In Silico Evaluation of natural bioactive compounds targeting against RgpB of *Porphyromonas gingivalis*

Chandni Krishnan *, Rohit Ruhal

School of Bio Sciences and Technology, Vellore Institute of Technology, Vellore, 632014, Tamil Nadu, India

*Presenter email: chandni.krishnan2022@vitstudent.ac.in

Corresponding author email: rohit.r@vit.ac.in

Abstract

Oral health issues are a global concern. Dysbiosis in the healthy oral microbiome can lead to a variety of diseases, both acute and chronic. Among these are dental caries, periodontitis, and gingivitis. *Porphyromonas gingivalis*, a black-pigmented oral anaerobe found in subgingival plaque, is responsible for chronic periodontitis. This bacterium damages the tooth supporting tissues during the acute phase and these can cause systemic diseases as well. The use of bioactive compounds derived from plants for oral disease prevention is becoming increasingly common. The primary objective is to investigate these bioactive compounds as potential inhibitors of Arg-specific cysteine proteinase gingipain R (RGPB), a virulent protein unique to *Porphyromonas gingivalis*. *Rosmarinus officinalis* is chosen as it contains a wide variety of bioactive chemicals that target several oral disease pathways. It's a promising natural agent for oral health. Its polyphenols exhibit potent antibacterial, anti-inflammatory, and antioxidant qualities, especially rosmarinic acid, carnosic acid etc... These substances aid in the prevention of gingival inflammation, the reduction of oxidative stress, and the inhibition of harmful bacteria that are primary causes of dental caries and periodontitis, The screening is done for 30 compounds. Moreover, molecular docking studies, along with ADMET assessments, drug likeliness evaluations, and analyses of bioavailability properties, were conducted, revealing that the optimal binding affinity score of -9.2 for a phenolic diterpene compound and further this compound was subsequently subjected to a molecular dynamic simulation lasting 100 nanoseconds, demonstrating a strong inhibitory potential that could mitigate disease progression and be incorporated into oral hygiene products such as mouthwashes or toothpaste. Future research should focus on experimental validation and formulation strategies to facilitate its application in infection control.

Keywords: Oral illness; Periodontal diseases; *Porphyromonas gingivalis*, RgpB protein