

## Supporting Information

*Rec. Nat. Prod.* 12:2 (2018) 190-194

### Antileishmanial Activity of a New ent-Kaurene Diterpene Glucoside Isolated from Leaves of *Xylopia excellens* R.E.Fr. (Annonaceae)

Danielle C. de Alencar, Felipe M. A. da Silva, Richardson A. de Almeida,  
Emmanoel V. Costa, Lívia M. Dutra, Andersson Barison,  
Helito Volpato, Celso V. Nakamura, Hector H. F. Koolen,  
Afonso Duarte L. de Souza and Maria Lúcia B. Pinheiro\*

<sup>1</sup>Departamento de Química, Universidade Federal do Amazonas, 69077-000, Manaus, AM, Brasil

<sup>2</sup>Centro de RMN, Universidade Federal do Paraná, 81531-990, Curitiba, PR, Brasil

<sup>3</sup>Laboratório de Inovação Tecnológica no Desenvolvimento de Fármacos e Cosméticos, Universidade

Estadual de Maringá, 87020-900, Maringá, PR, Brasil

<sup>4</sup>Metabolomics and Mass Spectrometry Research Group,, Universidade do Estado do Amazonas, 69050-010, Manaus, AM, Brasil

Table of Contents	Page
<b>Table S1.</b> <sup>1</sup> H NMR data for compound <b>1</b> .	<b>2</b>
<b>Figure S1.</b> HR-MS spectrum of compound <b>1</b> .	<b>3</b>
<b>Figure S2.</b> IR spectrum of compound <b>1</b> .	<b>3</b>
<b>Figure S3.</b> <sup>1</sup> H NMR spectrum of compound <b>1</b> in CD <sub>3</sub> OD at 600 MHz.	<b>4</b>
<b>Figure S4.</b> <sup>13</sup> C NMR spectrum of compound <b>1</b> in CD <sub>3</sub> OD at 125 MHz.	<b>4</b>
<b>Figure S5.</b> <sup>1</sup> H- <sup>13</sup> C correlation map from HSQC NMR experiment of compound <b>1</b> in CD <sub>3</sub> OD at 600 and 150 MHz.	<b>5</b>
<b>Figure S6.</b> <sup>1</sup> H- <sup>13</sup> C correlation map from HMBC NMR experiment of compound <b>1</b> in CD <sub>3</sub> OD at 600 and 150 MHz.	<b>5</b>
<b>Figure S7.</b> <sup>1</sup> H NMR spectrum and 1D NOE experiments of compound <b>1</b> in CDCl <sub>3</sub> at 600 MHz.	<b>6</b>

**Table S1.** <sup>1</sup>H NMR data for compound **1**

Position	CDCl <sub>3</sub>	CD <sub>3</sub> OD
	$\delta_{\text{H}}$ mult. ( <i>J</i> in Hz)	$\delta_{\text{H}}$ mult. ( <i>J</i> in Hz)
<b>1</b>	0.82 m	0.80 m
	1.78 m	1.81 m
<b>2</b>	1.63 m	1.40 m
	1.41 m	1.19 m
<b>3</b>	1.20 m	1.68 m
	1.38 m	1.38 m
<b>4</b>	-	-
<b>5</b>	1.51 m	1.60 m
<b>6</b>	1.52 m	1.52 dt (13.0 and 1.8)
	1.99 m	2.10 m
<b>7</b>	3.44 m	3.47 m
<b>8</b>	-	-
<b>9</b>	1.41 m	1.47 m
<b>10</b>	-	-
<b>11</b>	1.52 m	1.58 m
	1.54 m	
<b>12</b>	1.71 m	1.74 d (11.9)
	1.47 m	1.45 m
<b>13</b>	2.67 m	2.62 m
<b>14</b>	1.90 m	1.93 m
	1.16 m	1.16 m
<b>15</b>	2.25 m	2.37 m
	2.26 m	
<b>16</b>	-	-
<b>17</b>	4.77 m	4.74 m
	4.81 m	4.77 m
<b>18</b>	0.85 s	0.87 s
<b>19</b>	0.81 s	0.83 s
<b>20</b>	1.02 s	1.07 s
<b>1'</b>	4.39 d (7.7)	4.28 d (7.7)
<b>2'</b>	3.39 m	3.87 m
<b>3'</b>	3.37 m	3.46 m
<b>4'</b>	3.61 m	3.44 m
<b>5'</b>	3.57 m	3.53 dd (9.7 and 7.7)
<b>6'</b>	3.79 m	3.65 m
	3.86 m	3.72 m

