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Functional and Structural Diversity of Lipopeptide Biosurfactants in the Inhibition of Atrazine, Mancozeb, and Monocrotophos: Structural Insights for Bioremediation Purposes

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ABSTRACT

Biosurfactants, dynamic biomolecules synthesized by microorganisms, possess unique characteristics such as enhanced biodegradability and reduced toxicity. Their production has seen a surge alongside their applications in agriculture, bioremediation, therapeutics, and various industrial sectors. Atrazine, monocrotophos, and mancozeb act as herbicides, insecticides, and fungicides, respectively, fulfilling agricultural needs in weed, insect, and fungal control. This study aims to investigate the impact of lipopeptide biosurfactants on atrazine, monocrotophos, and mancozeb through molecular docking analyses, conducting docking simulations, our goal was to understand the interactions between lipopeptide biosurfactants and these agricultural chemicals. Our findings revealed significant docking interactions between lipopeptide biosurfactants and atrazine, monocrotophos, and mancozeb, suggesting potential inhibitory effects. These results are consistent with previous in vitro studies. This study represents the initial exploration of docking studies focusing on the interactions between lipopeptides and pesticides.

Keywords: *Atrazine, Biosurfactants, Mancozeb, Monochrotophous, Iturin A, and Surfactin.*

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1. Introduction

Pesticides encompass a range of organic and inorganic compounds utilized to control pests [7; 16] or eliminate weeds, playing a significant role in global crop production [6; [38]. However, their extensive use has led to various environmental issues, impacting both animal and human health [11; 31]. In recent years, heightened concern has arisen regarding the detection of pesticides in soil and water bodies, particularly regarding the accumulation of toxic metabolites in plants and organisms [10; 39]. Three pesticides—namely, atrazine, mancozeb, and monocrotophos—have seen widespread application in agriculture. Atrazine (2-chloro-4-ethylamino-6-isopropylamino-s-triazine), a polar herbicide, has been extensively used for nonselective weed control in industrial and non-cropped land, as well as for selective weed control in crops such as corn, sorghum, sugarcane, and pineapple [24;25]. Mancozeb, a non-systemic agricultural fungicide belonging to the dithiocarbamate family, is employed to control various fungal diseases across a wide range of field crops, fruits, nuts, vegetables, and ornamentals (Mehrasebi et al., 2015; 41]. However, it has been associated with adverse effects on human health and the environment. Its mechanism involves the inactivation of amino acids by reacting with sulfhydryl groups, ultimately disrupting lipid metabolism, respiration, and adenosine triphosphate production [37].

Monocrotophos, an organophosphate insecticide extensively used in cotton crops, demonstrates broad-spectrum toxicity and is applied for both systemic and contact actions across various crops such as citrus, olives, rice, maize, sorghum, sugar cane, sugar beet, peanuts, potatoes, green peas, soybeans, vegetables, ornamentals, strawberries, bananas, melons, and tobacco [14]. Its degradation in soil and water is influenced by environmental factors, with its half-life ranging from 131 days at acidic pH to 30 days at neutral pH at 25 °C in the absence of light [4]. Microorganisms and their metabolites offer a safe, cost-effective, and highly efficient method for the bioremediation of pesticide-contaminated sites [1;8;13;17]. Although microbial degradation is well-documented, the use of biosurfactants for degradation is still emerging. Biosurfactants, surface-active agents that reduce interfacial tension, hold promise for enhancing biodegradation and solubilization of environmental contaminants. Various microorganisms, including species of Bacillus, Mycobacterium, Nocardia, Pseudomonas, and Rhodococcus, are known to produce biosurfactants [9; Gudiña et al., 2016).

