Volume 3, Number 2, 2026 Pages 983-991

Bioscience Insights

ISSN: 3080-3489 (Print)
ISSN: 3080-3497 (Online)

BiosciInsights.com

COMPUTATIONAL SCREENING OF THE BIOACTIVE METABOLITE 2,6-DIMETHOXYPHENOL FROM SALVADORA PERSICA IDENTIFIED BY GC–MS AGAINST DRUG-RESISTANT ESCHERICHIA COLI AND STAPHYLOCOCCUS AUREUS

Abbas Shahid[1*], Bahaaeldin Anwer[2], Muhammad Shahbaz[3], Zinayyera Subhani[4], Tooba Chaudhary[5], Amina Noreen[6]

*[*1]Department of Basic & Applied Chemistry, University of Central Punjab, Lahore, Pakistan.*
[2]Faculty of Pharmacy, Al-Azhar University, Assiut, Egypt.
[3]Institute of Biochemistry & Biotechnology, University of Veterinary and Animal Sciences (UVAS), Lahore, Pakistan.
[4]Research and Development Section, Sarkar Health Care, Sargodha, Pakistan.
[5]Department of Biochemistry, University of Agriculture Faisalabad. Pakistan.
[6]Department of Zoology, University of Agriculture Faisalabad. Pakistan.

[*1]sh.abbas.shahid@gmail.com

https://doi.org/10.5281/zenodo.23119188

Abstract

Background: Antimicrobial resistance has increased the need for new antibacterial candidates from natural sources. Salvadora persica is a medicinal plant with reported antibacterial effects due to its rich phytochemical contents. Methods: Methanolic extract of S. persica was profiled using GC–MS for identification of bioactive metabolites. 2,6-dimethoxyphenol was chosen for computational analysis, based on its occurrence and reported antimicrobial relevance. The three-dimensional structure of the ligands was obtained from PubChem, whereas the DNA gyrase B structures from Escherichia coli (PDB: 1KZN) and Staphylococcus aureus (PDB: 3G7B) were downloaded from the Protein Data Bank. AutoDock Vina software was used for molecular docking and Discovery Studio Visualizer and PyMOL software was used for structural and interaction analysis. Results: GC–MS analysis revealed a number of metabolites, 2,6-dimethoxyphenol (12.6%) being the highest peak. Molecular docking showed good predicted binding of 2,6-dimethoxyphenol to both bacterial DNA gyrase B targets. The binding affinity of the compound was −5.3 kcal/mol for E. coli GyrB (1KZN) and −4.3 kcal/mol for S. aureus GyrB (3G7B). The ligand was placed in the expected binding sites of both target proteins. Conclusion: These results show that the compound 2,6-dimethoxyphenol is a promising compound that computationally was predicted to be antibacterial and could interact with bacterial DNA gyrase B, which is also known as GyrB. More favorable binding under the applied docking conditions is indicated by the greater predicted affinity towards E. coli GyrB. These computational studies need to be further confirmed in vitro using specific biochemical assays and further antibacterial studies.

Article Information

Article History

Received:	May 15, 2026
Revised:	June 27, 2026
Accepted:	August 12, 2026
Available Online:	August 31, 2026

Keywords:
S. persica; 2,6-Dimethoxyphenol; GC–MS; Molecular Docking; DNA Gyrase B; *E. coli*; *S. aureus*; Antibacterial Activity.

INTRODUCTION

Antimicrobial resistance (AMR) has become one of the greatest threats to global public health, with an estimated 4.95 million deaths caused by drug resistant bacterial infection in the world during a single year, and the escalation is predicted in the coming decades (Tang *et al.*, 2023) (Shahid *et al.*, 2023b). Multidrug-resistant *E. coli* and methicillin-resistant *S. aureus* (MRSA) remain in the top two most important pathogens on the World Health Organization's Bacterial Priority Pathogens List, where they are known for their ability to develop resistance to β-lactams, fluoroquinolones and other first-line antibiotics (Birlutiu and Birlutiu, 2025). The problem of an inadequate pipeline for discovering antibiotics and the lack of rapidity in the clinical translation of novel synthetic scaffolds has brought plant-derived bioactive metabolites back into the spotlight as alternative or complementary antibacterial leads. *S. persica* L. Miswak or arak is a shrub which is traditionally used for medicinal applications and its root, stem and leaf extracts have been used as an oral hygiene tool in South Asia, Middle East and North Africa (Shahid *et al.*, 2022). In addition to its dental applications, the phytochemical and pharmacological studies have revealed that the extracts of *S. persica* exhibit a wide range of antibacterial properties against a variety of Gram-positive and Gram-negative bacteria, including multidrug-resistant clinical isolates (Afzal *et al.*, 2024). The extracts of *S. persica* have been analysed using gas chromatography–mass spectrometry (GC–MS) and various secondary metabolites have been identified, such as thiocyanate, sterols, fatty acid esters and phenolic compounds, among which several have been found to have antimicrobial and membrane-disruptive effects, respectively (Shahid *et al.*, 2023a).

