Supporting Information

Transition-metal-catalyzed straightforward synthesis of N-trifluoromethyl indoles from 2-alkynylaryl isothiocyanates or 2-alkynylanilines†

Jianquan Hong,*a Chongbin Wei,a Ruilong Feng,a Kui Zhao,a Yi Zhu,a Chunxiang Li,a Xifei Chen,a Xinxin Gong,a Dejing Yin,b Changge Zheng*a

aKey Laboratory of Synthetic and Biological Colloids, Ministry of Education, School of Chemical and Material Engineering, Jiangnan University, Wuxi, Jiangsu 214122, P. R. China

bSchool of Biotechnology, Jiangnan University, Wuxi, Jiangsu 214122, P. R. China
# Table of Contents

1. General Information........................................................................................................S3
2. General procedure for synthesis of N-trifluoromethyl indoles ....................................S3
3. Modification of complex natural product and pharmaceutical molecules...............S6
4. Synthesis of compounds 3bk and 3bp on 5.0 mmol scale ............................................S7
5. Test on desulfurization-fluorination/cyclization of some alkynyl arylamines ..........S7
6. Identification of byproduct in the synthesis of N-trifluoromethyl indole 3aa ........S11
7. Characterization data for the products ........................................................................S11
8. Mechanism study .........................................................................................................S28
9. $^1$H NMR, $^{13}$C NMR and $^{19}$F NMR spectra of the products.................................S30
10. HRMS analysis reports for the new compounds.......................................................S104
11. Crystal data and structure refinement for the products.............................................S146
12. Checkcif report for the products ..............................................................................S149
13. References..................................................................................................................S154
1. General Information

Unless otherwise noted, all commercially available materials were purchased from Energy Chemical and used without further purification. Column chromatography was carried out on silica gel 60 (200–300 mesh). Thin-layer chromatography (TLC) was performed using 60 mesh silica gel plates and visualized with short-wavelength UV light (254 nm). $^1$H NMR, $^{13}$C NMR, $^{19}$F NMR were all recorded using CDCl$_3$ as a solvent on a Bruker 400 MHz spectrometer at 298 K (400 MHz for $^1$H, 100 MHz for $^{13}$C, and 376 MHz for $^{19}$F). Chemical shifts ($\delta$) were measured in ppm relative to TMS $\delta = 0$ for $^1$H or to chloroform $\delta = 77.0$ for $^{13}$C as an internal standard. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dq = doublet of quartets, m = multiplet). Coupling constant $J$ was reported in hertz (Hz).

2. General procedure for synthesis of N-trifluoromethyl indoles

Method A

\[
\begin{align*}
\text{R}^1\text{NCS} + \text{AgF} & \rightarrow \text{R}^2\text{NCF}_3 \\
\text{R}^1\text{RhCl}(\text{PPh}_3)_3 & \text{CH}_3\text{CN, N}_2, 45 \, ^\circ\text{C}
\end{align*}
\]

To an oven-dried 25 mL Schlenk tube equipped with a stir bar were added 2-alkynyl aryl isothiocyanate (0.5 mmol, 1.0 equiv.), AgF (3.2 equiv.), RhCl(PPh$_3$)$_3$ (1 mol%). The Schlenk tube was evacuated and refilled with N$_2$ (three times). CH$_3$CN (5 mL) was then added by syringe. The reaction mixture was required to heat to 45 °C and then stirred for 3 h under N$_2$. After cooling to room temperature, the reaction mixture was diluted with ethyl acetate, filtered through a plug of celite and wash with ethyl acetate, then concentrated under vacuum and purified by silica gel flash column chromatography (200-300 mesh) using petroleum ether (60-90 °C) as eluent.

**Table S1. Optimization of the reaction conditions**

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst</th>
<th>Base</th>
<th>Solvent</th>
<th>Temp/°C</th>
<th>Yield/%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>-</td>
<td>CH$_3$CN</td>
<td>45</td>
<td>63</td>
</tr>
<tr>
<td>2</td>
<td>-</td>
<td>-</td>
<td>CH$_3$OH</td>
<td>45</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>-</td>
<td>DMSO</td>
<td>45</td>
<td>20</td>
</tr>
<tr>
<td>4</td>
<td>-</td>
<td>-</td>
<td>DMF</td>
<td>45</td>
<td>45</td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>-</td>
<td>Dioxane</td>
<td>45</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>-</td>
<td>-</td>
<td>CH$_2$Cl$_2$</td>
<td>45</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>-</td>
<td>-</td>
<td>THF</td>
<td>45</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>-</td>
<td>-</td>
<td>NMP</td>
<td>45</td>
<td>20</td>
</tr>
<tr>
<td>9</td>
<td>-</td>
<td>-</td>
<td>Cyclohexane</td>
<td>45</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>-</td>
<td>-</td>
<td>Toluene</td>
<td>45</td>
<td>0</td>
</tr>
</tbody>
</table>
Method B

\[
\text{To an oven-dried 25 mL Schlenk tube equipped with a stir bar were added 2-alkynyl arylamine (0.5 mmol, 1.0 equiv.), AgSCF}_3 \ (1.5 \text{ equiv.}), KI \ (1.5 \text{ equiv.}), \text{AgF (5.0 equiv.), Cul (20 mol%) and 2,2'-Bipyridine (20 mol%)}.
\]

The Schlenk tube was evacuated and refilled with N\textsubscript{2} (three times). CH\textsubscript{3}CN (5 mL) was then added by syringe. The reaction mixture was required to heat to 50 °C and then stirred for 4 h under N\textsubscript{2}. After cooling to room temperature, the reaction mixture was diluted with ethyl acetate, filtered through a plug of celite and wash with ethyl acetate, then concentrated under
vacuum and purified by silica gel flash column chromatography (200-300 mesh) using petroleum ether (60-90 °C) as eluent.

**Table S2. Optimization of the reaction conditions**

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst</th>
<th>Ligand</th>
<th>Solvent</th>
<th>Temp./°C</th>
<th>Yield/%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>-</td>
<td>CH₃CN</td>
<td>25</td>
<td>58</td>
</tr>
<tr>
<td>2</td>
<td>-</td>
<td>-</td>
<td>THF</td>
<td>25</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>-</td>
<td>DMF</td>
<td>25</td>
<td>Trace</td>
</tr>
<tr>
<td>4</td>
<td>-</td>
<td>-</td>
<td>DMSO</td>
<td>25</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>-</td>
<td>DCE</td>
<td>25</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>-</td>
<td>-</td>
<td>DME</td>
<td>25</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>-</td>
<td>-</td>
<td>CH₃CN</td>
<td>25</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>-</td>
<td>-</td>
<td>CH₃CN</td>
<td>25</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>-</td>
<td>RuCl₂</td>
<td>CH₃CN</td>
<td>25</td>
<td>52</td>
</tr>
<tr>
<td>10</td>
<td>-</td>
<td>RhCl(PPh₃)</td>
<td>CH₃CN</td>
<td>25</td>
<td>37</td>
</tr>
<tr>
<td>11</td>
<td>-</td>
<td>Pd(OAc)₂</td>
<td>CH₃CN</td>
<td>25</td>
<td>46</td>
</tr>
<tr>
<td>12</td>
<td>-</td>
<td>CuI</td>
<td>CH₃CN</td>
<td>25</td>
<td>66</td>
</tr>
<tr>
<td>13</td>
<td>-</td>
<td>CuCl</td>
<td>CH₃CN</td>
<td>25</td>
<td>22</td>
</tr>
<tr>
<td>14</td>
<td>-</td>
<td>CuBr</td>
<td>CH₃CN</td>
<td>25</td>
<td>28</td>
</tr>
<tr>
<td>15</td>
<td>-</td>
<td>CuOAc</td>
<td>CH₃CN</td>
<td>25</td>
<td>Trace</td>
</tr>
<tr>
<td>16</td>
<td>-</td>
<td>Cu(OAc)₂</td>
<td>CH₃CN</td>
<td>25</td>
<td>Trace</td>
</tr>
<tr>
<td>17</td>
<td>-</td>
<td>CuCl₂</td>
<td>CH₃CN</td>
<td>25</td>
<td>Trace</td>
</tr>
<tr>
<td>18</td>
<td>-</td>
<td>CuF₂</td>
<td>CH₃CN</td>
<td>25</td>
<td>46</td>
</tr>
<tr>
<td>19</td>
<td>-</td>
<td>Cu(TFA)₂</td>
<td>CH₃CN</td>
<td>25</td>
<td>17</td>
</tr>
<tr>
<td>20</td>
<td>1,10-Phen</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>36</td>
</tr>
<tr>
<td>21</td>
<td>2,2'-Bipyridine</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>76</td>
</tr>
<tr>
<td>22</td>
<td>PPh₃</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>48</td>
</tr>
<tr>
<td>23</td>
<td>Tricyclohexyl Phosphine</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>44</td>
</tr>
<tr>
<td>24</td>
<td>DPEPhos</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>46</td>
</tr>
<tr>
<td>25</td>
<td>4,4'-Bipyridine</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>12</td>
</tr>
<tr>
<td>26</td>
<td>4,4'Di-Tert-Butyl-2,2'-Dipyridyl</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>22</td>
</tr>
<tr>
<td>27</td>
<td>2,2':6',2''-Terpyridine</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>16</td>
</tr>
<tr>
<td>28</td>
<td>5,5'-Dimethyl-2,2'-Dipyridyl</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>25</td>
<td>38</td>
</tr>
<tr>
<td>29</td>
<td>2,2'-Bipyridine</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>30</td>
<td>64</td>
</tr>
<tr>
<td>30</td>
<td>2,2'-Bipyridine</td>
<td>Cul</td>
<td>CH₃CN</td>
<td><strong>50</strong></td>
<td><strong>88</strong></td>
</tr>
<tr>
<td>31</td>
<td>2,2'-Bipyridine</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>70</td>
<td>83</td>
</tr>
<tr>
<td>32</td>
<td>2,2'-Bipyridine</td>
<td>Cul</td>
<td>CH₃CN</td>
<td>50</td>
<td>Trace</td>
</tr>
</tbody>
</table>

*Method C*

---

*a* Reaction conditions: 2-phenylethynyl aniline (0.10 mmol, 1.0 equiv), AgSCF₃ (0.15 mmol, 1.5 equiv), KI (0.15 mmol, 1.5 equiv), AgF (0.5 mmol, 5 equiv), catalyst (0.02 mmol, 20 mol%), ligand (0.02 mmol, 20 mol%), solvent (2 mL), N₂, Temp., 4 h. *b* Reaction yield determined by ¹⁹F NMR spectroscopy using 4,4'-difluorobiphenyl as internal standard based on 2-phenylethynyl aniline. *c* KBr instead of KI. *d* KCl instead of KI. *e* Under air.
To an oven-dried 10 mL Schlenk tube equipped with a stir bar were added 2-alkynyl aryl isothiocyanate (0.5 mmol, 1.0 equiv.), AgF (3.2 equiv.), CuI (1 mol%) and 2,2'-bipyridine (1 mol%). The Schlenk tube was evacuated and refilled with N\textsubscript{2} (three times). CH\textsubscript{3}CN (1.5 mL) was then added by syringe. The reaction mixture was required to heat to 45 °C and then stirred for 6 h under N\textsubscript{2}. After cooling to room temperature, the reaction mixture was diluted with ethyl acetate, filtered through a plug of celite and wash with ethyl acetate, then concentrated under vacuum and purified by silica gel flash column chromatography (200-300 mesh) using petroleum ether (60-90 °C) as eluent.

3. Modification of complex natural product and pharmaceutical molecules

(1) 2-Alkynyl aryl isothiocyanates 1ay and 1bn corresponding to products 3ay and 3bn were prepared according to the literature procedures.\textsuperscript{1-4} 2-Alkynyl arylamines 2ag' and 2bp corresponding to products 3ag' and 3bp were prepared according to the literature procedures.\textsuperscript{5-7}

(2) Target products were prepared according to the general procedure.
4. Synthesis of compounds 3bk and 3bp on 5.0 mmol scale

To an oven-dried 50 mL Schlenk tube equipped with a stir bar were added 1-isothiocyanato-2-(phenylethynyl)-4-(trifluoromethyl)benzene 1bk (5.00 mmol, 1.520 g, 1.0 equiv.), AgF (16.00 mmol, 2.020 g, 3.2 equiv) and RhCl(PPh3)3 (0.05 mmol, 0.046 mg, 1 mol%). The Schlenk tube was evacuated and refilled with N2 (three times). CH3CN (25 mL) was then added by syringe. The reaction mixture was required to heat to 45 °C and then stirred for 3 h under N2. After cooling to room temperature, the reaction mixture was diluted with ethyl acetate, filtered through a plug of celite and was with ethyl acetate, then concentrated under vacuum and purified by silica gel flash column chromatography (200-300 mesh) using petroleum ether (60-90 °C) as eluent. to afford N-trifluoromethyl indole 3bk (1.299 g, 79%).