Biosurfactants are classified based on molecular weight (low and high molecular weight) and chemical composition (glycolipids, phospholipids, polymeric microbial surfactants,

lipopeptides, and lipoproteins) [3; 30]. Lipopeptides, a type of biosurfactant, consist of a fatty acid linked to amino acids by a peptide bond. They exhibit complex structures and include surfactin, iturin, and fengycin, with Bacillus species such as *B. subtilis, B. licheniformis, B. amyloliquefaciens*, and *B. brevis* being primary producers [19; 28]. Surfactin and iturin, prominent among the cyclic lipopeptides, exhibit remarkable potency in the degradation of agricultural pesticides. Their efficacy lies in their ability to efficiently break down pesticide compounds, aiding in the remediation of pesticide-contaminated environments. Surfactin, characterized by its heptapeptide structure linked internally with a β-hydroxy fatty acid, possesses a unique capacity to interact with a wide range of pesticide molecules. This interaction facilitates the breakdown of pesticides into less harmful byproducts, thereby reducing their environmental impact [18; 27], the cyclic lactone ring formed within the surfactin structure enhances its stability and effectiveness in pesticide degradation, making it a potent agent for bioremediation efforts. Similarly, iturin, with its heptapeptide structure linked to a β-amino fatty acid chain, demonstrates exceptional efficacy in pesticide degradation. The variation in the length of the fatty acid chain allows iturin to interact with different types of pesticide molecules, facilitating their breakdown into non-toxic components, the small molecular size of iturin enhances its mobility and accessibility to pesticide contaminants in soil and water, further augmenting its effectiveness as a bioremediation agent [5; 15].

Numerous experimental studies have documented the effectiveness of lipopeptide biosurfactants in degrading agricultural pesticides. A comprehensive understanding of their mode of action remains elusive. This study addresses this gap by delving into the intricate mechanisms underlying the degradation process facilitated by lipopeptide biosurfactants. Our investigation centers on elucidating the specific mode of action through which these biosurfactants target and break down pesticides. The identifying and characterizing the binding sites and active amino acids crucial to the degradation process, we aim to provide a detailed insight into the molecular interactions driving this phenomenon. This knowledge holds significant implications for advancing pesticide remediation strategies and environmental sustainability efforts.

2. Methodology

Structure Building and Optimization

The chemical structures of atrazine, monocrotophos, and mancozeb were built using ChemSketch 12.0.1 software. Hydrogen atoms were added to each molecule to ensure accurate representation of their chemical properties. The structures were optimized to their lowest energy configurations using the software's built-in optimization tools, which is crucial for realistic docking simulations.

Selection of Lipopeptides

In the study, the biosurfactants iturin A and surfactin were chosen for their well-documented bioremediation capabilities. These lipopeptides are known to be produced by various strains of Bacillus spp., and numerous studies have reported their effectiveness in enhancing the degradation of environmental pollutants. The structures of iturin A and surfactin were built and optimized using ChemSketch 12.0.1 software. This software allows for the creation and refinement of molecular structures, ensuring accurate representation of the lipopeptides' chemical composition and geometry, hydrogen atoms were added to the structures to enhance their accuracy, as they play a crucial role in determining the spatial arrangement and interactions of atoms within molecules. An employing ChemSketch 12.0.1 for structure building and optimization, the study aimed to ensure that the molecular models of iturin A and surfactin accurately reflected their real-world counterparts. While the specific strains or sources of these biosurfactants were not explicitly mentioned in the paper, the use of iturin A and surfactin, which are well-known and widely studied lipopeptides produced by Bacillus spp., adds credibility to the findings.

Molecular Docking Analysis

Docking Software

Gold version 3.0.1 was utilized for the molecular docking studies. This software is known for its robust algorithms and accuracy in predicting ligand-receptor interactions.

Docking Protocol

Alpha Shape Theory and Discrete Flow Theory: These advanced computational geometry methods were employed to analyze the molecular surfaces and interactions. Alpha Shape Theory: Used to define and describe the shapes and topologies of the binding sites, identifying atoms that form the pockets, pocket openings, and buried cavities within the biosurfactants.

Discrete Flow Theory: Applied to model the surface flow of the molecules, providing detailed information on pocket and cavity volumes and areas, which are essential for understanding how well the pesticide molecules can fit and bind within these sites.

Binding Pocket Analysis

The software identified atoms lining the pockets where the pesticide molecules could potentially bind. It also mapped pocket openings and buried cavities to understand the accessibility and depth of these binding sites.

