IDENTIFICATION OF NOVEL TL 15 PEPTIDE TARGET IN PORPHYROMONAS GINGIVITIS AND PROPOSING INHIBITOR AGAINST HEME-BINDING

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INTRODUCTION:

This study focuses on the identification of a novel TL 15 peptide target in Porphyromonas gingivalis, exploring its potential as a therapeutic target against heme-binding. The aim is to propose an inhibitor that could disrupt this interaction, offering new insights into combating Porphyromonas gingivitis-related pathogenesis.

Porphyromonas gingivalis is a bacterium commonly associated with periodontal diseases, including gingivitis. To identify a novel TL 15 peptide target in Porphyromonas gingivalis and propose an inhibitor against heme-binding, extensive research and experimentation would be required. This involves conducting studies on the bacterium's genetic and proteomic makeup to identify potential targets, such as surface proteins or enzymes involved in heme-binding. Once a potential target is identified, the next step would be to design an inhibitor against heme-binding.By elucidating the role of the TL 15 peptide in Porphyromonas gingivalis and its connection to heme-binding, this research aims to contribute to a deeper understanding of the molecular mechanisms underlying periodontal diseases. The proposed inhibitor against heme-binding holds promise for developing targeted therapeutic strategies, potentially advancing treatment options for individuals affected by Porphyromonas gingivitis.

MATERIALS AND METHODS:

1) Toxinored and Peptide Ranker:

Toxinpred is an in silico method, which is developed to predict and design toxic/non-toxic peptides and PeptideRanker I server or the prediction o bioactive peptides

2) Peptide characteristics: structural characterisation of peptides is done

3) Helical wheel diagram: Helical wheels are a standard way to predict protein sequence segments with either helical or non-helical potential.

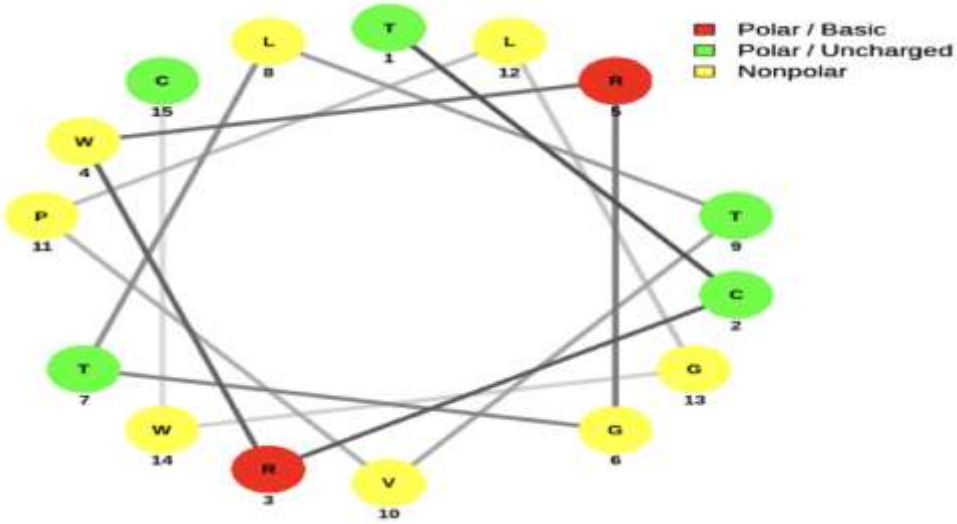
4) Peptide Protein Docking: Peptide docking is to treat the protein and the peptide input conformations as rigid and to perform exhaustive rigid-body docking

5) 5)Zebrafish larvae toxicity: Zebrafish can be used to assess the toxicity of drug candidates in early screening assays, sometimes in a high-throughput manner. Due to their small size and transparency, such tests require a small mass of test article, very little lab space.

and data can be collected non-invasively over time invivo

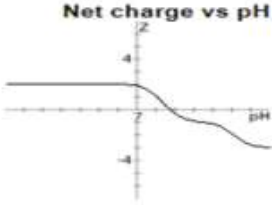
RESULTS:

