

of these experiments in a manner that is compatible with the current high throughput crystallisation (HTPX) robotics available at the EMBL Hamburg outstation. The additional opportunities for crystal detection using ANS-based fluorescence are also now available for external users who wish to submit their samples to the EMBL HTPX.

[1] Groves, M.R., Muller, I.B., Kreplin, X. & Muller-Dieckmann, J. *Acta Crystallogr D Biol Crystallogr*. **2007** Apr; 63 (Pt 4): 526-535

Keywords: crystallization; UV fluorescence; image analysis

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Dehydration-Induced Phase Transition in D-xylose Isomerase. Francesco Gramiccia^a, Céline Besnard^b, Yves Pellegrinelli^a, Sebastian Basso^a, Marc Schiltz^a.
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D-xylose isomerase, which causes the isomerization of glucose to fructose, has a large market in the food industry because of its application in the production of high-fructose corn syrup. In order to fully understand and control the activity of the protein a good knowledge of the structural response of the protein to changes in the environmental conditions is necessary. Since proteins function in aqueous media and nearly half of the volume of protein crystals is occupied by water, protein-water interactions are of great interest.

We have now identified a dehydration-induced phase transition in D-xylose isomerase from streptomyces rubiginosus. The transition, characterized using both powder and single crystal diffraction, occurs at room temperature for relative humidity around eighty percent. After the transition, the crystal recovers its crystalline state and diffracting power. The symmetry is reduced from space-group I222 to its subgroup P2₁2₁2 but the effects of this symmetry break on the structure are subtle. The decrease of the unit-cell volume by more than 15 percent produces more pronounced and interesting structural rearrangements in the crystal.

[1] Gummow R.J., Liles D.C., *Mat. Res. Bull.*, **1993**, 28, 1293. [2] Grirrane, A.; Pastor, A.; Galindo, A.; Ienco, A.; Mealli, C. *Chem. Commun.* **2003**, 512.

Keywords: protein X-ray crystallography; phase transitions and structure; isomerases

FA1-MS09-P07

Crystallization and Structure of Two Bovine Insulin Derivatives. Biserka Prugovečki^a, Ivica Đilović^a, Dubravka Matković-Čalogović^a. ^aDepartment of Chemistry, Faculty of Science, University of Zagreb, Zagreb, Croatia.
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Insulin is a polypeptide hormone, produced by the β -cells in

the pancreas, that regulates carbohydrate metabolism and it also takes part in the metabolism of fat and proteins. Insulin is structured as two polypeptide chains, chain A consists of 21 and chain B of 30 amino acids. Bovine insulin differs in sequence from human insulin at residues A8, A10 and B30. There are three forms of insulin hexamers. These forms of insulin are used in therapeutic preparations for the control of diabetes.

The crystal structure of T₆ bovine insulin was described by Smith et al in 2005 [1]. It has been known for many years that native insulin is in the T₃R₃ form in the crystals grown in high chloride ion concentrations [2].

This work presents crystallization of two bovine insulin derivatives: in high iodine and bromine concentrations. Structural investigations on bovine bromo- and iodo-derivatives show that these halogen atoms are bound to the zinc ions. Crystals were grown by the hanging drop vapour diffusion crystallisation method. Single crystal diffraction data were collected on laboratory instrument at 100 K. The investigated insulin derivatives belong to the R3 rhombohedral space group with cell parameters $a = 79.73 \text{ \AA}$, $c = 36.34 \text{ \AA}$ and $a = 79.25 \text{ \AA}$, $c = 36.97 \text{ \AA}$ for the bromo- and iodo-derivative, respectively. Conformation of the insulin molecule and coordination of Zn-ions will be discussed.

[1] Smith, G. D., Pangborn, W. A., Blessing, R. H. *Acta Cryst.*, **2005**, D61, 1476. [2] Kaarsholm, N. C., Ko H. C., Dunn M. F. *Biochemistry*, **1989**, 28, 4427.

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FA1-MS09-P08

Arabidopsis SET-domain Proteins with Different Histone Methyltransferase Activity. Mohammad Aminur Rahman^a, Silje Veie Sandvik^a, Tage Thorstensen^a, William Davies^a, Reidunn B. Aalene^a.
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Proteins containing a conserved SET domain catalyze the methylation of lysine residues on histone tails, and influences chromatin structure. The SET-domain proteins of Arabidopsis can be grouped in the same evolutionarily conserved subclasses as found in Drosophila and mammals [1], i.e. E(Z), TRX, ASH1 and Su(VAR)3-9, that have specificities for different lysine substrates. Different SET domain proteins may also differ in product specificity, i.e. they can add one, two or three methyl groups on a given lysine residue. The structures of more than ten SET domains have been solved [2], but they do not cover all substrate and product specificities. We aim at solving the structure of the Arabidopsis SUV4, for which a novel HMTase specificity was demonstrated in that monomethylated histone H3K9 is its preferred substrate in vitro [3], and for ASH1 and ASH2 of the ASH1 class. For the latter two Arabidopsis proteins HMTase activity against H3 has been demonstrated. Although the specific target lysine(s) and product specificity