ELECTRONIC SUPPORTING INFORMATION (ESI)

Design and synthesis of sugar-triazole based uracil appended sugar-imine derivatives – An application in DNA binding studies

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Table 1 Spectral data and optimization of reaction condition of sugar-triazole derivatives, 6-9

<table>
<thead>
<tr>
<th>Compound No.</th>
<th>R</th>
<th>Time (h)</th>
<th>Yield (%)</th>
<th>(\delta_{\text{Ano-H}}) /ppm</th>
<th>(\delta_{\text{Ald-H}}) /ppm</th>
<th>(\delta_{\text{Trz-H}}) /ppm</th>
<th>(\delta_{\text{Trz-C}}) /ppm</th>
<th>(\Delta(\delta_{C4}-\delta_{C5}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>-H</td>
<td>24</td>
<td>85</td>
<td>5.91-5.88</td>
<td>10.48</td>
<td>7.92</td>
<td>121.5, 144.1</td>
<td>23</td>
</tr>
<tr>
<td>7</td>
<td>-OCH(_3)</td>
<td>26</td>
<td>79</td>
<td>5.89-5.86</td>
<td>9.86</td>
<td>7.91</td>
<td>144.0, 121.7</td>
<td>22</td>
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<tr>
<td>8</td>
<td>-Cl</td>
<td>20</td>
<td>74</td>
<td>5.90-5.87</td>
<td>10.39</td>
<td>7.91</td>
<td>143.6, 121.6</td>
<td>22</td>
</tr>
<tr>
<td>9</td>
<td>-OH</td>
<td>24</td>
<td>83</td>
<td>5.91-5.88</td>
<td>9.98</td>
<td>7.88</td>
<td>144.4, 121.2</td>
<td>23</td>
</tr>
</tbody>
</table>

Table 2 Spectroscopic data and optimization of reaction condition of sugar-imine derivatives, 11-14

<table>
<thead>
<tr>
<th>Entry</th>
<th>R</th>
<th>Time (h)</th>
<th>Yield (%)</th>
<th>(\delta_{\text{Ano-H}})/ppm, (J_{\text{H,H,H}}) Hz</th>
<th>(\delta_{\text{Trz-H}}) /ppm</th>
<th>(\delta_{\text{Imin-H}}) /ppm</th>
<th>(\delta_{\text{Imin-C}}) /ppm</th>
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<tbody>
<tr>
<td>11</td>
<td>-H</td>
<td>1</td>
<td>56</td>
<td>5.79, 9.0</td>
<td>7.27</td>
<td>7.61</td>
<td>165</td>
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<tr>
<td>12</td>
<td>-OCH(_3)</td>
<td>3</td>
<td>58</td>
<td>5.58, 9.3</td>
<td>7.69</td>
<td>8.01</td>
<td>168</td>
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<tr>
<td>13</td>
<td>-Cl</td>
<td>3</td>
<td>35</td>
<td>5.60,(^a)</td>
<td>7.67</td>
<td>7.93</td>
<td>167</td>
</tr>
<tr>
<td>14</td>
<td>-H</td>
<td>4</td>
<td>52</td>
<td>5.60-5.53,(^*)</td>
<td>7.50</td>
<td>8.01</td>
<td>167</td>
</tr>
</tbody>
</table>

\(^a\)Peaks merged with saccharide proton, \(^*\)merged with alkene proton
General procedure for the synthesis of O-propargylated derivative, 2-5

To the corresponding hydroxy benzaldehydes (1 mmol) in dry DMF, (5 mmol) anhydrous K$_2$CO$_3$ was added and stirred for 10 minutes. To the reaction mixture was added propargyl bromide (1.2 mmol) and stirred for 24 hours. After the completion of the reaction, work up was done using chloroform. The organic layer was evaporated and the product was purified using silica gel column chromatography.

Spectral data of 2-(prop-2-ynyloxy)-1-benzaldehyde (2):
Pale yellow solid; Mp: 64-66 °C; Yield: 0.12 g (75%); $^1$H NMR (300 MHz, CDCl$_3$): δ 10.49 (s, 1H, -CHO), 7.87 (d, J = 7.8 Hz, 1H, Ar-H), 7.61-7.55 (m, 1H, Ar-H), 7.14-7.07 (m, 2H, Ar-H), 4.9 (s, 2H, -OCH$_2$), 2.57 (t, J = 2.4 Hz, 1H, -C≡CH); $^{13}$C NMR (75 MHz, CDCl$_3$): δ 189.5, 159.8, 135.7, 128.6, 125.5, 121.7, 113.2, 77.7, 76.5, 56.4.

