A SESQUITERPENE LACTONE FROM Saussurea amara

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From the epigeal part of Saussurea amara (L.) DC., collected in the Central Tien Shan, by extraction with water followed by chromatography on silica gel with elution by chloroform we have isolated a sesquiterpene lactone in the form of a colorless viscous liquid with the composition $C_{19}H_{22}O_6 \cdot H_2O$, $[\alpha]_D^{20}$ +105.1° (c 3.36; ethanol). Its IR spectrum has the following absorption bands (λ_{max}, cm^{-1}): 3490 (OH), 3470-3360 (H_2O), 1760 (γ-lactone), 1715 (OCO-C=C), 1660 and 1645 (C=C). Hydrolysis of the lactone (I) isolated gave a dihydroxylactone (II) with the composition $C_{15}H_{18}O_4$, also in the form of a viscous liquid, which, like the initial substance, did not crystallize when it was treated with various solvents. With acetic anhydride in pyridine, compound (II) formed a diacetate with the composition $C_{19}H_{22}O_6$, again a noncrystalline product. Consequently, (I) consisted of an ester of an acid $C_4H_6O_3$ with a sesquiterpene hydroxylactone $C_{15}H_{18}O_4$.

On comparing the constants of compound (I) and the features of its IR and NMR spectra with literature information, we found that they were close to those for saupirin from S. pulchella Fisch. [1] and cynaropicrin from Cynara scolymus L. [2, 3] and Centaurea americana [4]. The difficulty in identifying (I) was that, as mentioned above, compounds (I) and (II) were noncrystalline substances while cynaropicrin itself is also noncrystalline and deacylcynaropicrin is a crystalline substance; saupirin and deacylsaupirin are crystalline substances. In view of this, we silylated (II). The silyl derivative so obtained had the same melting point (115-117°C) as the corresponding derivative of cynaropicrin. The NMR spectra of these derivatives were also close [4].

In a detailed study of the NMR spectra of (I) taken in various solvents ($CDCl_3$, Py-d_5, DMSO-d_6) and a comparison of them with literature information on the NMR spectrum of cynaropicrin (in DMSO-d_6) we found that (I) was identical with cynaropicrin: multiplets at 6.18 and 5.91 ppm, signals of vinyl protons in the acyl group; doublets at 6.01 and 5.51 ppm, signals of the protons of an exocyclic methylene conjugated with a lactone ring; broadened doublets at 5.06 and 4.81 ppm, signals of the protons of an exocyclic methylene in a five-membered ring; a broadened singlet at 5.20 ppm, signal of one of the protons of an exocyclic methylene in a seven-membered ring (the signal of the second proton is superposed on the signal of a hemiacyl proton in the form of a multiplet at 5.15 ppm); and a broadened triplet at 4.34 ppm, signal of a lactone proton.

Thus, the substance that we have isolated from S. amara is cynaropicrin.

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