Supplementary Data

N-(Isobutyl)-3,4-methylenedioxy Cinnamoyl Amide

Aboagye Kwarteng Dofuor 1,2, Samuel Kwain 3, Enoch Osei 3, Gilbert Mawuli Tetevi 3, Laud Kenneth Okine 1,2, Mitsuko Ohashi 4, Theresa Manful Gwira 1,2,* and Kwaku Kyeremeh 3,*

1 West African Center for Cell Biology of Infectious Pathogens, University of Ghana, P.O. Box LG 54 Legon-Accra, Ghana; akdofuor@st.ug.edu.gh (A.K.D.); lnokine@ug.edu.gh (L.K.O.)
2 Department of Biochemistry, Cell and Molecular Biology, University of Ghana, P.O. Box LG 54, Legon-Accra, Ghana
3 Marine and Plant Research Laboratory of Ghana, Department of Chemistry, School of Physical and Mathematical Sciences, University of Ghana, P.O. Box LG 56, Legon-Accra, Ghana; kwainsamuel75@gmail.com (S.K.); kofiosei0591@gmail.com (E.O.); gilberttet@gmail.com (G.M.T.);
4 Department of Parasitology, Noguchi Memorial Institute for Medical Research, University of Ghana, P.O. Box LG 581, Legon-Accra, Ghana; mikkvip@tmd.ac.jp
* Correspondence: tmanful@ug.edu.gh (T.M.G.); kkyeremeh@ug.edu.gh (K.K.); Tel.: +233-204752176 (T.M.G.); +233-504829778 (K.K.)
Table of Contents

Figure S1. High resolution mass spectrometry ion chromatogram for FD fraction of Zanthoxylum zanthoxyloides. ......................................................................................................................... 3

Figure S2. Mass spectrometry fragmentation ions for Armatamide................................................................................. 4

Figure S3. Proposed mass spectrometry fragmentation structures for Armatamide. ................................................. 5

Figure S5. Mass spectrometry fragmentation ions for tortozanthoxylamide. ................................................................. 7

Figure S6. Proposed mass spectrometry fragmentation structures for tortozanthoxylamide. ......8

Figure S7. Mass spectrometry fragmentation ions for lanyuamide I-III analogue. .............................................. 9

Figure S8. Proposed mass spectrometry fragmentation structures for lanyuamide I-III analogue. ................................................................. 10

Figure S9. $^1$C-NMR spectrum of tortozanthoxylamide (1) in CDCl$_3$.................................................................11

Figure S10. $^1$H-NMR spectrum of tortozanthoxylamide (1) in CDCl$_3$. .................................................................12

Figure S11. HSQC spectrum of tortozanthoxylamide (1) in CDCl$_3$. .................................................................13

Figure S12. COSY spectrum of tortozanthoxylamide (1) in CDCl$_3$. .................................................................14

Figure S13. HMBC spectrum of tortozanthoxylamide (1) in CDCl$_3$. .................................................................15

Figure S14. TOCSY spectrum of tortozanthoxylamide (1) in CDCl$_3$. .................................................................16

Figure S15. T-ROESY spectrum of tortozanthoxylamide (1) in CDCl$_3$. .................................................................17

Figure S16. Flow chart of the modified Kupchan solvent partitioning process. .........................................................18

Table S1. Mean percentage cell count at cell cycle phases of T. brucei subsp. brucei. ........................................ 19

Table S2. Effects of FD fractions on cell viability of T. brucei subsp. brucei................................................................. 19
Figure S1. High resolution mass spectrometry ion chromatogram for FD fraction of *Zanthoxylum zanthoxyloides*.
**Figure S2.** Mass spectrometry fragmentation ions for Armamide.
Figure S3. Proposed mass spectrometry fragmentation structures for Armatamide.
Figure S4. High resolution mass spectrometry ion chromatogram for tortozanthoxylamide (1).
Figure S5. Mass spectrometry fragmentation ions for tortozanthoxylamide.
Figure S6. Proposed mass spectrometry fragmentation structures for tortozanthoxylamide.