Volume and Area Calculations

Pocket and cavity volumes and areas were calculated to quantify the available binding space within the lipopeptides. These measurements are crucial for determining the capacity of the lipopeptides to accommodate the pesticide molecules.

Mouth-Opening Assessment

The docking software assessed the mouth-opening areas and circumferences of the identified pockets. This information provided insights into how the pesticide molecules enter and interact within the binding pockets of iturin A and surfactin.

Binding Orientation and Affinity

The docking simulations generated multiple binding orientations for atrazine, monocrotophos, and mancozeb with iturin A and surfactin. The most favorable binding orientations were selected based on the scoring functions provided by the Gold software, which considers factors such as hydrogen bonding, van der Waals forces, and hydrophobic interactions.

Interaction Mapping

Detailed interaction maps were produced to visualize the specific atoms and functional groups involved in the binding process. These maps highlighted key interactions, such as hydrogen bonds, hydrophobic contacts, and electrostatic interactions between the lipopeptides and the pesticide molecules.

Comparative Analysis
The binding affinities of atrazine, monocrotophos, and mancozeb to iturin A and surfactin were compared. This comparative analysis provided insights into the relative efficacy of each lipopeptide in binding and potentially neutralizing the different pesticide molecules.

Docking method
Docking studies were conducted using the GOLD (Genetic Optimization of Ligand Docking) software, which employs a genetic algorithm (GA) to allow partial flexibility of the compounds and full flexibility of the ligands. This approach facilitated the docking of atrazine, monocrotophos, and mancozeb with the lipopeptides iturin A and surfactin, focusing on analyzing their interactions with the residues of the biosurfactants through detailed molecular mechanics calculations. The parameters chosen for the GA included a population size of 100, a selection pressure of 1.1, and 10,000 operations. Additionally, a single island with a niche size of 2 was utilized, along with operator parameters set to 100 for crossover, 100 for mutation, and 10 for migration. Default cutoff values were employed, with 3.0 Å for hydrogen bonds and 6.0 Å for van der Waals interactions.

Docking Configuration
During the docking process, the default algorithm speed was selected to ensure a balance between computational efficiency and accuracy. The ligand binding site for each docking experiment was defined within a 10 Å radius from the centroid of the binding pocket. Each inhibitor was subjected to 100 poses to explore a wide range of potential binding conformations. An early termination criterion was employed, allowing the docking process to stop if the top three bound conformations of a ligand were within 1.5 Å Root Mean Square Deviation (RMSD) of each other, indicating convergence towards a stable binding mode.

Interaction Analysis
After docking, the individual binding poses of each ligand were carefully examined to understand the specific interactions between the ligands and the residues of iturin A and surfactin. This detailed analysis included: Hydrogen Bonding: Identification and examination of hydrogen bonds formed between the ligands and specific residues. Van der Waals Interactions: Analysis of van der Waals forces that contribute to the overall binding affinity. Electrostatic Interactions: Evaluation of electrostatic interactions that play a role in stabilizing the ligand-receptor complex.

Gold Score fitness function
GOLD Score Components and Adjustment
The GOLD Score, a pivotal component of the docking methodology, relies on a force field-based scoring function comprising four fundamental components: Protein-Ligand Hydrogen Bond Energy (External H-Bond): This component quantifies the energy associated with hydrogen bonding interactions between the protein and ligand molecules. Protein-Ligand Van der Waals Energy (External VDW): This component measures the van der Waals interactions between the protein and ligand, contributing to the overall binding affinity. Ligand Internal Van der Waals Energy: This component represents the van der Waals interactions within the ligand molecule itself. Ligand Intra molecular Hydrogen Bond Energy: This component accounts for the energy associated with hydrogen bonding interactions within the ligand molecule.

Adjustment for Hydrophobic Interactions
In the computation of the total fitness score, the External VDW score undergoes a multiplication by a factor of 1.375. This adjustment, an empirical correction, aims to enhance hydrophobic interactions between the protein and ligand molecules. An amplifying the contribution of van der Waals interactions, particularly those involving hydrophobic contacts, this adjustment promotes more favorable protein-ligand interactions.

