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Evaluating binding affinity and toxicity profile of GC14 as potential peptide against phosphotransferase system enzyme PtxA of *Streptococcus mutans*.

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Abstract

Background: *Streptococcus mutans (S. mutans)* is a major etiological agent of dental caries due to its ability to metabolize carbohydrates, produce acids, and form biofilms on tooth surfaces. The phosphotransferase system (PTS), particularly the PtxA protein, plays an important role in carbohydrate transport and bacterial metabolism, contributing to bacterial survival and virulence. Targeting metabolic proteins using antimicrobial peptides represents a promising alternative therapeutic strategy to control *S. mutans* without promoting antibiotic resistance.

Methods: In the present study, the antimicrobial peptide GC14 was computationally evaluated for its therapeutic potential against *S. mutans*. The peptide was analyzed for toxicity using the ToxinPred server and biological activity using the Peptide Ranker tool. Physicochemical properties including molecular weight, net charge, hydrophobicity, and isoelectric point were determined using peptide property analysis tools. Structural characteristics were examined using a helical wheel plot. Molecular docking analysis was performed using the HPEPDOCK server to evaluate the interaction between GC14 and the phosphotransferase system protein PtxA. Additionally, protein–protein interaction network analysis was performed to understand the biological role of the target protein.

Results: The toxicity prediction indicated that GC14 is non-toxic and suitable for biological applications. The peptide showed a high biological activity prediction score, suggesting strong functional potential. Physicochemical analysis revealed that GC14 possesses typical antimicrobial peptide characteristics, including amphipathic nature and favorable charge distribution. Molecular docking demonstrated strong binding affinity between GC14 and the PtxA protein, indicating stable peptide–protein interaction. Protein interaction network analysis showed that PtxA is associated with multiple metabolic and cellular pathways in *S. mutans*.

Conclusion: Overall, the findings suggest that GC14 is a promising antimicrobial peptide candidate that may inhibit *S. mutans* by targeting metabolic pathways through interaction with the PtxA protein. Further experimental studies are required to validate its antimicrobial and anti-biofilm activity.

Keywords: Antimicrobial peptide, GC14, *S. mutans*, Molecular docking, protein-protein interaction

1. Introduction

The development of dental caries is closely linked to the metabolic activity and biofilm-forming ability of *Streptococcus mutans (S. mutans)*, a major cariogenic bacterium in the oral cavity [1]. The organism survives in the oral environment by efficiently transporting and metabolizing dietary carbohydrates, which are converted into organic acids that contribute to enamel demineralization. One of the important systems involved in carbohydrate uptake in S. mutans is the phosphotransferase system (PTS), a multi-component transport system that regulates sugar transport and metabolism. Proteins involved in this system play an essential role in bacterial growth, energy metabolism, and biofilm formation [2]. Among these proteins, the phosphotransferase enzyme PtxA is considered important for carbohydrate transport and metabolic regulation, making it a potential molecular target for antimicrobial intervention [3–5].

Traditional antimicrobial therapies used to control oral pathogens often face limitations such as development of resistance, disruption of normal oral microbiota, and reduced effectiveness against biofilms [6]. These challenges have encouraged researchers to explore alternative antimicrobial strategies that are more selective and less prone to resistance development [7]. Antimicrobial peptides (AMPs) have emerged as promising candidates due to their ability to interact with bacterial membranes, proteins, and metabolic pathways [8]. Their small size, structural diversity, and multiple mechanisms of action make them suitable for targeting bacterial virulence and survival pathways rather than simply killing bacteria through conventional antibiotic mechanisms [9].

With the advancement of computational biology, peptide design and drug discovery have increasingly shifted toward in silico approaches. Computational tools allow researchers to design peptides, evaluate their toxicity and biological activity, predict physicochemical properties, and study peptide–protein interactions through molecular docking [10]. These approaches significantly reduce experimental time and cost while improving the efficiency of identifying potential therapeutic molecules. Molecular docking studies, in particular, help predict binding affinity and interaction stability between peptides and target proteins, providing insight into possible mechanisms of inhibition [11].

Therefore, in this study, the antimicrobial peptide GC14 was evaluated using computational approaches to determine its potential as a therapeutic candidate against *S. mutans*. The peptide was analyzed for toxicity, predicted biological activity, physicochemical characteristics, and structural properties. Furthermore, molecular docking analysis was performed to study the interaction between the GC14 peptide and the phosphotransferase system protein PtxA, followed by protein interaction network analysis to understand the biological significance of the target protein. This study aims to explore the potential of GC14 as a peptide-based inhibitor targeting metabolic and virulence-associated pathways in *S. mutans*.

