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In-Silico Evaluation Of Anti-Acne Property Of *Syzygium (S.) Aromaticum*

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ABSTRACT

Acne vulgaris is a common inflammatory skin diseases seen in all age types, caused by the bacteria *Propionibacterium acnes*. *Syzygium (S.) aromaticum* (clove) is an aromatic plant with rich volatile compounds and antioxidants showing high antimicrobial properties mainly anti-acne property. In recent years, computational databases and methods have been shown to be an invaluable resource for research in the field of dermatology and skin health. The structural diversity of plant-derived phytochemicals with antiacne properties against receptor bacterial proteins involved in acne signaling pathways is facilitated by molecular docking studies. The present study reports the protein-ligand interaction of *P. acnes* bacterial protein and several phytochemicals present in *S. aromaticum* which acts as ligands. Thus the authors have made an effort to evaluate the anti-acne properties various phytochemicals against the

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predominant proteins of bacteria, *P. acnes.* Among the selected phytochemicals, Dillapiol showed the highest binding affinity with most number of Hydrogen bonds.

Key words: *Propionibacterium acnes, Syzygium (S.) aromaticum,* anti-acne, dermatology, molecular docking

1. Introduction

Acne vulgaris, often known as acne, is a chronic inflammatory and recurring skin disorder that affects 10% of people worldwide. It is a disease of the pilosebaceous unit and is astoundingly the ninth most frequent disease in the world. The condition has a complex origin, is initially brought on during adrenarche in susceptible people, and can have modest to quite severe symptoms [1]. Additionally, the illness might persist or manifest itself for the first time in adulthood for an increasing number of people, particularly females. Acne may have substantial social and psychological repercussions, even if it is not life-threatening. These effects are typically more noticeable when the condition is severe and scarring develops [2].

According to conventional knowledge, there are four primary processes that lead to the development of acne within a follicle: androgen-induced hyperseborrhea, follicular hypercornification, colonization and proliferation of Propionibacterium acnes, and induction of a local innate immune response. Following these modifications, a normal follicle or pore develops into a microcomedo, an uninflamed (open and closed comedones), and an inflamed lesion that is undetectable and subclinical (papule, pustule, or nodule) [3, 4].

In order to prove a causal impact, Koch's postulates cannot be met because P. acnes is a normal component of the human microbiota. Thus, circumstantial evidence for a role in the aetiology of inflammatory acne is mostly based on the finding that antimicrobial therapies are effective for the relief of symptoms [5, 6, 7]. The claim that the benefits of antibiotics are primarily attributable to their anti-inflammatory action is also refuted by the fact that non-response to antibiotic therapy is frequently associated with the development of antibiotic-resistant strains. Furthermore, it has been demonstrated that individuals with severe types of acne have greater antibody titres to the bacteria than do individuals in healthy controls.

Syzygium (S.) aromaticum, also known as clove, is a dried flower bud from the Myrtaceae family that was once only grown on the Maluku islands in Indonesia. However, in recent years, it has grown all over the world [8]. The antibacterial, antiviral, anticarcinogenic, and antifungal properties of a few fragrant herbs, such as cinnamon, oregano, clove, thyme, and mint, have been well-documented in several papers [9]. But due to its strong antibacterial and antioxidant properties, clove has drawn a lot of interest from cooks. Due to the presence of several chemical ingredients in high quantities that have antioxidant action, clove is believed to be useful in preventing a variety of degenerative disorders [10, 11]. According to pharmacological research, the primary source of phenolic molecules like hydroxybenzoic acids, flavonoids, hydroxyphenyl propene, hydroxycinnamic acids, and eugenol

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(C10H12O2)—the main bioactive molecule—as well as gallic acid derivatives like hydrolyzable tannins, which are present in significant amounts in the fresh plant—is clove. The flavonoids quercetin and kaempferol, as well as phenolic acids such ferulic, caffeic, ellagic, and salicylic acids, are also present in clove [12]. Eugenol, eugenol acetate, and -cariofileno make up the up to 18% of essential oil found in clove flower buds. The taste and aroma of cloves may be detected in clove oil, which is colourless or pale yellow. The variations in CEO composition and content are primarily influenced by pre-treatments, variety, agro-ecological conditions, and extraction techniques [13].

