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STRUCTURAL MODELING AND MOLECULAR DOCKING OF CELLULASE FAMILY GLYCOSYL HYDROLASE ENZYME FROM *BACILLUS STERCORIS* FOR ENHANCED BIODEGRADTION OF CHLOROGUAIACOLS DERIVATIVES

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Abstract

Chlorinated guaiacol compounds, commonly released from industrial effluents, are known for their environmental persistence and toxicity. While various microbial species have been studied for pollutant degradation, the enzymatic potential of Bacillus stercoris remains largely unexplored. This study addresses that gap by evaluating, through in silico methods, the biodegradation capability of a B. stercoris-derived cellulase family glycosyl hydrolase enzyme against selected chloroguaiacols. The enzyme's sequence was retrieved from NCBI and subjected to detailed structural and physicochemical analysis. Tertiary structure modeling using AlphaFold3, followed by validation with MolProbity and ERRAT, confirmed structural reliability. Molecular docking studies using PyRx and CB-Dock2 revealed that chloroxylenol exhibited the highest binding affinity (–6.2 kcal/mol), supported by strong interactions with active site residues through hydrogen bonds, π-π stacking, and hydrophobic forces. Toxicity profiling via ProTox-3 confirmed the environmental risk posed by these compounds, especially their hepatotoxic and neurotoxic effects. Overall, the findings provide novel insights into the underutilized enzymatic potential of B. stercoris, supporting its relevance in future enzyme-based bioremediation strategies.

Keywords: *AlphaFold3, Bacillus stercoris, Environmental toxicity, Cellulase family glycosyl hydrolase, Chloroguaiacols, Molecular docking, ProTox-3*

INTRODUCTION

Environmental contamination by chlorinated phenolic compounds, particularly chloroguaiacols, has become a growing concern due to their persistence, toxicity, and widespread occurrence in industrial effluents (1). These compounds are commonly released during the processing of wood pulp, paper bleaching, and pesticide manufacturing. Once introduced into the environment, they can accumulate in aquatic and terrestrial ecosystems, posing serious risks to human health and biodiversity. Their chemical stability and resistance to natural degradation processes make them particularly challenging to remove through conventional treatment methods (2).

In response to these challenges, microbial enzymes particularly those produced by *Bacillus* species have shown remarkable potential in environmental cleanup strategies (3). In this study, a cellulase family glycosyl hydrolase enzyme derived from *Bacillus stercoris* was selected due to the species' known resilience and enzymatic versatility in harsh conditions (4). These enzymes possess the capability to catalyze the breakdown of complex organic pollutants, including chlorinated compounds, through hydrolytic activity. Investigating the structural and functional characteristics of this enzyme provides valuable insights into its bioremediation potential. The use of computational tools for structural prediction and functional annotation

allows for an efficient, cost-effective evaluation of the enzyme's suitability for environmental applications (5).

In this study, an integrated in silico approach was employed to characterize a cellulase family glycosyl hydrolase enzyme, including analysis of its physicochemical properties, structural modeling, and post-translational modification sites. The enzyme's tertiary structure was predicted and validated using AlphaFold and MolProbity tools, providing a robust model for subsequent molecular docking studies. Additionally, its transmembrane topology and potential regulatory modifications were examined to better understand its interaction environment and functionality. This thorough characterization establishes a solid foundation for its application in pollutant-binding analysis.

To evaluate the enzyme's interaction potential with common chloroguaiacols, molecular docking simulations were performed using PyRx and CB-Dock2. A series of six chloroguaiacol compounds were selected from the PubChem database based on environmental relevance. Their docking scores and interaction profiles were analyzed to identify the most promising candidates for enzyme-mediated degradation. Furthermore, the toxicity of these compounds was predicted using ProTox-3 to assess their potential health impacts. The findings of this study aim to support future efforts in enzyme-based pollutant mitigation and environmental health risk assessment.