2. Materials and Methods

2.1 Peptide Design and Structural Visualization: The antimicrobial peptide used in this study was designed using computational approaches targeting the surface protein antigen I/II of *S. mutans*, which is an important virulence factor responsible for adhesion and biofilm formation [12]. The peptide sequence was generated through *in silico* peptide design tools. The structural representation and visualization of the peptide were performed using the PepDraw server, which provides structural illustrations and information related to amino acid composition and predicted molecular characteristics.

b. *In Silico* Toxicity Assessment

The toxicity of the designed peptide was evaluated using the ToxinPred server, an online computational tool used for predicting peptide toxicity. The prediction is based on amino acid composition, physicochemical parameters, and machine learning algorithms. The peptide sequence was analyzed and classified as either toxic or non-toxic, providing a preliminary safety evaluation for potential therapeutic application [13].

2.3 Prediction of Biological Activity and Availability: The potential biological activity of the designed peptide was assessed using the Peptide Ranker tool. This server predicts the likelihood of a peptide being biologically active by comparing the sequence features with datasets of experimentally validated bioactive peptides. A higher probability score indicates a greater chance of biological activity and functional relevance [14].

2.4 Analysis of Physicochemical Characteristics: Various physicochemical parameters of the peptide, including molecular weight, net charge, hydrophobicity, and isoelectric point, were calculated using peptide analysis tools. These properties are important for understanding peptide

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stability, solubility, and interaction potential with microbial membranes and proteins, and are commonly used in antimicrobial peptide screening studies.

2.5 Helical Wheel Structure Analysis

The structural arrangement and amphipathic properties of the peptide were examined using a helical wheel projection method [15]. This approach provides a visual representation of how hydrophobic and hydrophilic residues are distributed along an alpha-helical structure, which is a critical feature influencing the interaction of antimicrobial peptides with bacterial targets.

2.6 Molecular Docking Analysis

To investigate the binding interaction between the designed peptide and the antigen I/II protein of *S. mutans*, molecular docking analysis was performed [16]. The three-dimensional structure of the target protein was retrieved from the PDB and processed to remove non-essential components prior to docking. The interaction study was conducted using the HPEPDOCK server, which predicts the binding orientation and interaction energy of protein–peptide complexes. The docking outcomes were evaluated based on binding affinity values and the presence of interactions such as hydrogen bonds, hydrophobic contacts, and electrostatic forces.

2.7 Protein–Protein Interaction Network Analysis

To further understand the functional context of antigen I/II, a protein–protein interaction network was constructed using the STRING database [17]. The protein sequence was used as input, and the network was generated by integrating data from experimental findings, co-expression studies, and computational predictions. This analysis provided insights into the involvement of antigen I/II in biological processes such as adhesion, biofilm development, and virulence.

3. Results

3.1 Toxicity Assessment of GC14: The toxicity profile of the GC14 peptide was evaluated using an in-silico prediction approach. The analysis classified GC14 as a non-toxic peptide, indicating that it is unlikely to produce harmful biological effects. This finding supports its potential suitability for therapeutic applications (**Figure 1**).

3.2 Evaluation of Predicted Biological Activity: The functional potential of GC14 was assessed using a peptide activity prediction tool. The peptide demonstrated a high activity probability score, suggesting a strong likelihood of exhibiting biological function. This result indicates that GC14 may possess effective antimicrobial properties (**Figure 1**).

3.3 Physicochemical Characterization of GC14: Analysis of the physicochemical properties (**Figure 2**) showed that GC14 falls within the typical range observed for antimicrobial peptides. Parameters such as number of residues (14 amino acid), molecular weight (1637.89 g/mol), net charge of 0.9 at pH 7, extinction coefficient of 11380 $M^{-1}cm^{-1}$, and isoelectric point (pH of 8.11) were consistent with features required for antimicrobial activity. The peptide displayed an amphipathic nature and a favorable charge distribution, both of which are important for interaction with bacterial membranes and proteins. Additionally, GC14 exhibited good solubility, further supporting its applicability as a bioactive peptide.

