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Membrane sorting between secretory and endocytic organelles is predominantly controlled by small carrier vesicles or tubules that are layered on their cytoplasmic faces by specific protein coats. Recently we have begun studies of a novel putative membrane coat complex termed retromer. Retromer contains five subunits, Vps35, Vps26, Vps29, Snx1 and Snx2 and is responsible for tubule-based retrieval of proteins from the endosomal system to the Golgi, for example recycling mannose-6-phosphate receptors that traffic lysosomal hydrolases from the TGN to endosomes. We have determined the crystal structure of the mammalian retromer subunit Vps29, showing that it has structural similarity to divalent metal-containing phosphoesterases. However, although Vps29 can coordinate metals in a similar manner it has no detectable phosphatase activity *in vitro*, suggesting a novel specificity or function. We show that Vps29 and Vps26 bind directly to distinct regions of Vps35 and together form a high affinity heterotrimeric sub-complex. Mutagenesis reveals the structural basis for interaction of Vps29 with Vps35 and subsequent membrane association of Vps29 *in vivo*. Furthermore, we demonstrate that a conserved hydrophobic surface distinct from the primary Vps35 binding site can mediate assembly of the Vps29p-Vps26p-Vps35p sub-complex with sorting nexins in yeast, and mutation of either site results in a defect in retromer-dependant membrane trafficking.

Keywords: membrane trafficking, protein phosphatases, X-ray structure

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Crystallization of Molybdate-Binding Protein of Xanthomonas citri

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We report the crystallization and prelliminary data of the periplasmic molybdate-binding protein (ModA) of the plant pathogen *Xanthomonas citri*, responsible for the cancer disease affecting citrus plants. Structures of molybdate transporters have been solved in other species including *Escherichia coli* and *Azotobacter vinelandii* [1, 2], however, no ortholog derived from plant-associated bacteria have been reported so far. The 26 kDa protein has been overproduced in *E. coli*, purified, and crystallized in complex with Na_2MoO_4. The crystallization of ModA using the sitting-drop vapour-diffusion method with PEG 4000 as precipitant is described. Crystals belong to the orthorhombic space group $P222_1$, with unit-cell parameters a = 68,16, b = 172,21, c = 112,05. A X-ray diffraction data were collected to a maximum resolution of 1,7 Å using a synchrotron-radiation source. Structure refinement is in progress. The ongoing biochemical characterization in combination with the structural analysis, will assist the elucidation of the structure-activity relationship in regulating the uptake of molybdate in *Xanthomonas*.

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Keywords: ModA protein, Xanthomonas citri, crystallization

MS38 CONTROLLED BUILDING OF CRYSTALS FROM NON-COVALENT INTERACTIONS

Chairpersons: Christer Aakeroy, Alessia Bacchi

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Understanding and Using Solution Chemistry to Direct Crystal Nucleation

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Our understanding of non-covalent interactions which determine crystal packing in the solid state has progressed enormously over the last years due largely to the explosion in numbers of crystal structure determinations and their availability via the Cambridge Structural Database. In the context of *controlled* building of crystals however, this information is not enough, we also have to consider the interactions which exist in the solution phase at the time of nucleation. Such information can be gleaned from a number of sources: thermodynamic and colligative data (eg solubility, freezing point depression); UV/vis spectroscopy; vibrational spectroscopies; NMR; and neutron scattering.

This paper reports on the use of these techniques in understanding the key interactions in highly concentrated solutions of urea, benzoic acid, tetrolic acid, sulfamerazine and 2,6dihydroxybenzoic acid. In many cases there is a clear link between solvent mediated self assembly and the resulting crystal structures.

Keywords: nucleation, solutions, chemistry

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Molecular Tectonics : from Tectons to Networks

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Molecular crystals are compact and periodic entities. They are defined by the nature of their molecular components and interactions between them in the solid state. Although a crystal is described by translation of the unit cell into three directions of space, one may describe it as a network by considering intermolecular interactions as specific recognition patterns. The approach dealing with such an analysis is called molecular tectonics [1]. The latter is based on tectons which are construction units bearing within their backbone assembling programmes. The design and formation of molecular networks with predefined dimensionality and connectivity may be ensured by the nature and localisation of recognition sites within the structure of tectons.

The strength of molecular tectonics is related to the fact that not only it allows to describe a given crystal in terms of networks but, also and more interestingly, this approach allows to conceive molecular networks through the specific design of tectons [2].

A variety of tecons and molecular networks based on diverse intermolecular interactions will be presented.

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Keywords: tectons, networks, chemistry

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Testing the Reliability of the Self-complementary Noncovalent Interactions: Supramolecular Implications and Supramolecular Design

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Noncovalent interactions play a special role in supramolecular chemistry, which has been defined by Lehn [1] as “chemistry beyond the molecule”. Noncovalently assisted synthetic procedures are used to assemble various types of supramolecular species. These syntheses rely on the stabilization provided by noncovalent interactions between recognition sites incorporated within precursors. As a recognition motif utilized to guide the synthesis, various types of noncovalent interactions can be used. These are, specifically, hydrogen bonds (H-bonds), stacking interactions, electrostatic interactions, hydrophobic interactions, charge-transfer interactions, and metal coordination [2]. Unconventional polymers composed of covalent and noncovalent bonds differ dramatically from standard, conventional polymers with just covalent bonds. They posses novel physical, optical, electrochemical, photochemical, biological, and catalytic properties. Targeted synthesis of macro- and supramolecular structures of various sizes, shapes, and functionality has now become possible. Supramolecular chemitry offers incredible applications in various