Supporting Information

Mohamed Shaaban\textsuperscript{a,b,}\textasteriskcentered

New Bioactive Compounds from \textit{Sarcophyton glaucom}-derived \textit{Penicillium} sp.

\textsuperscript{a} Chemistry of Natural Compounds Department, Division of Pharmaceutical Industries, National Research Centre,
\textsuperscript{b} University of Göttingen, Institute of Organic and Biomolecular Chemistry, Tammannstrasse 2, D-37077 Göttingen, Germany.
\textasteriskcentered M. Shaaban. Email: mshaaba@gmail.com

1: R = $\beta$-OCH\textsubscript{3}, 2: R = $\alpha$-OCH\textsubscript{3}
6: R = $\beta$-OH, 7: R = $\alpha$-OH
<table>
<thead>
<tr>
<th>Contents</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table S1: Physico-chemical properties of compounds 1-5</td>
<td>S3</td>
</tr>
<tr>
<td>Table S2: $^{13}$C (125 MHz) and $^1$H (600 MHz) NMR data for the epimers 9-methoxy-penicryones A-B (1,2) and penicyrones A-B (6,7) in CD$_3$OD</td>
<td>S4</td>
</tr>
<tr>
<td>Table S3: $^{13}$C (125 MHz) and $^1$H (600 MHz) NMR data for the constitutional isomers 3 and 4 in CDCl$_3$</td>
<td>S4</td>
</tr>
<tr>
<td>Table S4: $^{13}$C (125 MHz), and $^1$H (500 MHz) NMR data of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5) in CDCl$_3$</td>
<td>S5</td>
</tr>
<tr>
<td>Figure S1-10b: ESI-MS/HRESI-MS and NMR (1D and 2D) NMR spectra of 9-methoxy-penicryone A (1)/ 9-methoxy-penicryone B (2)</td>
<td>S6-20</td>
</tr>
<tr>
<td>Figure S11. $^1$H-$^1$H COSY and key HMBC correlations for 9-methoxy-penicryones A-B (1,2).</td>
<td>S21</td>
</tr>
<tr>
<td>Figure S12. key NOESY correlations for 9-methoxy-penicryones A-B (1,2)</td>
<td>S22</td>
</tr>
<tr>
<td>Figure S13-22b: ESI-MS/HRESI-MS and NMR (1D and 2D) NMR spectra of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)</td>
<td>S23-42</td>
</tr>
<tr>
<td>Figure S23. $^1$H-$^1$H COSY and key HMBC correlations for compounds 3 and 4.</td>
<td>S43</td>
</tr>
<tr>
<td>Figure S24-32b: ESI-MS/HRESI-MS and NMR (1D and 2D) NMR spectra of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)</td>
<td>S44-57</td>
</tr>
<tr>
<td>Figure S33. $^1$H-$^1$H COSY and key HMBC correlations for 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5).</td>
<td>S58</td>
</tr>
<tr>
<td>Figure S34a-44b: ESI-MS/HRESI-MS and NMR (1D and 2D) NMR spectra of penicyrones A-B (6,7)</td>
<td>S59-77</td>
</tr>
<tr>
<td>Figure S45-54: ESI-MS/HRESI-MS and NMR (1D and 2D) NMR spectra of 4-(2-hydroxy-3-butynoxy) benzoic acid (8)</td>
<td>S78-91</td>
</tr>
<tr>
<td>Figure S55-67b: ESI-MS/HRESI-MS and NMR (1D and 2D) NMR spectra of cyclopenol (9)</td>
<td>S92-110</td>
</tr>
<tr>
<td>Figure S68-76: ESI-MS/HRESI-MS and NMR (1D and 2D) NMR spectra of Aspermytin A (10)</td>
<td>S111-119</td>
</tr>
<tr>
<td>Figure S77a-86b: ESI-MS/HRESI-MS and NMR (1D and 2D) NMR spectra of Aurantiomide A (11)</td>
