coding sequence of Zymomonas mobilis QC (ZmQC) was cloned and expressed. The recombinant ZmQC shows QC activity and its 1.7Å resolution crystal structure confirmed its close relationship to the plant QC enzymes. The bacterial ZmQC protein exhibits a five β-propeller fold with a cation, presumably calcium, in its core. The β-propeller consists of a five-fold repetition of four stranded antiparallel β-sheets arranged around a central axis to form a central tunnel connecting both sides of the molecule. The propeller is stabilized through a ¨ Velcro ¨ motif that tethers the toroidal structure but lacks any disulfide bridges present in the related plant enzymes. The putative active center of ZmQC, occupied in the crystal by a glycerol molecule, is lined by the residues E46, E90, W104, W130, W175, N175 and K244. The three trytophans form a square pocket juxtaposed by the other catalytically relevant residues E46, E90 and K244.

Keywords: Alzheimer disease, bacterial glutaminyl cyclase, pyroglutamate

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Optical separation of rimantadine and *in silico* prediction of chiral selectivity of M2 protein

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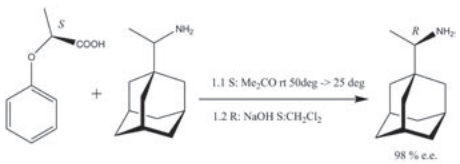
Racemic rimantadine possesses some N-methyl-D-aspartate (NMDA) antagonistic properties and is used as an antiparkinsonic drug. Rimantadine is also an orally administered antiviral drug used to treat and prevent influenza A infection. Genetic studies suggest that the virus M2 protein, a proton channel, plays an important role in the susceptibility of influenza A virus to inhibition by rimantadine. The production of chiral amines has great importance in the pharmaceutical industry, such as chiral switch. An aqueous solution of racemic compound and optically pure 2-phenoxypropionic acid [PPA] has been applied in the diastereomer salt separation.[1)] In this study, we focus on synthesis of chiral rimantadine, and clarify the inherent structures of R-rimantadine HCl and its diastereomer salt with R-PPA by X-ray analysis. From in silico prediction study of the enantiomers, it reveals that R-rimantadine has the higher inhibition activity of M2 protein than S-rimantadine and its derivative, adamantadine.



1) T Watadani, S Nunomura, Y. Takahashi and I Fujii, Jpn. Kokai Tokkyo Koho, 2008024666.

Keywords: molecular mechanics dynamics, chiral drugs, single-crystal X-ray analysis

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Validation of charge density refinements and application to molecules of biological interest

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The electronic properties of the macrolide antibiotic roxithromycin (1) that interacts with the nucleotides of the peptidyl transferase cavity of the bacterial ribosome [1] are investigated. A high resolution dataset of (1) was collected with synchrotron radiation. The experimental charge density was determined by least-squares refinements (program XD [2]) using the rigid pseudoatom formalism of Hansen and Coppens [3]. The multipole model was based on one generated by the program INVARIOMTOOL [5]. Differences between experimental- and invariom model [4] electron density were calculated on a grid. The refined multipole parameters model the electron density in the crystal (including packing effects and hydrogen bonding), but can also model disorder. (1) provides a good example that minor disorder can easily escape the attention of the examiner. However, slight differences in the electronic density tend to result in pronounced differences in the electrostatic potential. Since we hope to shed light on biological function of the molecule on the electronic level, the calculated difference density is used to validate the experimental charge density. A closely related problem in charge density refinements is over-parametrisation, which can be indicated by RFree. Results for both validation procedures are reported.

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Keywords: charge density analysis, electrostatic properties, disorder

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High-pressure crystallisation of antibiotic molecules

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The application of high pressure is a powerful method for exploring the polymorphic behaviour of simple molecular compounds.[1, 2] Direct compression of either single crystals or powders, and crystal growth from the melt are two methods that have been successfully used to prepare new polymorphs.[3] The recent development of the experimental technique for in situ high-pressure growth of single crystals from solution has allowed a wider range of compounds to be studied including small-molecule pharmaceuticals and energetic materials, and has enabled the preparation of new solvates and hydrates.[2] We have tested and extended the technique to the study of larger, more complex compounds of biological importance, namely antibiotics, with chemical formulae comprising more than 15 non-H atoms. Materials crystallised in the 0.1 - 2.0 GPa pressure range have been identified and characterised by in situ X-ray diffraction. Monitoring and understanding the effects of pressure on antibiotics is an important step towards understanding the phenomenon of polymorphism in terms of observed and favourable intermolecular

interactions and crystal packing motifs.
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2 Fabbiani F. P. A.; Pulham, C. R. Chem. Soc Rev. 2006, 35, 932-942.
3 See for example: Moggach, S. A.; Marshall, W. G.; Parsons, S. Acta Cryst. 2006, B62, 815-825; Allan, D. R.; Clark, S. J. Phys. Rev. B: Condens. Matter Mater. Phys. 1999, 60, 6328－6334.