5. Test on desulfurization-fluorination/cyclization of some alkynyl arylamines

To an oven-dried 50 mL Schlenk tube equipped with a stir bar were added ethyl 4-amino-3-(phenylethynyl)benzoate 2bp (5.00 mmol, 1.326 g, 1.0 equiv.), KI (7.5 mmol 1.245 g, 1.5 equiv.), AgSCF3 (7.5 mmol, 1.567 g, 1.5 equiv.), AgF (25 mmol, 3.171 g, 5 equiv.), CuI (1 mmol, 0.190 g, 20 mol%) and 2,2′-Bipyridine (1 mmol, 0.156 g, 20 mol%). The Schlenk tube was evacuated and refilled with N2 (three times). CH3CN (30 ml) was then added by syringe. After cooling to room temperature, the reaction mixture was diluted with ethyl acetate, filtered through a plug of celite and was with ethyl acetate, then concentrated under vacuum and purified by silica gel flash column chromatography (200-300 mesh) using petroleum ether (60-90 °C) as eluent to afford N-trifluoromethyl indole 3bp (1.222 g, 77%).

5. Test on desulfurization-fluorination/cyclization of some alkynyl arylamines

To an oven-dried 10 ml Schlenk tube equipped with a stir bar were added KI (0.15 mmol 24.9 mg, 1.5 equiv.), AgSCF3 (0.15 mmol, 31.33 mg, 1.5 equiv.), AgF (0.5 mmol,
63.4 mg, 5 equiv.), CuI (0.02 mmol, 3.82 mg, 20 mmol%) and 2,2′-Bipyridine (0.02 mmol, 3.12 mg, 20 mol%). The Schlenk tube was evacuated and refilled with N₂ (three times). CH₃CN (30 ml) and methyl 3-(2-aminophenyl)propiolate 2ah' (0.1 mmol, 11.71 mg, 1.0 equiv.) was then added by syringe. The reaction mixture was required to heat to 50 °C and then stirred for 4 h. After cooling to room temperature, the raw product was analyzed by ¹⁹F NMR using 4,4′-difluorobiphenyl (-115.0 ppm) as internal standard. The target product 3ah' (-55.6 ppm)⁸ was observed in 10% yield.

To an oven-dried 10 ml Schlenk tube equipped with a stir bar were added KI (0.15 mmol 24.9 mg, 1.5 equiv.), AgSCF₃(0.15 mmol, 31.33 mg, 1.5 equiv.), AgF (0.5 mmol, 63.4 mg, 5 equiv.), CuI (0.02 mmol, 3.82 mg, 20 mmol%) and 2,2′-Bipyridine (0.02 mmol, 3.12 mg, 20 mol%). The Schlenk tube was evacuated and refilled with N₂ (three times). CH₃CN (2 mL) and 2-((trimethylsilyl)ethynyl)aniline 2ai' (0.1 mmol, 1.0 equiv. 18.9 mg) was then added by syringe. The reaction mixture was required to heat to 50 °C and then stirred for 4. After cooling to room temperature, the raw product was analyzed by ¹⁹F NMR using 4,4′-difluorobiphenyl (-115.0 ppm) as internal standard. The product 3ah' (-55.6 ppm) instead of 3ai' was observed in 18% yield. The signal of TMSF can also be observed at -156.6 ppm in ¹⁹F NMR spectrum (Due to the volatility of this compound, the intensity of the signal is relatively weak in the spectrum).
To an oven-dried 10 ml Schlenk tube equipped with a stir bar were added methyl 3-(2-aminophenyl)propiolate 2aj' (0.1 mmol, 17.51 mg, 1.0 equiv.), KI (0.15 mmol 24.9 mg, 1.5 equiv.), AgSCF$_3$ (0.15 mmol, 31.33 mg, 1.5 equiv.), AgF (0.5 mmol, 63.4 mg, 5 equiv.), CuI (0.02mmol, 3.82 mg, 20 mmol%) and 2,2'-Bipyridine (0.02mmol, 3.12 mg, 20 mol%). The Schlenk tube was evacuated and refilled with N$_2$ (three times). CH$_3$CN (30 ml) was then added by syringe. The reaction mixture was required to heat to 50 °C (or 90 °C) and then stirred for 4 h. After cooling to room temperature, the raw product was analyzed by $^{19}$F NMR using 4,4'-difluorobiphenyl (-115.0 ppm) as internal standard. The target product was observed with a yield of 0.1%.
6. Identification of byproduct in the synthesis of N-trifluoromethyl indole 3aa

![Chemical structure of 3aa with reagents](image)

To an oven-dried 50 mL Schlenk tube equipped with a stir bar were added 1aa (5.00 mmol, 1.180 g, 1.0 equiv.), AgF (16.00 mmol, 2.020 g, 3.2 equiv) and RhCl(PPh$_3$)$_3$ (0.05 mmol, 0.046 mg, 1 mol%). The Schlenk tube was evacuated and refilled with N$_2$ (three times). CH$_3$CN (25 mL) was then added by syringe. The reaction mixture was required to heat to 45 °C and then stirred for 3 h under N$_2$. After cooling to room temperature, the reaction mixture was diluted with ethyl acetate, filtered through a plug of celite and was with ethyl acetate, then concentrated under vacuum and purified by silica gel flash column chromatography (200-300 mesh) using petroleum ether (60-90 °C) and ethyl acetate as eluent to afford 3aa (0.913 g, 70%) and 3′aa (0.145 g, 6%).

3′aa: $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.64 (dd, $J$ = 7.7, 1.5 Hz, 1H), 7.60–7.52 (m, 4H), 7.50 (dd, $J$ = 7.7, 1.5 Hz, 1H), 7.41 (ddd, $J$ = 14.3, 7.1, 1.6 Hz, 4H), 7.35 (qd, $J$ = 5.2, 4.7, 2.6 Hz, 6H), 7.18 (td, $J$ = 7.7, 1.6 Hz, 1H), 7.06 (td, $J$ = 7.6, 1.2 Hz, 1H), 6.95 (d, $J$ = 8.0 Hz, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -44.95 (s, 1F), -54.47 (d, $J$ = 14.3 Hz, 3F).

7. Characterization data for the products

![Chemical structure of 2-phenyl-1-(trifluoromethyl)-1H-indole (3aa)](image)

2-phenyl-1-(trifluoromethyl)-1H-indole (3aa). Following the general procedure of Method A, compound 3aa was synthesized and isolated as a colorless oil (0.105 g, 80%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.093 g, 71%) via Method B. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.79–7.69 (m, 1H), 7.69–7.62 (m, 1H), 7.57 (dd, $J$ = 6.5, 2.8 Hz, 2H), 7.52–7.44 (m, 3H), 7.43–7.30 (m, 2H), 6.69–6.61 (m, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.82 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 139.4 (s), 136.0 (s), 132.4 (s), 129.6 (s), 129.3 (s), 128.8 (s), 128.2 (s), 124.4 (s), 123.0 (s), 121.1 (s), 120.7 (q, $J$ = 263.2 Hz), 113.2 (q, $J$ = 4.3 Hz), 109.8 (s). HRMS (ESI) $m/z$ calcd. for C$_{15}$H$_{10}$F$_3$NH (M+H)$^+$: 262.0838; found: 262.0835.
2-(4-methoxyphenyl)-1-(trifluoromethyl)-1H-indole (3ab). Following the general procedure of Method A, compound 3ab was synthesized and isolated as a colorless solid (0.090 g, 62%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless solid (0.092 g, 66%) via Method B. mp 77-79 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.70–7.64 (m, 1H), 7.61 (d, $J = 7.3$ Hz, 1H), 7.45 (d, $J = 8.6$ Hz, 2H), 7.37–7.32 (m, 1H), 7.29 (td, $J = 7.5$, 0.9 Hz, 1H), 7.02–6.94 (m, 1H), 6.57 (s, 1H), 3.88 (s, 3H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.86 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 160.1 (s), 139.3 (s), 135.9 (s), 131.0–130.8 (m), 129.3 (s), 124.8–124.5 (m), 124.1 (s), 122.9 (s), 120.9 (s), 120.8 (q, $J = 261.5$ Hz), 113.7 (s), 113.1 (q, $J = 4.5$ Hz), 109.4 (s), 55.4 (s). HRMS (ESI) m/z calcd. for C$_{16}$H$_{12}$F$_3$NOH (M+H)$^+$: 292.0944; found: 292.0946.

NCF$_3$OMe

2-(3-methoxyphenyl)-1-(trifluoromethyl)-1H-indole (3ac). Following the general procedure of Method A, compound 3ac was synthesized and isolated as a yellow oil (0.090 g, 62%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a yellow oil (0.074 g, 51%) via Method B. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.71–7.65 (m, 1H), 7.63 (d, $J = 7.2$ Hz, 1H), 7.36 (td, $J = 8.4$, 1.6 Hz, 2H), 7.30 (td, $J = 7.5$, 1.1 Hz, 1H), 7.12 (d, $J = 7.6$ Hz, 1H), 7.08 (s, 1H), 7.00 (ddd, $J = 8.3$, 2.6, 0.9 Hz, 1H), 6.63 (s, 1H), 3.87 (s, 3H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.86 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 159.3 (s), 139.2 (s), 136.0 (s), 133.6 (s), 129.2 (d, $J = 3.9$ Hz), 124.4 (s), 123.0 (s), 122.2–121.9 (m), 121.1 (s), 120.7 (q, $J = 261.6$ Hz), 115.2 (s), 114.5 (s), 113.2 (q, $J = 4.3$ Hz), 109.8 (s), 55.4 (s). HRMS (ESI) m/z calcd. for C$_{16}$H$_{12}$F$_3$NOH (M+H)$^+$: 292.0944; found: 292.0949.

NCF$_3$MeO

2-(2-methoxyphenyl)-1-(trifluoromethyl)-1H-indole (3ad). Following the general procedure of Method A, compound 3ad was synthesized and isolated as a colorless oil (0.073 g, 50%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.070 g, 48%) via Method B. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.70–7.65 (m, 1H), 7.63 (d, $J = 7.8$ Hz, 1H), 7.45 (td, $J = 8.2$, 1.7 Hz, 1H), 7.39 (dd, $J = 7.4$, 1.7 Hz, 1H), 7.35 (td, $J = 8.4$, 7.8, 1.3 Hz, 1H), 7.28 (td, $J = 7.7$, 1.0 Hz, 1H), 7.04 (td, $J = 7.5$, 0.9 Hz, 1H), 6.97 (d, $J = 8.3$ Hz, 1H), 6.60–6.53 (m, 1H), 3.81 (s, 3H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -53.52 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 158.1 (s), 135.7 (d, $J = 22.4$ Hz), 131.6 (s), 130.7 (s), 129.2 (s), 124.0 (s), 122.6 (s), 121.8 (s), 121.0 (s), 120.5 (q, $J = 261.5$ Hz), 120.3
(s), 112.7 (q, J = 4.5 Hz), 110.5 (s), 109.1 (s), 55.5 (s). **HRMS (ESI) m/z** calcd. for C_{16}H_{12}F_{3}NOH (M+H)^+: 292.0944; found: 292.0956.

![NCF3](image1)

**2-(p-tolyl)-1-(trifluoromethyl)-1H-indole (3ae).** Following the general procedure of **Method A**, compound 3ae was synthesized and isolated as a yellow oil (0.107 g, 78%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a yellow oil (0.095 g, 69%) via **Method B**.

**1H NMR** (400 MHz, CDCl_3) δ 7.62–7.56 (m, 1H), 7.55–7.50 (m, 1H), 7.33 (d, J = 8.0 Hz, 2H), 7.29–7.24 (m, 1H), 7.22 (dd, J = 7.6, 1.1 Hz, 1H), 7.20–7.15 (m, 2H), 6.51 (s, 1H), 2.36 (s, 3H).

**19F NMR** (376 MHz, CDCl_3) δ -49.83 (s, 3F).

**13C NMR** (101 MHz, CDCl_3) δ 139.6 (s), 138.8 (s), 136.0 (s), 129.6–129.4 (m), 129.3 (s), 128.9 (s), 124.2 (s), 123.0 (s), 121.0 (s), 120.7 (q, J = 263.4 Hz), 113.2 (q, J = 4.4 Hz), 109.5 (s), 21.5 (s). **HRMS (ESI) m/z** calcd. for C_{16}H_{12}F_{3}NH (M+H)^+: 276.0995; found: 276.0996.

![NCF3](image2)

**2-(m-tolyl)-1-(trifluoromethyl)-1H-indole (3af).** Following the general procedure of **Method A**, compound 3af was synthesized and isolated as a colorless oil (0.105 g, 76%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent.

**1H NMR** (400 MHz, CDCl_3) δ 7.71–7.65 (m, 1H), 7.64–7.60 (m, 1H), 7.39–7.29 (m, 5H), 7.29–7.25 (m, 1H), 6.61 (s, 1H), 2.44 (s, 3H).

**19F NMR** (376 MHz, CDCl_3) δ -49.87 (s, 3F).

**13C NMR** (101 MHz, CDCl_3) δ 139.6 (s), 138.8 (s), 136.0 (s), 129.6–129.4 (m), 129.3 (s), 128.9 (s), 124.2 (s), 123.0 (s), 121.1 (s), 120.7 (q, J = 263.3 Hz), 113.2 (q, J = 4.3 Hz), 109.7 (s), 21.5 (s). **HRMS (ESI) m/z** calcd. for C_{16}H_{12}F_{3}NH (M+H)^+: 276.0995; found: 276.0989.

![NCF3](image3)

**2-(o-tolyl)-1-(trifluoromethyl)-1H-indole (3ag).** Following the general procedure of **Method A**, compound 3ag was synthesized and isolated as a yellow oil (0.076 g, 55%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent.

**1H NMR** (400 MHz, CDCl_3) δ 7.71–7.67 (m, 1H), 7.66–7.63 (m, 1H), 7.38 (dtd, J = 8.3, 5.8, 5.3, 1.5 Hz, 3H), 7.32 (td, J = 7.6, 1.1 Hz, 2H), 7.27 (t, J = 7.4 Hz, 1H), 6.58–6.50 (m, 1H), 2.25 (s, 3H).

**19F NMR** (376 MHz, CDCl_3) δ -51.95 (s, 3F).

**13C NMR** (101 MHz, CDCl_3) δ 138.1 (d, J = 34.9 Hz), 135.4 (s), 131.9 (s), 130.9 (s), 129.9 (s), 129.3 (d, J = 5.4 Hz), 125.4 (s), 124.2 (s), 122.9 (s), 121.0 (s), 120.6 (q, J = 263.3 Hz),...
112.9 (q, \( J = 4.1 \) Hz), 109.3 (s), 20.0 (s). **HRMS (ESI) m/z** calcd. for C_{16}H_{12}F_{3}NH (M+H)^+: 276.0995; found: 276.0982.

2-(4-ethylphenyl)-1-(trifluoromethyl)-1H-indole (3ah). Following the general procedure of Method A, compound 3ah was synthesized and isolated as a colorless oil (0.108 g, 75%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.72–7.67 (m, 1H), 7.65–7.60 (m, 1H), 7.46 (d, \( J = 8.0 \) Hz, 2H), 7.39–7.34 (m, 1H), 7.31 (t, \( J = 7.3 \) Hz, 3H), 6.61 (s, 1H), 2.76 (q, \( J = 7.6 \) Hz, 2H), 1.33 (t, \( J = 7.6 \) Hz, 3H). \(^{19}\)F NMR (376 MHz, CDCl\(_3\)) \( \delta \) -49.83 (s, 3F). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 145.0 (s), 139.6 (s), 136.0 (s), 129.7 (s), 129.5 (d, \( J = 1.1 \) Hz), 129.3 (s), 127.7 (s), 124.2(s), 123.0 (s), 121.0 (s), 120.7 (q, \( J = 261.6 \) Hz), 113.2 (q, \( J = 4.4 \) Hz), 109.6 (s), 28.8 (s), 15.5 (s). **HRMS (ESI) m/z** calcd. for C_{17}H_{14}F_{3}NH (M+H)^+: 290.1151; found: 290.1151.

2-(4-propylphenyl)-1-(trifluoromethyl)-1H-indole (3ai). Following the general procedure of Method A, compound 3ai was synthesized and isolated as a colorless oil (0.114 g, 75%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.038 g, 25%) via Method B. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.73–7.65 (m, 1H), 7.66–7.59 (m, 1H), 7.44 (d, \( J = 8.0 \) Hz, 2H), 7.38–7.32 (m, 1H), 7.31 (dd, \( J = 7.6, 1.0 \) Hz, 1H), 7.26 (d, \( J = 8.2 \) Hz, 2H), 6.60 (s, 1H), 2.86–2.41 (m, 2H), 1.73 (m, \( J = 7.4 \) Hz, 2H), 1.01 (t, \( J = 7.3 \) Hz, 3H). \(^{19}\)F NMR (376 MHz, CDCl\(_3\)) \( \delta \) -49.84 (s, 3F). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 143.5 (s), 139.6 (s), 136.0 (s), 129.7 (s), 129.5 – 129.3 (m), 129.3 (s), 128.3 (s), 124.2 (s), 123.0 (s), 120.7 (q, \( J = 261.8 \) Hz), 113.2 (q, \( J = 4.4 \) Hz), 109.5 (s), 38.0 (s), 24.6 (s), 14.0 (s). **HRMS (ESI) m/z** calcd. for C_{18}H_{16}F_{3}NH (M+H)^+: 304.1308; found: 304.1310.

2-(4-fluorophenyl)-1-(trifluoromethyl)-1H-indole (3aj). Following the general procedure of Method A, compound 3aj was synthesized and isolated as a colorless oil (0.089 g, 64%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.101 g, 72%) via Method B. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.71–7.65 (m, 1H), 7.62 (d, \( J = 7.3 \) Hz, 1H), 7.49 (dd, \( J = 8.5, 5.4 \) Hz, 2H), 7.41–7.26 (m, 2H), 7.18–7.08 (m, 2H), 6.60 (s, 1H). \(^{19}\)F NMR (376 MHz, CDCl\(_3\)) \( \delta \) -49.89 (s, 3F), -112.57 (s, 1F). \(^{13}\)C NMR (101 MHz,
CDCl₃ δ 163.2 (d, J = 248.6 Hz), 136.0 (s), 131.5 – 131.2 (m), 129.1 (s), 124.5 (s), 123.1 (s), 121.1 (s), 120.7 (q, J = 263.1 Hz), 115.8 (d, J = 21.8 Hz), 113.2 (q, J = 4.4 Hz), 110.0 (s). HRMS (ESI) m/z calcd. for C₁₅H₉F₄NH (M+H)^+: 280.0744; found: 280.0738.

2-(3-fluorophenyl)-1-(trifluoromethyl)-1H-indole (3ak). Following the general procedure of Method A, compound 3ak was synthesized and isolated as a colorless oil (0.098 g, 70%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.061 g, 44%) via Method B. ¹H NMR (400 MHz, CDCl₃) δ 7.71–7.65 (m, 1H), 7.63 (d, J = 7.6 Hz, 1H), 7.43–7.35 (m, 2H), 7.34–7.28 (m, 2H), 7.24 (d, J = 9.5 Hz, 1H), 7.15 (td, J = 8.5, 2.6, 1.0 Hz, 1H), 6.64 (s, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ -49.92 (s, 3F), -113.14 (s, 1F). ¹³C NMR (101 MHz, CDCl₃) δ 162.4 (d, J = 246.6 Hz), 137.8 (d, J = 2.3 Hz), 136.1 (s), 134.3 (d, J = 7.6 Hz), 129.8 (d, J = 8.5 Hz), 129.1 (s), 125.4 (dd, J = 2.8, 1.3 Hz), 124.7 (s), 123.2 (s), 121.3 (s), 120.6 (q, J = 261.8 Hz), 116.5 (d, J = 22.5 Hz), 115.8 (d, J = 21.1 Hz), 113.2 (q, J = 4.3 Hz), 110.4 (s). HRMS (ESI) m/z calcd. for C₁₅H₉F₄NH (M+H)^+: 280.0744; found: 280.0745.

2-(2-fluorophenyl)-1-(trifluoromethyl)-1H-indole (3al). Following the general procedure of Method A, compound 3al was synthesized and isolated as a colorless oil (0.073 g, 52%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.049 g, 35%) via Method B. ¹H NMR (400 MHz, CDCl₃) δ 7.71–7.66 (m, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.50–7.42 (m, 2H), 7.38 (td, J = 8.4, 7.8, 1.3 Hz, 1H), 7.34–7.28 (m, 1H), 7.23 (td, J = 7.6, 1.0 Hz, 1H), 7.18 (t, J = 9.0 Hz, 1H), 6.67 (s, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ -52.61 (d, J = 5.1 Hz, 3F), -112.86 (q, J = 5.1 Hz, 1F). ¹³C NMR (101 MHz, CDCl₃) δ 160.6 (d, J = 249.4 Hz), 135.9 (s), 132.4 (s), 132.0 (d, J = 1.9 Hz), 131.1 (d, J = 8.1 Hz), 129.1 (s), 124.6 (s), 124.0 (d, J = 3.7 Hz), 123.0 (s), 121.2 (s), 120.5 (q, J = 262.6 Hz), 120.4 (d, J = 15.7 Hz), 115.6 (d, J = 21.6 Hz), 112.9 (q, J = 3.7 Hz), 110.7 (s). HRMS (ESI) m/z calcd. for C₁₅H₉F₄NH (M+H)^+: 280.0744; found: 280.0735.

2-(4-chlorophenyl)-1-(trifluoromethyl)-1H-indole (3am). Following the general procedure of Method A, compound 3am was synthesized and isolated as a colorless
solid (0.074 g, 50%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless solid (0.075 g, 51%) via Method B. mp 23-24 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.71 – 7.64 (m, 1H), 7.62 (d, $J = 7.8$ Hz, 1H), 7.48 – 7.40 (m, 4H), 7.36 (ddd, $J = 8.4, 7.3, 1.4$ Hz, 1H), 7.30 (td, $J = 7.6, 1.0$ Hz, 1H), 6.61 (s, 1H).

$^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.88 (s, 3F).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 138.0 (s), 136.1 (s), 135.0 (s), 130.9 – 130.7 (m), 129.1 (s), 128.5 (s), 124.6 (s), 123.2 (s), 121.2 (s), 120.6 (q, $J = 263.5$ Hz), 113.2 (q, $J = 4.3$ Hz), 110.2 (s). HRMS (ESI) m/z calcd. for C$_{15}$H$_9$ClF$_3$NH (M+H)$^+$: 296.048; found: 296.0433.

**2-(3-chlorophenyl)-1-(trifluoromethyl)-1H-indole (3an).** Following the general procedure of Method A, compound 3an was synthesized and isolated as a colorless oil (0.102 g, 69%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.70–7.65 (m, 1H), 7.63 (d, $J = 7.8$ Hz, 1H), 7.52 (s, 1H), 7.44–7.34 (m, 4H), 7.31 (td, $J = 7.7, 0.9$ Hz, 1H), 6.63 (s, 1H).

$^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.93 (s, 3F).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 137.7 (s), 136.1 (s), 134.1 (d, $J = 10.1$ Hz), 129.6–129.5 (m), 129.5 (s), 129.1 (s), 127.8 (d, $J = 1.3$ Hz), 124.8 (s), 123.2 (s), 121.3 (s), 120.6 (q, $J = 261.8$ Hz), 113.2 (q, $J = 4.3$ Hz), 110.5 (s). HRMS (ESI) m/z calcd. for C$_{15}$H$_9$ClF$_3$NH (M+H)$^+$: 296.0448; found: 296.0438.

**2-(2-chlorophenyl)-1-(trifluoromethyl)-1H-indole (3ao).** Following the general procedure of Method A, compound 3ao was synthesized and isolated as a colorless solid (0.087 g, 59%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 70-71 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.72–7.63 (m, 2H), 7.51 (dd, $J = 8.0, 1.1$ Hz, 1H), 7.49–7.27 (m, 5H), 6.62 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -52.47 (s, 3F).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 135.4 (s), 135.2 (s), 132.3 (s), 131.6 (s), 130.6 (s), 129.5 (s), 129.0 (s), 126.4 (s), 124.6 (s), 123.0 (s), 121.3 (s), 120.4 (q, $J = 261.5$ Hz), 112.8 (q, $J = 3.7$ Hz), 110.0–110.0 (m). HRMS (ESI) m/z calcd. for C$_{15}$H$_9$ClF$_3$NH (M+H)$^+$: 296.0448; found: 296.0441.

**2-(4-bromophenyl)-1-(trifluoromethyl)-1H-indole (3ap).** Following the general procedure of Method A, compound 3ap was synthesized and isolated as a colorless oil
(0.116 g, 68%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.070 g, 41%) via Method B. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.69–7.64 (m, 1H), 7.62 (d, $J = 7.8$ Hz, 1H), 7.60–7.56 (m, 2H), 7.41–7.34 (m, 3H), 7.30 (td, $J = 7.6$, 1.0 Hz, 1H), 6.61 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.87 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 138.0 (s), 136.1 (s), 131.5 (s), 131.3 (s), 131.2–131.0 (m), 129.1 (s), 124.7 (s), 123.2 (d, $J = 2.4$ Hz), 121.2 (s), 120.6 (q, $J = 261.8$ Hz), 113.2 (q, $J = 4.3$ Hz), 110.2 (s). HRMS (ESI) m/z calcd. for C$_{15}$H$_9$BrF$_3$NH (M+H)$^+$: 339.9943; found: 339.9914.

2-(2-bromophenyl)-1-(trifluoromethyl)-1H-indole (3aq). Following the general procedure of Method A, compound 3aq was synthesized and isolated as a colorless solid (0.099 g, 58%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 68-69 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.73–7.63 (m, 3H), 7.45 (dd, $J = 7.5$, 1.8 Hz, 1H), 7.42–7.36 (m, 2H), 7.36–7.29 (m, 2H), 6.62 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -52.18 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 136.7 (s), 135.2 (s), 133.7 (s), 132.7 (s), 132.4 (s), 130.7 (s), 129.0 (s), 127.0 (s), 125.2 (s), 124.6 (s), 123.0 (s), 121.4 (s), 120.4 (q, $J = 261.7$ Hz), 112.8 (q, $J = 3.7$ Hz), 110.1 (s). HRMS (ESI) m/z calcd. for C$_{15}$H$_9$BrF$_3$NH (M+H)$^+$: 339.9943; found: 339.9943.

1-(trifluoromethyl)-2-(4-(trifluoromethyl)phenyl)-1H-indole (3ar). Following the general procedure of Method A, compound 3ar was synthesized and isolated as a colorless solid (0.122 g, 74%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 46-47 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.75–7.61 (m, 6H), 7.39 (t, $J = 7.5$ Hz, 1H), 7.32 (t, $J = 7.4$ Hz, 1H), 6.67 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.90 (s, 3F), -62.69 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 137.6 (s), 136.3 (s), 136.0 (s), 130.9 (q, $J = 32.6$ Hz), 129.8 (s), 129.1 (s), 125.3 (q, $J = 3.7$ Hz), 125.0 (s), 124.2 (q, $J = 270.4$ Hz), 123.4 (s), 121.4 (s), 120.6 (q, $J = 261.7$ Hz), 113.3 (q, $J = 4.2$ Hz), 110.9 (s). HRMS (ESI) m/z calcd. for C$_{16}$H$_9$F$_6$NH (M+H)$^+$: 330.0712; found: 330.0710.

