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Issue Article

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MOLECULAR DOCKING STUDIES OF INDOLE-3-ACETIC ACID AND ITS ZINC(II) COMPLEX WITH THE TIR1 AUXIN RECEPTOR

Abstract: *Indole-3-acetic acid (IAA) is one of the most important natural auxins involved in plant growth regulation, cell elongation, differentiation, and developmental processes. The biological activity of auxins is mainly associated with their recognition by auxin receptor proteins, among which TIR1 (Transport Inhibitor Response 1) plays a key role in auxin-dependent signaling pathways. In the present study, molecular docking analysis was carried out to investigate the interaction of free indole-3-acetic acid and its zinc(II) coordination complex with the TIR1 receptor protein. The zinc(II) complex contains one Zn(II) ion coordinated by two IAA ligands in a monodentate mode and one monoethanolamine molecule acting as a chelating ligand. Blind docking was performed using the CB-Dock2 server to identify the most favorable binding cavities and ligand-binding poses. The docking results showed that free IAA interacts with the TIR1 receptor with a best docking score of -6.8 kcal/mol, whereas the Zn(II) complex demonstrated a significantly stronger binding affinity with a best docking score of -8.8 kcal/mol. The enhanced binding of the Zn(II) complex may be related to the presence of two IAA fragments, increased molecular size, additional donor groups, and a more preorganized coordination structure around the zinc center. These results indicate that coordination of IAA with Zn(II) may modify and enhance its interaction with the TIR1 auxin receptor.*

Key words: *Indole-3-acetic acid, IAA, auxin, TIR1 receptor, zinc complex, monoethanolamine, molecular docking, CB-Dock2, binding energy.*

Language: *English*

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Introduction

Auxins are a major class of plant hormones that regulate numerous physiological and developmental processes, including cell elongation, apical dominance, root formation, vascular differentiation, and tropic responses. Among natural auxins, indole-3-acetic acid (IAA) is considered the most common and biologically active compound. Its activity is closely related to its ability to interact with specific receptor proteins and initiate auxin-dependent signaling pathways [1, 2, 9].

One of the most important auxin receptors is TIR1 (Transport Inhibitor Response 1), which functions as a component of the SCF-TIR1 ubiquitin ligase complex. Binding of auxin to the TIR1 receptor promotes the recognition and degradation of AUX/IAA repressor proteins, thereby activating auxin-responsive gene expression. Therefore, the molecular interaction between IAA and the TIR1 receptor is of significant interest for understanding auxin perception at the molecular level [3].

Metal coordination is an effective approach for modifying the structural and biological properties of organic ligands. Zinc is an essential microelement in plants and participates in many biochemical processes, including enzyme activation, protein stabilization, and regulation of growth-related metabolic pathways. Coordination of IAA with Zn(II) may influence its molecular geometry, electronic distribution, and receptor-binding ability [10].

In this study, molecular docking analysis was performed to compare the binding behavior of free

IAA and its Zn(II) complex toward the TIR1 auxin receptor. The investigated zinc complex consists of one Zn(II) ion coordinated by two IAA ligands in a monodentate coordination mode and one monoethanolamine molecule forming a chelate ring. The main purpose of this work was to evaluate whether Zn(II) coordination can enhance the interaction of IAA with the TIR1 receptor.

Methods

The molecular structures of indole-3-acetic acid and its zinc(II) complex were prepared for docking calculations. The Zn(II) complex was considered as a coordination compound containing one zinc ion, two monodentate IAA ligands, and one chelating monoethanolamine molecule. The carboxylate oxygen atoms of IAA and donor atoms of monoethanolamine participate in the coordination environment around the zinc center.

The three-dimensional structure of the TIR1 auxin receptor protein was used as the macromolecular target. Molecular docking simulations were carried out using the CB-Dock2 server, which automatically detects possible binding cavities and predicts the most favorable ligand-binding poses. CB-Dock2 uses the AutoDock Vina scoring function and ranks the predicted poses according to calculated binding affinity values expressed in kcal/mol [3-5, 8].

For each ligand, several possible binding pockets were identified. The best docking pose was selected based on the lowest binding energy value. The predicted ligand-protein complexes were analyzed in terms of docking score, binding pocket location, and contact amino acid residues. Special attention was given to hydrogen-bonding interactions, hydrophobic contacts, van der Waals interactions, and possible electrostatic interactions between the ligand and receptor residues [6, 7].

