HOMODIMERIC STRUCTURE OF *B. JAPONICUM* D-NCAASE

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N-carbamoyl-D-amino acid amidohydrolase (EC. 3.4.22.12) or D-NCAase is an enzyme that catalyzes the formation of *D*-amino acids, widely used in β-lactam-like antibiotics development. Although it appears as a dimer and trimer forms of identical subunits (~34 kDa), D-NCAase crystal structure in *Agrobacterium radiobacter* was refined as homotetramer. Being *A. radiobacter* a pathogen, the focus of this work was to analyze the structure of the D-NCAase "*in silico*" in the Brazilian strain SEMIA 5079 of *Bradyrhizobium japonicum* (non-pathogenic organism). *A. radiobacter* D-NCAase structure (pdb 1FO6) was used as template in homology modeling experiments (Modeller 8v2) to obtain the monomeric, dimeric and tetrameric structures of the *B. japonicum* D-NCAase. Results were validated in PROCHECK and molecular dynamic (GROMACS 3.3.1) was used in further refinement. Molecular dynamics experiments in spc water box (82.000 atom system) were used to test the D-NCAase dimeric forms using the GROMOS96 53a6 force fields. Steepest-Descent algorithm (2,000 steps) was used in energy minimization, and production dynamic (5 ns, 312 K) ran with PME treatment of electrostatic. *B. japonicum* D-NCAase monomer structure preserved the fold of the described *A. radiobacter* structure, and based in a 25.000 $Å^2$ hydrophobic surface, our model formed a stable homodimer with calculated dissociation $\Delta^i G$=-37.4 kcal/M. Based in these results we propose the homodimeric structure of *B. japonicum* D-NCAase.

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