\)N\(_2\) 426.0773, found 426.0778.
6-methyl-3-(perfluorobutyl)-2-phenylimidazo[1,2-a]pyridine (3fc) White solid, 94 mg, Yield: 73%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.07 (s, 1H), 7.66 – 7.55 (m, 3H), 7.46 – 7.38 (m, 3H), 7.24 (d, $J$ = 9.3 Hz, 1H), 2.39 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 150.6, 145.9, 133.5, 130.2, 129.5, 128.6, 127.8, 126.1, 123.8, 123.7 – 123.4 (m), 119.6 – 118.3 (m), 117.3, 116.4 – 115.5 (m), 115.3 – 114.4 (m), 107.9 – 106.9 (m), 18.4. $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -80.4 – -81.4 (m, 3F), -105.4 – -106.4 (m, 2F), -121.3 – -122.1 (m, 2F), -125.5 – -126.4 (m, 2F). The spectral data were in accordance with the literature.$^{11}$

5-methyl-3-(perfluorobutyl)-2-phenylimidazo[1,2-a]pyridine (3gc) Yellow solid, m.p. 131.5-132.4 °C, 70 mg, Yield: 55%; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.64 (d, $J$ = 8.9 Hz, 1H), 7.55 – 7.47 (m, 2H), 7.44 – 7.37 (m, 3H), 7.32 (t, $J$ = 8.0 Hz, 1H), 6.80 (d, $J$ = 6.9 Hz, 1H), 2.75 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 154.0 (d, $J$ = 3.1 Hz), 149.6, 138.4, 135.2, 129.9, 128.5, 127.8, 127.6, 119.5 – 118.3 (m), 116.9, 116.4, 116.1 – 115.2 (m), 115.0 – 113.9 (m), 112.4 – 110.8 (m), 109.2 – 107.8 (m), 22.7 – 22.2 (m). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -80.5 – -81.7 (m, 3F), -93.6 – -94.7 (m, 2F), -118.4 – -119.8 (m, 2F), -125.7 – -126.9 (m, 2F). HRMS (EI) $m/z$: [M]$^{+}$ calcd for C$_{18}$H$_{14}$F$_{9}$N$_{4}$ 426.0773, found 426.0778.
6-methyl-3-(perfluorobutyl)-2-(p-tolyl)imidazo[1,2-a]pyridine (3hc) Yellow solid, m.p. 103.2-104.3 °C, 99 mg. Yield: 75%; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.05 (s, 1H), 7.61 (d, \(J = 9.2\) Hz, 1H), 7.50 (d, \(J = 7.7\) Hz, 2H), 7.28 – 7.15 (m, 3H), 2.39 (s, 3H), 2.36 (s, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 150.7, 145.9, 138.5, 130.6, 130.1, 129.4, 128.6, 123.6, 123.7 – 123.4 (m), 119.4 – 118.2 (m), 117.3, 116.5 – 115.4 (m), 115.3 – 113.9 (m), 112.5 – 110.5 (m), 107.8 – 106.8 (m), 21.2, 18.4. \(^{19}\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -80.5 – -81.4 (m, 3F), -105.6 – -106.3 (m, 2F), -121.3 – -122.0 (m, 2F), -125.7 – -126.3 (m, 2F). HRMS (EI) \(m/z\): [M]\(^+\) calcd for C\(_{19}\)H\(_{13}\)F\(_9\)N\(_2\) 440.0930, found 440.0934.

