Poncimarin, a New Coumarin from *Poncirus trifoliata* L.

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*A new coumarinic derivative (Poncimarin: C₁₇H₁₈O₅; m.p. 140°C) was isolated from unripe fruits of *Poncirus trifoliata* L. which from spectroscopic evidences was formulated as 7-(2,3-epoxy-3-methylbutyloxy)-8-(2,3-epoxy-3-methylbutyl) coumarin.

In a systematic study of the coumarinic components of *Poncirus trifoliata* L. (Fam. Rutaceae; subfam. Aurantioideae), we recently described the presence of the coumarins aurapten and 6-methoxy-7-geranyloxy coumarin ¹ and the furocoumarins isopimpinellin, prangenin and pragenin hydrate ² in addition to the already reported bergapten and imperatorin ³. From the roots of the same plant the unknown coumarin present in low amount in the unripe fruits. This coumarin, which we call poncitrin ⁴ was also isolated.

We are now reporting the characterization of a unknown coumarin present in low amount in the unripe fruits. This coumarin, which we call poncimarin, is formulated from the evidences reported here as 7-(2,3-epoxy-3-methylbutyloxy)-8-(2,3-epoxy-3-methylbutyl) coumarin (1).

Poncimarin (1) is an optically active \([\alpha]_D^{20} = -56.2^\circ\) \((\text{CHCl}_3, c 9.4)\), neutral coumarin, which crystallized from \(\text{CH}_2\text{OH}\) in white needles, m.p. 140°C, and showed violet-blue fluorescent to UV light. Elemental analysis yielded \(\text{C}_9\text{H}_8\text{O}_2\) and the molecular weight is 328.6 (calcd. 330.37) (osmometric method; \(\text{CHCl}_3\)). The UV absorption spectrum [(95% \(\text{CH}_2\text{OH}\)) \(\lambda_{\text{max}}\) \(\text{nm} (\log e)\) 320 (4.19); 255.5 (3.61); 246 (3.60); 235 (3.57); 216 (shoulder; 4.14) and \(\lambda_{\text{min}}\): 262 (3.28); 250.5 (3.55); 240.5 (3.54); 233 (3.56)] is very similar to that of osthol and auraptenol ⁶.

The IR spectrum (KBr) of poncimarin shows absorption at 1725 (vs), 1600 (s), 1500 (m) [coumarin system], 1390 and 1380 (m) >C—C—OH and 1250 (s) [epoxide] and 830 cm⁻¹ (s) [substituted benzene ring].

The \(\text{H}^1\)-NMR spectrum of poncimarin (90 Me: 'DCl₃; TMS internal standard) shows doublets at \(\delta\) 6.26 (1H; \(J = 9.5\) cps) and \(\delta\) 7.65 (1H; \(J = 9.5\) cps), assigned to \(\text{C}_9\) and \(\text{C}_8\) protons \(a\) and \(b\) respectively and doublets at \(\delta\) 6.90 (1H; \(J = 8.6\) cps) and \(\delta\) 7.37 (1H; \(J = 8.6\) cps) assigned to \(\text{C}_9\) and \(\text{C}_8\) ortho benzenic protons \(d\) and \(e\) respectively.

A four-line signal of \(\text{A}_2\) system centered at \(\delta\) 4.23 (2H) assigned to methylene \(e\). A broad multisignal absorption from \(\delta\) 3.0 to \(\delta\) 3.40 (4H) assigned to benzylic methylene \(g\) and to the epoxide protons \(f, h\). Four singlets at \(\delta\) 1.30; 1.39; 1.41; 1.51 (3H each) for the two geminal methyls.

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