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ISOLATION, STRUCTURE AND SYNTHESIS OF 4',5,6,7-TETRAHYDROXY-3'-METHOXYFLAVONE (BATATIFOLIN), A NEW FLAVONE FROM MIKANIA BATATIFOLIA DC.

Werner Herz and P. S. Santhanam

Department of Chemistry

Florida State University, Tallahassee, Florida 32306

and

H. Wagner, R. Höer, L. Hörhammer and L. Farkas*)

Institut für Pharmazeutische Arzneimittellehre der Universität München

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In the course of a systematic search for sesquiterpene lactones in the family Compositae we isolated from Mikania batatifolia DC. (tribe Eupatoriae) in small amount a flavone which was not identical with 3,4-dihydroxy-4',6,7-trimethoxyflavone (mikanin), obtained by Kiang and coworkers (1) from Mikania cordata (Burm. f.) B. L. Robinson. The new flavone (I) (batatifolin), mp 250 - 253°, λ_{max} 256, 274 and 352 nm, had one methoxyl group, gave a tetra-acetate of mp 201 - 203° and furnished on methylation 3',4',5,6,7-penta-methoxyflavone (sinensetin), (II), mp 166 - 168° (2).

The nmr spectrum (DMSO) of batatifolin had signals at δ 3.79 (OCH_3), 6.62s (H-8), 6.7s (H-3), 6.97 dbr (J = 8.5, H-5'), 7.45br (H-2') and 7.48 dbr (J = 8.5, H-6'), in agreement with this distribution of functional groups. Because of the green ferric chloride reaction and ultraviolet spectral measurements, batatifolin had to be either the 7- or 3'-monomethyl ether of 6-hydroxyluteolin (III) (3).

To establish the structure of batatifolin we first synthesized 7-methoxy-5,6,3',4'-tetrahydroxyflavone (IV) from 4,6-dimethoxy-2,5-di(3,4-dibenzyloxy)-benzoyloxyacetophenone. Baker-Venkataraman rearrangement, ring closure with

*) Permanent address, Hungarian Academy of Sciences, Budapest, Hungary.

ethanolic sulfuric acid, hydrolysis with sodium methoxide to 6-hydroxy-5,7-dimethoxy-3',4'-dibenzyloxy-flavone, debenzylation and partial demethylation of the methoxyl group at C-5 furnished IV which had mp 302 - 304°. This substance, which has since been synthesized by a different route by Krishnaswamy and coworkers (4) was not identical with batatifolin. The recent work (4) indicates that pedalitin (5) from Sesamum indicum L. possesses the structure of IV.

For the purpose of synthesizing the isomeric 3'-monomethyl ether of III. 3',4',5,6,7-pentahydroxy-flavone/pentaacetate (V) (3), was partially benzylated at C-4'- and C-7- and saponified with sodium methoxide to 4',7-dibenzyloxy-3',5,6-trihydroxyflavone. Partial methylation (at C-3') and hydrogenolysis yielded 3'-methoxy-4',5,6,7-tetrahydroxyflavone (I). Mp (201 - 203°) and nmr spectrum of synthetic I tetraacetate were identical with mp and nmr spectrum of the tetraacetate of batatifolin.

An Indian group (7) has recently isolated from Lippia nodifera (Verbenaceae) a non-crystalline flavone to which structure I was assigned. Because physical data and a test substance for comparison are lacking, the identity of their material with batatifolin has not yet been established.

Details of our study will be published shortly in Chemische Berichte.

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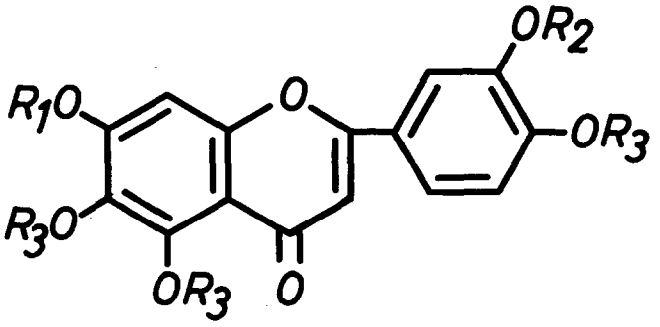

	R_1	R_2	R_3
I	H	CH_3	H
II	CH_3	CH_3	CH_3
III	H	H	H
IV	CH_3	H	H
V	CH_3CO	CH_3CO	CH_3CO

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