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Original Article

Anti-Bacterial Attributes of Phytochemicals from *Bougainvillaea spectabilis*: Computational Approach

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ABSTRACT

Background: The escalating issue of antibiotic resistance has spurred research into alternative antimicrobial agents, including phytochemicals from various plant sources. *Bougainvillaea spectabilis*, a plant renowned for its medicinal properties, is attracting attention for its potential antibacterial attributes. **Materials and Methods:** This study employs a computational approach to investigate the antibacterial potential of *B. spectabilis* phytochemical compounds derived from OSADHI and IMPPAT databases. Using advanced computational tools, we systematically screened and analyzed the phytochemical constituents of *B. spectabilis* for their ability to inhibit bacterial growth. An effective drug like phytochemicals screened by SwissADME and its target was identified. The molecular structure of quercetin was subjected to virtual docking experiments with bacterial target protein, single strand DNA binding protein. The binding affinity and interaction were assessed to predict the likelihood of antibacterial activity. To predict the possibility of antibacterial activity, the binding affinity and interaction were evaluated. **Results:** Several phytochemicals with antibacterial properties were discovered in our study. The binding affinity of quercetin was -6.81 kcal/mol, and it performs critical roles in bacterial growth and survival. This computational analysis sheds light on the possible antibacterial effects of phytochemicals derived from *B. spectabilis*. The results demonstrated additional experimental validation as well as the synthesis of novel antibacterial agents obtained from natural sources. **Conclusion:** This research contributes to ongoing efforts to prevent antibiotic resistance and lays the path for the identification of novel therapeutic alternatives to address bacterial infections by leveraging the power of computational tools.

Keywords: *Bougainvillaea spectabilis*, Phytochemical, Antibacterial activity, Quercetin, Single-stranded DNA binding protein.

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INTRODUCTION

The emergence and persistence of antibiotic-resistant bacterial strains have escalated into a global healthcare crisis, necessitating a concerted search for innovative antimicrobial strategies. Exploration of phytochemicals produced from various plant sources, which have shown potential as alternative agents to treat bacterial infections, is one intriguing area.[1] These naturally occurring chemicals contain a diverse spectrum of biological functions, including antibacterial characteristics, and have attracted the interest of researchers looking for new therapeutic possibilities.[2,3] *Bougainvillaea spectabilis*, a plant revered for its medicinal properties in ancient systems of medicine, has emerged as a prominent contender in the search for effective antibacterial drugs.

Bougainvillaea, a member of the Nyctaginaceae family, contains several species noted for their traditional medicinal purposes.[4] *B. spectabilis*, sometimes known as "paper flower," has drawn the curiosity of researchers due to its demonstrated therapeutic potential. The plant has historically been used to treat a variety of diseases, emphasising its medicinal value.[5,6] However, recent focus has shifted to using its phytochemical ingredients to treat bacterial infections. Computational strategies, like traditional approaches, have emerged as critical instruments in modern drug development efforts. *In silico* approaches predict the interactions between bioactive chemicals and their target proteins in a timely and cost-effective manner, allowing for a streamlined initial assessment of their potential biological activities.[7] A significant outcome of such computational studies is the sensible selection of candidate compounds for further experimental validation.[8,9]

The current study takes advantage of these synergistic features by using a computational approach to investigate the antibacterial potential of phytochemicals isolated from *B. spectabilis*. In particular, goes beyond empirical research to systematically screen and analyse the inhibitory effects of these phytochemicals

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on bacterial growth. The chemicals chosen are drawn from the biological databases, which contain a wide range of possible bioactive substances. The molecular interactions between these phytochemicals and bacterial target proteins using modern computational methods. The choice of a representative phytochemical, quercetin, serves as the focus point for virtual docking experiments with an important bacterial protein, the single-strand DNA binding protein.[10] The binding affinities and interaction kinetics are evaluated, revealing putative mechanisms causing antibacterial actions.

In a broader context, this study not only adds to the ongoing fight against antibiotic resistance but also shows the convergence of computational techniques and classical pharmacology. The collaboration of these disciplines has the potential to speed the identification of effective medication candidates while also expanding our understanding of the intricate molecular processes that drive antibacterial action. As a result, this research serves as a stepping stone towards the development of novel therapeutic alternatives for bacterial infections, thereby minimising the impending threat posed by antibiotic resistance.

