phosphatase which is distributed among eubacteria, archia and eukaryotes. In *E. coli*, it is necessary for survival during the stationary phase, but the physiological role of SurE is not clear. Crystal structures of SurE from *Thermotoga maritima* and *Pyrobaculum aerophilum* have been determined, which revealed that SurE forms a dimer that assembles into a tetramer.

We report here the crystal structures of SurE from *Thermus thermolhilus* HB8 ($SurE_{ther}$) in a few different space groups. The $SurE_{ther}$ structure consists of a globular Rossmann fold domain and a protruded domain that mediates tetramerization as so far-reported structures. However, the angle between the protruding domain and the Rossmann fold domain of $SurE_{ther}$ is different. As a result, the dimeric- and tetrameric-structures of $SurE_{ther}$ were quite different from the known SurE structures. We studied the self-associative properties of $SurE_{ther}$ in solution using the sedimentation equilibrium analytical ultracentrifugation. Phosphatase activity assays of $SurE_{ther}$ is in progress, and its substrate specificity seems to be strict compared to SurE from other species. The relationship between enzymatic property and the variant oligomeric structure of $SurE_{ther}$ will be discussed.

Keywords: protein crystallography structures, phosphatases, protein assembly

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Crystal Structure of *Mortierella vinacea* α-galactosidase I

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α-Galactosidase (E.C. 3.2.1.22) is an exoglycosidase that hydrolyzes an α-1,6-linked galactosyl residue from galacto-oligosaccharides and polymeric galacto-(gluco)mannans. α-Galactosidase I from *Mortierella vinacea* (α-Gal I) consists of 397 amino acid residues and it shows high activity to increase the yield of sucrose by eliminating raffinose, which prevents normal crystallization of beet sugar, and is sometimes referred to as raffinase. α-Gal I is considered to be a glycoprotein, resulting from the presence of its sugar chain. In addition, the gel filtration data shows that α-Gal I might exist as a tetramer in solution.

In order to understand the catalytic mechanism, we conducted structure analysis of this enzyme. Crystals of α-Gal I were obtained by the hanging drop vapour diffusion method using the polyethylene glycol 400 as a precipitant. Diffraction experiments were conducted at the Photon Factory, and the data up to 1.6 Å resolution were collected. Structure was determined by the molecular replacement method and the final model gave a crystallographic *R*-factor of 0.133 and an R_{free}-factor of 0.157. Owing to the high resolution X-ray data, four carbohydrate chains were observed in one α-Gal I molecule and their structures were identified to be high mannose type. α-Gal I seemed to form a tetramer around the crystallographic four-fold axis.

Keywords: α-galactosidase, glycoprotein, *Mortierella vinacea*

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Structural basis for Ca^{2+}-induced Activation of Human PAD4

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Peptidylarginine deiminase 4 (PAD4) is a Ca^{2+}-dependent enzyme that catalyzes the conversion of protein arginine residues to citrulline residues. PAD4 is expressed mainly in bloodstream granulocytes and present in the cell nucleus. The recent experimental evidence that PAD4 targets multiple arginine sites in histone H3 and H4, including those sites methylated by CARM1 (H3/Arg17) and PRMT1 (H4/Arg3), has attracted considerable attention to characterize the role of histone modifications in regulating gene transcription [1, 2].

On the other hand, a recent single-nucleotide polymorphism (SNP) analysis of the PAD4 (*PADI4*) gene has identified a specific haplotype linked to an increased susceptibility for rheumatoid arthritis in Japanese people [3].

Here we present the crystal structures of Ca^{2+}-free, Ca^{2+}-bound, and Ca^{2+}-substrates bound PAD4 [4]. PAD4 has five non-EF-hand Ca^{2+} binding sites and adopts an elongated shape, consist of N- and C-terminal domain. These structural data indicate that Ca^{2+} binding in C-terminal domain induces conformational changes that generate the active site cleft. Our findings identify a novel mechanism for enzyme activation by Ca^{2+} ions.

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Keywords: histone modification, citrullination, calcium binding

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The Crystal Structure of a Novel Subtilisin-like Alkaline Serine Protease, KP-43

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The crystal structure of an oxidatively stable subtilisin-like alkaline serine protease, KP-43 from *Bacillus* sp. KSM-KP43, with a C-terminal extension domain, was determined at 1.30-Å resolution. KP-43 consists of two domains, a subtilisin-like α/β domain and a C-terminal jelly roll β-barrel domain. The topological architecture of the molecule is similar to that of kexin and furin, which belong to the subtilisin-like proprotein convertases (SPCs), whereas the amino acid sequence and the binding orientation of the C-terminal β-barrel domain both differ in each case. Since the C-terminal domains of SPCs are essential for folding themselves, the domain of KP-43 is also thought to play such a role.

KP-43 is known to be an oxidation-resistant protease among the general subtilisin-like proteases. The structure analysis of oxidized form and the biochemical experiments have indicated that the oxidation of the methionine adjacent to the catalytic serine is not a dominant modification, but might alter the substrate specificities.

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Crystal Structure of Atypical Cytoplasmic ABC-ATPase SufC

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Biosynthesis of Fe-S clusters requires several specific proteins. The *suf* operon has been recently identified as a third system for the assembly of Fe-S clusters. The *suf* operon of *Eschrichia coli* comprises *suf*A, *suf*B, *suf*C, *suf*D, *suf*S, and *suf*E. Most of *suf* genes are conserved in various organisms, but the *suf* operon is seldom found in complete form. The most conserved *suf* genes are SufC and SufB. SufC is a cytoplasmic ABC-ATPase, probably the most essential Suf protein. SufC interacts with SufB and SufD in a stable complex, and the SufBCD complex interacts with other Suf proteins in the Fe-S cluster assembly.

We have determined the crystal structure of SufC from *Thermus thermophilus* HB8 in a nucleotide-free state and an ADP-Mg bound state at 1.7Å and 1.9Å resolution, respectively. The structure of SufC consists of two domains: the ABC αβ domain, which is structurally similar to the typical core fold of ABC-ATPase, and the α helical domain. In the ABC αβ domain, three residues following the end of