# Supplementary Material

# Antikinetoplastid activity of sesquiterpenes isolated from the zoanthid *Palythoa aff. clavata*

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## Table of Contents

**Figure S1.** Overlays of the detection of chromatin condensation by Vybrant® Apoptosis Assay Kit n°5, Hoechst 33342/Propidium Iodide, changes on the plasmatic membrane permeability by SYTOX® Green staining, and reactive oxygen species by CellROX® Deep Red Reagent in *Leishmania amazonensis*.

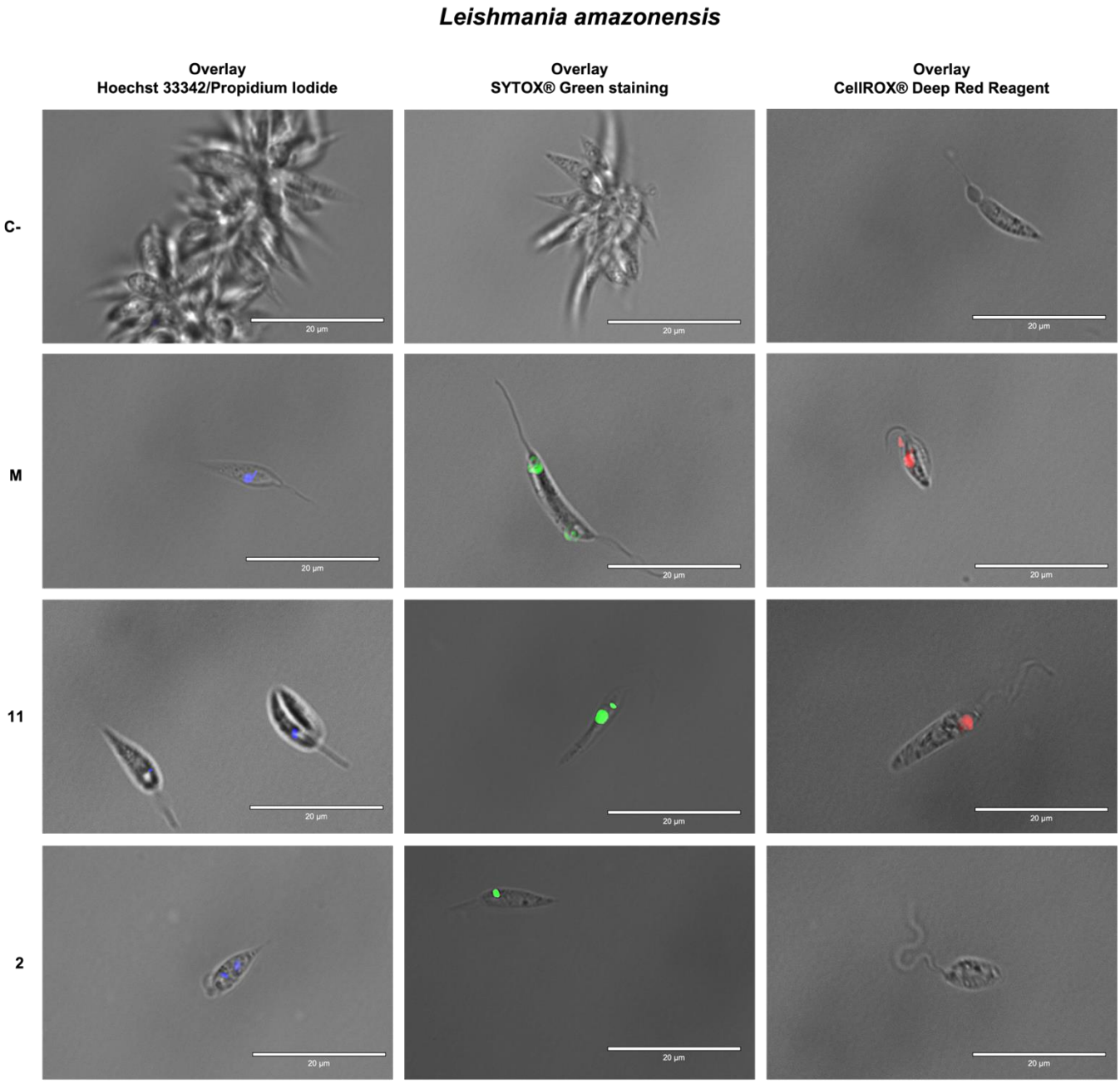


**Figure S2.** Overlays of the detection of chromatin condensation by Vybrant® Apoptosis Assay Kit n°5, Hoechst 33342/Propidium Iodide, changes on the plasmatic membrane permeability by SYTOX® Green staining, and reactive oxygen species by CellROX® Deep Red Reagent in *Leishmania donovani.*

