Pergamon

PII: S0031–9422(98)00069–7

Phytochemistry, Vol. 49, No. 4, pp. 1127–1128, 1998

Printed in Great Britain
0031–9422/98/$—see front matter

ACYL LUPEOLS FROM *CNIDOSCOLUS VITIFOLIUS*

ROSENEI L. BRUM, NELI K. HONDA, SONIA C. HESS, ALBERTO J. CAVALHEIRO† and FRANCO DELLE MONACHE*‡

Departamento de Quimica/CCET and Departamento de Ciencias do Ambiente, Universidade Federal de Mato Grosso do Sul, Caixa Postal 649, 79070-900, Campo Grande, MS, Brasil; † Instituto de Quimica, Universidade Estadual Paulista de Araraquara, Brasil; ‡ Centro Chimica dei Recettori del C.N.R., Istituto di Chimica, U.C.S.C., Largo Francesco Vito 1, 00168, Roma, Italia

(*Received* 8 *December* 1997)

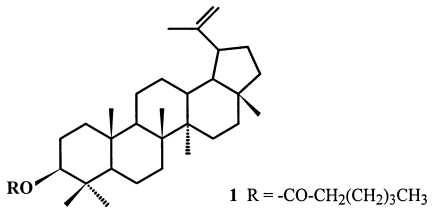
Key Word Index—*Cnidoscolus vitifolius*; Euphorbiaceae; acyl lupeols; lupeol hexanoate.

Abstract—In addition to 3-acetyl aleuritolic acid, 3β-acetyl-, cinnamoyl-, dihydrocinnamoyl-lupeol, a new ester of lupeol has been isolated from the stems of *Cnidoscolus vitifolius*. Its structure was established to be 3β-hexanoyl lupeol by spectroscopic methods. © 1998 Elsevier Science Ltd. All rights reserved

Cnidoscolus vitifolius is a latex-producing plant growing in the higher lands of the "pantanal" of Mato Grosso do Sul, Brazil. It is used in folk medicine for the treatment of callosities and cataract [1], and is known by the vernacular name of "cansançao". In this communication we report the isolation from the stems of *C. vitifolius* of 3-acetyl aleuritolic acid, a mixture of sterols, and four 3β-lupeol esters, one of which is a new compound.

RESULTS AND DISCUSSION

In addition to 3-acetyl aleuritolic acid and a mixture of sterols, the methylene dichloride extract of the stems yielded four acyl derivatives of lupeol (see Experimental). Three of them were identified by NMR techniques to be the known 3β-*O*-cinnamoyl, -dihydrocinnammoyl and -acetyl lupeols [2, 3]. The other ester is a new compound, and was assigned structure **1**. Compound **1** was obtained as a dextrorotatory powder. The ^{13}C NMR spectrum exhibited for the triterpene moiety the same signals as other acyl lupeols [2]. Additional signals were found for an ester function (δ 173.7), four methylenes (δ 34.8, 31.3, 24.8 and 22.3) and a methyl (δ 13.9), which agree for an hexanloyl group. Accordingly, the ^{1}H NMR spectrum showed a triplet ($J = 7.5$ Hz) at δ 2.29 for the methylene α to the carboxyl group. An homologous compound, lupeol heptanate, has been recently reported from *Acacia suma* (Leguminosaea) [4].



1 R = -CO-CH$_2$(CH$_2$)$_3$CH$_3$

EXPERIMENTAL

Plant material

Cnidoscolus vitifolius (Mill) Pohl was collected in Corumba (Mato Grosso do Sul, Brazil) and identified by Dr I. Cordeiro (Instituto Botanico de Sao Paulo) and Dr E. E. Dias (Herbario da UFMS em Campo Grande/MS-Brasil). A voucher specimen is deposited in herbarium CGMS under number 2352.

Extraction and isolation

The powdered air-dried stems (1.5 Kg) were extracted with cold CH_2Cl_2. Repeated CC on Silica gel (hexane with a gradient of Me_2CO or Et_2O) of the extract afforded compound **1** (40 mg), lupeol dihydrocinnamate (150 mg), lupeol cinnamate (35 mg), lupeol acetate (20 mg), 3-acetyl aleuritolic acid (125 mg) and a mixture of sterols (50 mg), successively.

Identification of known compounds

Lupeol-dihydrocinnamate, -cinnamate, -acetate [2, 3] and 3-acetyl aleuritolic acid [5] were identified by NMR data. The mixture of sterols (sitosterol, cam-

* Author to whom correspondence should be addressed.

pesterol and stigmasterol) was analysed by GC/MS with co-injection with authentic samples.

Lup-20(29)-en-3β-O-hexanoate (**1**)

$C_{36}H_{60}O_2$. FAB-MS m/z (rel. int.): 523 $[M-H]^-$ (5), 425 $[M-C_6H_{11}O]^-$ (10), 409 $[M-C_6H_{11}O_2]^-$ (50), 99 $[C_6H_{11}O]^-$ (50); Mp 130–1°C; $[\alpha]_D$ +31.8 (1.0; $CHCl_3$); IR (KBr, cm^{-1}): 1705. ^1H NMR (300 MHz, $CDCl_3$): δ 4.68 and 4.57 (*br s*, H_2-29), 4.47 (*dd*, H-3), 2.37 (*m*, H-19), 2.29 (*br t*, $J = 7.5$ Hz; H_2-2′), 1.68 (*s*, Me-30), 1.02 (*s*, Me-27), 0.94 (*s*, Me-26), 0.86–0.84 (Me-23, Me-24, Me-25, Me-6′), 0.79 (*s*, Me-28). ^{13}C NMR (75 MHz, $CDCl_3$): δ 173.7 (C-1′), 151.0 (C-20), 109.3 (C-29), 80.6 (C-3), 55.3 (C-5), 50.3 (C-9), 48.3 (C-18), 48.0 (C-19), 43.0 (C-17), 42.8 (C-14), 40.8 (C-8), 40.0 (C-22), 38.3 (C-1), 38.0 (C-13), 37.8 (C-4), 37.1 (C-10), 35.5 (C-16), 34.8 (C-2′), 34.2 (C-7), 31.3 (C- 4′), 29.8 (C-21), 27.9 (Me-23), 27.4 (C-15), 25.1 (C-12), 24.8 (C-3′), 23.7 (C-2), 22.3 (C-5′), 20.9 (C-11), 19.3 (Me-30), 18.2 (C-6), 18.0 (Me-28), 16.6 (Me-24), 16.2 (Me-25), 15.9 (Me-26), 14.5 (Me-27), 13.9 (Me-6′).

Acknowledgements—The authors are grateful to G. A. Damasceno Jr. and A. A. P. da Silva for the collection of the plant material, and to Drs I. Cordeiro and E. E. Dias for the botanical identification. Thanks are due to PROPP/UFMS for financial support.

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