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Crystal structure of the laminin-binding protein Lpb of *Streptococcus pyogenes*

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The crystal structure of the laminin-binding protein Lbp (Spy2007) of *Streptococcus pyogenes* has been determined to 2.45 Å resolution. According to recent studies, Lbp mediates adhesion of the major human pathogens *S. pyogenes* and *S. agalactiae* to the human basal lamina glycoprotein laminin. It has been shown to be essential in in vitro models of adhesion and invasion. In this study, *lbp* from *S. pyogenes* strain M1 was cloned, expressed in *E. coli* as a $(His)_6$-tagged protein and purified by IMAC. Recombinant Lbp yielded crystals belonging to the monoclinic space group $P2_1$ and of good diffraction quality. The structure of Lbp to a resolution of 2.45 Å was solved by molecular replacement using an ensemble of search models from homologous proteins and was refined to an R_{cryst} of 18.6 % and R_{free} of 24.7 %. The structure consists of a long helical backbone connecting two lobes which enclose a cobalt ion in a characteristic histidine/glutamate metal binding site. It is largely similar to that of homologous proteins, which are implicated in metal transport, but is among the first bacterial laminin-binding proteins to be determined. The crystal structure of Lbp will allow further investigations into the molecular basis of laminin-binding by human pathogens and give new insight into host-pathogen interactions. As Lbp is immunogenic and conserved in all S. pyogenes strains, its structure may guide development of an efficient vaccine.

Keywords: structural biology of bacterial pathogenesis, adhesion, metalloprotein structures

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Structural studies of isopropylmalate synthase from Mycobacterium tuberculosis.

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Although tuberculosis (TB) is a curable disease under present treatments, it is still a global threat largely due to the vast number of people infected with Mycobacterium tuberculosis in developing countries. Furthermore, the global impact of TB is widening due to an increasing prevalence of multi-drug resistant strains. New drugs, particularly ones that operate by alternative pathways from current regimens, are vital. The leucine biosynthetic pathway is essential for M. tuberculosis survival, and is not found in humans, making it an attractive target for the design of new anti-TB drugs. The three-dimensional structure of isopropylmalate synthase (IPMS), which catalyses the first committed step in this pathway, has been determined at high resolution atomic detail by X-ray crystallography using multiwavelength anomalous dispersion methods. A range of additional structures has been obtained by co-crystallisation or by soaking crystals with additives. These structures include complexes with: native substrate (ketoisovalerate); product analogue (citrate); competitive inhibitor (3-bromopyruvate); and feedback inhibitor (leucine). This repertoire of IPMS structures, together with the unliganded form, can be complemented with functional, mutagenic, and bioinformatic analyses to provide a general mechanism for activity and a sound template for the design of inhibitors specifically targeting IPMS.

Keywords: branched-chain amino acid biosynthesis, aldol-condensation reaction, active-site structure

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Structural studies of the glucuronate-xylulose pathway implicated in diabetic complications

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Diabetes mellitus is one of the world's foremost health concerns. Much of the pathology caused by the disease is due to the complications of sustained hyperglycemia. The seven-step glucuronate-xylulose (GX) pathway is over activated in diabetics. GX activity results in the depletion of D-chiro-inositol, a molecule pivotal in insulin signalling, and also of the protective osmolyte, myo-inositol. This pathway is only partially biochemically and structurally characterized. The three-dimensional structure of myo inositol oxygenase (MIOX), the enzyme that catalyses the first committed step in the GX pathway, has recently been determined at the University of Auckland, New Zealand. Inhibition of this pathway is an attractive target for the development of a novel class of therapeutics to treat diabetic complications. Our aims are to extend this investigation by (1) studying human MIOX with inhibitors and as part of a complex with the second member of the pathway, D-glucuronate reductase (aldehyde reductase-1), and by (2) investigating the three uncharacterized members of the GX pathway; L-gulonate dehydrogenase, dehydro-L-gulonate carboxylase and xylulokinase. An overview of the project and current progress will be presented.

Keywords: diabetes, inositol, glucuronate-xylulose pathway

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New polymorphs of Pigment Red 53:2

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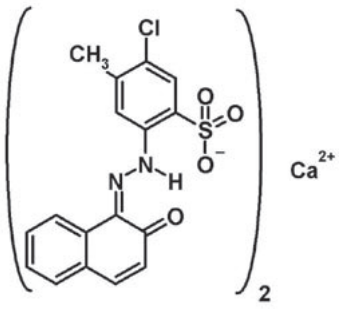
Pigment Red 53:2 is an industrial organic lake red azo pigment. It is synthesised by diazotation of 2-amino-5-chloro-4-methyl-benzenesulfonic acid with subsequent coupling on β-naphthole and final treatment with CaCl2 [1]. The pigment precipitates as a nanocrystalline powder, which is hardly soluble in water and all solvents. An extensive polymorph screening was performed using different synthetic methods and various re-crystallisation procedures. The new polymorphs show orange, red and brown

colours. All polymorphs were characterised by X-ray powder diffraction, DSC and DTA/TG. Additionally, temperature-dependent X-ray powder diffraction was used to determine the phase transitions, which occur upon heating.

