Crystal data: S.G. Orthorhombic P2₁₂₁₂₁, a=12.925(3), b=14.160(4), c=22.970(6) Å, C₄₂H₆₀O₁₂.Cl₂.H₂O, Ω=99.9, D=1.202 Mg/m³, Z=4, Mo-Kα radiation: R=0.093 and wR=0.083 for 3007 FT>2.0 (Fo).


Cardenolides constitute one of the several groups of pant secondary compounds that are sequestered by phytophagous insects for defense against predation. Most members of the genus Asclepias (Asclepiadaceae) produce the cardiotonics 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, C₂₇H₃₅O₁₂·2H₂O, is crystallized in orthorhombic space group P2₁2₁2₁ with Z=8. The cell parameters are: a=28.98(7), b=12.567(4), c=14.705(5) Å, R=0.064 and wR=0.066. In the two independent molecules b, 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-Cl hydrogen bond interactions.

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PS-04.01.16 UNCOMPLEXED IONOPHORE ANALOGS-CRYSTAL STRUCTURE OF MODIFIED 25-CROWN-7 ETHER.
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Crown ether macrocycles undergo conformational changes when complexed with various metal salts. The conformation of complexes are 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 180° 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 intramolecular interactions. The 25-Crown-7 ether crystallizes in space group P1 with a=10.890(1), b=10.945(1), c=10.556(1) Å, α=90, β=107.985(1), γ=104.15(1), P=0.727(1) mm⁻¹ and Dc=3.182 cm⁻³ for Z=2. The structure was solved by an R-index of 0.046. Three of these angles in the macrocycle take up gauche conformation in contrast to the usual all trans conformation. The crystal structure is stabilized by intramolecular van der Waals forces and C-H...Cl hydrogen bonds and C-H-C-C interactions. Stacking of the pyridazine rings is a noticeable stacking feature in the crystal lattice. Other structural details will also be presented.

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

In China there are three kinds of calacaceae Tripterygium Wilfordii Hook.f., that is Tripterygium Wilfordii Hook.f., Tripterygium hypoglaucum Hutch and Tripterygium Suipate at Takeda, which are distributed in Southwest China, South China and Northeast China. At the beginning of 30's Chinese scientist Zhao Chengyu first isolated Tripterygium 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, antifebrility and immuno-suppressive 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, antifebrility and immuno-suppression. The crystal structures of Triptolid, Triptolide, Triplopidol, Triplopidolide, Triplolide, Triplolide derivatives 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 analyzed 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.