

Molecular Modeling of the Allergen Arginine Kinase From The Venom of the Wasp
Polistes lanio lanio.

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Allergy to Hymenoptera venom is a classical IgE-mediated disease. Arginine kinase (AK) is a novel allergen identified both in crustaceans muscles and in Hymenoptera venoms. *Polistes* wasps are found in Southeast Brazil, where cause many stinging accidents. Four different isoforms of AK were identified during the proteomic analysis of *P. lanio lanio* venom. The complete sequences of these allergens were obtained by using the combination of *in gel* proteolytic digestions and mass spectrometry peptide sequencing, revealing a few polymorphic differences between them. All the isoforms were very conserved in relation to the AK from crustaceans. The aim of the present investigation was the structural characterization of these allergens. The molecular modeling was performed using restrained-based modeling, implemented in the program MODELLER. The AK from crab muscle (PDB: 1RL9) was used as template; a total of 1000 models were generated for each isoform model and the final models were selected based on stereochemical quality. The programs PROCHECK and WHATCHECK were 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. All the models presented all these parameters with acceptable values. All the four models presented two globular domains, in which first in N-terminal region is α -helical, while the C-terminal region consists of an eight-stranded antiparallel β -sheet flanked by seven α -helices. Supported by: **BIOprospecTA-FAPESP/CNPq**.

Key words: arginine kanase; molecular modeling; allergen; wasp venom