

STRUCTURAL INSIGHTS INTO THE HIGH PROTEOLYTIC ACTIVITY OF  
BJUSSUSP-I – A SERINE PROTEASE FROM *BOTHROPS JARARACUSSU*  
VENOM – OBTAINED BY THE ANALYSIS OF A THEORETICAL MODEL

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Snake venom serine proteases (SVSPs) are enzymes which affect the haemostatic system and belong to the trypsin family S1 (clan SA). Their actions on many components of the coagulation cascade and other systems and cells cause a disorder of the haemostatic system, contributing thus for the immobilization and death of the preys. A theoretical model of BjussuSP-I, a high-catalytic SVSP isolated from the *Bothrops jararacussu* venom, was built using threading techniques and submitted to a molecular dynamics (MD) simulation in order to improve the initial quality of the model and to obtain insights into the functional mechanisms of this molecule. The “open” disposition of 37, 60, 70, 99, 148, 174, and 218-loops in the theoretical model could explain part of the high proteolytic activity of BjussuSP-I since such conformation seems favoring the contact of the substrates with the catalytic site triad formed by the residues His57, Asp102, and Ser195. In addition, the good quality of the final theoretical BjussuSP-I model obtained after the MD simulation shows the potential importance of the acquired information to the understanding of the features relative to BjussuSP-I and other serine proteases.

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