3.4 Structural Orientation Analysis : The spatial arrangement of amino acid residues in GC14 was examined using a helical wheel projection (**Figure 3**). The results revealed a clear amphipathic α-helical configuration, characterized by the segregation of hydrophobic and hydrophilic residues. This structural feature is commonly associated with membrane-active peptides and suggests that GC14 may effectively interact with bacterial membranes and target proteins.

3.5 Peptide–Protein Interaction Analysis : Docking analysis demonstrated a strong interaction between GC14 and the target protein. The obtained docking score was highly negative, indicating a stable binding conformation and favorable interaction. The binding pattern suggests that GC14 may associate with functionally important regions of the target protein, potentially disrupting its role in bacterial adhesion and biofilm formation (**Figure 4**).

3.6 Functional Interaction Network of Target Protein: The interaction network analysis of the target protein (**Figure 5**) revealed multiple associations with proteins involved in key bacterial processes. These interacting partners are linked to functions such as adhesion, virulence, DNA replication, and cellular maintenance. The central positioning of the target protein within this network highlights its importance in regulating pathogenic mechanisms, further supporting its relevance as a therapeutic target.

4. Discussion

Dental caries remains strongly associated with the metabolic activity and biofilm-forming capacity of *S. mutans*, making metabolic enzymes and transport systems attractive targets for antimicrobial intervention [18,19]. In the present study, the antimicrobial peptide GC14 was computationally evaluated for its interaction with the phosphotransferase system protein PtxA, which plays a role in carbohydrate transport and bacterial metabolism. Targeting metabolic pathways rather than only adhesion-related proteins represents an alternative strategy to reduce bacterial survival and acid production, thereby potentially limiting biofilm formation and cariogenic activity.

The toxicity prediction results indicated that GC14 is non-toxic, which is an important characteristic for therapeutic peptides. Recent studies on antimicrobial peptide design have emphasized the importance of balancing antimicrobial activity with low cytotoxicity toward host cells [20,21]. Several computationally designed peptides targeting oral pathogens have demonstrated similar non-toxic profiles while maintaining antimicrobial activity, suggesting that rational peptide design approaches can successfully produce safe therapeutic candidates. Therefore, the non-toxic nature of GC14 supports its potential for further experimental validation [22,23]. The predicted biological activity score of GC14 suggests that the peptide has a high probability of functional activity. Previous studies using peptide activity prediction tools have reported that peptides with higher activity scores often demonstrate effective antimicrobial or anti-biofilm activity in experimental conditions. This indicates that GC14 may possess antimicrobial properties similar to other short antimicrobial peptides that target bacterial proteins or membranes [24].

Physicochemical analysis showed that GC14 possesses characteristics commonly associated with antimicrobial peptides, including appropriate molecular weight, net positive charge, hydrophobicity, and amphipathic nature. These properties are important for peptide interaction with bacterial membranes and proteins. Many antimicrobial peptides reported in earlier studies exhibit similar physicochemical profiles, which allow them to penetrate bacterial membranes, bind to intracellular targets, or interfere with enzyme function. The helical wheel plot further supported the amphipathic alpha-helical structure of GC14, which is a structural feature frequently observed in membrane-active and protein-binding antimicrobial peptides [25,26].

The molecular docking analysis demonstrated a strong binding interaction between GC14 and the PtxA protein, indicating the possibility of stable peptide–protein complex formation. Strong docking interactions between antimicrobial peptides and bacterial target proteins have been reported in several recent computational studies, where peptides were designed to inhibit enzymes involved in metabolism, adhesion, or biofilm formation. Binding of peptides to metabolic enzymes can interfere with substrate transport, enzyme activity, or regulatory processes, ultimately affecting bacterial growth and virulence. Therefore, the interaction between GC14 and PtxA suggests that the peptide may disrupt carbohydrate transport or metabolic pathways in *S. mutans*, which could reduce acid production and biofilm development [27,28].

Protein–protein interaction network analysis further showed that PtxA is functionally associated with proteins involved in bacterial metabolism, DNA replication, and cellular processes. This indicates that the target protein plays a central role in bacterial survival and metabolic regulation. Similar network analyses in previous studies have shown that targeting proteins with multiple functional interactions can have broader effects on bacterial physiology and virulence. Therefore, targeting PtxA may indirectly affect multiple metabolic and virulence-related pathways in *S.*

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mutans [29].Overall, the computational findings from this study suggest that GC14 possesses several important characteristics of potential antimicrobial peptides, including low predicted toxicity, favorable physicochemical properties, amphipathic structure, and strong binding interaction with a metabolically important bacterial protein. Compared with previous antimicrobial peptide studies targeting adhesion proteins or membrane structures, this study highlights the potential of targeting metabolic transport proteins such as PtxA as an alternative anti-cariogenic strategy. However, further in vitro and in vivo studies are necessary to validate the antimicrobial activity, biofilm inhibition potential, and therapeutic applicability of the GC14 peptide.

