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Effect of Soil Zinc Concentration on Plants Growth: Molecular Modelling and Docking of Interactions between Plant Proteins and Zinc Ions

Sadiya Alka[1]*, Habeebat Adekilekun Oyewusi[2], Mohammed Jibrin Ndeji[3], Ali Timothy Gandu[4], Habeebulahi Ajibola Adekilekun[5], Zinat Suleiman Mohammed[6] and Muhammad Jamilu Dauda[1]

[1]Department of Medical Biochemistry, Faculty of Basic Medical Sciences, College of Medical Science, Abubakar Tafawa Balewa University, P.M.B. 0248, Bauchi, Bauchi State, Nigeria.
[2]Department of Science Laboratory Technology (Biochemistry Unit), School of Science and Computer Studies, The Federal Polytechnic, P.M.B. 5351, Ado-Ekiti, Ekiti State, Nigeria.
[3]Department of Microbiology, Faculty of Natural Sciences, Ibrahim Badamasi Babangida University, P.M.B. 11, Lapai, Niger State, Nigeria.
[4]Department of Science Laboratory Technology, Nuhu Bamalli Polytechnic, P.M.B. 1061, Zaria, Kaduna State, Nigeria.
[5]Department of Pharmacology and Toxicology, Faculty of Medicine, Kampala International University, Western Campus, P.O. Box 71, Ishaka-Bushenyi, Uganda.
[6]Department of Biochemistry, Faculty of Science, Bauchi State University Gadau, P.M.B. 065, Gadau, Bauchi State, Nigeria.

*Corresponding author:
Sadiya Alka
Department of Biochemistry,
Faculty of Science,
Abubakar Tafawa Balewa University,
P.M.B. 0248, Bauchi,
Bauchi State,
Nigeria.
Email: Salka@atbu.edu.my

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ABSTRACT

This study examines plant-soil interactions involving zinc (Zn), focusing on the physiological effects on plant development and the molecular interactions between plant proteins and metal ions. About 2 kg of soil mixed with gravel (1.5:1 v/v) were placed in pots, and seeds of sunflower (*Helianthus annuus*), amaranth (*Amaranthus* spp.), cowpea (*Vigna unguiculata*), and groundnut (Arachis hypogaea) were sown and irrigated for two weeks. Seedlings were treated with a 500 ppm zinc sulfate solution, and shoots, leaves, and roots were separated for length and weight measurements. Zinc concentration in digested tissues was determined using atomic absorption spectroscopy (AAS). Computational modeling and molecular docking were performed using PubChem data and structural tools such as Chimera, Phyre2, and PyMOL. The BbZIP protein structure was modeled, and active sites were predicted using COACH-D, while CAVER Web 1.0 identified quantum tunnel pathways. Phytochemical analysis revealed the presence of bioactive compounds, including flavonoids, tannins, steroids, and saponins. Treated plants exhibited reduced growth compared to the controls, with significant zinc accumulation in the soil, shoots, and roots. The highest Zn concentration (315 ppm) occurred in groundnut roots. Five major binding poses were identified, involving catalytic residues Met91, Leu92, Phe94, Ala95, Ala96, Pro210, Glu211, Ala214, Gly93, and others. Molecular docking showed a binding affinity of –3.8 kcal/mol and an inhibition constant (Ki) of 247.81 mM. The BbZIP–Zn complex was stabilized by four hydrogen bonds (Ala96, Ala290, Ser236, Leu294). Overall, this study highlights the critical role of zinc in plant stress responses and development through physiological and molecular mechanisms.

INTRODUCTION

In global environments, soil naturally contains zinc (Zn), a crucial component of many metabolic pathways and essential for plant growth. Nevertheless, potentially toxic zinc levels in soils can alter plant growth, mineral nutrition, photosynthetic and respiratory rates, and reactive oxygen species production by plants [1]. Zn can enter soils through various processes, including the application of Zn-contaminated sewage sludges, excessive application of Zn-containing fertilizers, smelter and incinerator emissions, rock weathering, and the dispersal of wastes from mining and volcanoes [2]. The scientific community has begun

to pay more attention to the consequences of Zn on plants and its crucial function in agricultural sustainability, as a result of growing environmental concerns, as well as the narrow gap between Zn therapeutic and toxicity in plants [3]. Less research has shown how adequate Zn supplies can alter the drought tolerance of various crops such as wheat, sunflower, tomato, and red cabbage.

