

## A New Lupane from the Resin of *Boswellia carterii*

Jin Yun ZHOU\*, Rui CUI

Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union  
Medical College, Beijing 100050

**Abstract:** A new lupane-type triterpene was isolated from the resin of *Boswellia carterii* Birdw. Based on the spectral methods, its structure was elucidated as lup-20(29)-ene-3 $\alpha$ -acetoxy-24-oic acid.

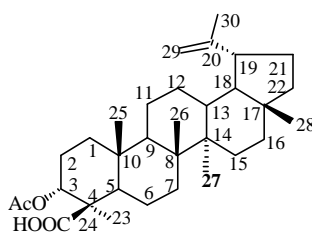
**Keywords:** Lupane, triterpenoid, *Boswellia carterii*.

Olibanum, a resin produced by *Boswellia carterii* Birdw which grows in Somalia and Ethiopia, is a traditional Chinese medicine. It invigorates the circulation of blood and relieves pain from injuries and tumors. In the previous chemical research, cembrane diterpenoids<sup>1,2</sup>, ursane and oleanane triperpenoids<sup>3-8</sup> were reported. A systematic study of the chemical constituents and antitumor activities of the resin led to the isolation of a new lup-type triterpene compound.

Compound **1**, obtained as colorless needles, mp 271-273°C (MeOH),  $[\alpha]_D^{25} +15.5$  (c 0.12, MeOH), has the molecular formula C<sub>32</sub>H<sub>50</sub>O<sub>4</sub> according to the EIMS ion peak at  $m/z$  498 and <sup>13</sup>CNMR spectrum (**Table 1**). The <sup>1</sup>HNMR spectrum showed five methyl groups ( $\delta$  0.78, 0.79, 0.99, 1.06, 1.21) and one isopropenyl group ( $\delta$  1.68, s;  $\delta$  4.57 and 4.69 d, J = 2.0 Hz). In the HMBC spectrum, the H-29 correlated to C-19 and the H-19 correlated with C-30, C-20 and C-29, which indicated that C-19 bore an isopropenyl group. Hence compound **1** should be a lupane triterpenoid. An acetyl group ( $\delta_H$  2.09,  $\delta_C$  21.20 and 170.35) and a carboxy group ( $\delta_C$  182.69) were also observed in the <sup>1</sup>H and <sup>13</sup>CNMR spectra, respectively (**Table 1**). The EIMS of **1** exhibited important fragments at  $m/z$  279, 219 (279-AcOH), 175(219-CO<sub>2</sub>), 218, 203 and 189. This fragmentation pattern revealed that the acetoxy and carboxy groups might be located at rings A and B<sup>9</sup>. The locations of an acetoxy group at C-3 and a carboxy group at C-4 $\beta$  were substantiated by the HMBC spectrum, in which the correlation of the H-3 to C-23 and the acetyl carbonyl carbon ( $\delta$  170.35), as well as that of H-23 with the carboxy carbon ( $\delta$  182.69) were observed. A small coupling constants (t, J = 3.0 Hz) between H-3 and H-2 pointed to equatorial disposition of H-3, hence the acetoxy group is axially oriented ( $\alpha$ -face). A careful comparison of <sup>13</sup>CNMR spectrum data of **1** with those of acetyl-11-keto- $\beta$ -boswellic acid<sup>10</sup> showed that the structure of the two compounds in ring A are very similar and confirmed that in compound **1** the acetoxy and carboxy groups are located at C-3 $\alpha$  and C-4 $\beta$ , respectively.

\* E-mail: jinyunzhou@imm.ac.cn

The relative stereochemistry of **1** was elucidated by NOE spectroscopy. The NOE between the H-19 and the Me-28 suggested that the isopropenyl group is in the  $\alpha$ -position. The acetoxy and carboxy groups located at C-3 $\alpha$  and C-4 $\beta$  were further supported by the NOE of H-3 to Me-23 and H<sub>2</sub>-2. Compound **1** was therefore assigned as lup-20(29)-ene-3 $\alpha$ -acetoxy-24-oic acid.

**1****Table 1** <sup>1</sup>H (500 Hz) and <sup>13</sup>CNMR (125 Hz) data of compound **1** ( $\delta$  ppm, CDCl<sub>3</sub>)

C	$\delta_H$	$\delta_C$	C	$\delta_H$	$\delta_C$
1	1.09 (m), 1.49 (m)	34.38 t	17		43.01 s
2	1.61 (m), 2.13 (m)	23.68 t	18	1.38 (m)	48.74 d
3	5.27 (t, J = 3.0)	73.27 d	19	2.38 (dt, J = 11.0, 6.0)	47.93 d
4		46.74 s	20		150.87 s
5	1.41 (m)	50.50 d	21	1.34 (m), 1.92 (m)	29.83 t
6	1.65 (m), 1.88 (m)	21.32 t	22	1.19 (m), 1.36 (m)	39.97 t
7	1.37 (m), 1.42 (m)	34.06 t	23	1.21 (s)	23.64 q
8		40.80 s	24		182.69 s
9	1.34 (m)	49.68 d	25	0.78 (s)	13.35 q
10		37.67 s	26	1.06 (s)	15.89 q
11	1.23 (m), 1.24 (m)	21.08 t	27	0.99 (s)	14.63 q
12	1.10 (m), 1.67 (m)	25.17 t	28	0.79 (s)	18.01 q
13	1.64 (m)	38.01 d	29	4.57, 4.69 (d, J = 2.0)	109.33 t
14		42.90 s	30	1.68 (s)	19.29 q
15	1.03 (m), 1.69 (m)	27.42 t	OCOCH <sub>3</sub>	2.09 (s)	21.20 q
16	1.37 (m), 1.46 (m)	35.54 t	OCOCH <sub>3</sub>		170.35 s

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