Crystal Structure of Sulfotransferase from *Mycobacterium Tuberculosis* H37Rv

<u>Yoshimitsu Kakuta</u>, Shotaro Tanaka, Yuuji Moriizumi, Makoto Kimura, *Department of Bioscience and Biotechnology, Faculty of Agriculture, Kyushu University, Fukuoka, Japan.* E-mail: kakuta@agr.kyushu-u.ac.jp

We determined the crystal structure of Mycobacterium tuberculosis H37Rv sulfotransferase (STF1). STF1 was crystallized in two conditions: neutral (pH 7.1) and acidic (pH 4.6). Diffractions of these crystals were observed up to 1.5 Å of resolution with synchrotron radiation at SPring-8. The phase was determined with MIR-AS and with molecular replacement. STF1 structure has 1 beta sheet with 5 parallel strands and 22 helices. PAPS binding structural motif (5'-PSB loop and 3'-PB) was conserved. STF1 forms unique structures, one at the amino terminal and another at between the PAPS binding motifs. The amino terminal structure forms 3-helical alphabundle formation, and may stabilize the monomeric conformation of STF1. The inserted structures between the PAPS binding motifs covered on acceptor-binding pocket. Alignment of primal structures with STF1 and other mycobacterial ST homologues revealed high similarity all through the sequences. The conservation of key amino acid residues for sulfation (containing the PAPS binding motifs) suggests that other mycobacterial STs will also perform ST reaction, and moreover, form the characteristic structures like as STF1.

[1] Tanaka S., Moriizumi Y., Kimura M., Kakuta Y., Acta. Cryst., 2005, F61, 33.

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