Zn is involved in protein synthesis and energy production [4]. Although the toxicity of Zn in plants is less common than its deficiency, most research focuses on increasing Zn availability in the tissues of crop plants. Therefore, it is reported that Zn phytotoxicity occurs frequently in soils that are acidic and have been amended with sludge. Due to the imbalance in Reactive Oxygen Species (ROS) production, the risk of zinc pollution in soil can endanger plants by causing oxidative stress [5]. Higher Zn concentrations are toxic to plants, reducing cell division and elongation, which affects the plant's phytochemicals and has consequences for biomass creation [6].

Plants grown in contaminated soil may contain different amounts and types of phytochemicals than plants grown in clean soil. Phytochemical analysis of plants growing in zinc (Zn)-contaminated soil can help determine the impact of heavy metal pollution on the quantity and quality of phytochemicals in the plants. However, some phytochemicals that have been found to be affected by Zn contamination include Phenolic and Flavonoid compounds, which are large groups of phytochemicals with antioxidant properties, and carotenoids, a collection of pigments responsible for the orange, red, and yellow colors of many vegetables and fruits. the analysis of phytochemicals in plants grown in Zn-contaminated soil can provide useful information about the actions of heavy metal pollution on the potential effect on man and even plant health.

The computational prediction of the three-dimensional structure of protein-protein or protein-ligand complexes, as well as the interaction between heavy metal transporters and heavy metal ions, can shed light on the efficiency and selectivity of these transporters. Plants utilize a variety of transporters to convey heavy metals from the root to the shoot or to sequester them within the vacuole in smaller portions, thereby reducing their toxicity [7]. Overall, protein docking is a valuable tool for investigating the molecular pathways underlying plant responses to heavy metal stress. Understanding the specificity, affinity, and stability of these interactions can aid in the development of innovative schemes for increasing plant tolerance to heavy metal stress [8]. This can be accomplished by anticipating the three-dimensional structures of protein-protein or protein-ligand complexes.

At the molecular level, the inhibition of the photosynthetic system is linked to significant alterations in the structure and abundance of chloride. Zn can substitute for Mg^{2+} inside the Chl structure, which affects light-harvesting complex (LHCII) performance [4]. Zinc is necessary for plants to produce tryptophan, which is an essential amino acid in the creation of auxin, indoleacetic acid. Therefore, through its indirect action on auxins, zinc also controls plant development. Protein synthesis is inhibited by Zn deficiency, primarily due to a decrease in ribonucleic acid (RNA). This is due to decreased Zn polymerase activity, decreased ribosome structural integrity, and increased RNA degradation. The significant lessening in growth rate caused by protein formation inhibition in Zn deficiency thus results in lower consumption of carbohydrate, which leads to reduction of photosynthesis, which is advantageous for greater free oxygen radicals production; if these are not separated, the Zn deficiency indication becomes more noticeable, especially under high radiation intensity [9].

Through their roots, plants are able to take in very small amounts of ionic substances from the soil and form potent coordination bonds with heavy metal ions that are present in a wide range of plant materials [10]. The cell walls of plants contain lipids and proteins with high chemical attraction for heavy metal ions, including amino groups, carboxylate, and hydroxyl groups [10]. By complexing the metal ions with an electron pair, these groups can bind heavy metals in solution. In this study, we attempted to increase Zn concentrations above the limit, and the effects on the growth of four different plants and secondary metabolites were investigated. Furthermore, in the context of plant response to heavy metal stress, molecular docking can be adopted to evaluate the interactions between heavy metal ions and plant proteins, as well as the interactions between plant proteins implicated in heavy metal decontamination pathways and plant bioactive components, and the potential to adsorb Zn by those bioactive components via complexation.

The novelty of this study lies in the integration of physiological evaluation of plant growth under varying soil zinc concentrations with molecular modeling and docking approaches in order to elucidate, at the atomic level, the interaction of zinc ions with key plant proteins involved in metal uptake, detoxification, and homeostasis. This dual experimental–computational strategy provides a mechanistic insight into zinc–protein affinity and its role in modulating plant growth under metal stress conditions.

MATERIALS AND METHODS

Soil Sample Preparation

The soil was obtained from Bauchi State University, Gadau. The soil was mixed with a small amount of gravel (1.5 v/v) to provide aeration for the plant's roots, and 2 kg of the soil mixture was placed in a pot with various holes (20 cm in diameter and 15 cm in length).

