Supporting Information

A Radical-Promoted Site-Specific Cross Dehydrogenative Coupling of Heterocycles with Nitriles

Zhong-Quan Liu* and Zejiang Li

State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, P. R. China

E-mail: liuzhq@lzu.edu.cn

General Information

Typical procedure

Modification of the typical reaction conditions

Competing Kinetic Isotope Effect (KIE) experiment

Radical trapping by addition of 2, 6-DTBP

Physical data and references for the following products

Copies of the $^1$H NMR, $^{13}$C NMR, $^{19}$F NMR, $^{135}$DEPT

General Information

$^1$H and $^{13}$C NMR spectra were recorded on a Bruker advance III 400 spectrometer in CDCl$_3$ with TMS as internal standard. Mass spectra were determined on a Hewlett Packard 5988A spectrometer by direct inlet at 70 eV. High-resolution mass spectral analysis (HRMS) data were measured on a Bruker Apex II. Element analysis (EA) data were measured on a Vario EL. All products were identified by $^1$H and $^{13}$C NMR, $^{19}$F NMR, $^{135}$DEPT NMR, MS, HRMS. The starting materials were purchased from Energy Chemicals, Alfa Aesar, Acros Organics, J&K Chemicals, Adamas, or Aldrich and used without further purification.

Typical procedure

Reaction of Acetonitriles with heterocycles: A mixture of heterocycles (1 equiv, 0.20 mmol), acetonitriles (7 mL), CuCl (10 mol%, 0.02 mmol), and DCP (3 equiv, 0.60 mmol) was heated at 110 °C, 115 °C or 130 °C (the measured temperature of the oil bath) under nitrogen condition
for 12 h in a sealed tube (15 mL). After the reaction finished, the mixture was evaporated under vacuum and purified by column chromatography to afford the desired product.

**Modification of the typical reaction conditions**

![Chemical Structure Diagram]

<table>
<thead>
<tr>
<th>Entry</th>
<th>CH$_3$CN (mL)</th>
<th>Initiator (mol%)</th>
<th>Peroxide (equiv)</th>
<th>T (°C)</th>
<th>t (h)</th>
<th>Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>40</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>CuI(10)</td>
<td>DTBP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>CuI(10)</td>
<td>BPO(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>CuI(10)</td>
<td>TBHP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>CuI(10)</td>
<td>TBBP(3)</td>
<td>110</td>
<td>12</td>
<td>39</td>
</tr>
<tr>
<td>6</td>
<td>5</td>
<td>CuI(10)</td>
<td>TBCP(3)</td>
<td>110</td>
<td>12</td>
<td>29</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(1)</td>
<td>110</td>
<td>12</td>
<td>6</td>
</tr>
<tr>
<td>8</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(2)</td>
<td>110</td>
<td>12</td>
<td>25</td>
</tr>
<tr>
<td>9</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(4)</td>
<td>110</td>
<td>12</td>
<td>29</td>
</tr>
<tr>
<td>10</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(5)</td>
<td>110</td>
<td>12</td>
<td>18</td>
</tr>
<tr>
<td>11</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>50</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>12</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>80</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>13</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>120</td>
<td>12</td>
<td>38</td>
</tr>
<tr>
<td>14</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>130</td>
<td>12</td>
<td>35</td>
</tr>
<tr>
<td>15</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>3</td>
<td>22</td>
</tr>
<tr>
<td>16</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>6</td>
<td>23</td>
</tr>
<tr>
<td>17</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>18</td>
<td>41</td>
</tr>
<tr>
<td>18</td>
<td>5</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>24</td>
<td>27</td>
</tr>
<tr>
<td>19</td>
<td>1</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>6</td>
</tr>
<tr>
<td>21</td>
<td>3</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>26</td>
</tr>
<tr>
<td>22</td>
<td>6</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>42</td>
</tr>
<tr>
<td>23</td>
<td>7</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>52</td>
</tr>
<tr>
<td>24</td>
<td>8</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>44</td>
</tr>
<tr>
<td>25</td>
<td>10</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>26</td>
<td>CH$_3$CN(5) + t-Butanol(2)</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>30</td>
</tr>
<tr>
<td>27</td>
<td>7</td>
<td>CuF$_2$(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>46</td>
</tr>
<tr>
<td>28</td>
<td>7</td>
<td>Cu(OAc)$_2$(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>27</td>
</tr>
<tr>
<td>29</td>
<td>7</td>
<td>CuBr(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>42</td>
</tr>
<tr>
<td>30</td>
<td>7</td>
<td>CuCl(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>53</td>
</tr>
<tr>
<td>31</td>
<td>7</td>
<td>CuCl(5)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>33</td>
</tr>
<tr>
<td>32</td>
<td>7</td>
<td>CuCl(20)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>18</td>
</tr>
<tr>
<td>33</td>
<td>7</td>
<td>CuCl(50)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>34</td>
<td>7</td>
<td>TBAI(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>5</td>
</tr>
<tr>
<td>35</td>
<td>7</td>
<td>Cu₂O(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>30</td>
</tr>
<tr>
<td>36</td>
<td>7</td>
<td>Cu(acac)₂ (10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>44</td>
</tr>
<tr>
<td>37</td>
<td>7</td>
<td>Cu(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>6</td>
</tr>
<tr>
<td>38</td>
<td>7</td>
<td>-</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>39</td>
<td>7</td>
<td>CuSO₄·5H₂O(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>42</td>
</tr>
<tr>
<td>40</td>
<td>7</td>
<td>CuO(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>41</td>
<td>7</td>
<td>CuCl₂·2H₂O(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>43</td>
</tr>
<tr>
<td>42</td>
<td>7</td>
<td>NiCl₂·2H₂O(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>40</td>
</tr>
<tr>
<td>43</td>
<td>7</td>
<td>FeCl₃ (10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>35</td>
</tr>
<tr>
<td>44</td>
<td>7</td>
<td>Co(acac)₂ (10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>5</td>
</tr>
<tr>
<td>45</td>
<td>7</td>
<td>Mn(OAc)₂(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>46</td>
<td>7</td>
<td>Cu(OOTf)₂(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>8</td>
</tr>
<tr>
<td>47</td>
<td>7</td>
<td>TTF-OMe(10)</td>
<td>-</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>48</td>
<td>7</td>
<td>CuCl(10)</td>
<td>H₂O₂(3)</td>
<td>R.T.</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>49</td>
<td>7</td>
<td>FeCl₃(10)</td>
<td>H₂O₂(3)</td>
<td>R.T.</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>50</td>
<td>7</td>
<td>Ferrocene (10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>26</td>
</tr>
<tr>
<td>51</td>
<td>7</td>
<td>CuNO₃(PPh₃)₂(10)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>28</td>
</tr>
<tr>
<td>52</td>
<td>7</td>
<td>CuI(10)+TFA(20)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>22</td>
</tr>
<tr>
<td>53</td>
<td>7</td>
<td>CuI(10)+1,10-phen(20)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>54</td>
<td>7</td>
<td>CuI(10)+TMEDA(20)</td>
<td>DCP(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>55</td>
<td>7</td>
<td>AgNO₃(20)</td>
<td>K₂S₂O₇(3)</td>
<td>110</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>56</td>
<td>7</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>105</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>57</td>
<td>7</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>115</td>
<td>12</td>
<td>30</td>
</tr>
<tr>
<td>58</td>
<td>7</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>120</td>
<td>12</td>
<td>26</td>
</tr>
<tr>
<td>59</td>
<td>7</td>
<td>CuI(10)</td>
<td>DCP(3)</td>
<td>130</td>
<td>12</td>
<td>16</td>
</tr>
<tr>
<td>60</td>
<td>7</td>
<td>CuCl(10)</td>
<td>DCP(3)</td>
<td>105</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>61</td>
<td>7</td>
<td>CuCl(10)</td>
<td>DCP(3)</td>
<td>115</td>
<td>12</td>
<td>55</td>
</tr>
<tr>
<td>62</td>
<td>7</td>
<td>CuCl(10)</td>
<td>DCP(3)</td>
<td>120</td>
<td>12</td>
<td>28</td>
</tr>
<tr>
<td>63</td>
<td>7</td>
<td>KI(10)</td>
<td>DCP(3)</td>
<td>115</td>
<td>12</td>
<td>Trace</td>
</tr>
<tr>
<td>64</td>
<td>7</td>
<td>NaI(10)</td>
<td>DCP(3)</td>
<td>115</td>
<td>12</td>
<td>Trace</td>
</tr>
</tbody>
</table>

