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Three-dimensional Structure of Human FKBP52
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FKBP family proteins are immunophilins which process peptidyl-prolyl isomerase (PPIase) domain and they can all bind FK506, a macrolide immunosuppressant. FKBP52 is a FKBP protein, which can be separated into four domains. The first (FK1) and the second (FK2) domains are similar with FKBP12. The third domain includes three tetratricopeptide repeat (TPR) motives and the forth domain contains calmodulin binding-site.

We have overexpressed and purified FKBP52 full-length and three segments of FKBP52, including FKBP52-FK1, N(1-260) and C(145-459). The crystals of FKBP52-FK1, N(1-260), C(145-459) have been obtained, as well as the complex of C(145-459) and a C-terminal pentapeptide MEEVD from Hsp90. The three dimensional structure of FKBP52 has been defined based on the crystal structures of N(1-260) and C(145-459). The structures have indicated the pattern of natural substrates binding to the active site of PPIase and the reason why the FKBP52-FK506 complex is not able to inhibit calcineurin activity, and has interpreted why FK2 has no PPIase activity. The functional differences between FKBP52 and FKBP51 have been clarified by comparing their structures. A hormone-signaling model based on FKBPs / Hsp90 / hormone receptor complex assembly has been proposed and FKBP51 is regarded as a negative feedback factor of FKBP52 in hormone signaling.
Keywords: FKBP52, PPIase, hormone receptor complex

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Structural Investigations of GFP-like Proteins
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Green Fluorescent Protein (GFP) from *A.Victoria* is an 11 stranded β-barrel protein with a cyclic tri-peptide chromophore. Encoded by a single gene, GFP is self folding and has an autocatalytic mechanism of chromophore formation.

The intrinsic pigmentation and fluorescence properties of GFP-like proteins arise from their all-protein chromophores, with their differing spectral properties due to their unique chromophore structures and environments of each protein. Understanding GFP-like protein structure and related function is of fundamental interest.

The GFP-like proteins under investigation include a highly fluorescent, moderately fluorescent and two non fluorescent proteins, eqFP611, HcRed, KFP and Rtms5 respectively. All of which have strong sequence and structural homology to both GFP and a red fluorescent protein from *Discosoma* coral (DsRed). I have solved high resolution crystal structures of KFP, eqFP611 and HcRed. From structural comparisons between previously solved structures, Rtms5, DsRed and GFP.

By the detailed investigation of several GFP-like proteins through their structural determination and characterization I am gaining an understanding of the dynamic nature of the GFP-like protein family. It is anticipated that we will expand the current understanding of chromophore structure in conjunction with related protein fluorescence, subsequently aiding the development of novel GFP-like protein applications.
Keywords: GFP, protein cyrstallography, chromophore structure

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Crystal Structure of Heme Binding Enolase P46 from *Bacteroides fragillis*
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The anaerobic gram-negative bacterium *Bacteroides fragilis* is frequently found in intestines and is known to cause intra-abdominal infections. A 46 kDa heme binding protein (P46) from *B. fragilis* was found to be induced in iron restricted condition [1]. The sequence of P46 shows it to be an enolase, an enzyme in glycolysis. Enolase forms dimers or octamers and the crystal structure of enolase from human, yeast, *Escherichia coli* and *Streptococcus pneumoniae* are known. But their structures do not explain heme binding to P46.

To investigate heme binding mechanism, we solved the crystal structure of P46 at 2.6 Å resolution. P46 forms an octamer in the crystal structure and solution. Furthermore, we measured the affinity of P46 for heme using surface plasmon resonance and found that the dissociation constant is 2.65 μM.

[1] Otto B.R, et al., *Infect Immun*., 1996, **64**, 4345.
Keywords: enolase, heme binding protein, bacteroides

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Structural Studies of the Disulfide Oxidoreductases DsbA from *Xylella fastidiosa*
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The first member of the disulfide oxidoreductases (DsbA) family was identified and characterized in *Escherichia coli* as a periplasmic protein involved in disulfide bond formation. It was also shown that the DsbA protein assists the correct folding of exported proteins containing disulfide bonds and in *Vibrio cholerae* a member of this family is required for the functional maturation of secreted virulence factors. *Xylella fastidiosa* is a phytopathogenic bacterium that causes serious diseases in a wide range of economically important crops. *X. fastidiosa* genome analysis revealed the presence of two members of the DsbA family (from now named DsbA1 and DsbA2). Furthermore, a sequence alignment showed that the active site regions of DsbA1 and DsbA2 differ from each other by one residue, usually considered important for the enzymatic activity. The purified proteins DsbA1 and DsbA2 were submitted to crystallization trials. Crystals of DsbA1 were obtained and X-ray diffraction data were collected at the Brazilian Synchrotron Light Laboratory. Best crystals diffracted to 2.2 Å resolution and belong to space group C2 with unit cell parameters a= 200.06 Å, b= 41.24 Å, c= 79.97 Å and β= 96.17°. DsbA1 crystals were also obtained after protein incubation with a reducing agent and diffracted up to 1.9 Å. The quick cryo-soaking technique was applied and some data sets were collected from heavy atom-derivative crystals. Attempts to solve the structure using the SIRAS and MIRAS methods are in progress. Circular Dichroism and Fluorescence experiments are being performed in order to obtain complementary structural data.
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Keywords: xylella fastidiosa, disulfide oxidoreductase, X-ray diffraction data

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Structure of MntC from Cyanobacteria
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We have determined the crystal structure of the MntC solute