Phytochemistry, 1971, Vol. 10, pp. 1971 to 1972. Pergamon Press. Printed in England.

PINNATERIN, A NEW COUMARIN FROM THE ROOTS OF *RUTA PINNATA**

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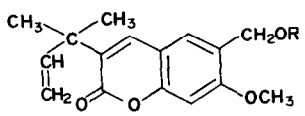
(*Received* 24 *November* 1970)

Abstract—The structure has been determined of pinnaterin (I), a new coumarin from the roots of *Ruta pinnata* L. fil.

THE SPECTROSCOPIC data presented here indicate structure I for the hydroxycoumarin of m.p. 130–132°, isolated earlier.[2] Its empirical formula is $C_{16}H_{18}O_4$, it forms a monoacetate (II), and its UV spectrum is identical to that of gravelliferone methyl ether. Since we have not found it described in the literature, we propose to name it pinnaterin (I).



I R=H
II R=Ac

The NMR (see Table 1) and mass spectra of I and II are in accord with the proposed structures. The fact that the protons —CH_2—OH in I appear at lower field than the corresponding ones in *p*-hydroxybenzyl alcohol (τ 5·61)[3] may be due to an anisotropic effect originating from the association between the hydrogen of the OH and the oxygen of the OMe group. This would impede any action of the hydroxymethyl group on H_5. This association disappears upon acetylation, the NMR spectrum of compound II showing the normal signal of a methoxyl at C_7; under the influence of the ester group, the peak of the H_5 is shifted to lower field by 0·03 ppm.

* Part XIX in the series "New Sources of Natural Coumarins".[1]

[1] Part XVIII: A. G. GONZÁLEZ, R. ESTÉVEZ and I. JARAIZ, *Anal. Quím.* **66**, 1017 (1970).
[2] A. G. GONZÁLEZ and R. ESTÉVEZ, *Phytochem.* in press.
[3] Sadtler Standard Spectra, NMR No. 4996M.

TABLE 1. τ-VALUES IN $CDCl_3$ (AT 100 MHz)

Compound	H_4	H_5	H_8	OMe	$-CH_2OH$	$-CH_2O\underline{H}$	Me_2C	$CH_2=CH-$	$CH_2=C\underline{H}-$
I	2·44 s	2·58 s	3·18 s	6·03 s	5·25 s	6 29 s	8 50 s	4·80 m 4·93 m	3 78 q
II	2·45 s	2·55 s	3·18 s	6 06 s	4·78 s*	7·85 s†	8 46 s	4·80 m 4·94 m	3·78 q

* $-CH_2OAc$
† $-CH_2O-COCH_3$.

Mass spectrum of I: molecular ion at *m/e* 274 ($C_{16}H_{18}O_4$ required 274); prominent ions at *m/e* 259 (M^+-Me), 246 (M^+-CO), 231 (M^+-Me,-CO), 215 (M^+-CH_2OH, -CO), 205 (M^+-$Me_2C-CH=CH_2$), 201 (M^+-3Me,-CO), 115 (M^+-$Me_2C-CH=CH_2$, -OMe,-CO, -CH_2OH; 100%), 69 ($Me_2\overset{+}{C}-CH=CH_2$), 41 ($CH_2=\overset{+}{C}-Me$; 98%).

Mass spectrum of II: molecular ion at *m/e* 316 ($C_{18}H_{20}O_5$ required 316); prominent ions at *m/e* 301 (M^+-Me; 100%), 289 (M^+-$CH_2=CH-$; 91%), 273 (M^+-Me,-CO), 257 (M^+-OCOMe), 247 (M^+-$Me_2C-CH=CH_2$), 243 (M^+-CH_2OCOMe), 219 (M^+-$Me_2C-CH=CH_2$, -CO), 215 (M^+-CH_2OCOMe,-CO), 69 ($Me_2C^+-CH=CH_2$).

Acknowledgements—The authors thank Dr. C. Pascual, Physikalisch-chemisches Institut, Universitat Basel, for the NMR and mass spectra. One of us (I.J.) thanks the Ministerio de Educación y Ciencia for financial help granted from 'Formación del Personal Investigador'.

Phytochemistry, 1971, Vol 10, pp. 1972 to 1973. Pergamon Press. Printed in England.

SALICACEAE

7-*O*-METHYLAROMADENDRIN FROM *POPULUS ALBA*

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(*Received* 28 *September* 1970)

Abstract—The 7-*O*-methylether of 4',5,7-trihydroxyflavanon-3-ol has been isolated from *Populus alba* L.

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† Supported by the Swiss National Foundation for Scientific Research.