MATERIALS AND METHODS

Collection and drug-likeness of phytocompounds

The Online Structural and Analytics-based Database for Herbs of India (OSADHI)[11] and Indian Medicinal Plants, Phytochemistry And Therapeutics 2.0 (IMPPAT)[12] databases were searched for bioactive phytochemicals derived from *B. spectabilis*. The database was built using detailed features such as canonical smiles, molecular weight, molecular formula, number of donors and acceptors for hydrogen bonds, and logP values of selected phytocompounds acquired from the PubChem Chemical compounds database. On the SwissADME (http://www.swissadme.ch/), the drug similarity score of phytocompounds was predicted using "Lipinski's rule of five model".[13]

Target identification

The canonical smiles of the selected phytochemicals were entered with a probability score of >0.4 into the AntiBacPred database, "a public, online-accessible, and experimentally determined antibacterial activity database," to find phytocompounds targeting antibacterial activity.[14]

Homology modelling, validation, and active site determination

In the current investigation, bio-actives putative phytocompound, namely Quercetin (IMPHY004619) 3D structure derived from IMPPAT. The X-ray crystal structure Single-Stranded DNA-Binding Protein (PDB ID: 6BHW) was obtained from the RCSB Protein Data Bank (https://www.rcsb.org/).

Docking studies

Molecular docking is a computational approach that may be used to build the interaction between phytochemicals and target proteins at an atomic level, followed by predicting the best confirmation that fits the protein binding site. AutoDock vina was used to do molecular docking investigations with possible targets.[15] The compounds were created utilising POAP and 5000 minimization steps with the MMF94 force field. AutoDock Tools was used to assign grid boxes based on the active sites of the target proteins. The exhaustiveness of the molecular docking method was set to 50. Higher exhaustiveness improves accuracy by increasing the number of steps in the search for an ideal docked position with the lowest binding energy.

RESULTS

Selection of phytocompounds

From the OSADHI and IMPPAT databases, 42 bioactive phytocompounds from *B. spectabilis* were identified (Table 1). These phytoconstituents were identified as alkaloid, terpene, and steroid compounds. The effective 9 molecules were selected based on the SWISS-ADME analysis, these showed good Estimated SOLubility (ESOL) Class, Silicos-IT Class, Blood-Brain Barrier (BBB), and Gastrointestinal (GI) absorption rank.

Target identification and their drug-likeness

The names of potential targets' microorganisms were found in the AntiBacPred database. We isolated nine candidate *B. spectabilis* pharmaceuticals (Table 2) that were projected to target thirty bacterial organisms (Table 3). Herbal medication is normally administered orally, where it is digested, distributed, metabolised, and ejected to the intended organ or tissue based on ADME analysis (Figure 1). As probable active phyto components for binding, phytocompounds that satisfy the demand were chosen. Similarly, surface proteins and enzymes were the most commonly targeted antibacterial protein compounds. The total drug-like properties of the proposed phytocompounds. Among them, quercetin (Figure 2a) is thought to influence single-stranded DNA-binding protein (Figure 2b) expression. But other molecules don't shown interaction with microbial proteins.

Docking research

Molecular docking was used to find the best conformation and study potential ligand interactions at the target protein's active sites, as well as to assess potential inhibitory effects on the target protein. A range of computer-aided drug design approaches have been used to investigate the potential therapeutic molecules derived from medicinal plants. However, molecular docking appears to be a cost-effective method for analysing ligand interactions with specific receptors as well as predicting the orientation of molecules in the binding sites of the chosen protein target. Molecular docking studies were carried out to find

Table 1: List of *B. spectabilis* phytocompounds from OSADHI and IMPPAT databases.