* Reaction conditions: 2-phenylfuran (1 equiv, 0.20 mmol), acetonitrile as solvent, sealed tube, unless otherwise noted. * Isolated yields.
Competing Kinetic Isotope Effect (KIE) Experiment:

At low conversion (38%): $K_\text{H}/K_\text{D} = 4.7$.

$^1H$ NMR
**Note:** The value of $k_H/k_D$ was calculated from the $^1$H NMR spectra above which should be the mixture of compound a and b (the KIE scheme). The sum of the integral of a and b at chemical shift 3.78 was integrated as 3.00 (both a and b keep the same single bond hydrogen). Compound a has 2 hydrogen atoms at chemical shift 3.86, while b has no H atoms. The amount of a could be defined as 1.65, on the other hand, the sum of a and b is 2.00, so the amount of b is 0.35 ($2.00 - 1.65 = 0.35$). As a result, $k_H / k_D = 1.65 / 0.35 = 4.7$.

**Radical trapping by addition of 2,6-DTBP:**

Physical data and references for the following products:

All known compounds are determined by $^1$H NMR, $^{13}$C NMR and $^{19}$F NMR, MS analysis and compared with which were cited in the following references, and the new compounds were further confirmed by HRMS and/or element analysis.
References:

Physical data for the following products:

1a. 2-(5-(hydroxymethyl)furan-2-yl)acetonitrile
A yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 2/1).

\[ \text{HO} \overset{\text{CN}}{\text{O}} \]

\textbf{1H NMR (400 MHz, CDCl}_3\text{)}: \delta 6.29 (d, J = 3.2 Hz, 1H), 6.27 (d, J = 3.2 Hz, 1H), 4.59 (s, 2H), 3.76 (s, 2H), 1.79 (s, 1H).
\textbf{13C NMR (100 MHz, CDCl}_3\text{)}: \delta 154.7, 143.0, 115.3, 109.3, 109.0, 57.3, 17.6.
\textbf{HRMS (ESI, m/z):} Calculated for C\textsubscript{2}H\textsubscript{11}N\textsubscript{2}O\textsubscript{2} (M+NH\textsubscript{4})\textsuperscript{+} 155.0815, found 155.0811.

1b. 2-(5-(hydroxydiphenylmethyl)furan-2-yl)acetonitrile
A yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 5/1).

\[ \text{Ph} \overset{\text{CN}}{\text{O}} \]

\textbf{1H NMR (400 MHz, CDCl}_3\text{)}: \delta 7.36 – 7.29 (m, 10H), 6.29 (d, J = 2.8 Hz, 1H), 5.89 (d, J = 3.2 Hz, 1H), 3.75 (s, 2H), 3.04 (s, 1H).
\textbf{13C NMR (100 MHz, CDCl}_3\text{)}: \delta 158.6, 144.1, 143.3, 128.1, 127.8, 127.1, 115.3, 110.9, 109.0, 77.9, 17.7.
\textbf{HRMS (ESI, m/z):} Calculated for C\textsubscript{19}H\textsubscript{15}NO\textsubscript{2}Na (M+Na\textsuperscript{+}) 312.0995, found 312.1001.

1c. 2-(5-([1,1’-biphenyl]-2-yl)(hydroxy)methyl)furan-2-yl)acetonitrile
A yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 5/1).

\[ \text{Ph} \overset{\text{CN}}{\text{O}} \]
\[1^1\text{H NMR (400 MHz, CDCl}_3\text{)}: \delta 7.70 (dd, J = 7.6, 1.2 \text{ Hz, 1H}), 7.46 - 7.42 (m, 1H), 7.41 - 7.36 (m, 4H), 7.29 - 7.24 (m, 3H), 6.25 (d, J = 3.2 \text{ Hz, 1H}), 6.00 (d, J = 3.2 \text{ Hz, 1H}), 5.82 (s, 1H), 3.72 (s, 2H), 2.27 (s, 1H).\]

\[1^3\text{C NMR (100 MHz, CDCl}_3\text{)}: \delta 156.9, 142.8, 141.1, 140.2, 137.7, 130.0, 129.2, 128.2, 128.1, 127.9, 127.4, 127.2, 115.4, 109.2, 109.1, 66.7, 17.6.\]

\[\text{HRMS (ESI, m/z): Calculated for C}_{19}\text{H}_{19}\text{N}_2\text{O}_2 (M+NH}_4^+ 307.1441, \text{ found 307.1438.}\]

1d. 2-(5-phenylfuran-2-yl)acetonitrile

A red solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).

\[1^1\text{H NMR (400 MHz, CDCl}_3\text{)}: \delta 7.65 (d, J = 7.2 \text{ Hz, 2H}), 7.39 (t, J = 7.6 \text{ Hz, 2H}), 7.29 (t, J = 7.2 \text{ Hz, 1H}), 6.61 (d, J = 3.2 \text{ Hz, 1H}), 6.41 (d, J = 3.2 \text{ Hz, 1H}), 3.84 (s, 2H).\]

\[1^3\text{C NMR (100 MHz, CDCl}_3\text{)}: \delta 154.6, 142.2, 130.1, 128.7, 127.8, 123.7, 115.4, 110.6, 105.9, 17.7.\]

\[\text{HRMS (ESI, m/z): Calculated for C}_{12}\text{H}_{10}\text{NO (M+H)}^+ 184.0757, \text{ found 184.0760.}\]

1e. 2-(5-(4-methoxyphenyl)furan-2-yl)acetonitrile

A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1); m.p.: 93-95 °C.

\[1^1\text{H NMR (400 MHz, CDCl}_3\text{)}: \delta 7.57 (d, J = 8.8 \text{ Hz, 2H}), 6.92 (d, J = 8.8 \text{ Hz, 2H}), 6.46 (d, J = 3.2 \text{ Hz, 1H}), 6.38 (d, J = 3.2 \text{ Hz, 1H}), 3.84 (s, 3H), 3.83 (s, 2H).\]

\[1^3\text{C NMR (100 MHz, CDCl}_3\text{)}: \delta 159.3, 154.7, 141.5, 125.2, 123.2, 114.2, 110.5, 104.3, 55.3, 17.7.\]

\[\text{HRMS (ESI, m/z): Calculated for C}_{13}\text{H}_{12}\text{NO}_2 (M+H)}^+ 214.0863, \text{ found 214.0861.}\]

1f. 2-(4-(4-methoxyphenyl)furan-2-yl)acetonitrile

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).
\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 7.43 (d, } J = 1.6 \text{ Hz, 1H), 7.27 (d, } J = 8.8 \text{ Hz, 2H), 6.97 (d, } J = 8.8 \text{ Hz, 2H), 6.51 (d, } J = 2.0 \text{ Hz, 1H), 3.84 (s, 3H), 3.82 (s, 2H).} \]

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 7.98 (d, } J = 8.4 \text{ Hz, 2H), 7.41 (d, } J = 8.8 \text{ Hz, 2H), 6.47 (d, } J = 3.2 \text{ Hz, 1H), 6.35 (d, } J = 3.2 \text{ Hz, 1H), 5.26 (s, 2H), 3.78 (s, 2H).} \]

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 6.30 (dd, } J = 7.2, 3.2 \text{ Hz, 2H), 4.49 (q, } J = 12.8 \text{ Hz, 2H), 3.78 (dd, } J = 11.6, 2.8 \text{ Hz, 1H), 3.76 (s, 2H), 3.42 (dd, } J = 11.6, 6.0 \text{ Hz, 1H), 3.16 (dq, } J = 8.8, 2.8 \text{ Hz, 1H), 2.80 (t, } J = 4.8 \text{ Hz, 1H), 2.61 (dd, } J = 4.8, 2.8 \text{ Hz, 1H).} \]