\[
\begin{align*}
\text{2-methylpropan-1-amine} & \quad \text{C}_{14}\text{H}_{18}\text{NO}_{3}^{+} \\
248.1281 & \quad \text{C}_{10}\text{H}_{7}\text{O}_{3}^{+} \\
175.0390 & \quad \text{C}_{9}\text{H}_{9}\text{O}_{2}^{+} \\
149.0597 & \quad \text{C}_{9}\text{H}_{7}\text{NO}^{+} \\
145.0522 & 
\end{align*}
\]
Figure S7. Mass spectrometry fragmentation ions for lanyuamide I-III analogue.
Figure S8. Proposed mass spectrometry fragmentation structures for lanyuamide I-III analogue.
Figure S9. $^{13}$C-NMR spectrum of tortozanthoxylamide (1) in CDCl$_3$. 
Figure S10. $^1$H-NMR spectrum of tortozanthoxylamide (I) in CDCl₃.
Figure S11. HSQC spectrum of tortozanthoxylamide (1) in CDCl₃.
Figure S12. COSY spectrum of tortozanthoxylamide (1) in CDCl₃.
Figure S13. HMBC spectrum of tortozanthoxylamide (1) in CDCl₃.
Figure S14. TOCSY spectrum of tortozanthoxylamide (1) in CDCl₃.
Figure S15. T-ROESY spectrum of tortozanthoxylamide (1) in CDCl₃.
Figure S16. Flow chart of the modified Kupchan solvent partitioning process.
**Table S1.** Mean percentage cell count at cell cycle phases of *T. brucei* subsp. *brucei*.

<table>
<thead>
<tr>
<th>COMPOUNDS</th>
<th>COMPOUNDS</th>
<th>COMPOUNDS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PERCENTAGE CELL COUNT (MEAN ± SEM)</td>
<td>PERCENTAGE CELL COUNT (MEAN ± SEM)</td>
</tr>
<tr>
<td></td>
<td>G0/G1 Phase</td>
<td>S Phase</td>
</tr>
<tr>
<td>Negative control</td>
<td>62.2 ± 0.7</td>
<td>13.1 ± 0.2</td>
</tr>
<tr>
<td>Tortozanthoxylamide</td>
<td>56.2 ± 0.9</td>
<td>19.4 ± 0.9</td>
</tr>
</tbody>
</table>

**Table S2.** Effects of FD fractions on cell viability of *T. brucei* subsp. *brucei*.

<table>
<thead>
<tr>
<th>FD, Subsequent fractions, and Standard</th>
<th>MEAN IC50 ± SE (µg/ml)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FD</td>
<td>7.9 ± 0.1</td>
</tr>
<tr>
<td>C1</td>
<td>11.2 ± 0.7</td>
</tr>
<tr>
<td>C2</td>
<td>13.4 ± 0.5</td>
</tr>
<tr>
<td>C3</td>
<td>9 ± 1</td>
</tr>
<tr>
<td>C4</td>
<td>2.0 ± 0.2</td>
</tr>
<tr>
<td>C5</td>
<td>6 ± 1</td>
</tr>
<tr>
<td>C6</td>
<td>10 ± 1</td>
</tr>
<tr>
<td>C7</td>
<td>17 ± 3</td>
</tr>
<tr>
<td>C8</td>
<td>8.9 ± 0.7</td>
</tr>
<tr>
<td>C9</td>
<td>19 ± 2</td>
</tr>
<tr>
<td>C10</td>
<td>28 ± 1</td>
</tr>
<tr>
<td>C11</td>
<td>54 ± 8</td>
</tr>
<tr>
<td>DA</td>
<td>0.53 ± 0.04</td>
</tr>
</tbody>
</table>

Mean IC<sub>50</sub> and standard errors (SE) were calculated from three different experiments. DA=Diminazene aceturate was used as a positive control.