Sl. No.	Phytochemicals	PubChem/ IMPPAT ID	SMILES
OSADHI			
1.	Cis-3-Hexenyl Salicylate	5371102	CC/C=CCCOC(=O)C1CCCCC1O
2.	Dehydroionene	6429341	CC1=C(C(CC=C1)(C)C)/C=C/C=C
3.	Propyl Palmitate	75232	CCCCCCCCCCCCCCCC(=O)OCCC
IMPPAT			
4.	Isophytol	IMPHY000112	C=CC(CCCC(CCCC(CCCC(C)C)C)C)(O)C
5.	Lauric acid	IMPHY003016	CCCCCCCCCCCC(=O)O
6.	Methyl salicylate	IMPHY003050	COC(=O)C1CCCCC1O
7.	alpha-Santalol	IMPHY004049	C/C(=C/CCC1(C2CC3C1(C3C2)C)C)/CO
8.	Verbenone	IMPHY004077	CC1=CC(=O)C2CC1C2(C)C
9.	Methyl linolenate	IMPHY004399	CC/C=CC/C=CC/C=CCCCCCCCC(=O)OC
10.	alpha-Ionone	IMPHY005569	CC(=O)/C=C/C1C(=CCCC1(C)C)C
11.	hydroxy hexanoate	IMPHY006314	CCCC(CC(=O)OCC)O
12.	Hexanal	IMPHY006347	CCCCCC=O
13.	Isobutyric acid	IMPHY006907	CC(C(=O)O)C
14.	Methyl palmitate	IMPHY006971	CCCCCCCCCCCCCCCC(=O)OC
15.	Furfural	IMPHY007041	O=CC1CCCO1
16.	Heptanal	IMPHY007186	CCCCCCC=O
17.	2-Heptadecanone	IMPHY008305	CCCCCCCCCCCCCCCC(=O)C
18.	Butyl acetate	IMPHY008972	CCCCOC(=O)C
19.	Ethyl palmitate	IMPHY009624	CCCCCCCCCCCCCCCC(=O)OCC
20.	Methyl 2-methylbutyrate	IMPHY009863	CCC(C(=O)OC)C
21.	Dihydroedulan II	IMPHY010385	CC1CCC2C(CC=CC2(O1)C)(C)C
22.	Toluene	IMPHY010995	CC1CCCCC1
23.	4-Carvomenthenol	IMPHY011396	CC1=CCC(CC1)(O)C(C)C
24.	Terpinolene	IMPHY011599	CC1=CCC(=C(C)C)CC1
25.	Pulegone	IMPHY011884	C[C@@H]1CCC(=C(C)C)C(=O)C1
26.	(Z)-2-hexenal	IMPHY011976	CCC/C=CC=O
27.	Linalool	IMPHY012058	C=CC(CCC=C(C)C)(O)C
28.	o-Xylene	IMPHY012070	CC1CCCCC1C
29.	Phytol	IMPHY012712	OC/C=C(/CCC[C@@H](CCC[C@@H](CCCC(C)C)C)C)C
30.	2-Furanmethanol, 5-ethenyltetrahydro-alpha, alpha, 5-trimethyl-, cis-	IMPHY012920	C=C[C@@]1(C)CC[C@H](O1)C(O)(C)C
31.	Carvomenthone	IMPHY013764	CC1CCC(CC1=O)C(C)C
32.	Aromadendrene	IMPHY014817	CC1CCC2C1C1C(C1(C)C)CCC2=C
33.	alpha-Copaene	IMPHY015123	CC1=CCC2C3C1C2(CCC3C(C)C)C
34.	cis-3-Hexenyl salicylate	IMPHY015566	CC/C=CCCOC(=O)C1CCCCC1O
35.	Dehydroionene	IMPHY015605	C=C/C=C/C1=C(C)C=CCC1(C)C
36.	Butyl formate	IMPHY015853	CCCCOC=O
37.	Propyl palmitate	IMPHY016832	CCCCCCCCCCCCCCCC(=O)OCCC

Sl. No.	Phytochemicals	PubChem/ IMPPAT ID	SMILES
38.	Quercetin	IMPHY004619	OC1CC(O)C2C(C1)OC(C(C2=O)O)C1CCC(C(C1)O)O
39.	Isorhamnetin	IMPHY008724	COC1CC(CCC1O)C1OC2CC(O)CC(C2C(=O)C1O)O
40.	D-Pinitol	IMPHY015039	COC1[C@H](O)[C@@H](O)C([C@@H]([C@@H]1O)O)O
41.	Flavylium	IMPHY002588	C1CCC(CC1)C1CCC2C([O+]1)CCCC2
42.	o-Dihydroxyphenol	IMPHY005691	OC1C=CC=CC1(O)O

Table 2: List of selected effective phytocompounds with their ADME.

