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(Research Article)

Molecular docking study on the interaction between fatty acid and retinol binding protein of root knot nematode and indole-3-acetic acid for nematicide action

Somnath Waghmare [1, *], Shivprasad Tingare [2], Sandip Badgujar [3] and Balde Govind [3]

[1] *Department of Zoology, Nowrosjee Wadia College, Pune, Maharashtra, India- 411 001.*
[2] *Department of Zoology, Shri Shiv Chhatrapati College, Junnar, Pune, Maharashtra, India-410502.*
[3] *Department of Zoology, N.T.V. S's G. T. Patil Arts, Commerce & Science College, Nandurbar, Maharashtra, India- 425412.*

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Abstract

The root-knot nematode (RKN) Meloidogyne javanica is present in plant roots and destroys numerous economically important plants which include cereals, vegetables, grape wine, and some ornamental plants. Fatty acid and retinol-binding protein (FAR) are important in the development of nematodes in their respective hosts. Therefore, FAR is of major interest as a target for drug development. The three-dimensional structure of the FAR protein was predicted using the MODELLER 9.24, and the homology modeling based predicted model was further validated using the PROCHECK analysis tool. The metabolic product of Fusarium oxysporum a fungus endophytes indole-3-acetic acid was found to bind at the active sites of fatty acid and retinol-binding protein of Meloidogyne javanica with lowest binding energy -6.4 Kcal/mole. The molecular docking interactions analysis of FAR protein with the ligand indole-3-acetic acid using AutoDock Vina allows us to detect the specific amino acid residues like Leu- 59, Asp-72, and Lys-120. Within the FAR proteins binding pockets these amino acids play a crucial role in the ligand-binding process and show the affinity towards ligand. The FAR protein model generated through the homology modeling approach along with structural insights gained from molecular docking analysis will promote the indole-3-acetic acid as a potent nematicide and a novel molecule for the rational drug design process. The present study contributes to the understanding mechanism of the nematicide effect of indole-3-acetic acid. Based on our InSilico findings we hypothesize that indole-3-acetic acid can be inhibitory effects on root-knot nematodes.

Keywords: Docking; Root knot nematodes; FAR; Indole-3-acetic acid; Binding energy

1. Introduction

Nematodes are the pathogenic parasites of plants and animals including humans, while some nematodes are free-living ones. Roundworms hold major global ecological and economic challenges [1]. Around 30,000 nematodes species have been identified and classified with an expected one million nematode species population supposed to exist [2]. Root-knot nematodes are potential pathogens of many economically important plant species. *Meloidogyne javanica* is one of the most substantial polyphagous nematode pests in the agricultural system in different parts of the word. The production and yield quality of plants get impacted highly by the infestation of root-knot nematodes. Approximately, 3000 wild and cultivated plant species have been described to be affected by these parasites [3]. Root-knot nematodes (RKN) are dispersed in different geographical conditions like tropical, subtropical, and temperate regions. Root-knot nematodes, 226 species belonging to 43 families, including some weed species, are known to act as hosts [4].

Fatty acid and retinol-binding (FAR) proteins, secreted by all trophic assemblies of nematodes, have long been recognized for their probable function in host immunomodulation development[5]. In the drug development process

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[*] Corresponding author: Somnath Waghmare

FAR proteins are of key interest for numerous reasons. As i) They play a significant role in foraging fatty acids and retinol for the existence of the parasite [6]. ii) By compromising the host's defensive immune response FAR may induce localized depletion of essential lipids such as oxylipins [7]. iii) FAR are located at the host-parasite interface [8]. iv) The structure of the FAR protein is exceptional to the nematode and is unlike that of any other recognized family of lipid-binding proteins [6]. Altogether above functions of proteins support that nematode restricted family of FAR proteins plays a key function in the host-parasite relationship [8]

There is an urgent need of finding natural product-based alternatives to control agricultural nematode pests to replace the biohazardous synthetic nematicides. The fungal endophyte *Fusarium oxysporum* secrets the various metabolites, amongst them a very popular phytohormone indole-3-acetic acid (IAA) plays a very critical role in initiating the plant resistance for various stimulus. Indole-3-acetic acid performs a dual role either as it kills the nematode parasites or by stimulating the defense mechanism of the plant against the nematode. These phyto-compounds like indole-3-acetic acid may act as an important lead molecule in the process of eco-friendly new nematicides design [9].

In-depth *in silico* analyses of FAR protein inhibition and protein-ligand interaction of the models were completed with high binding affinity. In the present study docking interactions between structural models of the fatty acid and retinol-binding protein and indole-3-acetic acid has been performed this molecular docking study helps for deciding strategies for developing drugs for nematode control.

