structure. The large domain shows (βα)8 barrel motif and the small domain suggests structural similarity to cyclophilin A.

Keywords: structural genomics, high-resolution protein structures, domain structure

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A High-efficiency, Low-cost Platform for Structural Genomics Studies at Peking University

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A high-throughput, high-efficiency and low-cost platform based on Beckman-Coulter robotic system Biomek FX for structural genomics has been set up. Several projects of structural genomics are in processing. Now, the platform has a capacity to process more than 1000 genes/year for structural and functional analyses. *B. Subtilis,* a model ogranism for Gram-positive bacteria and *S. Mutans,* the primary pathogen of dental caries were selected as our main target sources. So far, more than 450 *B. subtilis* and 250 *S. mutans* proteins and some proteins from other sources were selected as targets for this platform, the selected targets are mainly related to important metabolism pathways, and/or of potential for drug design. Up to 2005 Jan., 20 protein structures from the selected targets were determined, among them, eight structures were determined ab-initio. The application of beamline at **BSRF** (Beijing Synchrotron Radiation Facilities) and the ***OASIS-2004*** program have been crucial components for the operation of our platform. The use of SAD (single-wavelength anomalous diffraction) phasing methods combined with direct methods in ***OASIS-2004*** has increased the efficiency significantly, 5 out of 8 ab-initio determined structures have been solved this way.

Keywords: structural genomics, BSRF, OASIS-2004

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Progress in the Whole Cell Project of a Model Organism, *Thermus thermophilus* HB8

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One of the long-term goals of structural and functional genomics is the interpretation of all fundamental biological phenomena at atomic resolution. An extremely thermophilic bacterium, *Thermus thermophilus* HB8, is a promising model organism for structural and functional studies, because of the small genome size, the availability of genetic tools for functional analysis, and the thermostability of its proteins. Toward this aim, the "Whole Cell Project" of this bacterium is currently in progress (http://www.thermus.org/). The complete genome sequence identifies approximately 2,200 ORFs, and about 2,000 expression plasmids have been constructed. The target proteins were overproduced in *E. coli*, purified, crystallized, and characterized by X-ray crystallography, through which about 200 protein structures have been solved. As part of functional studies, we have constructed the gene disruption plasmids using the thermostable selective marker (kanamycin resistance) and analyzed mRNA by the DNA microarray system.

Keywords: structural genomics, functional genomics, *Thermus thermophilus*

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Structural Proteomics of Proteins Coded by the *cag* PAI of *Helicobacter pylori*

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H. pilory is a Gram-negative bacterium that colonizes the stomach of probably half of the human population. It is associated with gastritis, peptic ulcers and mucosa-associated lymphoid tissue lymphomas. Many factors contribute to the virulence of *H. pylori* [1]. Among them, the enzyme urease, the Neutrophil Activating Protein, NAP [2] and the secreted protein toxin VacA. However, the major genetic difference in HP isolates is the presence or absence of a specific pathogenicity island, named *cag*-PAI. It is a 40-kb locus that contains about 30 ORFs, whose function is unknown, with few exceptions.

We have cloned, expressed, and purified several proteins of the *cag* pathogenicity island of *H. pylori*. They all have been expressed in *E. coli.* We have already solved the structure of CagZ, using the Se-Met method [3] and the structure will be described in detail. We have also obtained crystals of a second protein, CagS, and its structure determination is in progress, along with crystallization tests on other *cag* proteins. Our final goal is to determine, in collaboration with other groups [4], most of the proteins coded by the *cag*-PAI island.

[1] Covacci, et al., *Science*, 1999, **284**, 1328. [2] Zanotti, et al., *J. Mol. Biol*., 2002, 323, 125-130. [3] Cendron L., Seydel A., Angelini A., Battistutta R., Zanotti G., *J. Mol. Biol.*, 2004, **340**, 881. [4] *The Helicopter Structural and Molecular Biology Consortium.*

Keywords: structural genomics, bacterial pathogenesis, MAD phasing

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Trying To Deduce Function From Structural Variability And Conservation

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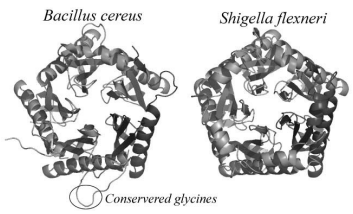
A comparative case is presented for two similar proteins from *Shigella flexneri* and *Bacillus cereus* which are homologs of the *E. coli* protein ybjQ. These two proteins are members of the COG0393, a widely conserved family of proteins in bacteria and archaea that are functionally uncharacterized. All members of the sequence family are about 100 residues. The two examples presented are both homopentamers and have 54% sequence identity. Despite the high sequence identity, the *B. cereus* protein contains regions of structural variation. A sequence alignment of the protein family reveals a pair of conserved glycines at residues 44 and 45. These conserved glycines are located in a loop that it is a region of structural variation in the *B. cereus* protein. This area of structural variation has been predicted as a region of disorder from the DisEMBL server which may be important to the function of these proteins.



Keywords: structural genomics, conformational change, macromolecular structure

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Comprehensive Structure-based Functional Analysis on Transcription Factors

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