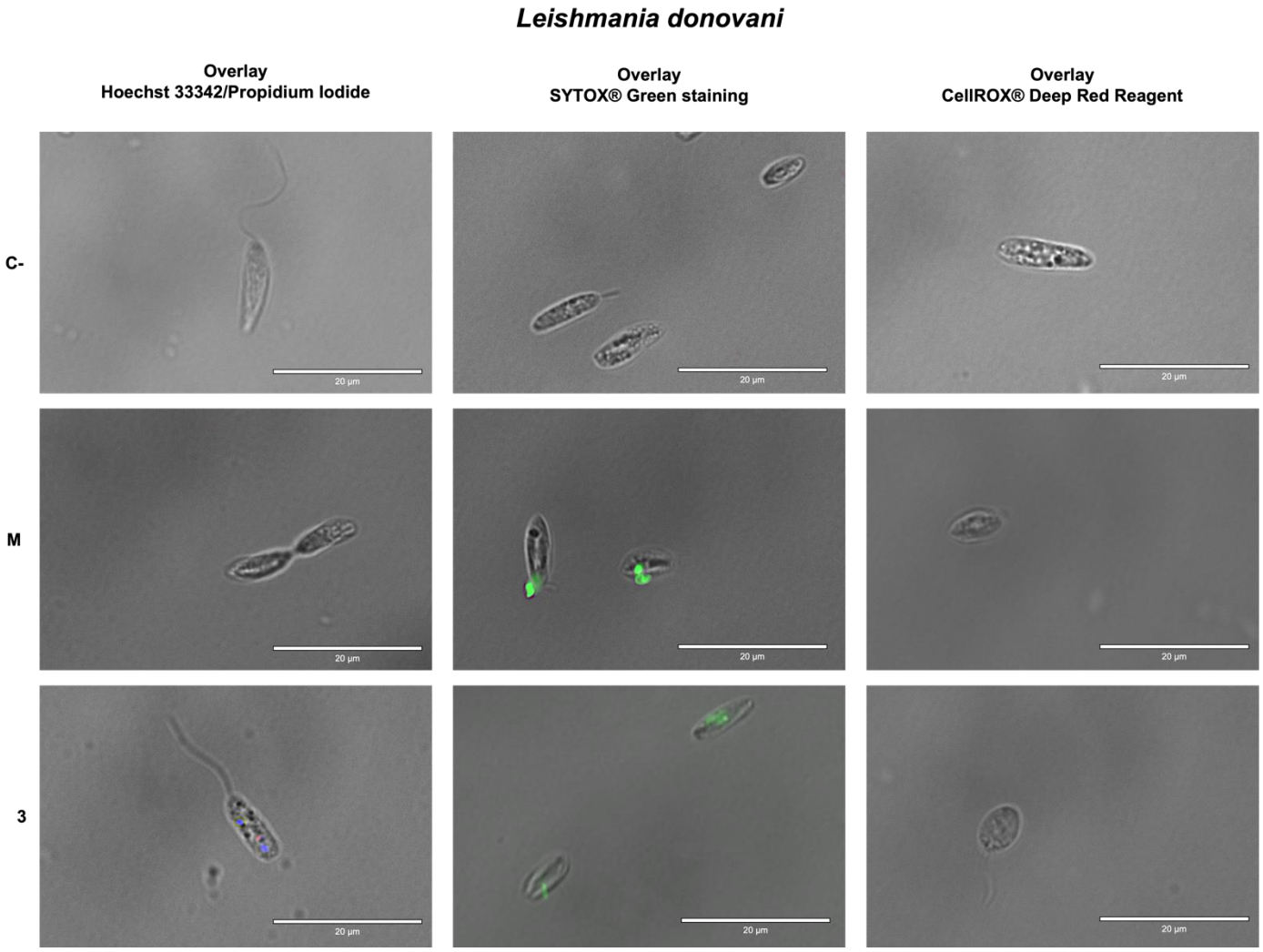


**Figure S3.** Overlays of the detection of chromatin condensation by Vybrant® Apoptosis Assay Kit n°5, Hoechst 33342/Propidium Iodide, changes on the plasmatic membrane permeability by SYTOX® Green staining, and reactive oxygen species by CellROX® Deep Red Reagent in *T. cruzi*.