2-(4-nitrophenyl)-1-(trifluoromethyl)-1H-indole (3as). Following the general procedure of Method A, compound 3as was synthesized and isolated as a yellow solid
(0.081 g, 53%) via silica gel flash column chromatography using petroleum ether/ethyl acetate (petroleum ether:ethyl acetate = 100:1) as eluent. This compound can also be obtained as a yellow solid (0.061 g, 40%) via Method B. mp 108-110 °C. \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 8.35–8.26 (m, 2H), 7.67 (dd, \(J = 15.0, 8.2\) Hz, 3H), 7.45–7.36 (m, 1H), 7.38–7.29 (m, 1H), 6.74 (s, 1H). \textsuperscript{19}F NMR (376 MHz, CDCl\textsubscript{3}) \(\delta\) -49.87 (s, 3F). \textsuperscript{13}C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta\) 147.9 (s), 138.8 (s), 136.6 (d, \(J = 13.4\) Hz), 130.3–130.0 (m), 129.0 (s), 125.4 (s), 123.6 (s), 121.6 (s), 120.5 (q, \(J = 262.1\) Hz), 113.4 (q, \(J = 4.1\) Hz), 111.8 (s). HRMS (ESI) \(m/z\) calcd. for C\textsubscript{15}H\textsubscript{9}F\textsubscript{3}N\textsubscript{2}O\textsubscript{2}H (M+H)\(^+\): 307.0689; found: 307.0682.

4-(1-(trifluoromethyl)-1H-indol-2-yl)benzonitrile (3at). Following the general procedure of Method A, compound 3at was synthesized and isolated as a colorless solid (0.100 g, 70%) via silica gel flash column chromatography using petroleum ether/ethyl acetate (petroleum ether:ethyl acetate = 50:1) as eluent. This compound can also be obtained as a colorless solid (0.109 g, 76%) via Method B. mp 101-102 °C. \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.73 (d, \(J = 8.5\) Hz, 2H), 7.69–7.66 (m, 1H), 7.63 (t, \(J = 7.4\) Hz, 3H), 7.42–7.37 (m, 1H), 7.35–7.29 (m, 1H), 6.69 (s, 1H). \textsuperscript{19}F NMR (376 MHz, CDCl\textsubscript{3}) \(\delta\) -49.90 (s, 3F). \textsuperscript{13}C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta\) 137.1 (s), 136.9 (s), 136.4 (s), 132.1 (s), 130.1–129.8 (m), 129.0 (s), 125.3 (s), 121.5 (s), 120.5 (q, \(J = 262.1\) Hz), 118.6 (s), 113.3 (q, \(J = 4.2\) Hz), 112.5 (s), 111.4 (s). HRMS (ESI) \(m/z\) calcd. for C\textsubscript{16}H\textsubscript{9}F\textsubscript{3}N\textsubscript{2}H (M+H)\(^+\): 287.0791; found: 287.0784.

2-(3,5-bis(trifluoromethyl)phenyl)-1-(trifluoromethyl)-1H-indole (3au). Following the general procedure of Method A, compound 3au was synthesized and isolated as a colorless oil (0.093 g, 47%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.97 (d, \(J = 6.9\) Hz, 3H), 7.71–7.67 (m, 1H), 7.66 (d, \(J = 7.8\) Hz, 1H), 7.41 (dd, \(J = 8.4, 1.3\) Hz, 1H), 7.37–7.31 (m, 1H), 6.76 (s, 1H). \textsuperscript{19}F NMR (376 MHz, CDCl\textsubscript{3}) \(\delta\) -50.06 (s, 3F), -63.00 (s, 6F). \textsuperscript{13}C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta\) 136.5 (s), 135.7 (s), 134.5 (s), 131.9 (q, \(J = 33.7\) Hz), 129.9–129.1 (m), 128.9 (s), 125.6 (s), 123.7 (s), 123.2 (q, \(J = 271.1\) Hz), 122.6 (p, \(J = 3.8\) Hz), 121.6 (s), 120.6 (q, \(J = 261.8\) Hz), 113.4 (q, \(J = 4.2\) Hz), 112.1 (s). HRMS (ESI) \(m/z\) calcd. for C\textsubscript{17}H\textsubscript{8}F\textsubscript{9}NH (M+H)\(^+\): 398.0586; found: 398.0583.
2-(thiophen-3-yl)-1-(trifluoromethyl)-1H-indole (3av). Following the general procedure of Method A, compound 3av was synthesized and isolated as a colorless oil (0.107 g, 80%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.64 (d, $J = 8.3$ Hz, 1H), 7.58 (d, $J = 7.5$ Hz, 1H), 7.45 (dd, $J = 2.9$, 1.0 Hz, 1H), 7.36 (dd, $J = 5.0$, 3.0 Hz, 1H), 7.25 (dd, $J = 14.1$, 6.8 Hz, 2H), 6.63 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -50.23 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 135.9 (s), 134.0 (s), 132.1 (s), 129.0 (s), 129.0 – 128.6 (m), 125.4 (s), 125.3 (s), 124.4 (s), 123.0 (s), 121.0 (s), 120.7 (q, $J = 261.3$ Hz), 113.1 (q, $J = 4.7$ Hz), 109.9 (s). HRMS (AP) m/z calcd. for C$_{13}$H$_8$F$_3$NS (M$^+$): 267.0430; found: 267.0330.

2-cyclohexyl-1-(trifluoromethyl)-1H-indole (3aw). Following the general procedure of Method A, compound 3aw was synthesized and isolated as a colorless oil (0.104 g, 78%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.64–7.57 (m, 1H), 7.56–7.50 (m, 1H), 7.31–7.18 (m, 2H), 6.45 (s, 1H), 2.85 (s, 1H), 2.11 (t, $J = 9.7$ Hz, 2H), 1.89 (dd, $J = 5.3$, 2.5 Hz, 2H), 1.81 (ddt, $J = 11.1$, 3.0, 1.4 Hz, 1H), 1.45 (p, $J = 11.7$ Hz, 5H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -51.35 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 146.2 (s), 135.3 (s), 129.4 (s), 123.4 (s), 122.5 (s), 121.2 (q, $J = 260.2$ Hz), 120.5 (s), 112.7 (q, $J = 5.1$ Hz), 104.6 (s), 37.1 (q, $J = 2.9$ Hz), 34.3 (s), 26.8 (s), 26.3 (s). HRMS (AP) m/z calcd. for C$_{15}$H$_{16}$F$_3$N [M$^+$]: 267.1380, found 267.1235.

2-hexyl-1-(trifluoromethyl)-1H-indole (3ax). Following the general procedure of Method A, compound 3ax was synthesized and isolated as a colorless oil (0.102 g, 76%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.035 g, 26%) via Method B. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.63–7.56 (m, 1H), 7.53 (dd, $J = 6.8$, 1.8 Hz, 1H), 7.24 (pd, $J = 7.2$, 6.7, 1.4 Hz, 2H), 6.43 (s, 1H), 2.84 (t, $J = 7.7$ Hz, 2H), 1.77 (p, $J = 7.5$ Hz, 2H), 1.42 (ddq, $J = 33.4$, 7.1, 3.2 Hz, 6H), 1.01–0.88 (m, 3H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -51.89 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 140.3 (s), 135.6 (s), 129.3 (s), 123.4 (s), 122.5 (s), 121.1 (q, $J = 260.0$ Hz), 120.4 (s), 112.5 (q, $J = 4.8$ Hz), 106.3 (s), 31.8 (s), 29.2 (s), 28.4 (s), 28.0 (q, $J = 3.2$ Hz), 22.8 (s), 14.2 (s). HRMS (AP) m/z calcd. for C$_{15}$H$_{18}$F$_3$NH (M+H)$^+$: 270.1470; found: 270.1477.
7-((1-(trifluoromethyl)-1H-indol-2-yl)methoxy)-2H-chromen-2-one (3ay).
Following the general procedure of Method A, compound 3ay was synthesized and isolated as a colorless solid (0.140 g, 78%) via silica gel flash column chromatography using petroleum ether/ethyl acetate (petroleum ether:ethyl acetate = 20:1) as eluent. mp 113-114 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.61 (dd, $J$ = 14.8, 8.7 Hz, 3H), 7.43–7.32 (m, 2H), 7.30–7.25 (m, 1H), 6.92 (d, $J$ = 7.5 Hz, 2H), 6.79 (s, 1H), 6.27 (d, $J$ = 9.5 Hz, 1H), 5.28 (s, 2H). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -53.21 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 154.7 (s), 150.1 (s), 142.2 (s), 134.9 (s), 131.1 (s), 127.9 (s), 127.1 (s), 124.1 (s), 121.9 (s), 120.5 (s), 112.6 (s), 112.2 (s), 111.6 (q, $J$ = 261.4 Hz), 111.5 (q, $J$ = 4.2 Hz), 109.8 (s), 100.9 (s), 62.5 (q, $J$ = 3.4 Hz). HRMS (AP) m/z calcd. for C$_{19}$H$_{12}$F$_3$NO$_3$ (M)$^+$: 359.0769; found: 359.0766.

2-(4-(tert-butyl)phenyl)-1-(trifluoromethyl)-1H-indole (3az). Following the general procedure of Method B, compound 3az was synthesized and isolated as a colorless solid (0.095 g, 60%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 52-54 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.65 (d, $J$ = 8.21 Hz, 2H), 7.59 (d, $J$ = 7.9 Hz, 1H), 7.43 (s, 4H), 7.36–7.26 (m, 2H), 6.57 (s, 1H), 1.37 (s, 9H). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -49.32 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 151.76 (s), 139.43 (s), 135.85 (s), 129.93–128.66 (m), 124.98 (s), 124.04 (s), 122.80 (s), 119.49 (q), 120.85 (s), 113.01 (q, $J$ = 4.4 Hz), 109.44 (s), 34.72 (s), 31.31 (s). HRMS (AP) m/z calcd. for C$_{19}$H$_{18}$F$_3$NH (M+H)$^+$: 318.1480; found: 318.1481.

2-[[1,1'-biphenyl]-4-yl]-1-(trifluoromethyl)-1H-indole (3aa'). Following the general procedure of Method B, compound 3aa' was synthesized and isolated as a colorless solid (0.067 g, 40%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 114-115 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.66 (dt, $J$ = 5.6, 3.5 Hz, 5H), 7.63–7.56 (m, 3H), 7.47 (t, $J$ = 7.6 Hz, 2H), 7.41–7.26 (m, 3H), 6.64 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) δ -49.27 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 140.94 (d, $J$ = 108.1 Hz), 138.98 (s), 135.99 (s), 131.14 (s), 129.85–129.66 (m), 129.17 (s), 128.87 (s), 127.64 (s), 126.94 (d, $J$ = 36.8 Hz), 124.27 (s), 122.93 (s), 120.97 (s), δ
120.60 (q, $J = 263.2$ Hz), 113.08 (q, $J = 4.3$ Hz), 109.82 (s). HRMS (AP) m/z calcd. for C$_{21}$H$_{14}$F$_3$NH (M+H)$^+$: 338.1157; found: 338.1142.

methyl 4-(1-(trifluoromethyl)-1H-indol-2-yl)benzoate (3ab'). Following the general procedure of Method B, compound 3ab' was synthesized and isolated as a colorless solid (0.120 g, 75%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 54-55 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.10 (d, $J = 8.4$ Hz, 2H), 7.60 (dd, $J = 13.7$, 7.9 Hz, 4H), 7.33 (dtd, $J = 26.4$, 7.3, 1.2 Hz, 2H), 6.66 (s, 1H), 3.95 (s, 3H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.41 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 166.65 (s), 138.05 (s), 136.45 (d, $J = 51.9$ Hz), 130.22 (s), 129.42 – 129.20 (m), 129.01 (s), 124.73 (s), 123.15 (s), 121.20 (s), $\delta$ 120.48 (q, $J = 263.6$ Hz), 113.14 (q, $J = 4.2$ Hz), 110.64 (s), 52.26 (s). HRMS (AP) m/z calcd. for C$_{17}$H$_{12}$F$_3$NO$_2$H (M+H)$^+$: 320.0898; found: 320.0898.

2-(3,5-difluorophenyl)-1-(trifluoromethyl)-1H-indole (3ac'). Following the general procedure of Method B, compound 3ac' was synthesized and isolated as a colorless solid (0.030 g, 20%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 56-58 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.63 (dd, $J = 15.7$, 8.1 Hz, 2H), 7.40 – 7.33 (m, 1H), 7.29 (t, $J = 7.5$ Hz, 1H), 7.04 (d, $J = 5.9$ Hz, 2H), 6.88 (tt, $J = 8.9$, 2.3 Hz, 1H), 6.64 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -109.18 (s, 2F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 163.74 (d, $J = 12.9$ Hz), 161.26 (d, $J = 13.1$ Hz), 136.51 (t, $J = 2.8$ Hz), 136.08 , 135.07 (d, $J = 10.7$ Hz), 128.74 (s), 124.11 (d, $J = 172.7$ Hz), 121.30 (s), $\delta$ 119.02 (q), 113.16 (q, $J = 4.3$ Hz), 112.73–112.33 (m), 104.22 (t, $J = 25.2$ Hz). HRMS (AP) m/z calcd. for C$_{15}$H$_{12}$F$_3$NO$_2$H (M+H)$^+$: 298.0655; found: 298.0652.

