Short Communication

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PROSOPOL STRUCTURE: A RE-INVESTIGATION

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INTRODUCTION

Reinvestigation of the structure of "Prosopol" isolated from *Prosopis glandulosa* was undertaken from a spectroscopic point of view. Early report about some chemical constituents of this plant was published in 1968 [1]. In this report it is suggested that prosopol is a new natural compound, which contains saturated cyclic rings. Our spectral investigations strongly indicate that the extracted chemical called prosopol is in fact n-triacontanol [2].

So under chemical ionisation conditions (NH_3) we determined that molecular ion is 438, and not 420 as shown by the routine mass spectrum: we observed an ion at *m/e* 456 (100 %) which is a characteristic of the chemically ionised molecular ion $(M + NH_4)^+$ [3]. Moreover, exact mass measurements indicate that peak 420 represents a $C_{30}H_{60}$ moiety and not $C_{29}H_{56}O$ as suggested before [1]. Of course, in the routine mass spectrum, fragment ion 420 results from the loss of water, which is a well known process for long chain alcohols [4]. This is also confirmed by the presence of an intense metastable ion at *m/e** 402.74 corresponding to this feature. Further, a long chain alcohol structure is in agreement with the observed numerous peak groups of 14 mass units, for which the intensity is increasing as the weight of fragments is decreasing.

Elemental analysis was also reperformed and is found to be in fairly good agreement with a molecular formula $C_{30}H_{62}O$. So we propose that prosopol has a $CH_3(CH_2)_{28}CH_2OH$ structure which is n-triacontanol.

This structure is consistent with the 60 MHz NMR spectrum. Despite the low solubility of prosopol in usual NMR solvents, it is possible to observe a very low intensity triplet (J=6Hz) at δ 3.62 corresponding to the absorption of methylenic protons of a $-CH_2OH$ group. Another low intensity triplet is observed at δ 0.83 (J=6.5Hz) for the protons of only one methyl group. Moreover, the overall appearance of ^1H NMR spectrum prosopol looks exactly like the one of 1-octadecanol [5], characterised by a strong signal (singlet) at δ 1.23 ppm.

EXPERIMENTAL

Melting point is uncorrected. NMR spectrum was recorded on VARIAN EM 360 A instrument with TMS as internal reference; chemical shifts were measured in ppm (δ). Mass spectra were obtained on a VARIAN MAT CH 5 instrument at 70 eV with a direct insertion. Exact mass was determined on a VG instrument 7070 F, working on electronic impact at 70 eV with a direct insertion (200°, resolution 10,000, sweeping rate : 10 sec per ten units). Mass chemical ionisation was performed on a VG-Micro Mass 305 at 200° with direct insertion and chemical ionisation of NH_3.

Prosopol was isolated from *Prosopis glandulosa* as reported [1]. m.p. 82.5–83.5° (Petroleum ether, Lit. 86.5° [2]. It analysed for $C_{30}H_{62}O$ (Found: C, 81,.90; H, 14.22; O, 3.39 % M^+, 420. Calculated for $C_{30}H_{62}O$: C, 82.11; H, 14.24; O, 3.65 %) *m/e* : 420 (M^+ 29 %) 406 (2), 392 (34), 378 (2), 364 (6), 350 (1), 349 (2), 336 (3), 335 (3), 321 (3), 308 (3), 307 (3), 293 (3), 279 (3), 265 (4), 251 (4), 237 (5), 223 (5), 209 (6), 195 (6), 181 (8), 168 (5), 167 (9), 154 (6), 153 (12), 152 (6), 141 (5), 140 (6), 139 (18), 138 (7), 127 (6), 126 (8), 125 (24), 124 (9), 113 (8), 112 (12), 111 (39), 110 (10), 99 (10), 98 (15), 97 (63), 96 (26), 95 (8), 85 (29), 84 (18), 83 (63), 82 (46), 81 (11), 71 (44), 70 (23), 69 (49), 68 (28), 67 (11), 58 (5), 57 (76), 56 (24), 55 (50), 54 (6), 43 (58), 42 (8), 41 (24), 40 (100 %). Exact mass (Found : 420.46867; calculated for $C_{30}H_{60}$; 420.469476) Mass chemical ionisation of NH_3 : 457 (34 %), 456 (100), 454 (8), 442 (3), 429 (13), 428 (42). ^1H NMR ($CDCl_3$) δ 0.83 (t, 3H), δ 1.0–1.9 (m, 57 H, with strong absorption at δ 1.23), δ 3.62 (t, 2H).

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