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A NEW TYPE OF TRITERPENE FROM *TRICHOCEREUS PACHANOI*

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ABSTRACT.—A new triterpene, pachanol A [**1**], which has a novel skeleton, was isolated from the hydrolysate of an MeOH extract of *Trichocereus pachanoi* (Cactaceae).

We have been interested in triterpenes of cacti and have isolated several known and unknown triterpenes from *Hertrichocereus beneckei* Backbg. and *Trichocereus bridgesii* Britt. & Rose (1). Now we report the isolation and structural determination of a new triterpene, pachanol A [**1**], from *Trichocereus pachanoi* Britt. & Rose (Cactaceae). This compound possesses a new skeleton named pachanane. The structure of pachanol A [**1**] was determined by single-crystal X-ray diffraction, and the result is reported together with its assigned nmr data.

The MeOH extract of *T. pachanoi* was hydrolyzed with 3.5% HCl, and the precipitates were chromatographed on a Si gel column with $CHCl_3$/MeOH to obtain pachanol A, which was recrystallized from $CHCl_3$/MeOH as colorless needles, mp >300°, $C_{30}H_{44}O_4$ (*m/z* calcd 468.3241, found 468.3233). The molecular structure is illustrated in Figure 1. The structure illustrated in Figure 1 was confirmed on the basis of DEPT, ^{1}H-^{1}H, ^{1}H-^{13}C COSY, and ^{1}H-^{13}C long range COSY. The nmr assignments are summarized in Table 1.

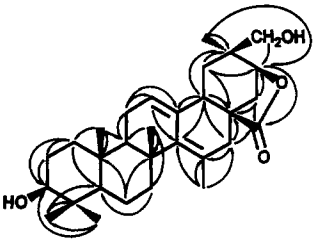

FIGURE 1. The COLOC correlations (^{1}H→^{13}C) for pachanol A [**1**].

CRYSTAL REFINEMENT DATA.[1]—$C_{30}H_{44}O_4$, M_r 468, orthorhombic, space group $P2_12_12_1$ (No. 19), a=28.415(11), b=13.602(6), c=6.477(9) Å, V=2503 (4) Å^3, D_c=1.244 g·cm^{-3}; 1533 unique diffractometer data measured at ca. 295 K [2θ max 100°; 2θ/ω scan mode, monochromatic CuKα radiation (λ 1.5418 Å)], 1312 with $F>3\sigma(F)$ considered observed and used in the block-matrix least-squares refinement without absorption correction (μ_{cu}=5.1 cm^{-1}; specimen 0.50×0.15×0.10 mm). Anisotropic thermal parameter refinement for C and O; contribution of H ignored; R=0.094. An ORTEP drawing of **1** is shown in Figure 2.

EXPERIMENTAL

PLANT MATERIAL.—*T. pachanoi* was cultivated in the Research Institute of Evolutionary Biology, Setagaya-ku, Tokyo, Japan, and in Izu Natural History Park, Itoh, Shizuoka, Japan. This cactus was botanically identified by Dr. Hiroshi Yuasa.

[1]Atomic coordinates for this structure have been deposited with the Cambridge Crystallographic Data Centre and can be obtained on request from Dr. Olga Kennard, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK.

TABLE 1. Nmr Assignments for Pachanol A [**1**].