2. Material and Methods

The fatty acid retinol-binding protein sequence (190 aa) of the plant-parasitic nematode *M. javanica* (UniProt Id. UniProtKB - L0ARN5) was retrieved from the UniProtKB Knowledgebase database [10]. The MODELLER 9.24 tool [11] was used to predict the tertiary structure of a fatty acid retinol-binding protein from the plant-parasitic nematode *M. javanica*. The protein BLAST tool was used to select the template for building the model by considering the PDB database identity more than 30%. The PROCHECK server of the PDBSum database [12] was used to predict, evaluate, and validate the homology build model of the FAR protein.

The docking of indole-3-acetic acid into the binding sites of fatty acid retinol-binding protein was discovered using the AutoDock Vina tool, which has been a proven tool for analysis of molecular interactions [13].

2.1. Preparation of protein for docking

The three-dimensional protein structure of a fatty acid retinol-binding protein from RKN *M. javanica* was built by using the homology modeling approach and the generated protein model was validated by various validation tools like PROCHECK server of PDBsum database (Fig. 01). FAR protein preparation for docking was done by removing all the removing water molecules and all non-protein molecules. All the docking calculations were completed by using the AutoDock Vina. FAR protein structure was improved by adding polar hydrogen's and kept the protein firm in the docking process, whereas all the torsional bonds of ligand were set free by ligand molecule in AutoDock vina tools.

2.2. Preparation of ligand for docking

The conjugate acid of indole-3- acetate ligand i.e. indole-3-acetic acid was retrieved from the PubChem database [14] (Fig. 02). The optimized ligand molecule was docked with the refined fatty acid and retinol-binding proteins of root-knot nematode using the AutoDock Vina.

The binding positions of protein and ligand were identified and authentication of the docking accuracy was done by docking the indole-3-acetic acid into its binding sites of fatty acid and retinol-binding protein. The AutoDock vina binding affinities of the indole-3-acetic acid into fatty acid and retinol-binding protein was estimated by the binding free energies in kcal/mol, the number of hydrogen bonds, and RSMD values.

2.3. Molecular Docking

Molecular docking interactions between fatty acid and retinol-binding protein of root-knot nematode and phytohormone indole-3-acetic acid were done by using Autodock Vina suite using a grid spacing of 0.375A^0, the grid points in x,y and z-axis were set to 30X30X30 A^0., and grid coordinate at centre= 4.052444, centre y= 29.866222, centre= 23.482667. The Lamarckian genetic algorithm search was used [15] and the generated results of protein-ligand interaction were studied by using the binding energies, and the number of hydrogen bonds interactions. A docking analysis consisting of 100 simulations was completed for the ligand. Docking analysis was based on free binding energies, RMSD values, perfectly bind ligand molecules were then ranked according to their increasing docking energies.

Figure 1 The modelled structure of Fatty acid and retinol binding protein from root knot nematode *M.javanica*

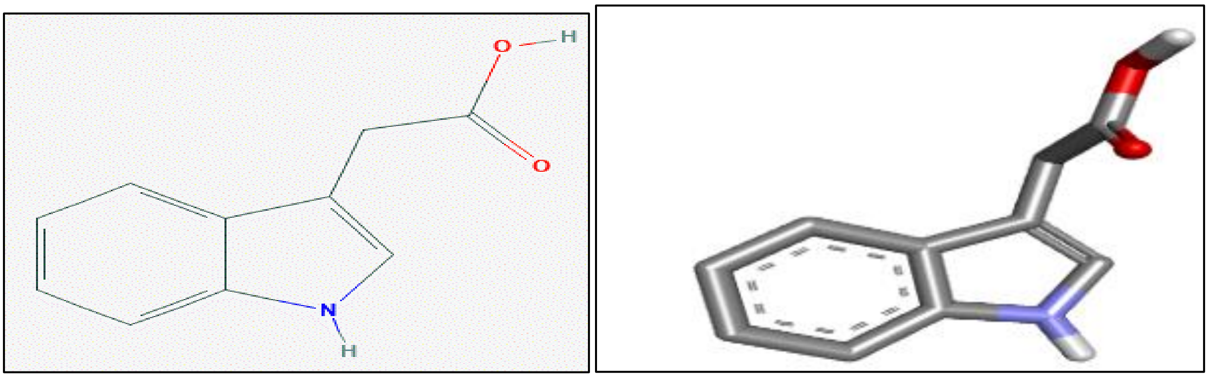
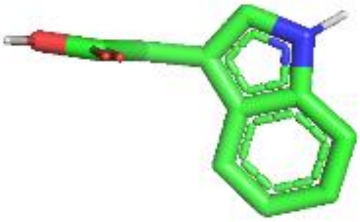