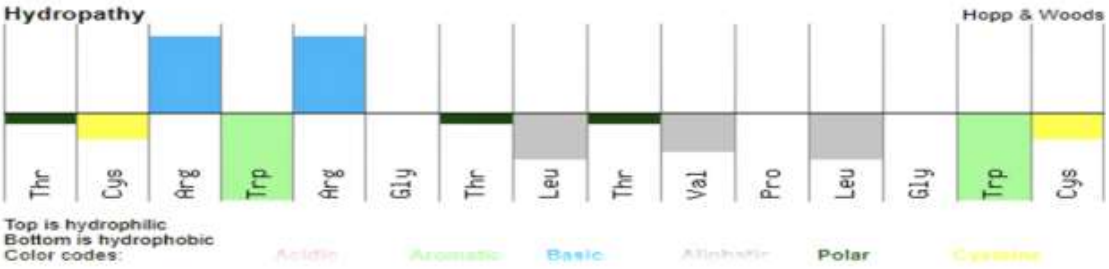
Peptide Bioavailability (Peptide ranker)	0.79

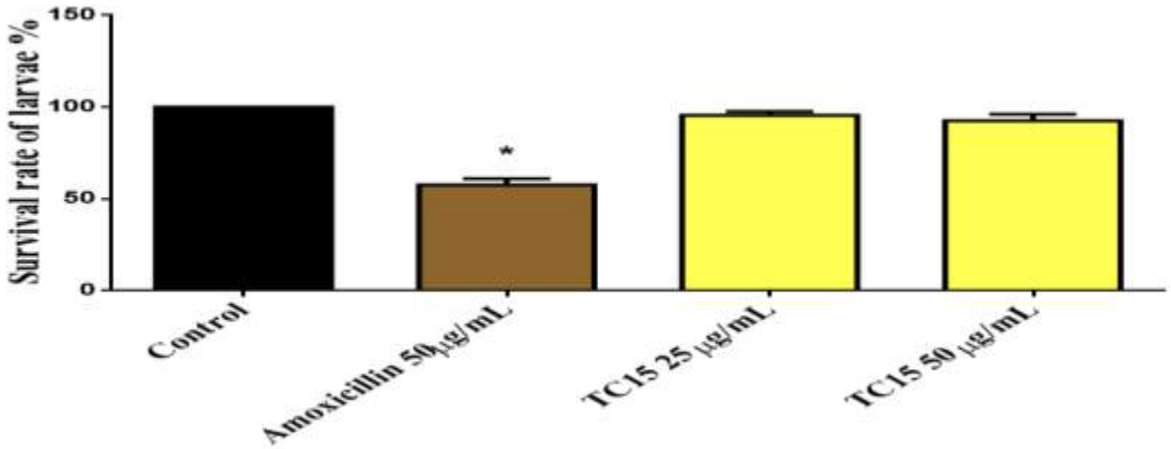


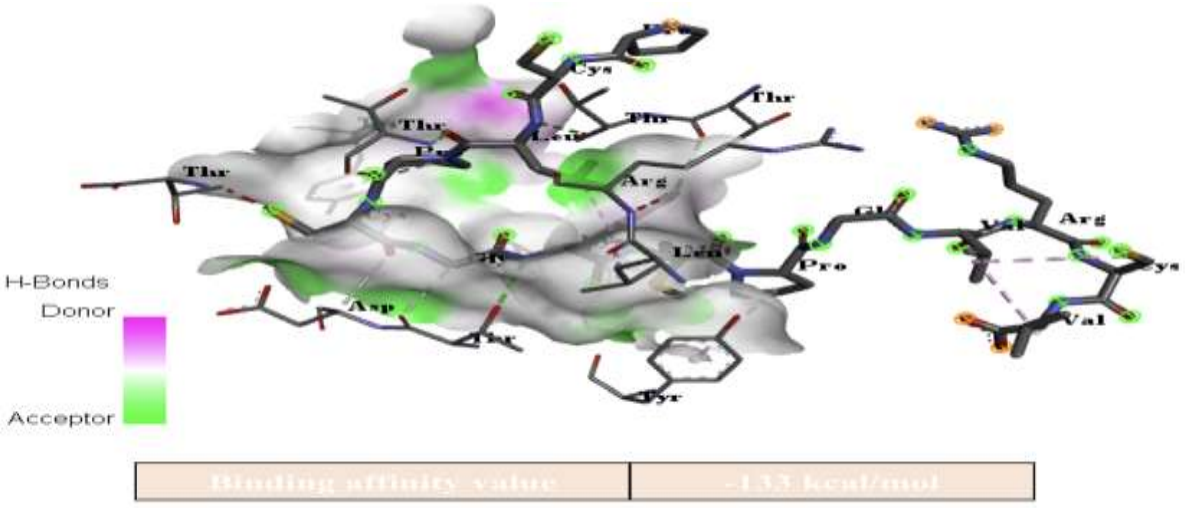
Physiochemical properties

Number of residues:	15
Molecular weight:	1749.07 g/mol
Extinction coefficient:	11380 $M^{-1}cm^{-1}$
Iso-electric point:	pH 8.76
Net charge at pH 7:	1.9
Estimated solubility:	Poor water solubility.









Binding affinity value	-13.3 kcal/mol

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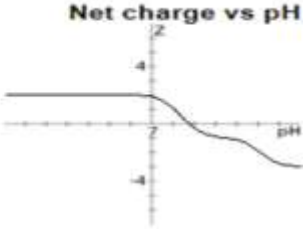
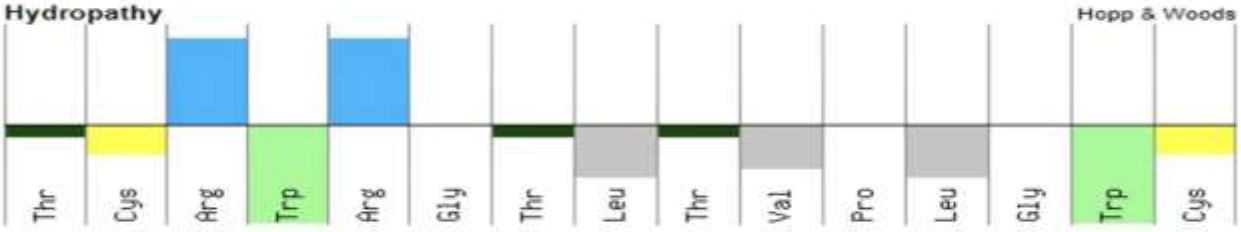
Net charge vs pH



Hydropathy

Hopp & Woods



Top is hydrophilic
Bottom is hydrophobic
Color codes: Acidic Aromatic Basic Aliphatic Polar Cysteine

DISCUSSION:

The development of a targeted inhibitor against heme-binding in Porphyromonas gingivalis has the potential to provide a novel therapeutic strategy for treating gingivitis and preventing the progression to more severe periodontal diseases. However, it's worth noting that the process of identifying a specific target and designing an effective inhibitor can be challenging and time-consuming. Extensive research, collaboration, and validation studies are necessary to ensure the success of such a project.it's crucial to analyze the findings and their implications. The identification of the TL 15 peptide as a potential target in Porphyromonas gingivalis presents an opportunity to delve into its significance in the context of periodontal diseases.The interaction between TL 15 and heme-binding becomes a focal point, as disrupting this interaction could have therapeutic benefits. Assessing the feasibility and specificity of the proposed