Spectral data of 2-methoxy-4-(prop-2-ynyloxy)-1-benzaldehyde (3):
Pale yellow solid; Mp: 86-88 °C; Yield: 0.16 g (84%); $^1$H NMR (300 MHz, CDCl$_3$): δ 9.88 (s, 1H, -CHO), 7.49-7.45 (m, 2H, Ar-H), 7.15 (d, J = 8.1 Hz, 1H, Ar-H), 4.87 (d, J = 2.4 Hz, 2H, -OCH$_2$), 3.95 (s, 3H, -OCH$_3$), 2.57 (t, J = 2.3 Hz, 1H, -C≡CH); $^{13}$C NMR (75 MHz, CDCl$_3$): δ 190.8, 152.2, 150.1, 131.0, 126.2, 112.7, 109.6, 77.0, 76.6, 56.6, 56.0.

Spectral data of 5-chloro-2-(prop-2-ynyloxy)-1-benzaldehyde (4):
Yellow solid; Mp: 60-62 °C; Yield: 0.14 g (74%); $^1$H NMR (300 MHz, CDCl$_3$): δ 10.41 (s, 1H, -CHO), 7.81 (s, 1H, Ar-H), 7.51 (d, J = 9.0 Hz, 1H, Ar-H), 7.09 (d, J = 9.0 Hz, 1H, Ar-H), 4.83 (d, J = 2.4 Hz, 2H, -OCH$_2$), 2.59 (t, J = 2.4 Hz, 1H, -C≡CH); $^{13}$C NMR (75 MHz, CDCl$_3$): δ 188.2, 158.1, 135.2, 128.1, 127.5, 126.5, 115.0, 77.2, 76.9, 56.8.

Spectral data of 3-(prop-2-ynyloxy)-1-benzaldehyde (5):
Yield 0.13 g, (81%); $^1$H NMR (300 MHz, CDCl$_3$): δ 9.97 (s, 1H, -CHO), 7.52-7.44 (m, 3H, Ar-H), 7.28-7.23 (m, 1H, Ar-H), 4.76 (d, J = 2.4 Hz, 2H, -OCH$_2$), 2.57 (t, J = 2.4 Hz, 1H, -C≡CH); $^{13}$C NMR (75 MHz, CDCl$_3$): δ 192.0, 158.1, 137.8, 130.2, 124.1, 122.1, 113.6, 77.9, 76.2, 56.0.

$^1$H NMR, $^{13}$C NMR, DEPT-135, Mass spectrum are available in the ESI
Contents

Figure 1: $^1$H NMR spectrum (300 MHz, CDCl$_3$) of compound 2.
Figure 2: $^{13}$C NMR spectrum (75 MHz, CDCl$_3$) of compound 2.
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Figure 6: $^{13}$C NMR spectrum (75 MHz, CDCl$_3$) of compound 4.
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Figure 8: $^{13}$C NMR spectrum (75 MHz, CDCl$_3$) of compound 5.
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Figure 15: $^1$H NMR expansion spectrum (300 MHz, CDCl$_3$) of compound 8.
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Figure 2 $^{13}$C NMR spectrum (75 MHz, CDCl$_3$) of compound, 2
Figure 3 $^1$H NMR spectrum (300 MHz, CDCl$_3$) of compound, 3.
Figure 4 $^{13}$C NMR spectrum (75 MHz, CDCl$_3$) of compound, 3
Figure 5 $^1$H NMR spectrum (300 MHz, CDCl$_3$) of compound, 4.
Figure 6 $\text{^{13}C}$ NMR spectrum (75 MHz, CDCl$_3$) of compound, 4.
Figure 7 $^1$H NMR spectrum (300 MHz, CDCl$_3$) of compound, 5.
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Figure 9 $^1$H NMR spectrum (300 MHz, CDCl$_3$) of compound, 6.
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Figure 25 Mass spectrum of compound, 12.

Calc. exact mass, 532.19
m/z found, 533.20 [M+H]^+
Figure 26 $^1$H NMR spectrum (300 MHz, CDCl$_3$) of compound, 13.
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Docking Studies:

Figure 30 Hydrogen bonding interaction of compounds (a) 6, (b) 11, (c) 7, (d) 12, (e) 8, (f) 13.