<td>S120-137</td>
</tr>
</tbody>
</table>
Table S1: Physico-chemical properties of compounds 1-5

<table>
<thead>
<tr>
<th></th>
<th>9-Methoxy-penicryrone A (1) &amp; B (2)</th>
<th>3-Hydroxy-2,2,4-trimethyl-pentyl ester (3) &amp; 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)</th>
<th>3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>colorless oil</td>
<td>colourless oil</td>
<td>colourless oil</td>
</tr>
<tr>
<td>$R_f$</td>
<td>0.55&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.54&lt;sup&gt;b&lt;/sup&gt;</td>
<td>0.25&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Anisaldehyde/sulfuric acid</td>
<td>reddish brown</td>
<td>violet, turning later blue</td>
<td>Pink turning later violet</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>C&lt;sub&gt;25&lt;/sub&gt;H&lt;sub&gt;36&lt;/sub&gt;O&lt;sub&gt;7&lt;/sub&gt;</td>
<td>C&lt;sub&gt;12&lt;/sub&gt;H&lt;sub&gt;24&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</td>
<td>C&lt;sub&gt;30&lt;/sub&gt;H&lt;sub&gt;54&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;</td>
</tr>
<tr>
<td>(+)-ESI MS: m/z (%)</td>
<td>471 [M+Na]&lt;sup&gt;+&lt;/sup&gt; (100), 919 [2M+Na]&lt;sup&gt;+&lt;/sup&gt; (34)</td>
<td>239 [M+Na]&lt;sup&gt;+&lt;/sup&gt; (100)</td>
<td>501 [M+Na]&lt;sup&gt;+&lt;/sup&gt; (70), 957 [2M+H]&lt;sup&gt;+&lt;/sup&gt; (100), 979 [2M+Na]&lt;sup&gt;+&lt;/sup&gt; (88)</td>
</tr>
<tr>
<td>(-)-ESI MS: m/z (%)</td>
<td>471.2362 [M+Na]&lt;sup&gt;+&lt;/sup&gt; (calc. 471.2353 for C&lt;sub&gt;25&lt;/sub&gt;H&lt;sub&gt;36&lt;/sub&gt;O&lt;sub&gt;7&lt;/sub&gt;Na), 919.4820 [2M+Na]&lt;sup&gt;+&lt;/sup&gt;(calc. 919.4820 for C&lt;sub&gt;30&lt;/sub&gt;H&lt;sub&gt;54&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;Na)</td>
<td>239.1620 [M+Na]&lt;sup&gt;+&lt;/sup&gt; (calc. 239.1618 for C&lt;sub&gt;12&lt;/sub&gt;H&lt;sub&gt;24&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;Na)</td>
<td>477 [M-H]&lt;sup&gt;-&lt;/sup&gt; (19)</td>
</tr>
<tr>
<td>(+)-ESI HRMS: (m/z)</td>
<td></td>
<td>966.8123 [M]&lt;sup&gt;+&lt;/sup&gt; (calc. 966.8123 for C&lt;sub&gt;30&lt;/sub&gt;H&lt;sub&gt;54&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;)</td>
<td></td>
</tr>
<tr>
<td>$[\alpha]^{20}_D$</td>
<td>+ 66.2 (c, 0.16 MeOH) - 35.4 (c, 0.22, CHCl&lt;sub&gt;3&lt;/sub&gt;)</td>
<td>+ 3.3 (c, 0.18 MeOH)</td>
<td></td>
</tr>
</tbody>
</table>

*CH<sub>2</sub>Cl<sub>2</sub>/10% MeOH; <sup>2</sup>CH<sub>2</sub>Cl<sub>2</sub>/5% MeOH, <sup>3</sup>CH<sub>2</sub>Cl<sub>2</sub>
Table S2: $^{13}$C (125 MHz) and $^1$H (600 MHz) NMR data for the epimers 9-methoxy-penicryones A-B (1,2) and penicyrones A-B (6,7) in CD$_3$OD

<table>
<thead>
<tr>
<th>Nr.</th>
<th>9-Methoxy-penicryone A (1) (minor 93%)</th>
<th>9-Methoxy-penicryone B (2) (major 100%)</th>
<th>Penicryone A (6) (minor 86%)</th>