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 159.1, 142.6, 137.5, 129.0, 124.4, 115.6, 114.4, 112.0, 55.3, 16.4.} \]

\[ \text{HRMS (ESI, m/z): Calculated for C}_{13}\text{H}_{12}\text{NO}_2 (M+H)^+ 214.0863, found 214.0860.} \]

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 159.1, 142.6, 137.5, 129.0, 124.4, 115.6, 114.4, 112.0, 55.3, 16.4.} \]

\[ \text{HRMS (ESI, m/z): Calculated for C}_{14}\text{H}_{10}\text{ClNO}_3\text{Na(M+Na)}^+ 298.0241, found 298.0237.} \]

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 152.1, 143.4, 115.3, 110.8, 109.2, 70.8, 64.9, 50.7, 44.2, 17.6.} \]

\[ \text{HRMS (ESI, m/z): Calculated for C}_{10}\text{H}_{11}\text{NO}_3\text{Na(M+Na)}^+ 216.0631, found 216.0627.} \]

A light yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).

A light yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 3/1).
**ii. 2-(5-(hydroxydiphenylmethyl)thiophen-2-yl)acetonitrile**

A yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 5/1).

![Diagram of 2-(5-(hydroxydiphenylmethyl)thiophen-2-yl)acetonitrile]

**$^{1}H$ NMR (400 MHz, CDCl$_3$):** δ 7.36 – 7.31 (m, 10H), 6.91 (d, $J = 3.6$ Hz, 1H), 6.61 (d, $J = 3.6$ Hz, 1H), 3.85 (s, 2H), 2.95 (s, 1H).

**$^{13}C$ NMR (100 MHz, CDCl$_3$):** δ 153.0, 145.9, 131.0, 128.1, 127.8, 127.1, 126.8, 126.6, 116.7, 80.1, 18.8.

**HRMS (ESI, m/z):** Calculated for C$_{19}$H$_{15}$NOSNa (M+Na$^+$) 328.0767, found 328.0772.

**2a. 2-(1-methyl-1H-indol-2-yl)acetonitrile**

A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1); m.p.: 99-101 °C.

![Diagram of 2-(1-methyl-1H-indol-2-yl)acetonitrile]

**$^{1}H$ NMR (400 MHz, CDCl$_3$):** δ 7.59 (d, $J = 8.0$ Hz, 1H), 7.32 (d, $J = 8.0$ Hz, 1H), 7.28 – 7.24 (m, 1H), 7.16 – 7.12 (m, 1H), 6.54 (s, 1H), 3.89 (s, 2H), 3.76 (s, 3H).

**$^{13}C$ NMR (100 MHz, CDCl$_3$):** δ 137.9, 127.6, 127.1, 122.3, 120.7, 120.1, 116.0, 109.1, 102.3, 29.8, 16.7.

**MS(EI): m/z(%):** 170(100.0), 169(94.3), 144(39.0), 128(10.0), 115(13.6).

**2b. 2-(1,5-dimethyl-1H-indol-2-yl)acetonitrile**

A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1); m.p.: 110-112 °C.

![Diagram of 2-(1,5-dimethyl-1H-indol-2-yl)acetonitrile]

**$^{1}H$ NMR (400 MHz, CDCl$_3$):** δ 7.36 (s, 1H), 7.20 (d, $J = 8.4$ Hz, 1H), 7.08 (dd, $J = 8.4, 1.2$ Hz, 1H), 6.44 (s, 1H), 3.86 (s, 2H), 3.72 (s, 3H), 2.44 (s, 3H).

**$^{13}C$ NMR (100 MHz, CDCl$_3$):** δ 136.3, 129.4, 127.5, 127.3, 123.9, 120.3, 116.0, 108.8, 101.7, 29.8, 21.3, 16.7.

**HRMS (ESI, m/z):** Calculated for C$_{12}$H$_{13}$N$_{2}$ (M+H$^+$) 185.1073, found 185.1071.

**2c. 2-(1,4-dimethyl-1H-indol-2-yl)acetonitrile**

A light yellow solid after purification by flash column chromatography (petroleum ether/ethyl...
acetate = 10/1); m.p.: 112-114 °C.

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta 7.19 - 7.14 (m, 2H), 6.94 (dd, J = 6.0, 1.2 Hz, 1H), 6.55 (s, 1H), 3.88 (s, 2H), 3.73 (s, 3H), 2.54 (s, 3H). \]

\[ \text{C NMR (100 MHz, CDCl}_3\text{): } \delta 137.7, 130.2, 127.0, 122.4, 120.3, 116.0, 106.8, 100.8, 29.9, 18.6, 16.7. \]

HRMS (ESI, m/z): Calculated for C\(_{12}\)H\(_{13}\)N\(_2\) (M+H\(^+\)) 185.1073, found 185.1070.

2d. 2-(1,7-dimethyl-1H-indol-2-yl)acetonitrile
A light yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1); m.p.: 145-146 °C.

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta 7.41 (d, J = 8.0 Hz, 1H), 6.99 (t, J = 7.2 Hz, 1H), 6.94 (d, J = 7.2 Hz, 1H), 6.50 (s, 1H), 3.99 (s, 3H), 3.84 (s, 2H), 2.78 (s, 3H). \]

\[ \text{C NMR (100 MHz, CDCl}_3\text{): } \delta 136.8, 128.0, 127.9, 125.4, 121.0, 120.2, 118.8, 116.1, 102.9, 32.9, 20.2, 17.0. \]

HRMS (ESI, m/z): Calculated for C\(_{12}\)H\(_{13}\)N\(_2\) (M+H\(^+\)) 185.1073, found 185.1070.