Hector\_16\_pos #1 RT: 0.01 AV: 1 NL: 7.68E6  
T: FTMS + p APCI corona !pi Full ms [100.00-1500.00]

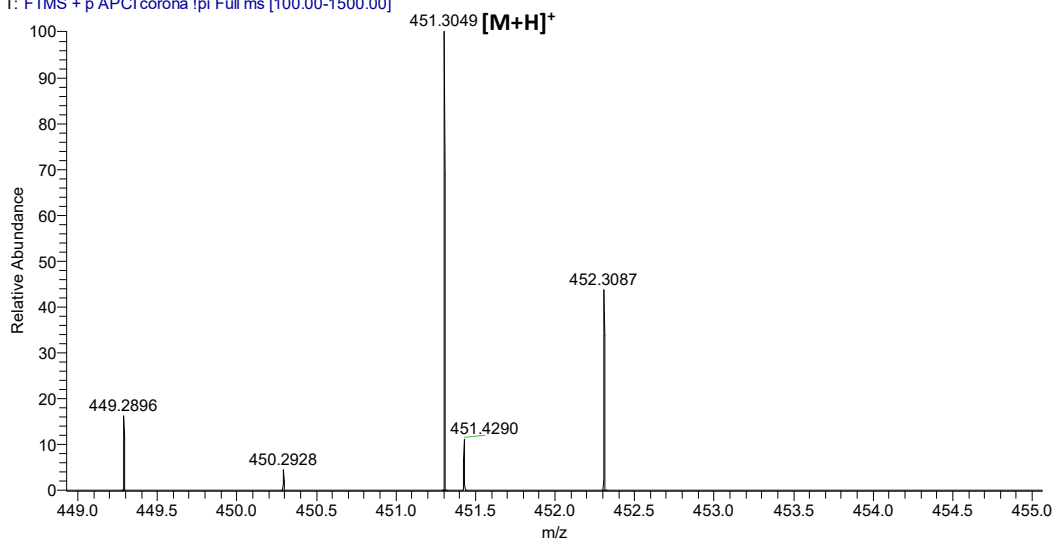


Figure S1. HR-MS spectrum of compound 1.

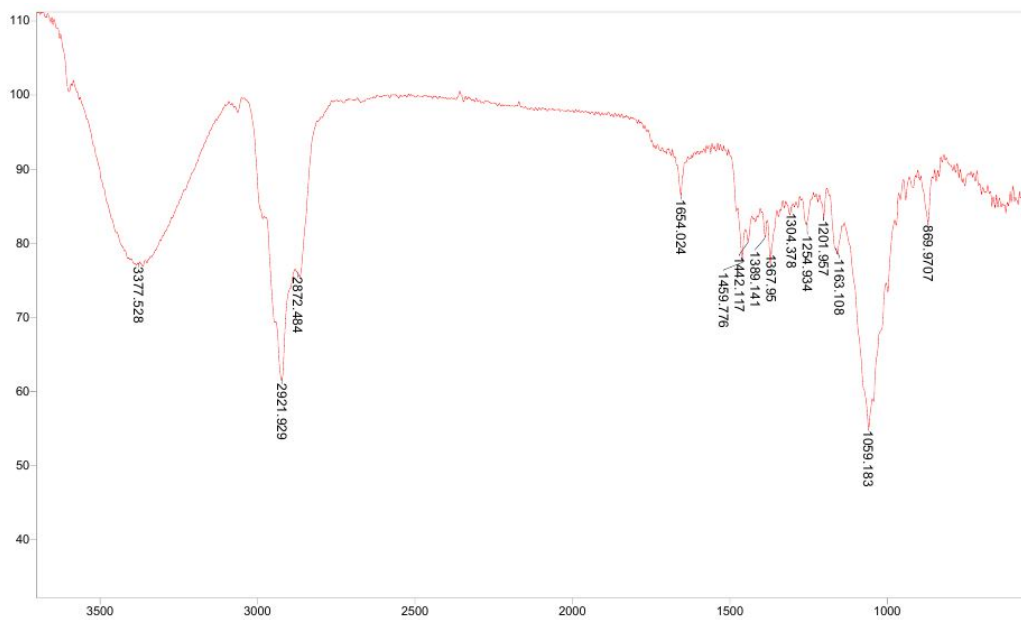


Figure S2. IR spectrum (KBr) of compound 1.

