Biochemical and Structural Analyses of the Alkanesulfonate-Binding Protein From *Xanthomonas axonopodis* pv. *citri* and Interactions With Different Ligands

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Microorganisms require sulfur for growth, and obtain it either from inorganic sulfate or from organosulfur compounds. One of the mechanisms of transport of sulfate into the cell is catalyzed by ABC transporters, which in gram negative bacteria are formed by two integral membrane, two nucleotide-binding domains and one periplasmic ligand-binding protein responsible for affinity and specificity of the system. In the phytopathogenic bacteria *Xanthomonas axonopodis* pv*. citri* (*Xac*) the *ssuABCDE* operon was related to the alkanesulfonate transport. We describe the structural and biochemical characterization of the SsuA protein. Native crystals of SsuA were grown in presence of HEPES and diffracted at 2.0 Å resolution. NaI and $CsCl_3$ derivative crystals were obtained by quick cryo-soaking and the structure was solved by multiple isomorphous replacement anomalous scattering (MIRAS). SsuA is an α/β sandwich protein with two domains separated by a cleft where the HEPES was bound. Spectroscopic analyses of the protein in different pH and in the presence of alkanesulfonates revealed that SsuA was stable in neutral pH and suffered structural changes in presence of MOPS, CHES and MES. In the presence of these ligands, SsuA showed an increased thermal stability, as evidenced by thermal shift assays. Molecular modelling of interactions realized between SsuA and all ligands revealed the structural basis for increasing in the thermal stability. Comparison of *Xac* SsuA and orthologs also was carried.

key words: alkanesulfonate-binding protein, SsuA, ABC transporter
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