METHODOLOGY

RETRIEVAL OF FASTA SEQUENCE OF ENZYME

FASTA sequence of cellulase family glycosylhydrolase enzyme was retrieved from NCBI (National Center for Biotechnology Information) database. The NCBI database https://www.ncbi.nlm.nih.gov/ served as a reliable platform to access well-curated genetic information essential for sequence-based studies. It also provided integrated tools for basic analysis and functional annotation of the retrieved enzyme sequence (6).

PHYSIOCHEMICAL PROPERTIES ANALYSIS

Physiochemical properties of enzymewas predicted by using Expasy Protparam tool https://web.expasy.org/protparam/ . It analyzed molecular weight, total number of amino acid residues present with in enzyme, theoretical isoelectric point (pI), GRAVY, aliphatic index, and instability index. These factors were useful in evaluating the enzyme's overall stability, solubility in aqueous media, and potential for use in environmental applications (7).

SECONDARY STRUCTURE PREDICTION

Secondary structure of enzyme was predicted using GOR IV tool https://npsa.lyon.inserm.fr/cgi-bin/npsa_automat.pl?page=/NPSA/npsa_gor4.html. This tool is freely available and determine the number of alpha helix, beta strand and random coil present with in secondary structure of protein of cellulase family glycosylhydrolase (8).

TERTIARY STRUCTURE PREDICTION ANALYSIS

AlphaFold 3 https://alphafold.ebi.ac.uk/ server tool employed to predict the tertiary structure of enzyme, which provides highly accurate protein structure models. To evaluate the overall quality of the predicted protein's tertiary structure, the MolProbity server http://molprobity.biochem.duke.edu/ was used, providing detailed validation through a Ramachandran plot. Additionally, the ERRAT tool was employed to identify potential structural errors by analyzing non-bonded atomic interactions (9).Standardized protocols were followed to ensure accuracy and comparability with previous studies on camel morphology.

PREDICTION OF PROTEIN TRANSMEMBRANE TOPOLOGY

The TMHMM tool https://services.healthtech.dtu.dk/services/TMHMM-2.0/ was used to predict the transmembrane topology of the enzyme, helping identify potential membrane-spanning regions. It uses a hidden Markov model to distinguish between transmembrane helices and non-membrane regions. This

information is essential for understanding the protein's orientation and function within a membrane environment (10).

PROTEIN POST TRANSLATION MODIFICATION PREDICTION

The MusiteDeep https://www.musite.net/ tool was used to predict potential post-translational modification (PTM) sites in the protein sequence. It applies deep learning algorithms to identify specific modification patterns such as phosphorylation.

RETRIEVAL OF CHLOROGUAIACOLS COMPOUNDS

The PubChem database https://pubchem.ncbi.nlm.nih.gov was used to retrieve the 3D structures of various chloroguaiacol derivatives in SDF format, ensuring accurate and standardized chemical information for molecular analysis. The compounds used in this study include Tetrachloroguaiacol, 2-chloro-6-methoxyphenol, 4-chloro-2-methoxyphenol, 1-chloro-4-methoxybenzene, chloroxylenol, and 3-Chloro-5-methoxyphenol. PubChem also provided detailed physicochemical properties and molecular identifiers, which were essential for structure-based computational studies (12).

MOLECUAR DOCKING AND INTERACTION ANALYSIS

PyRx software was used to perform virtual screening of all selected compounds against the target protein. For identifying binding pockets and predicting cavity-based docking, CB-Dock2 https://cadd.labshare.cn/cb-dock2/index.php was employed. The resulting protein-ligand interactions, including hydrogen bonding, hydrophobic contacts, and van der Waals forces, were visualized and analyzed using Discovery Studio (13).

TOXICOLOGICAL ASSESSMENT OF POLLUTANTS

ProTox-3 https://tox.charite.de/protox3/ toxicity profiles of the selected compounds through an online platform. It provides insight into possible toxicological effects, such as hepatotoxicity, carcinogenicity, and cytotoxicity. The tool uses machine learning models trained on experimental data to estimate safety levels. This helped in assessing the environmental and biological risks of the studied pollutants (14).