inhibitor is essential, considering potential challenges and the broader landscape of antimicrobial strategies.Furthermore, discussing the translational aspects of the research, such as the applicability of the identified target and inhibitor in clinical settings, strengthens the practical implications of the study. Addressing any limitations, suggesting future directions for research, and emphasizing the broader impact on oral health contribute to a comprehensive discussion.

CONCLUSION: Successful development of an inhibitor against heme-binding in Porphyromonas gingivalis could have significant implications for the treatment and prevention of gingivitis and related periodontal diseases. However, it is important to recognise that this process is time-consuming, requiring expertise in molecular biology, biochemistry, and drug discovery.this study underscores the significance of the TL 15 peptide as a potential therapeutic target in Porphyromonas gingivalis-associated pathogenesis. The identified interaction with heme-binding presents a novel avenue for intervention in periodontal diseases.The proposed inhibitor against heme-binding demonstrates promise, although further investigations are warranted to optimize its efficacy and safety. This research contributes to the growing body of knowledge surrounding molecular mechanisms in periodontal diseases and lays the foundation for future studies aimed at developing targeted therapies.Ultimately, the findings presented here open new possibilities for advancing treatment strategies against Porphyromonas gingivitis, emphasizing the potential impact on oral health and offering avenues for continued exploration in the field.