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A NEW AROMATIC ESTER AND OTHER CONSTITUENTS OF *Salvia aucheri* var. *canescens*

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SUMMARY

The roots of an endemic *Salvia* species, *Salvia aucheri* var. *canescens* Boiss. and Heldr. have been investigated and a new aromatic ester together with two diterpenoids, a triterpenoid and a steroidal compound were isolated. The structures of the new and the known compounds were determined by spectral methods and by TLC comparision with authentic samples except for the new compound.

ÖZET

Salvia aucheri var. *canescens* Boiss. and Heldr. bitkisinin köklerinden yeni bir aromatik ester ile iki diterpenoit, bir triterpen ve bir steroidal bileşik izole edildi. Yeni ve bilinen bileşiklerin yapıları spektral yöntemlerle ve İTK'de bilinen numunelerle karşılaştırılarak açıklandı.

Key words: *Salvia aucheri* var. *canescens* Boiss. and Heldr.; Labiatae; aromatic ester; terpenoidal compounds.

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INTRODUCTION

There are 86 *Salvia* species grown in Turkey, half of these species are endemic 51). Since 1968, *Salvia* species have been investigated by our group for their flavonoids and terpenoidal compounds (2-6). *Salvia* species have been used as folk medicine in Turkey for their sedative, digestive, diuretic and antiperspirant activities (7). There are a number of investigations on the pharmacological activities (8, 9). In our studies the antibacterial (10, 11) and antitumor (12) activities were also established.

RESULTS and DISCUSSION

From the roots of *Salvia aucheri* var. *canescens* Boiss. and Heldr. a new aromatic ester (**1**) was isolated together with four known compounds. These were 7-acetylhorminone (**2**), horminone (**3**), ursolic acid (**4**) and β-sitosterol (**5**).

Compound 1; White crystaline compound, mp 59-60°C. The ^{1}H NMR spectrum of **1** showed two broad doublets in the aromatic region, at δ 7.07 (2H, br d, J=8 Hz, H-3' and H-5') and 6.76 (2H, br d, J=8 Hz, H-2' and H-6') and nine methylene triplets at δ 4.24 (2H, t, J=7 Hz, C-2 protons), 2.85 (2H, t, J=7 Hz, C-3 protons), 2.27 (2H, t, J=7 Hz, C-4 protons), 1.59 (12H, m, C_5 - C_{10} protons), and one methyl triplet at δ 0.89 (3H, t, J=7 Hz, C-11 protons). In the IR spectrum of **1** there was a phenolic hydroxyl group at 3350 cm^{-1}, an aliphatic chain at 2870 cm^{-1}, aromatic peaks were at 3030, 1580 cm^{-1} and an ester carbonyl group at 1730 cm^{-1}. The UV maximum 276 nm correlated the presence of substituted aromatic ring system. In the ^{13}C NMR and APT spectrum, there was an ester carbonyl group at 175.5 ppm (C-1), the carbon next to the hydroxyl group at 155.0 ppm (C-4'), a signal at 65.0 ppm indicated the methylene group next to an oxygen function (C-2), 35.0 ppm (C-3). The HRMS indicated a molecular formula ($C_{17}H_{26}O_3$) at **m/z** 278.1881. The spectral data showed that compound **1** was a p-hydroxybenzoyldeca ester.

Compound 2; 7-Acetylhorminone was a yellow crystaline compound with a melting point 185°C. The ^{1}H NMR spectrum indicated the presence of an isopropyl group at δ 3.16 (1H, septet, J=7 Hz, H-15), 1.18 (3H, d, J=7 Hz), 1.22 (3H, d, J=7 Hz) (H-16 and H-17) and the presence of three methyl groups at δ 0.88, 0.89, 1.17 (3H, s, of each). An aromatic signal at δ 7.12 (1H, br s), D_2O exchange showed that it was a hydroxyl group. An acetyl peak at δ 2.06 was observed. The UV maximum of **2** was at 405 nm indicating the quinoid character of this compound. The signal at 1650 cm^{-1} in the IR spectrum correlated a paraquinoid ring system at ring C, in addition at 1730, 1240 cm^{-1} an acetyl group was indicated. The ^{13}C NMR and APT spectra correlated the presence of the quinoid

system (183.2 ppm, for two carbonyl groups), ppm as well as an oxygen substituted carbon at 64.09 ppm (C-7), acetyl carbonyl at 170.05 ppm (C-21). The spectral data have shown that **2** could be 7-acetylhorminone (13-14), TLC comparisons with an authentic sample proved that compound **2** was 7-acetylhorminone.