2e. 2-(1,3-dimethyl-1H-indol-2-yl)acetonitrile
A red solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1); m.p.: 90-92 °C.

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta 7.54 (d, J = 7.6 Hz, 1H), 7.30 - 7.27 (m, 1H), 7.25 - 7.23 (m, 1H), 7.15 - 7.11 (m, 1H), 3.84 (s, 2H), 3.77 (s, 3H), 2.31 (s, 3H). \]

\[ \text{C NMR (100 MHz, CDCl}_3\text{): } \delta 137.1, 127.6, 123.4, 122.5, 119.4, 118.9, 116.0, 109.8, 109.0, 29.9, 13.8, 8.8. \]

HRMS (ESI, m/z): Calculated for C\(_{12}\)H\(_{13}\)N\(_2\) (M+H\(^+\)) 185.1073, found 185.1072.

2f. 2-(5-fluoro-1-methyl-1H-indol-2-yl)acetonitrile
A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate =
5/1); m.p.: 101-103 °C.

\[
\text{H NMR (400 MHz, CDCl}_3\text{): } \delta 7.24 - 7.22 (m, 1H), 7.21 (t, J = 3.6 Hz, 1H), 7.00 (td, J = 9.2, 2.4 Hz, 1H), 6.49 (s, 1H), 3.87 (s, 2H), 3.74 (s, 3H).
\]

\[
\text{C NMR (100 MHz, CDCl}_3\text{): } \delta 159.2, 156.9, 134.5, 129.2, 127.3, 127.2, 115.7, 110.8, 110.6, 109.9, 109.8, 105.6, 105.4, 102.2, 102.1, 30.1, 16.8.
\]

\[
\text{F NMR (376 MHz, CDCl}_3\text{): } \delta \text{ -124.27 (td, } J = 9.4, 4.1 \text{ Hz, 1F).}
\]

\[
\text{HRMS (ESI, m/z): Calculated for C}_{11}\text{H}_{10}\text{FN}_2\text{(M+H)}^+ 189.0823, \text{found 189.0822.}
\]

2g. 2-(5-chloro-1-methyl-1H-indol-2-yl)acetonitrile
A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 5/1); m.p.: 118-120 °C.

\[
\text{H NMR (400 MHz, CDCl}_3\text{): } \delta 7.54 - 7.53 (m, 1H), 7.23 - 7.18 (m, 2H), 6.47 (s, 1H), 3.87 (s, 2H), 3.73 (s, 3H).
\]

\[
\text{C NMR (100 MHz, CDCl}_3\text{): } \delta 136.3, 129.0, 128.0, 125.8, 122.6, 120.0, 115.6, 110.2, 101.9, 30.0, 16.7.
\]

\[
\text{HRMS (ESI, m/z): Calculated for C}_{11}\text{H}_{10}\text{ClN}_2\text{(M+H)}^+ 205.0527, \text{found 205.0525.}
\]

2h. 2-(5-bromo-1-methyl-1H-indol-2-yl)acetonitrile
A red solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 5/1); m.p.: 107-109 °C.

\[
\text{H NMR (400 MHz, CDCl}_3\text{): } \delta 7.70 (d, J = 1.6 Hz, 1H), 7.32 (dd, J = 8.4, 1.6 Hz, 1H), 7.17 (d, J = 8.8 Hz, 1H), 6.47 (s, 1H), 3.87 (s, 2H), 3.73 (s, 3H).
\]

\[
\text{C NMR (100 MHz, CDCl}_3\text{): } \delta 136.6, 128.9, 128.7, 125.2, 123.2, 115.6, 113.4, 110.7, 101.8, 30.0, 16.7.
\]

\[
\text{HRMS (ESI, m/z): Calculated for C}_{11}\text{H}_{10}\text{BrN}_2\text{(M+H)}^+ 249.0022, \text{found 249.0019.}
\]
2i. methyl 2-(cyanomethyl)-1-methyl-1H-indole-5-carboxylate

A yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 3/1).

\[ \text{MeO}_2\text{C} \backslash \text{N} \]

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.34 (s, 1H), 7.96 (d, $J = 8.4$ Hz, 1H), 7.32 (d, $J = 8.8$ Hz, 1H), 6.64 (s, 1H), 3.93 (s, 3H), 3.91 (s, 2H), 3.79 (s, 3H).

$^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ 167.9, 140.3, 129.2, 126.6, 123.7, 123.6, 122.3, 115.6, 108.9, 103.8, 51.9, 30.1, 16.8.

HRMS (ESI, m/z): Calculated for C$_{13}$H$_{13}$N$_2$O$_2$ (M+H)$^+$ 229.0972, found 229.0975.

2j. 2-(3-(2-methoxyethyl)-1-methyl-1H-indol-2-yl)acetonitrile

A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1); m.p.: 85-87 °C.

\[ \text{O} \backslash \text{N} \]

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.55 (d, $J = 8.0$ Hz, 1H), 7.31 (d, $J = 8.4$ Hz, 1H), 7.27 – 7.23 (m, 1H), 7.15 – 7.11 (m, 1H), 3.92 (s, 2H), 3.78 (s, 3H), 3.54 (t, $J = 6.4$ Hz, 2H), 3.32 (s, 3H), 2.99 (t, $J = 6.4$ Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 137.0, 126.9, 125.2, 122.3, 119.5, 118.6, 116.4, 111.4, 109.2, 72.8, 58.8, 29.9, 25.0, 14.2.

