de Tecnologia Química e Biologica, Universidade Nova de Lisboa (Portugal) [c]*California Institute of Technology, Pasadena, (California) 91125.* E-mail: lpereira@itqb.unl.pt

FoxE is a protein belonging to the foxEYZ operon of sp. Strain SW2. This protein is known to confer light-dependent Fe(II) oxidation activity by itself and thus to allow for Fe(II) based anoxygenic photosynthesis[1]. This protein is estimated have 25kDa (259 residues) and two haem-c binding sites. It is believed to reside on theperiplasm and to stimulate Fe(II) oxidation directly by serving as an Fe(II)oxidoreductase.

Crystallization trials of FoxE were performed on a robot using nanoscale drops andcommercial crystallization screens. Best diffracting crystals were obtained at 293 K in 1.2 M sodium/potassium phosphate pH=7 with copper chloride as additive. Crystals were cryo protected by plunging them into mother liquor containing 25% v/v glycerol. Diffraction data was recorded at ESRF at 100 K in beamline ID23-1/2, using radiation near the iron absorption edge.

The collected dataset was processed with XDS, the phase problem was solved by Single Anomalous Dispersion method (SAD) using the HKL2MAP and the SHELXC/D/E suite.

FoxE crystals belonged to the spacegroups P3121 (trigonal) and P43212 (tetragonal). The trigonal crystal diffracted to an higher resolution with up to 2.4Ã… resolution (I/sigI=1.9 at the highest resolution shell, 2.54-2.44Ã…). The data set obtained had a global multiplicity of 32.2, Rsym=13% and Rpim=3%. The collected data contained anomalous signal up to 3.7Ã… resolution (self-anomalous CC above 30%), and since six centres were found in the anomalous substructure, one could deduce that the crystal asymmetric unit contained three FoxE molecules (crystal solvent content of 52%).

SHELXE was used to trace the main chain of the protein (610 out of 777 in the asymmetric unit). Coot and phenix were used for real and reciprocal space refinement (NCS and TLS restrains used) with a final Rwork/Rfree of 0.2227/0.2397. The final model of the trimer presents good stecheometry and only four Ramachandran outliers, as assessed by MolProbity. The Trimer formation implies 31% of surface area occlusion and the minimum distance between redox centres (two hemes and one disulfur bridge) is ca. 18 Angstroms.

[1] L.R. Croal, Y. Jiao, D.K. Newman. *Journal of Bacteriology* **2007**, *189,* 1774-1782

Keywords: photosynthesis, heme, SAD

MS01.P12

Acta Cryst. (2011) A**67,** C219

Crystal structure of zinc-finger domain of Nanos and its functional implications

Hiroshi Hashimoto,[a] Kodai Hara,[a] Asami Hishiki,[a] Shigeta Kawaguchi,[a] Takuya Yoshizawa,[a] Satoru Unzai,[a] Yutaka Tamaru,[b] Toshiyuki Shimizu,[c] Mamoru Sato,[a] [a]*Graduate School of Nanobioscience, Yokohama City University.* [b]*Graduate School of Bioresources, Mie University.* [c]*Graduate School of Pharmaceutical Sciences, The University of Tokyo (Japan).* E-mail: hash@tsurumi.yokohama-cu.ac.jp

Translational control of mRNAs is crucial in developmental processes including cell division, cell-fate determination and embryonic axis establishment in early embryogenesis. Most types of translational control are mediated by a sequence in the 3' untranslated region (3'-UTR) and are achieved by the interaction of various regulatory factors such as RNA-binding proteins. Nanos is a highly conserved RNA-binding protein in higher eukaryotes and functions as a key regulatory protein in translational control using a 3'-UTR during the development and maintenance of germ cells. In combination with Pumilio, Nanos represses the translation of maternal hunchback mRNA in the early *Drosophila* embryo, thereby governing abdominal segmentation. Nanos and Pumilio also have a variety of functions in the primary germ cells (PGCs). Nanos is essential for the development of PGCs. One of the regulatory targets of Nanos and Pumilio in PGCs is thought to be Cyclin B mRNA, Pumilio and Nanos directly bind to an element in the 3'-UTR to repress its translation. Although studies have revealed important functions of Nanos, neither the atomic structure of Nanos nor the structural basis of the interaction between Nanos and RNA has been reported.