RESULTS

RETRIEVAL OF FASTA SEQUENCE OF ENZYME

A FASTA sequence of cellulase family glycosyl hydrolase was retrieved from NCBI with accession number of WP_418657264.1.

PHYSIOCHEMICAL PROPERTIES ANALYSIS

The cellulase family glycosyl hydrolase consists of 499 amino acid with a molecular weight of 54,997.49 Daltons. The protein has a slightly higher number of positively charged residues (56), including arginine and lysine, compared to negatively charged residues (54), such as aspartic acid and glutamic acid. This slight difference contributes to the overall theoretical isoelectric point (pI) of 8.10, suggesting the protein will carry a net positive charge in environments with pH values below this point. The instability index of 27.62 classifies the protein as stable, suggesting it can maintain its structural integrity in vitro without rapid degradation. The aliphatic index is 75.87, reflecting the relative volume occupied by aliphatic side chains, and this moderately high value is associated with enhanced thermal stability, often beneficial for industrial enzymes. Lastly, the GRAVY (Grand Average of Hydropathicity) score of -0.578 indicates that the protein is overall hydrophilic, favoring interaction with water molecules, which is typical for enzymes that act in aqueous environments such as cellulases.

SECONDARY STRUCTRE PREDICTION

The secondary structure prediction of the cellulase family glycosyl hydrolase enzyme, based on the GOR IV method, reveals a well-structured and functionally diverse folding pattern. Out of the total 499 amino acids, approximately 97 residues (19.44%) are arranged into alpha helices, contributing to the

enzyme's structural stability. Around 141 residues (28.26%) form extended strands or beta sheets, which are typically involved in the formation of the enzyme's core structure. The majority of the protein, about 261 residues (52.30%), are present as random coils, suggesting flexible regions that may play a role in substrate binding, active site accessibility, or conformational changes during enzymatic activity. This combination of structural elements reflects the dynamic yet stable nature of the enzyme, necessary for its biological function.

TERTIARY STRUCTURE ANALYSIS

The tertiary structure of the cellulase family glycosyl hydrolase enzyme was was predicted using AlphaFold3, a powerful deep learning-based approach known for generating high-quality protein structural models (Fig. 1a). The predicted structure was then validated using a Ramachandran plot, which helps assess the stereochemical quality of protein models by analyzing backbone dihedral angles (Fig. 1b). The results showed that 93.0% of the residues were located in the favored regions, while 98.0% fell within the allowed regions, indicating a reliable and well-folded structure. Only a small number of residues (10 in total) were identified as outliers, including some common flexible or borderline residues such as Lysine (Lys), Arginine (Arg), Valine (Val), Isoleucine (Ile), Leucine (Leu), and Alanine (Ala). Notable outlier positions included Ala27, Glu338, and Gln350. To further ensure structural reliability, the model was evaluated using ERRAT (Fig. 2), which analyzes the statistics of non-bonded interactions between atoms. The protein achieved a high overall quality factor of 97%, confirming that the tertiary structure is of excellent quality and suitable for further functional and docking studies.