Figure 2 Structure of indole-3-acetic acid

3. Results and discussion

The docking interaction between the indole-3-acetic acid with fatty acid and retinol-binding protein of root-knot nematode *M javanica* was discovered using the widely accepted powerful molecular recognition tool AutoDock vina molecular docking study software. The molecular docking approaches are widely used for predicting the binding models of proteins to the total of energies of ligands [16]. The AutoDock Vina tool is used for the prediction of affinity, binding positioning, and binding activity of the ligand indole-3-acetic acid towards our plant root nematode target fatty acid and retinol-binding protein. The calculated RMSD values, lowest docked energy and free energy of binding sites are considered for the docking analysis. The RMSD values with upper boundaries and lowest boundaries along with the affinity of binding sites created on 09 different shapes of complementarity are shown in table no. 01

Table 1 Docking results of Indole-3-acetic acid molecule docked with fatty acid and retinol binding protein

Mode	Affinity(kcal/mol)	Distance from best mode		Lead molecule
		RMSDL.B.	RMSDU.B.	
1	-6.4	0.000	0.000	
2	-6.3	3.010	4.802	
3	-6.1	1.997	2.841	
4	-6.1	3.008	4.923	
5	-6.0	1.454	2.659	
6	-6.0	3.065	4.510	
7	-6.0	3.341	4.151	
8	-5.8	2.817	3.491	
9	-5.8	2.173	2.962	

The total internal energy, torsion free energy, intermolecular energy and unbounded systems energy is summed up to calculate the free binding energy. Docking analysis of protein and ligand interactions shown in the indole-3-acetic acid binding site are the hydrogen bonds with Leu-59 (H bonds 2.40 A^{o}), Asp-72 (H bonds 2.88 A^{o}) and Lys-120 (H bonds 2.21 A^{o}), whereas Ala-63 (Pi-alkyl 4.49 A^{o}), Val-62 (Pi-alkyl 4.89 A^{o}), Leu-79 (Pi-alkyl 4.80 A^{o}), Ala-75 (Pi-sigma bond 3.80 A^{o}), Pro-124 (Pi-alkyl 5.26 A^{o})interactions also noticed. The best docking pose of protein ligand interactions with maximum hydrogen 03 bonds are shown in fig.03. the best docking pose with protein ligand interaction in 2D diagram is shown in Fig 04.

