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IN SILICO COMPUTATIONAL ANALYSIS OF POTENTIAL INTERACTION OF DENTAL MATERIALS AGAINST *AGGREGATIBACTER ACTINOMYCETEMCOMITANS*

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ABSTRACT:
Aggregatibacter actinomycetemcomitans is a Gram-negative facultative anaerobic bacterium strongly associated with aggressive periodontitis and chronic periodontal infections. Colonization of oral microorganisms around dental restorative materials and prostheses may contribute to periodontal destruction. The present study aimed to evaluate the potential interaction of dental material (Austenitic steel) against *Aggregatibacter actinomycetemcomitans* through molecular docking analysis.An in silico molecular docking study was performed using the target protein of *Aggregatibacter actinomycetemcomitans*(PDB ID: 2Y3M). The protein was prepared by removing water molecules and co-crystallized ligands, followed by the addition of polar hydrogen atoms and Kollman charges. Austenitic steel was used as the ligand, and molecular docking was carried out using AutoDock 4.2.6. The docked complex was analyzed using Discovery Studio Visualizer to evaluate binding affinity and molecular interactions.Molecular docking demonstrated a binding affinity of −3.9 kcal/mol for Austenitic steel against the target protein of *Aggregatibacter actinomycetemcomitans*. Residual interactions included Lys-85 and Phe-78, while hydrophobic and van der Waals interactions involved Gln-86 and Ala-82, suggesting moderate molecular interaction between the material and bacterial target. The findings suggest that Austenitic steel exhibits a measurable interaction with the target protein of *Aggregatibacter actinomycetemcomitans*, indicating potential antimicrobial or inhibitory behavior. Although the binding affinity was moderate, these results support further experimental investigations to validate the clinical implications of dental material interactions with periodontal pathogens.

KEYWORDS: In silico analysis; Molecular docking; *Aggregatibacter actinomycetemcomitans*; Dental materials; Austenitic steel; Periodontitis; AutoDock; Antimicrobial activity.

1.INTRODUCTION:

In silico identification for potential hits has become a popular approach in computer-aided drug discovery. This approach is able to narrow down the search of potential lead compound from a huge number of compound databases to select potential hits by using high-throughput molecular docking(1); or to elucidate the mechanistic interaction of potential hits which helps in rationalisation or optimisation of bioactivity(2)In silico methods have had a significant impact on a number of toxicological sciences subdisciplines. Genetic toxicology, carcinogenicity, cardiotoxicity, hepatotoxicity, toxicokinetics, pharmacogenomics, non-clinical safety assessment of pharmaceuticals, safety of indirect food additives, and xenobiotic metabolism are just a few examples. Although early computer software programmes for compartmental modelling of pharmacokinetic data were widely recognised in the 1990s, in recent years, in silico methods have impacted emerging 'omics' sciences and have drawn particular attention given the advanced computer methods that are now available. Proteomics, metabolomics, and systems biology (pathway analysis) all rely heavily on computer platforms for data analysis and presentation. In silico (Q)SAR and SAR models for predicting discrete effects in chemical toxicology research are useful(3).

Microbiological and host factors influence the pathogenicity of the microorganism. A *actinomycetemcomitans* colonisation is aided by several virulence factors, colonisation, invasion, and destruction of periodontal tissues. Patients who use traditional fixed prostheses are at an increased risk of colonisation by periodontopathogenic microorganisms at the union interface between the prosthesis and the teeth. For the attachment of the prostheses to the teeth, various cements are used(4). This A.*actinomycetemcomitans* genotype significantly correlates with the onset of periodontal disease in infected Africans(5).In any case, ongoing information demonstrate that whenever periodontitis has created, the personality of the periodontal contamination might change over the long haul from a disease basically connected with A. *actinomycetemcomitans* into a more anaerobic, polymicrobial contamination(6).

Aggregatibacter actinomycetemcomitans is a Gram-negative, facultative anaerobe, non motile bacterium that is often found in association with localised aggressive periodontitis, a severe infection of the periodontium. It is also suspected to be involved in chronic periodontitis.*Aggregatibacter actinomycetemcomitans* (A.a) is an exogenous bacterium that causes true infections and is spread among people who have been exposed to it. It is linked to periodontitis in young people. It occurs in 90% of cases of locally aggressive periodontitis and 30-50% of cases of severe adult periodontitis. It is capable of producing virulence factors(7).Dental cements with antimicrobial activity can actively contribute to the prevention of periodontal disease. The results of this study were very useful from a scientific standpoint, as they show statistically significant values for the tested cements, with zinc phosphate cement and glass ionomer cement being positive and resin cement being negative for antibacterial activity(8).

