Modeling and Molecular Docking of the largest subunit of the Ribulose-1,5-Bisphosfate Carboxylase/Oxygenase (RuBisCO) from Alkalinema sp. CACIAM 70d

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Riblose -1,5- bisphosphate carboxylase/oxygenase (EC 4.1.1.39, RuBisCO) is the most abundant protein in the world and is considered the major enzyme involved in the photosynthesis process and can be found in most autotrophic organisms like photosynthetic bacteria, cyanobacteria, algae and plants. RuBisCO is classified in four distinct forms: Forms I, II, III and IV. The form I of RuBisCO is a hexadecameric protein structure with eight copies of both large and small polypeptides in an $(L_2)_4(S_4)_2$ structure codified by *rbcL* e *rbcS* genes, respectively. This form is the predominant RuBisCO found in nature and it is present in Cyanobacteria, algae and plants. To unravel the structure and function of this enzyme in Cyanobacteria, this study aimed to construct a three-dimensional model (3D) of the large subunit of a Cyanobacterium from the 'Coleção Amazônica de Cianobactérias e Microalgas' – LTB/UFPA. The amino acid sequence was obtained from a genomic study of cyanobacterium Alkalinema sp. CACIAM 70d isolated from superficial water of Tucuruí Hydropower Plant Reservoir, Pará State, Brazil. The mold selection was chosen using Blast tool included in the PDB database. The best identity with RuBisCO from the *Synechococcus* PCC6301 (PDB ID: 1RBL.A). The three dimensional structure was generated through Modeller 9.10 and subsequently validated by the Ramachandran plot, Verify3D, Anolea and the Root Mean Square Deviation (RMSD). Finally, Molegro Virtual Docking was used for an analysis of molecular docking (MD) to evaluate the substrate in the catalytic site fitting. The obtained structure showed 15 β-sheets and 19 α-helix. The Ramachandran plot showed 98.28 of residues within energetically favorable regions and 89.29% of residues showed positive value in the 3D-1D evaluation. Individual residues analysis done by Anolea resulted in a few regions with high energy and the obtained RMSD value was 0.194. The map of electrostatic potential revealed similarity between the molecules regarding to their charge distributions, with low electron density even to the active site region. The best conformation obtained in MD process showed MolDock and Rerank scores -124,222 and -91.5559, respectively, significantly similar to those obtained for the template that showed values -135.27 and -96.8823. Furthermore showed the main interactions already described, highlighting those with Lys167, Lys169 and His290 residues, as well as with magnesium ion. The highest structural conservation, including electrostatic charges and interactions presented by the obtained model, classifies it positively, been contributing to studies that aims to optimize the carboxylase activity of RuBisCO and cyanobacteria biomass exploitation.