Radopholus similis, a migratory endoparasitic nematode that cause massive necrosis of plant tissues and destruction in host plants. The search for new nematode control molecules, particularly those of natural origin are of great urgency and importance. Phenylpropanoids belong to a major group of secondary metabolites produced by plants, mainly in defense response to biotic or abiotic stresses; literatures shows that chemical constituents of this family have bioactive compounds that can substitute current synthetic nematicides. But its efficacy and mode of action have not been demonstrated scientifically. In the present study, compounds from metabolic pathways of phenylpropanoid biosynthesis in black pepper (Piper nigrum L.) have been screened for nematicidal and potential target inhibiting activity towards burrowing nematode, R. similis and the mechanism of inhibition of novel targets has been studied with molecular docking. The 3D structures of phenylpropanoid biosynthesis related phytochemicals were used as ligands. Available eight novel target protein (β-1, 4, endoglucanase, calreticulin-1, xylanase, cathepsin B-like cysteine proteinase, cathepsin S-like cysteine proteinase, cytochrome c-oxidase subunit III, glutathione S-transferase and transthyretin-like protein 3 precursor) of nematode associated with parasitic lifestyles and survival were selected.
Virtual Screening and in vitro Assay to Explore Novel Inhibitors from Black Pepper against Potential Targets of Radopholus similis as target molecule. Potential binding sites on each protein surfaces were predicted and screened phenylpropanoids have been docked to modeled targets of R. similis to assess their molecular interaction, binding energy and consequently their inhibitory activity. The docking results showed that thirteen phenylpropanoids possess similar dock score and hydrogen bond interactions, compared to current inhibitors and nematicides. Screening of these compounds in an in vitro assay showed that eight among the thirteen phenylpropanoids (syringaldehyde, salicylic acid, catechol, ferulic acid, coumaric acid, caffeic acid, tannic acid and N-vanillylnonanamide) caused maximum mortality to R. similis at 200ppm. Ferulic acid at 250ppm and 500ppm reduced R. similis population in infected black pepper in green house study. Hence the compounds represent promising starting points as lead compounds of natural origin that inhibit R. similis; this provides possibility to further exploit these compounds in nematode management. The study also helps in understanding various aspects of phenylpropanoid pathways that can be manipulated for in-situ production and enhancement of these compounds.

References

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Radopholus similis; burrowing nematode; black pepper; in vitro assay; phenylpropanoid pathway; molecular docking; molecular modeling; in silico prediction; virtual screening.