MS12-P5 **Structural Analysis of Nur and Zur from *Streptomyces coelicolor*.** Sangmin Lee, Young Jun An, Min-Kyu Kim, Chang-Sook Jeong, Sun-Shin Cha. *Marine and Extreme Genome Research Center, Korea Ocean Research and Development Institute, Ansan, 426-744, Republic of Korea*
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Various transition metal ions are essentially required for the cell growth and survival of almost all organisms. However, excess or lack of transition metal ions are very harmfulness. Thus, cells exploit highly sensitive metal ion-binding regulators to achieve homeostasis. In the present study, we describe the Crystal structure of (Nickel uptake regulator) Nur and (Zinc uptake regulator) Zur from *Streptomyces coelicolor* at 2.4-Å resolution. These two enzyme belongs to the ferric uptake regulator (Fur) family and controls expression of genes in response to available nickel or zinc. First, Nur is a nickel responsive transcription factor that controls nickel homeostasis and antioxidative response. It contains a unique nickel-specific metal site in addition to a nonspecific common metal site. The identification of the 6-5-6 motif of the Nur recognition box and a Nur/DNA complex model reveals that Nur mainly interacts with terminal bases of the palindrome on complex formation. This contrasts with more distributed contacts between Fur and the n-1-n type of the Fur-binding motif. seconds, Zur is zinc responsive transcription factor containing zinc-binding sites (C-,M- and D-sites). Mutations of the three sites differentially affected sporulation and transcription of target genes, such that C- and M-site mutations inhibited sporulation and derepressed all target genes examined, whereas D-site mutations did not affected sporulation and derepressed only a sensitive gene. Biochemical and spectroscopic analyses of representative metal site mutants revealed that the C-site serves a structural role, whereas the M- and D- sites regulate DNA-binding activity as an on-off switch and a fine-tuner, respectively. According to their crystal structures, the Fur-family members are homodimeric proteins that share the same topology, However, the local structures of metal binding sites and their dimeric conformations differ significantly from one another.

Keywords: Nickel uptake regulator; Zinc uptake regulator; DNA binding

MS12-P6 **Structure, electrostatics and complexation of immune receptors and ligands.** Tereza Skálová,[a] Kristýna Kotýnková, [b,c] Jarmila Dušková,[a] Jindrich Hašek,[a] Tomáš Koval,[d] Petr Man,[b,c] Pavel Hanc,[b,c] Ondrej Vanek,[b,c] Karel Bezouška,[b,c] Jan Dohnálek,[a] *[a]Inst. of Macromolecular Chemistry AS CR, v.v.i., Heyrovského nám. 2, 16206 Praha 6, Czech Republic, [b]Dpt. of Biochemistry, Faculty of Science, Charles University Prague, Hlavova 8, 12840 Praha 2, Czech Republic, [c]Inst. of Microbiology AS CR, v.v.i., Vídenská 1083, 14220 Praha 4, Czech Republic, [d]Inst. of Physics AS CR, v.v.i., Na Slovance 2, 182 21 Praha 8, Czech Republic*
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Natural killer cells (NK cells) belong to lymphocytes, besides more familiar B and T-lymphocytes. They comprise 5-10% of lymphocytes in blood and their role in the immune system is to discover and kill cells with cancer and cells infected by viruses. NK cells have a number of receptors on their surface, which are used for contact with other cells and for initiation of the cytotoxic response. Protein Clr-g, a target of this structural study, is a part of immune system of mouse. It is a ligand of NK receptor NKR-P1F. Clr-g occurs in dendritic cells and macrophages. The extracellular part of Clr-g was expressed, purified and crystallized and its structure was solved at 1.95 Å resolution using X-ray diffraction data measured at Bessy II of the Helmholtz Zentrum Berlin. The overall fold of mouse Clr-g is the fold typical of C-type lectin like proteins. Mouse Clr-g forms dimers and is most similar to human CD69. An interesting crystal contact was found in the crystal structure: N-terminus of the extracellular part of Clr-g binds to neighbour dimer in the crystal, and thus shows feasibility of peptide binding into the central pocket of the dimer. Mutual orientation of monomers in the dimer is slightly different than in the CD69 structure. However, moderate variability in orientations of monomers was found also among single structures of CD69. It seems that this difference gives testimony about flexibility in dimer formation and not about differences between mouse Clr-g and human CD69. Electrostatic potential was computed for several proteins structurally and functionally related to mouse Clr-g and surprisingly big differences were found.

This work was supported by the Grant Agency of the Academy of Sciences of the Czech Republic (KJB101120805), the Czech Science Foundation (310/09/1407, 303/09/0477, 305/09/H008, 305/07/1073 and 207/10/1040), by Charles University Prague (263209/2011, 265214/2012, and project UNCE #42)).

Keywords: immune system; NK receptors; C-type lectin like fold