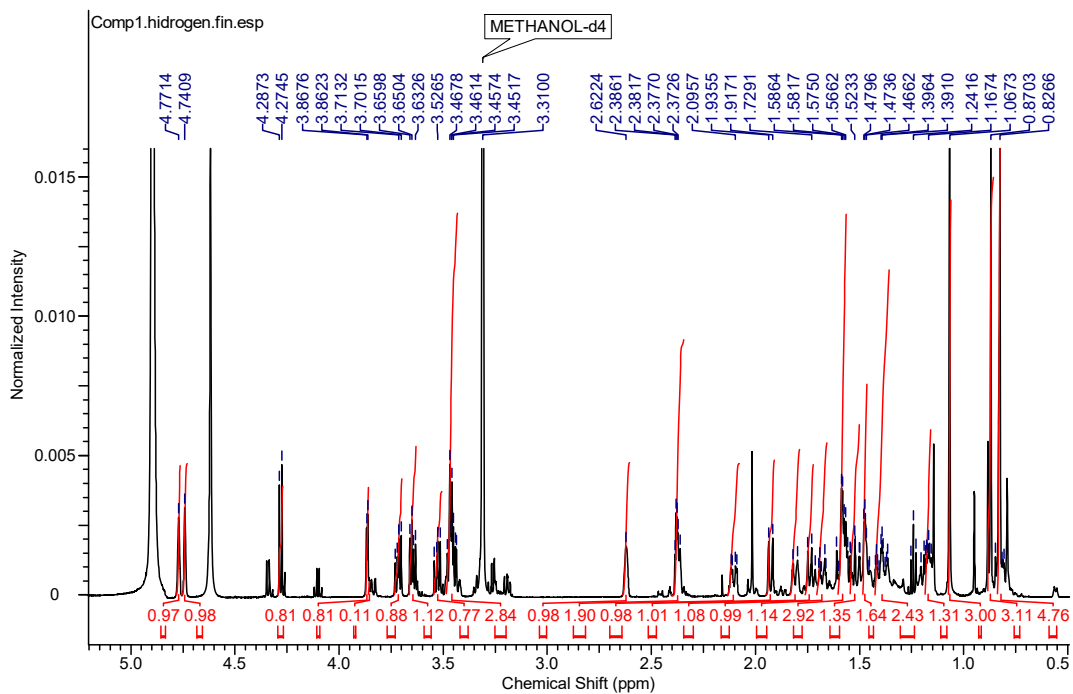


Figure S3.  $^1\text{H}$  NMR spectrum of compound 1 in  $\text{CD}_3\text{OD}$  at 600 MHz.

