A NEW XANTHONE COMPOUND FROM *Centaurium erythraea*. IV

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From the roots of *Frasera caroliniensis* Walt. we have previously isolated a tetrasubstituted xanthone with the 1,3,4,5-type of substitution: 1,3-dihydroxy-4,5-dimethoxyxanthone [1]. We have now isolated a new xanthone compound, 1,4-dihydroxy-3,5-dimethoxyxanthone from the epigeal part of *Centaurium erythraea* Rafn.

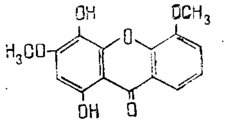
From a chloroform extract by rechromatography on silica gel with elution by chloroform, a crystalline substance was isolated with the formula $C_{15}H_{12}O_6$, M^+ 228, mp 249-251°C (from MeOH), of xanthone nature.

In the UV spectrum of the substance five absorption maxima were observed: λ_{max}^{MeOH} (nm), 244, 254, 274, 309, 364; + NaOAc 240, 255, 264, 284, 308, 362; + NaOAc/H_3BO_3 243, 254, 273, 309, 364; + $AlCl_3$, 245, 267, 284, 340, 420; + $AlCl_3$/HCl 246, 267, 283, 338, 420; + NaOMe 241, 264, 283, 330, 396.

The PMR spectrum of the compound (0 — TMS, δ, deuteropyridine, ppm) contained the signals of four aromatic protons: 6.24 (s, 1H, H-2); 7.84 (q, J_1 = 8 Hz, J_2 = 3 Hz, 1H) corresponding to H-8; and 7.44 (q, J_1 = 8 Hz, J_2 = 3 Hz, 1H) and 7.2 (t, ΣJ = 16 Hz, 1H) relating to H-6 and H-7, respectively. In the 3.74 (s, 3H, OCH_3) and 3.96 (s, 3H, OCH_3) regions there were the signals of two methoxy groups. In the PMR spectrum of the acetate of the substance (δ, $CDCl_3$, ppm), at 2.48 and 2.54 (s, 3H each, $-OCOCH_3$) there were the signals of two acetyl groups, and two methoxy groups at 3.88 (s, 3H, OCH_3) and 4.04 (s, 3H, OCH_3). The signal of the methoxy group at 4.04 corresponds to position 3 [2]. The position of the second methoxy group was determined from the mass spectrum. Thus, the mass spectrum contained, in addition to the molecular peak M^+ 288 (100%), a peak with m/z 273 (100%), corresponding to M — 15. The presence of this peak is characteristic for xanthones containing a methoxy group in position 5 [3]. To prove the 1,3,4,5-type of substitution, the initial compound was methylated with diazomethane. This gave 1-hydroxy-3,4,5-trimethoxyxanthone, $C_{16}H_4O_6$, M^+ 302, mp 185-186°C (sublimation of the compound).

The UV spectrum of the methylated compound had four absorption maxima: λ_{max}^{MeOH} (nm) 239, 263, 330, 364; + NaOAc 263, 330, 363; + NaOAc/H_3BO_3 263, 330, 364; + $AlCl_3$ 240, 278, 334, 374; + $AlCl_3$/HCl 240, 278, 334, 374; + NaOMe 243, 276, 338, 410. One hydroxy group in the molecule of the compound is present in position 1, as was shown by the UV spectrum with $AlCl_3$ from the bathochromic shift of the long-wave maximum [4]. The second hydroxy group was present in position 4, which follows from the negative Gibbs test [3].

On the basis of what has been stated, it may be concluded that the substance has the structure of 1,4-dihydroxy-3,5-dimethoxyxanthone and is a new xanthone compound



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