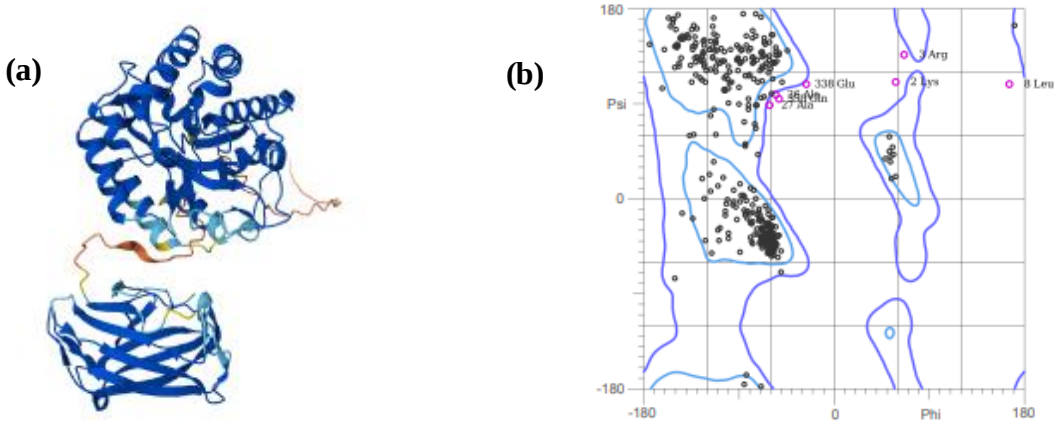


Fig. 1 (a). Tertiary structure of cellulase family glycosyl hydrolase enzyme; **(b).** Ramachandran plot of enzyme

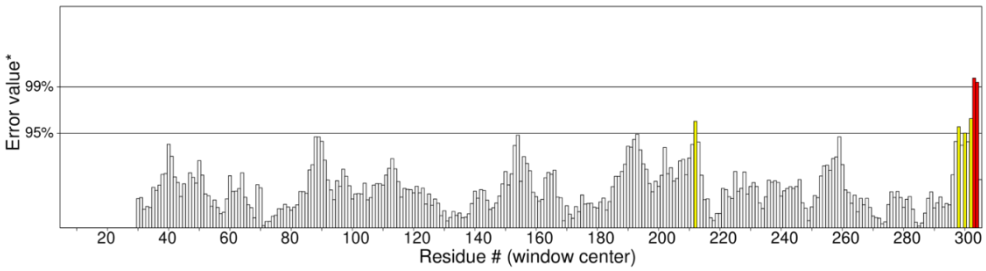


Fig. 2. ERRAT showing structure quality

PREDICTION OF PROTEIN TRANSMEMBRANE TOPOLOGY

The transmembrane topology prediction of suggests that the protein contains a single transmembrane helix. The first six amino acids are located on the cytoplasmic (inside) side of the membrane. The transmembrane helix spans from residue 7 to 29, indicating the region embedded within the lipid bilayer. The remaining residues, from 30 to 499, are positioned on the extracellular (outside) side, suggesting the functional domain of the protein lies outside the membrane (Fig. 3).

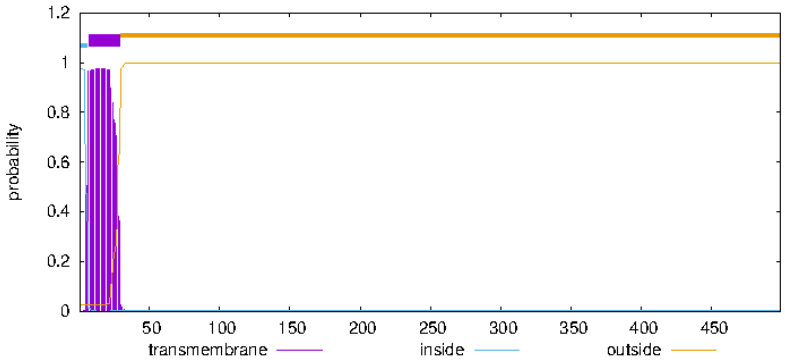


Fig. 3. Transmembrane topology prediction cellulase family glycosyl hydrolase

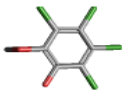
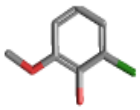
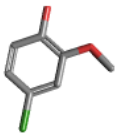
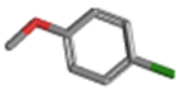
PROTEIN POST TRANSLATION MODIFICATION PREDICTION

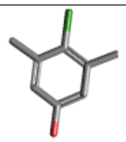
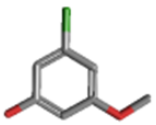
The Post-translational modification (PTM) analysisof the protein using the MusiteDeep tool revealed several potential regulatory sites. Phosphorylation sites were predicted at residues such as threonine (T34, T332), serine (S43, S287, S335), and tyrosine (Y408, Y433), indicating possible involvement in signal transduction or enzyme regulation. Glycosylation was suggested at threonine (T204), serine (S264), and asparagine residues (N292, N381, N415), which may contribute to protein folding, stability, or secretion. Ubiquitination was predicted at lysines K33, K109, K249, and K442, implying potential roles in protein turnover or degradation. In addition, acetylation sites were identified at K113, K377, K387, and K439, which could influence protein activity or interaction. No potential sites were detected for SUMOylation or methylation, suggesting these modifications may not be significant for this protein's function.

