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A Novel Triterpenoid from *Petasites tricholobus*

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Abstract: A novel triterpenoid, D:B-friedoursane-3α, 16α-dihydroxy-7α, 8α-epoxy-5(10)-ene, named petatrichol A, was isolated from the roots of *Petasites tricholobus* Franch.. Its structure was elucidated by spectroscopic methods, especially 2DNMR techniques.

Keywords: *Petasites tricholobus*, Compositae, triterpenoid, petatrichol A.

Some genus of *Petasites* was used as folk medicine in China for detoxification, detumescence and treatment of viper bite[1]. In order to find the medical value, we studied the chemical constituents of *Petasites tricholobus*. A novel triterpenoid compound **1**, possessing a migrated ursane skeleton with $\Delta^{5,10}$ double bond and 7, 8 - epoxy in the molecule, was isolated from this plant. Its structure elucidation was reported here.

Compound **1**, m.p. 186 – 187 °C, $[\alpha]_D^{17}$ + 43 (*c* 0.2, $CHCl_3$), was isolated as white powder. Its EIMS spectrum showed the molecular ion peak at *m/z* 456, combined with the ^1H and ^{13}CNMR (DEPT) data, the molecular formula was deduced to be $C_{30}H_{48}O_3$.

Figure 1 Compound **1** and the key correlations observed in NOESY spectrum of **1**

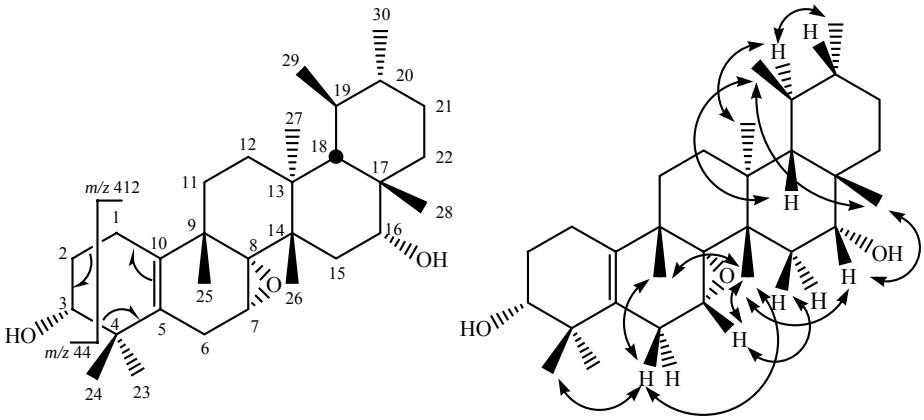

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Table 1 ^{1}H (400MHz), $^{13}CNMR$ (100MHz), DEPT data and HMBC correlations of compound **1** ($CDCl_3$, TMS, δ_{ppm})*

No.	δ_H	δ_C	DEPT	HMBC
1	2.02 (m), 1.96 (m)	20.9	CH_2	C-10
2	1.64 (m), 1.60 (m)	26.7	CH_2	C-10, C-1, C-3, C-4
3	3.50 (dd, *J* = 6.4/4.4 Hz)	75.2	CH	
4	—	39.0	C	
5	—	126.4	C	
6	2.62, 2.24 (brd, *J* = 17.4 Hz)	26.1	CH_2	C-5, C-7, C-8
7	3.16 (brd, *J* = 3.2 Hz)	51.3	CH	C-5, C-8
8	—	67.1	C	
9	—	40.1	C	
10	—	134.9	C	
11	1.39 (m), 1.35 (m)	28.7	CH_2	
12	1.49 (m), 1.43 (m)	28.5	CH_2	
13	—	40.4	C	
14	—	42.3	C	
15	1.59 (m), 1.13 (m)	32.8	CH_2	C-14, C-16
16	3.75 (dd, *J* = 12.8/5.2 Hz)	77.2	CH	
17	—	37.9	C	
18	1.25 (m)	53.5	CH	C-29
19	1.10 (m)	35.7	CH	C-27, C-30
20	1.61 (m)	31.9	CH	
21	1.58 (m), 1.16 (m)	28.9	CH_2	
22	1.86 (m), 1.64 (m)	26.7	CH_2	
23	1.05 (s)	26.0	CH_3	C-3, C-4, C-5, C-24
24	0.94 (s)	22.2	CH_3	C-3, C-4, C-5, C-23
25	1.20 (s)	26.0	CH_3	C-8, C-9, C-10, C-11
26	1.24 (s)	20.9	CH_3	C-8, C-13, C-14, C-15
27	1.01 (s)	16.9	CH_3	C-12, C-13, C-14, C-18
28	1.23 (s)	35.2	CH_3	C-16, C-17, C-18, C-22
29	1.02 (d, *J* = 6.0 Hz)	25.1	CH_3	C-18, C-19, C-20
30	0.93 (d, *J* = 6.0 Hz)	22.6	CH_3	C-19, C-20, C-21

