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*NOTE*

# Isolation and Characterization of 5-Ethylhentriacontane and Nonacosane from *Salvia plebeia*

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Two aliphatic compounds isolated from aerial parts of *Salvia plebeia* have been characterized as 5-ethylhentriacontane and nonacosane by spectral data and chemical studies.

**Key Words: Salvia plebeia, 5-Ethylhentriacontane, Nonacosane**

*Salvia plebeia* R. Br. belongs to family Labiatae and is commonly known as "Bhu-Tulasi" in Hindi. The aerial parts (leaves and stem) of this plant are used as diuretic, astringent and anthelmintic[1, 2]. Except isolation of Salvia coccin and epoxy-Salvia coccin[3] (a diterpene), no detailed chemical investigation of aerial parts has been undertaken earlier. We have isolated two aliphatic compounds 5-ethylhentriacontane and nonacosane (**1** and **2**) from the ethanolic extract of aerial parts of *Salvia plebeia.*

Compound **1** was isolated as white crystals (m.p. 62–63°C). Its mass spectrum displayed a molecular ion peak [$M^+$] at m/z 464 which suggested its molecular formula as $C_{33}H_{68}$. It did not respond to test for unsaturation. IR spectrum showed no characteristic peak for unsaturation and functions. Band at 720 $cm^{-1}$ suggested the presence of a long aliphatic chain[4]. It was confirmed by the appearance of a large number of ion peaks at a systematic interval of fourteen mass units in the mass spectrum[5]. Thus compound **1** could be inferred to be 5-ethylhentriacontane, an aliphatic hydrocarbon.

The $^1H$ NMR spectrum of the compound showed the signal centred at δ 0.80 (9H, t) for three methyl groups (two terminal and one side chain methyl groups). Appearance of a one proton unresolved signal at δ 1.45 was attributed to a methine proton suggesting the presence of a side chain[5]. A fifty eight proton broad singlet at δ 1.20 indicated the presence of twenty nine methylene units in identical environment. The appearance of an intense peak at m/z 435 corresponding to $[M-29]^+$ in the mass spectrum suggested the presence of an ethyl side chain. Ion peaks at m/z 57, 407, 99, 365, 113, 351 and 421 of considerable intensities led to the location of ethyl side chain at C-5. On the basis of the foregoing account, compound **1** was characterised as 5-ethylhentria contane.

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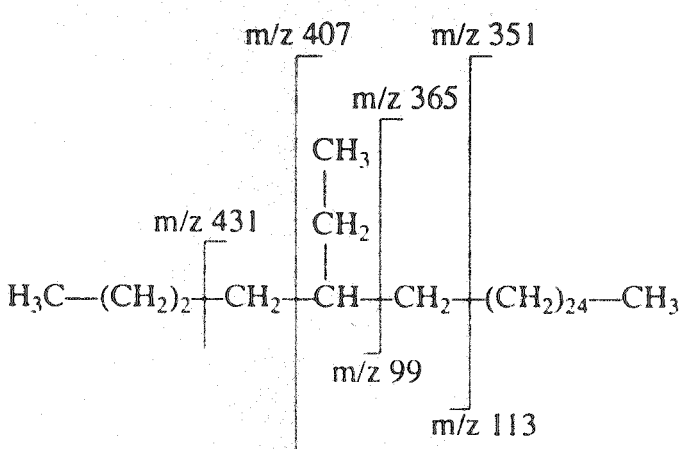
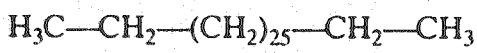
Compound nonacosane (**2**) was obtained as white crystals (m.p. 51–52°C). The molecular ion peak [$M^+$] at m/z 408 suggested its molecular formula as $C_{29}H_{60}$. Absorption bands at 725 and 710 $cm^{-1}$ in IR spectrum indicated the presence of a long aliphatic chain. IR spectrum showed no other typical peak for unsaturation and functions. A large number of ion peaks with a uniform difference of fourteen mass units in the mass spectrum confirmed the presence of a long aliphatic chain. On the basis of these facts, compound **2** may be concluded to be an aliphatic hydrocarbon.