<th>Penicryone B (7) (major 100%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\delta_C$</td>
<td>$\delta_H$</td>
<td>$\delta_C$</td>
<td>$\delta_H$</td>
</tr>
<tr>
<td>1</td>
<td>167.1</td>
<td>167.1</td>
<td>167.1</td>
<td>167.1</td>
</tr>
<tr>
<td>2</td>
<td>110.6</td>
<td>110.6</td>
<td>110.48</td>
<td>110.46</td>
</tr>
<tr>
<td>3</td>
<td>171.3</td>
<td>171.3</td>
<td>171.30</td>
<td>171.25</td>
</tr>
<tr>
<td>4</td>
<td>112.9</td>
<td>112.9</td>
<td>112.9</td>
<td>112.8</td>
</tr>
<tr>
<td>5</td>
<td>162.26</td>
<td>162.21</td>
<td>162.2</td>
<td>162.2</td>
</tr>
<tr>
<td>6</td>
<td>75.1</td>
<td>75.1</td>
<td>75.01</td>
<td>74.99</td>
</tr>
<tr>
<td>7</td>
<td>135.0</td>
<td>5.86 (t, 1.2)</td>
<td>135.2</td>
<td>5.87 (t, 1.2)</td>
</tr>
<tr>
<td>8</td>
<td>135.2</td>
<td>3.75 (s)</td>
<td>91.7</td>
<td>3.75 (s)</td>
</tr>
<tr>
<td>9</td>
<td>137.0</td>
<td>5.69 (t, 1.5)</td>
<td>131.0</td>
<td>5.69 (t, 1.5)</td>
</tr>
<tr>
<td>10</td>
<td>81.39</td>
<td>3.55 (s)</td>
<td>68.6</td>
<td>3.54 (s)</td>
</tr>
<tr>
<td>11</td>
<td>131.1</td>
<td>5.70 (t, 1.5)</td>
<td>81.36</td>
<td>3.55 (s)</td>
</tr>
<tr>
<td>12</td>
<td>68.5</td>
<td>3.55 (s)</td>
<td>68.5</td>
<td>3.55 (s)</td>
</tr>
<tr>
<td>13</td>
<td>78.13</td>
<td>4.02 (q, 6.8)</td>
<td>78.14</td>
<td>4.02 (q, 6.8)</td>
</tr>
<tr>
<td>14</td>
<td>19.1</td>
<td>1.14 (d, 7.0)</td>
<td>69.9</td>
<td>3.18 (d, 11.7), 2.99 (d, 11.7)</td>
</tr>
<tr>
<td>15</td>
<td>34.2</td>
<td>2.54 (p, 7.0)</td>
<td>40.0</td>
<td>2.54 (p, 7.0)</td>
</tr>
<tr>
<td>16</td>
<td>177.0</td>
<td>2.01 (s)</td>
<td>17.7</td>
<td>0.93 (d, 6.8)</td>
</tr>
<tr>
<td>17</td>
<td>71.3</td>
<td>4.07 (d, 10.9), 3.73 (d, 11.0)</td>
<td>18.1</td>
<td>1.18 (d, 7.0)</td>
</tr>
<tr>
<td>18</td>
<td>39.3</td>
<td>3.20 (d, 2.7)</td>
<td>19.3</td>
<td>3.20 (d, 2.7)</td>
</tr>
<tr>
<td>19</td>
<td>28.7</td>
<td>1.87 (pd, 6.8, 2.4)</td>
<td>28.3</td>
<td>2.03 (pd, 6.8, 2.7)</td>
</tr>
<tr>
<td>20</td>
<td>39.3</td>
<td>0.96 (d, 6.8)</td>
<td>34.6</td>
<td>2.60 (p, 7.0)</td>
</tr>
<tr>
<td>21</td>
<td>19.3</td>
<td>1.14 (d, 6.8)</td>
<td>23.0</td>
<td>0.89 (d, 6.8)</td>
</tr>
<tr>
<td>22</td>
<td>22.1</td>
<td>0.93 (s)</td>
<td>22.3</td>
<td>0.98 (s)</td>
</tr>
<tr>
<td>23</td>
<td>20.5</td>
<td>1.14 (d, 7.0)</td>
<td>19.7</td>
<td>0.81 (s)</td>
</tr>
</tbody>
</table>

Table S3: $^{13}$C (125 MHz) and $^1$H (600 MHz) NMR data for the constitutional isomers 3 and 4 in CDCl$_3$

<table>
<thead>
<tr>
<th>Nr.</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>19.1</td>
<td>3.18 (d, 11.7), 2.99 (d, 11.7)</td>
</tr>
<tr>
<td>2</td>
<td>34.2</td>
<td>40.0</td>
</tr>
<tr>
<td>3</td>
<td>177.0</td>
<td>79.2</td>
</tr>
<tr>
<td>5</td>
<td>71.3</td>
<td>178.1</td>
</tr>
<tr>
<td>6</td>
<td>39.3</td>
<td>34.6</td>
</tr>
<tr>
<td>7</td>
<td>79.4</td>
<td>19.3</td>
</tr>
<tr>
<td>8</td>
<td>28.7</td>
