KN01

Conformational Change and Assembly of Proteins into Amyloid fibrils Elisabeth Sauer-Eriksson[a], Anders Karlsson, Anders Olofsson, Malin Lindhagen-Persson, Anders Öhman *Umeå Centre for Molecular Pathogenesis, Umeå University, Sweden.* E-mail: liz@ucmp.umu.se

Keywords: amyloid, conformational change, protein structure

Self-assembly and deposition of proteins into amyloid fibrils and plaques have currently been linked to around 20 different human diseases. The best known examples of such disorders are Alzheimer's disease and prion diseases. Amyloid contains extremely insoluble protein fibrils (50-150 Å) that share similar morphological features but comprise many different proteins with no obvious sequence similarity. Amyloid formation and deposition are complex processes yet to be fully understood. Evidence from numerous in vitro studies shows that amyloid formation is a multistep process involving amyloidogenic intermediates. Structural and biophysical studies on amyloid-forming proteins are pursued with the aim to elucidate further information about the structural composition of amyloid and amyloid-forming intermediates. In this talk I will review some of our work with reference to three amyloidogenic proteins: amyloid-β-peptide, medin, and transthyretin.

KN02

Software for the refinement of aperiodic and incommensurate structures Václav Petříček[a], Michal Dušek[a], Lukáš Palatinus[ab], [a]*Institute of Physics, Praha, Czech Republic,* [b]*Ecole Polytechnique Fédérale de Lausanne, Laboratoire de Cristallographie, Lausanne, Switzerland* E-mail: petricek@fzu.cz

Keywords: modulated crystal structures, structure analysis, superspace theory

The refinement of modulated structures requires a specific modification of traditional refinement programs to account for additional satellite reflections. The most natural and effective way is application of the superspace theory developed by DeWolff, Jansen & Janner [1] which makes possible to apply symmetry and generalize all formulas for calculation of structure factors. Then modulated structures are described by the same set of parameters (atomic occupancies, coordinates and displacement parameters) but they can are now a periodic functions of the actual position of atom in the crystal. This new periodicity can be generally incommensurate with the basic translation periodicity. The basic ideas and several examples of application will be presented in the first part of the lecture. Modulation functions for occupancy in many cases have non-continuous character. Then a special function called *crenel* is to be used [2]. A new numerical method, based on using orthogonalized polynomials enhancing stability of the refinement, has been recently included into the new JANA2006. Typical examples will document main advantages of this approach.

The program Superflip written by L.Palatinus, based on the new progressive method for solution of modulated structures *charge flipping* [3], prove to be the best way how to solve even strongly modulated structures. Jana2006 allows applying of this method by direct calling of the Superflip.
The new Jana2006 can also be used for refining of magnetic structures. It can be applied even for combination of nuclear and magnetic modulations in the crystal.
The last new option in Jana2006 is possibility to combine data from different sources. Several sets of powder data and single crystal data from neutron and X-ray diffraction can be refined simultaneously.

[1] Wolff de P.M.; Janssen T; Janner A. *Acta Cryst.* A37, (1981), 625.
[2] Petříček, V.; van der Lee; A. & Evain, M. (1995). *Acta Cryst.* A51, 529.
[3] Palatinus L. *Acta Cryst.* (2004). A60, 604.

KN03

Cutting and Moving DNA Miquel Coll, *Institut de Recerca Biomèdica & Institut de Biologia Molecular (CSIC), Josep Samitier 1-5, Barcelona, Spain.*
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Keywords: Protein-DNA complexes, DNA translocation, Bacterial conjugation, Horizontal gene transfer

Mechanisms of horizontal gene transfer in bacteria are typically categorized into transduction, transformation and conjugation. Transduction is mediated by bacteriophages, which may incorporate fragments of the host bacterial DNA and transfer them into the infected hosts. Natural transformation consists in the uptake of portions of naked DNA. Finally, conjugation is the unidirectional transfer of single-stranded plasmidic DNA from a donor bacterium cell to a recipient cell. Conjugation endows bacteria with a mechanism for the rapid acquisition of new genetic information. Rampant antibiotic resistance among pathogens is a troubling consequence of this microbial capacity. DNA transfer across cell membranes requires sophisticated machinery formed by a number of proteins that first perform the DNA processing and then its transmembrane transport. Although bacterial conjugation was discovered in the 40s, only now are we unveiling the molecular mechanisms behind it. In particular, structural biology [1] is providing a detailed view of the molecular architecture of several of the pieces involved, showing their evolutionary relationship with DNA replication and protein transport systems.

[1] Gomis-Rüth, F.X. & Coll, M. (2006) Cut and Move: Protein Machinery for DNA Processing in Bacterial Conjugation. *Curr. Op. Str. Biol.* 16, 744-52.

KN04

Hydrophobic dipeptides as building blocks for the construction of nanoporous organic materials Carl Henrik Görbitz, *Department of Chemistry, University of Oslo, Norway.* E-mail: c.h.gorbitz@kjemi.uio.no

Keywords: dipeptides, microporous materials, supramolecular chemistry

In the last few years dipeptides with two hydrophobic residues (hydrophobic dipeptides) have emerged as an unexpected source of stable microporous organic materials. Supramolecular self-assembly of the rather