Results and Discussion

Molecular docking is a useful computational method for predicting the interaction between biologically active molecules and target proteins. In this study, docking calculations were performed for free indole-3-acetic acid and its Zn(II) complex with the TIR1 auxin receptor. The obtained results revealed noticeable differences in their binding affinities and interaction patterns [4, 6].

Free IAA was docked into the TIR1 receptor using blind docking. The docking results showed five possible binding cavities. Among them, the second binding pocket demonstrated the most favorable binding pose, with a docking score of -6.8 kcal/mol. The binding site was located in chain B of the receptor and included amino acid residues such as Cys53, Tyr54, Ala55, Val56, Ser57, Pro58, Ala59, Gly91, Tyr92, Val93, Pro95, Trp96, Ala99, Met115, Ala563, Gly564, Pro565, Arg566, Phe567, and Asp568.

The presence of aromatic and hydrophobic residues such as Tyr92, Trp96, Met115, and Phe567 suggests that hydrophobic and van der Waals interactions contribute to the stabilization of IAA in the receptor cavity. In addition, polar residues such as Ser57, Arg566, and Asp568 may participate in hydrogen-bonding or electrostatic interactions with the carboxylate group of IAA. These interactions are important for the accommodation of IAA within the TIR1 binding pocket. The corresponding docking pose of IAA in the TIR1 binding cavity is presented in Fig. 1.

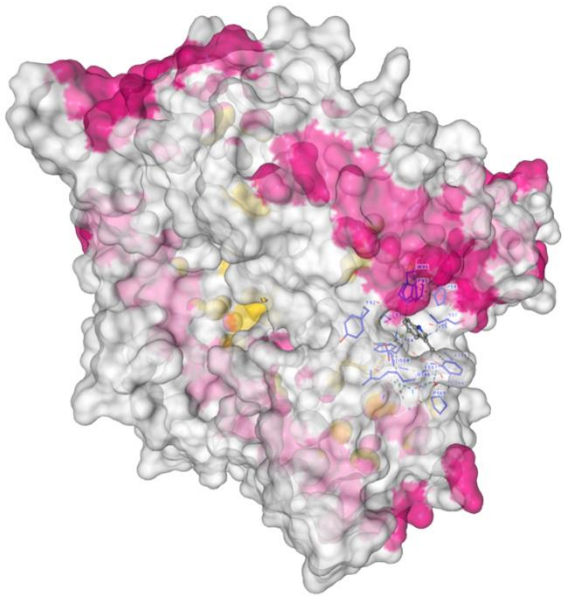

Fig. 1. Docked pose of indole-3-acetic acid in the binding cavity of the TIR1 auxin receptor.

The Zn(II) complex showed a stronger predicted interaction with the TIR1 receptor. According to the docking results, five binding pockets were also detected for the complex. The best docking pose was found in pocket 1, with a binding score of -8.8 kcal/mol. Other predicted poses also showed favorable binding energies of -8.5, -8.4, -8.1, and -7.9 kcal/mol, indicating stable accommodation of the Zn(II) complex in different receptor cavities. The most favorable binding conformation of the Zn(II) complex is illustrated in Fig. 2.

The most favorable binding site of the Zn(II) complex involved the following amino acid residues in chain B: His78, Phe79, Phe82, Leu84, Pro347, Pro350, Phe351, Leu378, Phe380, Arg403, Leu404, Cys405, Ile406, Ile407, Glu408, Pro409, Arg436, Ser438, Leu439, Ser440, Ser462, Val463, Ala464, Phe465, Glu487, and Arg489.

The binding pocket contains several hydrophobic and aromatic residues, including Phe79, Phe82, Phe351, Phe380, Leu378, Ile406, Ile407, Val463, and Phe465. These residues may stabilize the Zn(II) complex through hydrophobic and van der Waals interactions. At the same time, polar and charged residues such as Arg403, Glu408, Arg436, Ser438, Ser440, Glu487, and Arg489 can form hydrogen-bonding and electrostatic contacts with the carboxylate and hydroxyl groups of the coordinated ligands.