Optimization of Fitness Function
The fitness function, including the adjustment for hydrophobic interactions, has undergone meticulous optimization to ensure accurate prediction of ligand binding positions. This optimization process enhances the reliability and predictive power of the docking simulations, thereby improving the overall quality of the results. The fine-tuning the scoring function and incorporating empirical corrections, the docking methodology achieves greater accuracy in identifying energetically favorable binding poses.
GoldScore = S (hb_ext) + S (vdw_ext) + S (hb_int) + S (vdw_int)
Where S (hb_ext) is the protein-ligand hydrogen bond score, S (vdw_ext) is the protein-ligand van der Waals score, S (hb_int) is the score from intramolecular hydrogen bond in the ligand and S (vdw_int) is the score from intramolecular strain in the ligand.

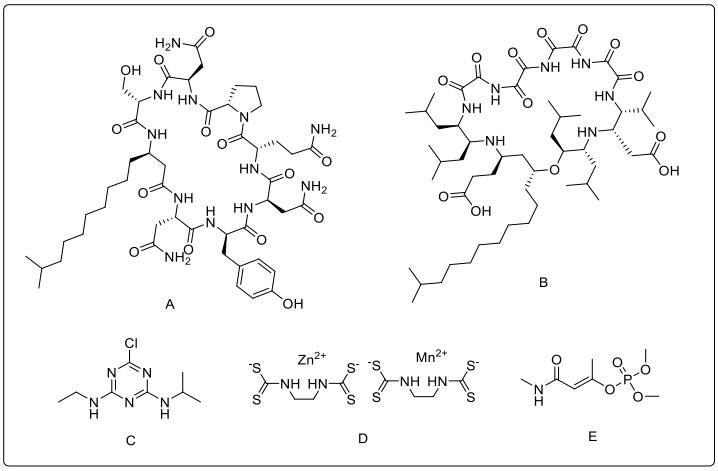

Fig. 1. Structures of biosurfactants: A) Iturin A; B) Surfactin and agriculture chemicals: C) Atrazine; D) Mancozeb; E) Monochrotophous

3. Results

Following the acquisition of the structures, hydrogen atoms were added to facilitate the development of possible binding interactions. Subsequent binding analysis revealed the uniformity of binding pockets across all chains, with the largest binding pocket selected for further docking studies. Given the cyclic nature of Iturin A and Surfactin structures, representative conformations were chosen for the docking investigations. Docking experiments were conducted using the GOLD software, with evaluations based on the GoldScore fitness functions. The Gold fitness score was favored over the Chemscore fitness function due to its slight superiority in performance. This preference was based on the assessment of various scoring metrics, ultimately selecting the Gold fitness score for its marginally better predictive capabilities in the context of our docking studies.

Molecular Docking Study of Iturin A
The docked conformations of atrazine and mancozeb with iturin A are illustrated in Fig. 2, showcasing the presence of all ligands within the binding pocket.

Across all docked ligands, interactions between oxygen atoms and the enzyme were observed, along with hydrogen-bonding interactions within the active site. Notably, common hydrogen-bonding interactions were identified between all docked ligands and iturin A within the binding pocket. Specific hydrogen-bonding interactions within the docked conformations of iturin A and surfactin, as well as surrounding atoms in the binding pocket, were further investigated. Fig. 2A highlights four robust hydrogen-bonding interactions between the hydroxyl group (N7) of atrazine and hydrogen atoms of iturin A. Specifically, hydrogen atoms H71, H74, H78, and H90 of iturin A participated in bonding with atrazine. Similarly, in the docked mancozeb complex, four hydrogen bonds were formed between the sulfur groups (S5 and S6) of mancozeb and hydrogen atoms H71, H74, H78, and H90 of iturin A (Fig. 2B). In contrast, the docked Monocrotophos-iturin A complex exhibited six hydrogen bonds with iturin A. These interactions comprised hydrogen bonding between the sulfur group (O13) of Monocrotophos and hydrogen atoms H78 and H71 of iturin A, the sulfur group (O1) of Monocrotophos and hydrogen atom H91 of iturin A, and the sulfur group (O3) of Monocrotophos and hydrogen atom H90 of iturin A (Fig. 2C)