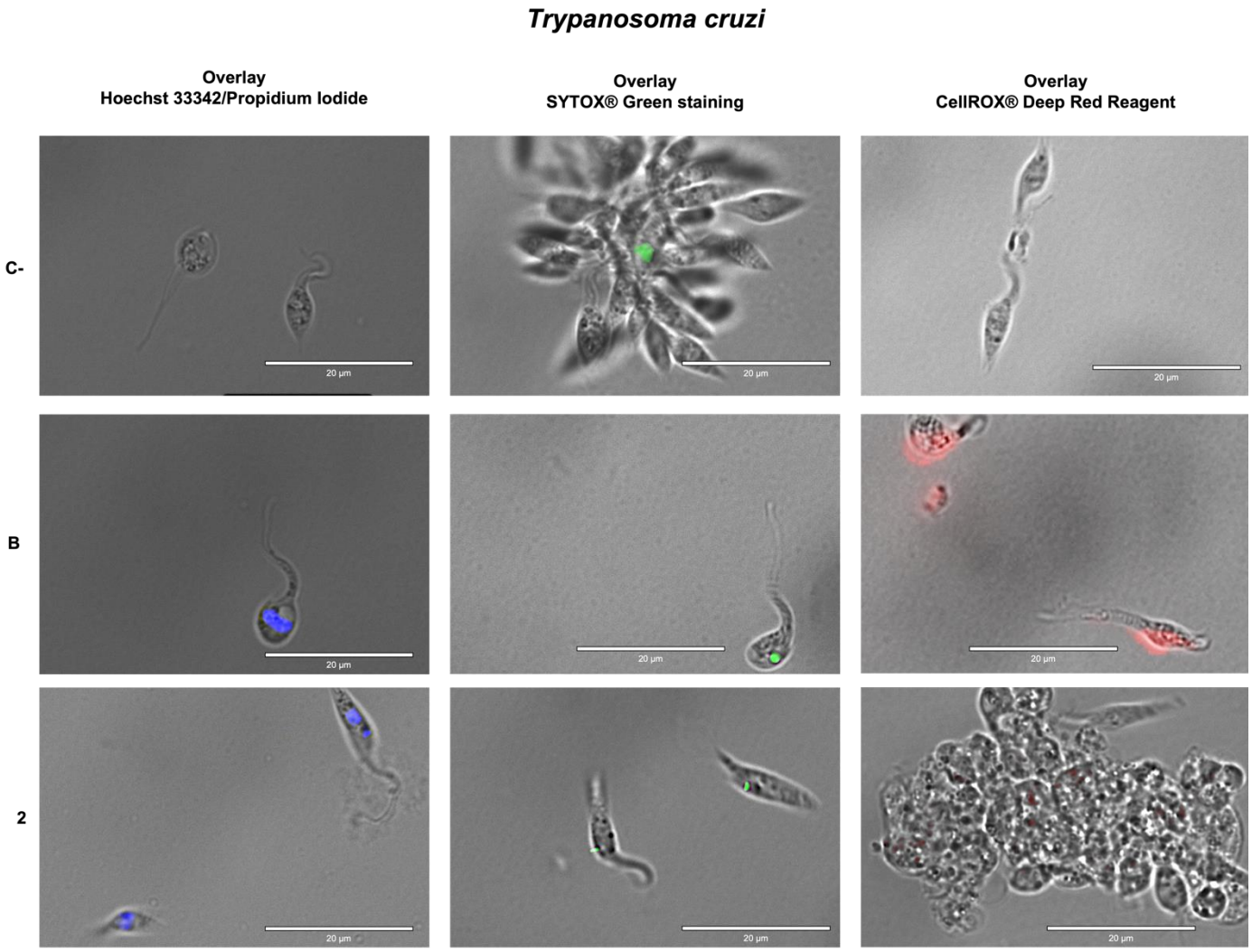
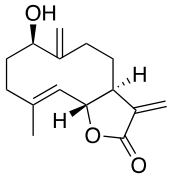
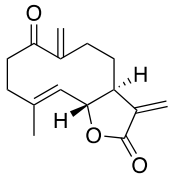


