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A NOVEL PENTACYCLIC TRITERPENOID ISOLATED FROM CARALLUMA ATTENUATA ROOT

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ABSTRACT

From the root of *Caralluma attenuata* belonging to the family *Asclepiadaceae*, a novel pentacyclic triterpeniod was isolated. The structure was elucidated on the basis of spectroscopic data. This is the first report of such novel pentacyclic triterpeniod from *Caralluma attenuata* root.

KEYWORDS: Caralluma attenuata, Asclepiadaceae, pentacyclic triterpenoid.

INTRODUCTION

In the course of our investigation on the chemical constituents of *Carallumas* we have isolated a number of triterpenoids and flavanoids. Isolation and characterization of oxypregnane glycosides, [1,2] pregnane glycosides, ^[1,2] triterpene saponins, ^[10] flavanoids, ^[11] pregnane esters, ^[12] bisdesmosidic glycosides, ^[13,14] flavone glycosides ^[15] were earlier reported from the same genus. In this report we report the structural elucidation of a novel pentacyclic triterpenoid derivative from *Caralluma attenuata*.

EXPERIMENTAL

The plant material of *Caralluma attenuata* was collected in Tirumala forests during Nov-2009.

MPs uncorr. IR v_{max}^{KBr} , UV $\lambda_{\text{max}}^{EtOH}$, ¹HNMR \square ppm, 300 MHz CDCl₃, ¹³C NMR \square ppm, CC and TLC on silica gel.

2.1 Spectral Data

2.1.1 U.V $\lambda_{\text{max}}^{EtOH}$ 281 nm

2.1.2 IR v_{max}^{KBr} 3442.02, 2919.20, 2849.43, 1737.16, 1463.03, 1463.03, 1382.16, 1261.84, 1168.99, 1100.34, 1020.19, 801.58, 719.47 cm⁻¹

2.1.3 ¹HNMR δ 5.30, 4.05, 3.60, 3.59, 2.35217, 2.333, 1.63723, 1.6180, 1.5955, 1.5681, 1.3021, 1.2544, 1.20244, 1.0117, 0.89751, 0.88134, 0.86383, 0.84590, 0.80608, 0.68149, 0.07045 ppm.

2.1.4 ¹³C NMR δ140.736, 138.322, 129.288, 121.719, 77.333, 77.017, 76.699, 71.831, 64.419, 56.879, 55.973, 51.247, 50.168, 42.270, 37.265, 34.428, 33.888, 31.927, 31.628, 29.710, 29.453, 29.368, 29.266, 29.173, 28.664,

25.948, 25.041, 24.731, 21.086, 22.694, 21.086, 19.394, 14.112 ppm

2.1.5 MASS [M⁺] m/Z 413, 391, 279, 193, 177, 167, 149, 133, 105, 71, 57

2.2 Extraction and isolation

The air dried roots of *Caralluma attenuata* were powdered and extracted with n-hexane, benzene, acetone and methanol in a soxhlet extractor.

n-Hexane extract (28gms) was subjected to column chromatography using silica gel (10-40 μ mesh). It is eluted with hexane:benzene 1:1 fraction yielded a white crystalline solid MP 136^{0} C (3.75mg) with Rf 0.67 (benzene as developing solvent). This was recrystallised from benzene and analysed by spectral data.

3.1 RESULTS AND DISCUSSIONS

The compound was isolated as white crystalline needles with melting point 139^{0} C and analysed for $C_{28}H_{44}O_{2}$ ([M+] m/z = 412).

The compound showed positive test for steroid (Libermann Burchard reaction). The IR spectrum showed bands at $\nu_{\rm max}^{\it KBr}$ 3442 cm $^{-1}$ (-OH group) and a weak band at 1600 and 1650 cm $^{-1}$ indicating the presence of conjugated homodiene system. This is further confirmed by the presence of two olefinic proton signals at δ 5.30 and $^{13}{\rm C}$ signals at δ 129.28, 121.71, 138.3, 140.7 ppm along with UV spectrum at $\lambda_{\rm max}^{\it EtOH}$ 281nm. $^{[16]}$

The characteristic ring protons ranging from $\delta 0.6$ - $\delta 1.8$ ppm indicated the presence of pentacyclic triterpenoid with olean diene skeleton. [17]

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A one proton downfield signal at $\delta 3.6$ (1H,d) and 4.05 (1H,t) ppm indicated the presence of a secondary and primary hydroxyl group accounting for all oxygens in the molecule.

The 1 HNMR spectrum showed presence of δ 0.89775, 0.80608, 0.84590, 0.86383 and 0.8813 ppm indicated the presence of five angular methyl groups. [18]

The ^{13}C NMR values at δ 138.3, 129.2, 121.7 and 140.7 ppm supported the presence of conjugated double bond in ring C.

The 13 C signals at δ 71.83 and 64.41 indicated the presence of secondary and primary hydroxyl group respectively. Peaks at δ 3.6 and 4.05 (t) indicated the presence of CH₂OH group. [21]

This accounts for all the carbons and oxygens in the molecular formula and the partial structure of the molecule can be assigned as

The IR frequency at $v_{max}^{\textit{KBr}}$, 1463-1382 indicated the presence of gem dimethyl groups which is further supported by ^{13}C values at δ 34.42 and δ 24.73 for gem dimethyl group $^{[20]}$.

The presence of olean type of skeleton indicates the position of angular methyl groups. All the methyls are attached to tertiary carbon atoms.

Thus, the structure of the compound is given as

This is further proved by mass spectral fragmentation as shown in the scheme-I

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Thus, the triterpenoid is which is the first report from *Caralluma attenuata* and is the first of its kind. The IUPAC name of the isolated compound is 1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14b-octadecahydro-4-(hydroxymethyl)-4,6a,6b,11,11-pentamethylpicen-3-ol

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