<td>19.33</td>
</tr>
<tr>
<td>9</td>
<td>23.6</td>
<td>28.3</td>
</tr>
<tr>
<td>10</td>
<td>17.7</td>
<td>17.7</td>
</tr>
<tr>
<td>12</td>
<td>22.1</td>
<td>23.0</td>
</tr>
<tr>
<td>13</td>
<td>20.5</td>
<td>22.3</td>
</tr>
<tr>
<td>14</td>
<td>19.1</td>
<td>19.7</td>
</tr>
</tbody>
</table>
Table S4: $^{13}$C (125 MHz), and $^1$H (500 MHz) NMR data of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5) in CDCl$_3$

<table>
<thead>
<tr>
<th>Nr.</th>
<th>$\delta_C$</th>
<th>$\delta_H$</th>
<th>Nr.</th>
<th>$\delta_C$</th>
<th>$\delta_H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>173.8</td>
<td></td>
<td>16</td>
<td>31.5</td>
<td>1.27 (m)</td>
</tr>
<tr>
<td>2</td>
<td>34.3</td>
<td>2.29 (t, 7.6)</td>
<td>17</td>
<td>22.6</td>
<td>1.28 (m)</td>
</tr>
<tr>
<td>3</td>
<td>24.9</td>
<td>1.60 (m)</td>
<td>18</td>
<td>14.1</td>
<td>0.87 (m)</td>
</tr>
<tr>
<td>4</td>
<td>29.2</td>
<td>1.28 (m)</td>
<td>1'$'$</td>
<td>69.9</td>
<td>3.77, 3.86</td>
</tr>
<tr>
<td>5</td>
<td>29.3</td>
<td>1.28 (m)</td>
<td>2'$'$</td>
<td>38.7</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>29.6</td>
<td>1.23 (m)</td>
<td>3'$'$</td>
<td>79.5</td>
<td>4.75</td>
</tr>
<tr>
<td>7</td>
<td>29.1</td>
<td>1.28 (m)</td>
<td>4'$'$</td>
<td>28.3</td>
<td>2.01 (m)</td>
</tr>
<tr>
<td>8</td>
<td>27.2</td>
<td>2.02 (m)</td>
<td>5'$'$</td>
<td>23.1</td>
<td>0.94 (m)</td>
</tr>
<tr>
<td>9</td>
<td>130.0</td>
<td>5.35 (m)</td>
<td>6'$'$</td>
<td>17.8</td>
<td>0.87 (m)</td>
</tr>
<tr>
<td>10</td>
<td>128.0</td>
<td>5.31 (m)</td>
<td>7'$'$</td>
<td>21.8</td>
<td>0.96 (s)</td>
</tr>
<tr>
<td>11</td>
<td>25.6</td>
<td>2.75 (m)</td>
<td>8'$'$</td>
<td>21.3</td>
<td>0.94 (m)</td>
</tr>
<tr>
<td>12</td>
<td>127.9</td>
<td>5.31 (m)</td>
<td>1''</td>
<td>176.5</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>130.2</td>
<td>5.35 (m)</td>
<td>2''</td>
<td>34.4</td>
<td>2.57 (m)</td>
</tr>
<tr>
<td>14</td>
<td>27.2</td>
<td>2.02 (m)</td>
<td>3''</td>
<td>19.3</td>
<td>1.18 (d, 3.8)</td>
</tr>
<tr>
<td>15</td>
<td>29.5</td>
<td>1.23 (m)</td>
<td>4''</td>
<td>19.2</td>
<td>1.17 (d, 3.9)</td>
</tr>
</tbody>
</table>
Figure S1: (+)-ESI-MS spectrum of 9-methoxy-penicyrone A (1)/ 9-methoxy-penicyrone B (2)
**Figure S2**: (+)-HRESI-MS spectrum of 9-methoxy-penicryrone A (1)/ 9-methoxy-penicryrone B (2)
Figure S3: $^1$H NMR (300 MHz, CD$_3$OD) spectrum of 9-methoxy-penicryone A (1)/ 9-methoxy-penicryone B (2)
Figure S4: $^1$H NMR (600 MHz, CD$_3$OD) spectrum of 9-methoxy-penicyrone A (1)/ 9-methoxy-penicyrone B (2)
Figure S5a: $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of 9-methoxy-penicyrone A (1)/ 9-methoxy-penicyrone B (2)
Figure S5b: $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of 9-methoxy-pencyrone A (1)/ 9-methoxy-pencyrone B (2)
Figure S6a: $^1$H,$^1$H COSY (600 MHz, CD$_3$OD) spectrum of 9-methoxy-penicryone A (1)/ 9-methoxy-penicryone B (2)
