contact. *Ec*RlmI also a methyltransferase synthesizes m5C 1962 of 23S rRNA. *Ec*RlmI forms dimer in both solution and crystal[1], *Sa*RlmL-C exists as monomer in crystal . In the structure of *Sa*RlmL-C, *S*-adenosylhomocysteine from *E.coli* was found in MTase domain, and located next to deep cleft by three domains. Conserved residues in each domains are concentrated in deep cleft can be considerd as possible RNA binding site. Finally we propose the RNA binding model of *Sa*RlmL-C different from of *Ec*RlmI.

[1] S. Sunita, K.L. Tkaczuk, E. Purta, J.M. Kasprzak, S. Douthwaite, J.M. Bujnicki, J. Sivaraman, *J Mol Biol.* **2008**, *383(3)*, 652-666.

Keywords: rRNA, methyltransferase

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Structures of engineered phytases

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Phytate (inositol hexaphosphate), that is found in cereals, acts as an anti-nutritive factor in animal feed. Phytase acts on phytate to remove phosphate and eliminate its anti-nutritive effect. Native phytase suffers from insufficient thermal stability for animal feed formulation making an engineered more thermal stable phytatse highly desirable. We have determined the three-dimensional structures of native along with a first and second generation engineered *Buttiaxella* phytase to better understand what structural elements were modified to achieve this thermal stability. The native enzyme has been crystallized in space group $P2_12_12_1$ and determined to 1.8 Å, one variant crystallized in a triclininc form with two molecules in the symmetric unit, was determined at 2.05 Å and a second variant having an additional amino acid substitutions was also crystallized in space group $P2_12_12_1$ and determined to 1.8 Å. These variants were achieved with programs of directed evolution. The analysis of these changes lead to a short set of guidelines that appear to have general applicability for rational engineering thermal stability in these and other enzymes of commercial interest.

Keywords: phytase, protein engineering

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Highlights from the macromolecular x-ray crystallography facility at pennsylvania state university (a) crystal structures of bacterial expansin in complex with cellohexoase and β-glucan (b) solution scattering and crystal structure of sorbitol dehydrogenase with a substrate (c) computation model of human ron receptor and its juxta-membrane domain and (d) model of phospholipase a2 with procyanidins

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This research is in collaboration with various groups at Penn State University **(a)** With the Cosgrove lab, we have solved the crystal structure of an expansin, encoded by the *yoaJ* gene of Bacillus subtilis in complex with polysaccharides, cellohexoase and β-glucan. Although the polysaccharide-binding surface was expected to span the two domains of the protein, it is seen to bind only to the carbohydrate-binding domain. The sugars trigger a dimer formation in the crystal packing with the conserved residues Trp125, Trp126 and Tyr157 from both monomers stacking against the carbohydrate rings. The structures point to a non-enzymatic function for expansin action.

(b) The crystal structure of sheep liver sorbitol dehydrogenase (slSDH) has been determined using the crystal structure of human sorbitol dehydrogenase (hSDH) as a molecular-replacement model. slSDH crystallized in space group I222 with one monomer in the asymmetric unit. A conserved tetramer that superposes well with that seen in hSDH (despite belonging to a different space group) and obeying the 222 crystal symmetry is seen in slSDH. An acetate molecule is bound in the active site, coordinating to the activesite zinc through a water molecule. Glycerol, a substrate of slSDH, also occupies the substrate-binding pocket together with the acetate designed by nature to fit large polyol substrates. The substrate-binding pocket is seen to be in close proximity to the tetramer interface, which explains the need for the structural integrity of the tetramer for enzyme activity. Small-angle X-ray scattering in collaboration with the Gillilan group at CHESS, was used to identify the quaternary structure of the tetramer of slSDH in solution.

(c) Mutation studies done in the Hankey lab have identified residues in the juxta-membrane (JM) segment crucial for human Ron receptor activation and repression. Analysis of conserved residues and electrostatic surface of human Ron kinase domain combined with the crystal structures of other related receptors has enabled building of models for the active and the autoinhibited structural fold of the JM domain. The autoinhibited form of other receptor protein kinases indicates JM approaches the active site from the front end of the nucleotide binding pocket and binds in the substrate binding region. We predict that a short acidic JM-C helix could position itself in the substrate binding region interacting with the activation and P-loops of the active site and a longer JM-D helix could interact with the alpha-C helix of the N-lobe maintaining the human Ron receptor in its inactive conformation. In the active state the JM region could undergo significant conformational changes and move out of the substrate binding region.

(d) Studies in the Lambert lab on cocoa, apple and cinnamon procyanidins have shown them to be potent inhibitors of key digestive enzymes phospholipase A2, lipase and α-amylase. Models of procyanidins of various sizes were built into the active site of phospholipase A2 guided by the dozens of available ligand-bound crystal structures. A 7-mer of procyanidin was the biggest ligand that could fit in the large active site tunnel and have favorable interactions with the protein residues.

Keywords: Expansin, Dehydrogenase, Ron

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Study on Crack of Yb:YAG Laser Crystal

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The 5at.% Yb3+-doped YAG crystal was grown by the Czochraski method, and the crystal growth process was investigated. the optimal process parameters were determined as follows: The crystal growing rate for Shoulder growth and equal-diameter growth were 0.8mm/h and 1mm/h, respectively. The optimal Rotation speed of this crystal was 15rad/min, and the axial temperature gradient was 0.01−0.05ºC/mm. The impact factors to crystal growth were analyzed theoretically, such as growth rate, rotation speed, thermal effect and crystal size

Keywords: Yb:YAG crystal, Czochralski method, Crack analysis