**Table S1.** Physical and spectroscopic data of compounds **1** and **2** [NMR: $CDCl_3$, 500 MHz, 298K]




Artemorin (**1**)



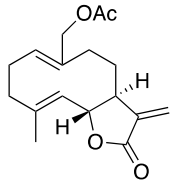

Anhydroartemorin (**2**)

| nº C | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) |
|---|---|---|---|---|---|---|---|---|
| **1** | 78.3 | 3.97 | m | - | 204.9 | - | - | - |
| **2** | 32.2 | 1.95 – 1.98 | m | - | 35.3 | 2.54 | m | - |
| | | 2.15 – 2.20 | m | | | 3.16 | m | - |
| **3** | 36.1 | 1.95 – 1.98 | m | - | 38.3 | 2.36 | ddd | 2.9, 8.7, 9.3 |
| | | 2.15 – 2.20 | m | | | 2.54 | m | - |
| **4** | 141.1 | - | - | - | 143.0 | - | - | - |
| **5** | 122.8 | 5.22 | d | 14.2 | 125.3 | 5.09 | d | 10.0 |
| **6** | 80.3 | 4.40 | m | - | 81.2 | 4.33 | dd | 9.7, 10.0 |
| **7** | 43.3 | 2.81 | m | - | 49.9 | 2.54 | m | - |
| **8** | 25.6 | 2.30 (2H) | m | - | 28.1 | 2.54 (2H) | m | - |
| **9** | 31.1 | 1.62 | m | | 29.1 | 1.42 | m | - |
| | | 2.30 | m | - | | 2.24 | m | - |
| **10** | 157.9 | - | - | - | 142.4 | - | - | - |
| **11** | 145.9 | - | - | - | 136.6 | - | - | - |
| **12** | 165.0 | - | - | - | 169.5 | - | - | - |
| **13** | 118.1 | 5.45 | d | 3.5 | 119.2 | 5.48 | d | 3.5 |
| | | 6.17 | d | 3.2 | | 6.22 | d | 3.5 |
| **14** | 110.7 | 4.87 | s | - | 123.8 | 5.66 | s | - |
| | | 5.21 | s | - | | 5.82 | s | - |
| **15** | 17.8 | 1.72 | s | - | 17.1 | 1.76 | s | - |

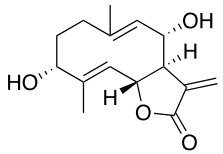
**$[\alpha]^{25}_D$** +70.0 (*c* 0.08, $CHCl_3$)
**IR $\nu_{max}$:** 3340, 2918, 2849, 1758, 1667 and 1446 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{20}O_3Na$ $[M+Na]^+$; *m/z* 271.1307 (Calcd. 271.1310)

**$[\alpha]^{25}_D$** +60.0 (*c* 0.02, $CHCl_3$)
**IR $\nu_{max}$:** 2924, 2852, 1765,1712, 1668 and 1454 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{18}O_4Na$ $[M+Na]^+$; *m/z* 269.1198 (Calcd. 269.1154)

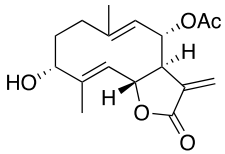
**Table S2.** Physical and spectroscopic data of compounds **3-5** [NMR: $CDCl_3$, 500 MHz, 298K]




*cis,trans*-Costunolide-14-acetate (**3**)




Tatridin A (**4**)




Tatridin A acetate (**5**)

