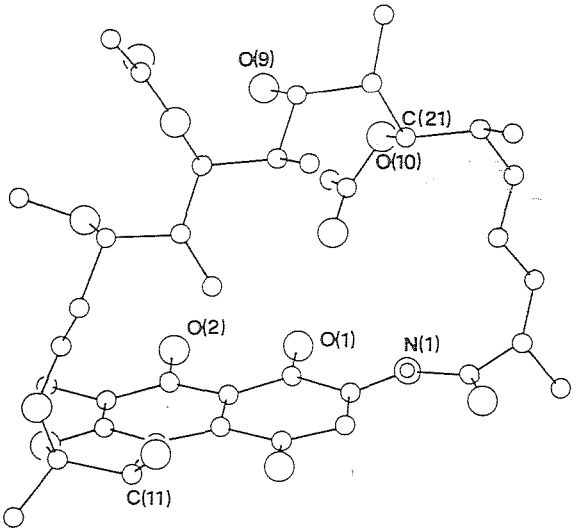
Crystal Data: S.G. P 2_1, a=11.860, b=9.139, c=20.423 Å, β=90.72° ,$C_{39}H_{49}NO_{13}.CH_3OH.H_2O$, F.W.=789.85, Dc=1.20 g.cm^{-3} for Z=2; Mo-K_α radiation.



In spite of the chemical substitution on position 21 of the ansa-chain and the reduction on position 11 of the chromophore rings, the conformation of the molecule is comparable with that of the other rifamycins. Further conformational and structural features will be discussed.

03.1–7 CAN THE CLATHRATES OF BINAPHTYL-DICARBOXYLIC ACID SERVE AS STRUCTURAL MODELS FOR THE RELATIONS IN THE ACTIVE SITE OF NATIVE SERINE PROTEASES?

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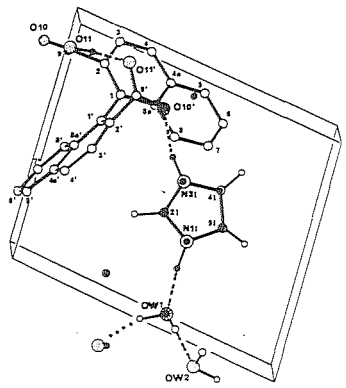
THE USE OF INCLUSION COMPOUNDS AS MODEL ENZYMES IS A RECOGNIZED APPROACH IN BIOORGANIC CHEMISTRY (Dugas,H., Penney,C. *Bioorganic Chemistry*, Springer, 1981). 1,1'-BINAPHTYL-2,2'-DICARBOXYLIC ACID (*BNDA*) HAS BEEN SHOWN TO ACT AS A VERSATILE COORDINATO-CLATHRATE HOST (Weber, *press*). THEREFORE WE ATTEMPTED TO GET COMPLEXES OF *BNDA* WITH *imidazole* BOTH IN AQUEOUS AND WATER-FREE MEDIA. THE STRUCTURE OF THE CRYSTALS OBTAINED FROM AN AQUEOUS SOLUTION (*Figure*) SHOWED SIMILARITY BOTH IN FORMAL STOICHIOMETRY (*BNDA:imidazole:2H$_2$O*) AND SPATIAL ARRANGEMENT (Δ-0.3 Å FOR SEVEN FITTED ATOMS) OF THE FUNCTIONS CORRESPONDING TO *Asp102, His57 and 2 internal water* FOUND IN THE NATIVE CRYSTALS OF *SGPA* (James,M.N.G., Sielecki,A., 1983, *Private communication*). A FURTHER POINT OF THIS STUDY IS ALSO ILLUSTRATED IN THE *Figure*, WHICH SHOWS THAT A PROTON IS TRANSFERRED FROM THE *-COOH* MIMICKING THE ROLE OF *Asp102* TO THE IMIDAZOLE RING IMITATING *His57* IN THE PROTEIN. THE WHOLE PROCESS SEEMS TO BE ATTENUATED BY THE PRESENCE OF THE WATER MOLECULES WHICH FORM CHAINS OF HYDROGEN BONDS TO DIFFERENTLY CHARGED MOIETIES THUS RENDERING FURTHER (ELECTROSTATIC) RESEMBLANCE TO THE SITUATION FOUND IN MANY SERINE PROTEASES (Kossiakoff,A.A., Spencer,S.A., 1981, *Biochemistry*, 20, 6462-6474.



Csöregh, Stensland, Czugler, *J.Amer.Chem.Soc., in the*

Crystal data: Form (I) $C_{22}H_{13}O_4^-.C_3H_5N_2^+.2H_2O$, triclinic $P\bar{1}$, Z = 2, R = 0.028 for 1975 obs. data

Form (II) $C_{22}H_{14}O_4.C_3H_4N_2$, monoclinic $P2_1/c$, Z = 4, R = 0.096 for 924 obs. data.

03.1–8 THE CRYSTAL STRUCTURES OF DI- AND TRIMETHOXYLATED 1,4-PHENANTHRENE QUINONES WITH DIFFERENT ALLERGENIC POTENCY.

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The first naturally occurring 1,4-phenanthrene quinone (PQ) with sensitizing potency, separated from the orchid Cypripedium calceolus L., has been identified by X-ray analysis and named cypripedin (2,8-Dimethoxy-7-hydroxy-1,4-PQ). Its two independent molecules showed slightly different conformations in the crystalline state (Schmalle & Hausen, Nat. Wiss. (1979) 66, 527). In order to study their sensitizing properties and cross-reactivities, a series of 12 cypripedin related PQs have been synthesized and used for sensitizing experiments in guinea pigs. As it was not possible to identify the position of one methoxy group in the quinonoid ring system by spectroscopic methods, X-ray structure determination has been performed for three PQs:

3,7,8-Trimethoxy-1,4-PQ (I)
3,5,8- " " (II)
3,8-Dimethoxy- " (III).
5,8- " -10-hydroxy-1,4-PQ (IV) was identified as a by-product of the quinone synthesis. All synthetic PQs are strong sensitizers if not being substituted in the C(2) and C(3) position of the quinonoid ring.The