

Comparative modeling of *Gluconacetobacter diazotrophicus* proteins involved in plant- bacteria association

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The gram-negative endophytic bacterium *Gluconacetobacter diazotrophicus* is found in plants such as sugarcane, pineapple, coffee and sweet potato. This bacterium fixes atmospheric nitrogen, produces plant growth-promoting hormones and bacteriocins and helps solubilization of zinc compounds. The *G. diazotrophicus* PAL5 genome [Refseq: NC_010125] has about 3778 protein sequences. We study proteins that could be involved during plant-bacteria association. From these, 32 proteins were denoted as outer membrane proteins and 34 as secretion system proteins. In addition, we decided to examine another 14 proteins predicted as extracellular by PSORTb. These 80 proteins were analyzed by MHOLline, a computational workflow for structural genomic projects. MHOLline combines a specific set of programs for comparative modeling approach. The first result showed that 30 three-dimensional models can be constructed by MHOLline (e-value>0.00001, identity>25% and coverages between sequences>70%), comprising 18 outer membrane proteins, 7 secretion systems proteins and 5 extracellular proteins. Analysis with bioinformatics programs showed that 16 proteins with excellent stereochemistry quality should be studied in the future by docking and molecular dynamics (MD) simulations. These proteins have different function, most of them (11) form long pores for multidrug efflux and protein export. Also, there are proteins belong to the secretion systems (2), one levansucrase, one inner membrane lipoprotein and one component of the response regulator transcription systems. We focus in these proteins that are probably involved in signaling and recognition in plant-bacteria association.

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