

# MOSCHATOL - A NEW COUMARIN FROM THE ROOTS OF *Ferula moschata*

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From an acetone extract of the roots of *Ferula moschata* (Reinsch) K.-Pol., in addition to conferol [1] [ $R_f$  0.32 on Woelm DS silica gel, petroleum ether-ethyl acetate (1:1)], by chromatography on alumina and subsequent preparative thin-layer chromatography on silica gel in the petroleum ether-ethyl acetate (1:1) system we have isolated a substance isomeric with conferol having  $R_f$  0.27, composition  $C_{24}H_{30}O_4$  ( $M^+$  382), mp 78-80°C (from ether, Kofler),  $[\alpha]_D^{20}$  -77.4° (c 0.2; ethanol), which we have called moschatol.

It follows from the UV spectrum of moschatol [ $\lambda_{max}^{EtOH}$  214, 242, 252, 325 nm ( $\log \epsilon$  4.20; 3.62; 3.51; 4.14)] that it is an umbelliferone derivative, and the IR spectrum (Fig. 1) shows the presence of a hydroxy group ( $3400\text{ cm}^{-1}$ ).

The NMR spectrum of moschatol (taken on a Varian HA-100D instrument,  $CCl_4$ , 0 - HMDS) shows the following signals ( $\delta$ , ppm): 0.79 (s, 3H), 0.83 (s, 3H), 0.92 (s, 3H) ( $CH_3-C-$ ) 1.60 (3H), broadened signal ( $CH_3-C=C$ ); 5.42 (1H), broadened signal ( $H-C=C$ ); 3.14 (q, 1H),  $J_{aa}=9\text{ Hz}$ ,  $J_{ae}=6\text{ Hz}$  ( $H-C-OH$ ); 3.91 (q,  $J_{gem}=10\text{ Hz}$ ,  $J_{vic}=6\text{ Hz}$ ), 4.09 (q,  $J_{gem}=10\text{ Hz}$ ,  $J_{vic}=4\text{ Hz}$ ) ( $Ar-O-CH_2-CH$ ); 6.06 (d, 1H),  $J=9.3\text{ Hz}$  ( $C_3-H$ ); 7.45 (d, 1H),  $J=9.3\text{ Hz}$  ( $C_4-H$ ); 7.20 (d, 1H),  $J=9\text{ Hz}$  ( $C_5-H$ ); 6.70 (1H) ( $C_8-H$ ); and 6.66 (1H) ( $C_6-H$ ).

The NMR spectrum of moschatol is similar to that of conferol [1], but the nature of the splitting of the signal of the proton geminal to the hydroxy group shows that in this compound the hydroxyl is equatorial. It follows from the completely analogous fragmentation of moschatol and of conferol on mass spectrometry that these compounds are stereoisomers.

Thus, moschatol is a stereoisomer of conferol in which the hydroxyl is present in the equatorial position.

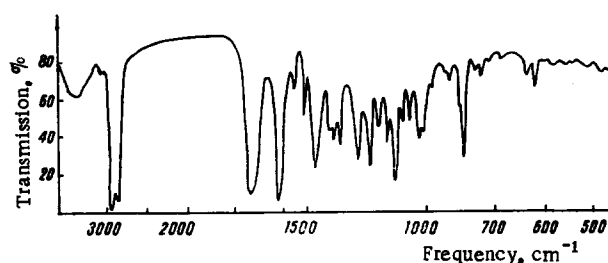


Fig. 1. IR spectrum of moschatol (mull in paraffin oil).

## LITERATURE CITED

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