recessive juvenile parkinsonism (AR-JP). Parkin contains a unique ubiquitin-like domain in its N-terminus designated Uld which is assumed to be a interaction domain with the Rpn 10 subunit of 26S proteasome. To elucidate the structural and functional role of Uld in parkin at the atomic level, the X-ray crystal structure of murine Uld was determined and a molecular dynamics simulation of wild Uld and its five mutants (K27N, R33Q, R42P, K48A and V56E) identified from AR-JP patients were performed. Crystals of Uld were obtained by the hanging-drop vapor-diffusion method using NaCl as a precipitant. Diffraction data were collected to 1.65Å resolution. The structure of Uld was determined by the single-wavelength anomalous diffusion (SAD) method using an iodinated derivative. The final model gave the R-factor of 0.195 and R_{free}-factor of 0.244. Murine Uld consists of two α helices and five β strands, and its overall structure is essentially the same as that of human ubiquitin with a 1.22 Å rmsd for the backbone atoms. The MD simulations showed the K27N and R33Q mutations increase the structural fluctuation of these β strands including the α1 helix. Reversely, the V56E mutant restricted the spatial flexibility at the periphery of the short α2 helix by the interactions between the polar atoms of Glu56 and Ser19 residues.

Keywords: Parkin, ubiquitin-like domain, molecular dynamics simulation

P04.22.418

Acta Cryst. (2008). A**64**, C361

Structural and functional whole-cell project for the model organism, *Thermus thermophilus* HB8

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This research project aims to understand all fundamental biological phenomena at an atomic-resolution, on the basis of molecular structures and functions. Towards this aim, we selected the extremely thermophilic organism, *Thermus thermophilus* HB8, as a model organism, because many of the approximately 2,200 genes encoded in its genome have been selected during evolution and are common to many organisms. However, about 500 of the genes (proteins) are functionally-uncharacterized. As a first step to obtain functional clues about these proteins, we determined their three-dimensional structures. Based on the structures, we inferred the molecular functions of about 60% of them and intensively characterized several family proteins, such as the house-cleaning NUDIX hydrolases, metallo-beta-lactamases and DNA repair proteins. While we have continued to solve the structures of other uncharacterized proteins for their functional inference, we have also been exploring their functions by functional genomics analyses (mRNA, protein and metabolite) in combination with gene disruption and stress-perturbation. For example, we found that cyclic AMP receptor protein (CRP), which is known as a global transcriptional factor, regulates 22 genes, including ones presumably involved in host defense (1 characterized and 21 uncharacterized), whereas one of the CRP family proteins functions in stationary phase, and regulates 14 genes related to energy and redox metabolism (3 characterized and 11 uncharacterized). We also found that about 40 genes of unknown function display altered mRNA expression upon metal stress. All of the plasmids for protein expression and gene disruption prepared in our laboratory are now available from the RIKEN BioResource Center (see http://www.thermus.org/).

Keywords: structural genomics, functional genomics, systems biology

P04.22.419

Acta Cryst. (2008). A**64**, C361

X-ray crystal structure of a hypothetical Sua5 protein from *Sulfolobus tokodaii* strain 7

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The Sua5-yciO-yrdC domain proteins are widely distributed in prokaryotes and eukaryotes. One of the proteins in this family, *Escherichia coli* YrdC, preferentially binds to double-stranded RNA and DNA. It has been predicted to be a rRNA maturation factor. Sua5 consists of an N-terminal YrdC domain and a C-terminal Sua5 domain. The *sua5* gene was first identified in *Saccharomyces cerevisiae* as a suppressor of a translation initiation defect of the iso-1-cytochrome c (*cyc1*) gene. The function and 3D structure of Sua5 remain to be elucidated. In the present study, we determined the crystal structure of Sua5 (ST1526) from thermoacidophilic archaeon *Sulfolobus tokodaii* strain 7, which exhibits 49.7% similarity to *S. cerevisiae* Sua5. The overall fold of the N-terminal yrdC domain of *Sulfolobus* Sua5 is similar to that of *E. coli* YrdC, the *Z*-score being 21.3 and the r.m.s.d. value being 2.4 Å. A large concave surface exhibiting a positive electrostatic potential, which is similar to that in YrdC, was found in Sua5. Interestingly, excess electron density that might be due to an *E. coli*-derived nucleotide was observed on this concave surface. The C-terminal Sua5 domain consists of three α-helices and five β-strands, which adopt a Rossmann fold. A structure similarity database search using the DALI server revealed that the closest structure was that of *Methanocaldococcus jannascii* HypB, a GTP-binding protein that regulates metal binding. Thus, the three-dimensional structure of Sua5 showed that both the N- and C-terminal domains might be involved in nucleotide binding or metabolism, which is supported by the observation that Sua5 showed ATP hydrolysis activity, AMP being produced.

Keywords: nucleotide, Rossmann fold, translation factor

P04.22.420

Acta Cryst. (2008). A**64**, C361−362

Characterization of metal ions and protein oligomeric states in JCSG structures

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