Pot experiment

The experiment was conducted in a greenhouse in order to assess the tolerance of four plant species—sunflower (*Helianthus annuus*), amaranthus (*Amaranthus sp.*), cowpea (*Vigna unguiculata*), and groundnut (*Arachis hypogaea*)—to zinc (Zn) stress. Only uniform and healthy seeds were selected, and they were sown in plastic pots containing 2 kg of homogenized loamy soil mixed with a small amount of washed gravel to enhance aeration and drainage. The soil was pre-moistened with distilled water. Then, the soils were allowed to equilibrate for two weeks before exposure to metals. The plants were subjected to zinc treatment using a 500 ppm zinc sulfate ($ZnSO_4 \cdot 7H_2O$) stock solution after two weeks of germination and seedling establishment. Control pots received an equal volume of distilled water to maintain similar hydration levels. Treatments were arranged in a completely randomized design (CRD) with three replicates per plant species and treatment group (n = 3).

All pots were maintained under greenhouse conditions with an ambient temperature of 25–30 °C, relative humidity of 65–70%, and a natural light photoperiod. These conditions were designed to simulate natural growth environments and minimize external variability. The experiment continued for four weeks following Zn exposure, during which plants were regularly monitored for growth and any visible signs of stress, such as chlorosis or stunted development. This methodology aligns with the procedures reported by [3].

Harvest and Analysis

After four weeks of zinc treatment, plants were carefully uprooted to prevent mechanical damage to the roots, and soil samples were collected to determine residual zinc concentration. Plant growth parameters—including root length, shoot length, and stem diameter—were measured using a precision vernier caliper (±0.01 mm). Fresh biomass of roots, shoots, and leaves was recorded immediately after harvest. Samples were then oven-dried at 70 °C until a constant weight was achieved to determine dry biomass accumulation. Following drying, the plant tissues (roots, shoots, and leaves) were finely ground using a stainless steel mill to obtain a homogeneous powder for elemental analysis. Approximately 0.5 g of each ground sample was digested in an aqua regia mixture ($HCl:HNO_3$, 3:1 v/v) on a hot plate until the solution became clear. The resulting digests were filtered through Whatman No. 42 filter paper and diluted to a final volume of 50 mL with deionized water. Zinc concentration in both plant and soil digests was determined using Atomic Absorption Spectrophotometry (AAS; PerkinElmer AAnalyst 400), following standard methods described by [11].

Phytochemical screening

Preliminary phytochemical screening of crude extracts was conducted to identify the presence of major secondary metabolites that may contribute to metal tolerance mechanisms. The screening was performed using standard qualitative protocols [7,12]. For tannin detection, 0.2 g of each crude extract was boiled in distilled water, filtered, and treated with three drops of 5% ferric chloride ($FeCl_3$); the appearance of a blue-black or greenish precipitate indicated the presence of tannins. Flavonoids were tested by dissolving 0.5 g of extract in 5 mL of 10% NaOH and subsequently adding 3 mL of 2 M HCl; the development and subsequent disappearance of a yellow coloration confirmed the presence of flavonoids.

Steroids were identified using the Liebermann–Burchard reaction, where 1 g of extract was mixed with 2 mL of acetic anhydride and 2 mL of concentrated sulfuric acid. The formation of a blue, green, or red color signified the presence of steroids. For alkaloids, 0.2 mL of extract was treated with two drops of Wagner's reagent, and the development of a pale reddish-brown precipitate indicated positive results. Saponins were detected by mixing 2 mL of extract with 2 mL of distilled water and shaking vigorously; the persistent froth that filled the entire tube was indicative of saponin presence. All phytochemical tests were performed in triplicate, and qualitative results were expressed using the intensity notation system: + (trace), ++ (moderate), and +++ (high). The assays were designed to provide reproducible indicators of secondary metabolite activity relevant to plant defense, aligning with the findings of [12], who emphasized the protective roles of phenolic and flavonoid compounds in mitigating oxidative damage during metal stress.

Molecular Modeling and Docking

Ligand Library and Protein Preparation

The three-dimensional structure of zinc was acquired from the PubChem database and subsequently optimized using Chimera version 1.10.2. The refined structure was exported in PDB format for molecular docking purposes. The crystal structure of the zinc-binding protein BbZIP was retrieved from the Protein Data Bank (PDB ID: 7Z6M). Further refinement, including structural optimization and energy minimization, was performed using Phyre2 [13]. Visualization and preparation of the BbZIP protein structure were carried out with PyMOL [14].