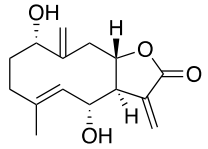
| nº C | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **1** | 97.6 | 6.00 | d | 9.2 | 35.2 | (α) 2.30 | dd | 6.1, 11.6 | 35.3 | (α) 2.30 | dd | 6.7, 12.3 |
| | | | | | | (β) 1.93 | dd | 6.1, 11.6 | | (β) 1.91 | m | - |
| **2** | 31.2 | 1.79 | m | - | 27.2 | (α) 1.74 | m | - | 27.3 | (α) 1.76 | dd | 6.7, 12.1 |
| | | 2.15 | m | - | | (β) 2.00 | dd | 6.2, 12.0 | | (β) 2.03 | dd | 6.7, 12.1 |
| **3** | 37.2 | 2.31 (2H) | m | - | 66.7 | 4.39 | m | - | 66.9 | 4.40 | m | - |
| **4** | 140.7 | - | - | - | 142.2 | - | - | - | 142.9 | - | - | - |
| **5** | 123.2 | 5.18 | d | 9.5 | 126.8 | 5.33 | d | 10.2 | 126.4 | 5.33 | d | 9.7 |
| **6** | 79.3 | 4.66 | dd | 9.5, 9.5 | 74.0 | 4.54 | dd | 9.4, 10.2 | 74.1 | 4.62 | dd | 9.4, 9.7 |
| **7** | 43.9 | 2.76 | dddd | 3.2, 5.8, 5.9, 9.5 | 52.3 | 2.80 | ddd | 3.1, 9.4, 10.3 | 49.2 | 3.03 | dd | 9.4, 9.9 |
| **8** | 25.4 | 1.69 | m | - | 71.1 | 4.47 | dd | 3.4, 10.3 | 73.1 | 5.39 | dd | 9.9, 10.6 |
| | | 1.95 | m | - | | | | | | | | |
| **9** | 31.6 | 2.14 | m | - | 129.9 | 4.99 | d | 10.3 | 126.0 | 4.87 | d | 10.6 |
| | | 2.31 | m | - | | | | | | | | |
| **10** | 157.9 | - | - | - | 135.2 | - | - | - | 137.9 | - | - | - |
| **11** | 135.3 | - | - | - | 135.9 | - | - | - | 136.9 | - | - | - |
| **12** | 170.1 | - | - | - | 169.3 | - | - | - | 169.1 | - | - | - |
| **13** | 118.9 | 5.46 | d | 3.2 | 123.6 | 6.21 | d | 3.1 | 122.9 | 5.75 | d | 3.3 |
| | | 6.19 | d | 3.2 | | 6.31 | d | 3.1 | | 6.29 | d | 3.3 |
| **14** | 87.1 | 4.09 | d | 3.0 | 15.6 | 1.78 | s | - | 15.6 | 1.90 | s | - |
| | | 4.20 | d | 3.0 | | | | | | | | |
| **15** | 16.6 | 1.83 | s | - | 16.7 | 1.83 | s | - | 16.7 | 1.83 | s | - |
| | 169.6 (C=O) | - | - | - | - | 1.47 (OH) | d | 3.0 | 169.8 (C=O) | - | - | - |
| | 21.1 (Me-O-) | 2.09 | s | - | - | 1.65 (OH) | d | 3.4 | 21.0 (Me-O-) | 2.09 | s | - |

**$[\alpha]^{25}_D$** +38.3 (*c* 0.06, $CHCl_3$)
**IR $\nu_{max}$:** 2925, 2852, 2360, 1766, 1667 and 1445 $cm^{-1}$
**ESI-HRMS:** $C_{17}H_{22}O_5Na$ $[M+Na]^+$; *m/z* 329.1357 (Calcd. 329.1365)

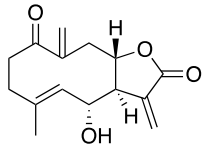
**$[\alpha]^{25}_D$** -33.3 (*c* 0.03, $CHCl_3$)
**IR $\nu_{max}$:** 3363, 2918, 2849, 2360, 1759 and 1666 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{20}O_4Na$ $[M+Na]^+$; *m/z* 287.1259 (Calcd. 287.1259)

**$[\alpha]^{25}_D$** -+26.7 (*c* 0.06, $CHCl_3$)
**IR $\nu_{max}$:** 3374, 2918, 2850, 1771, 1667and 1438 $cm^{-1}$
**ESI-HRMS:** $C_{17}H_{22}O_5Na$ $[M+Na]^+$; *m/z* 329.1368 (Calcd. 329.1365)

**Table S3.** Physical and spectroscopic data of compounds **6** and **7** [NMR: $CDCl_3$, 500 MHz, 298K]



Tanachin (**6**)



