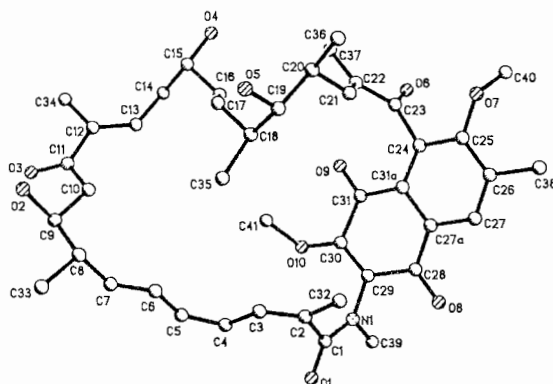


04-Crystallography of Biological Small Molecules

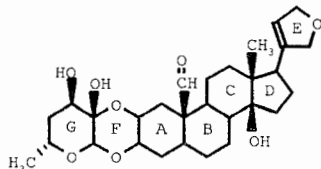
129



Crystal data: S.G. Orthorhombic $P2_12_12_1$, $a=12.925(3)$, $b=14.160(4)$, $c=23.970(6)$ Å, $C_{43}H_{53}NO_{10} \cdot CH_3OH \cdot H_2O$, $F_w=793.9$, $D_c=1.202$ Mg/m³, $Z=4$, Mo-K α radiation; $R=0.093$ and $wR=0.083$ for 3002 $F_o \gg 2.0$ (F_o).

PS-04.01.15 CRYSTAL STRUCTURE OF CALACTIN, A CARDENOLIDE FROM ASCLEPIAS LINARIA By T. Hernández-Quiroz*, M. Soriano-García, A. Rodríguez-Romero, C. Valencia, L. Hernández and F. Aguirre. Instituto de Química Universidad Nacional Autónoma de México, Delegación Coyoacán, México D.F. 04510, México and Area de Productos Naturales, Departamento de Biotecnología, Universidad Autónoma Metropolitana-Unidad Iztapalapa, Delegación Iztapalapa, México D.F. 09340, México.

Cardenolides constitute one of the several groups of plant secondary compounds that are sequestered by phytophagous insects for defense against predation. Most members of the genus *Asclepias* (Asclepiadaceae) produce the cardiac steroids at varying concentrations. The molecular structure is determined from the X-ray data and confirms the structure previously assigned on the basis of chemical and spectroscopic evidence. The title compound, $C_{27}H_{39}O_9 \cdot 2H_2O$, is crystallized in orthorhombic space group, $P2_12_12$ with $Z=8$. The cell parameters are: $a=29.868(7)$, $b=12.567(4)$, $c=14.705(5)$ Å, $R=0.064$ and $R_w=0.066$. In the two independent molecules rings A, B, C, F and G have chair conformations, ring D adopts an envelope conformation and ring E is almost flat. The A/B, B/C, A/F and C/D, F/G ring junctions are *trans* and *cis*, respectively. The crystal structure is stabilized by a three-dimensional network of hydrogen bonds and a number of C-H...O hydrogen bond interactions.



Funding for this project is provided by the National Research Council of Mexico, CONACyT, grant 1304-E9205.

PS-04.01.16

UNCOMPLEXED IONOPHORE ANALOGS-CRYSTAL STRUCTURE OF MODIFIED 25-CROWN-7 ETHER

M.Elizabeth Sobhia and K.K.Chacko

Department of Crystallography and Biophysics, University of Madras, Madras - 600 025, India.

Crown ether macrocycles undergo conformational changes when complexed with various metal salts. The conformation of complexes are often quite different for different salts but in general they all feature the O atoms directed towards the cavity of the macrocycle and the C and H atoms on the periphery. But uncomplexed crown ethers often adopt a more elongated conformation with methylene groups pointing into and filling the cavity. This is usually accomplished by rotation about the bonds to give torsion angles which differ markedly from the expected $\pm 60^\circ$ for C-C bonds. But only a very small number of C-O torsion angles are usually affected to a major extent when the macrocycle geometry is deformed in order to optimize specific ligand-substrate or intraligand interactions. The 25-Crown-7 ether crystallizes in space group $P1$ with $a = 10.809(1)$, $b = 10.945(1)$, $c = 10.256(1)$ Å, $\alpha = 107.85(1)^\circ$, $\beta = 104.15(1)^\circ$, $\gamma = 87.27(1)^\circ$ and $D_c = 1.318$ g/cm³ for $Z=2$. The structure was solved and refined to an R-index of 0.049. Three torsion angles in the macrocycle take up gauche conformation in contrast to the usual anti conformation. The crystal structure is stabilized by intramolecular van der Waals forces and C-H...O and C-H...N types of interaction. Stacking of the pyridine rings is a noticeable packing feature in the crystal lattice. Other structural details will also be presented.

PS-04.01.17 STRUCTURE AND FUNCTION STUDY ON DITERPENOID LACTONE IN TRIPTERYGIUM WILFORDII HOOK.F. BY Y.Lu*, Z.Y. Tian, Q.T. Zheng, Institute of Materia Medica, Chinese Academy of Medical Sciences, Beijing, 100050, China

In china there are three kinds of celastraceae *Tripterygium Wilfordii* Hook.f., that is *Tripterygium Wilfordii* Hook.f., *Tripterygium hypoglaucum* Hutch and *Tripterygium Sprague et Takeda*, which are distributed in Southwest China, South China and Northeast China.

At the beginning of 30's Chinese scientist Zhao Chenggu first isolated Tripterine from the root to *Tripterygium wilfordii* Hook.f and its structure was determined. Up to now, nearly 20 diterpenoid compounds have been found, which have anti-inflammatory, antitumor, antifertility and immunosuppressive properties. In 1972 Kupchan et al isolated three diterpenoid compounds and found that these compounds have protective action or antitumor activity. The research group in our country showed that these compounds exhibited various biological activities including anti-inflammatory, antitumor, antifertility and immunosuppression.

The crystal structures of Triptolide, Triptidiolide, Triptolidenol, Triptriolide, Triptchlorolide, Triptdioltonide, 16-Hydroxytriptolide and their derivatives have been determined by X-ray diffraction techniques. The structural and conformational properties with bond lengths, bond angles and torsion angles are analysed systematically. Molecular mechanical calculations have been carried out to optimize conformation and structure in solution. The stereostructure-activity relationship is discussed by molecular graphics method.