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

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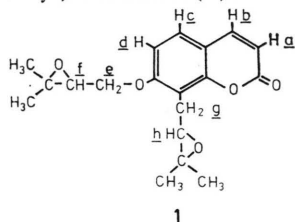
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Poncirus trifoliata, Rutaceae, New Coumarin,
NMR chemical shift

A new coumarinic derivative (Poncimarín; $C_{19}H_{22}O_5$; 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-methyl butyloxy)-8-(2,3-epoxy-3-methyl butyl) 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 coumarin¹ and the furocoumarins isopimpinellin, prangenin and pragenin hydrate² in addition to the already reported bergapten and imperatorin³. From the roots of the same plant the coumarins seselin, marmesin⁴ and poncitrin⁵ were 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 poncimarín, is formulated from the evidences reported here as 7-(2,3-epoxy-3-methylbutyloxy)-8-(2,3-epoxy-3-methylbutyl) coumarin (**1**).



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¹ A. Guiotto, P. Rodighiero, and U. Fornasiero, Z. Naturforsch. **29** c, 201 [1974].

² A. Guiotto, P. Rodighiero, and U. Fornasiero, Z. Naturforsch. **28** c, 260 [1973].

³ D. L. Dreyer, J. Org. Chem. **30**, 749 [1965].

Poncimarín (**1**) is an optically active $[\alpha]_D^{25} - 56.2^\circ$ ($CHCl_3$, c 9.4), neutral coumarin, which crystallized from CH_3OH in white needles, m.p. 140 °C, and showed violet-blue fluorescent to UV light. Elemental analysis yielded $C_{19}H_{22}O_5$ and the molecular weight is 328.6 (calcd. 330.37) (osmometric method; $CHCl_3$). The UV absorption spectrum [(95% C_2H_5OH) λ_{max} nm (log ϵ) 320 (4.19); 255.5 (3.61); 246 (3.60); 235 (3.57); 216 (shoulder; 4.14) and λ_{min} : 262 (3.28); 250.5 (3.55); 240.5 (3.54); 233 (3.56)] is very similar to that of osthonol and auraptenol⁶.

The IR spectrum (KBr) of poncimarín shows absorption at 1725 (vs), 1600 (s), 1500 (m) [coumarin system], 1390 and 1380 (m) $\left[\begin{array}{c} O \\ >C-C< \\ &CH_3 \\ &CH_3 \end{array} \right]$ 1250 (s) [epoxide] and 830 cm^{-1} (s) [substituted benzene ring].

The H^1 -NMR spectrum of poncimarín (90 Mc; $CDCl_3$; TMS internal standard) shows doublets at δ 6.26 (1H; $J=9.5$ cps) and δ 7.65 (1H; $J=9.5$ cps), assigned to C_3 and C_4 protons **a** and **b** respectively and doublets at δ 6.90 (1H; $J=8.6$ cps) and δ 7.37 (1H; $J=8.6$ cps) assigned to C_6 and C_5 *ortho* benzenic protons **d** and **c** respectively.

A four-line signal of AB_2 system centered at δ 4.23 (2H) assigned to methylene **e**. A broad multi-signal absorption from δ 3.0 to δ 3.40 (4H) assigned to benzylic methylene **g** and to the epoxide protons **f**, **h**. Four singlets at δ 1.30; 1.39; 1.41; 1.51 (3H each) for the two geminal methyls.

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⁴ a) T. Tomimatsu, J. Pharmac. Soc. Japan **88**, 643 [1968].

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⁶ W. L. Stanley, A. C. Waiss, Jr., R. E. Lundin, and S. Vannier, Tetrahedron **21**, 89 [1965].



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