2.MATERIALS AND METHODS:

The molecular docking studies of the compounds (Steel and nickel) and the positive control (xxx) were performed using the AutoDock 4.2.6 software (Allouche, 2011). The same protocols to our previous works were used (Bitew et al., 2021, Lemilemu et al., 2021, Damena et al., 2022). Briefly, the PDB file for xxxxx was downloaded from the Protein Data Bank with a resolution of 2.4 Å (Xie et al., 2017b). The co-crystallized substrate and water molecules were removed from the receptor using the MGL 1.5.6 software. After cleaning the protein, only polar hydrogens were added together with the Kollman charges. Non-polar hydrogen atoms were merged and Gasteiger partial atomic charges were assigned to the molecules. Standard docking parameters for all the light and metal atoms were used. The grid box was constructed using 120, 120, and 120 pointing in the x, y, and z dimensions, respectively, with a grid point spacing of 0.375 Å. The center grid box was set at -12.055, -10.491, and 5.964 Å for the x, y, and z centers, respectively. Lamarckian genetic algorithm (LGA) program (Morris et al., 1998) with an adaptive whole method search in the AutoDock was selected and set at 100, which generated one hundred different conformations for each of the molecules (Ördög and Grolmusz, 2008). The conformers with the lowest binding free energies were used for the visualization of the interactions between the active amino acids and the molecules using the Discovery Studio software.

Swiss ADME: The ligands were subjected for physicochemical and pharmacokinetic (ADME) evaluation using SwissADME (Daina et al., 2017). The protocol to predict physicochemical properties, pharmacokinetic and drug likeness evaluation, and BOILED egg model of the metal complexes and the ligands were conducted according to our previous work (Lemilemu et al., 2021, Bitew et al., 2021, Damena et al., 2022).

3.RESULTS:

3.1 Protein Preparation

FIGURE 1

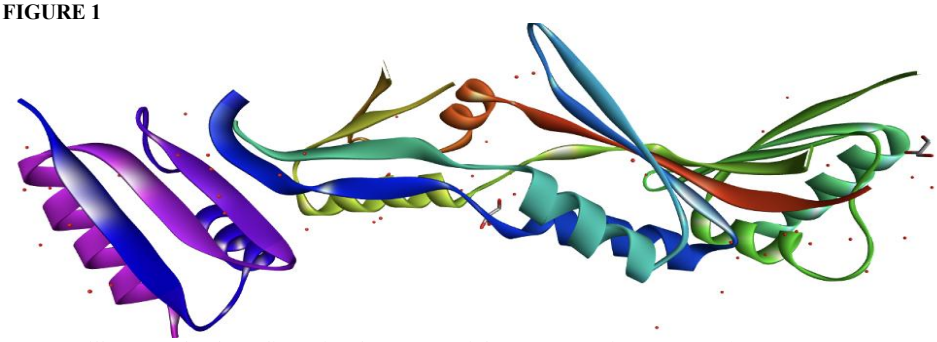

Figure 1 illustrates the three-dimensional structure of the target protein (*Aggregatibacter actinomycetemcomitans*, PDB ID: 2Y3M) before and after protein preparation for molecular docking analysis. The upper image represents the original protein structure obtained from the Protein Data Bank, while the lower

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image shows the prepared protein after removal of water molecules and unwanted co-crystallized ligands. Polar hydrogen atoms and charges were added to optimize the receptor for molecular docking and improve binding interaction analysis.

FIGURE 2

3.2 Prepared Protein

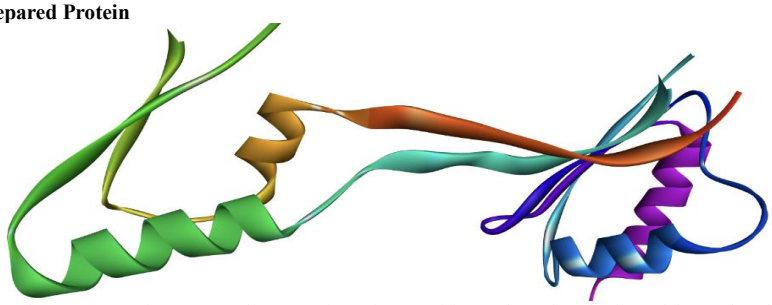

Figure 2 demonstrates the structural preparation of Austenitic steel used as the ligand for molecular docking analysis. The molecular arrangement of constituent elements, including iron (Fe), nickel (Ni), and carbon components, was prepared and optimized to ensure appropriate geometry and stability before docking with the target protein. Proper ligand preparation is essential for accurate prediction of receptor–ligand interactions during computational analysis.