Prediction of Binding Pocket Sites

The active sites and key catalytic residues of the target proteins were identified using the COACH-D algorithm, available at the Yang Lab website (https://yanglab.qd.sdu.edu.cn/COACH-D/) [15]. Additionally, potential quantum tunnels were mapped using CAVER Web 1.0 (https://loschmidt.chemi.muni.cz/caverweb/). COACH-D results were validated to ensure accurate active site prediction, which was subsequently analyzed for quantum tunnel characteristics via CAVER Web 1.0. This dual-step approach facilitated the identification of plausible ligand pathways within the BbZIP protein structure.

Molecular Docking

Molecular docking was performed using the Lamarckian Genetic Algorithm (LGA) implemented in AutoDock 4.2 [16,17]. The LGA approach, which supports protein-ligand rigid-flexible docking, allowed for up to 250,000 energy evaluations and 27,000 generations. Mutation and crossover rates were set at 0.02 and 0.8, respectively. The workflow involved grid generation, protein screening, and ligand optimization. The optimized 3D structures of BbZIP (PDB ID: 7Z6M) and zinc were input into AutoDock 4.2 for blind docking. A grid box with dimensions of 91 × 91 × 91 Å and a spacing of 1.0 Å was centered at coordinates -18.11 × 41.70 × 121.91 to define the docking search space for BbZIP. Docking parameters adhered to those reported in prior studies [18]. AutoDock calculated binding free energy values using the following equation:

$$\Delta G_{bind} = \Delta G_{vdw+hbond+desolv} + \Delta G_{elec} + \Delta G_{total} + \Delta G_{tor} - \Delta G_{unb} \quad (1)$$

where ΔG_{bind} is free binding energy as estimated, and $\Delta G_{vdw+hbond+desolv}$ represents sum of the energies repulsed and dispersed (ΔG_{vdw}), hydrogen bond (ΔG_{hbond}), and desolvation (ΔG_{desolv}). ΔG_{total} stands for 'final overall internal energy', ΔG_{tor} is torsional free energy, ΔG_{unb} is "unbounding energy of the system, and ΔG_{elec} is electrostatic energy.

RESULTS AND DISCUSSION

Phytochemical Analysis of Plant Crude Extracts

The results of the earliest investigation of the crude extract, which include a phytochemical assessment to determine the key plant components under Zn stress, are presented in **Tables 1** and **2**. As shown in **Table 1**, various phytochemicals, including flavonoids, tannins, steroids, and saponins, were present in all extracts compared to the control. The + sign indicated the presence of phytochemicals. These findings align with the results of numerous other studies, which have suggested that the plant defense mechanisms of this plant, including its anti-inflammatory characteristics, are derived from secondary metabolites found in plants (Khare et al., 2020). They have developed a unique defense mechanism that utilizes a diverse range of secondary metabolites to help them cope with various stress situations.

The plant's developmental stage, contaminant type and concentration, and the plant's response to metal toxicity all have an effect. Following heavy metal treatment, phenolics, in particular flavonoids, can undergo peroxidase oxidation and participate in the H_2O_2-scavenging phenolic/ASC/POX system [19]. Heavy metal toxicity occurs through three primary mechanisms: (1) the generation of Reactive Oxygen Species (ROS) via autoxidation and the Fenton reaction, which is commonly associated with transition metals such as copper and

iron; (2) the obstruction of essential functional groups in biomolecules, which is typically caused by non-redox-reactive heavy metals like cadmium and mercury; and (3) the displacement of critical metal ions from biomolecules, which can occur with a variety Flavonoids are known to form compounds with heavy metals, which may strengthen the plant's defense mechanisms against heavy metal-induced stress.

Table 1. Phytochemical screening of the treatment plant.

Plant constituents	Sunflower			Amaranthus			Cowpea			Peanut		
	L	R	S	L	R	S	L	R	S	L	R	S
Alkaloid	++	+++	+	++	++	++	++	++	+	+++++++		
Tannins	++	++	+	++	+++	+	+++++		+	++	++	+
Steroids	+++	+	+	+	++	++	+++++		++	+	+++	+
Saponins	+	+	++	+	+	++	+	+	+++	++	++	++
Flavanoid	+++	++	+	+++	++	+	++	++	+	+	++	++

Table 2 . Phytochemical screening of control plant after treatment.