*assigned by HSQC and HMBC spectrum

The ^{1}H and $^{13}CNMR$ (DEPT) spectrum of **1** displayed the signals of six tertiary methyls, two secondary methyls, eight methenes, six methines (three of them were connected with oxygen) and eight quarternary carbons, which indicated that compound **1** was a pentacyclic triterpenoid possessing a tetrasubstituted double bond (δ_C 126.4,134.9, C), two methines connected with hydroxy (δ_H 3.50, 3.75 and δ_C 75.2, 77.2) and an epoxide group (δ_H 3.16 and δ_C 67.1 C, 51.3 CH) (**Table 1**). The IR spectrum also revealed the presence of hydroxy (3380 cm^{-1}) and double bond (1665 cm^{-1}).

The skeleton of compoud **1** was constructed by the correlations of eight methyls in HMBC spectrum (**Table 1**). In the HMBC spectrum, the correlations of H-1 (δ_H 2.02, 1.96) with C-10 (δ_C 134.9), H-2 (δ_H 1.64, 1.60) with C-10 (δ_C 134.9), C-1 (δ_C 20.9), C-3 (δ_C 75.2), C-4 (δ_C 39.0), CH_3-23 (δ_H 1.05) with C-3 (δ_C 75.2), C-5 (δ_C 126.4), CH_3-24 (δ_H 0.94) with C-3 (δ_C 75.2), C-5 (δ_C 126.4) and H-6 (δ_H 2.62, 2.24) with C-5 (δ_C 126.4) indicated that a double bond was between C-5 and C-10 and a hydroxyl group was located at C-3. The fragment peaks in EIMS at *m/z* 412 (1), 44 (17) and 43 (100), which were caused by RDA cleavage (**Figure 1**), further confirmed the presence of the

5(10)-ene structure. The correlations of H-7 (δ_H 3.16) with C-8 (δ_C 67.1), and H-6 (δ_H 2.62, 2.24) with C-7 (δ_C 51.3), C-8 (δ_C 67.1) confirmed that the epoxide group was between C-7 and C-8, and the correlations of CH_3-28 (δ_H 1.23) with C-16 (δ_C 77.2), H-15 (δ_H1.13, 1.59) with C-16 (δ_C 77.2) indicated that the second hydroxyl group was at C-16. The coupling contants of H-3 (dd, J = 6.4/4.4 Hz), H-16 (dd, J = 12.8/5.2 Hz) and H-7 (brd, J = 3.2 Hz) showed the presence of α-hydroxy at C-3, C-16 and 7α, 8α-epoxy. The correlations of H-7 (δ_H 3.16) with CH_3-26 (δ_H 1.24) in NOESY spectrum further supported the α configuration of epoxy. The 25, 26, 28, 29 methyls and H-18 were on β side, which can be deduced from the cross peaks in NOESY spectrum (**Figure 1**). The correlations between H-19 and 27, 30 methyls, at the same time, not having correlation between 26 and 27 methyls indicated that 27 and 30 methyls were on α side. The skeleton of **1** and relative configurations of these methyls were the same as that of rhoiptelenol[2,3]. Based on the above evidence, compound **1** was determined as D:B-friedoursane-3α, 16α-dihydroxy-7α, 8α-epoxy-5(10)-ene, and named as petatrichol A.

Acknowledgments

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References

1. Jiangsu New Medical Collage, *Chinese Medicine Dictionary*, Shanghai People's Publishing House. Shanghai, **1977**, p. 2483.
2. J. Kitajima, M. Arai, Y. Tanaka, *Chem. Pharm. Bull*., **1994**, *42* (3), 608.
3. Z. H. Jiang, R. H. Zhou, K. Masuda, H. Ageta, *Phytochemistry*, **1995**, *40* (1), 219.

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