Three-Dimensional Modelling of Honeybee Venom Allergenic Proteases: Relation to Allergenicity

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Z. Naturforsch. **66 c**, 305 – 312 (2011); received July 23, 2010/March 14, 2011

Api SI and Api SII are serine proteases of the honeybee venom containing allergenic determinants. Each protease consists of two structural modules: an N-terminal CUB (Api SI) or a clip domain (Api SII) and a C-terminal serine protease-like (SPL) domain. Both domains are connected with a linker peptide. The knowledge about the structure and function of Api SI and Api SII is limited mainly to their amino acid sequences. We constructed 3-D models of the two proteases using their amino acid sequences and crystallographic coordinates of related proteins. The models of the SPL domains were built using the structure of the prophenoloxidase-activating factor (PPAF)-II as a template. For modelling of the Api SI CUB domain the coordinates of porcine spermadhesin PSP-I were used. The models revealed the catalytic and substrate-binding sites and the negatively charged residue responsible for the trypsin-like activity. IgE-binding and antigenic sites in the two allergens were predicted using the models and programs based on the structure of known epitopes. Api SI and Api SII show structural and functional similarity to the members of the PPAF-II family. Most probably, they are part of the defence system of *Apis mellifera*.

Key words: Honeybee Venom, Allergenic Proteases, Protein Modelling