Compound name	Phytochemicals	ESOL Class	Silicos-IT class	BBB permeant	GI absorption
Molecular 1	Phytol	Very soluble	Soluble	Yes	High
Molecular 2	2-Furanmethanol, 5-ethenyltetrahydro-alpha,alpha,5-trimethyl-, cis-	Very soluble	Soluble	Yes	High
Molecular 3	Carvomenthone	Very soluble	Soluble	Yes	High
Molecular 4	Aromadendrene	Very soluble	Soluble	Yes	High
Molecular 5	cis-3-Hexenyl salicylate	Very soluble	Soluble	Yes	High
Molecular 6	Dehydroionene	Very soluble	Soluble	Yes	High
Molecular 7	Butyl formate	Very soluble	Soluble	Yes	High
Molecular 8	Propyl palmitate	Very soluble	Soluble	Yes	High
Molecular 9	Quercetin	Very soluble	Soluble	Yes	High

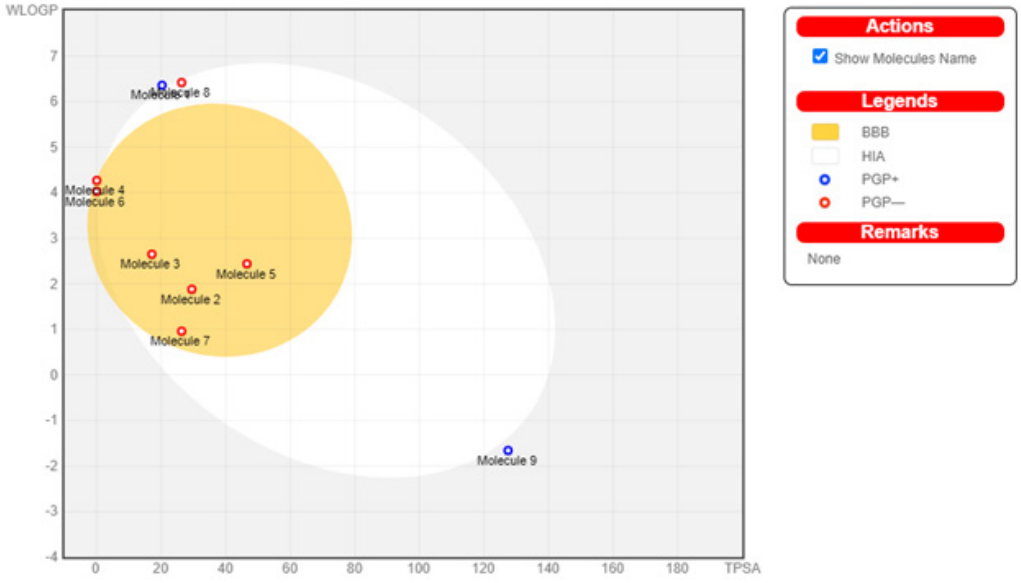

Figure 1: Effective phytocompounds ADME analysis by Boiled Egg method.

the probable binding of *B. spectabilis* compounds with specified therapeutic targets of antibacterial action (Figure 3).

Docking findings were examined for ligand and receptor based on docking energy and contact of each ligand with functional residues of single-stranded DNA-Binding Protein (6BHW). Hydrogen bonding and Van der Waals are the primary interactions found between the ligand and target proteins. Quercetin formed two hydrogen bonds with the amino acid residues ARG55, GLN78 and seven Van der Waals interactions with PHE37, THR53, GLN57, ARG76, GLN96, ALA97, GLU98