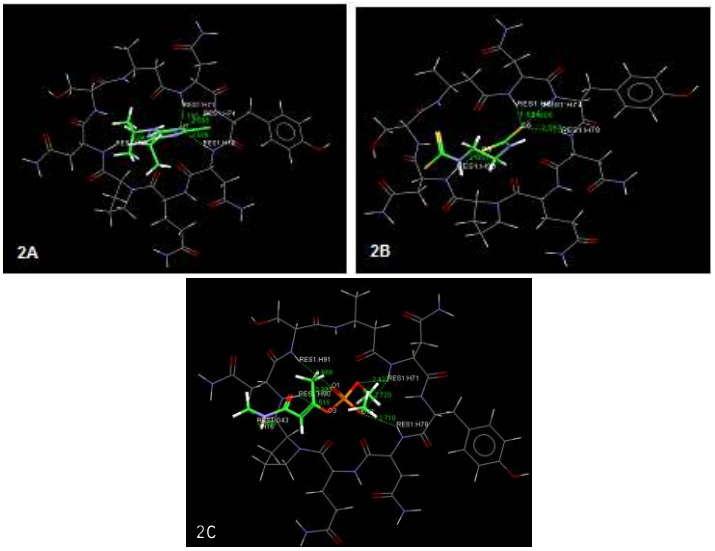

Fig. 2 (A-C). Iturin A docked with atrazine, Mancozeb, and Monochrotophous

The analysis of the docked conformations revealed distinct docking scores for iturin A in complex with atrazine, Monochrotophous, and mancozeb. Specifically, the docking score for iturin A with atrazine was determined to be 35.24 K.cal/mol, with Monochrotophous at 33.94 K.cal/mol, and with mancozeb at 31.86 K.cal/mol. This quantitative assessment highlighted that atrazine exhibited a higher affinity towards iturin A compared to both mancozeb and Monochrotophous, indicative of a stronger interaction between atrazine and iturin A. These findings underscore the differential binding affinities of iturin A towards various pesticide compounds, with atrazine demonstrating the highest affinity. Such insights into the binding preferences of iturin A towards different pesticides contribute to a deeper understanding of the molecular interactions underlying the potential bioremediation of pesticide-contaminated environments.

Table 1: Docking score of iturin A with atrazine and mancozeb

Fitness	S(hb_ext)	S(vdw_ext)	S(hb_int)	S(int)	Ligand name
35.24	3.45	24.24	0.00	-2.84	Atrazine
33.94	10.41	26.00	0.00	-3.62	Mancozeb
31.86	5.15	23.84	0.00	-2.84	Monochrotophous

3.2 Molecular docking study of surfactin

During the docking of atrazine, Monochrotophous, and mancozeb into the binding site of surfactin, hydrogen bond interactions were observed, indicating potential binding affinity between these pesticide compounds and surfactin. Specifically, in the case of atrazine docking, a hydrogen bond was identified between the oxygen group (O15) of surfactin and the hydrogen atom (H15) of atrazine (Fig. 3A). Similarly, when mancozeb was docked into the surfactin binding site, four hydrogen bonds were observed. These hydrogen bonds were formed between the sulfur atoms (S5, S9, and S10) of mancozeb and hydrogen atoms of surfactin (Fig. 3B). Furthermore, during the docking of Monochrotophous into the surfactin binding site, three hydrogen bonds were identified. These hydrogen bonds involved interactions between the oxygen groups (O11, O1) and hydrogen atom (H16) of Monochrotophous, and specific residues (H102, H145, and O73) of surfactin, respectively (Fig. 3C). These observations provide insights into the potential molecular interactions between surfactin and pesticide compounds, suggesting their ability to bind within the surfactin binding site and form hydrogen bond interactions. Such interactions may have implications for the role of surfactin in pesticide bioremediation and warrant further investigation into the mechanism of action underlying these interactions.