2. Materials and methods

2.1.Protein preparation

The RCSB Protein Data Bank was used to retrieve the three-dimensional crystal structures of the target protein, Propionibacterium acnes surface sialidase with PDB ID 7LBU, which is implicated in a number of antimicrobial pathways [14]. The data bank's 7LBU structure had a resolution of 2.11 Å. Before the molecular docking study, all of the water molecules and pre-existing molecules that were already bound to the proteins were removed. PyRx 0.8 virtual screening software was used to clean the target proteins structures, limit energy consumption, compute Gasteiger charges, and add polar hydrogen.

2.2.Protein binding site prediction

The GalaxyWEB server, which offers surface pockets and inner cavities of the provided protein PDB file, was used to retrieve the proteins potential binding sites [15]. The binding pockets' volume and surface area are also measured by this service. The docking program selects and specifies the residues that are highlighted in the sequence of the chosen pocket.

2.3.Ligand optimization

The 3D structure of the screened phyto constituents were obtained and downloaded as PDB file from the IMPPAT: Indian Medicinal Plants, Phytochemistry and Therapeutics database.

2.4.Molecular Docking

Based on binding free energies, binding affinity, and compounds with significant hydrophobic interactions and hydrogen bonds, molecular docking approach was used to evaluate which plant molecule interacted with the chosen microbial target the best. The phyto-compounds that target the bacterial proteins were molecularly docked using PyRx 0.8 software. The chosen binding residues of the protein, to which the ligands were docked, were surrounded by a grid box [16]. Nine docked poses of each ligand to the active site of the cancer target protein were created, and they were then ordered in descending order according to their negative binding energy values. The BIOVIA discovery studio visualizer tool was used to examine these compounds in further detail.

3. Results

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3.1.Protein preparation

The *Propionibacterium acnes* bacterial protein with PDB ID 7LBU was visualized using UCSF Chimera, a visualization software and is represented in the Figure.

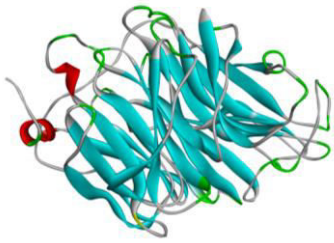
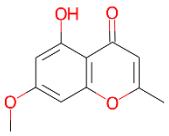
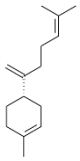
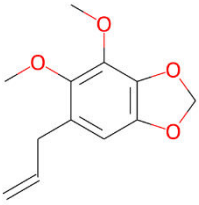
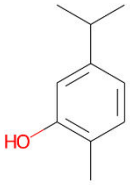


Figure1: Crystal structure of the Propionibacterium acnes surface sialidase

3.2.Ligand Optimization

Table1. The structure of the screened phytoconstituents

IMPPAT Phytochemical identifier	Phytochemical name	Structure
IMPHY000239	Eugenin	
IMPHY000399	beta-Bisabolene	
IMPHY001144	Dillapiol	
IMPHY001246	Carvacrol	

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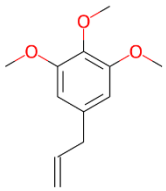
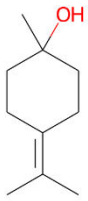
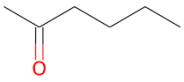
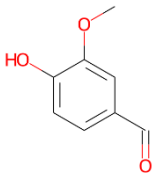
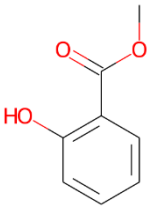
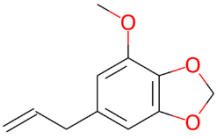
IMPHY001351	Elemicin	
IMPHY001816	gamma-Terpineol	
IMPHY001861	2-Hexanone	
IMPHY001931	Vanillin	
IMPHY003050	Methyl salicylate	
IMPHY003398	Myristicin	

3.3.Protein binding site prediction

The binding pocket residues of the protein which is responsible for the protein-ligand interaction were obtained using GalaxyWEB. The obtained residues were 121R, 122I, 140R, 185D, 209F, 257F, 312D, 313E, 329R, 395R and 423Y.