In this study, we present the first, to our knowledge, crystal structure of the zinc-finger domain of zebrafish Nanos (residues 59–159), which includes the two conserved zinc-finger motifs. Our study also reveals that the two CCHC motifs actually bind zinc ions and that the zinc-finger domain of Nanos adopts a novel structure. Furthermore, we reveal a conserved basic surface that is responsible for RNA binding. Our results provide the structural basis for further studies to clarify Nanos function.

[1] H. Hashimoto, K. Hara, A. Hishiki, S. Kawaguchi, N. Shichijo, K. Nakamura, S. Unzai, Y. Tamaru, T. Shimizu, M. Sato, *EMBO Rep.*, **2010**, *11*, 848-853.

Keywords: structure, protein, RNA

MS01.P13

Acta Cryst. (2011) A**67,** C219

Structural Characterization of the [Co^{II}(TPP)(18-C-6)$_2$] Complex

Yassin Belghith,[a] Mohamed Salah Belkhiria,[a] Grzegorz Bujacz,[b] Anna Bujacz,[b] Habib Nasri[a] [a]*Laboratoire de Physico-Chimie des Matériaux, Faculté des Sciences de Monastir, Avenue de l'environnement, 5019 Monastir Tunisia.* [b]*Institute of Technical Biochemistry Technical, University of Lodz Stefanowskiego 4/10, 90-924 Lodz, (Poland).* E-mail: yassinbelghith@gmail.com

This work concerns the synthesis, the spectroscopic and the X-ray molecular structural characterization of a new six-coordinated cobalt(II) porphyrin derivative: bis(18-C-6) (tetraphenylporphyrinato)cobalt(II) complex ([Co^{II}(TPP)(18-C-6)$_2$]). The UV-visible spectrum of this species presents a Soret band at 412 nm and the IR spectrum exhibits a strong stretching frequencies at 1102 cm^{-1} attributed to the ν(O-C) of the ether crown 18-C-6.

The X-ray structural analysis shows that the complex [Co^{II}(TPP)(18-C-6)$_2$] crystallizes in the triclinic system (space group P-1). Crystal data for this complex: a = 10.262(2) Å, b = 11.250(2) Å, c = 11.815(2) Å, α = 104.180 (0) °, β = 106.100 (0) °and γ = 108.489 (0) °, Z= 2, R_1=0.0056, WR_2=0.181 and S=1.042. The title compound is a polymer where the cobalt(II) is bonded to two oxygen atoms of two trans coordinated ether crown 18-C-6. The Co^{II}—O(18-C-6) is 2.406 (2) Å is slightly longuer than the related species bis-THF derivative [Co^{II}(F_{28}TPP)(THF)$_2$] (octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphinato) [1] for which the distance Co^{II}—O(THF) = 2.31(1) Å.

[1] R.Crescenzi, E.Solari, C. Floriani, A.Chiesi-Villa, C.Rizzoli *Inorg.Chem.* **1996**, *35,* 2413.

Keywords: cobalt(II) porphyrin, Bis(18-crown-6) cobalt complexe

MS01.P14

Acta Cryst. (2011) A**67,** C219-C220

Refinement of the Vault particle using DEN protocols with NCS constraints

Arnau Casañas,[a] Núria Verdaguer,[a] Ignasi Fita,[a,b] [a]*Institut de*

Biología Molecular de Barcelona (CSIC), (Spain). [b]*RB Barcelona. Parc Científic de Barcelona, Baldiri i Reixac 10, 08028-Barcelona, (Spain).* E-mail: acacri@ibmb.csic.es

The Vault particle, with an astounding molecular weight of 13 MDa, is the largest Ribonucleoprotein described. Although its function is still unclear, it has been related to cell signalling, proliferation and immune responses. The Vault complex shows an overall barrel-shaped structure organized in two identical moieties, each consisting of thirty-nine copies of the major vault protein MVP. Earlier data indicated that Vault particles can dissociate at acidic pH.

