Molecular Modeling Studies of Nitrogenase's Conformational Protection Mechanisms in *Gluconacetobacter diazotrophicus* and *Azotobacter vinelandii*

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G. diazotrophicus is a nitrogen-fixing bacterium found in plants such as sugarcane and coffee. Although its respiratory system requires a high flux of O_2 to work properly, high concentrations of oxygen inactivate the nitrogenase complex, which is responsible for the biological nitrogen fixation. Different metabolic approaches of protection against nitrogenase inactivation were described. A mechanism of conformational protection of nitrogenase has been reported in *A. vinelandii*, other nitrogen-fixing bacterium, through interaction between a FeSII protein and the Fe-protein (one of the two subunits of nitrogenase complex). In such complex, nitrogenase is inactive, but protected against the harmful effects of O_2. It has been proposed that a similar mechanism of protection also takes place in *G. diazotrophicus.* Analysis of the whole *G. diazotrophicus* genome showed a single gene presenting the fer2 ferredoxin domain, the same as the FeSII from *A. vinelandii*, which was then denoted as the putative FeSII protein from *G. diazotrophicus*. This work intends to understand the possible mechanism of interaction between FeSII and Fe-protein. First, the three-dimensional models of both *A. vinelandii's* and *G. diazotrophicus'* FeSII proteins were built trough comparative modeling. Subsequently, docking calculations were carried out to identify low energies complexes. These complexes were further simulated through Molecular Dynamics (MD) to gain insights about their affinities, contacts and stabilities. Preliminary results suggests that the homodimer models of FeSII of *G. diazotrophicus* interacts mainly by electrostatic forces and MD analysis have shown that the dimer was stable throughout 10ns dynamics. The interaction between FeSII proteins and Fe-proteins will be further analyzed using a similar computational procedure.

Keywords: Bioinformatics, nitrogen fixation, FeSII

Acknowledgements: Capes, CNPq and Faperj.