

Antibiofilm activity of Phytochemicals against of *Staphylococcus aureus* Biofilm forming Protein - *In silico* study

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Abstract

Biofilms are the syntrophic consortia of microbial sessile colonies that remain adhered to the biotic and abiotic surface with the help of self-secreted polymeric substances known as extracellular polymeric substances (EPS). The biofilms developed by the group of Gram-positive bacteria help them to survive within extremes of environmental conditions. This paper, *in-silico* studies were performed on biofilm forming proteins to study the role of various phytochemicals in eradication of biofilm formation by *Staphylococcus aureus*. It was observed that nimbin showed maximum interaction with the biofilm forming proteins of *S. aureus*.

Keywords: Biofilm, *S. aureus*, phytochemicals, molecular interaction, antibiofilm

1. Introduction

Biofilms are formed by the adherent group of sessile communities of micro-organisms those remain embedded by a matrix of extracellular polymeric substance (EPS). The adherent cells stick to biotic and abiotic surfaces with the help of extracellular polymeric substances (1). The EPS not only provides nourishment to the developing sessile cells but also prevents the penetration of drugs resulting in the development of multi-drug or antimicrobial resistance (2). *Staphylococcus aureus* is Gram-positive, potent nosocomial and biofilm forming microbial species that possesses the ability to adhere on both biotic and abiotic surfaces and result in the development of potent nosocomial infections (3,4). This has resulted in the development of alternative therapeutics for the purpose of preventing the biofilm associated chronic infections (5). This work emphasizes on the use of

alternative therapeutics comprising of phytochemicals in treating biofilm associated chronic infections by *S. aureus*.

2. Materials and methods

2.1. Docking

Docking has been done between the bioactive compounds against the biofilm forming protein of *S. aureus* using AutoDock Vina (6). The interaction between the proteins has been checked.

3. Results and Discussion

The molecular docking interactions showed that nimbin showed maximum inhibition of the biofilm forming protein of *S. aureus* in comparison to other phytochemicals that interacted with the protein. (Table 1, Figure 1).

Table 1: Binding energy of the molecular docking interaction between the biofilm forming protein and phytochemicals

Organism	Biofilm forming protein	Phytochemical	Binding Energy (Kcal/mole)
<i>Staphylococcus aureus</i>	3TIP	Curcumin	-6.00
		Eugenol	-4.09
		Quercetin	-5.75
		Nimbin	-6.26
		Gingerol	-5.62

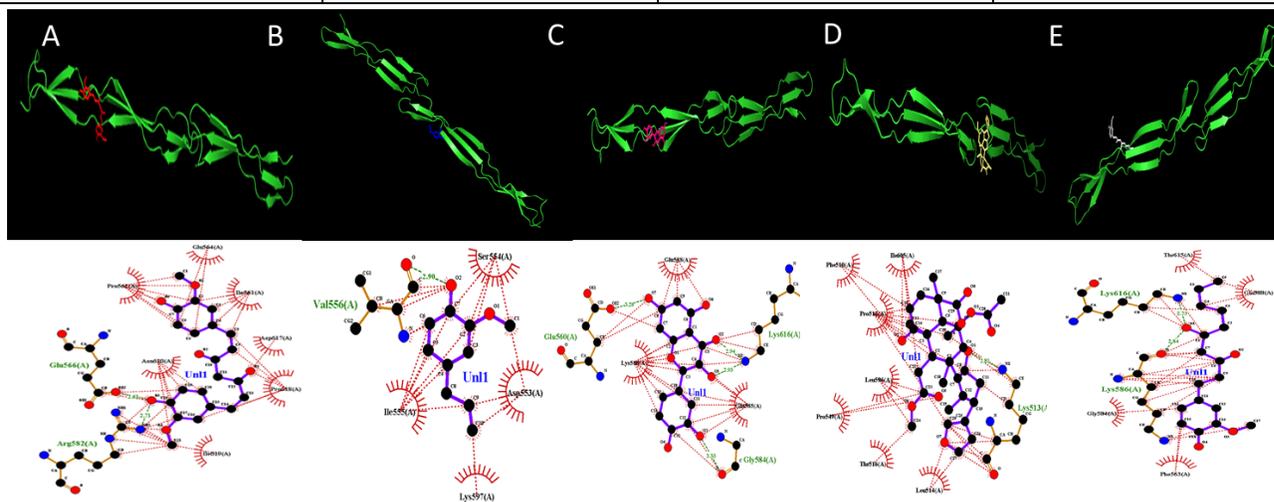


Figure 1: Molecular docking interaction of the biofilm forming proteins of *S. aureus* with the phytochemicals.

4. Conclusion

The study showed nimbin showed maximum interaction with the biofilm forming proteins of *S. aureus*. This depicts that phytocompounds can be used as alternate therapeutics in the inhibition of the biofilm formed by major organisms.

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