RETRIEVAL OF CHLOROGUAIACOLS COMPOUNDS

The PubChem database was utilized to retrieve detailed information on various chloroguaiacol compounds, which are recognized as significant environmental pollutants. These compounds were selected based on their relevance to industrial waste and persistence in the environment. Table I provides a summary of the selected pollutants, including their compound names, molecular weights, PubChem Compound IDs (CIDs), and their predicted tertiary structures.

Table I. List of selected pollutants

Pollutants	Compound CID	Molecular weight	3D Structure
Tetrachloroguaiacol	17343	261.899 g/mol	
2-chloro-6-methoxyphenol	93421	158.58 g/mol	
4-chloro-2-methoxy phenol	28050	158.58 g/mol	
1-Chloro-4-methoxybenzene	12167	142.58g/mol	

Chloroxylenol	2723	156.61 g/mol	
3-Chloro-5-methoxyphenol	103339	158.58 g/mol	

MOLECUAR DOCKING AND INTERACTION ANALYSIS

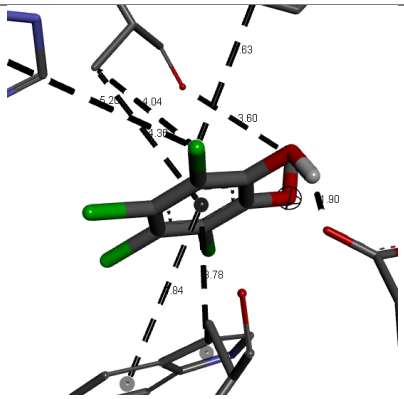
The Virtual screening of selected environmental pollutants was carried out using PyRx to predict their binding affinity towards the target enzyme. The initial docking results were further validated through pocket-specific docking using the CB-Dock2 tool, enhancing the reliability of binding site predictions. Among the screened compounds, chloroxylenol exhibited the strongest binding affinity with a binding energy of –6.2 kcal/mol, indicating a higher likelihood of stable interaction with the target enzyme. Other compounds showed the following binding energies: tetrachloroguaiacol (–5.5 kcal/mol), 2-chloro-6-methoxyphenol (-5.0kcal/mol), 4-chloro-2-methoxyphenol (–5.4 kcal/mol), 3-chloro-5-methoxyphenol (–5.0 kcal/mol), and 1-chloro-4-methoxybenzene (–4.6 kcal/mol). These values suggest varying degrees of interaction strength, with chloroxylenol being the most promising ligand for further evaluation. To gain deeper insights into the nature of these interactions, molecular docking poses were visualized, and protein-ligand interactions were analyzed. The interaction profiles, including hydrogen bonding and hydrophobic interactions, are summarized in Table II, detailing the key amino acid residues involved in stabilizing the pollutant-enzyme complexes.

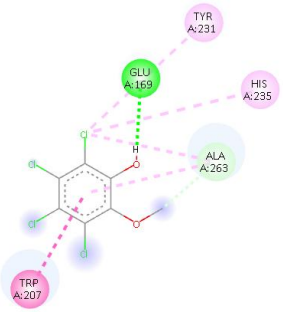
Table II. Molecular docking interaction analysis of selected pollutants with the target enzyme

