Rani et al. (2017) Can J Biotech, Volume 1, Special Issue, Page 34
https://doi.org/10.24870/cjb.2017-a21

Canadian Journal of Biotechnology

ISSN 2560-8304
Poster Presentation OPEN ACCESS

Category: Bioinformatics

Screening of phytochemicals from selected plants with antifungal properties against RXLR effector protein Avr3a11 in *Phytophthora capsici*

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Abstract

Phytophthora Capsici is a fungal plant pathogen which causes significant damage to broad range of commercial & medicinally valuable plants like black pepper, tomato, watermelon, etc. Chemical compounds like fungicides are commonly used against *Phytophthora* infections. Prolonged inhalation of fungicides by humans, leads to neural & visual disturbances & lung infections. They can also permanently silence or reprogram normal genes that last for several generations & are very harmful to the environment too. An alternative to chemical control of fungal pathogens is by introducing phytochemicals, which are potentially active against *Phytophthora capsici.*

The study involves computational screening of phytochemicals with antifungal activity of plants against Avr3a11 in *P. Capsici.* Avr3a11 is an RXLR effector protein which functions as a virulence factor when recognised by plant immune receptors. The functional domain in Avr3a11 interacts with Resistance (R) proteins of the plant thereby triggering ETI (Effector Triggered Immunity) in plants. The phytochemicals from Turmeric, Garlic and Neem were used as ligand molecules. The 3D structure of Avr3a11 was retrieved from PDB (PDB id: 3ZR8) & the ligand structures collected from PubChem. Molecular docking was carried out in *Discovery studio* package to assess the binding energy of the phytochemicals with Avr3a11 in its functional domain. The phytochemical Alliin from garlic showed significant binding interactions with the target-Avr3a11 compared to the commonly used fungicides, indicating that Alliin can act as a potential inhibitor of Avr3a11. An *in vitro* assay of the plant extracts on *phytohthora capsici* also gives a validation of the docking study. This study provides insight into the potential use of phytochemicals to effectively combat the Phytophthora infections in plants.

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Citation: Rani, J.R., Aswathy, T.R., Kumar, M.S., Nair, A.S. and Soniya, E.V. SHIVGAMI : Screening of phytochemicals from selected plants with antifungal properties against RXLR effector protein Avr3a11in *Phytophthora capsici* [Abstract]. In: Abstracts of the NGBT conference; Oct 02-04, 2017; Bhubaneswar, Odisha, India: Can J biotech, Volume 1, Special Issue, Page 34. https://doi.org/10.24870/cjb.2017-a21