2-(4-methoxyphenyl)-3-(perfluorobutyl)imidazo[1,2-a]pyridine (3ic) White solid, 115 mg. Yield: 87%; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.28 (d, \(J = 7.0\) Hz, 1H), 7.69 (d, \(J = 9.0\) Hz, 1H), 7.56 (d, \(J = 8.2\) Hz, 2H), 7.34 (t, \(J = 7.9\) Hz, 1H), 7.02 – 6.85 (m, 3H), 3.83 (s, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 160.1, 150.6, 146.8, 130.8, 127.0, 126.1 – 125.8 (m), 125.6, 119.3 – 118.4 (m), 118.0, 116.5 – 115.4 (m), 115.3 – 114.1 (m), 113.7, 113.4, 112.6 – 111.1 (m), 107.8 – 106.8 (m), 55.1. \(^{19}\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -80.2 – -81.6 (m, 3F), -105.5 – -106.8 (m, 2F), -121.0 – -122.4 (m, 2F), -125.2 – -126.8 (m, 2F). The spectral data were in accordance with the literature.\(^1\)
2-(4-fluorophenyl)-8-methyl-3-(perfluorobutyl)imidazo[1,2-a]pyridine (3jc) White solid, m.p. 80.7-81.8 °C, 115 mg, Yield: 87%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.17 (d, $J$ = 7.0 Hz, 1H), 7.63 – 7.52 (m, 2H), 7.18 (d, $J$ = 7.0 Hz, 1H), 7.15 – 7.07 (m, 2H), 6.87 (t, $J$ = 7.0 Hz, 1H), 2.66 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 163.2 (d, $J$ = 246.4 Hz), 149.3, 147.3, 131.6 (d, $J$ = 8.4 Hz), 129.7 (d, $J$ = 3.5 Hz), 128.3, 126.0, 123.9 – 123.5 (m), 119.3 – 118.4 (m), 117.8 – 117.0 (m), 116.5 – 115.4 (m), 114.9 (d, $J$ = 21.8 Hz), 114.0, 112.4 – 110.9 (m), 108.9 – 107.7 (m), 17.1. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -80.8 – -81.2 (m, 3F), -105.8 – -106.2 (m, 2F), -113.2 (s, 1F), -121.5 – -122.1 (m, 2F), -125.7 – -126.3 (m, 2F). HRMS (EI) m/z: [M]$^+$ calcd for C$_{18}$H$_{10}$F$_{10}$N$_2$ 444.0679, found 444.0680.

\[
\text{\begin{figure}[h]
\centering
\includegraphics[width=0.2\textwidth]{image1}
\caption{Image 1}
\end{figure}}
\]

2-(4-chlorophenyl)-7-methyl-3-(perfluorobutyl)imidazo[1,2-a]pyridine (3kc) White solid, m.p. 76.5-77.7 °C, 113 mg, Yield: 82%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.16 (d, $J$ = 7.2 Hz, 1H), 7.54 (d, $J$ = 8.1 Hz, 2H), 7.46 (s, 1H), 7.39 (d, $J$ = 8.2 Hz, 2H), 6.79 (d, $J$ = 7.2 Hz, 1H), 2.44 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 149.5, 147.4, 138.7, 134.9, 132.0, 130.9, 128.2, 125.3 – 124.9 (m), 119.3 – 118.2 (m), 116.7, 116.5, 115.3 – 114.3 (m), 112.6 – 111.0 (m), 107.9 – 106.8 (m), 21.2. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -80.5 – -81.3 (m, 3F), -105.5 – -106.2 (m, 2F), -112.4 – -122.2 (m, 2F), -125.5 – -126.4 (m, 2F). HRMS (EI) m/z: [M]$^+$ calcd for C$_{18}$H$_{10}$ClF$_9$N$_2$ 460.0383, found 460.0385.

\[
\text{\begin{figure}[h]
\centering
\includegraphics[width=0.2\textwidth]{image2}
\caption{Image 2}
\end{figure}}
\]

2-(4-chlorophenyl)-8-methyl-3-(perfluorobutyl)imidazo[1,2-a]pyridine (3lc) Pale yellow solid,
m.p. 82.8-83.7 °C, 93 mg, Yield: 82%; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.17 (d, \(J = 7.0\) Hz, 1H), 7.55 (d, \(J = 8.1\) Hz, 2H), 7.41 (d, \(J = 8.1\) Hz, 2H), 7.18 (d, \(J = 6.9\) Hz, 1H), 6.88 (t, \(J = 7.0\) Hz, 1H), 2.66 (s, 3H). \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 149.0, 147.4, 134.9, 132.2, 131.0, 128.3, 128.2, 126.0, 124.0 – 123.5 (m), 119.3 – 118.2 (m), 116.8 – 115.5 (m), 115.3 – 114.3 (m), 114.1, 112.0 – 110.8 (m), 109.0 – 107.7 (m), 17.1. \(^19\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -80.5 – -81.5 (m, 3F), -105.5 – -106.6 (m, 2F), -121.3 – -122.2 (m, 2F), -125.4 – -126.6 (m, 2F). HRMS (EI) \(m/z\): [M]\(^+\) calcd for C\(_{18}\)H\(_{16}\)ClF\(_9\)N\(_2\) 460.0383, found 460.0390.

