

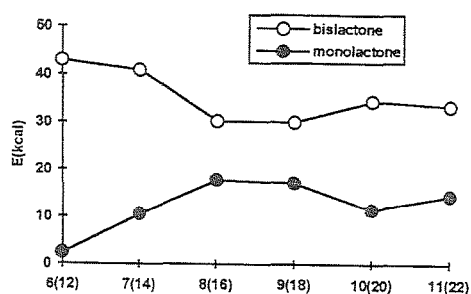
**PS05.05.04 A STUDY OF MONO- AND BISLACTONE RING FORMATION OF DEOXYCHOLIC ACID AND ITS NOR AND HOMO DERIVATIVES.** S.Stankovic, D.Lazar, K.Kuhajda and D.Miljkovic Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovica 4, 21000 Novi Sad, Serbia, Yugoslavia

The formation of 3 $\alpha$ -acetoxy-5 $\beta$ -cholano-bislactone (from 3-O-acetyl deoxycholic acid) was described in our earlier paper (1). In order to study further the lactonization processes in similar compounds, we have examined the chemical and structural features of 24-nor-5 $\beta$ -cholan-23-oic acid. The structure was determined by X-ray diffraction. Contrary to our earlier finding, in this case the monolactonization process occurred exclusively.

The pairs of molecules with 7-membered monolactone rings are related by a pseudo twofold axis, resembling molecules with 16-membered bislactone rings which possess the same element of symmetry.

Energetical examinations, applied to similar molecules containing 6- to 11 membered monolactone and 12- to 22- membered bislactone rings (obtained by modeling), are summarized in graphs. The relative energy minimum values, obtained by MMX calculations, show a dramatic change between molecules with 7- and 8-membered monolactone and, consequently 14- and 16-membered bislactone rings, which is in full agreement with our experimental results.

Conformational examinations show that the carbonyl oxygens from lactone moiety change their orientations from  $\alpha$ - to  $\beta$ -face between 14 and 16-membered bislactone rings.

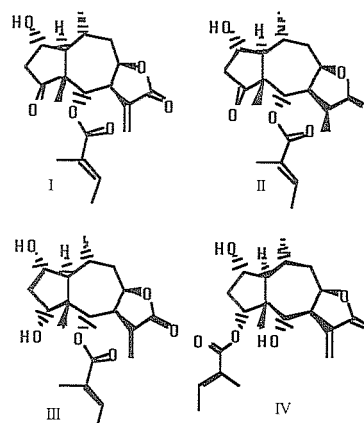


(1) S.Stankovic *et al.*, *J.Mol.Struc.*, **221** (1990), 271.

## Other Natural Products

**PS05.06.01 ARNIFOLIN AND RELATED NATURAL PRODUCTS.** Yen-Hsiang Liu<sup>1</sup>, Frank R. Fronczek<sup>1</sup> and Tom J. Schmidt<sup>2</sup>. <sup>1</sup>Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA; <sup>2</sup>Institut für Pharmazeutische Biologie der Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

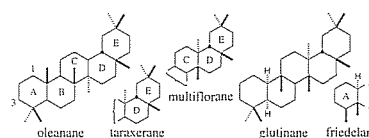
Several sesquiterpene lactones of the 10 $\alpha$ -methylpseudoguaianolide (=helenanolide) type compounds have been isolated from plants of the genus *Arnica*. This type of compound is thought to be responsible for the pharmacological activity of the *Arnica* species in phytomedicine. In this study, the crystal structures of arnifolin (I), 11 $\alpha$ -13-dihydroarnifolin (II), 2-deacetyl-6-O-tigloylchamissonolide (III), and 2-deacetyl-4-O-tigloylchamissonolide (IV) have been determined. Conformational study of the ring system shows that compounds I and II possess twist-chair conformations while compounds III and IV possess twist-boat conformations. Hydrogen bonding will also be discussed.



**PS05.06.02 CONFORMATIONAL STUDY ON SOME OLEANANE AND MIGRATED OLEANANE TRITERPENOIDS.** Tamiko Kiyotani, Yôko Arai and Hiroyuki Ageta, Showa College of Pharmaceutical Sciences Machida, Tokyo 194, Japan

Oleanane and migrated oleanane triterpenoids with an oxygen function at C-3 are distributed in many higher plants. In the course of chemotaxonomic study on ferns, we have reported some triterpenoid hydrocarbons belonging to the oleanane and migrated oleanane triterpenoids from only Polypodiaceae ferns.<sup>1)</sup> We also reported the conformational study on the related compounds by means of 2D-NMR and a molecular mechanics (MM2) calculation by Chem3D plus.<sup>2)</sup>

To confirm the conformations of the compounds, we applied an X-ray crystallographic analysis of them. As a result, an X-ray analysis indicates that the results obtained by 2D-NMR and MM2 calculation are applicable to solve their conformations. Oleanane and migrated oleanane triterpenoids:



1) Ageta, H & Arai, Y (1983). *Phytochemistry* **22**, 1801-1808.

2) Ageta, H., Arai, Y., Suzuki, H., Kiyotani, T. & Kitabayashi, M. (1995). *Chem. Pharm. Bull.* **43**, 198-203.