COMPARATIVE ANALYSIS OF THE THREE-DIMENSIONAL STRUCTURAL OF THE CRY23AA1 AND CRY51AA1 INSECTILE PROTEINS USING BIOINFORMATIC TOOLS.

Luis Angel Chicoma Rojas, Renato Farinacio, Eliana Gertrudes de Macedo Lemos

Private University Antenor Orrego & Paulista State University, Jaboticabal Campus

Abstract

Bacillus thuringiensis has been widely used as a bioinsecticide or in the genetic transformation of plants because of its ability to produce a wide variety of active toxins, such as Cry proteins. The use of computational methods for the study of the three-dimensional structures of Cry proteins allows a better understanding of their functionality and classification, for this reason, the objective of this work is to make a comparison between the tertiary structures of the Cry23Aa1 and Cry51Aa1 proteins, and their respective amino acid sequences, to identify the similarity between said biomolecules.The NCBI database was used to obtain the amino acid sequence of the Cry23Aa1 (GenBank: AAF76375.1) and Cry51Aa1 (GenBank: ABI14444.1) proteins. The SuperPose 1.0 program was used to perform a sequence alignment between proteins and identify their degree of identity and similarity. To obtain and display / edit the three-dimensional structures of Cry23A1 and Cry51Aa1, the SWISS-MODEL server and the Pymol 2.0 program were used, respectively. The electrostatic surface of both proteins was calculated with the APBS program (Adaptative Poisson-Boltzman Solver). Finally, to generate a matrix graph, a structural overlap was made between Cry23Aa1 and Cry51A1 with the Distance Difference Matrix (DDM) of SupePose 1.0 and structural alignment commands of Pymol 2.0. The results showed that at the amino acid sequence level the Cry23Aa1 and Cry51Aa1 proteins have a score, identity and similarity of 127.5, 20.8% (67/322) and 34.2% (110/322), respectively. At the level of three-dimensional structure, a Root-Mean-Square Deviation (RMSD) of 1.85 was identified, indicating a high similarity. Through computational biology tools it is possible to understand the differences that exist at the structural level of different molecules that are of interest, allowing a better classification of these.

Funding: