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Using Molecular Docking for Bioremedation of Environmental Toxins via Bacilus Sabtils

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Abstract

The escalating environmental pollution caused by diverse chemical contaminants poses significant challenges to ecosystem health and human well-being. In response, molecular docking emerges as a promising tool for designing effective bioremediation strategies. This study investigates the potential of *Bacillus subtilis* in degrading a spectrum of environmental toxins through molecular docking simulations. Twelve toxic compounds, including 1-(4-chlorophenyl)-3-(3,4-dichlorophenyl)urea, 2,3,4,5,6-pentachlorophenol, and 2,3,7,8-tetrachlorodibenzo-p-dioxin, were selected as ligands. By evaluating binding affinities, represented by docking score values ranging from -15.604645 to -7.805723, the interactions between these toxins and Bacillus subtilis enzymes were characterized. The results unveil promising interactions, suggesting the potential efficacy of Bacillus subtilis in bioremediating various environmental toxins. This research provides valuable insights into utilizing molecular docking as a predictive tool for bioremediation strategies, contributing to the sustainable management of environmental contaminants.

Keywords: environmental pollution; molecular docking; environmental toxin; *Bacillus subtilis,* laccase.

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1. Introduction

Bioremediation is an environmentally sound, advanced technology that uses natural biological processes to completely eliminate toxic contaminants[1]. Any process that uses microorganisms, fungi, green plants, or their enzymes to restore the natural environment that has been altered by pollutants to its original state [2]. Bioremediation techniques can generally be classified as in situ or ex situ [3]. On-site bioremediation involves treating contaminated materials on site while ex-site remediation involves removing contaminated materials for treatment elsewhere [4]. Some examples of bioremediation techniques are bioaeration [5], land cultivation [6], bioreactor [7], synthesis, bioaugmentation [8], radical filtration, biostimulation [9] and *in-silico* bioremediation [10]. Microorganisms that perform the function of bioremediation are known as bioremedies (bioaugmentation) [11]. However, not all contaminants can be easily treated by biological treatment using microorganisms. For example, heavy metals such as cadmium and lead are not easily absorbed or captured by organisms. Ingesting metals such as mercury into the food chain may make matters worse.

Bacteria are considered one of the most important microorganisms used in this process [12]. This is due to their ability to decompose organic materials, especially toxic ones. They are the main factor in the role of carbon, nitrogen, phosphorus, and sulfur in nature [13]. They maintain the continuity of these elements in the soil to an important and sufficient extent for the life of plants and animals, and they play an important role. Studies have also indicated that there are approximately 10 billion bacterial cells in every gram of soil that live in and around plant roots, known as the Rhizosphere [14]. These bacteria are famous for their ability to fix atmospheric nitrogen into beneficial substances for the plant. These bacteria are known for their rapid response and sensitivity to changes in the surrounding environmental conditions [15]. In addition, there are many bacterial strains that have the ability to produce hormones that stimulate plant growth and also stimulate the plant's immune system [16], which greatly contributes to reducing diseases that affect plants and increasing yields. If we talk about the role of bacteria specifically in treating oil waste stuck in the soil, it was actually able to achieve this goal brilliantly in a period not exceeding 42 days, as bacteria were used as a biological preparation that the production company called OBT, short for Oil biodegradation treatment.

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Bacillus subtilis, a Gram-positive, rod-shaped bacterium renowned for its versatility and adaptability, emerges as a promising candidate for bioremediation of aromatic toxins [17]. Aromatic toxins represent a diverse class of pollutants, including aromatic hydrocarbons, polycyclic aromatic hydrocarbons (PAHs), phenolic compounds, and aromatic amines, which pose significant environmental hazards due to their persistence, toxicity, and carcinogenicity [18].

In recent years, the application of molecular docking in the field of bioremediation has gained significant attention, particularly in optimizing the coating of laccase from Bacillus subtilis [19]. This literature survey aims to provide an overview of recent studies focusing on molecular docking techniques for understanding and enhancing the coating of Bacillus subtilis laccase, with a specific emphasis on bioremediation applications. The aim of using molecular docking for bioremediation by Bacillus subtilis laccase against aromatic environmental toxins is to elucidate and optimize the interaction between the enzyme and target pollutants at the molecular level. Molecular docking serves as a computational tool to predict the binding affinity, orientation, and stability of Bacillus subtilis laccase with aromatic toxins, thereby facilitating the design and optimization of bioremediation strategies. Specifically, the aims include:

2. Materials and Methods

The molecular docking simulations were performed using Molsoft ICM (Internal Coordinate Mechanics) [20], a comprehensive software package for structure-based drug design and molecular modeling. The software includes tools for protein modeling, ligand docking, virtual screening, and molecular dynamics simulations. Protein Structure Acquisition: The three-dimensional structure of the CotA laccase from the endospore coat of Bacillus subtilis (PDB:3ZDW) [21] was obtained from Protein Data Bank (PDB). Protein Preparation: The protein structure was prepared for docking by removing water molecules, adding missing hydrogen atoms, assigning protonation states, and optimizing side-chain conformations. Any co-crystallized ligands or ions were also removed, unless they were essential for the binding site definition.

Grid Generation: A docking grid was generated around the binding site of the protein to guide the docking simulations. The grid size and resolution were optimized based on the reference ligand binding mode and interactions.

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Ligand Database: A database of ligands or small molecules to be docked was prepared. These ligands sourced from PubChem database. Ligand Preparation: The ligands were prepared by assigning proper bond orders, adding hydrogen atoms, and generating 3D coordinates. Ionization states and tautomeric forms were also considered for accurate docking predictions.

Protein-Ligand Docking: The prepared protein and ligand structures were input into the Molsoft ICM software 3.8.7C [20] for docking simulations. The software utilizes an internal coordinate mechanics approach, considering both ligand flexibility and protein flexibility during the docking process.

Scoring Functions: Molsoft ICM employs scoring functions to evaluate and rank the binding poses generated during docking. These scoring functions take into account factors such as electrostatic interactions, van der Waals forces, hydrogen bonding, hydrophobic interactions, and solvation energies [22].

Docking Settings: Parameters such as docking algorithm, search space, energy cutoffs, and scoring preferences were set based on the specific requirements of the docking study. Multiple docking runs or ensemble docking approaches could be employed to enhance sampling and accuracy.

Pose Clustering: The generated docking poses were clustered based on structural similarity to identify distinct binding modes and consensus poses.

Scoring and Ranking: Docked poses were ranked based on their docking scores or binding energies, with lower scores indicating stronger binding affinity.

Visual Inspection: The top-ranked docking poses were visually inspected using molecular visualization tools within Molsoft ICM or external software for analyzing key interactions, hydrogen bonding patterns, and ligand-protein interactions.

Binding Mode Analysis: The binding modes of the ligands within the active site of the protein were analyzed to understand the molecular basis of ligand-receptor interactions and identify potential pharmacophore features.

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3. Results and Discussion

The database of environmental toxins was compiled, including a diverse pollutant of aromatic compounds found in environmental samples. Chemical structures of the environmental toxins were obtained from reputable databases and prepared for molecular docking. Ligands were optimized for computational analysis by minimizing energy and adding appropriate charges. The CotA laccase from *Bacillus subtilis* was chosen as the protein target due to its known enzymatic activity against phenolic and aromatic compounds [23], making it a potential candidate **for the degradation of environmental toxins**. Molecular docking studies were conducted to predict the binding affinity and mode of interaction between the environmental toxins and the active site of the CotA laccase. Molsoft icm docking algorithm and scoring function were employed to explore ligand-protein interactions. Several environmental toxins demonstrated favorable binding interactions with the active site residues of the CotA laccase, suggesting their potential as substrates for enzymatic degradation. These included phenolic compounds and aromatic pollutants.

Analysis of the docking complexes provided insights into the spatial orientation and binding modes of toxins within the active site pocket of the CotA laccase. Key interactions between the toxins and specific amino acid residues were identified. Therefore here, we examined the docking results between environmental toxins and CotA laccase.

3.1 Molecular docking of 1-(4-chlorophenyl)-3-(3,4-dichlorophenyl)urea and CotA laccase

The molecular docking study of 1-(4-chlorophenyl)-3-(3,4-dichlorophenyl)urea with CotA laccase resulted in a promising binding pose with notable interactions. The docking score was calculated to be -15.6046 kcal/mol, indicating a strong affinity between the ligand and the enzyme. The docking analysis revealed that the ligand forms multiple interactions within the active site of CotA laccase. The primary mode of interaction involves the formation of three hydrogen bonds between the urea moiety of the ligand and key amino acid residues of the enzyme **Figure 1**. These hydrogen bonds play a crucial role in stabilizing the ligand within the binding pocket's residues: Thr264 and Thr418, enhancing its affinity for the enzyme. The significant docking score of -15.6046 suggests a favorable energetically stable conformation of the ligand within the active site of CotA laccase.

The presence of multiple hydrogen bonds and hydrophobic interactions indicates a strong binding affinity and potential for the ligand to act as an effective inhibitor or substrate for the enzyme.

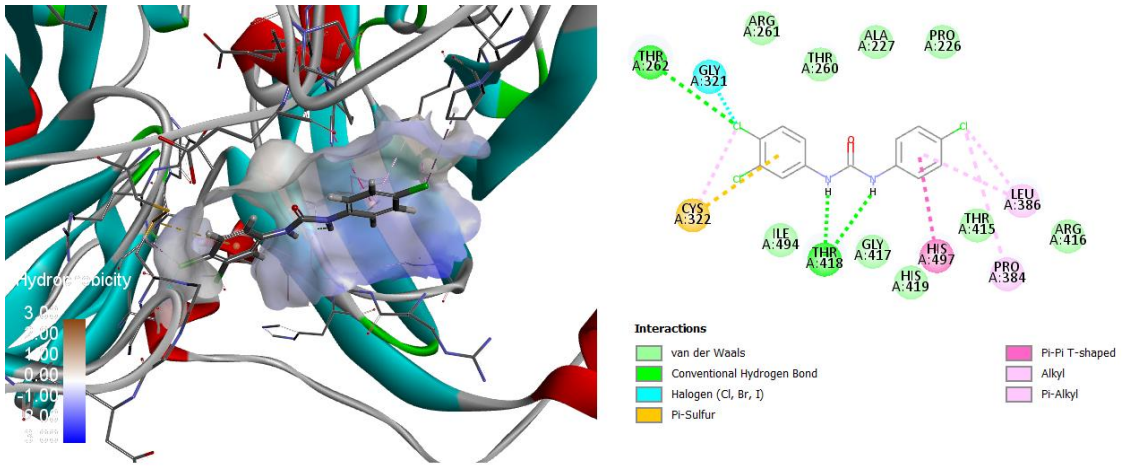

Figure 1: *The 3D and 2D interactions between CotA laccase and 1-(4-chlorophenyl)-3-(3,4-dichlorophenyl)urea*

3. 2 Molecular docking of 2,3,4,5,6-Pentachlorophenol and CotA laccase

The molecular docking study of 2,3,4,5,6-pentachlorophenol with CotA laccase revealed insightful details about the binding interactions between the ligand and the enzyme. The docking score obtained was "-15.2791", indicating a robust binding affinity between the ligand and the active site of CotA laccase.

Analysis of the docking results showed that 2,3,4,5,6-pentachlorophenol forms a stable complex within the active site of CotA laccase. The primary mode of interaction involves the formation of two hydrogen bonds between the phenolic hydroxyl groups of the ligand and Cys229 residue of the enzyme **Figure 2**. These hydrogen bonds play a pivotal role in anchoring the ligand within the binding pocket of the enzyme.

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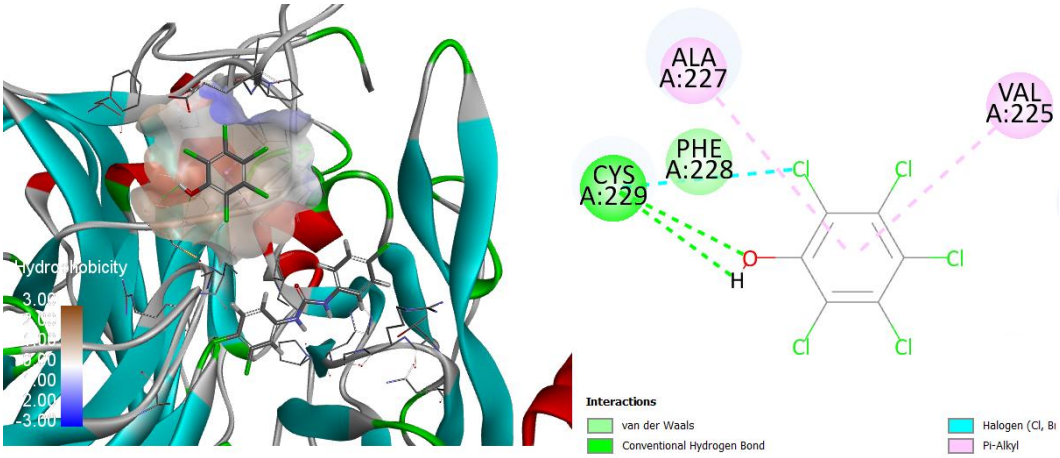

Figure 2: *The 3D and 2D interactions between CotA laccase and 2,3,4,5,6-Pentachlorophenol*

Given the potential toxicity of pentachlorophenol [24], understanding its interaction with CotA laccase is of particular interest for environmental remediation applications. The ability of the enzyme to bind and potentially degrade this compound could have implications for bioremediation strategies.

3.3 Molecular docking of 1,6-diisocyanatohexane and CotA laccase

The molecular docking study of 1,6-diisocyanatohexane with CotA laccase provides crucial insights into the binding interactions between the ligand and the enzyme's active site. The docking analysis resulted in a calculated docking score of "-15.0528 kcal/mol", indicating a strong and favorable binding affinity between the ligand and CotA laccase.

Analysis of the docking results reveals a stable binding pose of 1,6-diisocyanatohexane within the active site of CotA laccase. The primary mode of interaction involves the formation of three hydrogen bonds between the isocyanate groups of the ligand and specific amino acid residues of the enzyme (**Figure 3**). These hydrogen bonds are crucial for anchoring the ligand within the enzyme's binding pocket and stabilizing its conformation.

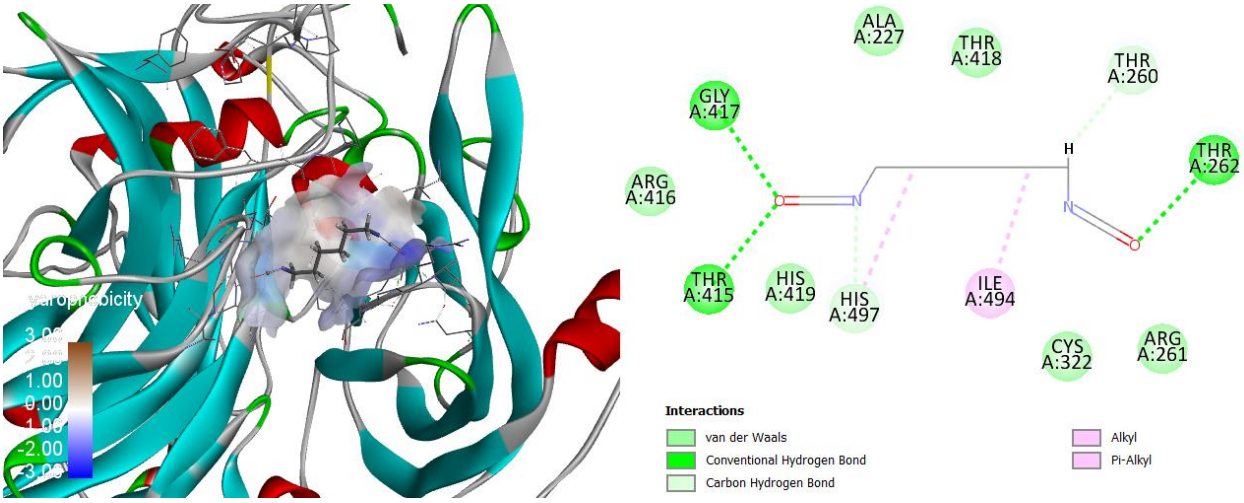

Figure 3: *The 3D and 2D interactions between CotA laccase and 1,6-diisocyanatohexane.*

The docking score of -15.0528 kcal/mol underscores the strong binding affinity of 1,6-diisocyanatohexane for CotA laccase. The presence of hydrogen bonds and hydrophobic interactions highlights the energetically favorable conformation of the ligand within the enzyme's active site. Given the potential toxicity of isocyanates [25], further investigation into the enzymatic degradation or modification of 1,6-diisocyanatohexane by CotA laccase is warranted. This could have significant implications for environmental and industrial safety, offering potential avenues for the bioremediation of isocyanate contaminants.

3.4 Molecular docking of 4-[1-(4-hydroxyphenyl)-1-methyl-ethyl]phenol and CotA laccase

The molecular docking study of 4-[1-(4-hydroxyphenyl)-1-methyl-ethyl]phenol with CotA laccase provides valuable insights into the binding interactions between the ligand and the enzyme's active site. The calculated docking score was "-12.6365 kcal/mol", indicating a favorable binding affinity between the ligand and CotA laccase.

Analysis of the docking results reveals that 4-[1-(4-hydroxyphenyl)-1-methyl-ethyl]phenol adopts a stable conformation within the active site of CotA laccase. The primary mode of interaction involves the formation of three hydrogen bonds between the hydroxyl groups of the ligand and Thr262 and Thr418 residues of the enzyme (**Figure 4**). These hydrogen bonds play a critical role in anchoring the ligand within the enzyme's binding pocket.

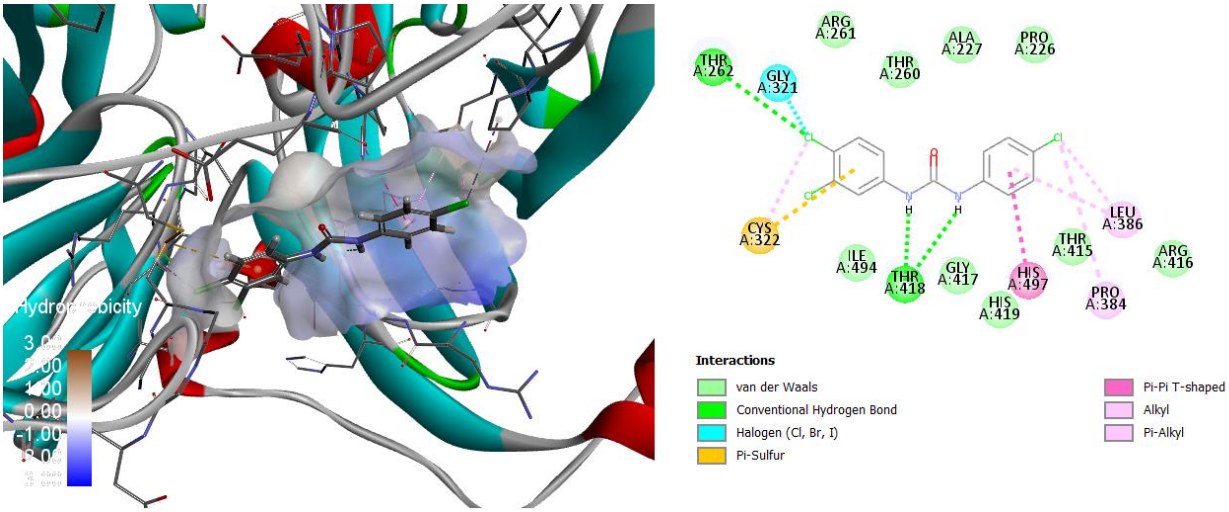

Figure 4: *The 3D and 2D interactions between CotA laccase and 4-[1-(4-hydroxyphenyl)-1-methyl-ethyl]phenol*

3.5 Molecular docking of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) and CotA laccase

The molecular docking study of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) with CotA laccase sheds light on the binding interactions between this environmental pollutant and the enzyme's active site. The calculated docking score was "-12.3935 kcal/mol", indicating a significant binding affinity between TCDD and CotA laccase.

Analysis of the docking results reveals that TCDD adopts a stable conformation within the active site of CotA laccase. Despite lacking traditional hydrogen bonding groups, TCDD forms various non-covalent interactions with specific amino acid residues of the enzyme. These interactions likely involve hydrophobic interactions due to the hydrophobic nature of TCDD's structure (**Figure 5**).

The primary mode of interaction observed involves hydrophobic interactions between the chlorinated aromatic rings of TCDD and the hydrophobic residues lining the active site of CotA laccase. These interactions contribute significantly to the stability of the TCDD-enzyme complex, enhancing the overall binding affinity.

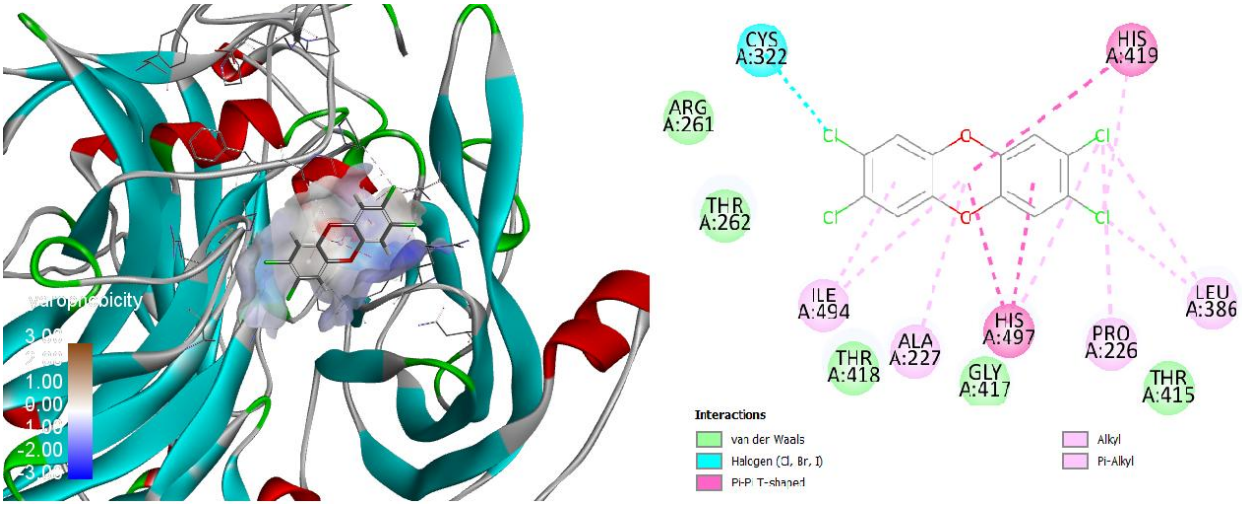

Figure 5: *The 3D and 2D interactions between CotA laccase and 4-[1-(4-hydroxyphenyl)-1-methyl-ethyl]phenol 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD)*

Understanding the binding mode of TCDD with CotA laccase is crucial for assessing the enzyme's potential role in TCDD degradation or detoxification. Enzymatic degradation of TCDD by CotA laccase could have significant implications for environmental remediation efforts, particularly in contaminated soil or water.