Pollutants	Interacting	Bond energy
Tetrachloroguaiacol	LEU 133	Van der waals
	HIS235	Carbon hydrogen bond
	ALA263	Conventional hydrogen bond
	GLU169	Pi pi stacked
	TRP207	Alkyl
		Pi-alkyl
2-chloror-6-methoxyphenol	TYR231	Van der waals
	THR234	Conventional hydrogen bond
	HIS235	Carbon hydrogen bond
	GLU169	Pi pi stacked
	TRP207	Pi-alkyl
	GLN209	Pi sigma
	HIS229	
	ALA263	
4-chloro-2-methoxyphenol	GLN209	Pi sigma
	LEU133	Alkyl
	HIS235	Pi alkyl
	GLU169	Conventional hydrogen bond
	TRP207	Carbon hydrogen bond
	TYR231	Van der waals
	ALA263	Pi pi stacked
chloroxylenol	TYR231	Pi sigma
	HIS235	Van der waals
	ALA263	pi pi stacked
	GLU169	Conventional hydrogen bond
	TRP207	
	GLN209	

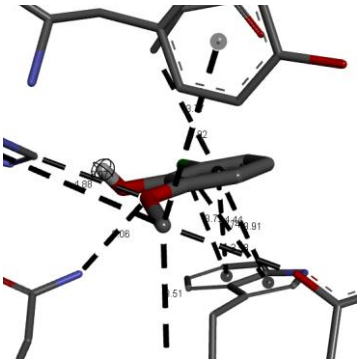
1-Chloro-4-methoxybenzene	LEU133	Pi sigma
	TYR231	Van der waals
	HIS235	Conventional hydrogen bond
	ALA263	pi pi stacked
	GLU169	Alkyl
	TRP207	Pi-alkyl
	GLN209	
3-Chloro-5-methoxyphenol	LEU133	Pi sigma
	TYR231	Van der waals
	GLU169	Conventional hydrogen bond
	GLU257	Carbon hydrogen bond
	TYR96	Alkyl
	LYS296	Pi-alkyl
	GLU298	
	HIS65	

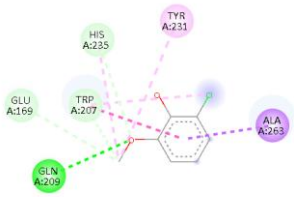
(a)





(b)





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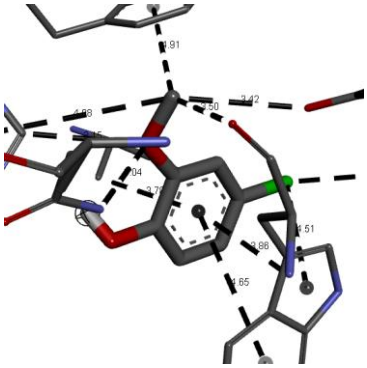

