

A New Sesquiterpene Lactone from *Ainsliaea bonatii*

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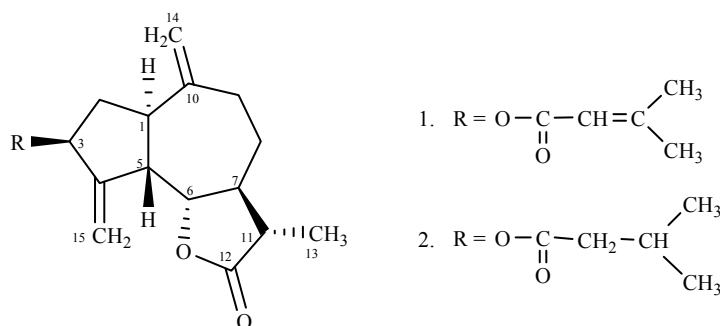
Abstract: A new sesquiterpene lactone, Ainsliaolide A, was isolated from *Ainsliaea bonatii*. The structure was determined on the basis of spectral data.

Keywords: *Ainsliaea bonatii*, sesquiterpene lactone, ainsliaolide A, diaspanolide A.

Ainsliaea bonatii Beauverd, a plant of Ainsliaea, is mainly distributed in the south-west of China, Southern and Eastern China¹. It has long been used in Tibetan folk medicine for the treatment of rheumatism, lumbago and gonitis². The chemical constituents of this species have not been reported previously. In our chemical investigation of this plant, we isolated a new sesquiterpene lactone from its EtOAc extract. Its structure was determined as 3 β -seneciyoxy-11 α -methyl-4 (15),10 (14)-guaiadien-12,6-olide, named ainsliaolide A, mainly by 1D and 2D NMR experiments. In this article, we report the isolation and structural identification of ainsliaolide A (**1**).

Compound **1** was isolated as white amorphous powder. $[\alpha]_D^{20} + 66.0$ (*c* 0.27, CHCl₃), mp 109–111 °C. Its positive ESIMS spectrum displays a quasimolecular ion [M+Na]⁺ at *m/z* 353 corresponding to a molecular formula of C₂₀H₂₆O₄ for compound **1**, which was confirmed by its HRESIMS spectrum (353.1762 [M+Na]⁺, calcd. 353.1728).

Figure 1 The structure of compound **1**



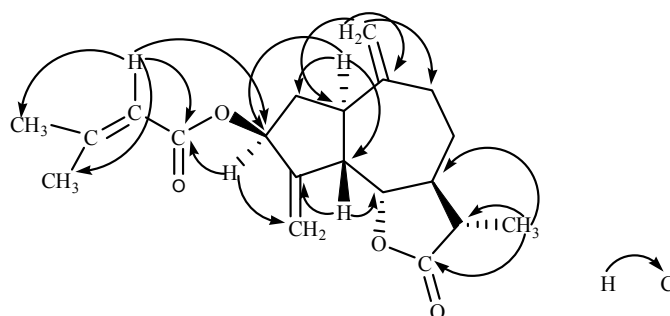
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The IR spectrum suggested the presence of a γ -lactone group (1770cm^{-1}) and an ester group (1730cm^{-1}). Its $^1\text{H-NMR}$ spectrum was quite similar to that of diaspanolide A (**2**)³, except for the ester moiety. Compound **1** has a seneciyoxy group which present two methyl signals at δ 1.89 (s, 3H, H-4'), 2.17 (s, 3H, H-5') and hydrogen signal of double band at δ 5.71 (s, 1H, H-2'). In the $^{13}\text{C-NMR}$ spectrum, twenty signals were observed, including three methyl signals at δ 13.2, 20.3 and 27.4 ppm, and two carbonyl signals at δ 178.4 and 166.3 ppm. We also find two carbonyl signals at δ 116.0 and 157.3 ppm in $^{13}\text{C-NMR}$. Furthermore, the signals of methyl (C-4', 5') were downfield shifted in comparison with that of diaspanolide A. In the HMBC spectrum, the correlation between H-3 and C-1' (δ 166.3) indicated that the seneciyoxy group is linked at C-3. The full assignments of all the proton and carbon signals in compound **1** were made by means of $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, $^1\text{H-}^1\text{H-COSY}$, HMQC, HMBC (**Figure 2**) and NOESY. The comparison of $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectrum data of compound **1** with that of diaspanolide A (**Table 1**) led to the establishment of the structure of compound **1** as 3 β -seneciyoxy-11 α -methy-4 (15), 10 (14)-guaidiene-12,6-olide.

Table 1 $^1\text{H-NMR}$ (500MHz) and $^{13}\text{C-NMR}$ (125MHz) data of compound **1** (CDCl_3 , TMS, δ ppm)

C	δ_{H}	δ_{C}	C	δ_{H}	δ_{C}
Aglycone moiety					
1	2.89 (m)	44.1 (d)	9	2.49 (m), 2.03 (m)	36.3 (t)
2	2.46 (m), 1.79 (m)	36.6 (t)	10		148.8 (s)
3	5.55 (dd, J = 6, 8)	73.8 (d)	11	2.20 (m)	42.1 (d)
4		148.8 (s)	12		178.4 (s)
5	1.93 (m)	50.4 (d)	13	1.22 (d, J = 7)	13.2 (q)
6	3.99 (t, J = 9)	83.9 (d)	14	4.91 (s)	113.5 (t)
7	2.81 (m)	50.0 (d)	15	5.26 (brt, J = 2), 5.38 (brt, J = 2)	112.9 (t)
8	2.11 (m), 1.31 (m)	32.4 (t)			
Ester moiety					
1		166.3 (s)	4	1.89 (s)	27.4 (q)
2	5.71 (s)	116.0 (d)	5	2.17 (s)	20.3 (q)
3		157.3 (s)			

Figure 2 The key correlation in HMBC spectrum of compound **1**



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