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A Computational Approach of Plant-Microbe Interactions

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Abstract—*Polygalacturonases (PGs) are secreted by phytopathogenic fungi or bacteria to degrade the plant cell wall homogalacturonan during plant infection. Polygalacturonase inhibiting proteins (PGIPs) are cell wall proteins that inhibit the pectin-depolymerizing activity of polygalacturonases. These ubiquitous inhibitors have a leucine-rich repeat structure that strongly conserved in monocot and dicot plants. The interaction with PGIP limits the destructive potential of polygalacturonases and might trigger the plant defence responses induced by oligogalacturonides. Structural information for PGIP-PG complex are being absent, we performed molecular modelling to gain insight into the mechanism of recognition and discrimination of PGs by PGIPs. We have built homology models of banana germplasm PGIP using the crystal structure of Phaseoulus vulgaries PGIP (pvPGIP) (1OGQ) as template. The banana PGIPs was then docked with Erwinia PG to elucidate the characteristics features of their interactions. We mutate the Phaseoulus vulgaries PGIP and elucidate the interaction with Erwinia PG. In order to investigate the role of PGIP-PG interactions, we have carried out a series of solvent Molecular Dynamics Simulations of 50 ns on banana PGIP (bPGIP), Ervinia PG (ecPG), bPGIP-ecPG complex, pvPGIP and pvPGIP-ecPG complex. van der Waals and eletrostatic interactions play an active role in PGIPs for proper recognition and discrimination of PGs. Docking studies reveal that bPGIPand pvPGIP interact with the residues constituting the active site of ecPG with implications that the proteins bind ecPG at its active site and thereby inhibit the enzyme.*