HRMS (ESI, m/z): Calculated for C$_{14}$H$_{17}$N$_2$O (M+H)$^+$ 229.1335, found 229.1334.

2k. 2-(2-(cyanomethyl)-1-methyl-1H-indol-3-yl)ethyl acetate

A red solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 5/1); m.p.: 90-91 °C.
1H NMR (400 MHz, CDCl₃): δ 7.58 (d, J = 8.0 Hz, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.29 (dd, J = 6.8, 1.2 Hz, 1H), 7.18 – 7.14 (m, 1H), 4.25 (t, J = 6.8 Hz, 2H), 3.91 (s, 2H), 3.81 (s, 3H), 3.08 (t, J = 6.8 Hz, 2H), 2.07 (s, 3H).

13C NMR (100 MHz, CDCl₃): δ 171.1, 137.2, 126.8, 124.9, 122.7, 119.8, 118.7, 116.0, 110.2, 109.3, 64.4, 30.0, 23.9, 21.0, 14.0.

HRMS (ESI, m/z): Calculated for C₁₅H₂₀N₃O₂ (M+NH₄)⁺ 274.1550, found 274.1549.

2l. methyl 2-(cyanomethyl)-1-methyl-1H-indole-3-carboxylate
A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 2/1); m.p.: 128-130 °C.

1H NMR (400 MHz, CDCl₃): δ 8.13 (d, J = 7.6 Hz, 1H), 7.38 (d, J = 7.6 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.31 – 7.28 (m, 1H), 4.57 (s, 2H), 3.97 (s, 3H), 3.86 (s, 3H).

13C NMR (100 MHz, CDCl₃): δ 165.7, 136.8, 134.6, 125.6, 123.7, 122.5, 115.3, 109.6, 105.7, 51.3, 30.3, 14.3.

HRMS (ESI, m/z): Calculated for C₁₃H₁₃N₂O₂ (M+H)⁺ 229.0972, found 229.0969.

2m. 2-(1-methyl-3-(2,2,2-trifluoro-1-methoxyethyl)-1H-indol-2-yl)acetonitrile
A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1); m.p.: 123-125 °C.

1H NMR (400 MHz, CDCl₃): δ 7.60 (d, J = 8.0 Hz, 1H), 7.38 (d, J = 8.4 Hz, 1H), 7.34 – 7.30 (m, 1H), 7.23 – 7.19 (m, 1H), 4.99 (q, J = 6.8 Hz, 1H), 4.22 (d, J = 18.0 Hz, 1H), 3.98 (d, J = 18.0 Hz, 1H), 3.85 (s, 3H), 3.50 (s, 3H).

13C NMR (150 MHz, CDCl₃): δ 137.0, 127.2, 126.6, 124.3(d, J = 281.9 Hz), 123.1, 120.8, 118.7, 115.5, 109.6, 104.9, 75.6(q, J = 32.6 Hz), 58.5, 30.0, 14.3.

19F NMR (376 MHz, CDCl₃): δ -76.79 (s, 3F).
HRMS (ESI, m/z): Calculated for C$_{14}$H$_{14}$F$_3$N$_2$O (M+H)$^+$ 283.1053, found 283.1058.

2n. 2-(1-ethyl-1H-indol-2-yl)acetonitrile
A yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1).

$^1$H NMR (400 MHz, CDCl$_3$): δ 7.59 (d, $J = 8.0$ Hz, 1H), 7.33 (d, $J = 8.0$ Hz, 1H), 7.27 – 7.22 (m, 1H), 7.15 – 7.11 (m, 1H), 6.54 (d, $J = 0.8$ Hz, 1H), 4.19 (q, $J = 7.2$ Hz, 2H), 3.88 (s, 2H), 1.42 (t, $J = 7.2$ Hz, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$): δ 136.8, 127.4, 126.9, 122.3, 120.8, 120.1, 116.1, 109.3, 102.5, 38.3, 16.6, 15.2.

HRMS (ESI, m/z): Calculated for C$_{12}$H$_{13}$N$_2$ (M+H)$^+$ 185.1073, found 185.1067.

2o. 2-(1-acetyl-1H-indol-2-yl)acetonitrile
A white solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1).

$^1$H NMR (400 MHz, CDCl$_3$): δ 7.66 (d, $J = 8.4$ Hz, 1H), 7.59 (d, $J = 8.0$ Hz, 1H), 7.38 – 7.34 (m, 1H), 7.32 – 7.28 (m, 1H), 6.83 (s, 1H), 4.23 (s, 2H), 2.84 (s, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$): δ 170.3, 135.8, 130.8, 129.2, 124.8, 123.6, 121.5, 116.7, 114.1, 111.4, 27.4, 20.9.

HRMS (ESI, m/z): Calculated for C$_{12}$H$_{14}$N$_3$O (M+NH$_4$)$^+$ 216.1131, found 216.1128.

2p. 2-(1-methyl-1H-pyrrolo[2,3-b]pyridin-2-yl)acetonitrile
A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 3/1); m.p.: 100-103 °C.