3.4.Analyzing Molecular Docking interactions

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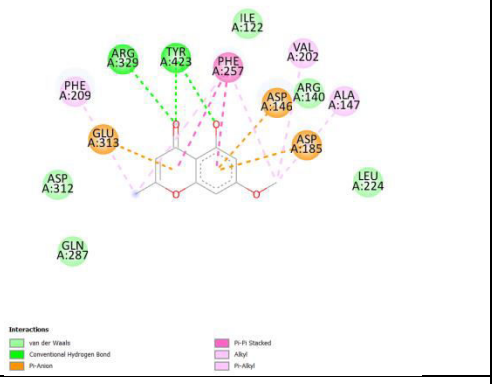
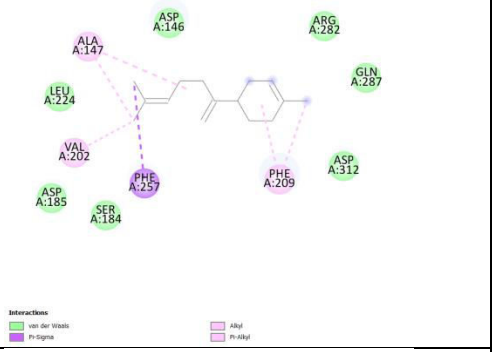
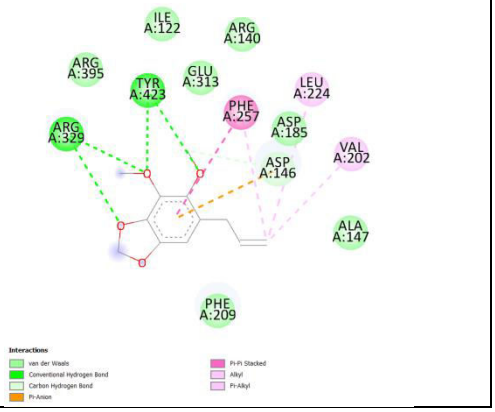
Table2. The 2D interactions between 7LBU with all the ligands analyzed using BIOVIA discovery studio visualizer

Protein ID	Plant name	Ligand name	Binding affinity	No. of H-bonds	Structure of interactions
7LBU	*Syzygium aromaticum*	Eugenin	-6.6	3	
		beta-Bisabolene	-6.4	0	
		Dillapiol	-6.4	4	

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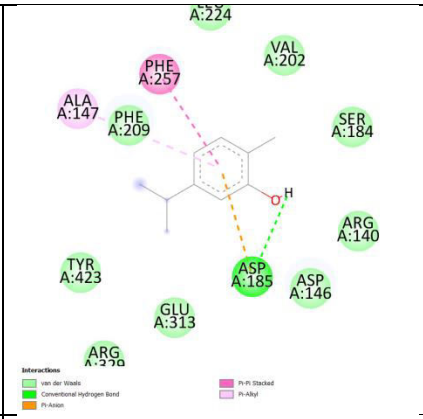
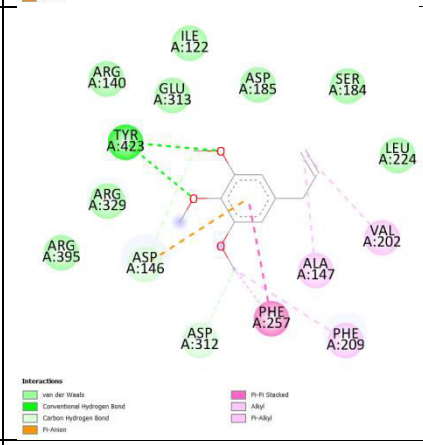
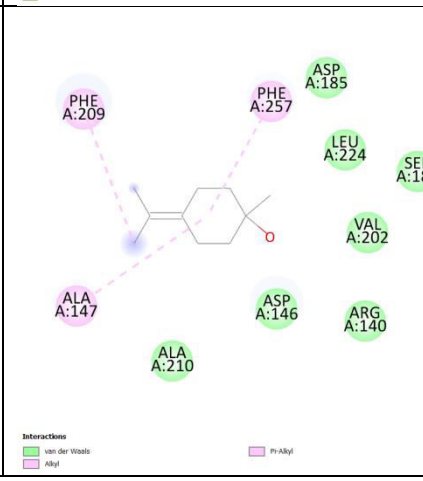
		Carvacrol	-6.5	1	
		Elemicin	-6.2	2	
		gamma-Terpineol	-5.7	0	