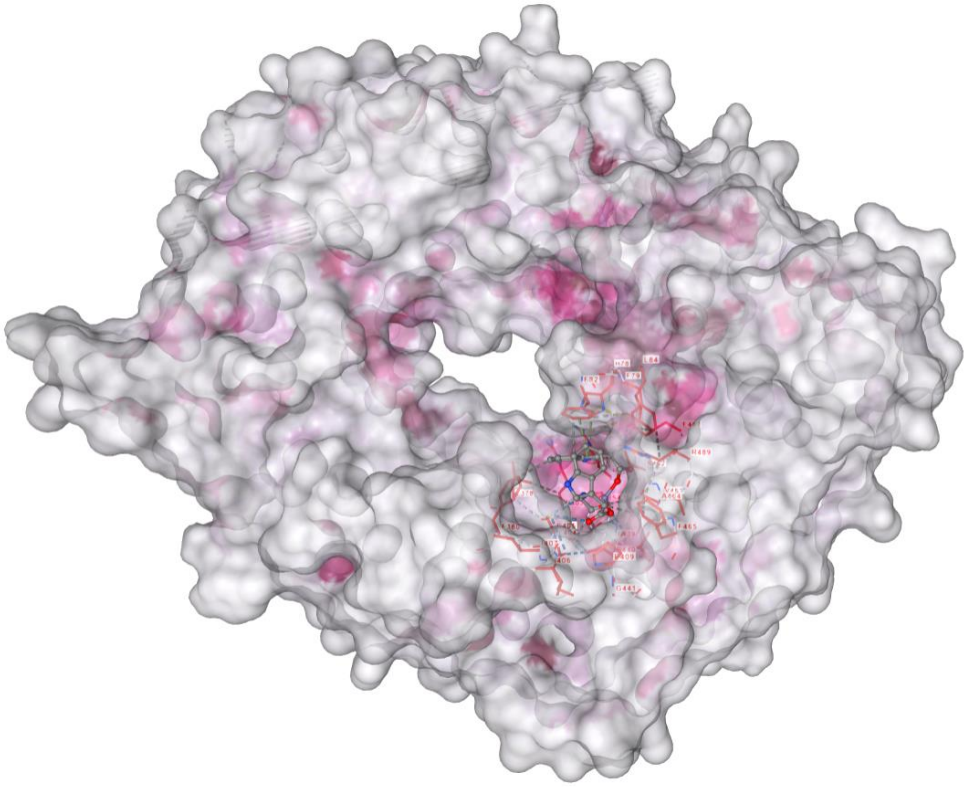

Fig. 2. Docked pose of the Zn(II) complex of indole-3-acetic acid with the TIR1 auxin receptor.

A comparison of the docking scores clearly shows that the Zn(II) complex binds more strongly to the TIR1 receptor than free IAA. The binding energy improved from -6.8 kcal/mol for free IAA to -8.8 kcal/mol for the Zn(II) complex. This difference may be explained by several structural factors. First, the Zn(II) complex contains two IAA fragments, which increases the number of possible contacts with the receptor surface. Second, monoethanolamine introduces additional donor atoms and hydroxyl functionality, which may participate in hydrogen bonding. Third, coordination around the zinc center may provide a more rigid and preorganized molecular conformation, allowing more favorable accommodation in the receptor pocket.

Thus, the docking data suggest that Zn(II) coordination changes the receptor-binding behavior of IAA and enhances its predicted affinity toward the TIR1 auxin receptor. Such an increase in binding affinity is important for the further design and evaluation of auxin-derived metal complexes with potential biological activity in plant systems. The comparative binding energies and main contact residues obtained for both compounds are summarized in Table 1.

Table 1. Binding energies and contact residues of IAA and its Zn(II) complex with the TIR1 receptor.

Compound	Best pocket	Binding energy, kcal/mol	Main contact residues
Indole-3-acetic acid	Pocket 2	-6.8	Cys53, Tyr54, Ser57, Tyr92, Trp96, Met115, Arg566, Phe567, Asp568
Zn(II)-IAA-monoethanolamine complex	Pocket 1	-8.8	His78, Phe79, Phe82, Leu84, Phe351, Leu378, Phe380, Arg403, Glu408, Arg436, Ser438, Ser440, Phe465, Glu487, Arg489

Conclusion

The molecular docking study demonstrated that both indole-3-acetic acid and its Zn(II) complex are able to interact with the TIR1 auxin receptor. Free IAA showed a favorable docking score of -6.8 kcal/mol, confirming its ability to bind within the receptor cavity. However, the Zn(II) complex exhibited a significantly stronger docking score of -8.8 kcal/mol, indicating enhanced predicted binding affinity, as shown in Table 1.

The improved binding of the Zn(II) complex can be associated with the presence of two IAA ligands, chelating monoethanolamine, and the coordination environment around the zinc ion. These structural features increase the number of possible interactions with amino acid residues in the TIR1 receptor cavity. The obtained results suggest that zinc coordination may enhance the receptor-binding properties of IAA derivatives and may be useful for further studies related to plant growth regulation and biologically active metal complexes of auxins.

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