



Functional Synergy Between Pathogenesis-Related Proteins for Sustainable Crop Protection

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Abstract

Pathogenesis-related (PR) proteins have been combined for effective plant disease control, yet their synergistic mechanisms remain unexplored at the molecular level. This study elucidates the molecular basis of synergism between thaumatin-like protein (TLP) and PR1 using computational (in silico) methods. Analyses encompassed physicochemical properties, subcellular localization predictions, topological and domain characterization, conserved motif identification, phylogenetic relationships, secondary and tertiary structure prediction, molecular docking and simulation of TLP and PR1 individually and combined with key fungal cell wall components. Physicochemical profiling indicated TLP as a neutral, hydrophobic, thermostable protein, while PR1 was acidic, hydrophilic, and thermostable. Both were predicted to localize extracellularly, with TLP exhibiting transmembrane topology and PR1 positioned externally. Docking simulations revealed superior binding affinities for the TLP-PR1 complex versus individual proteins against chitin, chitosan, glucan, and mannan. These computational insights highlight the synergistic chitinolytic mechanism of TLP-PR1, suggesting their co-expression could potentiate broad-spectrum antifungal defense and inform strategies for engineering durable plant resistance.

Keywords: *Thaumatococcus*-like protein (TLP), PR1 protein, Chitinolytic activity, Synergistic antifungal defense, Molecular docking.