TCDD is a highly toxic compound with widespread environmental and health implications [26]. Investigating its interaction with CotA laccase could lead to the development of enzyme-based strategies for TCDD detoxification, potentially mitigating its harmful effects.

3.6 Molecular docking of 1,3-dichloro-5-(3,5-dichlorophenyl)benzene and CotA laccase

The molecular docking study of 1,3-dichloro-5-(3,5-dichlorophenyl)benzene with CotA laccase provides insights into the potential binding interactions between the ligand and the enzyme's active site. The calculated docking score was "-11.2221 kcal/mol", indicating a significant binding affinity between the ligand and CotA laccase.

Analysis of the docking results reveals that 1,3-dichloro-5-(3,5-dichlorophenyl)benzene adopts a stable conformation within the active site of CotA laccase. The primary mode of interaction involves the formation of hydrophobic interactions between the chlorinated aromatic rings of the ligand and Arg416, Arg497, Ile494, Cys229 residues lining the enzyme's binding pocket (**Figure 6**).

The docking analysis provides valuable structural insights into the specific residues involved in the binding of 1,3-dichloro-5-(3,5-dichlorophenyl)benzene to CotA laccase. These insights can guide further experimental studies aimed at understanding the mechanism of ligand-enzyme interaction and optimizing the enzyme's activity against this compound.

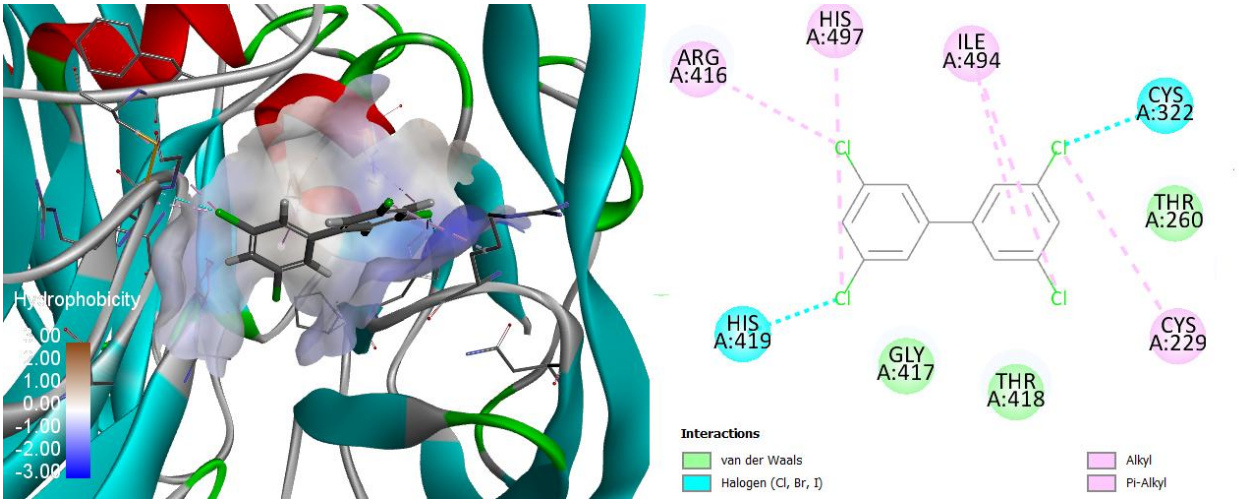

Figure 6: *The 3D and 2D interactions between CotA laccase and 1,3-dichloro-5-(3,5-dichlorophenyl) benzene.*

The presence of chlorinated aromatic rings in 1,3-dichloro-5-(3,5-dichlorophenyl) benzene suggests potential environmental toxicity. Investigating its interaction with CotA laccase could lead to insights into the enzyme's role in detoxification or degradation of similar pollutants.

3.7 Molecular docking of 1,2,3-trichloro-4-(2,3-dichlorophenyl)benzene and CotA laccase

The molecular docking study of 1,2,3-trichloro-4-(2,3-dichlorophenyl) benzene with CotA laccase provides valuable insights into the potential binding interactions between the ligand and the enzyme's active site. The calculated docking score was "-11.2221 kcal/mol", indicating a significant binding affinity between the ligand and CotA laccase.

Analysis of the docking results reveals that 1,2,3-trichloro-4-(2,3-dichlorophenyl) benzene adopts a stable conformation within the active site of CotA laccase. The primary mode of interaction involves the formation of hydrophobic interactions between the chlorinated aromatic rings of the ligand and His419, His497 and Cys322 residues lining the enzyme's binding pocket (**Figure 7**)

The obtained docking score of "-11.2221 kcal/mol" suggests a favorable and energetically stable binding between 1,2,3-trichloro-4-(2,3-dichlorophenyl) benzene and CotA laccase. The presence of hydrophobic interactions indicates a strong binding affinity, highlighting the potential of the ligand as an effective inhibitor or substrate.