![Diagram](image1)

4-(3-(perfluorobutyl)imidazo[1,2-a]pyridin-2-yl)benzonitrile (3mc) White solid, m.p. 122.3-122.9 °C, 106 mg, Yield: 81%; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.32 (d, \(J = 7.1\) Hz, 1H), 7.78 – 7.70 (m, 5H), 7.49 – 7.40 (m, 1H), 7.03 (t, \(J = 7.0\) Hz, 1H). \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 148.6, 147.1, 138.0, 131.8, 130.3, 127.8, 126.3 – 125.8 (m), 118.6, 118.4, 114.5, 112.7, 108.9 – 107.9 (m). \(^19\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -80.7 – -81.1 (m, 3F), -105.9 – -106.2 (m, 2F), -121.6 – -121.9 (m, 2F), -125.8 – -126.0 (m, 2F). HRMS (EI) \(m/z\): [M]\(^+\) calcd for C\(_{18}\)H\(_{16}\)ClF\(_9\)N\(_2\) 437.0569, found 437.0573.

![Diagram](image2)

3-(perfluorobutyl)-2-phenyl-6-(trifluoromethyl)imidazo[1,2-a]pyridine (3nc) White solid, m.p. 99.8-101.1 °C, 117 mg, Yield: 81%; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.64 (s, 1H), 7.84 (d, \(J = 9.5\) Hz, 1H), 7.55 (d, \(J = 8.1\) Hz, 2H), 7.41 (d, \(J = 8.1\) Hz, 2H), 7.18 (d, \(J = 6.9\) Hz, 1H), 6.88 (t, \(J = 7.0\) Hz, 1H), 2.66 (s, 3H). \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 149.0, 147.4, 134.9, 132.2, 131.0, 128.3, 128.2, 126.0, 124.0 – 123.5 (m), 119.3 – 118.2 (m), 116.8 – 115.5 (m), 115.3 – 114.3 (m), 114.1, 112.0 – 110.8 (m), 109.0 – 107.7 (m), 17.1. \(^19\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -80.5 – -81.5 (m, 3F), -105.5 – -106.6 (m, 2F), -121.3 – -122.2 (m, 2F), -125.4 – -126.6 (m, 2F). HRMS (EI) \(m/z\): [M]\(^+\) calcd for C\(_{18}\)H\(_{16}\)ClF\(_9\)N\(_2\) 460.0383, found 460.0390.
1H), 7.67 – 7.58 (m, 2H), 7.54 (d, J = 9.5 Hz, 1H), 7.49 – 7.40 (m, 3H). $^1$C NMR (100 MHz, CDCl$_3$) δ 152.6, 146.7, 132.5, 129.5, 129.3, 128.1, 125.1 – 124.7 (m), 124.4 (q, J = 269.8 Hz), 123.2 (q, J = 2.7 Hz), 119.0, 118.6 (q, J = 34.4 Hz), 117.7 – 116.6 (m), 116.4 – 115.4 (m), 115.1 – 113.9 (m), 112.5 – 110.7 (m), 109.9 – 108.7 (m). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -62.6 (s, 3F), -80.9 – -81.2 (m, 3F), -106.1 – -106.4 (m, 2F), -121.5 – -121.9 (m, 2F), -125.8 – -126.2 (m, 2F). HRMS (EI) m/z: [M]$^+$ calcd for C$_{18}$H$_{18}$F$_{12}$N$_2$ 480.0490, found 480.0497.

7-methoxy-3-(perfluorobutyl)-2-phenylimidazo[1,2-a]pyridine (3o) White solid, m.p. 142.8-143.3 ºC, 114 mg, Yield: 86%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.08 (d, J = 7.7 Hz, 1H), 7.64 – 7.56 (m, 2H), 7.45 – 7.36 (m, 3H), 6.95 (s, 1H), 6.63 (d, J = 7.7 Hz, 1H), 3.85 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 159.3, 150.9, 148.8, 133.4, 129.4, 128.6, 127.8, 127.0 – 125.6 (m), 119.2 – 118.4 (m), 117.9 – 116.8 (m), 116.4 – 114.3 (m), 112.4 – 110.8 (m), 108.8, 107.2 – 106.1 (m), 95.2, 55.5. $^{19}$F NMR (376 MHz, CDCl$_3$) δ -80.6 – -81.4 (m, 3F), -105.3 – -105.9 (m, 2F), -121.5 – -122.1 (m, 2F), -125.7 – -126.3 (m, 2F). HRMS (EI) m/z: [M]$^+$ calcd for C$_{18}$H$_{11}$F$_3$N$_2$O 442.0722, found 442.0729.