Plant constituents	Sunflower			Amaranthus			Cowpea			Peanut		
	L	R	S	L	R	S	L	R	S	L	R	S
Alkaloid	++	++	++	+	++	++	+	+	+	++++		+
Tannins	+	+	+	++	+	+	++	+	-	++	+	-
Steroids	+++	+	++	-	+	+	++	+	+	-	++	+
Saponins	+	+	+	-	++	+	+	-	+	+	+	+
Flavanoid	+++++		+	+	-	+	+	++	-	-	+	+

Plant Growth in the Presence of Zinc Contamination

According to the results in **Fig. 1**, plant growth is less than that of the control, which is consistent with the findings of all studies. Zinc stress affects metabolic processes and nutrient intake, potentially hindering plant growth. It frequently leads to decreased plant height and other difficulties with development [20]. Excessive zinc contamination in soil can adversely affect plant growth by disrupting the nutritional balance and leading to toxic symptoms [11,21]. It may cause the plant to grow more slowly, turn yellow in its leaves, and become less healthy overall.

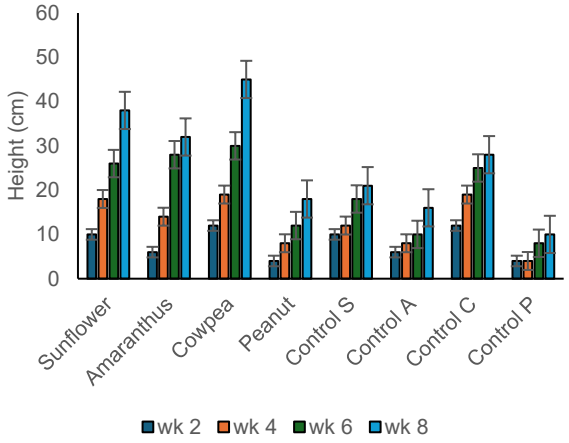


Fig. 1. Plant height after zinc treatment. Control S: sunflower control, Control A: amaranth control, Control C: cowpea control, Control P: peanut control. Error bars represent standard deviations of replicate measurements.

Zinc Content in Soil, Plant Root, and Shoot

The Zinc concentration in soil, root, and shoot is as displayed in **Fig. 2**. There was an elevated concentration of zinc bioaccumulated into the plant roots and shoots of the four plants grown on contaminated soils in comparison with the control sample plant. The concentration of Zn in the roots of sunflower, amaranthus, cowpea, and peanut was, respectively, 180 ppm, 200 ppm, 210 ppm, and 315 ppm, indicating that the Peanut root can bioaccumulate more Zn than the three other plants. The Zn concentration in the shoots of the four plants was 60 ppm, 100 ppm, 80 ppm, and 60 ppm, respectively. Thus, more Zn was bioaccumulated in the shoots of plants grown on Zn-contaminated soils compared to the 10 ppm recorded in the control. Plants utilize a variety of transporters to convey heavy metals from the root to the shoot or to sequester them within the vacuole in smaller portions, thereby reducing their toxicity [7]. The physical and biochemical apparatuses, such as symbiotic nitrogen fixation, root exudates, metal-chelating proteins, efficient transport systems, adaptive responses, and certain genetic factors, which are well-adapted for nutrient assimilation and storage, collectively enable these plants to efficiently accumulate zinc in their tissues [20,22,23].

Although this is essential for their growth, development, and nutritional quality, too much zinc in the plants could have a negative impact on the animals that feed on such plants. Potentially toxic levels of zinc in soils can alter plant growth, photosynthetic and respiration rates, mineral nutrition, and the amount of reactive oxygen species produced by plants [1]. Understanding these processes can help in breeding and engineering Plant species with enhanced zinc uptake, contributing to improved human nutrition and sustainable agriculture.