2-(thiophen-2-yl)-1-(trifluoromethyl)-1H-indole (3ad'). Following the general procedure of Method B, compound 3ad' was synthesized and isolated as a brown oil (0.094 g, 70%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.64 (d, $J = 8.3$ Hz, 1H), 7.58 (d, $J = 7.8$ Hz, 1H), 7.40 (d, $J = 6.0$ Hz, 1H), 7.36–7.29 (m, 1H), 7.29–7.22 (m, 2H), 7.10 (dd, $J = 5.1$, 3.7 Hz, 1H), 6.74 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.36 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 135.91 (s), 131.97 (s), 131.13 (s), 128.92–128.77 (m),
2-(naphthalen-1-yl)-1-(trifluoromethyl)-1H-indole (3ae'). Following the general procedure of Method B, compound 3ae' was synthesized and isolated as a colorless solid (0.089 g, 57%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 39-41 °C. \( ^1H \) NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.92 (dd, \( J = 18.1, 8.1 \) Hz, 2H), 7.70 (d, \( J = 8.6 \) Hz, 2H), 7.66 (d, \( J = 7.5 \) Hz, 1H), 7.59–7.47 (m, 3H), 7.47–7.30 (m, 3H), 6.69 (s, 1H). \( ^19F \) NMR (376 MHz, CDCl\(_3\)) \( \delta \) -51.21 (s, 3F). \( ^13C \) NMR (101 MHz, CDCl\(_3\)) \( \delta \) 136.67 (s), 135.66 (s), 133.34 (d, \( J = 5.7 \) Hz), 129.87 (s), 129.67 (s), 129.34 (s), 128.80 (s), 128.29 (s), 126.50 (d, \( J = 52.1 \) Hz), 125.84 (s), 124.95 (s), 124.42 (s), 123.06 (s), 121.17 (s), 119.81 (q, \( J = 263.5 \) Hz). 112.97 (q, \( J = 4.0 \) Hz), 110.84 (s). HRMS (AP) m/z calcd. for C\(_{13}\)H\(_8\)F\(_3\)NSH (M+H)+: 268.0408; found: 268.0401.

\[ \begin{align*} 
&\text{N} \\
&\text{CF}_3 \\
&\text{N} \\
&\text{CF}_3 \\
&\text{O} \\
\end{align*} \]

2-(phenanthren-9-yl)-1-(trifluoromethyl)-1H-indole (3af'). Following the general procedure of Method B, compound 3af' was synthesized and isolated as a colorless solid (0.103 g, 57%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 47-49 °C. \( ^1H \) NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.78 – 8.71 (m, 2H), 7.92 (d, \( J = 7.9 \) Hz, 1H), 7.86 (s, 1H), 7.76 – 7.62 (m, 6H), 7.56 – 7.51 (m, 1H), 7.44 – 7.37 (m, 1H), 7.37 – 7.31 (m, 1H), 7.25 (s, 1H), 6.76 (s, 1H). \( ^19F \) NMR (376 MHz, CDCl\(_3\)) \( \delta \) -51.43 (s, 3F). \( ^13C \) NMR (101 MHz, CDCl\(_3\)) \( \delta \) 136.81 (s), 135.67 (s), 130.94 (d, \( J = 8.0 \) Hz), 130.21 (s), 129.99 (s), 129.37 (s), 128.76 (s), 127.69 (s), 127.11 (d, \( J = 7.0 \) Hz), 126.80 (d, \( J = 28.0 \) Hz), 124.50 (s), 123.10 (s), 122.85 (d, \( J = 10.7 \) Hz), 121.23 (s), 120.62 (q, \( J = 263.4 \) Hz), 112.95 (q, \( J = 3.8 \) Hz), 110.87 (s). HRMS (AP) m/z calcd. for C\(_{23}\)H\(_{14}\)F\(_3\)NH (M+H)+: 362.1157; found: 362.1170.

\[ \begin{align*} 
&\text{N} \\
&\text{CF}_3 \\
&\text{O} \\
&\text{O} \\
\end{align*} \]

6-(1-(trifluoromethyl)-1H-indol-2-yl)-2H-chromen-2-one (3ag'). Following the general procedure of Method B, compound 3ag' was synthesized and isolated as a yellow solid (0.040 g, 24%) via silica gel flash column chromatography using petroleum ether/ethyl acetate (ether:ethyl acetate = 20:1) as eluent. mp 106-108 °C. \( ^1H \) NMR (400 MHz, CDCl\(_3\)) \( \delta \) 128.60 (s), 127.12 (d, \( J = 27.9 \) Hz), 124.72 (s), 122.94 (s), 121.05 (s), 120.51 (q, \( J = 263.3 \) Hz), 113.01 (q, \( J = 5.0 \) Hz), 111.54 (s). HRMS (AP) m/z calcd. for C\(_{13}\)H\(_8\)F\(_3\)NSH (M+H)+: 268.0408; found: 268.0401.
NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.74 (d, \(J = 9.6\) Hz, 1H), 7.70 – 7.59 (m, 4H), 7.38 (dd, \(J = 13.7, 7.8\) Hz, 2H), 7.31 (t, \(J = 7.4\) Hz, 1H), 6.64 (s, 1H), 6.49 (d, \(J = 9.5\) Hz, 1H). \(^{19}\)F NMR (376 MHz, CDCl\textsubscript{3}) \(\delta\) -49.39 (s, 3F). \(^{13}\)C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta\) 160.37 (s), 154.13 (s), 143.10 (s), 136.47 (d, \(J = 109.6\) Hz), 132.89 (s), 128.96 – 128.54 (m), 124.76 (s), 123.21 (s), 121.14 (s), 121.67 (q), 118.55 (s), 117.12 (d, \(J = 64.7\) Hz), 113.09 (q, \(J = 4.3\) Hz), 110.60 (s). HRMS (AP) \(m/z\) calcd. for C\textsubscript{18}H\textsubscript{10}F\textsubscript{3}NO\textsubscript{2}H [M+H]\textsuperscript{+}: 330.0742; found: 330.0759.

6-methyl-2-phenyl-1-(trifluoromethyl)-1H-indole (3ba). Following the general procedure of Method A, compound 3ba was synthesized and isolated as a colorless oil (0.084 g, 61%) via silica gel flash column chromatography using petroleum ether as eluent. This compound can also be obtained as a colorless oil (0.039 g, 28%) via Method B. \(^{1}\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.55–7.46 (m, 4H), 7.46–7.40 (m, 3H), 7.13 (d, \(J = 8.1\) Hz, 1H), 6.56 (s, 1H), 2.53 (s, 3H). \(^{19}\)F NMR (376 MHz, CDCl\textsubscript{3}) \(\delta\) -49.94 (s, 3F). \(^{13}\)C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta\) 138.8 (s), 136.5 (s), 134.4 (s), 132.6 (s), 129.5 (s), 128.6 (s), 128.2 (s), 127.1 (s), 124.6 (s), 120.7 (q, \(J = 261.4\) Hz), 120.7 (s), 113.3 (q, \(J = 4.2\) Hz), 109.7 (s), 22.1 (s). HRMS (AP) \(m/z\) calcd. for C\textsubscript{16}H\textsubscript{12}F\textsubscript{3}NH (M)\textsuperscript{+}: 276.0995; found: 276.1001.

5-methyl-2-phenyl-1-(trifluoromethyl)-1H-indole (3bb). Following the general procedure of Method A, compound 3bb was synthesized and isolated as a yellow oil (0.081 g, 59%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a yellow oil (0.045 g, 33%) via Method B. \(^{1}\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.54 (dd, \(J = 13.6, 7.0, 1.9\) Hz, 3H), 7.47–7.43 (m, 3H), 7.41 (s, 1H), 7.18 (dd, \(J = 8.5, 1.3\) Hz, 1H), 6.55 (s, 1H), 2.49 (s, 3H). \(^{19}\)F NMR (376 MHz, CDCl\textsubscript{3}) \(\delta\) -50.03 (s, 3F). \(^{13}\)C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta\) 139.5 (s), 134.3 (s), 132.7 (s), 132.6 (s), 129.7 – 129.3 (m), 128.7 (s), 128.2 (s), 125.8 (s), 120.9 (s), 120.8 (q, \(J = 261.3\) Hz), 112.9 (q, \(J = 4.2\) Hz), 109.6 (s), 21.4 (s). HRMS (ESI) \(m/z\) calcd. for C\textsubscript{16}H\textsubscript{12}F\textsubscript{3}NH (M+H)\textsuperscript{+}: 276.0995; found: 276.0995.

5-(tert-butyl)-2-phenyl-1-(trifluoromethyl)-1H-indole (3bc). Following the general procedure of Method A, compound 3bc was synthesized and isolated as a colorless oil (0.090 g, 57%) via silica gel flash column chromatography using petroleum ether (60-
90 °C) as eluent. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.60 (dd, \(J = 11.6, 1.9\) Hz, 2H), 7.50 (dd, \(J = 6.5, 2.9\) Hz, 2H), 7.46–7.40 (m, 4H), 6.58 (s, 1H), 1.42 (s, 9H). \(^19\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -50.03 (s, 3F). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 146.2 (s), 139.5 (s), 134.2 (s), 132.5 (s), 129.6 (s), 129.2 (s), 128.7 (s), 128.2 (s), 122.5 (s), 120.8 (q, \(J = 261.4\) Hz), 117.2 (s), 112.7 (q, \(J = 4.2\) Hz), 110.0 (s), 34.8 (s), 31.9 (s). HRMS (AP) \(m/z\) calcd. for C\(_{19}\)H\(_{18}\)F\(_3\)NH (M+H): 318.1470; found: 318.1479.

6-fluoro-2-phenyl-1-(trifluoromethyl)-1H-indole (3bd). Following the general procedure of Method A, compound 3bd was synthesized and isolated as a colorless oil (0.091 g, 65%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.57–7.48 (m, 3H), 7.49–7.41 (m, 3H), 7.41–7.35 (m, 1H), 7.11–6.99 (m, 1H), 6.58 (s, 1H). \(^19\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -50.24 (s, 3F), -116.99 (s, 1F). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 160.8 (d, \(J = 241.0\) Hz), 139.7 (d, \(J = 4.0\) Hz), 136.0 (d, \(J = 12.4\) Hz), 132.0 (s), 129.8–129.3 (m), 128.9 (s), 128.3 (s), 125.5 (s), 121.9 (d, \(J = 9.9\) Hz), 120.5 (q, \(J = 262.0\) Hz), 111.5 (d, \(J = 24.1\) Hz), 109.4 (s), 100.6 (dq, \(J = 28.5, 4.6\) Hz). HRMS (ESI) \(m/z\) calcd. for C\(_{15}\)H\(_9\)F\(_4\)NH (M+H): 280.0744; found: 280.0734.

5-fluoro-2-phenyl-1-(trifluoromethyl)-1H-indole (3be): Following the general procedure of Method A, compound 3be was synthesized and isolated as a colorless oil (0.108 g, 77%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless oil (0.081 g, 58%) via Method B. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.59 (ddd, \(J = 8.9, 4.1, 2.0\) Hz, 1H), 7.51 (dd, \(J = 6.6, 2.9\) Hz, 2H), 7.50–7.41 (m, 3H), 7.27 (dd, \(J = 8.6, 2.7\) Hz, 1H), 7.08 (td, \(J = 9.1, 2.6\) Hz, 1H), 6.59–6.55 (m, 1H). \(^19\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -50.10 (s, 3F), -120.68 (s, 1F). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 159.5 (d, \(J = 239.3\) Hz), 141.1 (s), 132.2 (d, \(J = 36.8\) Hz), 130.1 (d, \(J = 10.1\) Hz), 129.5 (d, \(J = 1.0\) Hz), 129.1 (s), 128.3 (s), 120.6 (q, \(J = 261.6\) Hz), 114.1 (dd, \(J = 9.3, 4.6\) Hz), 112.4 (d, \(J = 25.7\) Hz), 109.6 (d, \(J = 3.3\) Hz), 106.4 (d, \(J = 23.8\) Hz). HRMS (ESI) \(m/z\) calcd. for C\(_{15}\)H\(_9\)F\(_4\)NH (M+H): 280.0736; found: 280.0744.

6-chloro-2-phenyl-1-(trifluoromethyl)-1H-indole (3bf). Following the general procedure of Method A, compound 3bf was synthesized and isolated as a colorless oil
(0.096 g, 65%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. **1H NMR** (400 MHz, CDCl$_3$) $\delta$ 7.68 (s, 1H), 7.55–7.48 (m, 3H), 7.48–7.42 (m, 3H), 7.28 (dd, $J$ = 8.4, 1.8 Hz, 1H), 6.58 (s, 1H). **19F NMR** (376 MHz, CDCl$_3$) $\delta$ -49.97 (s, 3F). **13C NMR** (101 MHz, CDCl$_3$) $\delta$ 140.0 (s), 136.2 (s), 131.8 (s), 130.2 (s), 129.5 (s), 129.1 (s), 128.3 (s), 127.7 (s), 123.7 (s), 121.8 (s), 120.4 (q, $J$ = 263.9 Hz), 113.4 (q, $J$ = 4.7 Hz), 109.4 (s). **HRMS (ESI)** m/z calcd. for C$_{15}$H$_9$ClF$_3$NH (M+H)$^+$: 296.0448; found: 296.0437.