Recently, we solved the crystal structure of the Vault particle at 8 Å resolution, together with the 2.1 Å structure of the seven N-terminal domains (R1-R7) of MVP. The structure reveals the interactions that govern Vault association and provides an explanation for a reversible dissociation induced by low pH. [1]. This information complemented the 3.5Å X-ray structure of the vault particle, published at the beginning of 2009 by other authors [2], showing the MVP monomers folded into twelve distinct domains: nine repeat domains, a shoulder domain, a cap-helix and a cap ring. The comparison between the structures of R1-R7 and the equivalent region in the 3.5Å structure of the entire particle showed important discrepancies in the tracing of domains R1 and R2. Furthermore, in the structure reported by Tanaka et al., all the atomic positions and temperature factors of the 39 copies of MVP found in the crystal asymmetric unit were included explicitly in the refinement (PDB ids. 2ZU0, 2ZV4 and 2ZV5, with an averaged temperature factor of 121.4 Å2). In this report, refinement of the vault structure was performed using the DEN protocols as included in the Refine low-resolution package of CNS [3]. During refinement the 39-fold non-crystallographic symmetry was always strictly maintained with constrains applied to a single MVP monomer, which was generated as a hybrid model containing the R1R7 structure at the N-terminus (residues form Glu4 to Val380) and the coordinates corresponding to monomer A (PDB id: 2ZV4) at the C-terminus (residues from P381 to G814). The deposited structure factors of the 3.5 Å vault structure (PDB id: 2ZU0) were used as experimental data. Refinement was combined with averaging and solvent flattening with DM and the quality of the resulting maps was also enhanced by applying a negative Bsharp value in a resolution dependent weighting scheme (map sharpening).

This refinement suggests important movements in the N-terminus of the MVP structure during the closing of the two Vault halves and provides an improved view of the C-terminal region.

[1] J. Querol-Audí, A. Casañas, I. Usón, D. Luque, J.R. Castón, I. Fita, N. Verdaguer, *EMBO J.* **2009,** *4, 28(21),* 3450-7. *Epub* **2009**, *24*. [2] H. Tanaka, K. Kato, E. Yamashita, T. Sumizawa, Y. Zhou, M. Yao, K. Iwasaki, M. Yoshimura, T. Tsukihara *Science*. **2009**, *16 ,323(5912)*, 384-8. [3] A.T. Brunger et al, *Crystallography & NMR System (CNS), Acta Cryst.D54,* **1998** 905-921.

Keywords: vault, macromolecular crystallography

MS01.P15

Acta Cryst. (2011) A**67,** C220

Preparation and Characterization of the complex [Co^{III}(TpivPP)(4,4'-bipy)(Cl)]

Anissa Mansour,[a] Mohamed Salah Belkhiria,[a] Jean-Claude Daran,[b] Habib Nasri,[a] [a]*Département de Chimie, Faculte´ des Sciences de Monastir, Avenue de l'environnement, 5019 Monastir Tunisia.* [b] *Laboratoire de Chimie de Coordination, CNRS UPR 8241, 205 route de Norbonne, 31077 Toulouse,Cedex 04, (France).* E-mail: anissamansour@gmail.com