Position	$\delta^{13}C$ (C_5D_5N)	$\delta^{1}H$ (C_5D_5N)	Multiplicity (J in Hz)	^{1}H- ^{13}C Long-range correlations
1	39.1	0.92	m	C-3, C-5
		1.65	m	
2	28.3	1.83	m	
3	77.9	3.34	dd (5.7, 10.4)	
4	39.2			
5	54.5	0.89	d (11.9)	C-25
6	19.5	1.60	m	C-8, C-10
7	41.1	1.54	m	C-5, C-9, C-26
		2.57	m	
8	40.4			
9	55.4	1.28	m	
10	38.1			
11	22.9	2.09	m	C-12, C-13
		2.25	m	
12	124.0	5.99	bs	C-9, C-14
13	132.0			
14	140.0			
15	125.4			
16	42.4	1.96	d (18.7)	C-14, C-15, C-17,
		2.97	d (18.7)	C-18, C-28
17	45.2			
18	39.3	2.49	bs	
19	29.0	1.57	m	C-13, C-17, C-21,
		2.16	d (15.6)	C-29
20	38.7			
21	80.2	4.85	d (5.7)	
22	33.0	1.82	m	C-28
		2.43	d (11.9)	
23	28.6	1.26	s	C-3, C-4, C-5, C-24
24	16.4	1.06	s	C-5, C-23
25	16.6	0.95	s	C-5, C-9, C-10
26	19.0	1.09	s	C-7, C-8, C-9, C-14
27	23.8	1.86	s	C-14, C-15, C-16
28	180.3			
29	21.8	1.36	s	C-19, C-20, C-21
30	68.9	3.55	d (10.4)	C-21
		3.89	d (10.4)	

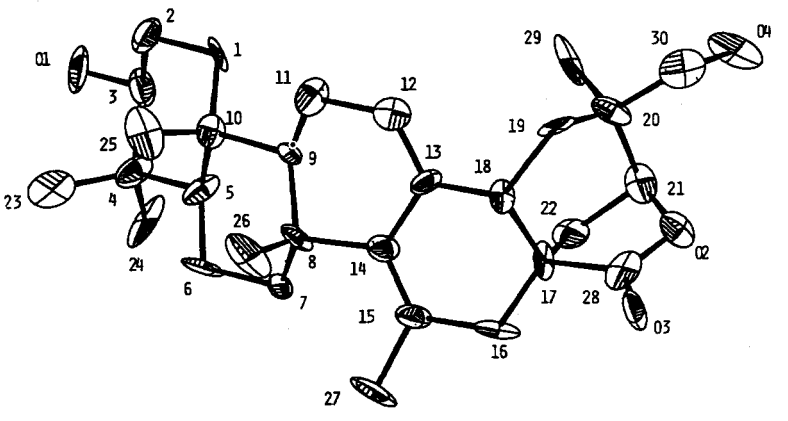

FIGURE 2. ORTEP drawing of **1**.

This specimen is deposited at the Research Institute of Evolutionary Biology, Setagaya-ku Tokyo, Japan.

INSTRUMENTS.—Mp was determined with a Yanagimoto MP micro mp apparatus. ^{1}H- and ^{13}C-nmr spectra were recorded using a JEOL GSX-400 (^{1}H 400 and ^{13}C 100 MHz) spectrometer in C_5D_5N with TMS as an internal standard. The chemical shifts are expressed in ppm (δ) (Table 1). The [α]D values were determined with a JASCO DIP-140 digital polarimeter. Cc was carried out on 70–230 mesh Si gel (Merck). Hrms and eims spectra were obtained using a JEOL JMS-DX 302.

EXTRACTION AND ISOLATION OF PACHANOL A [**1**].—Dry *T. pachanoi* (196.9 g) was extracted with $CHCl_3$ and then repeatedly with MeOH. The MeOH extract (12.9 g) was hydrolyzed with 3.5% HCl at 110° for 2.5 h. The precipitates (2.98 g) produced were subjected to cc on Si gel ($CHCl_3$/MeOH) and purified by hplc on a Si gel column (Nucleosil 60-5, 1×25 cm), eluted with $CHCl_3$-MeOH (50:1), resulting in pachanol A (15.0 mg). Crystallization from MeOH gave pachanol A [**1**]: mp >300° (dec), [α]D −89.0° (*c*=0.145; $CHCl_3$); ir ν max (KBr) 3500, 3450, 2950, 2900, 1740 cm^{-1}; uv λ max (MeOH) 255 (ε=8700); ^{1}H and ^{13}C nmr see Table 1; eims *m/z* $[M]^+$ 468 (93) 450 (30), 422 (32), 383 (100), 351 (38), 214 (29), 201 (59), 189 (35), 135 (27).

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LITERATURE CITED

1. K. Kinoshita, K. Koyama, and K. Takahashi, *J. Nat. Prod.*, **55**, 953 (1992).

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