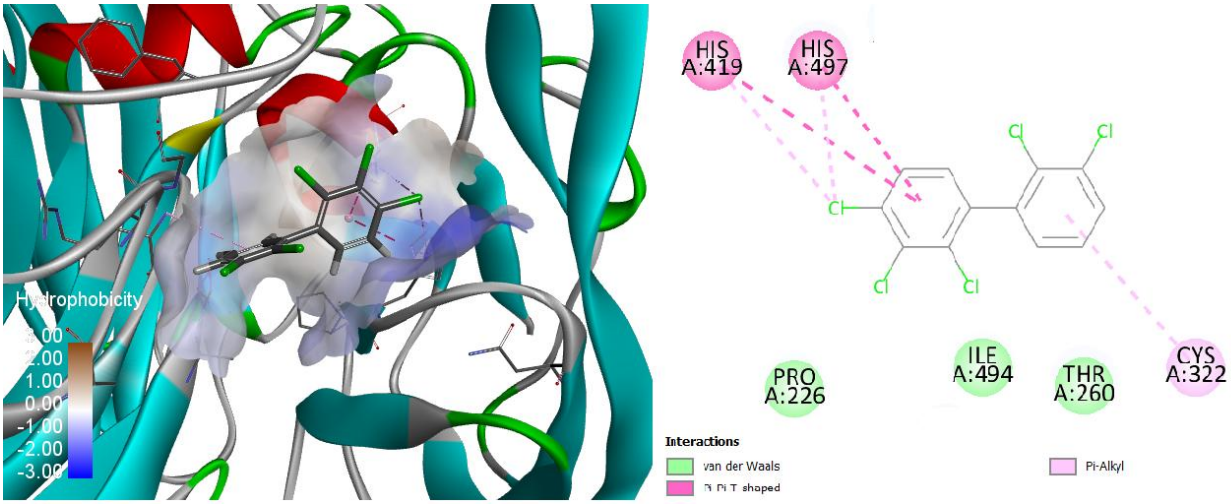

Figure 7: *The 3D and 2D interactions between CotA laccase and **1**,2,3-trichloro-4-(2,3-dichlorophenyl) benzene.*

The docking analysis provides valuable structural insights into the specific residues involved in the binding of 1,2,3-trichloro-4-(2,3-dichlorophenyl) benzene to CotA laccase. These insights can guide further experimental studies aimed at understanding the mechanism of ligand-enzyme interaction and optimizing the enzyme's activity against this compound.

The presence of chlorinated aromatic rings in 1,2,3-trichloro-4-(2,3-dichlorophenyl) benzene suggests potential environmental toxicity. Investigating its interaction with CotA laccase could lead to insights into the enzyme's role in detoxification or degradation of similar pollutants.

3.8 Molecular docking of 1,2-dichloro-4-(trifluoromethyl)benzene and CotA laccase

The molecular docking study of 1,2-dichloro-4-(trifluoromethyl)benzene with CotA laccase offers insights into the potential binding interactions between the ligand and the enzyme's active site. The calculated docking score was "-9.59908 kcal/mol", indicating a significant binding affinity between the ligand and CotA laccase.

Analysis of the docking results reveals that 1,2-dichloro-4-(trifluoromethyl)benzene adopts a stable conformation within the active site of CotA laccase. The primary mode of interaction involves the formation of hydrophobic interactions between the chlorinated and trifluoromethyl-substituted aromatic rings of the ligand and the residues (His497, Ile494, Ala227, His419) lining the enzyme's binding pocket. Further, hydrogen bonds were formed between the ligand and Gly417 and Thr415) (**Figure 8**).

The obtained docking score of "-9.59908 kcal/mol" suggests a favorable and energetically stable binding between 1,2-dichloro-4-(trifluoromethyl)benzene and CotA laccase. The presence of hydrophobic interactions indicates a strong binding affinity, highlighting the potential of the ligand as an effective inhibitor or substrate.

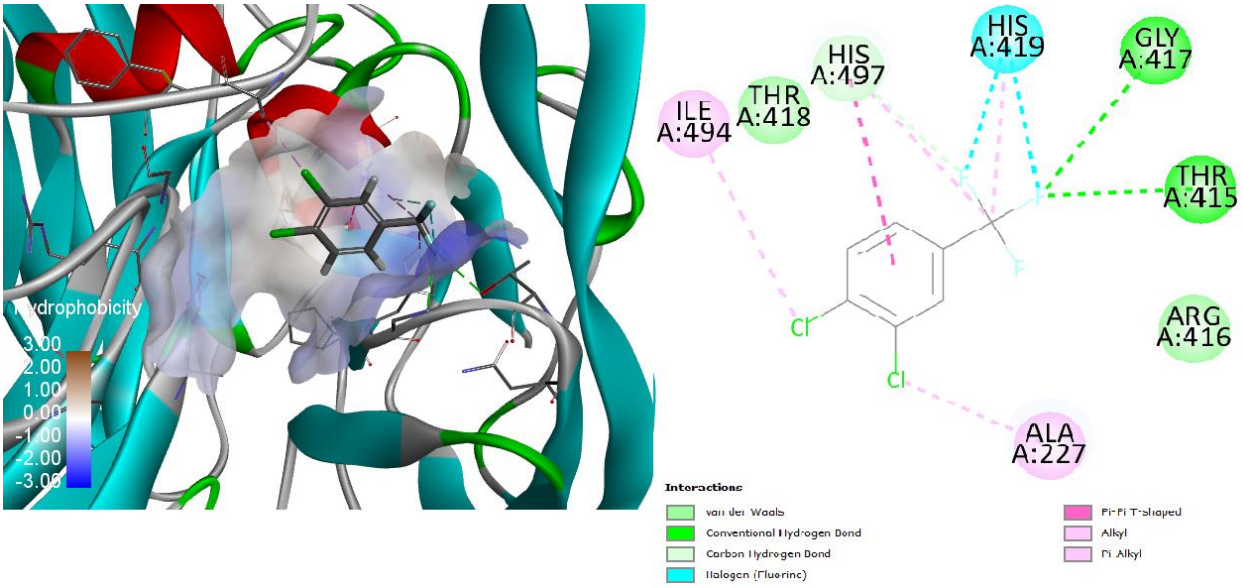

Figure 8: *The 3D and 2D interactions between CotA laccase and **1**,2-dichloro-4-(trifluoromethyl)benzene*

The docking analysis provides valuable structural insights into the specific residues involved in the binding of 1,2-dichloro-4-(trifluoromethyl)benzene to CotA laccase. These insights can guide further experimental studies aimed at understanding the mechanism of ligand-enzyme interaction and optimizing the enzyme's activity against this compound.

