KELLERIN – A NEW COUMARIN FROM THE ROOTS OF *Ferula kelleri*

V. B. Andrianova, Yu. E. Sklyar,
M. E. Perel'son, and M. G. Pimenov

UDC 547.9:582.89

From the neutral ethereal extract of the roots of Ferula kelleri K.-Pol., collected in Kirghizia, by preparative thin-layer chromatography on alumina in chloroform with subsequent rechromatography on silica gel in petroleum ether–ethyl acetate (1 : 1) we have isolated a new terpenoid coumarin with the composition $C_{26}H_{34}O_6$, mp 76-78°C (from ether, Kofler), $[\alpha]_D^{20}$ +66.4° (c 0.18; ethanol); M^+ 442, which we have called kellerin.

The UV spectrum of kellerin [$\lambda_{\max}^{\mathrm{EtOH}}$ (log ε), 215, 243, 253, 325 nm (4.17, 3.65, 3.49, 4.16)] shows that this compound is an umbelliferone derivative. The IR spectrum (Fig. 1) shows that it contains a free hydroxyl. On the basis of a comparison of these facts with the NMR spectrum (Table 1) for kellerin it is possible to put forward the probable structure (I). However, this does not exclude the possibility of the presence of an acetoxyl group in position 8 of the decalin residue and not in 6, as in (I).

TABLE 1. Parameters of the NMR Spectra of Kellerin and Its Derivatives (Varian HA-100D, 0 – HMDS)

Kellerin ($CDCl_3$)	Deacetylkellerin ($CDCl_3$)	Anhydrokellerin (CCl_4)	Assignment
0,84; s., 3H 0,87; s., 3H 1,26; s., 3H	0,81; s., 3H 0, 2; s., 3H 1,22; s., 3H	0,81; s., 3H 0,92; s., 3H 0,93; s., 3H	$CH_3-\overset{\vert}{\underset{\vert}{C}}-$
1,31; s., 3H	1,28; s., 3H	—	$\underline{CH_3}-C-OH$
1,71; s., 3H	—	1,70; s., 3H	CH_3 COO
—	—	1,70s., broadened 3H	$CH_3-C=C$
4,12; d. 28 Hz; 2H	4,01; q., 10,3 Hz, 3,0 Hz; 1H 4,16; q., 10,3 Hz, 3,4 Hz; 1H	3,81; q., 10,2 Hz, 1,6 Hz; 1H 4,08; q., 10,2 Hz, 6,0 Hz; 1H	$Ar-O-\underline{CH_2}-CH\langle$
4,58; s., $W_{\frac{1}{2}}$ 6,0Hz; 1H	3,15; q., 3,2 Hz; 2,0Hz; 1H	4,53; s., $W_{\frac{1}{2}}$ 6,0 Hz; 1H	$H-\overset{\vert}{\underset{\vert}{C}}-OR$ $R=CH_3COO$, H
—	—	5,42; s $W_{\frac{1}{2}}$ 6,4 Hz; 1H	$H-C=C$
6,19; d., 9,2 Hz; 1H	6,16; d. 9,3 Hz; 1H	6,04; d., 9,4 Hz; 1H	C_3-H
6,80; q, 9,2 Hz 2,5 Hz: 1H	6,76: q., 8,9 Hz, 2,5 Hz; 1H	6,67; q., 8,2 Hz; 2,3Hz; 1H	C_6-H
6,77; d., 2,5Hz; 1H	6,75; d., 2,5 Hz; 1H	6,73; d., 2,3 Hz; 1H	C_8-H
7,31; d. 9,2Hz; 1H	7,27; d., 8,9 Hz; 1H	7,22; d., 8,2 Hz; 1H	C_5-H
7,56; d. 9,2 Hz; 1H	7,53; d., 9,3 Hz; 1H	7,45; d., 9,4 Hz; 1H	C_4-H

All-Union Scientific-Research Institute of Medicinal Plants. Translated from Khimiya Prirodnykh Soedinenii, No. 6, pp. 795-796, November-December, 1973. Original article submitted December 3, 1972.

© 1975 Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording or otherwise, without written permission of the publisher. A copy of this article is available from the publisher for $15.00.

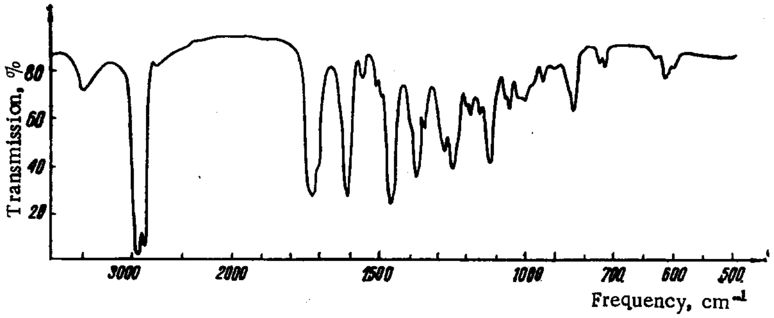
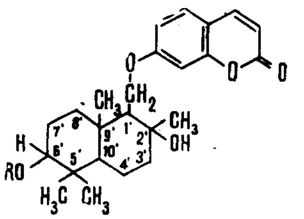


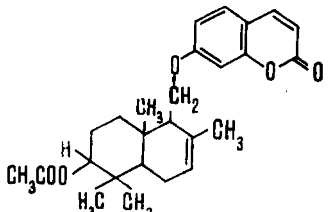
Fig. 1. IR spectrum of kellerin (mull in paraffin oil).

The alkaline hydrolysis of kellerin gave deacetylkellerin (II) with the composition $C_{24}H_{32}O_5$, mp 80-82°C. The dehydration of kellerin with thionyl chloride in pyridine formed anhydrokellerin (III), with the composition $C_{26}H_{32}O_5$, M^+ 424, a noncrystallizing oily substance. The NMR spectra of compounds (II) and (III) agree with the probable structure of kellerin (I).



I, R = CH_3CO

II, R = H



III

The structure (I) formally corresponds to that of samarcandin acetate [1]. However, deacetylkellerin and kellerin differ, respectively, from samarcandin and its acetate* in their physical constants (mp, IR spectra). It is not excluded that kellerin is a stereoisomer of samarcandin acetate.

LITERATURE CITED

1. N. P. Kir'yalov and S. D. Movchan, Khim. Prirodn. Soedin., 73 (1968).

---

* Samples of samarcandin and its acetate were kindly given to us by N. P. Kir'yalov and T. V. Bukreeva.