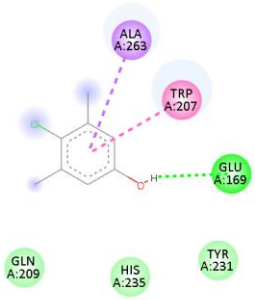

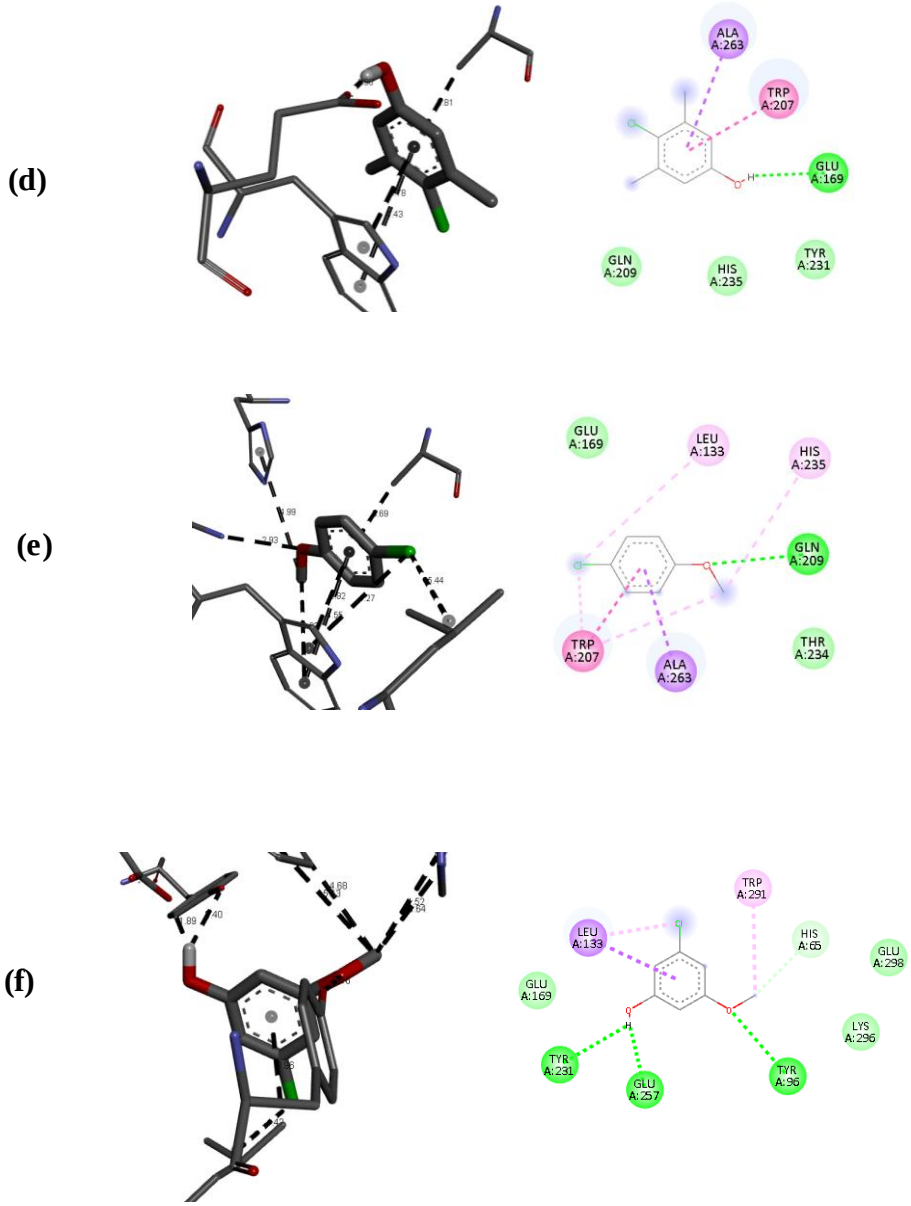

Fig. 5 (a). Bond length and 2D interaction of Tetrachloroguaiacol; **(b)** Bond length and 2D interaction of 2-chloror-6-methoxyphenol; **(c)** Bond length and 2D interaction of 4-chloro-2-methoxyphenol f; **(d)** Bond length and 2D interaction of chloroxylenol; **(e)** Bond length and 2D interaction of 1-Chloro-4-methoxybenzene; **(f)** Bond length and 2D interaction of 3-Chloro-5-methoxyphenol

TOXICOLOGICAL ASSESSMENT OF POLLUTANTS

The toxicological assessment of chloroguaiacol compounds was conducted using the ProTox-3 web-based platform. Specifically, it provides insights into various organ-specific toxicities, including hepatotoxicity, nephrotoxicity, neurotoxicity, and potential carcinogenicity. By analyzing structural similarities to known toxic compounds, ProTox-3 offers an early indication of safety risks, thereby aiding in the prioritization of environmentally relevant pollutants for further experimental validation. The predicted toxicity profiles of chloroguaiacol compounds, including their potential effects are summarized in Table III.