5. Conclusion

In conclusion, the present study computationally evaluated the antimicrobial peptide GC14 for its potential activity against *S. mutans* by targeting the phosphotransferase system protein PtxA, a key component involved in carbohydrate transport and bacterial metabolism. The peptide demonstrated favorable characteristics, including a non-toxic profile, high predicted biological activity, suitable physicochemical properties, and an amphipathic structural arrangement, all of which are important features of effective antimicrobial peptides. Molecular docking analysis further revealed strong binding affinity between GC14 and the target protein, suggesting the possibility of stable peptide–protein interaction that may interfere with metabolic processes essential for bacterial survival and biofilm formation. Additionally, protein interaction network analysis indicated the functional importance of the target protein in multiple bacterial pathways, further supporting its relevance as a therapeutic target. Overall, the findings suggest that GC14 may serve as a promising peptide-based therapeutic candidate against *S. mutans*, although further experimental validation through in vitro and in vivo studies is necessary to confirm its antimicrobial efficacy and clinical applicability.

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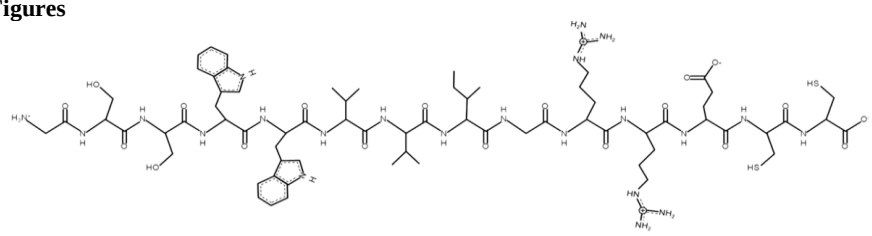
Figures



Peptide Toxicity (ToxinPred)	Non-toxic
Peptide Bioavailability (Peptide ranker)	0.92

Figure 1. Prediction of toxicity and biological activity of the GC14 peptide. In silico analysis of the GC14 peptide showing toxicity prediction using the ToxinPred server and biological activity prediction using the Peptide Ranker tool. The results indicate that the peptide is non-toxic and has a high probability of biological activity, suggesting its potential as a therapeutic antimicrobial peptide.

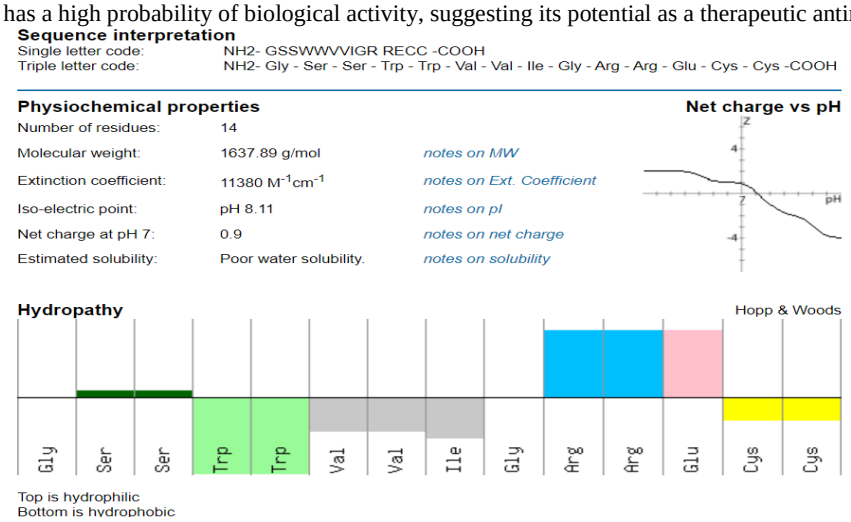


Figure 2. Physicochemical properties of the GC14 peptide. Physicochemical characterization of the GC14 peptide including molecular weight, net charge, hydrophobicity, isoelectric point, and solubility profile. These properties indicate that the peptide possesses characteristics typical of antimicrobial peptides and supports its potential interaction with bacterial membranes and proteins.