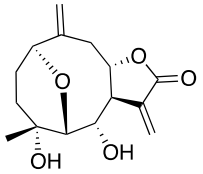
Tamirin (**7**)

| nº C | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) |
|---|---|---|---|---|---|---|---|---|
| **1** | 70.4 | 3.84 | m | - | 203.0 | - | - | - |
| **2** | 31.2 | (α) 2.17 | m | - | 36.5 | 2.55 | m | - |
| | | (β) 2.05 | ddd | 3.8, 8.8, 8.8 | | 3.28 | ddd | 5.4, 5.4, 8.6 |
| **3** | 34.4 | (α) 2.11 | m | - | 35.9 | 2.41 | ddd | 5.4, 5.6, 8.6 |
| | | (β) 2.26 | ddd | 3.3, 5.5, 8.8 | | 2.55 | m | - |
| **4** | 136.0 | - | - | - | 136.8 | - | - | - |
| **5** | 131.6 | 5.05 | d | 10.0 | 131.9 | 5.08 | d | 10.3 |
| **6** | 71.5 | 4.28 | ddd | 3.3, 10.0, 10.0 | 70.1 | 4.16 | ddd | 3.0, 10.3, 10.3 |
| **7** | 51.9 | 2.83 | ddd | 3.0, 6.5, 10.0 | 50.2 | 2.74 | ddd | 2.0, 9.7, 10.3 |
| **8** | 79.0 | 3.97 | m | - | 76.5 | 3.96 | m | - |
| **9** | 42.0 | (α) 2.39 | dd | 10.3, 14.0 | 40.1 | (α) 2.15 | dd | 11.7, 11,7 |
| | | (β) 2.96 | d | 14.0 | | (β) 3.42 | d | 11,7 |
| **10** | 146.7 | - | - | - | 146.3 | - | - | - |
| **11** | 137.1 | - | - | - | 135.6 | - | - | - |
| **12** | 170.0 | - | - | - | 169.6 | - | - | - |
| **13** | 125.7 | 6.20 | d | 3.0 | 126.2 | 6.17 | d | 2.0 |
| | | 6.37 | d | 3.0 | | 6.38 | d | 2.0 |
| **14** | 115.2 | 5.12 | sa | - | 125.2 | 5.79 | d | 1.8 |
| | | 5.17 | sa | - | | 5.83 | sa | - |
| **15** | 17.7 | 1.71 | s | - | 17.3 | 1.66 | s | - |
| | - | 1.73 (OH) | d | 3.3 | | | | |

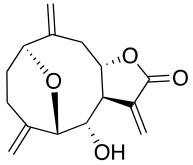
**$[\alpha]^{25}_D$** +0.8 (*c* 0.07, $CHCl_3$)
**IR $\nu_{max}$:** 3390, 2925, 2855, 1756, 1659 and 1446 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{20}O_4Na$ $[M+Na]^+$; *m/z* 287.1253 (Calcd. 287.1259)

**$[\alpha]^{25}_D$** -23.3 (*c* 0.06, $CHCl_3$)
**IR $\nu_{max}$:** 3444, 2922, 2851, 1758, 1672 and 1443$cm^{-1}$
**ESI-HRMS:** $C_{15}H_{18}O_4Na$ $[M+Na]^+$; *m/z* 285.1104 (Calcd. 285.1103)

**Table S4.** Physical and spectroscopic data of compounds **8** and **9** [NMR: $CDCl_3$, 500 MHz, 298K]



Isobadgerin (**8**)



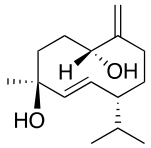
Dehydroxyisobadgerin (**9**)

