Analysis *in silico* of the chitin binding domains of legume vicilins and relationship with *Callosobruchus maculates* toxicity

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Chitin is a long-chain polymer of a β-1,4-*N*-acetyl-*D*-glucosamine residues, is the main component of the cell walls of fungi, the exoskeletons of arthropods, such as crustaceans and insects. Vicilins (7S storage proteins) from cowpea (*Vigna unguiculata*) and other legume seeds were shown to bind to chitin and have been implicated as antibiosis factors against insects, particularly the cowpea weevil, *Callosbruchus maculatus*. In this work, knowledge-based proteins modeling and substrate docking experiments as well as structural sequence comparisons were performed to identify vicilin chitin-binding domains in *V. unguiculata* and *Canavalia ensiformis*. Vicilin from *Glycine max*, protein of known three-dimensional structure, was used as the template to generate a model structure for vicilin. To build a model structure for vicilin of the *V. unguiculata*, automated protein homology-based molecular modeling software were used (SWISS-MODEL and PROCHECK) and 3D model for vicilin of the *C. ensiformis* and *G. max* were obtained from PDB. The structural model from *V. unguiculata* vicilin presented 86% homology and 0.36Å RMSD compared to structural model from *G. max* vicilin. Vicilins sequences alignment and chitin binding domains (Hevein domain – HD; R&R concensus motif found in insect cuticular proteins – R&R; β-conglicinine domain – CD) was done with the ClustalW program and localization of chitin domains were done using Pymol and SPdbV programs. Protein docking of the vicilin model with β-1,4-N-acetyl-D-glucosamine (GlcNac) was constructed using GRAMM program and visualized with PyMol and Ligand Explorer Programs. This structure revealed that two concerved domains R&R and CD occur in the vicilins from *G. max*, *C. ensiformis* and *V. unguiculata*. These conserved domains are believed to be involved in chitin binding. Hevein domain don't was found. Comparasion of amino acid conserved in chitin binding domains demonstred that CD can be associated to WD_{50} of the legumes vicilins to *C. maculatus*.
Key words: *In silico* analysis, chitin-binding domains, vicilins, *Callosobruchus maculatus*.