5-chloro-2-phenyl-1-(trifluoromethyl)-1H-indole (3bg). Following the general procedure of Method A, compound 3bg was synthesized and isolated as a colorless solid (0.109 g, 74%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless solid (0.064 g, 43%) via Method B. mp 61-63 °C. **1H NMR** (400 MHz, CDCl$_3$) $\delta$ 7.57 (dd, $J$ = 9.4, 1.9 Hz, 2H), 7.51 (dd, $J$ = 6.7, 2.9 Hz, 2H), 7.48–7.43 (m, 3H), 7.30 (dd, $J$ = 8.9, 2.1 Hz, 1H), 6.55 (s, 1H). **19F NMR** (376 MHz, CDCl$_3$) $\delta$ -49.98 (s, 3F). **13C NMR** (101 MHz, CDCl$_3$) $\delta$ 140.8 (s), 134.3 (s), 131.8 (s), 130.4 (s), 129.5 (d, $J$ = 1.1 Hz), 129.1 (s), 128.8 (s), 128.3 (s), 124.6 (s), 120.6 (s), 120.5 (q, $J$ = 262.1 Hz), 114.2 (q, $J$ = 4.5 Hz), 109.1 (s). **HRMS (ESI)** m/z calcd. for C$_{15}$H$_9$ClF$_3$NH (M+H)$^+$: 296.0448; found: 296.0438.

5-bromo-2-phenyl-1-(trifluoromethyl)-1H-indole (3bh). Following the general procedure of Method A, compound 3bh was synthesized and isolated as a colorless solid (0.122 g, 72%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent to afford the product. This compound can also be obtained as a colorless solid (0.122 g, 72%) via Method B. mp 57-59 °C. **1H NMR** (400 MHz, CDCl$_3$) $\delta$ 7.75 (d, $J$ = 1.9 Hz, 1H), 7.56–7.48 (m, 3H), 7.47–7.41 (m, 4H), 6.55 (s, 1H). **19F NMR** (376 MHz, CDCl$_3$) $\delta$ -49.95 (s, 3F). **13C NMR** (101 MHz, CDCl$_3$) $\delta$ 140.6 (s), 134.6 (s), 131.7 (s), 130.9 (s), 129.8–129.3 (m), 129.1 (s), 128.3 (s), 127.2 (s), 123.7 (s), 120.4 (q, $J$ = 262.2 Hz), 116.3 (s), 114.6 (q, $J$ = 4.5 Hz), 108.9 (s). **HRMS (AP)** m/z calcd. for C$_{15}$H$_9$BrF$_3$NH (M+H)$^+$: 339.9949; found: 339.9955.

5-nitro-2-phenyl-1-(trifluoromethyl)-1H-indole (3bi). Following the general procedure of Method A, compound 3bi was synthesized and isolated as a yellow solid
(0.110 g, 72%) via silica gel flash column chromatography using petroleum ether/ethyl acetate (petroleum ether:ethyl acetate = 100:1) as eluent. This compound can also be obtained as a yellow solid (0.031 g, 20%) via Method B. mp 84-86 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.54 (d, $J$ = 2.2 Hz, 1H), 8.23 (dd, $J$ = 9.2, 2.3 Hz, 1H), 7.73 (dd, $J$ = 9.2, 1.8 Hz, 1H), 7.49 (qd, $J$ = 6.6, 5.4, 3.3 Hz, 5H), 6.75 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.81 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 144.0 (s), 142.4 (s), 138.5 (s), 131.0 (s), 129.6 (s), 129.6–129.4 (m), 128.9 (s), 128.5 (s), 120.1 (q, $J$ = 265.0 Hz), 119.5 (s), 117.4 (s), 113.3 (q, $J$ = 4.8 Hz), 110.1 (s). HRMS (ESI) $m/z$ calcd. for $C_{15}H_9F_3N_2O_2H$ (M+H)$^+$: 307.0689; found: 307.0681.

N$_2$CF$_3$MeO$_2$C methyl 2-phenyl-1-(trifluoromethyl)-1H-indole-5-carboxylate (3bj). Following the general procedure of Method A, compound 3bj was synthesized and isolated as a colorless oil (0.118 g, 74%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.35 (s, 1H), 8.04 (d, $J$ = 8.8 Hz, 1H), 7.68 (d, $J$ = 8.7 Hz, 1H), 7.55–7.40 (m, 5H), 6.67 (s, 1H), 3.96 (s, 3H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.83 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 167.4 (s), 140.6 (s), 138.3 (s), 131.7 (s), 129.7–129.4 (m), 129.1 (s), 128.9 (s), 128.3 (s), 125.6 (s), 125.2 (s), 123.5 (s), 120.4 (q, $J$ = 262.5 Hz), 12.8 (q, $J$ = 4.5 Hz), 110.0 (s), 52.2 (s). HRMS (AP) $m/z$ calcd. for $C_{17}H_{12}F_3NO_2H$ (M+H)$^+$: 320.0893; found: 320.0997.

2-phenyl-1,5-bis(trifluoromethyl)-1H-indole (3bk). Following the general procedure of Method A, compound 3bk was synthesized and isolated as a colorless oil (0.115 g, 70%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.92 (s, 1H), 7.81–7.67 (m, 1H), 7.59 (dd, $J$ = 8.8, 1.4 Hz, 1H), 7.52 (dd, $J$ = 6.8, 2.9 Hz, 2H), 7.47 (dt, $J$ = 4.8, 2.1 Hz, 3H), 6.68 (s, 1H). $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -49.86 (s, 3F), -61.20 (s, 3F). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 141.1 (s), 137.2 (s), 131.6 (s), 129.6 (d, $J$ = 1.1 Hz), 129.3 (s), 128.8 (s), 128.4 (s), 125.6 (q, $J$ = 32.4 Hz), 124.8 (q, $J$ = 270.2 Hz), 121.1 (q, $J$ = 3.2 Hz), 120.4 (q, $J$ = 264.1 Hz), 118.7 (q, $J$ = 4.2 Hz), 113.4 (q, $J$ = 4.6 Hz), 109.7 (s). HRMS (ESI) $m/z$ calcd. for $C_{16}H_{10}F_6N$ (M+H)$^+$: 330.0712; found: 330.0717.
5-chloro-7-fluoro-2-phenyl-1-(trifluoromethyl)-1H-indole (3bl). Following the general procedure of Method A, compound 3bl was synthesized and isolated as a colorless solid (0.110 g, 70%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. This compound can also be obtained as a colorless solid (0.069 g, 44%) via Method B. mp 76-77 °C. 

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.54–7.49 (m, 2H), 7.48–7.41 (m, 3H), 7.40–7.33 (m, 1H), 7.13–7.06 (m, 1H), 6.55 (d, J = 1.9 Hz, 1H). 

$^{19}$F NMR (376 MHz, CDCl$_3$) δ -48.37 (d, J = 30.0 Hz, 3F), -123.17 (q, J = 30.0 Hz, 1F). 

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 150.2 (s), 147.7 (s), 142.5 (s), 133.4 (d, J = 4.2 Hz), 131.9 (s), 129.2 (s), 128.9 (d, J = 8.9 Hz), 128.8 – 128.6 (m), 128.5 (s), 122.2 (d, J = 10.6 Hz), 119.7 (q, J = 263.6 Hz), 116.5 (d, J = 4.0 Hz), 112.0 (d, J = 23.8 Hz), 109.0 (s). HRMS (AP) m/z calcd. for C$_{15}$H$_8$ClF$_4$NH (M+H)$^+$: 314.0354; found: 314.0392.

2-phenyl-3-(trifluoromethyl)-3H-benzo[e]indole (3bm). Following the general procedure of Method A, compound 3bm was synthesized and isolated as a colorless solid (0.092 g, 59%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 44-46 °C. 

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.18 (d, J = 7.9 Hz, 1H), 7.93 (d, J = 7.9 Hz, 1H), 7.76 (q, J = 8.5 Hz, 2H), 7.63–7.39 (m, 7H), 7.12 (s, 1H). 

$^{19}$F NMR (376 MHz, CDCl$_3$) δ -49.30 (s, 3F). 

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 138.1 (s), 132.6 (d, J = 11.1 Hz), 130.2 (s), 129.9–129.5 (m), 128.7 (d, J = 10.9 Hz), 128.2 (s), 127.4 (s), 126.6 (s), 125.2 (s), 125.0 (s), 124.8 (s), 123.2 (s), 120.6 (q, J = 262.3 Hz), 113.4 (q, J = 4.4 Hz), 108.3 (s). HRMS (AP) m/z calcd. for C$_{19}$H$_{12}$F$_3$NH (M+H)$^+$: 312.0995; found: 311.1061.

3-ethyl-3-(2-phenyl-1-(trifluoromethyl)-1H-indol-5-yl)piperidine-2,6-dione (3bn). Following the general procedure of Method A, compound 3bn was synthesized and isolated as a colorless solid (0.060 g, 30%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 123-124 °C. 

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.99 (s, 1H), 7.69–7.60 (m, 1H), 7.53–7.42 (m, 6H), 7.30–7.25 (m, 1H), 6.57 (s, 1H), 2.63 (dd, J = 15.8, 4.7 Hz, 1H), 2.54–2.38 (m, 2H), 2.36–2.23 (m, 1H), 2.06 (ddt, J = 41.5, 14.1, 7.3 Hz, 2H), 0.92 (t, J = 7.4 Hz, 3H). 

$^{19}$F NMR (376 MHz, CDCl$_3$) δ -49.94 (s, 3F). 

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 175.5 (s), 172.3 (s), 140.3 (s), 135.1 (s), 133.5 (s), 132.0 (s), 129.7 (s), 129.6–129.4 (m), 129.0 (s), 128.3 (s), 122.2 (s), 120.5
(q, J = 261.8 Hz), 119.0 (s), 113.7 (q, J = 4.4 Hz), 109.6 (s), 51.2 (s), 33.4 (s), 29.5 (s), 27.6 (s), 9.3 (s). **HRMS (AP) m/z** calcd. for C_{22}H_{19}F_{3}N_{2}O_{2}H (M+H)^+: 401.1477; found: 401.1474.

5,7-dichloro-2-phenyl-1-(trifluoromethyl)-1H-indole (3bo). Following the general procedure of **Method B**, compound 3bo was synthesized and isolated as a colorless solid (0.033 g, 20%) via silica gel flash column chromatography using petroleum ether (60-90 °C) as eluent. mp 80-82 °C. **^1H NMR** (600 MHz, CDCl₃) δ 7.53 (d, J = 8.1 Hz, 2H), 7.48–7.42 (m, 4H), 7.35 (s, 1H), 6.57 (s, 1H), 7.38 (dt, J = 24.4, 6.9 Hz, 2H), 6.77 (s, 1H). **^19F NMR** (565 MHz, CDCl₃) δ -42.90 (s, 3F). **^13C NMR** (151 MHz, CDCl₃) δ 143.81 (s), 133.56 (s), 132.59 (s), 132.43 (d, J = 1.8 Hz), 129.41 (s), 129.07 (s), 128.68 (s), 128.05 (s), 126.39 (s), 120.33 (s), 119.35 (s), 119.81 (q, J = 266.1 Hz). 109.33 (s). **HRMS (AP) m/z** calcd. for C_{15}H_{8}Cl_{2}F_{3}NH (M+H)^+: 330.0064; found: 330.0057.

ethyl 2-phenyl-1-(trifluoromethyl)-1H-indole-5-carboxylate (3bp). Following the general procedure of **Method B**, compound 3bp was synthesized and isolated as a colorless solid (0.138 g, 83%) via silica gel flash column chromatography using petroleum ether/ethyl acetate (petroleum ether:ethyl acetate = 100:1) as eluent. mp 41-42 °C. **^1H NMR** (600 MHz, CDCl₃) δ 8.34 (d, J = 1.7 Hz, 1H), 8.04 (d, J = 8.7 Hz, 1H), 7.67 (d, J = 7.0 Hz, 2H), 7.47 (dt, J = 33.3, 3.8 Hz, 3H), 6.66 (s, 1H), 4.42 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.1 Hz, 3H). **^19F NMR** (565 MHz, CDCl₃) δ -49.21 (s, 3F). **^13C NMR** (151 MHz, CDCl₃) δ 166.80 (s), 140.42 (s), 138.18 (s), 131.64 (s), 129.43 (s), 129.00 (s), 128.75 (s), 128.17 (s), 125.42 (d, J = 8.3 Hz), 123.27 (s), 120.28 (q, J = 264.1 Hz), 112.64 (q, J = 4.6 Hz), 109.92 (s), 60.97 (s), 14.40 (s). **HRMS (AP) m/z** calcd. for C_{18}H_{14}F_{3}NO_{2}H (M+H)^+: 334.1055; found: 334.1058.

8. Mechanism study

To an oven-dried 25 mL Schlenk tube equipped with a stir bar were added 2-alkynyl arylamine 2aa (0.5 mmol, 1.0 equiv.), AgSCF₃ (1.5 equiv.), KI (1.5 equiv.). The Schlenk tube was evacuated and refilled with dry nitrogen (three times). CH₃CN (5 mL)
was then added by syringe. The reaction mixture was required to heat to 50 °C and then stirred for 1 h under nitrogen. After cooling to room temperature, the reaction mixture was diluted with ethyl acetate, filtered through a plug of celite and was with ethyl acetate, then concentrated under vacuum and purified by silica gel flash column chromatography (200-300 mesh) using petroleum ether (60-90 °C) as eluent to afford 2-alkynyl arylisothiocyanate 1aa (0.102 g, 87% yield).

