

## A New Benzosesquiterpenoid Dimer from *Polyalthia cheliensis* Hu

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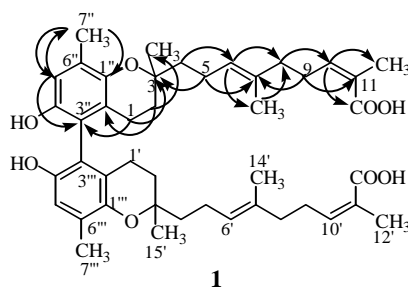
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**Abstract:** A new benzosesquiterpenoid dimer, 3'',3'''-bispolycerasoidol (**1**), along with its monomer, polycerasoidol, were isolated from the dried leaves of *Polyalthia cheliensis* Hu. The structure of **1** was established by spectroscopic methods.

**Keywords:** *Polyalthia cheliensis*, Annonaceae, bispolycerasoidol, benzosesquiterpenoid.

The genus plants *Polyalthia*, being rich in bioactive diterpenoids and alkaloids<sup>1,2</sup>, have been attracting much attention. *Polyalthia cheliensis* Hu is a bush mainly distributed in Xishuangbanna, Yunnan Province of China. The previous researches<sup>1</sup> reported the isolations of four clerodane diterpenes from the stem bark of this plants. Recent phytochemical work on its dried leaves results in the elucidations of a new benzosesquiterpenoid dimer, 3'', 3'''-bispolycerasoidol (**1**) and its monomer, a known benzosesquiterpenoid polycerasoidol<sup>2</sup>.

**Figure 1** The structure and HMBC of **1** (H→C)



**1**

Compound **1**, a brown gum,  $[\alpha]_D^{20.6} +16.5$  (*c* 0.21, CH<sub>3</sub>OH). High-resolution FABMS gave the  $[M+1]^+$  peak at *m/z* 715.4228 corresponding to the molecular formula C<sub>44</sub>H<sub>59</sub>O<sub>8</sub>  $[M+H]$  (calcd. 715.4209). The <sup>1</sup>H and <sup>13</sup>C NMR spectra of **1** were similar to those of polycerasoidol<sup>2</sup>, and the <sup>13</sup>C NMR spectrum of the former showed only 22 signals for four methyls, six methylenes, three methines and nine quaternary carbons, indicating that **1** was a dimer of polycerasoidol. Only one aromatic proton signal

( $\delta$  7.08) was observed in the  $^1\text{H}$  NMR spectra of **1**, and the  $^{13}\text{C}$  NMR signal at  $\delta$  114.1 for the C3'' of polycerasoidol was replaced by  $\delta$  121.8 in **1**, revealing that the C3'' and C3''' were connected. This linkage was further supported by 0.4 and 2.6 ppm of upfield shifts observed for C2'' and C4'', respectively (**Table 1**), and unambiguously signed by the analysis of the HMBC experiments, *i.e.* the  $^1\text{H}$ - $^{13}\text{C}$  long-range correlations between H1/H1' ( $\delta$  2.79) and the quaternary carbon at  $\delta$  121.8 (C3''/C3'''), H7''/H7''' ( $\delta$  2.32) and C1''/C1''' ( $\delta$  145.9), and C5''/C5''' ( $\delta$  117.1) (**Figure 1**). Besides, EIMS gave the main fragment peak at  $m/z$  358 corresponding the cleavage of the bond of C3'' and C3'''. Thus the structure of **1** was identified to be as shown.

**Table 1** The NMR data of compound polycerasoidol and **1**<sup>a</sup>

position	polycerasoidol		<b>1</b>	
	$^1\text{H}^b$	$^{13}\text{C}$	$^1\text{H}^b$	$^{13}\text{C}$
1 (1')	2.69 (m, 6.5, 2H)	21.7t	2.79 (m, 7.8, 2H)	21.6t
2 (2')	1.74 (dd, 6.5, 9.2), 1.60 (d, 7.3)	32.1t	1.74 (dd, 6.7, 10.2), 1.60 (d, 7.8)	31.8t
3 (3')	/	75.6s	/	75.0s
4 (4')	1.64 (t, 6.9, 2H)	39.9t	1.64 (t, 7.6, 2H)	39.5t
5 (5')	2.22 (t, 6.9, 2H)	22.9t	2.39 (m, 7.6, 2H)	22.9t
6 (6')	5.31 (t, 6.9)	125.6d	5.29 (t, 7.6)	124.6d
7 (7')	/	135.1s	/	135.5s
8 (8')	2.22 (t, 6.9, 2H)	40.3t	2.18 (t, 7.6, 2H)	40.3t
9 (9')	2.92 (dd, 6.9, 7.1, 2H)	28.8t	2.92 (dd, 7.1, 7.6, 2H)	28.7t
10 (10')	6.02 (t, 7.1)	141.9d	5.63 (t, 7.1)	132.7d
11 (11')	/	129.3s	/	135.0s
12 (12')	2.11 (s, 3H)	21.7q	2.14 (s, 3H)	22.5q
13 (13')	/	170.9s	/	173.2s
14 (14')	1.69 (s, 3H)	16.2q	1.63 (s, 3H)	16.1q
15 (15')	1.28 (s, 3H)	24.4q	1.25 (s, 3H)	24.8q
1'' (1'')	/	145.5s	/	145.9s
2'' (2'')	/	121.9s	/	121.5s
3'' (3'')	6.18 (s)	114.1d	/	121.8s
4'' (4'')	/	151.5s	/	148.9s
5'' (5'')	6.94 (s)	117.1d	7.08 (s)	117.1d
6'' (6'')	/	127.2s	/	126.1s
7'' (7'')	2.29 (s, 3H)	16.8q	2.32 (s, 3H)	16.5q

<sup>a</sup>  $^1\text{H}$ ,  $^{13}\text{C}$  NMR and HMBC spectra were obtained at 500 MHz, 125 MHz and 500 MHz, and recorded in  $\text{C}_5\text{D}_5\text{N}$  at room temperature, respectively.

<sup>b</sup> Coupling constants are presented in Hz. Unless otherwise indicated, all proton signals integrate to 1 H.

### Acknowledgment

This work was financially supported by the National Foundation for Outstanding Young Scientists to Prof. Xiao Jiang Hao (No. 39525025).

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Received 31 October, 2000