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The trifluoromethyl substitution in 1,2-dichloro-4-(trifluoromethyl)benzene adds a unique chemical property to the ligand. This could have implications for its interaction with CotA laccase and its potential applications in biocatalysis or enzyme-based transformations.

While chlorinated aromatic compounds are often associated with environmental concerns, the trifluoromethyl group in 1,2-dichloro-4-(trifluoromethyl)benzene introduces a different chemical aspect. Investigating its interaction with CotA laccase could provide insights into the enzyme's role in the degradation or modification of fluorinated compounds.

3.9 Molecular docking of 1,2-dichloro-4-(trifluoromethyl)benzene and CotA laccase

The molecular docking study of 1,2-dichloro-3-(2,4-dichlorophenyl) benzene with CotA laccase provides insights into the potential binding interactions between the ligand and the enzyme's active site. The calculated docking score was "-9.284 kcal/mol", indicating a significant binding affinity between the ligand and CotA laccase.

Analysis of the docking results reveals that 1,2-dichloro-3-(2,4-dichlorophenyl) benzene adopts a stable conformation within the active site of CotA laccase. The primary mode of interaction involves the formation of hydrophobic interactions between the chlorinated and dichlorophenyl-substituted aromatic rings of the ligand and the residues (His419, His497 and Cys332) as shown in **Figure 9**.

The obtained docking score of "-9.284 kcal/mol" suggests a favorable and energetically stable binding between 1,2-dichloro-3-(2,4-dichlorophenyl) benzene and CotA laccase. The presence of hydrophobic interactions indicates a strong binding affinity, highlighting the potential of the ligand as an effective inhibitor or substrate.

The docking analysis provides valuable structural insights into the specific residues involved in the binding of 1,2-dichloro-3-(2,4-dichlorophenyl)benzene to CotA laccase. These insights can guide further experimental studies aimed at understanding the mechanism of ligand-enzyme interaction and optimizing the enzyme's activity against this compound.

Chlorinated aromatic compounds [27], such as 1,2-dichloro-3-(2,4-dichlorophenyl)benzene, are often associated with environmental concerns due to their persistence and potential toxicity. Investigating its interaction with CotA laccase could lead to insights into the enzyme's role in the degradation or detoxification of similar pollutants.

Understanding the binding mode of 1,2-dichloro-3-(2,4-dichlorophenyl) benzene with CotA laccase provides insights into its potential as a substrate or inhibitor in enzyme-mediated processes. Further studies could explore its applications in biocatalysis or enzyme-based transformations.

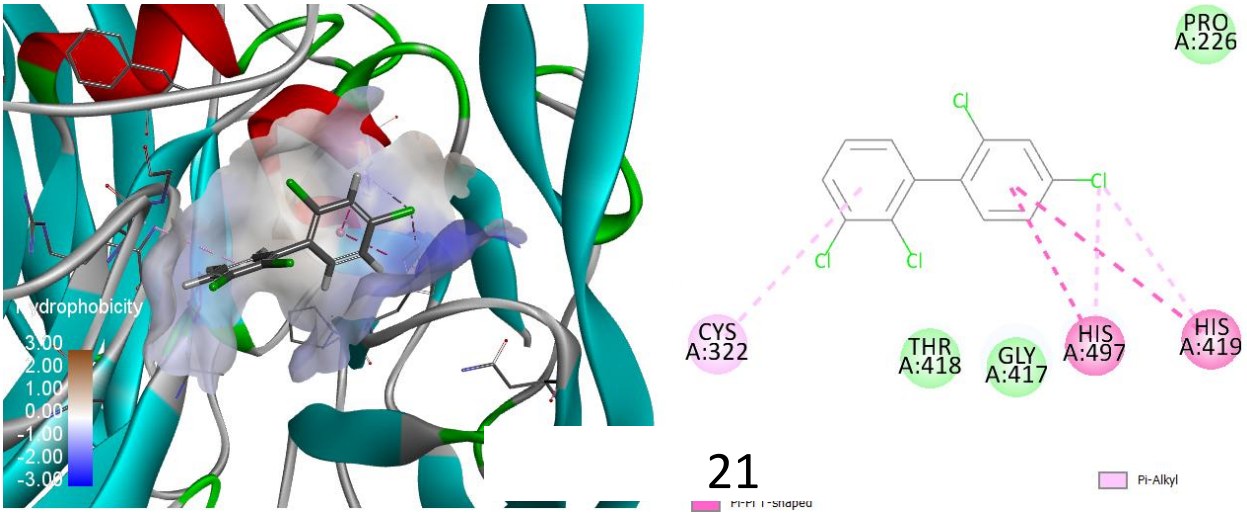

Figure 9: *The 3D and 2D interactions between CotA laccase and 1,2-dichloro-3-(2,4-dichlorophenyl) benzene.*

3.10 Molecular docking of 1,2,4-Trichloro-5-(2,4,5-trichlorophenyl) benzene and CotA Laccase

The molecular docking study of 1,2,4-trichloro-5-(2,4,5-trichlorophenyl)benzene with CotA laccase provides insights into the potential binding interactions between the ligand and the enzyme's active site. The calculated docking score was "-7.80572 kcal/mol", indicating a significant binding affinity between the ligand and CotA laccase.