To an oven-dried 25 mL Schlenk tube equipped with a stir bar were added 2-alkynyl arylisothiocyanate 1aa (0.5 mmol, 1.0equiv.), AgF (3.2 equiv.), TEMPO (4.0 equiv.), RhCl(PPh₃)₃ (1 mol%). The Schlenk tube was evacuated and refilled with dry nitrogen (three times). CH₃CN (5 mL) was then added by syringe. The reaction mixture was required to heat to 45 °C and then stirred for 3 h under nitrogen. After cooling to room temperature, the reaction mixture was diluted with dichloromethane. The raw product was analyzed by ¹⁹F NMR using 4,4′-difluorobiphenyl (-115.0 ppm) as internal standard. The final product 3aa is obtained with a yield of 60%.
9. $^1$H NMR, $^{13}$C NMR and $^{19}$F NMR spectra of the products

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

$^{19}$F NMR Spectrum of 3aa (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3aa (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3ab (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ac (400 MHz, CDCl$\text{_3}$)

$^{19}$F NMR Spectrum of 3ac (376 MHz, CDCl$\text{_3}$)
$^{13}$C NMR Spectrum of $3\text{ac}$ (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3ad (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ae (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3ae (376 MHz, CDCl$_3$)
**$^{13}$C NMR Spectrum of 3ae (101 MHz, CDCl$_3$)**

![C NMR Spectrum of 3ae](image)

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

![H NMR Spectrum of 3af](image)
$^{19}$F NMR Spectrum of 3af (376 MHz, CDCl$_3$)

13C NMR Spectrum of 3af (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ag (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3ag (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of $3\text{ag}$ (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3ah (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ai (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3ai (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3ai (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3aj (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ak (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3ak (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3ak (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3al (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3am (400 MHz, CDCl$_3$)

19F NMR Spectrum of 3am (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3am (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3an (101 MHz, CDCl$_3$)
\(^1\)H NMR Spectrum of 3ao (400 MHz, CDCl\(_3\)) 

\[^{19}\text{F} \text{NMR Spectrum of 3ao (376 MHz, CDCl}_3\])
$^{13}$C NMR Spectrum of 3ao (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3ap (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3aq (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3aq (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3aq (101 MHz, CDCl$_3$)

N
\[ \text{Br} \]
\[ \text{CF}_3 \]

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

N
\[ \text{CF}_3 \]

S55
$^{19}$F NMR Spectrum of 3ar (376 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of 3ar (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3as (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3as (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of $3\text{as}$ (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3at (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3au (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3au (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3au (101 MHz, CDCl$_3$)

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

13C NMR Spectrum of 3av (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3aw (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3aw (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3aw (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3ax (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ay (400 MHz, CDCl$_3$)

![](image)

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

![](image)
$^{13}$C NMR Spectrum of $3ay$ (101 MHz, CDCl$_3$)

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

13C NMR Spectrum of 3az (101 MHz, CDCl$_3$)
$^{1}$H NMR Spectrum of 3aa’ (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3aa’ (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3aa' (101 MHz, CDCl$_3$)

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

13C NMR Spectrum of 3ab' (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ac' (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3ac' (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3ac' (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3ad’ (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ae' (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3ae' (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3ae' (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3af' (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3ag′ (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3ag′ (376 MHz, CDCl$_3$)
13C NMR Spectrum of 3ag' (101 MHz, CDCl₃)

1H NMR Spectrum of 3ba (400 MHz, CDCl₃)
$^{19}$F NMR Spectrum of 3ba (376 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of 3ba (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3bb (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3bb (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3bb (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3bc (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3bd (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3bd (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3bd (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3be (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3bf (400 MHz, CDCl$_3$)

![$^1$H NMR Spectrum of 3bf (400 MHz, CDCl$_3$)](image1)

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

![$^{19}$F NMR Spectrum of 3bf (376 MHz, CDCl$_3$)](image2)
$^{13}$C NMR Spectrum of **3bf** (101 MHz, CDCl$_3$)

\begin{align*}
109.43 & \\
113.34 & \\
113.39 & \\
113.44 & \\
113.48 & \\
113.70 & \\
116.46 & \\
119.08 & \\
121.70 & \\
121.83 & \\
123.74 & \\
124.33 & \\
127.72 & \\
128.27 & \\
129.05 & \\
129.52 & \\
130.23 & \\
131.84 & \\
136.18 & \\
140.02 & \\
\end{align*}

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

\begin{align*}
1.00 & \\
1.01 & \\
3.05 & \\
2.10 & \\
1.99 & \\
6.55 & \\
7.29 & \\
7.29 & \\
7.31 & \\
7.32 & \\
7.44 & \\
7.44 & \\
7.45 & \\
7.45 & \\
7.46 & \\
7.46 & \\
7.47 & \\
7.47 & \\
7.48 & \\
7.48 & \\
7.49 & \\
7.50 & \\
7.51 & \\
7.52 & \\
7.53 & \\
7.55 & \\
\end{align*}
$^{19}\text{F NMR Spectrum of 3bg (376 MHz, CDCl}_3\text{)}$ 

$^{13}\text{C NMR Spectrum of 3bg (101 MHz, CDCl}_3\text{)}$
$^1$H NMR Spectrum of 3bh (400 MHz, CDCl$_3$)

1$^9$F NMR Spectrum of 3bh (376 MHz, CDCl$_3$)
13C NMR Spectrum of 3bh (101 MHz, CDCl₃)

1H NMR Spectrum of 3bi (400 MHz, CDCl₃)
$^{19}$F NMR Spectrum of 3bi (376 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of 3bi (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3bj (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3bj (376 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3bj (101 MHz, CDCl$_3$)

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

$^{13}\text{C}$ NMR Spectrum of $3\text{bk}$ (101 MHz, CDCl$_3$)
$^1\text{H NMR Spectrum of 3bl (400 MHz, CDCl}_3\text{)}$

$^{19}\text{F NMR Spectrum of 3bl (376 MHz, CDCl}_3\text{)}$
$^{13}$C NMR Spectrum of 3bl (101 MHz, CDCl$_3$)

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

$^{13}$C NMR Spectrum of 3bm (101 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3bn (400 MHz, CDCl$_3$)

$^{19}$F NMR Spectrum of 3bn (376 MHz, CDCl$_3$)
\[\begin{align*}
\text{\^{13}C NMR Spectrum of 3bn (101 MHz, CDCl}_3)\\
\end{align*}\]

\[\begin{align*}
\text{\^{1}H NMR Spectrum of 3bo (600 MHz, CDCl}_3)\\
\end{align*}\]
$^{19}$F NMR Spectrum of $3\text{bo}$ (565 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $3\text{bo}$ (151 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3bp (600 MHz, CDCl$_3$)

$^1$F NMR Spectrum of 3bp (565 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3bp (151 MHz, CDCl$_3$)

14.40 60.97 109.92 112.59 112.62 112.65 112.68 117.66 119.41 121.16 122.91 123.27 125.39 125.45 128.17 128.75 129.00 129.43 131.64 132.23 138.18 138.59 140.42 166.80
10. HRMS analysis reports for the new compounds

HRMS (ESI) spectra of 3aa
HRMS (ESI) spectra of 3ab
HRMS (ESI) spectra of 3ac
HRMS (ESI) spectra of 3ad
HRMS (ESI) spectra of 3ae
HRMS (ESI) spectra of $3\text{af}$
HRMS (ESI) spectra of 3ag
HRMS (ESI) spectra of 3ah
HRMS (ESI) spectra of 3ai
HRMS (ESI) spectra of 3aj
HRMS (ESI) spectra of 3ak
HRMS (ESI) spectra of 3al
HRMS (ESI) spectra of 3am
HRMS (ESI) spectra of **3an**
HRMS (ESI) spectra of 3ao
HRMS (ESI) spectra of 3ap
HRMS (ESI) spectra of 3aq
HRMS (ESI) spectra of 3ar
HRMS (ESI) spectra of 3as
HRMS (ESI) spectra of 3at
HRMS (ESI) spectra of 3au
HRMS (AP) spectra of 3av
HRMS (AP) spectra of 3aw
HRMS (AP) spectra of 3ax
HRMS (AP) spectra of 3ay

HRMS (AP) spectra of 3az
RMS (AP) spectra of 3aa'

HRMS (AP) spectra of 3ab'
HRMS (AP) spectra of 3ac’

HRMS (AP) spectra of 3ad’
HRMS (AP) spectra of 3ae$	extsuperscript{'}$

HRMS (AP) spectra of 3af$	extsuperscript{'}$
HRMS (AP) spectra of 3ag'

HRMS (AP) spectra of 3ba
HRMS (ESI) spectra of 3bb
HRMS (AP) spectra of 3bc
HRMS (ESI) spectra of **3bd**
HRMS (ESI) spectra of 3be
HRMS (ESI) spectra of 3bf
HRMS (ESI) spectra of 3bg
HRMS (AP) spectra of 3bh
HRMS (ESI) spectra of 3bi
HRMS (AP) spectra of 3bj
HRMS (ESI) spectra of 3bk
HRMS (AP) spectra of 3bl

HRMS (AP) spectra of 3bm
HRMS (AP) spectra of 3bn

HRMS (AP) spectra of 3bo
HRMS (AP) spectra of 3bp
11. Crystal data and structure refinement for the products

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Identification code</td>
<td>3am</td>
</tr>
<tr>
<td>Empirical formula</td>
<td>C15 H9 Cl F3 N</td>
</tr>
<tr>
<td>Formula weight</td>
<td>295.68</td>
</tr>
<tr>
<td>Temperature</td>
<td>100(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>1.54178 Å</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Monoclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>Cc</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>a = 5.9221(4) Å, b = 21.7851(16) Å, c = 10.0601(8) Å, α = 90°, β = 100.563(4)°, γ = 90°</td>
</tr>
<tr>
<td>Volume</td>
<td>1275.89(16) Å³</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Density (calculated)</td>
<td>1.539 Mg/m³</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>2.903 mm⁻¹</td>
</tr>
<tr>
<td>F(000)</td>
<td>600</td>
</tr>
<tr>
<td>Crystal size</td>
<td>0.15 x 0.20 x 0.25 mm³</td>
</tr>
<tr>
<td>Theta range for data collection</td>
<td>4.058 to 68.245°</td>
</tr>
<tr>
<td>Index ranges</td>
<td>-7≤h≤5, -26≤k≤25, -12≤l≤11</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>6340</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>1822 [R(int) = 0.0526]</td>
</tr>
<tr>
<td>Completeness to theta = 67.679°</td>
<td>100.0 %</td>
</tr>
<tr>
<td>Absorption correction</td>
<td>Multi-Scan</td>
</tr>
<tr>
<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
</tr>
<tr>
<td>Data / restraints / parameters</td>
<td>1822 / 2 / 181</td>
</tr>
<tr>
<td>Goodness-of-fit on F²</td>
<td>1.004</td>
</tr>
<tr>
<td>Final R indices [I≥2sigma(I)]</td>
<td>R1 = 0.0360, wR2 = 0.0859</td>
</tr>
<tr>
<td>R indices (all data)</td>
<td>R1 = 0.0407, wR2 = 0.0891</td>
</tr>
<tr>
<td>Absolute structure parameter</td>
<td>0.037(19)</td>
</tr>
<tr>
<td>Extinction coefficient</td>
<td>n/a</td>
</tr>
<tr>
<td>Largest diff. peak and hole</td>
<td>0.269 and -0.207 e.Å⁻³</td>
</tr>
</tbody>
</table>
Identification code 3aq
Empirical formula C15 H9 Br3 F3 N
Formula weight 340.14
Temperature 100(2) K
Wavelength 1.54178 Å
Crystal system Triclinic
Space group P-1
Unit cell dimensions
\[ a = 8.1764(6) \text{ Å}, \alpha = 86.542(2)^\circ \]
\[ b = 10.5249(7) \text{ Å}, \beta = 88.533(2)^\circ \]
\[ c = 15.2713(10) \text{ Å}, \gamma = 89.967(2)^\circ \]
Volume 1311.36(16) Å³
Z 4
Density (calculated) 1.723 Mg/m³
Absorption coefficient 4.521 mm⁻¹
F(000) 672
Crystal size 0.15 x 0.20 x 0.25 mm³
Theta range for data collection 2.900 to 68.317°
Index ranges -9≤h≤9, -12≤k≤12, -18≤l≤18
Reflections collected 17835
Independent reflections 4791 [R(int) = 0.0430]
Completeness to theta = 67.679° 99.9 %
Absorption correction Multi-Scan
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 4791 / 24 / 361
Goodness-of-fit on F² 1.003
Final R indices [I>2sigma(I)] R1 = 0.0317, wR2 = 0.0831
R indices (all data)  
R1 = 0.0333, wR2 = 0.0844

Extinction coefficient  
n/a

Largest diff. peak and hole  
0.807 and -0.546 e.Å

Identification code  
3ag'

Empirical formula  
C18 H10 F3 N O2

Formula weight  
329.27

Temperature  
100(2) K

Wavelength  
1.54178 Å

Crystal system  
Triclinic

Space group  
P-1

Unit cell dimensions  
a = 6.6165(5) Å  
β = 96.542(3)°

b = 10.3211(8) Å  
γ = 102.766(3)°

c = 10.9424(8) Å

Volume  
716.99(9) Å³

Z  
2

Density (calculated)  
1.525 Mg/m³

Absorption coefficient  
1.088 mm⁻¹

F(000)  
336

Crystal size  
0.028 x 0.097 x 0.26 mm³

Theta range for data collection  
4.106 to 68.360°

Index ranges  
-7<=h<=7, -12<=k<=12, -13<=l<=13

Reflections collected  
8757

Independent reflections  
2627 [R(int) = 0.0553]

Completeness to theta = 67.679°  
99.8 %

Absorption correction  
Multi-Scan

Refinement method  
Full-matrix least-squares on F²

Data / restraints / parameters  
2627 / 0 / 217

Goodness-of-fit on F²  
1.063

Final R indices [I>2sigma(I)]  
R1 = 0.0482, wR2 = 0.1258

R indices (all data)  
R1 = 0.0525, wR2 = 0.1303

Extinction coefficient  
n/a
12. Checkcif report for the products

**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 3am

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REVIEWER.