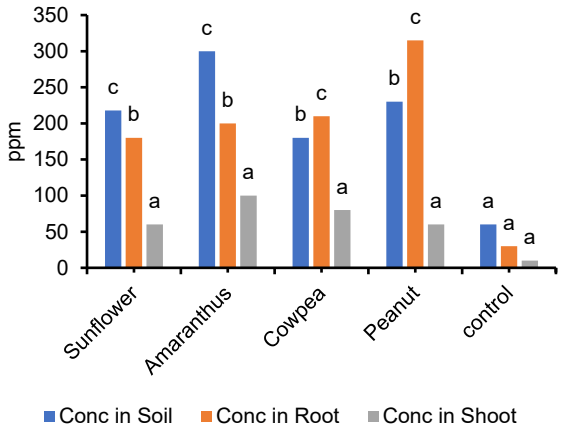
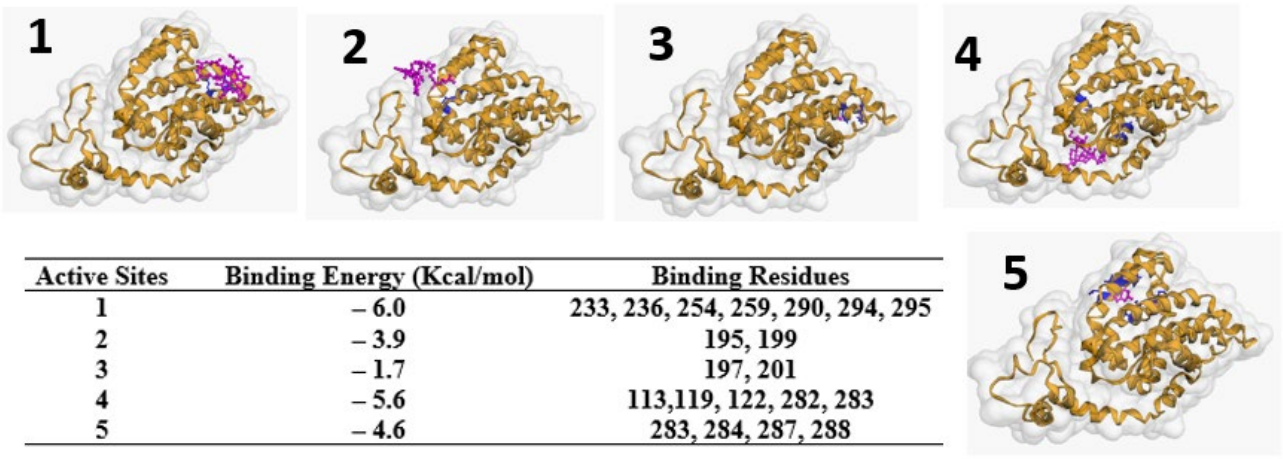


Fig. 2. Zinc concentration in soil, root, and shoot. Values starred with the same letters within a species do not significantly differ, according to Tukey's test ($p < 0.05$).

Computational Analysis

Zn is among the elements required for growth by plants, but it is lacking in most of the arable soil of the world [22]. The recognition of specific transporter proteins for various minerals has led to novel ideas for crop cultivation, particularly in transforming plants. Different experimental investigations have exploited the connection between the resistance to mineral deficiency and the overexpression of mineral transporters [24,25]; this relationship thus identified the affiliates of the ZIP proteins as prospective apparatuses for crop management and improvement, overexpressing the ZIP protein members in plants, and served as the potential marker molecules for the observation of the crop nutrient conditions [26]. Moreover, Zn distribution improvement can be used as a method for translocating Zn from the soil to the cytosol and for enhancing long-distance transport to sink sites, which can improve plant processes and even the quality of fruits in fruiting plants [26]. The ligand binding site prediction or active site of protein structure has several applications in the field of structural biology. Various techniques for detecting enzyme-binding sites have been developed over

decades, depending on the protein's geometrical, chemical, and structural features [15, . In this study, the binding active sites of the BbZIP protein were predicted using the COACH-D algorithm, which is based on deep convolutional neural networks. This machine learning-based server enables rapid visualization of results and provides accurate predictions that surpass the capabilities of other tools. The findings revealed multiple binding site orientations, with five distinct poses identified. Notably, the predicted binding affinities of these poses ranged from −6.0 to −1.7 kcal/mol, with the first pose exhibiting the lowest binding energy of −6.0 kcal/mol (**Fig. 3**). To validate the aforementioned results and ensure a comprehensive analysis, the first binding pose of the BbZIP protein was subjected to quantum tunneling analysis using the Caver 3 webserver [30,31]. The results revealed six tunnels with lengths and radii ranging from 0.9 Å to 26.9 Å and an average radius of 3.0 Å (**Fig. 4**). In terms of catalytic amino acids within the tunnels, tunnel 1 contained the fewest amino acids (Leu94, His177, Glu211, and Glu276), while tunnel 2 exhibited the highest number (Asp89, Leu92, Gly276, Val287, Pro279, Ala290, Thr291, Leu294, Gly93, Ile278, His286, and Glu287). Tunnel 3, by comparison, contained eight catalytic amino acids (Ala96, Leu100, Val273, Glu276, Val277, Leu294, Gly97, and Ser274) (**Fig. 4**). The results obtained showed that tunnels 4 and 5 showed the same catalytic amino acids, having Met91, Leu92, Phe94, Ala95, Ala96, Pro210, Glu211, Ala214, and Gly93. While Tunnel 6 showed Ala178, Leu179, Glu181, Ser236, Leu238, Met239, Glu240, Pro241, Gly182, and Gly237 (**Fig. 4**). It is worth mentioning that Alanine, Aspartate, Leucine, Glutamate, Valine, Threonine, Isoleucine, Histidine, Serine, Methionine, Phenylalanine and Proline are the predicted catalytic amino acids which were found in different position in all the predicted tunnels (**Fig. 4**). Therefore, the binding affinity and catalytic amino acids predicted by COACH-D algorithm and Caver 3 webserver for quantum tunnelling are further reconfirmed in the incoming section using molecular docking methods.



