Indole-Based Novel Small Molecules for the Modulation of Bacterial Signalling Pathways

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Supporting Information

1) Growth Inhibition Data
2) 1H and 13C NMR Spectrums of Synthesised Compounds
1) Growth Inhibition Data

Table 1: Percentage growth inhibition of the indole based AHLs as determined by reduction in OD$_{600}$ in the P$_{lasB}$::gfp reporter strain

<table>
<thead>
<tr>
<th>Compound</th>
<th>Concentration (µM)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>250</td>
</tr>
<tr>
<td>11a</td>
<td>6.19 ± 3.21</td>
</tr>
<tr>
<td>11b</td>
<td>7.50 ± 5.32</td>
</tr>
<tr>
<td>11c</td>
<td>7.28 ± 3.41</td>
</tr>
<tr>
<td>11d</td>
<td>14.99 ± 4.89</td>
</tr>
<tr>
<td>11e</td>
<td>0</td>
</tr>
<tr>
<td>14a</td>
<td>0</td>
</tr>
<tr>
<td>14b</td>
<td>0</td>
</tr>
<tr>
<td>14c</td>
<td>0</td>
</tr>
<tr>
<td>16a</td>
<td>6.96 ± 3.89</td>
</tr>
<tr>
<td>16b</td>
<td>0</td>
</tr>
<tr>
<td>16c</td>
<td>0</td>
</tr>
<tr>
<td>16d</td>
<td>0</td>
</tr>
<tr>
<td>16e</td>
<td>0</td>
</tr>
<tr>
<td>17a</td>
<td>0</td>
</tr>
<tr>
<td>17b</td>
<td>0</td>
</tr>
<tr>
<td>17c</td>
<td>5.92 ± 1.88</td>
</tr>
<tr>
<td>20a</td>
<td>0</td>
</tr>
<tr>
<td>20b</td>
<td>7.38 ± 2.12</td>
</tr>
<tr>
<td>20c</td>
<td>0</td>
</tr>
<tr>
<td>21a</td>
<td>0</td>
</tr>
<tr>
<td>21b</td>
<td>0</td>
</tr>
<tr>
<td>21c</td>
<td>0</td>
</tr>
<tr>
<td>Furanone 30</td>
<td>31.57 ± 3.87</td>
</tr>
</tbody>
</table>

Growth inhibition ± standard deviation of mean from at least two independent experiments. Compounds tested twice in duplicate. 0 = No growth inhibition
1) $^1$H and $^{13}$C NMR Spectrums of Synthesised Compounds

$^1$H NMR spectrum of Compound # 9

$^{13}$C NMR spectrum of Compound # 9
**1H NMR spectrum of Compound # 10**

![1H NMR spectrum](image1)

**13C NMR spectrum of Compound # 10**

![13C NMR spectrum](image2)
$^1$H NMR spectrum of Compound # 11a

$^{13}$C NMR spectrum of Compound # 11a
$^1$H NMR spectrum of Compound # 11b

$^{13}$C NMR spectrum of Compound # 11b
$^1$H NMR spectrum of Compound # 11c

$^{13}$C NMR spectrum of Compound # 11c
$^1$H NMR spectrum of Compound # 11d

$^{13}$C NMR spectrum of Compound # 11d
$^1$H NMR spectrum of Compound # 11e

$^{13}$C NMR spectrum of Compound # 11e
$^1$H NMR spectrum of Compound # 14a

$^{13}$C NMR spectrum of Compound # 14a
$^1$H NMR spectrum of Compound # 14b

$^{13}$C NMR spectrum of Compound # 14b
**H NMR spectrum of Compound # 14c**

\[ \text{structure image} \]

**13C NMR spectrum of Compound # 14c**

\[ \text{structure image} \]
$^1$H NMR spectrum of Compound # 16a

$^{13}$C NMR spectrum of Compound # 16a
$^1$H NMR spectrum of Compound # 16c

$^{13}$C NMR spectrum of Compound # 16c
$^{1}$H NMR spectrum of Compound # 16d

$^{13}$C NMR spectrum of Compound # 16d
\(^1\)H NMR spectrum of Compound \# 16e

\(^{13}\)C NMR spectrum of Compound \# 16e
$^1$H NMR spectrum of Compound # 17a

$^{13}$C NMR spectrum of Compound # 17a
\(^1\)H NMR spectrum of Compound \# 17b

\(^1\)C NMR spectrum of Compound \# 17b
**1H NMR spectrum of Compound # 17c**

![H NMR spectrum of Compound # 17c](image)

**13C NMR spectrum of Compound # 17c**

![13C NMR spectrum of Compound # 17c](image)
\(^1\)H NMR spectrum of Compound \# 19

\(^13\)C NMR spectrum of Compound \# 19
\(^1\)H NMR spectrum of Compound \# 20a

\(^13\)C NMR spectrum of Compound \# 20a
$^1$H NMR spectrum of Compound # 20b

$^{13}$C NMR spectrum of Compound # 20b
$^1$H NMR spectrum of Compound # 20c

\[ \text{Diagram of H NMR spectrum} \]

$^{13}$C NMR spectrum of Compound # 20c

\[ \text{Diagram of C NMR spectrum} \]
$^1$H NMR spectrum of Compound #21a

$^{13}$C NMR spectrum of Compound #21a
$^1$H NMR spectrum of Compound # 21b

$^{13}$C NMR spectrum of Compound # 21b
$^1$H NMR spectrum of Compound # 21c

$^{13}$C NMR spectrum of Compound # 21c