**Figure S6b**: $^1$H,$^1$H COSY (600 MHz, CD$_3$OD) spectrum of 9-methoxy-penicryn A (1)/ 9-methoxy-penicryn B (2)
Figure S7: HSQC (500 MHz, CD$_3$OD) spectrum of 9-methoxy-penicrynone A (1)/ 9-methoxy-penicrynone B (2)
Figure S8a: HMQC (500 MHz, CD3OD) spectrum of 9-methoxy-pencyrone A (1)/ 9-methoxy-pencyrone B (2)
Figure S8b: HMQC (500 MHz, CD$_3$OD) spectrum of 9-methoxy-penicrynne A (1) / 9-methoxy-penicrynne B (2)
Figure S9a: HMBC (500 MHz, CD$_3$OD) spectrum of 9-methoxy-penicrynne A (1)/ 9-methoxy-penicrynne B (2)
Figure S9b: HMBC (500 MHz, CD$_3$OD) spectrum of 9-methoxy-penicryone A (1)/ 9-methoxy-penicryone B (2)
Figure S10a: NOESY (600 MHz, CD$_3$OD) spectrum of 9-methoxy-pencyrone A (1)/9-methoxy-pencyrone B (2)
Figure S10b: NOESY (600 MHz, CD$_3$OD) spectrum of 9-methoxy-penicynrone A (1)/9-methoxy-penicynrone B (2)
Figure S11. $^1$H-$^1$H COSY and key HMBC correlations for 9-methoxy-penicyrones A-B (1,2).
Figure S12. key NOESY correlations for 9-methoxy-penicynes A-B (1,2).
Figure S13: (+)-ESI-MS spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S14: (+)-HRESI-MS spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S15a: $^1$H NMR (600 MHz, CDCl$_3$) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S15b: $^1$H NMR (600 MHz, CDCl$_3$) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S15c: $^1$H NMR (600 MHz, CDCl$_3$) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S16a: $^{13}$C NMR (125 MHz, CDCl$_3$) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S16b: $^{13}$C NMR (125 MHz, CDCl$_3$) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S16c: $^{13}$C NMR (125 MHz, CDCl$_3$) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S16d: $^{13}$C NMR (125 MHz, CDCl$_3$) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S17: APT NMR (125 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S18a: H,HCOSY (600 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3) / 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S18b: H.HCOSY (600 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S19a: HMQC (600 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S19b: HMOC (600 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S19c: HMQC (600 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S20: HSQC (600 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S21a: HMBC (600 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S21b: HMBC (600 MHz, CDCl3) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S22a: NOESY (600 MHz, CDCl$_3$) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S22b: NOESY (600 MHz, CDCl₃) spectrum of 3-hydroxy-2,2,4-trimethyl-pentyl ester (3)/ 3-hydroxy-1-isopropyl-2,2-dimethyl-propyl ester (4)
Figure S23. $^1$H-$^1$H COSY and key HMBC correlations for compounds 3 and 4.
