Homology Modeling of *Xanthomonas citri* Molybdate-binding Protein

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We propose a molecular model for molybdate-binding protein (ModA) of the plant pathogen *Xanthomonas citri* based on homology modeling using *Escherichia coli* ortholog as a template. Alignments of ModA amino acid sequences were carried out using the BLASTp, Psi-BLAST and ClustalW. The rigid and dynamic molecular modeling of *Xac* ModA protein were obtained with Modeller and Gromacs, respectively. The results and the model were analysed with Sting Millenium. The built model contains two nearly symmetrical domains separated by a hinge region where the substrate-binding site lies. The first domain consists of 5 α-helix (52 amino acids) and 5 β-sheets (26 amino acids) and the second domain has two more β-strands than the first. The Ramachandran plot for the models shows 95,59% residues in the favorable regions and none is in the disallowed regions, as calculated with the program PROCHECK. Values of rmsd for *Xac* ModA X *E. coli* and *Xac* ModA X *A.vinelandii* were 1.5A and 1.9A, respectively. Comparisons between *X. Citri* ModA model and the structure of the *E. coli* and *Azotobacter vinelandii* orthologs have been done.

The ongoing biochemical characterization in combination with the structural analysis will assist the elucidation of the structure-activity relationship in regulating the uptake of molybdate in *Xanthomonas*.

Keywords: ModA, ABC transport system, molecular modeling