Keywords: high-pressure polymorphism, crystal growth from solution, antibiotics

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Behaviour of the azido group in crystal structure of the intermediates of aminoglycoside antibiotics

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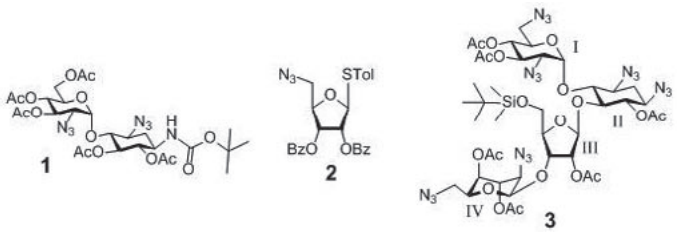
Aminoglycoside antibiotics are function through binding to specific sites in prokaryotic ribosomal RNA and affecting the fidelity of protein synthesis. Compounds **1-3** are the precursors of new derivatives of neomycin B and paromomycin. Conformational disorders of the azide groups at these compounds were observed. Compound **3** consists of pyranose (I and IV), furanose (III) and an aminocyclitol (II) rings joined together via glycosidic linkages. Compounds **1** and **2** are smaller by the number of the rings and of the azide groups. All azido groups are in a linear arrangement. In **2** it has usual geometry. The azide groups in **1** and **3** are significantly disordered. In **1** one of the azide group gave the ratio of 0.65:0.35 between the two positions, which lead to a significant distortion from the linearity. In **3** at least three from the six N_3 groups are disordered: in two the ratio between two possible conformations are 0.60:0.40 and in one- 0.80:0.20. For all of them the N=N=N angle is smaller than the literature value and most of the N=N bonds are shorter than usual bonds. Such a flexibility of the azido groups suggests that they are present in two resonance structures N=N=N and N-N≡N.



Keywords: difficult structures, antibiotics, azides

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Crystallography of steroids: A comparative analysis of geometrical features and hydrogen bonding

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Steriods are a class of biologically important organic compounds which have extensively been studied crystallographically for the last over fifty years. In view of the striking properties as exhibited by this class of materials, we have classified the cholestane (C27) into four types, viz. cholane, pregnane, androstane, oestrane, etc. and have carried out a detailed study on each of its classes to (i) compare selected bond distances and angles and their deviations from the accepted values vis-a-vis the substitutional group and X-H...A intra and intermolecular interactions, (ii) study asymmetry parameters and the importance of hybridization and ring fusions for the conformation of individual ring systems, (iii) investigate the incidence and role of X-H...A intra- and intermolecular interactions in molecular entities of this kind, (iv) prepare a database on d(H...A), D(X...A) and theta(X-H...A) range based on the cut-off criterion as proposed by Desiraju(1999), (v) study the effect of solvent on the properties of steriodal molecules and investigate the solvent-solute/solute-solvent and solvent-solvent interactions in a hydrogen bonded network. Some part of the work has been published in Acta Cryst B 2007, Z.Kristallographie, 2007., Journal of Chemical crystallography, 2007., Ind. J. Biochemistry and Biophysics 2007. A comprehensive presentation of the entire work will be made.

Keywords: crystallography, steroids, molecular structures

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Crystal and molecular structure of the diethyl ester of rhodoporphyrin

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Natural product plant porphyrins are a relatively underrepresented class in the structural databases. The current work reports the crystal and molecular structure of ethyl 8,13-diethyl-18-ethoxycarbonyl-3,7,12,17-tetramethylporphyrin-2-propionate (the diethyl ester of rhodoporphyrin) isolated from the leaves of the Thai traditional medicine plant, *Bridelia ovata* Decne, also commonly called *maka* in Thai. The structure determination was straightforward with a minor disorder of one ethyl group (refined occupancy ratio 0.77(1):0.23). The ethoxycarbonyl group is fixed to be coplanar with the porphyrin core by a concerted group of five intramolecular C－H···O interactions, while the ethyl propionate groups are oriented perpendicular to the porphyrin cores forming ribbons of intra- and inter-molecular C－H···O interactions. The other dominant packing feature is π···π stacking of the porphyrin planes, which are required to be parallel by symmetry. Experimental Data: From the leaves of *Bridelia ovata* Decne; intense violet plate crystals, recrystallized from hexane-dichloromethane solution; MP 194-196 ℃ . Crystal data: $C_{36}H_{42}N_4O_4$, *Mw*=594.74; 0.4 x 0.3 x 0.05 mm; triclinic *P*－1 (No. 2), *a*=9.409(2), *b*=12.589(2), *c*=14.683(2) Å, α=103.19(2), β=107.49(2), γ=103.40(2)°, *V*=1528.3 Å^3; *Z*=2, μ_{Cu}=0.68 mm^{-1}; d_{calc}=1.292 Mg m^{-3}; *T*=113 K; R_1(F)=0.084, *gof*=1.12.

Keywords: porphyrin, supramolecular structure, natural product

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Potassium salts of some ribonucleotides: AMP, IMP, CMP and UMP

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