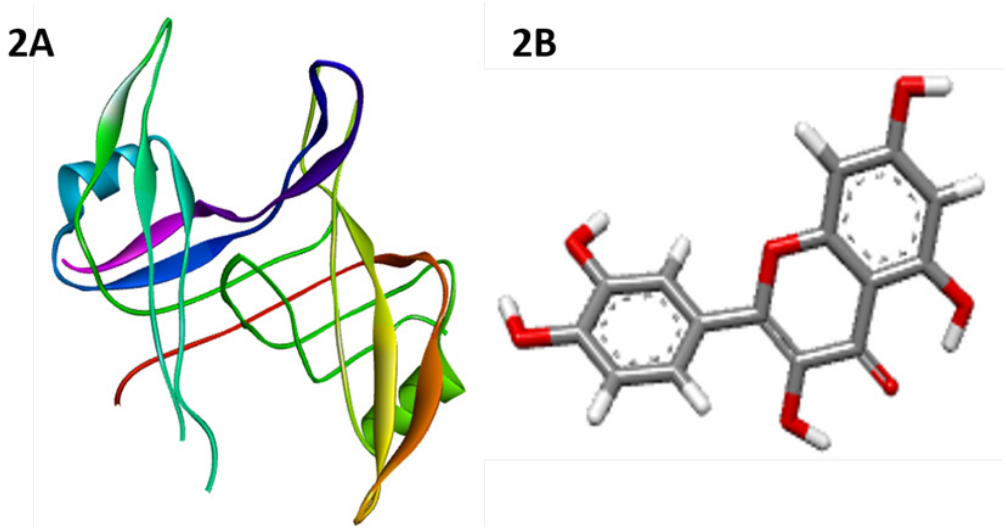

Figure 2: A) Three-dimensional structure of single-stranded DNA-Binding Protein (6BHW) (target) and 2B) quercetin (IMPHY004619) (ligand).

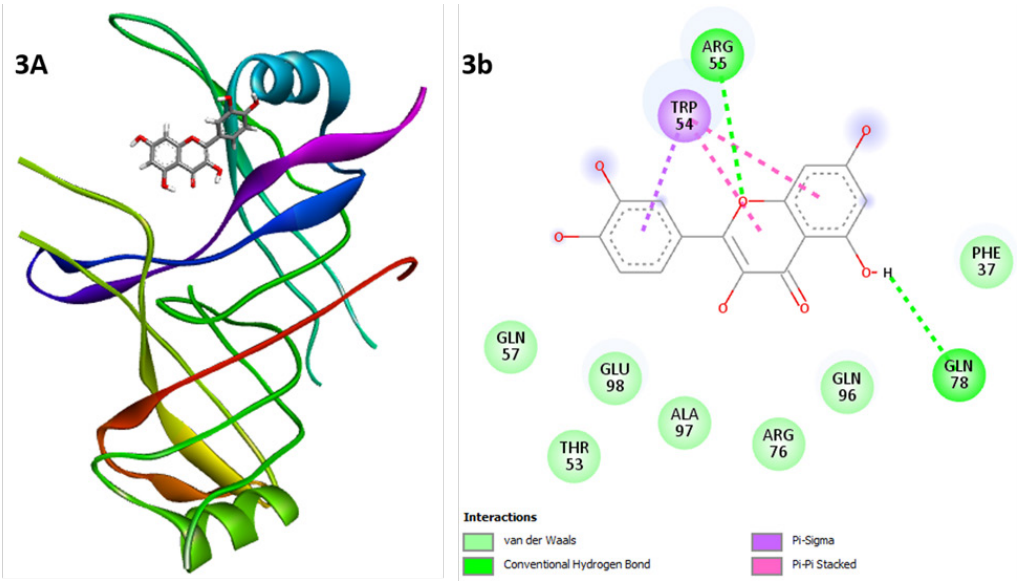

Figure 3: A) The interactions of the drug, quercetin with single-stranded DNA-Binding Protein in three-dimensional structure and B) active site of representation in two-dimensional structure in molecular docking analysis.

with a binding energy of -6.81 kcal/mol. Moreover, Pi-Sigma and Pi-Pi stacked interaction with TRP54.

DISCUSSION

This study, which employs a computational approach to investigate the antibacterial potential of phytochemicals from *B. spectabilis*, addresses several critical aspects. These include the selection of phytochemical candidates, their interactions with bacterial proteins, drug development implications, the significance of computational tools in furthering antibacterial research, and the broader context of antibiotic resistance.[6,16,17] The primary goal of this study is to identify phytochemicals from *B. spectabilis* with identifiable antibacterial activity. The hunt for alternative antimicrobial agents has become critical in the context of the rising antibiotic resistance problems.[18,19] Natural substances, particularly phytochemicals originating from plants, have piqued the interest of researchers due to their potential as novel antibacterial agents.[20] The findings of this study highlight the variety of phytochemicals found in *B. spectabilis* as well as their potential antibacterial properties. This plant's abundance of natural chemicals is a viable resource for fighting bacterial illnesses. The variety of these molecules indicates a wealth of chemical structures, each of which can interact specifically with bacterial proteins.[21]

Understanding the molecular interactions between chosen phytochemicals, such as quercetin, and bacterial target proteins, particularly the single-strand DNA binding protein, is at the centre of this research. The high binding affinity for quercetin

Table 3: Effective phytocompounds antibacterial activity analysed by AntiBac Pred database.