3-(perfluorobutyl)-2-(thiophen-2-yl)imidazo[1,2-a]pyridine (3p) White solid, m.p. 80.9-81.4 ºC, 98 mg, Yield: 78%; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.27 (d, J = 7.1 Hz, 1H), 7.70 (d, J = 9.1 Hz, 1H), 7.49 – 7.40 (m, 2H), 7.35 (t, J = 8.0 Hz, 1H), 7.14 – 7.06 (m, 1H), 6.91 (t, J = 7.0 Hz, 1H).
$^{13}$C NMR (100 MHz, CDCl$_3$) δ 146.7, 144.0, 135.0, 127.9, 127.8 – 127.6 (m), 127.6, 127.3, 126.1 – 125.7 (m), 119.3 – 118.4 (m), 117.9, 116.4 – 114.5 (m), 114.0, 112.6 – 111.4 (m), 109.5 – 108.1 (m), 106.9 – 105.9 (m). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -80.8 – -81.1 (m, 3F), -106.7 – -107.0 (m, 2F), -122.1 – -122.4 (m, 2F), -125.8 – -126.1 (m, 2F). HRMS (EI) m/z: [M]$^+$ calcd for C$_{15}$H$_9$F$_9$N$_2$S 418.0181, found 418.0186.

![Chemical structure](image)

3-(perfluorobutyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3q)

White solid, m.p. 113.1-113.8 ºC, 82 mg, Yield: 58% $^1$H NMR (400 MHz, CDCl$_3$) δ 7.86 (d, $J = 8.5$ Hz, 1H), 7.79 – 7.72 (m, 1H), 7.63 – 7.56 (m, 2H), 7.54 – 7.47 (m, 1H), 7.46 – 7.39 (m, 4H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 152.8, 152.0, 133.3, 132.8, 130.1, 129.6, 128.8, 127.8, 126.7, 125.5, 124.3, 119.3 – 118.1 (m), 117.2 – 116.2 (m), 115.7 – 115.3 (m), 114.9 – 113.9 (m), 113.4 – 113.0 (m), 111.8 – 110.6 (m). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -80.4 – -81.3 (m, 3F), -101.4 – -102.0 (m, 2F), -120.1 – -120.5 (m, 2F), -125.4 – -126.2 (m, 2F). HRMS (EI) m/z: [M]$^+$ calcd for C$_{19}$H$_9$F$_9$N$_2$S 468.0337, found 468.0342.

![Chemical structure](image)

2-phenyl-3,8-bis(trifluoromethyl)imidazo[1,2-a]pyridine (4)

Colorless oil, 4 mg, Yield: 4% $^1$H NMR (400 MHz, CDCl$_3$) δ 8.47 (d, $J = 7.0$ Hz, 1H), 7.77 – 7.67 (m, 3H), 7.51 – 7.41 (m, 3H), 7.08 (t, $J = 7.1$ Hz, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 149.1, 141.7, 132.2, 129.8, 129.3, 128.7 (q, $J = 4.1$ Hz), 128.2, 125.2 (q, $J = 5.2$ Hz), 122.3 (q, $J = 270.8$ Hz), 121.6 (q, $J = 266.3$ Hz), 120.0 (q, $J = 34.3$ Hz).
Hz), 112.3, 110.7 (q, J = 39.7 Hz). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -57.6, -63.4. HRMS (ESI) m/z: [M + H]$^+$ calcd for C$_{15}$H$_8$F$_6$N$_2$ 331.0665, found 331.0667.

