A New Triterpene from Cephalomappa sinensis

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Abstract: A new triterpene **1**, 1β , 2α , 3β -trihydroxylup-20 (29) -ene was isolated from *Cepha-lomappa sinensis*. The structure was elucidated mainly on the basis of 1D and 2D NMR spectral means.

Keywords: Triterpene, Cephalomappa sinensis, Euphorbiaceae.

Cephalomappa sinensis (Chun et How) Kosterm belongs to the family Euphorbiaceae. It is distributed in southwest and west of Guangxi Zhung Autonomous Region¹. Its fresh leaves are used as feeding stuff for cattle, horse, and sheep and can make them strong¹. Chemical constituents of this species have not been reported previously. In our research, a new triterpene was isolated from the ethanolic extract of its roots.

Compound 1 was obtained as colorless needles, mp 235-237°C. The EI-mass spectrum showed molecular ion peak at m/z 458. The 30 carbon signals observed in the ¹³C NMR and DEPT spectrum indicated that **1** was a triterpene having seven methyls, nine methylenes, eight methines and six quaternary carbons. Furthermore, the chemical shifts of three methine carbon signals (δ 83.5, 74.2, 80.0) suggested the presence of three hydroxyl groups. From these data, the empirical formula, $C_{30}H_{50}O_3$ was deduced. In the ¹H NMR spectrum, the appearance of a pair of olefinic proton signals (δ 4.68, 4.56) and an allylic methyl signal (δ 1.68), which are characteristic of an isopropenyl group, and six singlet methyl signals suggested a lupene skeleton triterpene². In the HMBC spectrum, carbon signals resonating at δ 80.0 (d), δ 38.9 (s), δ 53.1 (d) were correlated with two singlet methyl protons (δ 0.99, 0.81), indicating that these signals were assigned to C-3, C-4, C-5, respectively, and a hydroxyl group was located at $C-3^2$. The other two hydroxyl groups were determined to be at C-1 and C-2 on the basis of the fact that H-2 (δ 3.46) showed cross peak to H-3 (δ 3.04) and H-1 (δ 3.16) showed cross peak to H-2 in the 1 H- 1 H COSY spectrum. The configuration of the hydroxyl group at C-2 was determined to be α on the basis of the NOE interactions between H-2 and CH₃-25 in the NOESY spectrum. By analysis of the coupling constants between H-2 (1H, t, J = 7.6Hz) and H-1 (1H, d, J = 7.2Hz), H-3 (1H, d, J = 7.9Hz) and H-2, the configuration of the two hydroxyl groups at C-1 and C-3 were both determined to be β . Thus, **1** was elucidated as 1β, 2α , 3β-trihydroxylup-20(29)-ene. The assignments of ¹H and ¹³C NMR data are given in Table 1 and 2.

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Positi	on	Positio	on	Positi	on	Position	l	Position		Positi	on
1	83.5	6	17.9	11	23.8	16	35.7	21	29.9	26	16.4
2	74.2	7	34.3	12	25.3	17	43.1	22	40.1	27	14.5
3	80.0	8	41.8	13	37.8	18	48.5	23	28.4	28	18.1
4	38.9	9	51.8	14	43.1	19	48.0	24	16.2	29	109.5
5	53.1	10	43.7	15	27.6	20	150.8	25	13.4	30	19.3

Table 1 ¹³C NMR (125 MHz) data of **1** (δ in ppm)*

Table 2	¹ H NMR	(500 MHz)	data of 1	(δ in ppm, .	J in Hz)*
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Position		Position		Position		Position	
H-29a	4.68 (br s)	H-3	3.04 (d, 7.9)	Me-23	0.99 (s)	Me-27	0.96 (s)
H-29b	4.56 (s)	H-19	2.37 (dt, 4.8, 8.8)	Me-24	0.81 (s)	Me-28	0.79 (s)
H-1	3.16 (d, 7.2)	H-9	1.56 (m)	Me-25	0.98 (s)	Me-30	1.68 (s)
H-2	3.46 (t, 7.6)	H-5	o.75 (m)	Me-26	1.05 (s)		

*The data were measured in $CDCL_3$ with TMS as internal standard (Table 1 and 2).



Figure 1 Selected HMBC for 1

References

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