Abstract

Arcelin, a seed protein originally discovered in wild bean accession of *Lablab purpureus* was purified, characterized, and compared to phaseolin, the major seed protein of common bean *Phaseolus vulgaris*. There are several reports available for common bean arcelin from *P. vulgaris* and its defense mechanism against the stored product insect pests, but...
L. purpureus 
arcelin function is not yet studied well. To understand the molecular function of arcelin in L. purpureus 
the structural knowledge is essential. This work is an attempt to explore the molecular defense mechanism of L. purpureus 
arcelin based on homology modelling and binding pocket analysis to emphasize the structural and functional relationship. The structural template from P. vulgaris arcelin [1AVB] is selected for homology modelling of L. purpureus 
arcelin. The 3D structure of L. purpureus 
arcelin was generated using Modeller software. The best model is selected based on Ramachandran Plot, Errat and Energy minimization analysis (Steepest Descent). The overall quality of computed model showed 87.2 % amino acid residues under favored region with 93.5 % overall quality. The putative refined model of L. purpureus 
arcelin was deposited into Protein Model Data Base with ID: PM0076542. Deposited model is used for further active cavity analysis against carbohydrate (sugar) binding sites. These results will help further development of transgenic crops with arcelin for future integrated insect pest management (IPM) programme.

Reference

Comparative Modeling and Prediction of Carbohydrate Binding Pockets in 3-D Structure of Wild Pulse Lablab Purpureus Arcelin

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