A complex of atypical PKC and Par6 is a common regulator for cell-polarity related processes, which is an essential clue to evolutionary conserved cell-polarity regulation. Here, we determined the crystal structure of the aPKC and Par6 PB1 domain complex to a resolution of 1.5 Å. Both PB1 adopt a ubiquitin fold. aPKC PB1 presents an OPCA motif, 28 amino acid residues with acidic and hydrophobic residues, which interacts with the conserved lysine residue of Par6 PB1 in a front-and-back manner. Structural comparison of the aPKC and Par6 PB1 complex with the $p40^{phox}$ and $p67^{phox}$ PB1 complex, subunits of neutrophil NADPH oxidase, reveals that the specific interaction is achieved by tilting the interface so that the insertion or extension in the sequence is engaged in the specificity determinant. The PB1 domain develops the interaction surface on the ubiquitin fold to increase the versatility of molecular interaction.

Keywords: protein complex structure, domain structure, cell polarity

P.04.17.3

Acta Cryst. (2005). A**61**, C252

The Allergenic Non-specific Lipid Transfer Protein from Peach: Structural Studies

Nicola Pasquato[a], Claudia Folli[b], Silvia Folloni[b], Michele Cianci[c], Rodolfo Berni[b], John R. Helliwell[c], Giuseppe Zanotti[a], *[a]Department of Chemistry, University of Padova, 35131 Padova, Italy. [b]Department of Biochemistry and Molecular Biology, University of Parma, 43100 Parma, Italy. [c]Department of Chemistry, University of Manchester, Manchester M13 9PL, England.* E-mail: nicola.pasquato@unipd.it

A large number of proteins can bind small molecules with a poor solubility in water. The function of many of these proteins is to transport small molecules which would not be soluble in the biological environment. The ligands often present a strong lipophilic characters, as, for example, retinoids and fatty acids. In addition to the well known calycins, this group of protein includes the so-called non-specific lipid transfer proteins (*ns*-LTPs). They are plant proteins of about 9 kDa molecular mass, and they bind fatty acids, steroids and other types of lipids. However, their function has not been precisely defined as yet [1].

Our study is focused on the determination of the three dimensional structure of peach ns-LTP. Recently, several biological and medical studies have stimulated interest in the *ns*-LTP from peach. This protein, like others *ns*-LTPs, binds fatty acids, but it has been also identified as an important food allergen [2].

Despite its strong sequence similarity with others ns-LTPs whose structure is already known [3], its crystal structure determination was not straightforward. It required the measurement of synchrotron anomalous data with enhanced sulphur f´´ by using a synchrotron X-ray wavelength of 2Å from SRS MPW beamline 10. In addition a stronger <I/sig(I)> was then achieved using the APS undulator at SBC CAT. The molecular model is a single compact domain, made up by four *α-helices*, which form a hydrophobic pocket where the lipid is bound. The 3-D structure is strongly stabilized by four disulphide bridges. Possible immunogenic epitopes associated with the allergenic reaction will be proposed by this study.

[1] Kader J. C., *Annu. Rev Plant Physiol. Plant Mol. Biol.*, 1996, **47**, 627. [2] Salcedo G., Sanchez – Monge R., Diaz – Casado A., Barber D., *Clin. Exp. Allergy* 2004, **34**, 1336. [3] Han G. W., Lee J. Y., Song H. K., Chang C., Min K., Moon J., Shin D. H., Kopka M. L., Sawaya M. R., Yuan H. S., Kim T. D., Choe J., Lim D., Moon H. J., Suh S. W., *J. Mol. Biol.* 2001, **308**, 263.