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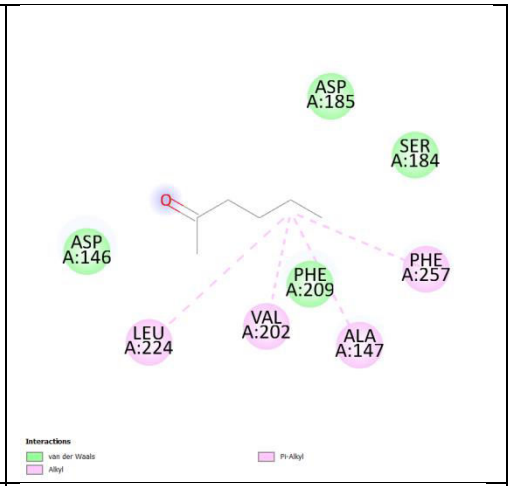
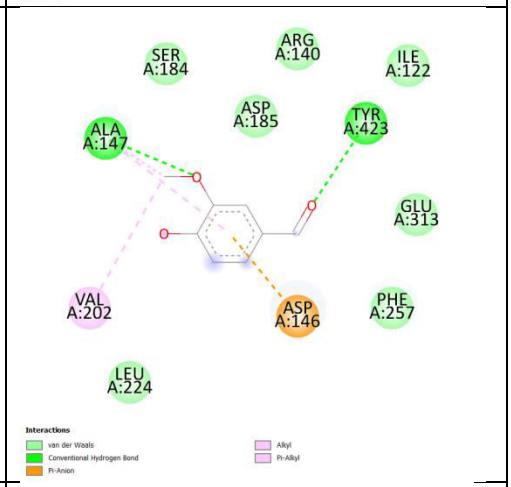
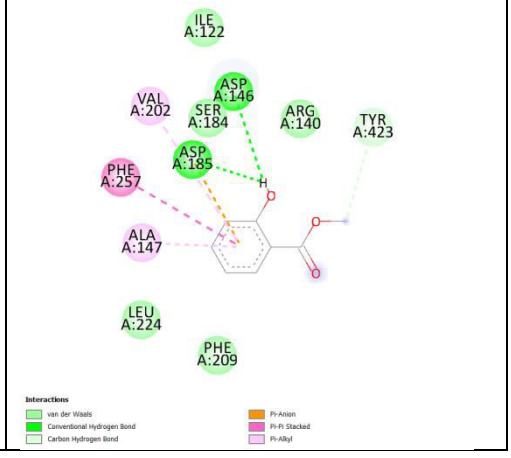
		2-Hexanone	-4.0	0	
		Vanillin	-5.2	2	
		Methyl salicylate	-6.0	2	

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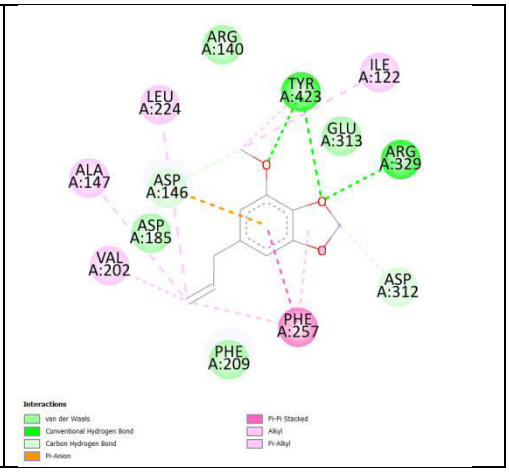
		Myristicin	-6.4	3	

Here we analyzed the interaction between 7LBU protein and selected phytochemicals. Dillapiol has 4 hydrogen bonds with ARG 329 and TYR 423 binding residues. Its exhibits a binding affinity of -6.4 kcal/mol. Eugenin has the 3 hydrogen bonds with ARG 329 and TYR 423 binding residues and its exhibits a binding affinity of -6.6 kcal/mol. Carvacrol has 1 hydrogen bond with ASP 185 binding residues and exhibits a binding affinity of -6.5 kcal/mol. Elemicin has 2 hydrogen bonds with TYR 423 binding residues and its exhibits a binding affinity of -6.2 kcal/mol. vanillin has 2 hydrogen bonds with ALA 147 and TYR 423 binding residues and its exhibits -5.2 kcal/mol binding affinity. Methyl salicylate has 2 hydrogen bonds TYR 423 and ARG 329. It's have a binding affinity of -6.4 kcal/mol.

4. Conclusion

This study was carried out to analyze the anti-acne properties of *Syzygium (S.) aromaticum*. Based on the molecular docking studies some phytochemical compounds have good interaction with the targeted protein. In comparison, to other ligands, the Dillapiol showed 4 hydrogen interactions with a binding affinity of -6.4 kcal/mol. Thus, Dillapiol shows good anti-microbial and anti-acne properties.

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