

function of the enzyme consists in catalytic oxidation of the primary alcohol in various oligosaccharides with the highest activity towards D-cellobiose (Kulys et al., 2001). Crystallization experiments were performed using Hampton Research Crystal Screen and Index solutions. Crystals show variable morphology depending on crystallization conditions and feature varying stability. The measured hexagon-shaped crystal grew with Jeffamine ED2001 as precipitant. X-ray diffraction data were collected at beamline BM14, ESRF in Grenoble using the MARMosaic 225 detector. The crystal diffracted up to 2.7 Å resolution, however, a rapid intensity fall off occurred beyond 3.5 Å resolution. The space group was indicated as *P*6<sub>2</sub>2<sub>2</sub>, with unit cell parameters *a* = *b* = 55.7 Å, *c* = 610.4 Å. The crystallographic symmetry was verified with program Pointless (Collaborative Computational Project, Number 4, 1994). Extensive molecular replacement trials with a model of 39% sequence identity (PDB code 1zr6) failed. The size of the molecule, size of the unit cell and high symmetry of the space group inadvertently resulted in significant overlaps of the 'solutions'. The real crystallographic symmetry is lower (subgroup of *P*6<sub>2</sub>2<sub>2</sub>) and one or more symmetry operators arise from twinning of the crystal. Further experiments to produce well diffracting crystals without twinning are in progress. Acknowledgement: This work was supported by GA AV CR, project IAA500500701 and by GA CR, project 305/07/1073.

Collaborative Computational Project, Number 4 (1994). *Acta Cryst.* D50, 760-763.

Kulys, J., Tetianec, L. & Schneider, P. (2001). *J. Mol. Catal. B: Enzym.* 13, 95-101.

Keywords: carbohydrate oxidase, crystallization, X-ray structure analysis

### P04.01.23

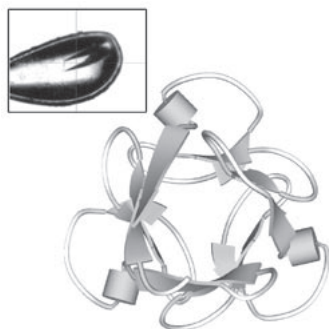
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#### Crystal structure of actinohivin; A novel anti-human immunodeficiency virus protein

Masaru Tsunoda<sup>1</sup>, Kaoru Suzuki<sup>1</sup>, Tsubasa Sagara<sup>1</sup>, Atsushi Takahashi<sup>1</sup>, Junji Inokoshi<sup>2</sup>, Satoshi Omura<sup>2,3</sup>, Takeshi Sekiguchi<sup>1</sup>, Akio Takenaka<sup>1</sup>, Haruo Tanaka<sup>1</sup>

<sup>1</sup>Iwaki Meisei University, Faculty of Pharmacy, 5-5-1 Chuodai-iino, Iwaki, Fukushima, 970-8551, Japan, <sup>2</sup>Kitasato University, 5-9-1 Shirokane, Minato-ku, Tokyo, 108-8641, Japan, <sup>3</sup>The Kitasato Institute, 5-9-1 Shirokane, Minato-ku, Tokyo, 108-8642, Japan, E-mail : masaru@iwakimu.ac.jp

Actionohivin (AH) is a protein found in a culture filtrate of the newly discovered genus actinomycete *Longispora albida*. AH is a potent anti-human immunodeficiency virus (HIV) protein that inhibits viral entry to cells by binding high-mannose-type saccharide chains of HIV gp120. Consisting of highly conserved sequence which has three-tandem repeats, it might belong to carbohydrate binding module (CBM) family 13. To confirm mechanisms of specific binding of sugar to AH and to provide new approach for activity improvement, it was examined by crystallization and X-ray diffraction. Single crystals were obtained for several months. Crystals were soaked in a solution of platinum and were diffracted at maximum resolution of 1.1Å. Single wavelength anomalous dispersion method was used for initial phase determination. The



crystal structure of AH has a pseudo threefold axis and consists of three domains which are analogous to each other. Three segments are consistent with highly conserved tandem repeats. The active site, LD and QXW motif, was positioned in central area of each segment.

Keywords: HIV drug design, high-resolution crystal structures, AIDS inhibitors

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#### Structural and functional analysis of an important *Pseudomonas aeruginosa* redox protein

Stephen R Shouldice<sup>1</sup>, Russell Jarrott<sup>1</sup>, Begona Heras<sup>1</sup>, Martin J Scanlon<sup>2</sup>, Jennifer L Martin<sup>1</sup>

<sup>1</sup>University of Queensland, Institute for Molecular Bioscience, 306 Carmody Rd, Building 80, Brisbane, Queensland, 4072, Australia, <sup>2</sup>Department of Medicinal Chemistry, Victorian College of Pharmacy, Monash University, Victoria 3052, Australia, E-mail : s.shouldice@imb.uq.edu.au

*Pseudomonas aeruginosa* is ubiquitous in soil and water and also occurs regularly on the surfaces of plants and occasionally animals. *P. aeruginosa* is an opportunistic human pathogen. It almost never infects healthy tissues, yet there is hardly a tissue that it cannot infect if defences are compromised in some manner. Therefore, *P. aeruginosa* is often responsible for nosocomial infections. To survive within a host, bacteria produce and secrete a variety of virulence factors. These are typically protein molecules that specifically influence host function and allow the bacterium to thrive. Even though each pathogenic species possesses a specific repertoire of virulence factors, a common feature of these molecules is that they are usually secreted to the surface of the cell or released into the extracellular environment to interact with host components. Often, these virulence factors contain disulfide bonds, which are incorporated to stabilize tertiary structure in a foreign environment. This involves the oxidation of two cysteine residues. It is now well established that the disulfide bond (Dsb) family of proteins catalyzes the formation of disulfide bonds in the bacterial periplasm. The key enzyme, DsbA, catalyzes disulfide bond formation by donation of its active-site disulfide to a folding protein substrate, via a mixed disulfide intermediate. The reduced DsbA produced by this reaction is then re-oxidized by the integral inner membrane protein DsbB. We have determined the 1.6 Å resolution crystal structure of the DsbA enzyme of *P. aeruginosa* (PaDsbA). Additional functional analysis of purified PaDsbA has enabled us to compare PaDsbA to previously characterized oxidoreductases. This information is vital to future studies aimed at combating this important pathogen.

Keywords: crystallographic structure determination, protein crystallography, protein biochemistry

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#### Crystallization of serine proteases for neutron single crystal structure determination

Taro Yamada<sup>1</sup>, Kenji Kawamura<sup>1</sup>, Yuki Onishi<sup>1</sup>, Takuya Ishikawa<sup>2</sup>, Katsuhiro Kusaka<sup>1</sup>, Ichiro Tanaka<sup>1</sup>, Nobuo Niimura<sup>1</sup>

<sup>1</sup>Ibaraki University, 4-12-1 Nakanarusawa, Hitachi, Ibaraki, 316-8511, Japan, <sup>2</sup>Kyoto University Research Reactor Institute, 2 Asashiro Nishi, Kumatori, Osaka, 590-0494, Japan, E-mail : taro@mx.ibaraki.ac.jp