References


4. NMR spectrum

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3aa

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3aa
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3aa

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ba
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ba

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ba
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ca

\[
\begin{array}{c}
\text{HNMR (400 MHz, CDCl$_3$) Spectrum of 3ca} \\
\includegraphics[width=0.5\textwidth]{hnmr_spectrum}
\end{array}
\]

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ca

\[
\begin{array}{c}
\text{^{13}C NMR (100 MHz, CDCl$_3$) Spectrum of 3ca} \\
\includegraphics[width=0.5\textwidth]{cnmr_spectrum}
\end{array}
\]
$^{19}\text{F NMR (376 MHz, CDCl}_3\text{)}$ Spectrum of 3ca

$^1\text{H NMR (400 MHz, CDCl}_3\text{)}$ Spectrum of 3da
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3da

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3da
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ea

![1H NMR spectrum](image)

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ea

![13C NMR spectrum](image)
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ea

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3fa
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3fa

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3fa
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ga

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ga
$^{19}\text{F NMR (376 MHz, CDCl}_3\text{)}$ Spectrum of 3ga

$^{1}\text{H NMR (400 MHz, CDCl}_3\text{)}$ Spectrum of 3ha
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ha

![C NMR Spectrum of 3ha]

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ha

![F NMR Spectrum of 3ha]
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ia

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ia
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ia

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ja
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of **3ja**

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of **3ja**
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ka

![NMR spectrum of 3ka](image1)

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ka

![NMR spectrum of 3ka](image2)
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ka

\[ \text{Diagram of 3ka} \]

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3la

\[ \text{Diagram of 3la} \]
\textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}) Spectrum of 3la

![13C NMR spectrum of 3la](image)

\textsuperscript{19}F NMR (376 MHz, CDCl\textsubscript{3}) Spectrum of 3la

![\textsuperscript{19}F NMR spectrum of 3la](image)
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ma

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ma
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ma

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3na
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3na

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3na
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 30a

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 30a
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3oa

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3pa
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3pa

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3pa
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3qa

\[ \text{N} \begin{array}{c}
\text{N}
\end{array} \text{S} \]

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3qa

\[ \text{N} \begin{array}{c}
\text{N}
\end{array} \text{S} \]
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3qa

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ra
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ra

\[ \text{Structure of 3ra} \]

\[ \text{Spectrum of 3ra} \]

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ra

\[ \text{Structure of 3ra} \]

\[ \text{Spectrum of 3ra} \]
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ab

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ab

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ab

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ab
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ab

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ac
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ac

![13C NMR spectrum of 3ac](image1)

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ac

![19F NMR spectrum of 3ac](image2)
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ad

![H NMR Spectrum]

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ad

![C NMR Spectrum]
$^{19}\text{F NMR (376 MHz, CDCl}_3\text{) Spectrum of 3ad}$

![F NMR spectrum of 3ad]

$^1\text{H NMR (400 MHz, CDCl}_3\text{) Spectrum of 3ae}$

![H NMR spectrum of 3ae]
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ae

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ae
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3bc

![H NMR spectrum of 3bc](image)

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3bc

![C NMR spectrum of 3bc](image)
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3be

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3cc
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3cc

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3cc
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3dc

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3dc
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of **3dc**

![$^{19}$F NMR Spectrum of 3dc](image)

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of **3ec**

![$^1$H NMR Spectrum of 3ec](image)
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ee

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ee
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3fc

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3fc
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3fc

![$^{19}$F NMR spectrum of 3fc](image)

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3gc

![$^1$H NMR spectrum of 3gc](image)
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ge

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ge
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3hc

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3hc
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3he

\[
\text{\begin{figure}
\centering
\includegraphics[width=\textwidth]{f_nmr_spectra.png}
\end{figure}}
\]

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ic

\[
\text{\begin{figure}
\centering
\includegraphics[width=\textwidth]{h_nmr_spectra.png}
\end{figure}}
\]
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3ic

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3ic
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of $3jc$

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of $3jc$
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3je

![F NMR Spectrum](image)

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3ke

![H NMR Spectrum](image)
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3kc

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3kc
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3lc

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3lc
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3le

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3mc
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3mc

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3mc
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3nc

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3nc
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3nc

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3oc
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 30c

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 30c
$^{1}{H}$ NMR (400 MHz, CDCl$_3$) Spectrum of 3pc

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3pc
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 3pe

![19F NMR Spectrum of 3pe](image)

$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 3qc

![1H NMR Spectrum of 3qc](image)
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of $3\text{qc}$

![Carbon NMR Spectrum](image)

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of $3\text{qc}$

![Fluorine NMR Spectrum](image)
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 4

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 4
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectrum of 4