Analysis of the docking results reveals that 1,2,4-trichloro-5-(2,4,5-trichlorophenyl) benzene adopts a stable conformation within the active site of CotA laccase. The primary mode of interaction involves the formation of hydrophobic interactions between the chlorinated and trichlorophenyl-substituted aromatic rings of the ligand and the Ala227, His497, Ile494, Ala320 in the enzyme's binding pocket (**Figure 10**).

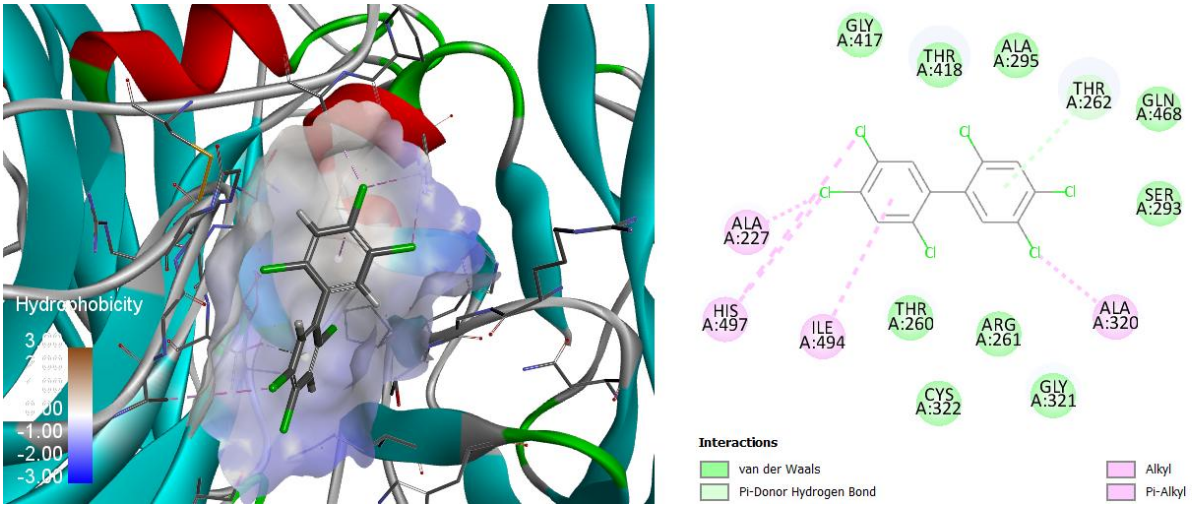

Figure 10*: The 3D and 2D interactions between CotA laccase and 1,2,4-trichloro-5-(2,4,5-trichlorophenyl) benzene.*

The obtained docking score of "-7.80572 kcal/mol" suggests a favorable and energetically stable binding between 1,2,4-trichloro-5-(2,4,5-trichlorophenyl) benzene and CotA laccase. The presence of hydrophobic interactions indicates a strong binding affinity, highlighting the potential of the ligand as an effective inhibitor or substrate.

The docking analysis provides valuable structural insights into the specific residues involved in the binding of 1,2,4-trichloro-5-(2,4,5-trichlorophenyl) benzene to CotA laccase. These insights can guide further experimental studies aimed at understanding the mechanism of ligand-enzyme interaction and optimizing the enzyme's activity against this compound.

Chlorinated aromatic compounds, such as 1,2,4-trichloro-5-(2,4,5-trichlorophenyl) benzene, are often associated with environmental concerns due to their persistence and potential toxicity. Investigating its interaction with CotA laccase could lead to insights into the enzyme's role in the degradation or detoxification of similar pollutants.

Understanding the binding mode of 1,2,4-trichloro-5-(2,4,5-trichlorophenyl) benzene with CotA laccase provides insights into its potential as a substrate or inhibitor in enzyme-mediated processes. Further studies could explore its applications in biocatalysis or enzyme-based transformations.

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4. Conclusion

Molecular docking serves as a valuable tool in the rational design and optimization of coatings for laccase from Bacillus subtilis in bioremediation applications. Through computational simulations, researchers can explore coating materials, optimize their structure, and gain mechanistic insights into laccase-coating interactions. Future research efforts leveraging molecular docking are poised to advance the development of tailored enzyme-coating systems, paving the way for more effective and sustainable solutions to environmental pollution.

Molecular docking study highlights the promising interaction of 1-(4-chlorophenyl)-3-(3,4-dichlorophenyl)urea, 2,3,4,5,6-pentachlorophenol, 1,6-diisocyanatohexane, 4-[1-(4-hydroxyphenyl)-1-methyl-ethyl]phenol, 2,3,7,8-tetrachlorodibenzo-p-dioxin, 1,3-dichloro-5-(3,5-dichlorophenyl)benzene, 1,2,3-trichloro-4-(2,3-dichlorophenyl)benzene, 1,2-dichloro-4-(trifluoromethyl)benzene, 1,2-dichloro-3-(2,4-dichlorophenyl)benzene and 1,2,4-trichloro-5-(2,4,5-trichlorophenyl)benzene with CotA laccase, laying the foundation for future investigations in the field of enzyme-ligand interactions and biocatalysis.

Molecular docking study demonstrates the strongest binding affinity of 21-(4-chlorophenyl)-3-(3,4-dichlorophenyl)urea with CotA laccase, highlighting the potential for this compound to act as a substrate or inhibitor. Further experimental validation and structural studies are warranted to explore the functional implications of these interactions and their applications in biocatalysis and environmental remediation efforts.

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