The $^1H$ NMR spectrum of the compound displayed six proton triplet at δ 0.80 for two terminal methyl groups. A fifty four proton broad singlet at δ 1.20 was assigned to twenty seven methylene units present in identical environment. Absence of signal for methine proton and additional methyl group in $^1H$ NMR and ion peak corresponding to side chain in the mass spectrum suggested straight aliphatic chain in the molecule. Thus compound **2** was characterized as nonacosane. Its identity was finally confirmed by comparing its m.p. with the literature value[6] 53°C.




**1**




**2**

*Salvia plebeia*, collected from nearby area of Gorakhpur (U.P.), India, in March 2004, was identified by Dr. S.K. Verma, Department of Botany, St. Andrews Post Graduate College, Gorakhpur (U.P.), India. A voucher specimen has been deposited in Deptt. of Chemistry, K.B.P.G. College, Mirzapur (U.P.) India.

All m.p.s are uncorrected. IR spectra were recorded in KBr on Perkin-Elmer-881 spectrophotometer. $^1H$ NMR spectra were recorded on a Bruker Wm instrument at 300 MHz in $CDCl_3$ with TMS as internal standard and mass spectra were measured with JEOL high resolution mass spectrometer. Silica gel G (Qualigens) was used for TLC.

**Isolation**

Aerial parts of *Salvia plebeia* were separated, air-dried and ground to a coarse powder (5.0 kg). It was thoroughly extracted with hot ethanol. The extract was filtered and the solvent was removed by distillation under reduced pressure to

yield a semi-solid mass (175 g). This was fractionated into hexane-soluble fraction (125 g) and insoluble fraction (50 g).

The hexane-soluble fraction (125 g) was chromatographed over a column of silica gel (2.5 kg). The column was eluted with *n*-hexane and *n*-hexane-chloroform mixture (3 : 1). The elution of the column was monitored by intermittent CO-TLC of effluent fractions (200 mL); chromatographically identical fractions were mixed together. Repeated fractional crystallization led to the isolation of two solid compounds in pure form.

**Compound 1:** Fractions 2–11 of *n*-hexane eluate yielded a residue which recrystallized from methanol into white crystals (60 mg), m.p. 62–63°C. IR $\nu(cm^{-1})$ (KBr) 2925, 2852, 1465, 1260, 1095, 1025, 805, 720; $^1H$ NMR ($CDCl_3$) $\delta$ 0.80 (9H, t, $J = 7.0$ Hz, 3 $CH_3$), 1.20 (58 H, br s, 29 $CH_2$), 1.45 (1H, Urs, —CH). MS (m/z) (rel. int.): 464 [$M^+$] (3.4%) 449 (3.6); 435 (4.4), 421 (2.6), 408 (2.2), 407 (2.5), –380 (1.8), 379 (2.5), 365 (1.9), 351 (1.9), 309 (1.9), 281 (2.4), 267 (2.5), 253 (2.9), 239 (2.8), 225 (3.3), 211 (3.7), 197 (3.6), 183 (4.1), 169 (5.0), 155 (6.5), 127 (9.9), 113 (11.2), 99 (13.8), 85 (50.6), 71 (85.0, 57 (100).

**Compound 2:** Fractions 2–8 of *n*-hexane-chloroform (3 : 1) eluate afforded a white mass which was recrystallized into white crystals (75 g), m.p. 51–52°C. IR $\nu(cm^{-1})$ (KBr) 2910, 2860, 1585, 1460, 1365, 1250, 1070, 800, 725, 710; $^1H$ NMR ($CDCl_3$) $\delta$ 0.80 (6 H, t, $J = 7.0$ Hz, $2CH_3$), 1.20 (54 H, br s, 27 $CH_2$); MS m/z (rel. int.) 408 [$M^+$] (2.0%), 351 (2.0), 337 (2.2), 309 (2.0), 267 (2.2), 253, (5.0), 211 (3.5), 169 (5.0), 127 (10.0), 99 (15.1), 85 (50.0), 71 (67.0), 57 (100).

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