| nº C | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) |
|---|---|---|---|---|---|---|---|---|
| **1** | 77.8 | 4.44 | m | - | 75.4 | 4.46 | dd | 5.1, 5.7 |
| **2** | 24.4 | (α) 1.67 | m | - | 26.9 | (α) 1.78 | dddd | 2.6, 5.0, 5.3, 15.7 |
| | | (β) 2.05 | m | - | | (β) 2.26 | dddd | 2.6, 5.1, 5.7, 15.7 |
| **3** | 38.0 | (α) 1.67 | m | - | 28.1 | (α) 2.46 | m | |
| | | (β) 2.05 | m | - | | (β) 2.35 | ddd | 5.0, 5.3, 15.7 |
| **4** | 70.8 | - | - | - | 144.2 | | | |
| **5** | 77.8 | 2.86 | sa | 2.2 | 73.0 | 3.49 | sa | - |
| **6** | 72.3 | 4.22 | dd | 8.4, 10.3 | 72.3 | 4.20 | ddd | 2.3, 6.8, 7.9 |
| **7** | 54.8 | 3.21 | ddd | 3.5, 9.5, 10.3 | 53.6 | 3.32 | ddd | 3.5, 7.9, 10.4 |
| **8** | 81.8 | 4.10 | dd | 9.5, 12.4 | 81.6 | 4.06 | dd | 10.4, 10.5 |
| **9** | 42.0 | (α) 2.45 | dd | 10.75, 12.46 | 42.8 | (α) 2.96 | d | 12.7 |
| | | (β) 2.95 | d | 12.45 | | (β) 2.62 | dd | 10.5, 12.7 |
| **10** | 145.1 | - | - | - | 149.9 | - | - | - |
| **11** | 127.8 | - | - | - | 139.2 | - | - | - |
| **12** | 169.0 | - | - | - | 169.2 | - | - | - |
| **13** | 121.0 | 6.02 | d | 3.14 | 121.4 | 6.07 | d | 3.5 |
| | | 6.21 | d | 3.55 | | 6.24 | d | 3.5 |
| **14** | 117.5 | 5.12 | d | 1.70 | 117.6 | 5.13 | d | 2.0 |
| | | 5.35 | sa | - | | 5.38 | sa | - |
| **15** | 21.7 | 1.52 | s | - | 107.1 | 4.95 | sa | - |
| | | | | | | 4.98 | d | 1.9 |
| | | | | | - | 2.03 (OH) | d | 6.8 |

**$[\alpha]^{25}_D$** -12.2 (*c* 0.09, $CHCl_3$)
**IR $\nu_{max}$:** 3362, 2921, 2851, 1766, 1660 and 1455 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{20}O_5Na$ $[M+Na]^+$; *m/z* 303.1209 (Calcd. 303.1208)

**$[\alpha]^{25}_D$** +60.0 (*c* 0.12, $CHCl_3$)
**IR $\nu_{max}$:** 3457, 2918, 2850, 1762, 1661 and 1436 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{18}O_4Na$ $[M+Na]^+$; *m/z* 285.1103 (Calcd. 285.1103)

**Table S5.** Physical and spectroscopic data of (-)-nephtediol (**10**) [NMR: $CDCl_3$, 500 MHz, 298K]

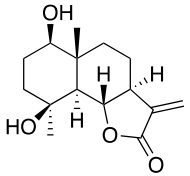



(-) Nephthediol (**10**)

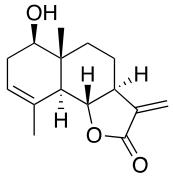
| C nº | $\delta^{13}C$ | $\delta^{1}H$ | mult. | *J* (Hz) |
|---|---|---|---|---|
| **1** | 78.3 | 3.94 | d | 8.7 |
| **2** | 28.3 | 1.62 | m | |
| | | 1.93 | m | |
| **3** | 38.5 | 1.43 | m | |
| | | 1.84 | m | |
| **4** | 72.3 | | | |
| **5** | 137.4 | 5.22 | d | 15.18 |
| **6** | 130.0 | 5.30 | dd | 9.5, 15.25 |
| **7** | 49.7 | 1.87 | m | |
| **8** | 29.5 | 1.55 | m | |
| | | 1.96 | m | |
| **9** | 28.2 | 1.82 | m | |
| | | 2.25 | dd | 12.0, 12.8 |
| **10** | 151.1 | | | |
| **11** | 32.3 | 1.50 | dd | 6.7, 13.5 |
| **12** | 20.5 | 0.84 | d | 6.7 |
| **13** | 20.6 | 0.89 | d | 6.7 |
| **14** | 111.4 | 4.90 | s | |
| | | 5.13 | s | |
| **15** | 23.9 | 1.27 | s | |

**$[\alpha]^{25}_D$** -70.0 (*c* 0.02, $CHCl_3$)
**IR $\nu_{max}$:** 3314, 2927, 2869, 1723, 1670 and 1454 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{26}O_2Na$; $[M+Na]^+$ *m/z* 261.1833 (Calcd. 261.1831)

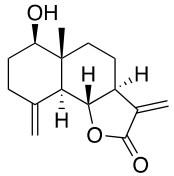
**Table S6.** Physical and spectroscopic data of compounds **11-13** [NMR: $CDCl_3$, 500 MHz, 29




4β−Hydroxyarbusculin A (**11**)




Santamarine (**12**)




