

Metabolic Pathways Analysis and Molecular Modeling of the Enzymes Responsible for Indole-3-acetic Acid Biosynthesis in *Gluconacetobacter diazotrophicus*

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Gluconacetobacter diazotrophicus is an endophytic nitrogen-fixing gram-negative bacterium, originally isolated from sugarcane. It was subsequently found in association with many other organisms, such as rice, sweet potato and coffee. It is known that the association with this bacterium propitiates several benefits to sugarcane. In addition to nitrogen fixation, it was shown that *G. diazotrophicus* promote plant growth by other mechanisms. Indeed, the ability of producing plant growth-promoting hormones, especially indole-3-acetic acid (IAA) is also of great importance. The objective of the present work was to unravel the pathways and the respective enzymes involved in the production of this hormone in *G. diazotrophicus*, and to build 3D models of these enzymes using comparative modeling. We could successfully identify, using similarity searches and multiple sequence alignments techniques, six enzymes that are significantly related with IAA biosynthesis and build models of good quality for all of them. Also, a key enzyme that acts in the indole-3-acetamide pathway wasn't found in *G. diazotrophicus*, suggesting that this organism is unable to produce IAA through this pathway. Analysis of the 3D models will permit a greater understanding of the role played by these enzymes, such as suggestion of mutations intending to optimization of the reactions. The identification of these enzymes will allow a better insight of their respective gene regulatory regions, being able to search for patterns and possible binding sites for transcription factors, aiming to propose a model for the transcriptional regulation of this hormone.

Keywords: *Bioinformatics; Gluconacetobacter diazotrophicus; plant growth-promoting hormones.*

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