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NOTES

Non-Saponifiable Components of *Xanthium Strumarium* Leaves (Linn.)

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The present paper deals with the isolation of a number of compounds from petrol fractions which were identified as β-sitosterol, β-amyrin, stigmasterol and *n*-octacosanol by spectral and chemical analysis.

Xanthium strumarium (Linn.)[1] is commonly known as *Gokhru* in Hindi and is mainly distributed in tropical and subtropical regions of the world[2]. The plant is used for the treatment of hydrophobia, rabbies, intermittent fevers and exhibits diuretic and antitumour activity[3].

The dried and crushed leaves of *Xanthium strumarium* (procured from M/s United Chemicals and Allied Products, Calcutta) were exhaustively extracted with methanol. The methanol extract was concentrated under reduced pressure. The greenish-brown mass obtained was successively refluxed with petrol, benzene and ethyl acetate and finally with acetone.

The petroleum ether and benzene fractions on TLC over Si-gel (pet-benzene, 5 : 5) were found to be identical and they were mixed.

The mixed fraction was subjected to co-chromatography over silica gel using *n*-hexane, petrol, benzene as eluents. The fractions when worked up gave compounds 1, 2, 3 and 4.

Compound 1. The fraction eluated from co-chromatography by pet-benzene (6 : 4) gave white crystals.

Molecular formula: $C_{30}H_{50}O$; m.pt. 198°C $[\alpha]_D^{25}$ + 80° ($CHCl_3$). IR spectrum showed bands at 3360 cm^{-1} (OH), 2960 cm^{-1} (C–H str), 1650 cm^{-1}, 1040–980 cm^{-1} (C=C).

^1H NMR ($CDCl_3$): 0.78 (s, 3H, Me); 0.83 (s, 3H, Me); 0.88 (s, 6H, 2Me); 0.95 (s, 3H, Me); 0.98 (s, 3H, Me) 1.0 (s, 3H, Me); 1.14 (s, 3H, Me); 1.08, 2.01, 3.01 (dd, J = 9 Hz and 7 Hz, 1 Hz $-CH_2$, –CH protons of cyclic and side chains); 4.88 (1 H, s, br, OH); 5.21 (1 H, m, olefinic protons). MS data: m/z $|M|^+$ – 426.

From these data and direct comparison with the authentic sample[3] the compound 1 was identified as β-amyrin.

Compound 2: The fraction eluated from CC by pet-benzene (3 : 7) mixture gave a white crystalline compound.

Molecular formula: $C_{29}H_{50}O$; m.pt. 136–137°C $[\alpha]_D^{28}$ – 45° ($CHCl_3$).

IR spectrum showed bands at 3390 cm^{-1} (OH); 2920 cm^{-1} ($-CH_3$–CH_2);

1635 cm^{-1} (C=CH stretching); 1455 cm^{-1} ($-CH_3$); 1385, 1125, 1045, 1040, 1020 cm^{-1} (steroidal nucleus); 995, 950 cm^{-1} (cyclopentane ring); 845, 800 cm^{-1} (C=CH deformation).

^1H NMR spectrum of the monoacetyl derivative of the sterol: 0.66 (s, 3H, C_{18}–Me); 0.82 (d, J = 7.0, 6H, C_{26}–Me and C_{27}–Me); 0.90 (t, 3H, C_{39}–Me); 0.92 (d, J = 3.0, 3H, C_{21}–Me); 0.98 (s, 3H, C_{18}–Me); 2.22 (s, 3H, C_3–OAc), 4.50 (m, 1H, C_3–H); 5.35 dd, J = 4.0, 8.0, 1H, C_6–H (vinyl proton). MS data: m/z $|M|^+$ 414.

On the basis of these spectral data compound 2 was identified as β-sitosterol.

Compound 3: It was eluated from petroleum ether.

Molecular formula: $C_{28}H_{58}O$, m.pt. 84°.

IR spectrum showed bands at 2960 cm^{-1} (C–H str. of methyl gp.), 2915 cm^{-1} (C–H str. of methylene gp., 3630 OH). ^1H-NMR ($CdCl_3$): 0.9 (T, 3H, Me); 1.3 (m, 2H, $-CH_2$). MS data: m/z $|M|^+$ 410.

On the basis of these spectral data compound 3 was identified as *n*-octacosanol.

Compound 4: It was eluated from pet-ether fraction as a crystalline compound.

Molecular formula: $C_{29}H_{52}O$, m.pt. 160°C $|\alpha|_D^{28}$ – 49 ($CHCl_3$).

IR spectrum of the compound showed bands at: 3388 cm^{-1} (OH); 2919 cm^{-1} ($-CH_3CH_2$); 1638 cm^{-1} (C=CH str) 1450 cm^{-1} ($-CH_3$); 993, 948 (cyclopentane ring); 884, 883 cm^{-1} (C=CH deformation). MS data: m/z $|M|^+$ – 416.

On the basis of the above data, co-chromatography and direct comparison with the authentic sample, the compound-4 was identified as stigmasterol.

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