

Biochemical and structural characterization of the molybdate transporter ModABC from the pathogenic bacteria *Xanthomonas axonopodis* pv. *citri*

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The periplasmic molybdate-binding protein (ModA) of *Xanthomonas axonopodis* pv. *citri* (*Xac*) determines the affinity of an ion-binding system responsible for the specific transport of molybdate in this phytopathogenic bacteria. The crystallographic structure of the *Xac* ModA protein was previously solved by our group and two ModA mutant proteins were expressed and structurally characterized. Spectroscopic analyses showed that the mutation D59A is important to maintain functional and structural features in the protein. The crystallographic structure of a second mutant protein (K127S) demonstrated to be very similar to the native protein structurally and functionally. Additionally, through fluorescence assays it was possible to determine the affinity of each mutant for the molybdate and carrying out the comparisons with the native protein. Moreover, molecular dynamics simulations of the ModA protein were performed in the presence and absence of molybdate and showed that the release mechanism of this ion-binding protein is coincident with data already described for other type of binding proteins. Additionally, with the aim of studying the interactions among molybdate transport proteins (ModA, ModB and ModC), we have explored the three-dimensional structure of the membrane protein (ModB) in complex with the ATPase-binding protein (ModC), both models obtained by homology modeling. The model for the *Xac* transporter showed conservation of the interacting regions when compared with other orthologs including *Archaeoglobus fulgidus*, which was used as the template. The comparison of the *Xac* molybdate transporter with other ABC transporters will be of great interest for the identification of similarities and differences among them regarding the interactions between: i) periplasmic protein and ligand and ii) periplasmic or cytoplasmic proteins and trans -membrane domains.

Key Words: molybdate, ModA, ModB, ModC, *Xanthomonas axonopodis* pv. *citri*.

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