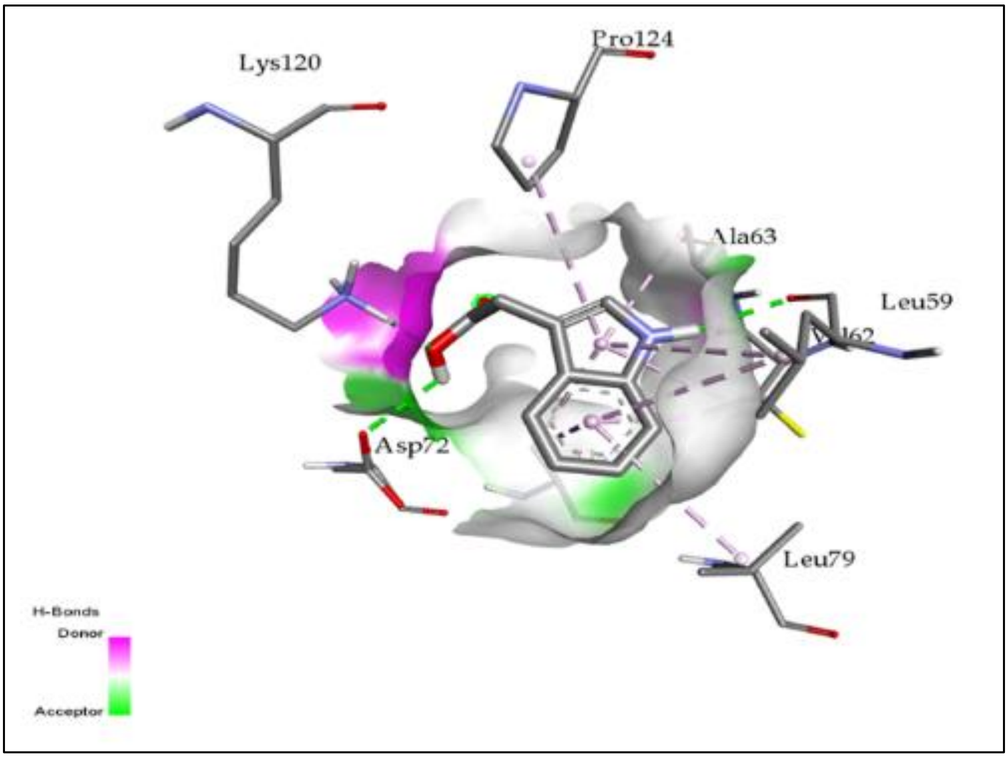


Figure 3 Molecular docking interactions of RKN M.javanica fatty acid and retinol binding protein with indole-3-acetic acid. FAR amino acids Leu-59, Asp-72, and Lys-120 forms hydrogen bonds with indole-3-acetic acid

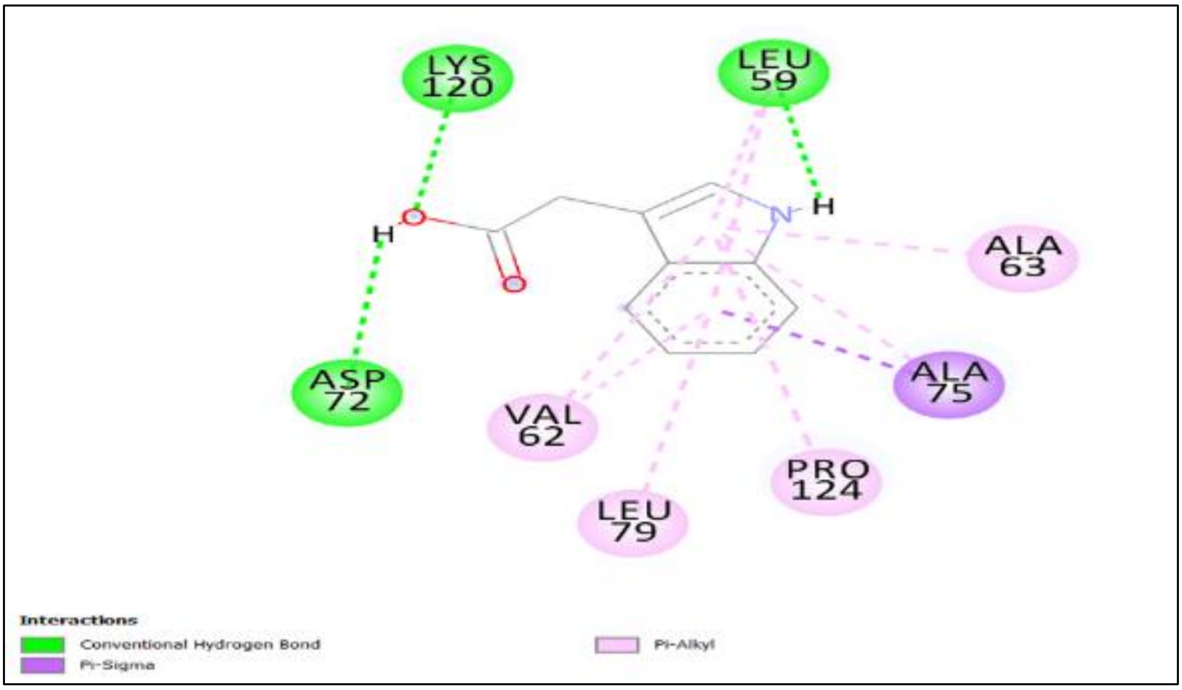


Figure 4 2D interactions between the FAR amino acid and indole-3-acetic acid

The molecular docking interactions from this prediction show that indole-3-acetic acid binds with fatty acid and retinol-binding protein of root-knot nematode and it also shows the inhibitory nature. So, we can use indole-3-acetic as a drug to control the root-knot nematodes. For drug designing, it is already knowing that inhibitory pathways have to be considered as a key drug target for nematode control. From this prediction analysis, we can hypothesize that indole-3-acetic acid plays an important function of inhibition of FAR protein activity which leads to the destruction of nematodes.

4. Conclusions

The outcomes of present molecular docking interactions undoubtedly show that *in silico* docking studies of indole-3-acetic acid along with fatty acid and retinol-binding protein of root-knot nematode *M. javanica* shows binding interactions and need further in-vitro studies on the synthesis of FAR protein inhibitor for treatment and control of root-knot nematodes.

Compliance with ethical standards

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Disclosure of conflict of interest

No conflict of interest to be disclosed.

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