Table III. Predicted organ-specific toxicological profiles of chloroguaiacol compounds

Chloroguaiacol compounds	Hepatotoxicity	Neurotoxicity	Nephrotoxicity	Respiratory toxicity	Cardiotoxicity
Tetrachloroguaiacol	Active	Active	Inactive	Active	Inactive
2-chloror-6-methoxyphenol	Active	Active	Inactive	Active	Inactive
4-chloro-2-methoxyphenol	Active	Active	Inactive	Active	Inactive

chloroxylenol	Active	Active	Inactive	Active	Inactive
1-Chloro-4-methoxybenzene	Active	Active	Inactive	Active	Inactive
3-Chloro-5-methoxyphenol	Active	Active	Inactive	Active	Inactive

DISCUSSION

The present study successfully employed an in silico approach to explore the structural and functional characteristics of a cellulase family glycosyl hydrolase enzyme derived from Bacillus stercoris, with a specific focus on its potential interaction with environmentally hazardous chloroguaiacol compounds. The physicochemical analysis revealed that the enzyme is relatively stable, hydrophilic, and thermally tolerant, suggesting that it can perform effectively under diverse environmental conditions (15). Structural predictions, validated through tools such as AlphaFold 3 and MolProbity, confirmed a well-folded protein model with high reliability, making it suitable for downstream docking analysis. These findings highlight the potential of *Bacillus stercoris* enzymes as viable candidates for environmental pollutant mitigation (16).

Molecular docking results demonstrated significant binding interactions between the enzyme and selected chloroguaiacols, particularly chloroxylenol, which exhibited the highest binding affinity among all tested compounds. The interactions were stabilized by hydrogen bonds, van der Waals forces, and π-π stacking, involving key active site residues. These interactions suggest a strong potential for the enzyme to bind and possibly degrade these toxic compounds. The presence of flexible regions in the enzyme's secondary structure further supports its ability to adapt to various ligands, enhancing substrate accessibility and catalytic efficiency. Such adaptability is essential for enzymes involved in bioremediation, where target pollutants may vary in structure and concentration. Toxicological profiling using the ProTox-3 tool revealed that most of the chloroguaiacol compounds exhibited organ-specific toxicity, particularly hepatotoxicity and neurotoxicity. This underscores the importance of identifying efficient biodegradation pathways to neutralize these pollutants before they can accumulate in ecosystems or pose risks to human health. The enzyme from Bacillus stercoris, through its structural compatibility and predicted binding efficiency, shows promise for further development into a bioscavenger system for chlorinated phenolic compounds. However, experimental validation of degradation potential and enzyme kinetics will be essential to translate these computational predictions into real-world applications.

In comparison to previous studies, enzymes from Bacillus species have been widely documented for their environmental applications (17). For instance, cellulase enzymes from *Bacillus subtilis* and *Bacillus licheniformis* have demonstrated notable efficiency in degrading industrial waste and lignocellulosic biomass (18) (19). However, limited literature exists on *Bacillus stercoris* specifically. Our study provides novel insight into its enzymatic potential, aligning with reports that emphasize the genus Bacillus as a valuable resource for pollutant-degrading enzymes due to its robust metabolic pathways and adaptability. Future studies should aim to express and purify this enzyme in vitro to evaluate its actual catalytic behavior against chloroguaiacols under varying pH and temperature conditions. A key limitation of this work is the absence of wet-lab validation, which is essential to confirm predicted interactions and assess degradation efficiency. Nonetheless, the findings offer a strong computational foundation for advancing enzyme-based environmental remediation strategies.

CONCLUSION

The study presents the first in silico investigation of a cellulase family glycosyl hydrolase enzyme from *Bacillus stercoris* for its potential to bind and degrade toxic chloroguaiacol pollutants. The strong docking affinity, particularly with chloroxylenol, highlights the enzyme's promising bioremediation capability. Structural analysis confirmed the enzyme's stability and adaptability, essential for environmental applications. Unlike previous work focused on common *Bacillus* strains, our study introduces *B. stercoris* as a novel candidate for pollutant detoxification. Future research should involve

cloning, expression, and kinetic validation of the enzyme under laboratory conditions. These findings lay the groundwork for developing enzyme-based solutions to mitigate persistent industrial contaminants.

Authors' contribution:

AY, AN, AS, MS, MAS, IM, EM, IT, MB, SFAS & ZA Research work; ES, SZ, LE & RP Conceptualization, data analysis and supervision.

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