Cobalt porphyrin species are specially used as models for hemoproteines and actually investigations concerning these species includes many areas such as organic reaction catalysis [1], [2] biosensors [3] and materials presenting non-linear optical activities.The (4,4'-bib yridine)(chlorido)(α,α,α,α-tetrakis(*o*-pivalamidophenyl)porphyrinato) cobalt(III) has been synthesized and characterized by UV-vis, IR and proton NMR spectroscopy which indicate, inter alia, that the cobalt ion presents the oxidation state III. The X-ray molecular structure shows that the Co(III) ion is hexa-coordinated by the four nitrogen atoms of the pyrrole rings of the TpivPP anion, the chlorido axial ligand on the pocket side of the porphyrin and the nitrogen atom of 4,4'-bipyridine ligand. The average cobalt-pyrrole nitrogen atoms is Co-N_p = 1.983 (2) Å, the Co—Cl and Co—N(bpy) bond lengths are respectively 2.230 (1)Å and 2.030 (3)Å. The compound [Co^{III}(TpivPP)(Cl)(4,4'-bipy)] crystallizes in the monoclinic space group C2/c with unit cell dimensions *a*=18,906(5) Å, *b*=19,112(6) Å, *c*=18,264(8) Å, *β*=92,112°. The structure was refined to *R*=4,61%, WR_2=13,78% and S=1,079 .

[1] S. Berner, H. Lidbaum, G. Ledung, J. Aahlund, K. Nilson, J. Schiessling, U. Gelius, J.-E. Baeckvall, C. Puglia, S. Oscarsson, *Applied Surface Sciences* **2007**, *253(18),* 7540-7548. [2] B. Wayland Bradford, Ch-H. Peng, X. Fu, Z. Lu, M. Fryd, *Macromolecules* **2006**, *39(24),* 8219-8222. [3] F. D'Souza, Y.Y. Hsieh, H. Wickman, W. Kutner *Electroanalysis*, **1997**, *9(14),* 1093-1101.

Keywords: porphyrins, single-crystal X-ray

MS01.P16

Acta Cryst. (2011) A**67,** C220-C221

Interaction of Alzheimer β-amyloid and metal complexes with lipid bilayers

Mario Suwalsky,[a] Silvia Bolognin,[b] Paolo Zatta,[b] [a]*Faculty of Chemical Sciences, University of Concepción, Concepción (Chile).* [b]*CNR-Institute for Biomedical Technologies, Department of Biology, University of Padova, Padova (Italy).* E-mail: msuwalsk@udec.cl

Alzheimer's disease is an age-related disorder characterized by progressive cognitive decline and neurodegeneration. One of the key features of this disease is the presence of amyloid plaques associated with neuritic degeneration [1]. The amyloid plaques are composed predominantly of 40-42-residue peptides, the amyloid β-peptide (βA), being the βA(1-42) the most toxic. Soluble βA peptides interact with cell membranes and have been proposed to affect membrane integrity leading to apoptosis. The molecular mechanisms of these interactions are still unclear. In the context of these observations we investigated the molecular mechanisms that might explain the abnormal accumulation of aluminum in the brains of patients with Alzheimer's disease.

There are reports indicating that Al(III) interacts with cell membranes inducing structural and functional perturbations. They might be due to: a) direct interaction of Al(III) with proteins forming ion channels, receptors and enzymes, b) induction of structural alterations in the membrane lipid bilayer, or c) action on the lipid-protein interfaces. To elucidate among these alternatives, and given the structural complexity of native cell membranes, we utilized molecular models consisting of bilayers of dimyristoylphosphatidylcholine (DMPC) and dimyristoyl-phosphatidylethanolamine (DMPE), representative of phospholipid classes located in the outer and inner monolayers of many cell membranes, respectively.

The capacity of βA and of its complexes with Al, Zn, Cu and Fe to perturb the multibilayer structures of DMPC and DMPE was evaluated by X-ray diffraction. In the context of these studies we report that βA, in our experimental conditions, did not alter any of the bilayer structures while the addition of the βA-Al complex deeply disordered that of DMPC membrane [2]. Our findings imply that Al, compared to the other βA-metal complexes tested could have a specifically relevant effect in enhancing βA toxicity. It is important to stress that, in our experimental conditions, it is not Al alone which causes such alterations but the