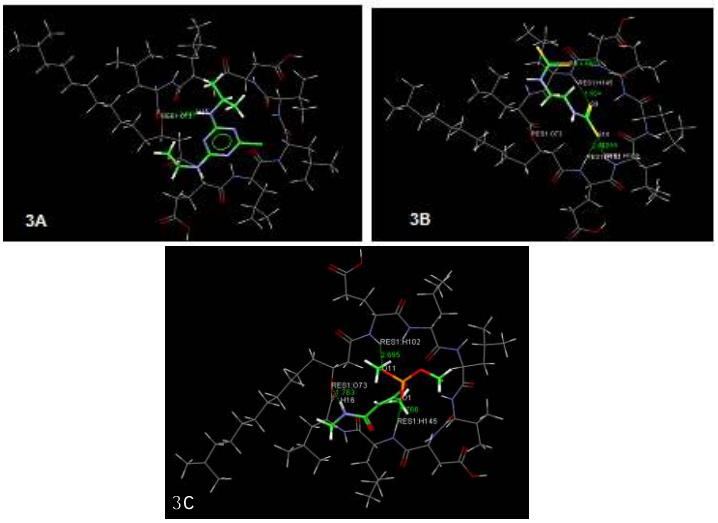

Fig. 3 (A-C). Surfactin docked with Atrazine, Mancozeb, and Monochrotophous

Upon analyzing the docked conformations, it was discerned that surfactin exhibited varying docking scores when bound to atrazine, Monochrotophous, and mancozeb. Specifically, the docking score for surfactin with atrazine was determined to be 42.54 K.cal/mol, with Monochrotophous at 36.47 K.cal/mol, and with mancozeb at 39.77 K.cal/mol. These quantitative evaluations indicated that atrazine displayed a higher affinity towards surfactin compared to both mancozeb and Monochrotophous, signifying a stronger binding interaction between atrazine and surfactin. These findings emphasize the differential binding affinities of surfactin towards different pesticide compounds, with atrazine exhibiting the highest affinity. Such insights into the binding preferences of surfactin towards various pesticides contribute to a better understanding of the potential role of surfactin in pesticide bioremediation processes.

Table 2: Docking score of surfactin with atrazine and mancozeb

Fitness	S(hb_ext)	S(vdw_ext)	S(hb_int)	S(int)	Ligand name
42.54	1.30	24.23	0.00	-2.77	Atrazine
39.77	7.24	25.95	0.00	-3.15	Mancozeb
36.47	6.14	24.05	0.00	-3.15	Monochrotophous

Within the realm of bio-surfactants, namely iturin A and surfactin, surfactin emerges as exerting the most potent inhibitory effect on atrazine, Monochrotophous, and mancozeb in comparison to iturin A. This observation underscores the superior efficacy of surfactin in mitigating the activity of these pesticide compounds.

In Table 3, detailed information regarding the atoms involved in bonding, their respective bond lengths, and the corresponding docking energies are provided. This comprehensive data elucidates the molecular interactions occurring between the bio-surfactants and the pesticide molecules, shedding light on the underlying mechanisms of inhibition. An analyzing the bonding patterns and associated energetics, a clearer understanding of the inhibitory potential of surfactin relative to iturin A can be gleaned. These insights contribute to the ongoing exploration of bio-surfactants as promising agents for pesticide bioremediation and underscore the importance of surfactin in this context.

Table 3: Molecules involved in docking of iturin A and surfactin

Bio-surfactant	Atoms	Molecule	No.of Hydrogen bonds	Bond length	Docking score (K.Cal/mol)
Iturin A	71(H) 74(H) 78 (H) 90 (H)	Atrazine (N7) N(5)	4	1.798 2.089 2.586 2.383	35.24
	71(H) 74(H) 78 (H) 90 (H)	Mancozeb(S6) S(5)	4	1.684 1.905 2.506 2.057	33.94
	78(H) 71(H) 71 (H) 91 (H) 90 (H)	Monochrotophous (O13) (O4) (O1) (O3)	5	2.720 2.710 2.420 2.668 2.510	31.86
Surfactin	15(H)	Atrazine(O73)	1	2.649	42.54
	147(H) 145(H) 102(H) 109(H)	Mancozeb (S5) (S9) (S10)	4	1.688 1.884 2.032 2.659	39.77
	102(H) 145 (H) 73 (O)	Monochrotophous (O11) (O1) H16	3	2.698 2.766 1.763	36.47