FIGURE 3:

3.3 Ligand Preparation

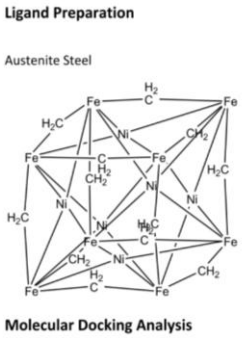

Figure 3 illustrates the molecular docking interaction between Austenitic steel and the target protein (PDB ID: 2Y3M) of *Aggregatibacter actinomycetemcomitans*. The figure represents the docked conformation of the ligand within the protein environment, demonstrating the possible binding orientation and interaction pattern. The molecular docking analysis suggests that Austenitic steel interacts with amino acid residues present in the receptor site, contributing to stabilization through non-covalent interactions.

FIGURE 4:

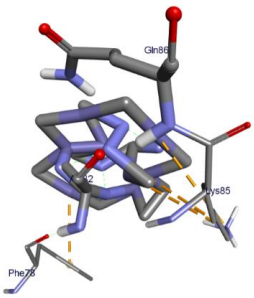

Figure 4 depicts the amino acid interaction map of Austenitic steel against the target protein of *Aggregatibacter actinomycetemcomitans*. The interaction diagram demonstrates the involvement of amino acid residues such as Lys-85, Phe-78, Gln-86, and Ala-82 in receptor–ligand stabilization. The interaction map highlights hydrophobic/pi-cation and van der Waals interactions, indicating the molecular basis for ligand binding and structural stabilization within the receptor site.

TABLE 1:

Interaction Table

Molecular docking scores and residual amino acid interactions of Austenite Steel against Protein (PDB ID: 2Y3M) of *Aggregatibacter actinomycetemcomitans.*

Ligands	Affinity (kcal/mol)	H-bond	Residual interactions	
			Hydrophobic/Pi-Cation	Van dar Waals
Austenite Steel	-3.9		Lys-85, Phe-78	Gln-86, Ala-82

Table 1 summarizes the molecular docking results of Austenitic steel against the target protein (PDB ID: 2Y3M) of *Aggregatibacter actinomycetemcomitans*. The ligand demonstrated a binding affinity score of **−3.9 kcal/mol**, indicating moderate interaction with the receptor protein. Residual interactions involved **Lys-85** and **Phe-78**, while **Gln-86** and **Ala-82** contributed through van der Waals interactions. These findings suggest the ability of Austenitic steel to establish molecular interactions with the bacterial target protein

4. DISCUSSION

Periodontal diseases continue to represent a major oral health burden, particularly due to their polymicrobial nature and destructive effects on periodontal tissues (9). Among periodontal pathogens, *Aggregatibacter actinomycetemcomitans* has been extensively associated with localized aggressive periodontitis and severe periodontal destruction (10). Its pathogenicity is attributed to several virulence factors including leukotoxin production, endotoxins, tissue invasion, and immune modulation, making it an important target for antimicrobial investigation(11).

The present study investigated the molecular interaction between Austenitic steel and *Aggregatibacter actinomycetemcomitans* using molecular docking analysis (12). In silico methods are increasingly recognized as valuable tools for predicting molecular interactions, identifying biological targets, and screening therapeutic compounds in a time- and cost-effective manner (13). Molecular docking provides insight into ligand–receptor compatibility by estimating binding affinity and identifying amino acid residues involved in intermolecular stabilization (14).

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In this study, Austenitic steel demonstrated a binding affinity of **−3.9 kcal/mol** against the target protein (PDB ID: 2Y3M). This result suggests a moderate degree of interaction between the material and bacterial protein (15). While the binding affinity observed was not highly negative compared with potent antimicrobial compounds, the interaction still indicates a measurable association that may contribute to biological influence under clinical conditions (16). The docking result suggests that Austenitic steel possesses the potential to interact with bacterial proteins and may interfere with microbial adherence or survival mechanisms .

5. CONCLUSION

The present in silico computational analysis demonstrated that Austenitic steel exhibits a measurable interaction against the target protein of *Aggregatibacter actinomycetemcomitans* (PDB ID: 2Y3M), with a docking affinity score of **−3.9 kcal/mol**. The interaction involved amino acid residues **Lys-85, Phe-78, Gln-86, and Ala-82**, suggesting stabilization through hydrophobic and van der Waals interactions. Although the binding affinity indicated a moderate interaction, the findings support the possibility that dental materials such as Austenitic steel may influence bacterial behavior and microbial colonization. Further experimental and clinical investigations are required to validate these computational findings and establish their practical relevance in restorative and periodontal dentistry.

AUTHOR CONTRIBUTIONS

Author 1: Kaviya Selvaraj carried out the study by collecting data and drafted the manuscript after performing the necessary statistical analysis and in the preparation of the manuscript.

Author 2: Rajlakshman aided in conception of the topic, designing the study and supervision of the study, correction and final approval of the manuscript.

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