

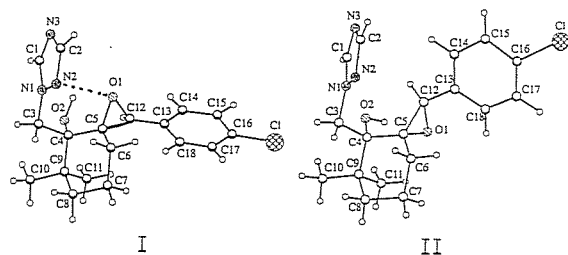
**PS05.06.03 CRYSTAL STRUCTURE OF THE TANNIN GERANIIN BASED ON CONVENTIONAL X-RAY AND ON SYNCHROTRON DATA.** Peter Luger, Manuela Weber, Freie Universität Berlin, Germany; Setsuo Kashino, Yoshiaki Amakura, Takashi Yoshida, Takuo Okuda, Okayama University, Japan; Gezina Beurskens, University of Nijmegen, The Netherlands; Zbigniew Dauter, EMBL Outstation c/o DESY, Hamburg, Germany

Geraniin,  $C_{41}H_{28}O_{27} \times 7H_2O$ , the main tannin from *Geranium thunbergii* Sieb. et Zucc. is one of the most popular folk medicines and also an official antidiarrhetic in Japan. Conventional X-ray diffractometer data at room temperature and room and low temperature (120K) synchrotron data (beam line X 1 1 at EMBL/DESY Hamburg with a MARRESEARCH imaging plate) were measured. The structure could not be determined with any of the currently distributed direct methods programs but was easily solved with DIRDIF using several conformers of the hexahydroxydiphenoyl group as input fragment into a vector search. Thus a 20 atom fragment was sufficient to solve this 75 (non H) atoms problem. A molecular structure was established where a cyclohexenetrione moiety attached to O-4 of a central glucose unit was in a hydrated six-membered hemiacetal-ring structure as expected from a solid state NMR study. Due to the high oligocyclic substitution the glucopyranosyl ring is in the unusual  ${}^1C_4$  conformation. Refinement of the low temperature synchrotron data allowed the identification of almost all hydrogens even at the seven water molecules so that a rather complex system of about thirty different hydrogen bonds can be studied in some details.

**PS05.06.04 X-RAY INVESTIGATION OF FUNGICID ACTIVITY OF OXIRAN CONTAINING TRIAZOLIL-ALKANES.** St. Malinovskii, M. Krimer. Institute of Chemistry Moldavian Acad. Sci. 277028 Kishinev.

Some of cycloalcanoles in the 1-(1H-1,2,4-triazol-1-ylmethyl) row display high biological activity. We have elaborated the stereospecific method of I and II oxiranes obtaining. (Selectivity of I formation is 100% and II - 96.5%). We have also elaborated some more diastereomeric oxirans III displaying fungicid activity.

The dependence of activity on conformation distinctions molecules was determined by X-ray method. Different positions of oxirane fragments concerning CC bond, different stabilization of the triazol cycle and different systems of H-bonds is the main cause diverse biology activity.



**PS05.06.05 CONFORMATIONAL CONSIDERATION OF NATURAL SESQUITERPENES GERMACRANE TYPE.** Bakhodir Tashkhodjaev and Mirsakadir K.Makhmudov, Institute of Chemistry of Plant Substances, 700170Tashkent, Kh. Abdullaev 77, Uzbekistan

On base our X-ray investigations of the crystal structure of the natural *E,E*-germacrane compounds and CSD data was shown that the realization conformers is depending on orientation of substitute in  $C_2$  and  $C_6$ . Germacrane are frequent occurrence among the natural sesquiterpenes. They contain flowing cyclodecadiene macrocycle. In according to Samek the cyclodecadiene may be in four conformation: chair-chair (a), boat-boat (b), chair-boat (c), boat-boat (d). The *E,E*-germacranes with 6 $\alpha$ -oxygen substitute is realized in (a) or (b) conformation. On the contrary, they are having 6 $\beta$ -oxygen substitute is realized in (c) or (d) conformation. The alternative of realization dies out, as a rule, when the oxygen group is appeared in  $C_2$  and depends on the its orientation. The configuration of endocyclic epoxy group is of crucial importance in realization of conformers. The reason of realization one in every four conformers of cyclodecadiene have been studied by molecular mechanics (MM) technique. In first approximation (by MM calculation) all mutual transitions (a-b-c-d) have been modelled by sequential torsion change around bonds  $C_3-C_4$  and  $C_9-C_{10}$ . The energetical barrier are estimated for non-substituted 6(7), 7(8) and germacrane lactone free.

**PS05.06.06 STRUCTURAL EFFECTS OF CONJUGATION IN THREE CYCLIC QUINASOLINE TYPE ALKALOIDS.** Kambarali K. Turgunov, Bakhodir Tashkhodjaev, Lev V. Molchanov, Khamidulla N. Aripov, Institute of Chemistry of Plant Substances, 700170-Tashkent, Kh.Abdullaev 77, Uzbekistan

Our investigations are devoted to the study of crystal structure of drug molecules- alkaloids quinasoline type. The threecyclic quinasolones-4 and quinasolines containing cycloalkane ring with different amount of methylene groups are sharply distinguished by the reactivity. In our mind, the properties of studied quinasoline type alkaloids are determined mainly by fine structure of part  $Car-N_1=C_2-N_3-C_4-Car$  of ring B, where pi-electronic system of double bonds and benzene ring create a pseudoaromatic system. The system is sensitively to little changes of their structures. We determined X-ray structure of 10 alkaloids polymethylenquinasolone-4 and quinasoline type and received a quantitative survey for distortions taking place.

Analysis of the geometry of the part  $Car-N_1-C_2-N_3-C_4=O$  shows a conjugation of electron pair of atoms  $N_1$  and  $N_3$  with pi-electronic system of aromatic ring and double bond  $C=O$  correspondingly. The conjugation n-pi are induced the atom  $N_3$  to transform into flat  $Nsp^2$  hybrid form. In these structures pi-electronic system of  $N=C$  bond is conjugated with electrons pair of atom  $N_3$ . The conjugation gives marked increasing of double bond  $N_1=C_2$  length and strong decreasing of the single bond  $N_3C_2$  compared with wellknown standarts. Analogical results were obtained on solvating forms of quinasoline alkaloids. In these compounds the comparison of bond lengths uncovers a shortening of the single bonds  $C_2-N_3$  and elongation of the double bonds  $N_1=C_2$ .