No syntax errors found. CIF dictionary: Interpreting this report

**Datablock: 3am**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0051 Å</th>
<th>Wave-length=1.54178</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=5.9221(4)</td>
<td>b=21.7851(16)</td>
</tr>
<tr>
<td></td>
<td>c=10.0601(8)</td>
<td>alpha=90</td>
</tr>
<tr>
<td></td>
<td>beta=100.563(4)</td>
<td>gamma=90</td>
</tr>
<tr>
<td>Temperature:</td>
<td>100 K</td>
<td></td>
</tr>
<tr>
<td>Volume:</td>
<td>1275.90(16)</td>
<td>1275.90(16)</td>
</tr>
<tr>
<td>Space group:</td>
<td>C c</td>
<td>C 1 c 1</td>
</tr>
<tr>
<td>Hall group:</td>
<td>C -2yc</td>
<td>C -2yc</td>
</tr>
<tr>
<td>Moletry formula</td>
<td>C15 H9 Cl F3 N</td>
<td>C15 H9 Cl F3 N</td>
</tr>
<tr>
<td>Sum formula:</td>
<td>C15 H9 Cl F3 N</td>
<td>C15 H9 Cl F3 N</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Dm. g cm-3</td>
<td>1.539</td>
<td>1.539</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Ns (mm-1)</td>
<td>2.903</td>
<td>2.903</td>
</tr>
<tr>
<td>F000</td>
<td>600.0</td>
<td>600.0</td>
</tr>
<tr>
<td>F000'</td>
<td>603.47</td>
<td>603.47</td>
</tr>
<tr>
<td>b,h,k,lim</td>
<td>7.26,12</td>
<td>7.26,12</td>
</tr>
<tr>
<td>Sym</td>
<td>233[1 1 1]</td>
<td>1822</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.033,0.647</td>
<td>0.533,0.753</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.461</td>
<td></td>
</tr>
<tr>
<td>Correction method:</td>
<td>Reported T Limits: Tmin=0.533 Tmax=0.753</td>
<td></td>
</tr>
<tr>
<td>AbeCorr = MULTI-SMN</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Data completeness=</td>
<td>1.55/0.78</td>
<td>Theta(max)= 68.250</td>
</tr>
</tbody>
</table>

R(reflections)= 0.0358 (1699)  wR2(reflections)= 0.0529 (1822)
S = 1.101  Npar= 182
The following ALERTS were generated. Each ALERT has the format
    test-name_ALERT-type_ALERT-level.
    Click on the hyperlinks for more details of the test.

**Alert level C**
- **FLATFLAT_ALERT_C Low Data / Parameter Ratio NX < 100 6.46 Note**
- **FLATFLAT_ALERT_C Low Bond Precision on C-C Bonds 0.05912 A**

**Alert level G**
- **FLATFLAT_ALERT_G ‘Haimaki’ ‘Deg as Compared to Neighbours’ CIF Check**
- **FLATFLAT_ALERT_G No InfoValue for _atom_site_solution.legacy Please Do!**
- **FLATFLAT_ALERT_G C Number C=C Bonds with Positive Residual Density 54 %**

**Alert level G**
- **FLATFLAT_ALERT_G C ‘Haimaki’ ‘Deg as Compared to Neighbours’ CIF Check**
- **FLATFLAT_ALERT_G No InfoValue for _atom_site_solution.legacy Please Do!**
- **FLATFLAT_ALERT_G C Number C=C Bonds with Positive Residual Density 54 %**

**Validation response form**

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF:

```plaintext
# start Validation Reply Form
  _vrf_VALID0_3xm
  
  PROBLEM: poor Data / Parameter Ratio NX < 100 6.46 Note
  RESPONSE:
  ...
  _VRF_VALID0_3xm

PROBLEM: Low Bond Precision on C=C Bonds 0.05912 A
  RESPONSE:
  ...
  
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these finer details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may arise. Consequently, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

**Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit to Acta Crystallographica Section C or E for IUCrData, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

**Publication of your CIF in other journals**

Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF submission.

---

PLATON version of 28/11/2022; check.def file version of 28/11/2022
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3aq

THIS REPORT IS FOR GUIDANCE ONLY. IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary interpreting this report

Datablock: 3aq

Bond precision: C-C = 0.0035 A  Wavelength=1.54178

Cell:

a=8.1764(6)  b=20.5249(7)  c=15.2713(10)

alpha=86.542(2)  beta=88.533(2)  gamma=89.967(2)

Temperature: 100 K

Volume 1311.16(16)  Calculated 1311.16(16)  Reported

Space group P -1

Hall group -P 1

Moisture formula C15 H9 Br F3 N

Sum formula C15 H9 Br F3 N

Z 4

Mu (mm-1) 4.521  4.521

I (max) 672.0  672.0

h,k,l (max) 9,12,18  9,12,18

R intl 0.0804  4791

Twin,Tmax 0.533,0.508  0.533,0.753

AbsCorr: MULTICR

Correction method: # Reported T Limits: Tmajo=0.533 Tmax=0.753

Data completeness= 0.997  Theta(max)= 68.320

R(reflections)= 0.0317  9551  wR2(reflections)=

Weighted R= 0.0317  9551  0.0810  4791

S = 1.054  Npar = 361
The following ALERTS were generated. Each ALERT has the format:
\texttt{test-name_ALERT-type_alert-level}.
Click on the hyperlink for more details of the test.

\textbf{Alert level C}

\begin{itemize}
  \item PLAT21_ALERT_2_C Atom P1 \hspace{1cm} has ADP max/min Ratio \ldots \hspace{1cm} 3.3 prolac
  \item PLAT21_ALERT_2_C Atom P4 \hspace{1cm} has ADP max/min Ratio \ldots \hspace{1cm} 3.6 prolac
  \item PLAT21_ALERT_2_C Low ‘Main Mol’ \& as Compared to Neighbors of
  \hspace{1cm} 0.00 Check
  \item PLAT21_ALERT_2_C Low ‘Main Mol’ \& as Compared to Neighbors of
  \hspace{1cm} 0.00 Check
  \item PLAT51_ALERT_3_C Missing P/P Rel between Tmn & Sth/I-
  \hspace{1cm} 0.400 \hspace{1cm} 4 Report
\end{itemize}

\textbf{Alert level G}

\begin{itemize}
  \item PLAT09_ALERT_2_G Number of Use or Uij Restrainted non-H Atoms \ldots \hspace{1cm} 4 Report
  \item PLAT27_ALERT_4_G The e.s.d.’s on the Cell Angles are Equal \ldots \hspace{1cm} (Note)
  \hspace{1cm} 0.002 Degree
  \item PLAT77_ALERT_1_G The CIF-Emended .res File Contains CIF2 Records \hspace{1cm} 1 Report
  \item PLAT52_ALERT_4_G A non-default SIO Restrains Value has been used \hspace{1cm} 0.0200 Report
  \item PLAT52_ALERT_1_G A non-default SIO Restrains Value has been used \hspace{1cm} 0.0200 Report
  \item PLAT57_ALERT_2_G Number of Least-Squares Parameters \hspace{1cm} 24 NoG
  \item PLAT51_ALERT_1_G No Info/Value for _atom_sites_solution_primary \hspace{1cm} Please Do!
  \item PLAT92_ALERT_1_G Average HSL Measurement Multiplicity \hspace{1cm} 3.7 Low
  \item PLAT99_ALERT_2_G Number C-C Bonds with Positive Residual Density \hspace{1cm} 3 Info
\end{itemize}

\textbf{Validation response form}

Please find below a validation response form (VRF) that can be filled in and posted into your CIF.

```
# start Validation Reply Form
\texttt{vrf\_PLAT21\_eq}
#
\textbf{PROBLEM:} Atom P1 \hspace{1cm} has ADP max/min Ratio \ldots \hspace{1cm} 3.3 prolac
\textbf{RESPONSE:} \ldots
/
\texttt{vrf\_PLAT24\_eq}
#
\textbf{PROBLEM:} Low ‘Main Mol’ \& as Compared to Neighbors of
\textbf{RESPONSE:} \ldots
/
\texttt{vrf\_PLAT91\_eq}
#
\textbf{PROBLEM:} Missing P/P Rel between Tmn & Sth/I-
\textbf{RESPONSE:} \ldots
/
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor
alerts point to easily fixed omissions, errors and omissions in your CIF or refinement strategy, so
attention to these fine details can be worthwhile. In order to resolve some of the more serious problems
it may be necessary to carry out additional measurements or structure refinement. However, the
purpose of your study may justifiy the reported deviations and the more serious of these should
normally be commented upon in the discussion or experimental section of a paper or in the
"special_details" field of the CIF. checkCIF was carefully designed to identify outliers and unusual
parameters, but every test has its limitations and alerts that are not important in a particular case may
appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing
attention. It is up to the individual to critically assess their own results and, if necessary, seek expert
advice.

\textbf{Publication of your CIF in IUCr journals}

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs
submitted for publication in IUCr journals (\textit{Acta Crystallographica, Journal of Applied
Crystallography, Journal of Synchrotron Radiation}); however, if you intend to submit to \textit{Acta
Crystallographica Section C} or \textit{Acta ICEData}, you should make sure that full publication checks are
run on the final version of your CIF prior to submission.

\textbf{Publication of your CIF in other journals}

Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF
submission.

\textit{PLATON version of 28/11/2022; checkCIF file version of 28/11/2022}
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3ag

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

**Datablock: 3ag**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0022 Å</th>
<th>Wavelength=1.54178</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=6.6165(5)</td>
<td>b=10.3211(8)</td>
</tr>
<tr>
<td></td>
<td>alpha=96.542(3)</td>
<td>beta=96.293(3)</td>
</tr>
<tr>
<td>Temperature:</td>
<td>100 K</td>
<td></td>
</tr>
<tr>
<td>Volume</td>
<td>717.00(9)</td>
<td>716.99(9)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C18 H10 F3 N O2</td>
<td>C18 H10 F3 N O2</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C18 H10 F3 N O2</td>
<td>C18 H10 F3 N O2</td>
</tr>
<tr>
<td>Mr</td>
<td>329.27</td>
<td>329.27</td>
</tr>
<tr>
<td>S</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Mo (mm-1)</td>
<td>1.088</td>
<td>1.088</td>
</tr>
<tr>
<td>F000</td>
<td>336.0</td>
<td>336.0</td>
</tr>
<tr>
<td>F000'</td>
<td>337.30</td>
<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>7,12,13</td>
<td>7,12,13</td>
</tr>
<tr>
<td>Nref</td>
<td>2633</td>
<td>2627</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.881, 0.970</td>
<td>0.667, 0.753</td>
</tr>
<tr>
<td>Twin'</td>
<td>0.754</td>
<td></td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.667 Tmax=0.753
AbsCorr = MULTI-SOON

Data completeness= 0.998          Theta(max)= 68.360

R(intreflections)= 0.0483( 2361)  wR2(reflections)= 0.1303( 2627)
S = 1.063                     Npar= 217

S159
The following ALERTS were generated. Each ALERT has the format
<test-name>_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

**Alert level C**
PLAT91_ALERT_C Missing POF Refl Between Thim & STh/L= 6.600 5 Report

**Alert level C**
PLAT154_ALERT_C The S.u.'s on the Cell Angles are Equal ...[Note] 0.003 Degree
PLAT903_ALERT_C No Info/Value for _atom_sites_solution_primary ... Please Co !
PLAT912_ALERT_C Missing # of POF Reflections Above STh/L= 6.600 2 Note
PLAT914_ALERT_C Average Bkl Measurement Multiplicity ............ 3.3 Low
PLAT915_ALERT_C Number C-C Bonds with Positive Residual Density. 3 Info
PLAT992_ALERT_C Bond & Actual _reobs_number.of.Values Differ by 2 Check

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
2 ALERT level D = General information/check it is not something unexpected
3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
7 ALERT type 5 Informative message, check

Validation response form
Please find below a validation response form (VRF) that can be filled in and posted into your CIF.

```bash
# start Validation Reply Form
  _vrf_PLAT911elog'
  PROBLEM: Missing POF Refl Between Thim & STh/L= 6.600 5 Report
  RESPONSE: ...
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit to Acta Crystallographica Section C or E or IUCrData, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/07/2023; check.def file version of 30/06/2023
13. References