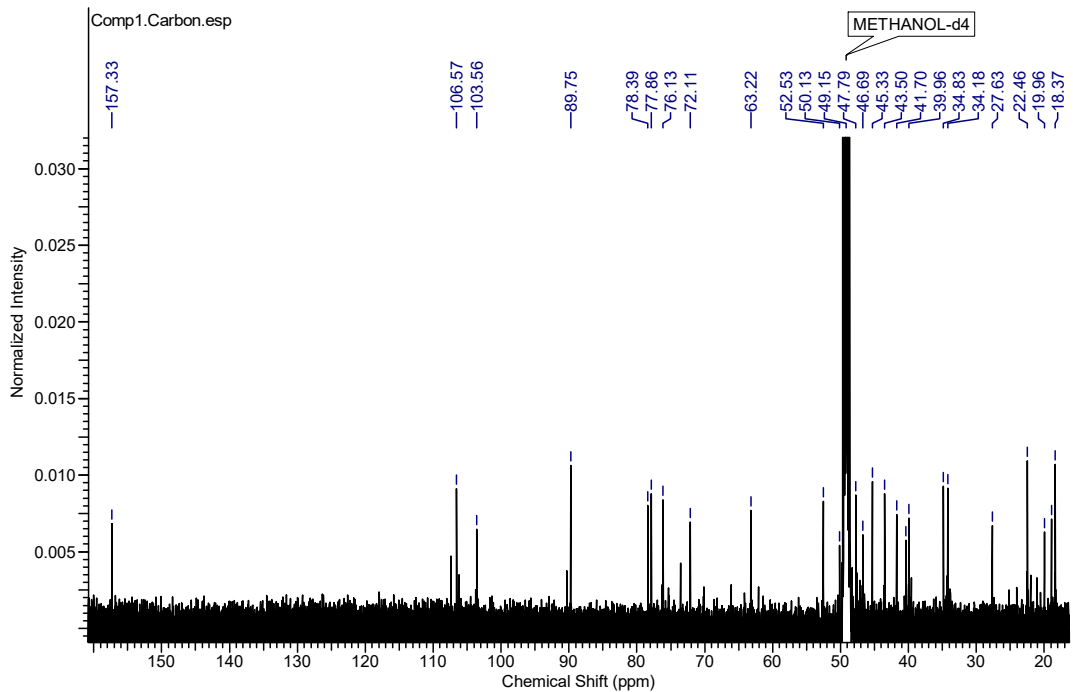
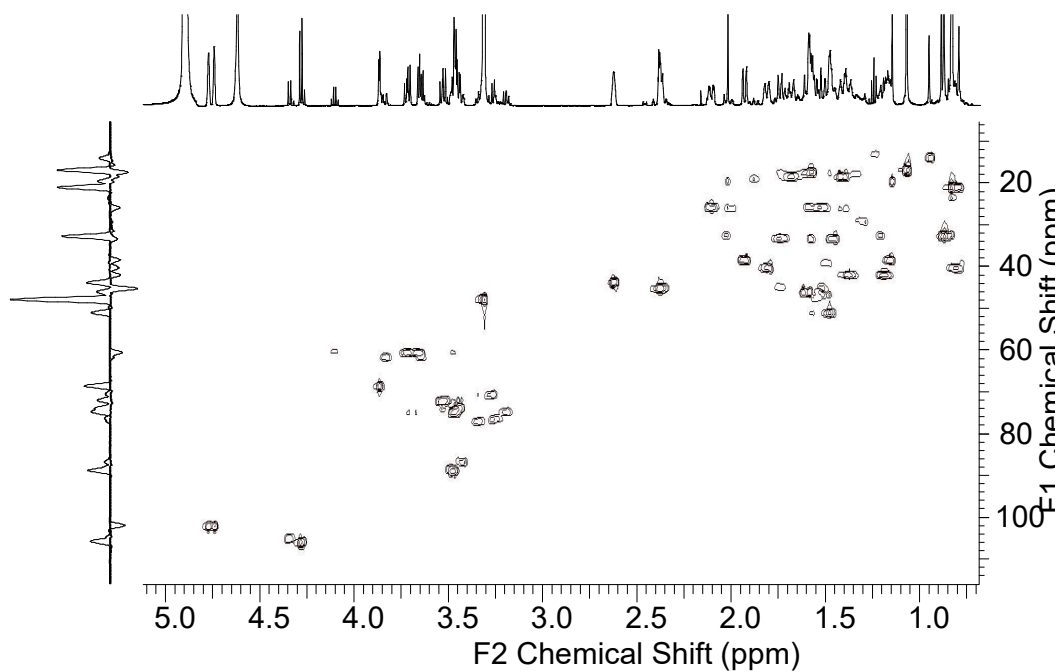
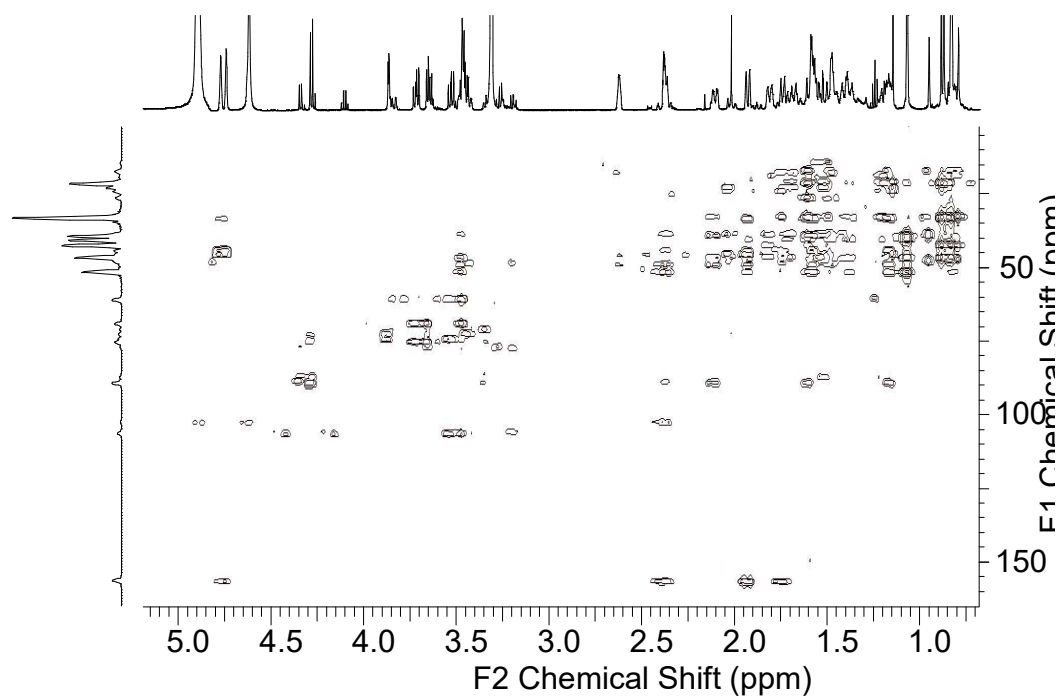