Active Sites	Binding Energy (Kcal/mol)	Binding Residues
1	– 6.0	233, 236, 254, 259, 290, 294, 295
2	– 3.9	195, 199
3	– 1.7	197, 201
4	– 5.6	113,119, 122, 282, 283
5	– 4.6	283, 284, 287, 288

Fig. 3. Different active site poses of BbZIP protein predicted by COACH-D by considering the binding energy (Kcal/mol) and the number of the amino acids involved at the docking region.

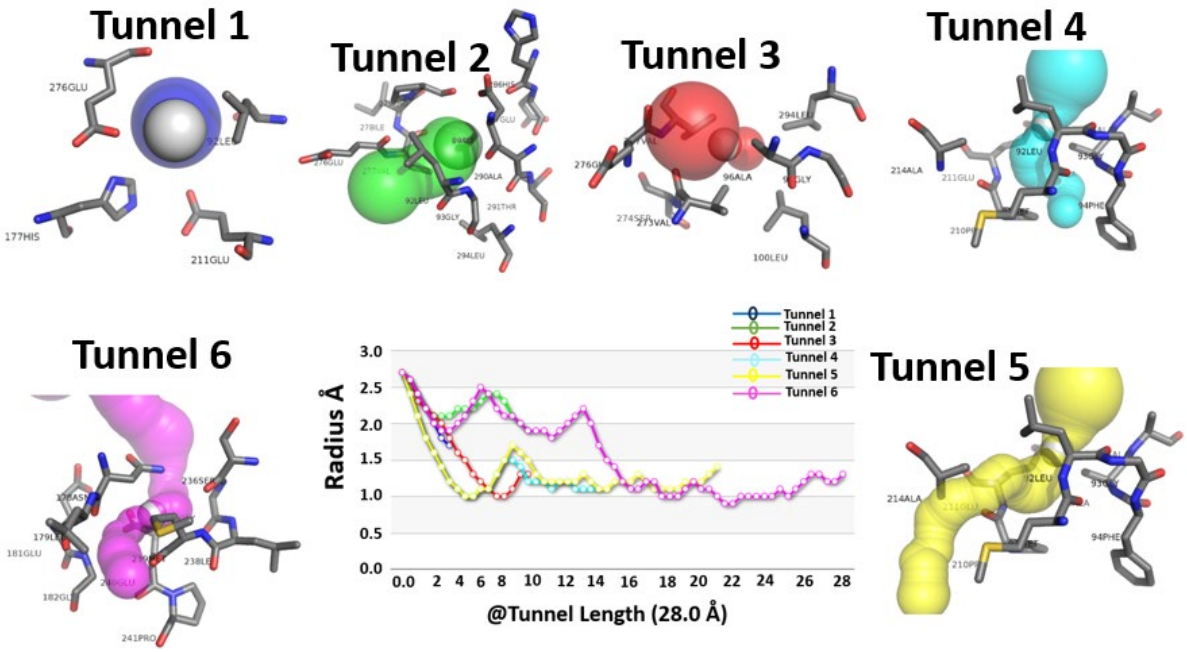


Fig. 4. Protein Tunnels demonstration along with the tunnel length (Å), radius (Å) of the six tunnels predicted for allocating any ligand in the docking position as well as catalytic amino acids involved in protein-ligand interaction.

Molecular docking simulation is a powerful tool for predicting the interaction mode between small ligands and biological macromolecules (receptors) at the molecular level [15,32]. Docking was performed to facilitate the population of likely coordination modes for the ligands at the binding site [33–35]. The coordination having lowest binding affinity, docking score and binding energy was considered spectacular. Docking outcomes were assessed further and revalidated by checking the interaction between the BbZIP protein and small molecules (Zinc metal). Zinc ions mitigate different effects on plant cells by interacting with functional groups or displacing other cations from binding sites. Plants thriving depend on Zn absorption, transportation, and distribution throughout the plant's intracellular cells and tissues. Therefore, molecular docking technology was utilized to forecast the possible docking sites between BbZIP protein and zinc metal. According to the rule of energy minimization, three binding conformations with the lowest energy were output to justify the docking mechanism between BbZIP protein and zinc metal.