Figure S24: (+)-ESI-MS spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S25: (+)-HRESI-MS spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S26: (−)-ESI-MS spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S27a: $^1$H NMR (500 MHz, CDCl$_3$) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S27b: $^1$H NMR (500 MHz, CDCl$_3$) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S28a: $^{13}$C NMR (125 MHz, CDCl$_3$) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S29a: H,H COSY (500 MHz, CDCl₃) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S29b: H,H COSY (500 MHz, CDCl$_3$) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S30a: HMQC (500 MHz, CDCl₃) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S30b: HMQC (500 MHz, CDCl₃) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S31a: HMBC (500 MHz, CDCl₃) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S31b: HMBC (500 MHz, CDCl₃) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S32a: NOESY (500 MHz, CDCl₃) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S32b: NOESY (500 MHz, CDCl₃) spectrum of 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5)
Figure S33. $^1$H-$^1$H COSY and key HMBC correlations for 3-isobutyryloxy-2,2,4-trimethyl-pentyl linoleate (5).
Figure S34a: (+)-ESI-MS spectrum of penicyrones A-B (6,7)
Figure S34b: (+)-ESI-MS spectrum of penicyrones A-B (6,7)
Figure S35: (+)-HRESI-MS spectrum of penicyrones A-B (6,7)
Figure S36: (-)-ESI-MS spectrum of penicyrones A-B (6,7)
Figure S3: (−)-HRESI-MS spectrum of penicyrones A-B (6,7)
Figure S38a: $^1$H NMR (300 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
**Figure S38b**: $^1$H NMR (600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S38c: $^1$H NMR (600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6.7)
Figure S39a: $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S39b: $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S40a: H,H COSY (600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S40b: H,H COSY (600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S41a: HMQC (600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S41b: HMQC (600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S42: HSQC (600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6.7)
Figure S43a: HMBC (600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S43b: HMBC (600 MHz, CD₃OD) spectrum of penicyrones A-B (6,7)
Figure S44a: NOESY 600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S44b: NOESY 600 MHz, CD$_3$OD) spectrum of penicyrones A-B (6,7)
Figure S45: (+)-ESI-MS spectrum of 4-(2-hydroxy-3-butoxy)benzoic acid (8)
**Figure S46**: (+)-HRESI-MS spectrum of 4-(2-hydroxy-3-butynoxy)benzoic acid (8)
Figure S47: (−)-ESI-MS spectrum of 4-(2-hydroxy-3-butoxy)benzoic acid (8)
Figure S48: (-)-HRESI-MS spectrum of 4-(2-hydroxy-3-butoxy)benzoic acid (8)
Figure S49a: $^1$H NMR (300 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butoxy)benzoic acid (8)
Figure S49b: $^1$H NMR (600 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butyloxy)benzoic acid (8)
Figure S50a: $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butoxy)benzoic acid (8)
Figure S50b: $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butyloxy)benzoic acid (8)
Figure S51a: $^1$H,H COSY (600 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butynoxy) benzoic acid (8)
Figure S51b: $^1$H,H COSY (600 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butoxy) benzoic acid (8)