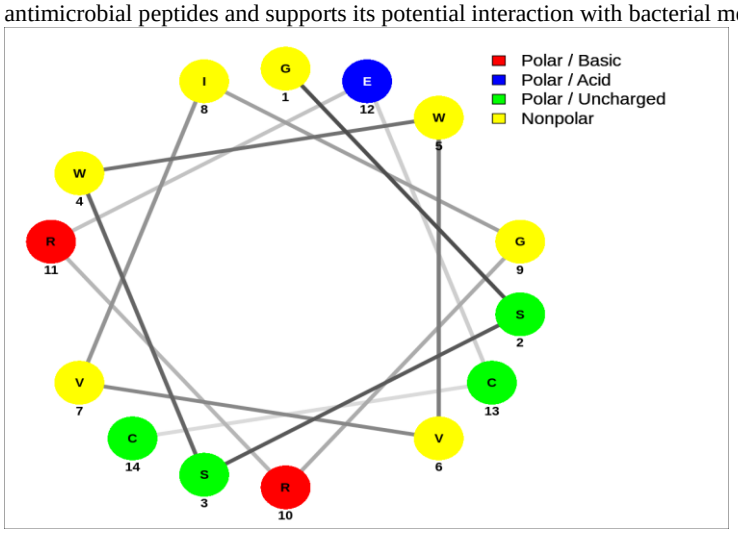


Figure 3. Helical wheel plot of the GC14 peptide. Helical wheel projection showing the spatial distribution of hydrophobic and hydrophilic amino acid residues in the GC14 peptide. The plot demonstrates an amphipathic α-helical structure, which is a characteristic feature of many membrane-active antimicrobial peptides.

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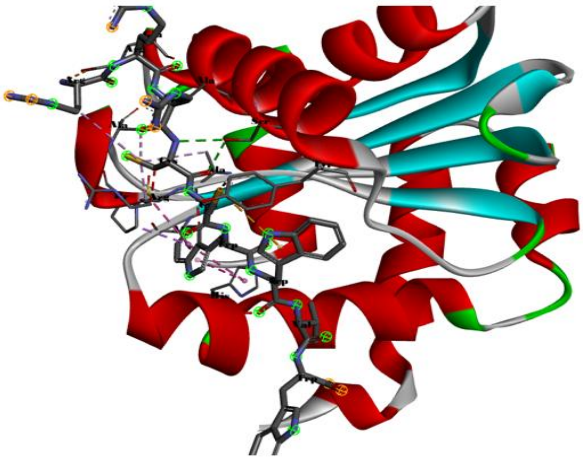

Binding affinity	-177 kcal/mol

Figure 4. **Molecular docking interaction between GC14 peptide and target protein.** Docking model showing the binding interaction between the GC14 peptide and the target protein. The peptide forms a stable complex with the protein through hydrogen bonding, hydrophobic interactions, and electrostatic interactions, indicating strong binding affinity and potential inhibitory activity.

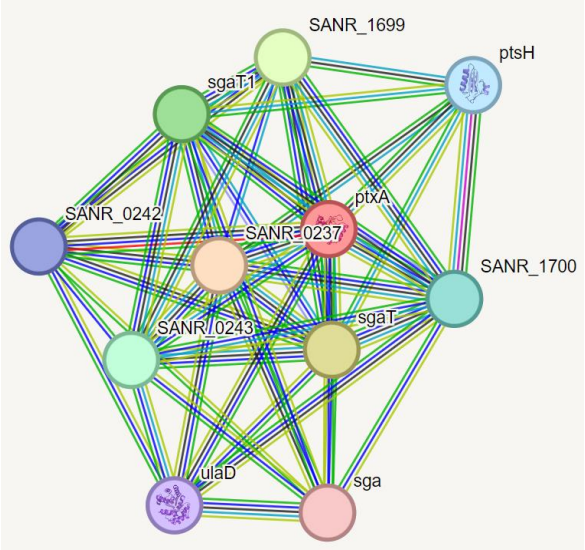

Figure 5. Protein-protein interaction network of the target protein. Protein interaction network generated using the STRING database showing the functional association of the target protein with other proteins involved in bacterial adhesion, virulence, DNA replication, and cellular processes. The network highlights the biological significance of the target protein in bacterial pathogenicity.