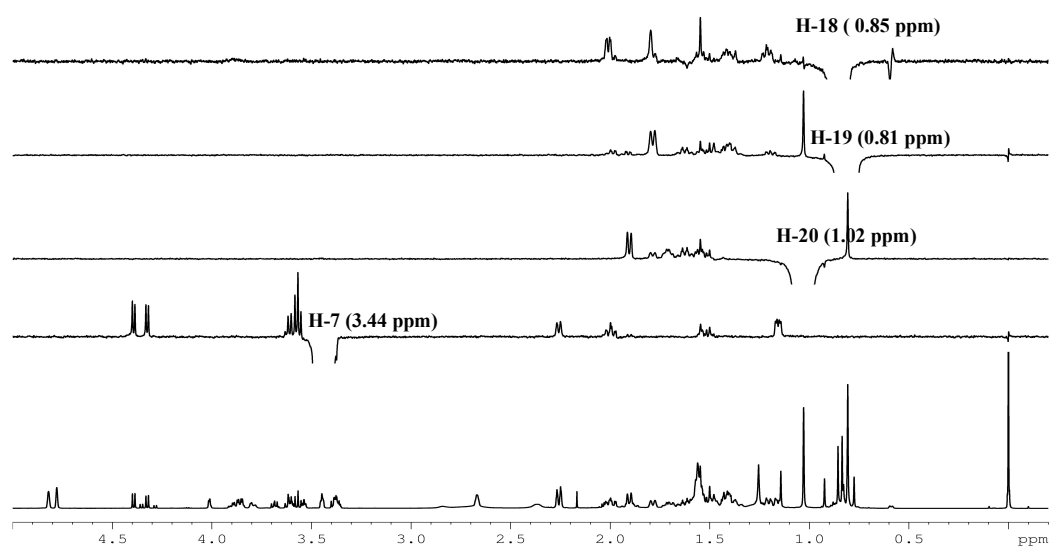
Figure S4.  $^{13}\text{C}$  NMR spectrum of compound 1 in  $\text{CD}_3\text{OD}$  at 125 MHz.



**Figure S5.**  $^1\text{H}$ - $^{13}\text{C}$  correlation map from HSQC NMR experiment of compound **1** in  $\text{CD}_3\text{OD}$  at 600 and 150 MHz.



**Figure S6.**  $^1\text{H}$ - $^{13}\text{C}$  correlation map from HMBC NMR experiment of compound **1** in  $\text{CD}_3\text{OD}$  at 600 and 150 MHz.



**Figure S7.** <sup>1</sup>H NMR spectrum and 1D NOE experiments of compound **1** in CDCl<sub>3</sub> at 600 MHz.