Keywords: ns-LTP, non specific lipid transfer protein, food allergen

P.04.17.4

Acta Cryst. (2005). A**61**, C252

LRRs: A platform to build a Protein Recognition Motif

Tom Garrett, Trevor Huyton, *Walter and Eliza Hall Institute, Parkville, Vic, Australia.* E-mail: tgarrett@wehi.edu.au

The leucine-rich repeat domains (LRRs) of cell-surface receptors often constitute the binding regions for small protein ligands. Examples are found in many types of medically important receptors, e.g. Insulin and growth-factor receptors, G-coupled protein receptors and Toll-like receptors. Thus they are important therapeutic targets.

The architecture of LRRs generally consists of a β-helix or solenoid with a prominent β-sheet down one face forming the ligand-binding surface. Side chains on this face are tightly packed to form a sterically well-defined surface with the chemical composition dictated by sequence. The opposite face shows considerable structural variability and here, the space occupied by the main chain appears to dictate the curvature of the ligand-binding face. Thus LRRs have a simple but elegant design, where the main chain provides a regular framework of variable size and shape and chemical nature of the site is under genetic control.

Now that a considerable number of these structures have been determined, with or without their ligands, a detailed analysis has revealed the factors which control the overall architecture for *ab initio* design of a protein-binding surface. Naturally-occurring augmentations of this standard architecture provide additional ways of creating a protein-docking site.

Keywords: receptor-ligand interactions, molecular recognition, protein engineering

P.04.18.1

Acta Cryst. (2005). A**61**, C252

Cracking of the Targeting Signal Embedded in Mitochondrial Presequences

Mayumi Igura[a], Takayuki Obita[a], Toyoyuki Ose[a], Toshiya Endo[b], Katsumi Maenaka[a], Daisuke Kohda[a], *[a]Medical Institute of Bioregulation, Kyushu University, Fukuoka. [b]Nagoya Univeristy, Nagoya, Japan.* E-mail: nmigura@bioreg.kyushu-u.ac.jp

Most mitochondrial proteins are synthesized in the cytosol as precursor proteins with a cleavable N-terminal presequences and are imported into mitochondria. Protein import into mitochondria is mediated by protein assemblies in the mitochondrial membranes. A subunit, Tom20, functions as a general protein import receptor by recognizing presequences of preproteins. Although no consensus sequence is found, Tom20 recognizes a wide variety of presequences.

To understand the structural basis of the presequence recognition, we determined the NMR and crystal structures of Tom20 in a complex with a presequence peptide. Note that the presequence was fixed to Tom20 via a designed intermolecular disulfide bond to obtain crystals. The bound presequence forms an amphiphilic a-helix. NMR titration experiments indicated the presence of a unique presequence binding site in Tom20, and defined a common five-residue pattern in different presequences. To refine this pattern, we introduced a new peptide library approach using the formation of an intermolecular disulfide bond. We propose that a presequence is regarded as a collective entity of short amino acid sequences that are recognized by several proteins including Tom20. The organization (position, order, and overlapping) of these binding segments is unique for each presequence. This view explains why no consensus sequences are found by simple sequence comparisons.

Keywords: protein transport, molecular recognition, crystallographic and NMR solution structures

P.04.19.1

Acta Cryst. (2005). A**61**, C252-C253

Crystal Structure of Decameric Peroxiredoxin (AhpC) from *Amphibacillus xylanus*

Ken Kitano[a,b], Akiko Kita[a], Toshio Hakoshima[b], Youichi Niimura[c], and Kunio Miki[a,d], *[a]Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto, Japan. [b]Structural Biology Laboratory, Nara Institute of Science and Technology, Ikoma, Japan. [c]Department of Bioscience, Tokyo University of Agriculture, Tokyo, Japan. [d]RIKEN Harima Institute/SPring-8, Hyogo, Japan.* E-mail: kkitano@is.naist.jp

Peroxiredoxins (Prxs), also referred to as AhpCs, are a ubiquitous family of antioxidant enzymes. Bacterial AhpC is recognized as the primary scavenger of endogenously generated hydrogen peroxides. AhpC purified from *Amphibacillus xylanus* shows extremely high scavenging activity for both hydroperoxide and alkyl hydroperoxide in