Modeled Structures and Molecular Dynamics of Plant Ureases

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Widely found in plants, fungi and bacteria, ureases (EC 3.5.1.5) are nickel-dependent enzymes which catalyze hydrolysis of urea to ammonia and carbon dioxide. It is known that microbial and plant ureases display several biological properties that are independent of their ureolytic activity, such as the activation of blood platelets, interaction with glycoconjugates and insecticidal activity. In plants and fungi, ureases are homopolymers of subunits with ~840 amino acids, forming hexamers or trimers. Bacterial ureases have two or three smaller subunits which align within the single chain of plants and fungi ureases with ~55% sequence identity. Since structures of plants and fungi ureases are yet not solved, models for a *C. ensiformi*s (jack bean) urease (JBU-IIB) and *G. max* (soybean) ubiquitous and embryo specific ureases were built via comparative molecular modeling with MODELLER9v4, using bacterial ureases structures as templates. Molecular dynamics studies of these structures, focused on possible differences and similarities among their dynamical behavior, were performed with GROMACS 3.3.1. Fully solvated enzymes were simulated for 10 ns using GROMOS96 force field, at 300K in a NTP ensemble. All three modeled ureases share the same overall structure with remarkable differences in their interdomain regions. Molecular dynamics trajectories showed the expected active site flaps flexibilities and maintenance of the active site organization throughout the simulation. It is also noteworthy that the different domains of the studied plant ureases seemed to move in an independent manner. These studies should help understanding the structural basis of biological properties of plant ureases (CAPES, CNPq, FINEP).
Keywords: comparative molecular modeling, molecular dynamics, ureases.