The ligand compound (Zn ion) was docked with the target protein (BbZIP) through AutoDock 4.2, thereby predicting the best position where ligands can bind. The AutoDock 4.2 docked consequences reveal the binding energy involved in the formation of the protein-ligand complex structure, as well as the generation of a detailed understanding of all outward molecular interactions responsible for their activity. The protein-ligand composite, Zn-BbZIP, showed the best binding affinity of –3.8 kcal/mol (**Table 3**). The outcome of other possible important thermodynamic parameters (such as Ki constant of inhibition, $\Delta G_{\text{total final total internal energy}}$, $\Delta G_{\text{tor torsional free energy}}$, $\Delta G_{\text{unb unbound system's energy}}$, $\Delta G_{\text{elec electrostatic energy}}$, and $\Delta G_{\text{vdw+hbond+desolv}}$ is the sum of dispersion and repulsion (ΔG_{vdw}), hydrogen bond (ΔG_{hbond}), and desolvation (ΔG_{desolv}) energy predicted for most stable docking conformations are summarized in **Table 3**.

Table 3. Important thermodynamic parameters generated from AutoDock 4.2.

Conformation	Zn-BbZIP complex
ΔG_{bind} (kcal/mol)	– 3.8
Ki (mM)	247.81
ΔG_{inter}	– 1.1
$\Delta G_{\text{vdw+hbond+desolv}}$	– 3.1
ΔG_{elec}	0.0
ΔG_{total}	0.0
ΔG_{tor}	0.27
ΔG_{unb}	0.0

The 2-dimensional interaction of the Zn-BbZIP complex was visualized by LigPlot v.1.4.5 program. The protein's amino acid residues interact with the ligand's compounds through hydrogen bonds. Zn shows interaction by forming four hydrogen bonds (**Fig. 5**). Zn-BbZIP complex also exhibits hydrogen bond interactions with Leu294, Ala96, Ser236, and Ala290 residues with no hydrophobic interaction. Similarly, the binding pocket of BbZIP protein with the Zn ligand, revealing hydrogen bond donors and acceptors, are represented well in **Fig. 5**. The results obtained from the docking studies have shown that the Zn ligand bind with the predicted active site of the BbZIP protein, as it was revealed by COACH-D algorithm and quantum tunnelling analysis (**Figs. 3** and **4**). A summary of the results obtained from docking of the studied Zn ion with BbZIP protein (PDB ID: 7Z6M) is summarized in **Table 2** and **Fig. 5**.

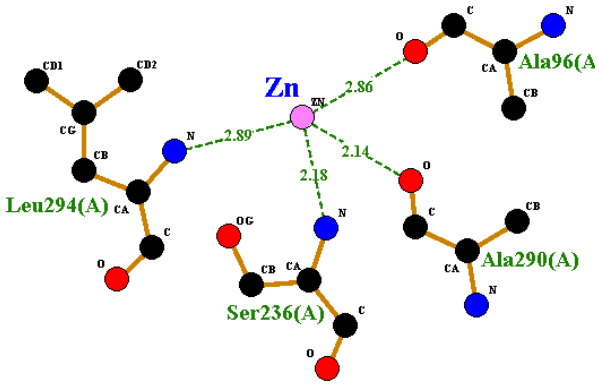


Fig. 5. Binding sites interaction and bond involved in docking of BbZIP protein with Zn ligands.

CONCLUSION

This study, conducted on the effect of soil Zinc concentration on plant growth, molecular modeling, and docking of interactions between plant proteins and Zinc ions, offers insight into the multifaceted role of zinc in plant life. The results indicate that soil zinc concentration has a significant impact on plant growth, affecting physiological parameters such as biomass production and the overall health of the entire plant. Both zinc deficiency and toxicity harmfully affect plant growth, highlighting the importance of maintaining an optimum zinc concentration in the soil. Zinc serves as a cofactor in many enzymatic reactions and is necessary for plants' metabolic activities and structural integration. Molecular docking and modeling clarified the connections between plant proteins and zinc ions, revealing critical insights into how zinc ions bind to specific sites on proteins. The structural scrutiny offered by the models underscores the importance of zinc in stabilizing protein structures and facilitating catalytic activities that are crucial for plant physiology. The findings from this study can inform the development of targeted agricultural interventions and breeding programs that focus on improving zinc uptake in crops. Further research should focus on the exploration of the genetic basis of zinc assimilation and metabolism in plants, as well as the potential biotechnological applications of these findings for crop improvement programs.

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