Reynosin (**13**)

| nº C | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) | $\delta^{13}$C | $\delta^{1}$H | m | *J* (Hz) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **1** | 78.3 | 3.46 | m | - | 75.0 | 3.68 | ddd | 5.0, 6.0, 10.0 | 78.1 | 3.53 | dd | 4.5, 11.5 |
| **2** | 28.5 | (α) 1.64 | m | - | 32.8 | (α) 1.97 | m | - | 31.2 | (α) 1.85 | m | - |
| | | (β) 1.76 | dd | 5.3, 12.0 | | (β) 2.40 | m | - | | (β) 1.57 | m | - |
| **3** | 38.0 | (α) 1.64 | m | - | 21.2 | 5.35 | d | 2.7 | 33.5 | (α) 2.14 | m | - |
| | | (β) 1.81 | dd | 3.0, 12.0 | | | | | | (β) 2.34 | ddd | 1.0, 5.1, 13.8 |
| **4** | 71.9 | - | - | - | 133.1 | - | - | - | 143.3 | - | - | - |
| **5** | 57.1 | 1.86 | d | 11.5 | 51.2 | 2.35 | d | 11.0 | 52.9 | 2.19 | d | 10.9 |
| **6** | 80.8 | 4.12 | dd | 11.5, 11.5 | 81.2 | 3.95 | dd | 11.0, 11.0 | 79.6 | 4.03 | dd | 10.9, 10.9 |
| **7** | 50.7 | 2.60 | dddd | 3.1, 3.3, 11.5, 11.5 | 51.0 | 2-50 | ddd | 3.2, 11.0, 12.8 | 49.4 | 2.54 | ddd | 3.1, 10.9, 11.2 |
| **8** | 22.0 | (α) 2.02 | ddd | 3.3, 11.5, 13.0 | 21.2 | (α) 2.10 | dddd | 3.9, 3.9, 6.4, 12.9 | 21.4 | (α) 2.09 | m | - |
| | | (β) 1.57 | m | - | | (β) 1.67 | dddd | 3.4, 12.8, 12.8, 12.9 | | (β) 1.60 | m | - |
| **9** | 39.1 | (α) 1.30 | m | - | 34.4 | (α) 1.31 | ddd | 3.9, 12.9, 12.9 | 35.5 | (α) 1.36 | ddd | 3.9, 13.1, 13.1 |
| | | (β) 2.01 | ddd | 3.3, 3.3., 13.0 | | (β) 2.06 | ddd | 4.0, 6.4, 12,9 | | (β) 2.10 | m | - |
| **10** | 42.1 | - | - | - | 40.5 | - | - | - | 42.9 | - | - | - |
| **11** | 138.9 | - | - | - | 138.5 | - | - | - | 139.1 | - | - | - |
| **12** | 171.3 | - | - | - | 170.6 | - | - | - | 170.5 | - | - | - |
| **13** | 118.0 | 5.46 | d | 3.1 | 116.7 | 5.41 | d | 3.2 | 117.0 | 5.42 | d | 3.1 |
| | | 6.13 | d | 3.1 | | 6.08 | d | 3.2 | | 6.09 | d | 3.1 |
| **14** | 13.9 | 0.98 | s | - | 11.0 | 0.88 | s | - | 11.6 | 0.82 | s | - |
| **15** | 24.1 | 1.37 | s | - | 23.2 | 1.84 | s | - | 110.1 | 4.87 | d | 1.0 |
| | | 3.09 (OH) | s | - | | 1.41 (OH) | d | 5.0 | | 4.99 | sa | - |

**$[\alpha]^{25}_D$** +15.0 (*c* 0.10, $CHCl_3$)
**IR $\nu_{max}$:** 3418, 2931, 2871, 1769, 1460 and 1411 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{22}O_4Na$; $[M+Na]^+$ *m/z* 289.1417 (Calcd. 289.1416)

**$[\alpha]^{25}_D$** +68.6 (*c* 0.07, $CHCl_3$)
**IR $\nu_{max}$:** 3347, 2918, 2848, 1762, 1439 and 1412 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{20}O_3Na$; $[M+Na]^+$ *m/z* 271.1315 (Calcd. 271.1310)

**$[\alpha]^{25}_D$** +82.0 (*c* 0.20, $CHCl_3$)
**IR $\nu_{max}$:** 3454, 2928, 2851, 1768, 1460 and 1413 $cm^{-1}$
**ESI-HRMS:** $C_{15}H_{20}O_3Na$; $[M+Na]^+$ *m/z* 271.1308 (calc. 271.1310)