$^1$H NMR (400 MHz, CDCl$_3$): δ 8.34 (dd, $J = 4.8$, 1.2 Hz, 1H), 7.87 (dd, $J = 8.0$, 1.2 Hz, 1H), 7.08 (dd, $J = 8.0$, 4.8 Hz, 1H), 6.52 (s, 1H), 3.92 (s, 2H), 3.88 (s, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$): δ 148.7, 143.4, 128.6, 128.5, 119.7, 116.4, 115.5, 100.1, 28.2, 17.0.
HRMS (ESI, m/z): Calculated for C_{10}H_{10}N_{3} (M+H)^{+} 172.0869, found 172.0864.

2q. 2-(1-methyl-5-(4-methylbenzoyl)-1H-pyrrol-2-yl)acetonitrile
A red solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1); m.p.: 100-102 °C.

\[
\begin{array}{c}
\text{O} \\
\text{I} \\
\text{N} \\
\text{CN}
\end{array}
\]

\[\text{^1H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 7.71 (d, } J = 8.0 \text{ Hz, 2H), 7.26 (d, } J = 8.0 \text{ Hz, 2H),} \\
6.67 (d, } J = 4.4 \text{ Hz, 1H), 6.23 (d, } J = 4.4 \text{ Hz, 1H), 3.98 (s, 3H), 3.77 (s, 2H), 2.43 (s, 3H).} \\
\text{^13C NMR (100 MHz, CDCl}_3\text{): } \delta \text{ 186.1, 142.4, 136.7, 132.3, 129.5, 129.1, 128.8,} \\
121.7, 115.4, 109.2, 33.1, 21.6, 16.5.} \\
\text{HRMS (ESI, m/z): Calculated for C}_{15}\text{H}_{15}\text{N}_{2}\text{O} (\text{M+H})^{+} 239.1179, \text{ found 239.1176.}
\]

2r. 4-methoxyphenyl 5-(cyanomethyl)-1-methyl-1H-pyrrole-2-carboxylate
A yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1); m.p.: 136-138 °C.

\[
\begin{array}{c}
\text{MeO} \\
\text{O} \\
\text{I} \\
\text{N} \\
\text{CN}
\end{array}
\]

\[\text{^1H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 7.15 (d, } J = 4.0 \text{ Hz, 1H), 7.08 (d, } J = 9.2 \text{ Hz, 2H),} \\
6.92 (d, } J = 9.2 \text{ Hz, 2H), 6.27 (d, } J = 4.0 \text{ Hz, 1H), 3.93 (s, 3H), 3.81 (s, 3H), 3.75 (s, 2H).} \\
\text{^13C NMR (100 MHz, CDCl}_3\text{): } \delta \text{ 159.8, 157.2, 143.8, 128.5, 123.3, 122.6, 118.4,} \\
115.4, 114.5, 109.5, 55.6, 32.7, 16.5.} \\
\text{HRMS (ESI, m/z): Calculated for C}_{15}\text{H}_{15}\text{N}_{2}\text{O}_{3} (\text{M+H})^{+} 271.1077, \text{ found 271.1075.}
\]

2s. tert-butyl 2-(cyanomethyl)-5-(4-methoxyphenyl)-1H-pyrrole-1-carboxylate
A blue liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 10/1).

\[
\begin{array}{c}
\text{O} \\
\text{I} \\
\text{N} \\
\text{CN}
\end{array}
\]

\[\text{^1H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ 7.20 (d, } J = 8.8 \text{ Hz, 2H), 6.90 (d, } J = 8.8 \text{ Hz, 2H),} \\
6.30 (d, } J = 3.6 \text{ Hz, 1H), 6.07 (d, } J = 3.6 \text{ Hz, 1H), 4.00 (s, 2H), 3.83 (s, 3H), 1.28 (s, 3H).} \\
\text{^13C NMR (100 MHz, CDCl}_3\text{): } \delta \text{ 159.8, 157.2, 143.8, 128.5, 123.3, 122.6, 118.4,} \\
115.4, 114.5, 109.5, 55.6, 32.7, 16.5.} \\
\text{HRMS (ESI, m/z): Calculated for C}_{15}\text{H}_{15}\text{N}_{2}\text{O}_{3} (\text{M+H})^{+} 271.1077, \text{ found 271.1075.}
\]
H).  

\(^{13}\text{C NMR (150 MHz, CDCl}_3\):} \quad \delta 159.0, 149.7, 136.6, 130.0, 127.2, 123.8, 117.2, 113.2, 112.2, 110.0, 84.7, 55.4, 27.4, 19.2.

HRMS (ESI, m/z): Calculated for C\textsubscript{18}H\textsubscript{21}N\textsubscript{2}O\textsubscript{3} (M+H)\textsuperscript{+} 313.1547, found 313.1548.

2s'. 2-(5-(4-methoxyphenyl)-1H-pyrrol-2-yl)acetonitrile

A red liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 5/1).

\(^{1}\text{H NMR (400 MHz, CDCl}_3\):} \quad \delta 8.35 (s, 1H), 7.39 (d, \( J = 8.8 \) Hz, 2H), 6.92 (d, \( J = 8.8 \) Hz, 2H), 6.31 (t, \( J = 3.2 \) Hz, 1H), 6.16 (t, \( J = 3.2 \) Hz, 1H), 3.83 (s, 3H), 3.81 (s, 2H).

\(^{13}\text{C NMR (150 MHz, CDCl}_3\):} \quad \delta 158.6, 133.4, 125.3, 118.8, 116.9, 114.4, 110.0, 109.9, 105.5, 55.3, 17.1.