4. Discussion

Biosurfactants play a pivotal role in enhancing the biodegradation of pesticides through various mechanisms such as micellar solubilization, emulsification, and facilitated mass transport [23]. The biodegradation of several pesticides often faces challenges due to their sorption and low solubility on soil surfaces. To address this issue, biosurfactants have been evaluated, and their effectiveness has been assessed through the determination of critical micelle concentration (CMC) values. For instance, the degradation of hexachlorocyclohexane (HCH) by Sphingomonas sp. NM05 was significantly enhanced by surfactant amendments, resulting in a 30% improvement in biodegradation [20]. An increased emulsification of HCH and n-hexadecane was observed, further indicating the effectiveness of surfactants in improving HCH degradation [35]. Similarly, the biodegradation of endosulfan, both in flask and soil culture conditions, was notably enhanced by a biosurfactant derived from Bacillus subtiris MTCC1427, resulting in a 30-40% increase in the rate of biodegradation [2]. These findings highlight the significant potential of biosurfactants in facilitating the removal of chemical pollutants from the environment, the use of biosurfactants for pesticide biodegradation has garnered considerable attention due to its effectiveness in enhancing the removal of chemical contaminants from the environment [21;41]. These studies underscore the importance of biosurfactants as valuable tools for sustainable environmental remediation strategies. To investigate the degradation of agrochemicals using biosurfactants, in silicon-binding studies were conducted to analyze the interaction of surfactin and iturin A with atrazine, mancozeb, and monocrotophos.

Biosurfactants represent a diverse class of compounds with multifaceted applications in environmental, industrial, and agricultural settings. While the study by Liu et al. (2016) provides valuable insights into the potential of biosurfactants for pesticide degradation, it is essential to contextualize these findings within the broader field of biosurfactant research, encompassing previous studies on similar interactions and exploring potential applications beyond molecular docking. Previous research has extensively investigated the role of biosurfactants in enhancing the biodegradation of various pollutants, including pesticides. For example, studies have demonstrated the effectiveness of biosurfactants in enhancing the degradation of pesticides such as chlorpyrifos, atrazine, and glyphosate. Biosurfactants facilitate the solubilization and dispersion of hydrophobic pesticides in aqueous environments, thereby improving their bioavailability to microbial degraders and enhancing degradation rates [34].

The biosurfactants have been explored for their potential applications beyond pesticide degradation. In the environmental remediation context, biosurfactants have shown promise in the bioremediation of hydrocarbon-contaminated soils and waters. Studies have demonstrated their ability to enhance the solubilization and biodegradation of petroleum hydrocarbons, polycyclic aromatic hydrocarbons (PAHs), and other recalcitrant pollutants [26;29]. Environmental remediation, biosurfactants have diverse applications in agriculture and biotechnology. They have been investigated for their potential in improving soil structure and fertility, enhancing plant growth and stress tolerance, and controlling plant pathogens and pests. Biosurfactants can act as biofertilizers, biopesticides, and biostimulants, offering sustainable alternatives to synthetic agrochemicals [32; 36].

The biosurfactants have gained attention in industrial sectors such as cosmetics, food processing, and pharmaceuticals, where they serve as eco-friendly alternatives to synthetic surfactants. They are used in formulations for personal care products, food emulsifiers, drug delivery systems, and microbial enhanced oil recovery (MEOR) processes [32-33]. The biosurfactant-mediated pesticide degradation, previous studies have elucidated the mechanisms underlying the interactions between biosurfactants and pesticides, including adsorption, emulsification, and enzymatic degradation. Biosurfactants can enhance pesticide degradation by increasing their solubility, bioavailability, and accessibility to microbial degraders, leading to accelerated degradation rates and reduced environmental persistence [25;34]. While molecular docking studies, such as those conducted by Liu et al. (2016), provide valuable insights into the potential interactions between biosurfactants and pesticides at the molecular level, it is essential to complement these findings with experimental studies to validate their efficacy under real-world conditions. Field trials, laboratory-scale experiments, and microbial consortia studies can provide a more comprehensive understanding of the role of biosurfactants in pesticide degradation and their potential applications in sustainable agriculture and environmental management.