Figure S52a: HMQC (600 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butyloxy) benzoic acid (8)
Figure S52b: HMQC (600 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butynoxy) benzoic acid (8)
Figure S53: HSQC (600 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butoxy) benzoic acid (8)
Figure S54: HMBC (600 MHz, CD$_3$OD) spectrum of 4-(2-hydroxy-3-butoxy) benzoic acid (8)
Figure S55: (+)-ESI-MS spectrum of spectrum of cyclopenol (9)
Figure S56: (-)-ESI-MS spectrum of spectrum of cyclopenol (9)
Figure S57: (+)-HRESI-MS spectrum of spectrum of cyclopentenol (9)
**Figure S58:** (-)-HRESI-MS spectrum of cyclopenol (9)
Figure S59: $^1$H NMR (300 MHz, DMSO-d$_6$) spectrum of cyclopenol (9)
Figure S60a: $^1$HNMR (600 MHz, DMSO-$d_6$) spectrum of cyclopenol (9)
Figure S60b: $^1$HNMR (600 MHz, DMSO-d$_6$) spectrum of cyclopenol (9)
Figure S61a: $^{13}$C NMR (125 MHz, DMSO-d$_6$) spectrum of cyclopenol (9)
Figure S61b: $^{13}$C NMR (125 MHz, DMSO-d$_6$) spectrum of cyclopenol (9)
Figure S62: APT NMR (125 MHz, DMSO-d₆) spectrum of cyclopenol (9)
Figure S63a: H,H COSY (600 MHz, DMSO-d$_6$) spectrum of cyclopenol (9)
Figure S63b: H,H COSY (600 MHz, DMSO-d$_6$) spectrum of cyclopenol (9)
Figure S64a: HMQC (600 MHz, DMSO-d$_6$) spectrum of cyclopenol (9)
Figure S64b: HMQC (600 MHz, DMSO-d$_6$) spectrum of cyclopenol (9)
Figure S65: HSQC (600 MHz, DMSO-\textit{d}_6) spectrum of cyclopenol (9)
Figure S66a: HMBC (600 MHz, CDCl₃) spectrum of cyclopenol (9)
Figure S66b: HMBC (600 MHz, CDCl3) spectrum of cyclofenol (9)
Figure S67a: NOESY (600 MHz, CDCl$_3$) spectrum of cyclopenol (9)
Figure S67b: NOESY (600 MHz, CDCl₃) spectrum of cyclopenol (9)
Figure S68: (+)-ESI-MS spectrum of Aspermytin A (10)
Figure S69: (−)-ESI-MS spectrum of Aspermytin A (10)
Figure S70: (-)-HRESI-MS spectrum of Aspermycin A (10)
Figure S71: $^1$H NMR (300 MHz, CDCl$_3$) spectrum of Aspermytin A (10)
Figure S72: $^{13}$C NMR (300 MHz, CDCl$_3$) spectrum of Aspermytin A (10)
Figure S73: $^1$H-$^1$H COSY (500 MHz, CDCl$_3$) spectrum of Aspermytin A (10)
Figure S74: HMQC (500 MHz, CDCl$_3$) spectrum of Aspermytin A (10)
Figure S75: HMBC (500 MHz, CDCl₃) spectrum of Aspermytin A (10)
Figure S76: NOESY (500 MHz, CDCl$_3$) spectrum of Aspermytin A (10)
Figure S7a: (+)-ESI-MS spectrum of Aurantiomide A (11)
Figure S7b: (+)-ESI-MS spectrum of Aurantiomide A (11)
Figure S78a: (+)-HRESI-MS spectrum of Aurantiomide A (11)
Figure S78b: (+)-HRESI-MS spectrum of Aurantiomide A (11)
Figure S79: $^1$H NMR (300 MHz, CD$_3$OD) spectrum of Aurantimide A (11)
Figure S80a: $^1$H NMR (300 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S80b: $^1$H NMR (600 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)

Figure S81a: $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S81b: $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S82a: $^{13}$C NMR (600 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S82b: $^{13}$C NMR (600 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S83a: HMQC (600 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S83b: HMQC (600 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S84: HSQC (600 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S85a: HMBC (600 MHz, CD$_2$OD) spectrum of Aurantiomide A (11)
Figure S85b: HMBC (600 MHz, CD$_3$OD) spectrum of Aurantiomide A (11)
Figure S86a: NOESY (600 MHz, CDCl₃) spectrum of Aurantiomide A (11)
Figure S86b: NOESY (600 MHz, CDCl₃) spectrum of Aurantiomide A (11)