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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 the periplasm 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 and commercial 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 space groups P3121 (trigonal) and P43212 (tetragonal). The trigonal crystal diffracted to a higher resolution with up to 2.4 Å... resolution ( $1/\sigma I = 1.9$  at the highest resolution shell, 2.54-2.44 Å...). The data set obtained had a global multiplicity of 32.2,  $R_{sym} = 13\%$  and  $R_{pim} = 3\%$ . The collected data contained anomalous signal up to 3.7 Å... 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 restraints used) with a final  $R_{work}/R_{free}$  of 0.2227/0.2397. The final model of the trimer presents good stereochemistry 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

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

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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.

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## MS01.P13

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**Structural Characterization of the [Co<sup>II</sup>(TPP)(18-C-6)<sub>2</sub>] Complex**  
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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<sup>II</sup>(TPP)(18-C-6)<sub>2</sub>]). 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<sup>-1</sup> attributed to the ν(O-C) of the ether crown 18-C-6.

The X-ray structural analysis shows that the complex [Co<sup>II</sup>(TPP)(18-C-6)<sub>2</sub>] 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,  $R_f = 0.0056$ ,  $WR_2 = 0.181$  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<sup>II</sup>—O(18-C-6) is 2.406 (2) Å is slightly longer than the related species bis-THF derivative [Co<sup>II</sup>(F<sub>28</sub>TPP)(THF)<sub>2</sub>] (octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrinato) [1] for which the distance Co<sup>II</sup>—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 complex

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### Refinement of the Vault particle using DEN protocols with NCS constraints

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