Protein-Protein Docking of Serine Proteinase of Nematodes with Plant Proteinase Inhibitors

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Root-knot nematodes are plant-parasitic nematodes on horticultural and agricultural crops; they cause damage on root of the plant. Generally the plant parasitic nematodes are controlled with the help of synthetic nematicides. Very high cost of nematicides and environment safety and concern has necessitated reducing the use of amount of nematicides for nematode control. So there is a need of effective, ecologically safe control methods. Biological

method is the securest way to solve these problems. Proteinases Inhibitors of various plants are used to control the proteolysis of nematodes by inhibiting gut Serine Proteinases. In present work the 3D models of Serine Proteinases as well as Proteinase Inhibitors generated using Modeller9v8 and I-Tasser server. These models were testified using several validation methods including Procheck, What-IF, ProSA, Errat and Verify-3D. All predicted structures validation score shows that geometric quality of the backbone conformation, residue interaction, residue contact and energy profile of the structure were well within the limits accomplished for reliable structures. Protein-Protein interacting surface patches was identified by PPi-pred. Site specific docking was performed by using ZDOCK server and backbone refinement of protein complex was performed in Fiber Dock server. Protein complexes having minimum energy was again docked in using Rosetta Dock server. Docking output parameter like energy score, number of forming Hydrogen bond, Van der walls interaction, Electrostatic potential etc. inferring that Serine Proteinase was inhibited by Proteinase inhibitors. The energy score, electrostatic potential map, key hotspot residues and hydrogen bonding shows that some of Serine Proteinase inhibitor was potent inhibitor in comparison to others. This study has been further helpful in understanding the mechanism of proteolysis by inhibition of Serine Proteinase and selecting potent inhibitor for transgenic plant development.