The docking results were in concordance with observed in vitro findings (data not shown), indicating that both iturin A and surfactin possess inhibitory activity against atrazine, mancozeb, and monocrotophos. Our investigations revealed that atrazine exhibited the highest docking interactions with both iturin A and surfactin, suggesting its potential for further investigation. The docking results supported the inhibitory activity of iturin A and surfactin. These biosurfactants were docked to the agrochemicals, and the results were interpreted accordingly. Surfactin demonstrated the strongest bonding with atrazine, mancozeb, and monocrotophos among the two biosurfactants, indicating their interaction through hydrogen bonds and potentially facilitating biodegradation. The role of biosurfactants in atrazine degradation was elucidated using the structures of surfactin and iturin A. Surfactin, being a macromolecule comprising lipid and protein moieties, exhibited a protein fraction representing proximal enzymes involved in pesticide metabolism. In the presence of biosurfactants, chemical compounds were transformed into their respective derivatives, rendering them nonfunctional in soil and water environments [25]. These findings underscore the potential of biosurfactants, particularly surfactin, in facilitating the degradation of agrochemicals and highlight their significance in environmental remediation efforts. Further exploration of biosurfactant-mediated degradation pathways could provide valuable insights into sustainable strategies for mitigating the impact of agricultural pollutants on ecosystems.

5. Conclusión

Based on the results obtained, it can be concluded that both iturin A and surfactin exhibit inhibitory effects on atrazine, monochrotophous, and mancozeb. Docking studies confirmed the binding affinity of iturin A and surfactin with these agrochemicals. Iturin A demonstrated docking scores of 35.24 K.cal/mol with atrazine, 31.86 K.cal/mol with monocrotophos, and 33.96 K.cal/mol with mancozeb. These results indicate that atrazine exhibited a higher affinity towards iturin A compared to monochrotopous and mancozeb. On the other hand, surfactin displayed docking scores of 42.54 K.cal/mol with atrazine, 36.47 K.cal/mol with monochrotopous, and 39.77 K.cal/mol with mancozeb. Similarly, atrazine exhibited a higher affinity towards surfactin compared to monochrotopous and mancozeb. Comparatively, when assessing the inhibitory effects of iturin A and surfactin, surfactin demonstrated the highest inhibitory effect on atrazine, monochrotopous, and mancozeb. These findings suggest that surfactin may be more effective in inhibiting the activity of these agrochemicals compared to iturin A. Overall, these results provide valuable insights into the potential of both iturin A and surfactin as inhibitory compounds against atrazine, monochrotopous, and mancozeb, with surfactin exhibiting superior inhibitory effects.

The term "initial exploration" implies that this paper marks the first attempt at conducting docking studies between lipopeptides and pesticides. However, to establish the novelty and importance of this investigation in the present scientific context, additional context and rationale are essential. For instance, the absence of prior docking studies between lipopeptides and pesticides underscores the novelty of this research endeavor, the potential complexity of molecular interactions between lipopeptides and pesticides, which may remain unexplored, highlights the significance of investigating these interactions. An elucidating such complexities, this study can pave the way for more effective pesticide degradation methods and the development of innovative bio-based pesticides. Furthermore, given the escalating concerns regarding pesticide residues and environmental contamination, emphasizing how this research addresses these issues can elevate its significance, the paper can comprehensively justify the significance of exploring docking studies between lipopeptides and pesticides in the current scientific landscape.

Data Availability: All data generated or analyzed during this study are included in this article.

Ethical approval: The author confirms that there are no ethical issues in the publication of the manuscript.

Human and animal rights: No animals/humans were used for studies that are the basis of this research.

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