Compound name	Bacterial Name
Molecule 1	*Staphylococcus simulans*
	Acinetobacter pittii
	Mycobacterium bovis BCG
	Klebsiella oxytoca
Molecule 2	*Mycobacterium mageritense*
Molecule 3	*Corynebacterium jeikeium*
	Mycobacterium ulcerans
	Staphylococcus simulans
	Staphylococcus simulans
	Propionibacterium acnes
Molecule 4	*Actinomyces viscosus*
	Streptococcus mutans
	Prevotella melaninogenica
	Prevotella intermedia
	Fusobacterium nucleatum
	Capnocytophaga ochracea
	Porphyromonas gingivalis
Molecule 5	*Staphylococcus lugdunensis*
	Prevotella oralis
	Lactobacillus plantarum
	Clostridium ramosum
	Staphylococcus saprophyticus
	Clostridium cadaveris
Molecule 7	*Klebsiella pneumoniae*
Molecule 8	*Streptococcus viridans*
Molecule 9	*Bacillus subtilis*
	Prevotella oralis
	Staphylococcus lugdunensis
	Lactobacillus plantarum
	Prevotella bivia

(-6.81) indicates a strong interaction, indicating that this phytochemical can interfere with critical processes in bacterial growth and survival. This discovery is consistent with prior research on the antibacterial activities of quercetin. Quercetin has been demonstrated to limit bacterial replication and survival by breaking bacterial cell membranes, blocking DNA gyrase, and interfering with numerous enzymatic processes.[10] As a result, the computational data in this study confirm and strengthen the body of evidence pointing to quercetin as a promising natural antibacterial agent.

The rise of antibiotic-resistant bacterial species has fueled the search for new therapeutic approaches.[22] Phytochemicals with strong antibacterial properties, such as quercetin, provide a ray of light in an otherwise bleak landscape of antibiotic resistance.[10] This study's computer technique accelerates the identification of such potential candidates, expediting the early phases of drug research. Quercetin's high affinity for the single-strand DNA binding protein implies that it could be used as a pioneer molecule in the development of antibacterial medications.[23] It is important to emphasise, however, that these computational discoveries should be confirmed through thorough experimental testing. Such empirical validation is essential for confirming the efficacy and safety of these phytochemicals in therapeutic settings.[24,25] Furthermore, structural modifications and optimisation of quercetin derivatives represent possible routes for improving antibacterial activity while minimising negative effects. Based on computational findings, this technique could lead to the production of more effective and selective antibacterial medicines obtained from natural sources.

CONCLUSION

This study sheds light on the antibacterial activity of phytochemicals derived from *B. spectabilis*. It accelerates the identification of interesting candidates for subsequent drug development efforts by using computational methodologies. This study highlights the synergy between computational and empirical methodologies, paving the door for the development of novel therapeutic options for bacterial infections while minimising the problem of antibiotic resistance.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ABBREVIATIONS

OSADHI: Online Structural and Analytics-based Database for Herbs of India; **IMPPAT:** Indian Medicinal Plants, Phytochemistry and Therapeutics 2.0; **DNA:** Deoxyribonucleic acid; **PDB:** Protein data bank; **ADME:** Absorption, Distribution, Metabolism, and Excretion.

SUMMARY

This research advances beyond phytochemical identification in B. glabra, evaluating 36 compounds for drug development potential. Utilizing predictive models and computational tools, key pharmacokinetic parameters and bioavailability are assessed. N-(1-Deoxy-1-fructosyl) phenylalanine emerges as a promising

antibacterial candidate, substantiated through the AntiBacPred database. This integrative approach optimizes candidate selection, highlighting the potential of natural compounds for therapeutic development, particularly in antibacterial applications.

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