Compound 3; Horminone, the ^1H NMR spectrum indicated the presence of an isopropyl group at δ 3.16 (1H, septet, J=7 Hz, H-15), 1.17 (3H, d, J=7 Hz), 1.16 (3H, d, J=7 Hz) (H-16 and H-17) and the presence of three methyl signals at δ 0.82, 0.89, 1.21 (3H, s, of each). In addition the presence of signals at δ 7.27 (1H, br s, 12-OH), 3.04 (1H, br s, 7-OH) D_2O exchange showed that these two signals were the hydroxyl groups. The UV maximum of **3** was at 409 nm and the signal at 1630 cm^{-1} in the IR spectrum indicated a paraquinoid ring system rather then an aromatic system at ring C. These spectral data have indicated that **3** could be horminone (15). Its comparison with authentic sample on TLC has proven that compound **3** is horminone.

Compound 4 and 5 were ursolic acid **4** and β-sitosterol 5 which were widely found in plant kingdom. Their structures were decided by UV; IR; and ^1H NMR; as well as by comparison with authentic samples on TLC plates.

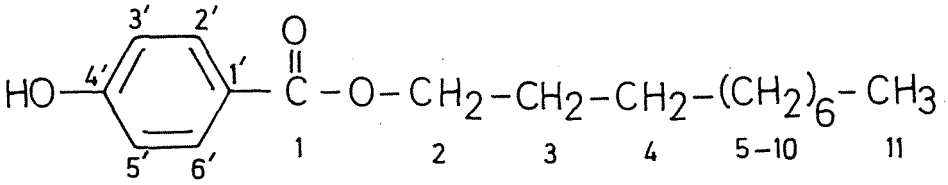
EXPERIMENTAL

General Experimental Procedures - Spectra were recorded with the following instruments: ^1H NMR and ^{13}C NMR on a Bruker AC 200 L; IR on a Perkin-Elmer 983; UV Varian Techtron 635; MS Kratos MS 30.

Plant Material - *Salvia aucheri* var. *canescens* Boiss. and Heldr. was collected from Ermenek-Karaman in July 1991. A voucher specimen is deposited in the Herbarium of the Faculty of Pharmacy, University of Marmara (MARE 3359).

Extraction and Isolation - Air dried roots were extracted with petroleum ether in a Soxhlet apparatus and concentrated to a small volume in vacuo. and re-extracted with acetone and ethanol. Both petroleum ether and acetone extracts were compared on TLC plates, since they were nearly the same the acetone extract was studied. Acetone extract was seperated in a silica gel column (5x70 cm). The column was eluted with petroleum ether and ethyl acetate using a gradient method followed by ethanol. The fractions were purified by preparative TLC, and the following compounds were obtained: compound **1** (30 mg), compound **2** (15 mg), compound **3** (20 mg), compound **4** (10 mg), compound **5** (15 mg). Aromatic ester: Mp 59-60°C. UV λ_{max}^{MeOH} nm: 276 (log ε 3.5), 230 (log ε

4.3). IR $\lambda_{max}^{CHCl_3}$ cm^{-1} : 3350, 3030, 2880, 2870, 2830, 1730, 1675, 1650, 1615, 1580, 1240, 840. ^1H NMR ($CDCl_3$) given in t he text. ^{13}C NMR ($CDCl_3$): 154.0 (C-1'), 116.5 (C-2' and C-6'), 130.1 (C-3' and C-5'), 155.0 (C-4'), 175.5 (C-1), 65.5 (C-2), 34.3 (C-3), 34.2 (C-4), 29.8 (C-5) (C-6) (C-7) (C-8) (C-9), 25.6 (C-10), 14.1 (C-11). HRMS m/z (rel. int.): 278.1881 ($C_{17}H_{26}O_3$) $[M]^+$ (8), 121 $[M-C_{10}H_{21}O]^+$ (100), 137 $[M-C_{10}H_{21}]^+$ (18).



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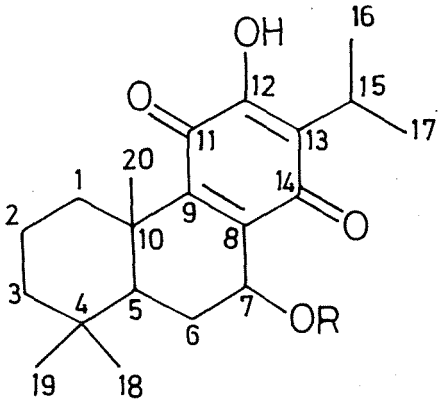

2 R = Ac

3 R = H

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