A TRITERPENE ACID FROM THE ROOTS OF Cephalaria kotschyi and C. nachiczevanica

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From chloroform extracts of the roots Cephalaria kotschyi Boiss. et Hoh. and C. nachiczevanica Bobr., family Dipsacaceae, we have isolated substance (I) with the composition $C_{30}H_{48}O_4$, mp 280-282°C (from ethanol) $[\alpha]_D^{20}$ + 65.7° (c 0.8; dimethylformamide). It consists of small white acicular crystals readily soluble in dimethylformamide and pyridine, and sparingly soluble in ethanol, chloroform, and diethyl ether, and water.

On the basis of the positive Salkowski and Lieberman—Burchard reactions and the presence of a maximum at 310 nm in the UV spectrum taken in concentrated sulfuric acid, (I) was assigned to the class of triterpene compounds (there was no inflection in the 300-305-nm region) of the β-amyrin series [1]. By a direct comparison it was shown that the UV absorption spectrum of the substance in concentrated sulfuric acid differed from those of β-amyrin derivatives described in the literature [2].

The IR spectrum of (I) showed absorption bands of an OH group (3420 and 3200 cm^{-1}) and of a carboxy carbonyl (1690 cm^{-1}). There is no keto group and no conjugated system in (I) (no maximum in the 220-400-nm region).

As the NMR spectrum shows (δ scale, HA-100D, deuteropyridine, 0 — HMDS), the molecule of (I) contains one double bond, probably of secondary-tertiary nature (weakly resolved triplet at 5.44 ppm, 1H).

The presence of a carboxy group in the compound was shown by the formation of a methyl ester (single in the NMR spectrum at 3.60 ppm, 3H). The acetylation of (I) with acetic anhydride in pyridine formed a monoacetate (II), $C_{32}H_{50}O_5$, mp 289-292°C (from aqueous ethanol).

The IR spectrum of the acetate showed the absorption bands of an OH group (3260 cm^{-1}), an ester group (1730 cm^{-1}), and a carboxy carbonyl (1710 cm^{-1}).

The NMR spectrum of (II) (solution in $CDCl_3$) showed a three-proton singlet at 2.02 ppm, and a geminal proton at a secondary hydroxyl, which appeared in the NMR spectrum of (I) at 3.40 ppm (multiplet, 1H), was shifted downfield in the spectrum of (II), as was to be expected, appearing in the form of a one-proton multiplet at 4.47 ppm. An olefinic proton was also shown in the spectrum of (II) (5.21 ppm, 1H).

Thus, the compound under investigation contains two hydroxy groups one of which is tertiary. The results of a comparison of the physicochemical properties of the acid and its derivatives with those of the triterpene acids described in the literature available to us [3, 4] permitted the conclusions that the acid isolated was apparently a new β-amyrin derivative.

LITERATURE CITED

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