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Reports on Structure Elucidation

Contents

TERPENOIDS

The absolute configuration of (–)-3-hydroxy-α-calacorene

pp 1304-1308

Robert D. Stipanovic*, Lorraine S. Puckhaber, Joseph H. Reibenspies, Howard J. Williams

We have established that (8R)-(-)-3-hydroxy- α -calacorene is found in the flowers of *Heterotheca inuloides*, while accumulation of the opposite enantiomer is induced in cold-shocked seedlings of cotton and kenaf.

Tirucallane triterpenes from the roots of Ozoroa insignis

pp 1309-1315

Yonghong Liu, Pedro Abreu*

Eight tirucallane triterpenes, methyl $3\alpha,24S$ -dihydroxytirucalla-8,25-dien-21-oate, methyl 3α -hydroxy-24-oxotirucalla-8,25-dien-21-oate, methyl 3α -hydroxy-25,26,27-trinor-24-oxotirucalla-8-en-21-oate, $3\alpha,25$ -dihydroxy-24-(2-hydroxyethyl)-tirucall-8-en-21-oic acid, $3\alpha,24S,25$ -trihydroxytirucall-8-en-21-oic acid, $3\alpha,24S,25$ -trihydroxytirucall-8-en-21-oic acid, and methyl $3\alpha,25$ -dihydroxytirucall-8-en-21-oate, together with α -elemolic acid methyl ester, were isolated from the roots of *Ozoroa insignis*. Their structures were elucidated on the basis of spectroscopic evidence.

3\alpha,25-Dihydroxy-24-(2-hydroxyethyl)-tirucall-8-en-21-oic acid (5)

Steroidal saponins from the fruits of Asparagus racemosus

pp 1316-1321

Debayan Mandal, Sukdeb Banerjee, Nirup B. Mondal, Ajit K. Chakravarty, Niranjan P. Sahu*

Three steroidal saponins, racemosides A (1), B (2) and C (3), were isolated from the methanolic extract of the fruits of *Asparagus racemosus*, and characterized as (25*S*)-5 β -spirostan-3 β -ol-3-O-{ β -D-glucopyranosyl (1 \rightarrow 6)-[α -L-rhamnopyranosyl (1 \rightarrow 6)- β -D-glucopyranosyl (25*S*)-5 β -spirostan-3 β -ol-3-O- α -L-rhamnopyranosyl (1 \rightarrow 6)- β -D-glucopyranosyl (1 \rightarrow 6)- β -D-glucopyranoside and (25*S*)-5 β -spirostan-3 β -ol-3-O-{ α -L-rhamnopyranosyl-(1 \rightarrow 6)-[α -L-rhamnopyranosyl (1 \rightarrow 4)]- β -D-glucopyranoside}, respectively, by spectrometric analysis and some chemical strategies.

1. R = rhm
$$\stackrel{6}{-}$$
 glu $\stackrel{1}{-}$ glu - 2. R = rhm $\stackrel{6}{-}$ glu $\stackrel{1}{-}$ glu - 3. R = rhm $\stackrel{4}{-}$ glu - rhm

Three ent-trachylobane diterpenes from the leaf exudates of Psiadia punctulata

Bernard F. Juma, Jacob O. Midiwo*, Abiy Yenesew, Peter G. Waterman, Matthias Heydenreich, Martin G. Peter

Three ent-trachylobane diterpenes, including 1, have been isolated from the leaf exudates of Psiadia punctulata and characterised as 6α,18,19-ent-trachylobantriol (1), 2α,18,19-enttrachylobantriol and 2β,6α,18,19-ent-trachylobantetraol. The structures were determined on the basis of spectroscopic evidence.

pp 1322-1325

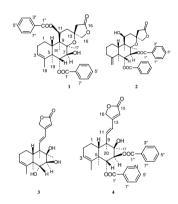
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neo-Clerodane diterpenoids from Scutellaria barbata with cytotoxic activities

Sheng-Jun Dai*, Jia-Yi Tao, Ke Liu, Yong-Tao Jiang, Li Shen

neo-Clerodane diterpenoids, named barbatins A-C (1-3), and the neo-clerodane diterpenoid nicotinyl ester, named scutebarbatine B (4), were isolated from Scutellaria barbata.



Aldingenin derivatives from the red alga Laurencia aldingensis

Luciana R. de Carvalho, Mutue T. Fujii, Nidia F. Roque, João Henrique G. Lago*

Three brominated bisabolene-type sesquiterpene derivatives, aldingenin B, C and D, together with cholesterol and palmitic acid, have been isolated from the red alga Laurencia aldingensis (Ceramiales, Rodophyta) and their structures elucidated by spectroscopic methods including NMR analysis.

Cytotoxic ent-kaurene diterpenoids from Isodon phyllostachys

Xian Li, Weilie Xiao, Jianxin Pu, Lili Ban, Yunheng Shen, Zhiying Weng, Shenghong Li, Handong Sun

Five ent-kaurene diterpenoids, phyllostachysins D-H (1-5), together with nine known compounds, rabdoloxins A-B (6-7), rabdoinflexin B (8), amethystoidin A (9), rabdokunmin D (10), macrocalyxin E (11), a flavonoid, 5,7-dihydroxy-4'-hydroxylflavone (12), oleanolic acid (13) and daucosterol (14), were isolated from the aerial parts of Isodon phyllostachys. Structures were elucidated on the basis of spectroscopic methods, especially the 2D-NMR spectroscopic analysis. All ent-kaurenoids were tested for their cytotoxic effects against K562 cells. Compound 9 was the most potent with an IC50 value of 0.69 µg/ml.