HRMS (ESI, m/z): Calculated for C\textsubscript{13}H\textsubscript{13}N\textsubscript{2}O (M+H)\textsuperscript{+} 213.1022, found 213.1020.

2t. (S)-2-(1,3-dimethyl-1H-indol-2-yl)butanenitrile

A light yellow liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).

\(^{1}\text{H NMR (400 MHz, CDCl}_3\):} \quad \delta 7.55 (d, \( J = 8.0 \) Hz, 1H), 7.30 (d, \( J = 8.0 \) Hz, 1H), 7.28 – 7.24 (m, 1H), 7.16 – 7.12 (m, 1H), 4.07 (t, \( J = 8.0 \) Hz, 1H), 3.81 (s, 3H), 2.35 (s, 3H), 2.20 – 2.09 (m, 1H), 2.00 – 1.89 (m, 1H), 1.10 (t, \( J = 7.6 \) Hz, 3H).

\(^{13}\text{C NMR (100 MHz, CDCl}_3\):} \quad \delta 137.1, 127.9, 127.8, 122.4, 119.4, 119.2, 118.8, 109.5, 109.0, 30.5, 29.4, 27.1, 11.9, 8.9.

HRMS (ESI, m/z): Calculated for C\textsubscript{14}H\textsubscript{17}N\textsubscript{2} (M+H)\textsuperscript{+} 213.1386, found 213.1384.

Tolmetin. 2-(1-methyl-5-(4-methylbenzoyl)-1H-pyrrol-2-yl)acetic acid

A light yellow solid after purification by flash column chromatography (petroleum ether/ethyl acetate = 1/1); m.p.: 160-161 °C.
$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.71 (d, $J = 8.0$ Hz, 2H), 7.24 (d, $J = 8.0$ Hz, 2H), 6.68 (d, $J = 4.0$ Hz, 1H), 6.13 (d, $J = 4.0$ Hz, 1H), 3.95 (s, 3H), 3.76 (s, 2H), 2.42 (s, 3H).
$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 186.1, 174.7, 142.0, 137.1, 133.8, 131.5, 129.5, 128.7, 122.4, 109.7, 33.2, 32.5, 21.5.
HRMS (ESI, m/z): Calculated for C$_{15}$H$_{15}$NO$_3$Na (M+Na)$^+$ 280.0944, found 280.0948.

2-(3,3',5,5'-tetra-tert-butyl-4'-hydroxy-4-oxo-1,4-dihydro-[1,1'-biphenyl]-1-yl)acetonitrile

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.01 (s, 2H), 6.58 (s, 2H), 5.25 (s, 1H), 3.00 (s, 2H), 1.42 (s, 18H), 1.27 (s, 18H).
$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 185.6, 153.3, 147.2, 142.1, 136.5, 128.8, 122.6, 116.4, 44.5, 35.0, 34.6, 30.1, 29.4, 27.5.
$^{13}$DEPT NMR (150 MHz, CDCl$_3$): $\delta$ 142.1, 122.5, 30.1, 29.4, 27.5.
HRMS (ESI, m/z): Calculated for C$_{30}$H$_{43}$NO$_2$Na (M+Na)$^+$ 472.3186, found 472.3173.
Copies of the $^1$H NMR, $^{13}$C NMR, $^{19}$F NMR, $^{135}$DEPT

1a- $^1$H NMR

1a- $^{13}$C NMR
1b-$^1$H NMR

1b-$^{13}$C NMR
1c-^1^H NMR

1c-^13^C NMR
$1\text{e}^{-1}H$ NMR

$1\text{e}^{-13}C$ NMR
$^{1}H$ NMR

$^{13}C$ NMR
$^{1}H$ NMR

$^{13}C$ NMR
$^{1}H$ NMR

$^{13}C$ NMR
2a-\textsuperscript{1}H NMR

2a-\textsuperscript{13}C NMR
2b-\textsuperscript{1}H NMR

2b-\textsuperscript{13}C NMR
$2e^{-1}{}^1\text{H NMR}$

$2e^{-13}{}^1\text{C NMR}$
2f$^1$H NMR

2f$^{13}$C NMR
2f-$^{19}$F NMR

2g-$^1$H NMR
$^{13}$C NMR

$^1$H NMR
2i-\textsuperscript{13}C NMR

2j-\textsuperscript{1H} NMR
2j-^{13}C NMR

2k-^{1}H NMR
$2m^{13}\text{C NMR}$

$2m^{19}\text{F NMR}$
$2n^{-1}{^1}H$ NMR

$2n^{-13}C$ NMR
2o-¹H NMR

2o-¹³C NMR
2p-\textsuperscript{1}H NMR

2p-\textsuperscript{13}C NMR
$2r^{-13}C$ NMR

![2r^{-13}C NMR spectrum](image)

$2s^{-1}H$ NMR

![2s^{-1}H NMR spectrum](image)
2s\textsuperscript{-13}C NMR

2s\textsuperscript{-1}H NMR
$2s^1$-^{13}C NMR

$2t^1$H NMR
$^{2t-13}C \text{ NMR}$

![$^{2t-13}C \text{ NMR}$ graph]

$^{1}H \text{ NMR}$

![$^{1}H \text{ NMR}$ graph]
Tolmetin-\(^{13}\)C NMR

trap-\(^{1}\)H NMR
trap$^{13}$C NMR

trap$^{135}$DEPT