HENTRIACONTANE FROM Scabiosa comosa

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The raw material - 1 kg of the epigeal part of Scabiosa comosa Fisch. ex Roem et Schult., family Dipsacaceae - after the extraction of the combined alkaloids was covered with chloroform at pH 7.0. The chloroform extract was decanted off and concentrated in vacuum to a syrupy consistency. The viscous extract was transferred to a column of alumina (Brockman activity II) and eluted with petroleum ether, 200-ml fractions being collected.

Fractions 2-10 yielded by recrystallization (from acetone) a substance with mp 68° C. Its IR spectrum showed the stretching vibrations of C-H bonds at 2850 and 2920 cm⁻¹, the deformation vibrations of the same bonds (C-H) at 1470 and 1380 cm⁻¹, and the vibrations of CH₂-CH₃ groups at 720 cm⁻¹. These vibrations are characteristic for saturated hydrocarbons [1]. The elementary analysis corresponded to the composition $C_{31}H_{64}$, M⁺ 436. The maximum peak was that of the ion M - 14, due to the splitting off of CH₂ groups. The loss of 15 mass units was also observed, which was confirmed by the appearance of an M - 15 peak [2, 3]. The NMR spectrum of the substance (JNM-4H-60, 60 MHz instrument, CDCl₃, internal standard TMS, δ scale) contained a narrow three-proton signal at 0.88 ppm, which characterizes the presence of a CH₃ group for saturated hydrocarbons, and a signal at 1.27 ppm - CH₂ [4].

On the basis of the facts given, we identified the substance as hentriacontane.

Fractions 11-19, by recrystallization from acetone, yielded white tabular crystals with mp 67°C. The elementary analysis corresponded to the empirical formula $C_{31}H_{64}$, M^{\dagger} 436. In the mass spectrum, a strong peak appeared at m/e 31, showing the presence of branching in this compound [2]. The NMR and IR spectra were also characteristic for saturated hydrocarbons. The results of the investigations show that the second substance is an isomer of hentriacontane.

The mass and NMR spectra were taken in VNIKhFI im. S. Ordzhonikidze [S. Ordzhonikidze All-Union Scientific-Research Institute of Pharmaceutical Chemistry] under the direction of Yu. N. Sheinker.

LITERATURE CITED

- L. Bellamy, Infrared Spectra of Complex Molecules, second ed., Methuen, London/Wiley, New York (1958).
- 2. R. Ryhage, S. Stallberg-Stenhagen, and E. Stenhagen, Arkiv. Kemi, 14, 259 (1959).
- 3. H. Budzikiewicz, C. Djerassi, and D. Williams, Interpretation of Mass Spectra of Organic Compounds, Holden-Day, San Francisco (1964).
- 4. J. Slomp and F. Mackellar, J. Am. Chem. Soc., 82, 999 (1960).

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