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PHENOLICS

Laurentixanthones A and B, antimicrobial xanthones from Vismia laurentii

pp 1341-1346

Jean Robert Nguemeving, Anatole Guy Blaise Azebaze, Victor Kuete, Nono Nono Eric Carly, Véronique Penlap Beng, Michèle Meyer, Alain Blond, Bernard Bodo, Augustin Ephrem Nkengfack*

Two xanthones derivatives, laurentixanthones A (1) and B (2) were isolated from *Vismia laurentii*. Their structures were determined by spectroscopic methods. They showed significant and selective antimicrobial activities against a wide range of microorganisms.

Pongamone A–E, five flavonoids from the stems of a mangrove plant, *Pongamia pinnata*

pp 1347-1352

Liya Li, Xiang Li, Cui Shi, Zhiwei Deng, Hongzheng Fu, Peter Proksch, Wenhan Lin*

Chemical investigation on the stems of the mangrove plant, *Pongamia pinnata*, resulted in the isolation and characterization of five pongamones A–E (1–5) together with 16 known flavonoid derivatives. Their structures were determined on the basis of spectroscopic analyses and by comparison of their spectroscopic data with those reported in the literature.

Geranylated phenolic constituents from the fruits of Artocarpus nobilis

pp 1353-1358

Lalith Jayasinghe*, G. Kalinga Rupasinghe, Noriyuki Hara, Yoshinori Fujimoto

Four geranylated phenolic constituents **4**, **5**, **8** and **9** besides six known chalcones and flavanones have been isolated from the fruits of *Artocarpus nobilis*. Some of these compounds showed strong radical scavenging activity against DPPH radical by spectrophotometric method.

GENERAL CHEMISTRY

Isolation and structure elucidation of cytotoxic polyacetylenes and polyenes from ${\it Echinacea~pallida}$

pp 1359-1364

Federica Pellati*, Samuele Calò, Stefania Benvenuti, Barbara Adinolfi, Paola Nieri, Michele Melegari

Two new dicarbonylic acetylenes (3, 4) and three known acetylenes (1, 2, 5) were isolated and characterized from the *n*-hexane extracts of *Echinacea pallida* roots. Compounds 1 and 2 exhibited low cytotoxicity on MIA PaCa-2 human pancreatic adenocarcinoma cells, while compounds 3–5 displayed moderate activity.

A galloylated cyanogenic glycoside from the Australian endemic rainforest tree *Elaeocarpus sericopetalus* (Elaeocarpaceae)

pp 1365-1371

Rebecca E. Miller*, Michael Stewart, Robert J. Capon, Ian E. Woodrow

A cyanogenic glycoside – 6'-O-galloylsambunigrin – has been isolated from foliage of the highly cyanogenic Australian tropical rainforest endemic *Elaeocarpus sericopetalus* (Elaeocarpaceae). This is the first published characterisation of a cyanogenic glycoside in the family Elaeocarpaceae.

Iridoid glycosides from Harpagophytum procumbens D.C. (devil's claw)

pp 1372-1377

Jin Qi, Ji-Jun Chen, Zhi-Hong Cheng, Jia-Hong Zhou, Bo-Yang Yu^* , Samuel X. Qiu

Two iridoid glycosides, harprocubine A and harprocubine B were isolated from tubers of *Harpagophytum prucumbens* D.C., along with nine known iridoid glycosides. Two of these compounds displayed marginal inhibition activity against macrophages respiratory burst following chemiluminescence method.

Rourinoside and rouremin, antimalarial constituents from Rourea minor

pp 1378-1384

Zhen-Dan He, Cui-Ying Ma, Ghee Teng Tan, Kongmany Sydara, Pamela Tamez, Bounhoong Southavong, Somsanith Bouamanivong, D. Doel Soejarto, John M. Pezzuto, Harry H.S. Fong*, Hong-Jie Zhang

Bioassay-directed fractionation of the CHCl₃ extract of the dried stems of *Rourea minor* (Gaertn.) Aubl. (Connaraceae) liana led to the isolation of two glycosides, rourinoside (1) and rouremin (2), as well as five known compounds. Compounds 1–3 showed weak *in vitro* activities against *Plasmodium falciparum*. Their structures and stereochemistry were elucidated by spectroscopic methods and selected enzyme hydrolysis.

Isotheasaponins B₁-B₃ from Camellia sinensis var. sinensis tea leaves

pp 1385-1389

Keiko Kobayashi, Toshiaki Teruya, Kiyotake Suenaga, Yoko Kobayashi, Hideki Masuda, Hideo Kigoshi*

Three saponins, isotheasaponins B_1 – B_3 , were isolated from the leaves of the tea plant *Camelia sinensis* var. *sinensis*, and their structures were determined by spectroscopic analysis.

Secondary metabolites from Opuntia ficus-indica var. saboten

pp 1390-1394

Muhammad Saleem, Hyoung Ja Kim, Chang Kyun Han, Changbae Jin, Yong Sup Lee *

Isorhamnetin glycoside (1) and ionol derivatives (2) and (3) were isolated from the butanol fraction of *Opuntia ficus-indica* var. *saboten* along with 15 known compounds. The absolute stereochemistries in compounds opuntiside A (2) and B (3) were established with the help of CD data analysis and comparison with the reported data in the literature.

Benzoic acid allopyranosides from the bark of Pseudolarix kaempferi

pp 1395-1398

Peng Liu, Hongzhu Guo*, Yin Tian, Qiao Wang, Dean Guo*

Two benzoic acid allopyranosides, pseudolaroside A and B, along with seven known compounds were isolated from the bark of *Pseudolarix kaempferi*. This is the first example of the presence of benzoic acid alloside derivatives in natural products.

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