

## ***In-Silico* Identification of Potential Targets for Sugarcane Smut Disease**

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### **Abstract**

Sugarcane (*Saccharum officinarum*) is a significant agro-industrial crop all over the world. It is polyploid crop with genomic size of 10GB. It is cultivated for its stalk in more than 119 countries, which accumulates sucrose. It contributes 60% of the raw sugar produced worldwide, the remaining comes from sugar beet. Sugarcane smut disease is caused by the fungus *Sporisorium scitamineum* that causes considerable yield losses. The symptoms for the sugarcane smut are black whip like structure instead of spindle leaves, emerging from the meristem, thin stalks, and leaves are more slender and much weaker. In present study potential targets were found against smut disease in sugarcane using subtractive genomic approaches. Molecular docking of drug target with available ligands helped to find a more suitable drug for sugarcane smut. The whole proteome of 11214 proteins of pathogen was retrieved from UniprotKB. Similar and repeated sequences were eliminated by CD-HIT server and only 8235 non-paralog sequences were obtained out of the total proteome. Homolog sequences were compared with host using NCBI-BLAST and 8079 non-homolog sequences were identified. DEG identified 452 essential proteins of pathogen. 3-D structures of two functional proteins ARL1-ADP-ribosylation factor and n-acetyltransferase were checked from Protein Data Bank but due to non-availability of their structures, 3D-Model of each protein was predicted using four homology modeling tools. Molecular docking was performed against the best selected protein model of ARL1-ADP-ribosylation factor with a library of 5000 phytochemicals and only ten compounds were selected which showed best interactions. Luteolin 7-O-beta-d-glucopyranoside compound was selected due to showing lowest RMSD and S-score with the target protein. Potential target identified in this study and docking results with different ligands can be developed more effective and suitable drug to eliminate the sugarcane smut disease caused by pathogen *S. scitamineum*.

**Key Words:** *Sporisorium scitamineum*, Proteome, Essential Proteins, Pathway analysis, Subcellular localization, Druggable targets, Docking