

Chemical Investigation of *Cedrus deodara* Stem-Bark-I Isolation and Structure of Branched Chain Fatty Acid Ethyl Ester

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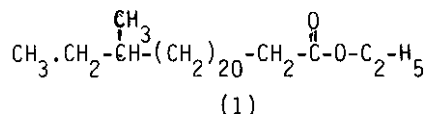
Summary: Isolation and structure determination of a new branched chain fatty acid ester is reported from the stem bark of *Cedrus deodara*. The structure of the compound was established to be ethyl 23-methyl-pentacosanoate on the basis of i.r., n.m.r. and mass spectral data.

Introduction

Cedrus deodara is a tall ever-green tree belonging to family Pinaceae [1]. It is grown in Northern parts of India and Pakistan. Flowering in October at the heights of 1500-3000 m in Dir, Chitral, Swat and some parts of Murree hills. The tree both wild and cultivated is a source of good quality timber. It is a soft wood with characteristic sweet odour and is extensively used for making furniture due to its termite repellent property. The exudate of wood obtained by heating in the absence of air was believed to be active against leprosy [2].

Like other plants belonging to this family and its other species *Cedrus deodara* is rich in terpenes. Quite a few sesquiterpenes and some flavonols have been reported in the literature [3-8] from this species but the structure of some of them are still unknown. This work was therefore undertaken to isolate and identify the unknown terpenes and also to investigate the presence of compounds other than terpenes in a systematic manner. This paper describes the isolation and structure of a new branched chain fatty acid ester for the first time from

the bark of this tree. The structure ethyl 23-methyl pentacosanoate (1) has been established on the basis of i.r., n.m.r. and mass spectral evidence.



The corresponding straight chain fatty acid ester has been reported in *Trichodesma indicum* [9]. The structure of ethylhexacosanoate ($\text{C}_{28}\text{H}_{56}\text{O}_2$) was based on i.r. and mass spectral data only.

Experimental

The stem bark and branches of the tree were collected from the forest of Patriata in Murree hills in October 1985. Air dried and powdered bark (3 kg) was thoroughly extracted with ethanol. The resinous mass (25 g, 0.83%) after evaporation (in vacuo) of ethanol was triturated with pet-ether 40-60°, ethylacetate and chloroform respectively in order to fractionate the material on the basis of solubility. First the pet-ether soluble portion was chromatographed

on t.l.c. with 95:5 benzene:chloroform silica gel HF 254. It showed ten spots. Then it was subjected to column chromatography using the same eluants thus collecting seven major fractions. Fractions 1 and 2 were oils, while 3,4,5 and 6 were semi-solids and 7 was a resinous material. Fraction 3 on preparative t.l.c. on silica gel HF 254 yielded a white solid, which melted at 52-53°C (on recrystallisation from acetone).

I.R. ν_{\max} . (KBr) 2970(s), 2850(s), 1720(s), 1450(m), 1370(m), 1180(m), 740-730(m) cm^{-1} . NMR CDCl_3 , 100MHz δ 0.85 (t, 3H, $\text{CH}_3\text{CH}_2\text{}$), 0.88 (d, 3H, CH_3CH), 1.1-1.5 a large signal overlapping OCH_2CH_3 and methylene protons of long chain, 4.1 (t, 2H, CH_2C), 4.1 (q, 2H, OCH_2CH_3).

M.S. m/z 424.42367 (M^+ , 6%, $\text{C}_{28}\text{H}_{56}\text{O}_2$), 396.39338 ($\text{C}_{26}\text{H}_{52}\text{O}_2$, 22%), 368.36203 ($\text{C}_{24}\text{H}_{48}\text{O}_2$, 10%), 353.3410 ($\text{C}_{23}\text{H}_{45}\text{O}_2$, 8%), 88.052571 ($\text{C}_4\text{H}_8\text{O}_2$, 100%), 57 (C_4H_9 , 75%).

Results and Discussion

A strong band at 1720 cm^{-1} in the infra-red spectrum corresponds to a saturated ester carbonyl group $\text{C}=\text{O}$ stretching vibration which is further confirmed by $\text{C}-\text{O}$ stretching at 1370 cm^{-1} . The presence of M-28 ion corresponding to formula $\text{C}_{26}\text{H}_{52}\text{O}_2$ confirms the presence of ethyl ester. The ion arises due to β -cleavage eliminating $\text{CH}_2=\text{CH}_2$. The base peak at m/z 88 also confirms the presence of ethyl ester group which is further substantiated by the presence of a triplet in the n.m.r. spectrum for

CH_3 -group (overlapped in the large methylene signal) and a quartet at δ 4.1 due to the methylene next to ester oxygen. The methylene next to carbonyl group is confirmed by the presence of a triplet comprising of two protons at δ 2.14. The position of branching and methyl substitution are confirmed by a methyl doublet at δ 0.88 and m/z 57 ion due to α -cleavage at the secondary carbon atom [10]. Moreover the appearance of the ion at m/z 353 also confirms the presence of a secondary methyl group. Thus, the structure I was assigned to this compound. Infra-red spectra were recorded on Pye Unicam Sp-1000 spectrophotometer as KBr discs.

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