

Structural characterization of the allergen hyaluronidase from the venom of the wasp *Polybia paulista* (Hymenoptera, Vespidae)

Pinto, J.R.A.S.; Santos, L.D.; Arcuri, H. A.; Dias, N.B.; Palma, M.S.
CEIS /Department of Biology /IBRC-UNESP, Rio Claro/SP.

The venoms of social Hymenoptera are studied to improve our understanding about the allergies caused by wasps, bees and ants. *Polybia paulista* is one of the most abundant social wasps of Southwest Brazil, causing many accidents every year. Hyaluronidase is known as one of the major allergens from Hymenoptera venoms. The aim of this study is the structural characterization of this enzyme. The hyaluronidase was purified from the venom of the wasp *P. paulista* and sequenced by combining proteolytic digestion, peptide mass spectrometry analysis and automated Edman degradation. The molecular modeling was performed by using restrained-based modeling, implemented in the program MODELLER. The hyaluronidase from the venom of *Vespula vulgaris* was used as template (PDB: 2ATM); a total of 1000 models were generated and the final model was selected based on stereochemical quality. The programs PROCHECK was used to check bond lengths, bond angles, peptide bonds and side-chain ring planarities, chirality, main-chain and side-chain torsion angles. VERIFY 3D program, which measures the compatibility of a protein model with its sequence using a 3D profile, also was used for model validation. The RMSD from ideal geometry was extracted for each model using the program X-PLOR. The model presented all these parameters with acceptable values. As the typical allergenic hyaluronidase the model presented seven α -helices and seven β -sheets covering respectively, 44% of and 10.7% of the sequence. The core of the molecule presents a barrel constituted of an alternation of β -sheets and α -helices in a $(\alpha/\beta)_5$ formation, characteristic of the glycosyl hydrolases.

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Key words: wasp venom; allergen; hyaluronidase