[1] W. Herbst, K. Hunger, Industrial Organic Pigments, 3rd ed., Wiley-VCH, Weinheim, 269-270 (2004).



Keywords: polymorphism, organic compound, X-ray powder diffraction

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Development of Vapochromic Organic Crystals for Monitoring Systems of Sick-House Syndrome Gases

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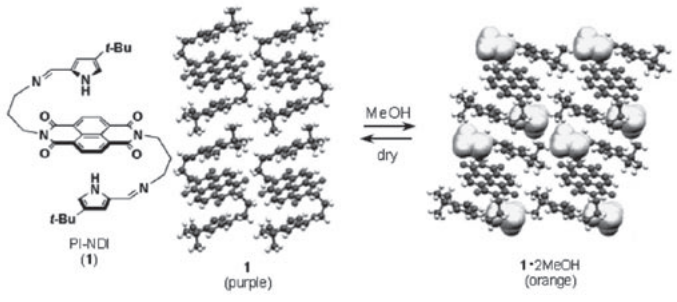
Growing public awareness of the potential risk from exposure to volatile organic compounds (VOCs) in ordinary environment has prompted us to develop organic sensing materials by crystal engineering. Of particular interest are vapochromic materials that show reversible color change in visible spectral regions upon exposure to VOCs. Porous organic crystal of PI-NDI (**1**) was obtained by recrystallization from MeOH and subsequent removal of the solvent *in vacuo*. These purple crystals exhibit vapochromic behavior upon exposure to a variety of organic vapor such as MeOH (orange), acetone (orange), toluene (red) and triethylamine (yellow). It is noteworthy that sick-house gases such as formaldehyde can be also absorbed efficiently with irreversible color change to yellow. Powder structure analysis using synchrotron X-ray at SPring-8 (BL19B2) revealed that controlled intensity of D-A interaction between the PI and NDI units is a key for the vapochromism.



Keywords: solid-state gas-sensors, powder structure determination, inclusion complexes

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Crystal engineering Intermolecular Hydrogen bond

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Crystal Engineering:
The rational design of supramolecular structure can be realized through crystal engineering based on relatively weak intermolecular forces. Among these forces, hydrogen bonding is the most common; however, other interactions including halogen-halogen or halogen-nitrogen have been used to organize molecules within the crystal. In particular, it is possible to define a supramolecular synthon as a structural unit within a supermolecule which can be formed and/or assembled by known or conceivable synthetic operations involving intermolecular interactions, by analogy with Corey`s definition of a synthon in traditional organic synthesis. To understand the design of crystal packing of substituted benzene compounds, we look to different supramolecular synthons, to determine if there is a relationship between the role of substitution pattern and differnt types of intermolecular interactions.
Intermolecular:
Intermolecular forces are forces that act between stable molecules or between functional groups of macromolecules. Intermolecular forces include momentary attractions between molecules, diatomic free elements, and individual atoms. They differ from covalent and ionic bonding in that they are not stable, but are caused by momentary polarization of particles. Because electrons have no fixed position in the structure of an atom or molecule, but rather are distributed in a probabilistic fashion based on quantum probability, there is a positive chance that the electrons are not evenly distributed and thus their electrical charges are not evenly distributed.
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Keywords: Crystal engineering, Intermolecular, Hydrogen bond

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Inorganic crystallography Geosciences

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Geosciences are the sciences of the earth, its stones, minerals and waterways. Geologists examine the history of minerals back to the origins of the planet, look at the development of the environment in recent decades, study the evolution of climate since the last Ice Age or deal with the question of why the dinosaurs died out. Geologists understand the process of sediment movement, how minerals are created, and the mineralogical constitution of the earth in the past, present and future. They are able to explain the origins of volcanoes and to forecast eruptions. Geosciences are a field study that deals with a great variety of topics. Geologists must understand the chemical composition of the waters, the physics of earthquakes and continental shifts, the evolution of life, the structures of precious stones but also the components of which the earth is made. Moreover, they must understand the impact of rain and snow on the mountains. In our society, the profession of geoscientist is a very important one,