In the GC–MS profiles of *S. persica*, 2,6-dimethoxyphenol (syringol) is among the phenolic compounds that have been detected repeatedly and has been reported to have measurable inhibitory activity against Gram-negative pathogens like *Pseudomonas aeruginosa* and *Acinetobacter baumannii* (Aliaño-González *et al.*, 2022) and to interfere in the bacterial ribosomal protein synthesis. Despite this preliminary evidence, the molecular basis of its antibacterial action specifically, its capacity to bind and inhibit essential bacterial enzymes has not been characterized against drug-resistant *E. coli* and *S. aureus* (Tariq *et al.*, 2026). Computational screening, specifically structure-based molecular docking of the compound against validated drug targets in bacteria (DNA gyrase B), provide a quick and efficient pathway to formulating mechanisms of action hypotheses that can then be confirmed in wet labs (Islam and Pillay, 2020).

In the present study, an in-silico structure-based screening workflow was thus combined with GC–MS based phytochemical profiling of a *S. persica* extract for the evaluation of the binding potential of 2,6-dimethoxyphenol with the drug resistant bacterial DNA gyrase B (gyrB) of *E. coli* and *S. aureus* using PubChem and Protein Data Bank (PDB) for ligand and target retrieval, AutoDock Vina for docking simulation and Discovery Studio Visualizer and PyMOL for post docking structural analysis.

The aims of this paper are: (i) to identify the GC–MS metabolite profile of the extract; (ii) to identify and retrieve the crystal structure of the bacterial enzymes targeted (iii) to perform molecular docking of 2,6-dimethoxyphenol against the target enzymes and to identify the ligand enzyme interactions; (iv) to characterize the ligand enzyme interactions and to give an idea about their plausibility as a natural antibiotic lead.

2. Literature Review

2.1 Antimicrobial Resistance and the Case for Phytochemical Leads

Over the last 25 years, the global burden of AMR in *Enterobacterales* and *S. aureus* has been steadily increasing, and most recently, structured reviews of the burden of AMR between 2000 and 2024 highlight that there are significant gaps in surveillance and treatment, especially in LMICs (Elsaman *et al.*, 2025). In 2024, the WHO's Bacterial Priority Pathogens List once again identified carbapenem-resistant *Enterobacterales* (CRE) and cephalosporin-resistant *Enterobacterales* (CRE) as priority targets, as well as MRSA, because there was a continued lack of progress in the discovery pipeline for truly novel antibacterial chemotypes (Bhatia, 2026). This gap has led to a significant focus on research involving plant secondary metabolites, which provide chemically diverse scaffolds that are often multi-target, and relatively low cost to be easily screened computationally prior to their synthesis or validation from an extraction scale.

2.2 S. persica: Phytochemistry and Antibacterial Activity

The antibacterial properties of *S. persica* extracts have been highlighted in several recent studies. The GC–MS profile of a extract of *S. persica* used in intracanal medicament, revealing 26 compounds which included mainly benzyl isothiocyanate and steroidal constituents, with a notable reduction in *Enterococcus faecalis* colony count similar to calcium hydroxide (Shahid *et al.*, 2023). Similar findings were obtained from a 2024 clinical-isolate study, which showed that *S. persica* extracts also exhibited concentration-dependent inhibitory effect against *S. aureus* and *E. coli*, that chitosan potentiated the activity of *S. persica* extracts against carbapenem-resistant *A. baumannii* (Kouteu *et al.*, 2024). Synergic effect of *S. persica* extract and chitosan nanoparticles has been proved against a panel of oropharyngeal Gram-positive, Gram-negative and fungal strains including *S. aureus* and *E. coli* reference strains in complementary work (Balto *et al.*, 2024). These studies validate *S. persica* as a phenolically rich and reliably effective antibacterial agent but have yet to identify or computationally query the mechanism of its phenolic compound 2,6-dimethoxyphenol against particular resistant Gram-positive and Gram-negative targets.

2.3 GC–MS-Guided Molecular Docking Against Bacterial Targets

The translation from GC–MS identified metabolites in plants to validated bacterial enzymes has become a standard step in structure-based virtual screening to generate mechanistic hypotheses. In 2026, fourteen constituents of Rosa damascena essential oil were identified using GC/MS and docked in the AutoDock Vina module with *E. coli* DNA gyrase B (PDB: 6F86) and *S. aureus* DNA gyrase (PDB: 3G7B), with the binding affinities for the top four reported as acceptable ADMET/Lipinski profiles, congruous with docking results from redocking studies (RMSD ≈ 1.0 Å) (Lebkiri *et al.*, 2026). Similarly, the AutoDock Vina docking of Rungia repens leaf extract with the *S. aureus* virulence regulator SarA showed that phthalic acid butyl undecyl ester is a good binder with a docking score of −10.0 kcal/mol which matches the zone-of-inhibition data (Balaji and Mahalingam, 2026). The same DNA gyrase B target class (PDB IDs: 3G7B, 6F86) was selected for essential-oil studies to rationalize activity against multidrug-resistant (MDR) *S. aureus* and *E. coli*, always with AutoDock Vina paired with Discovery Studio or PyMOL for visualization of interactions (Yuan and Hao, 2023). In the case of Hydrocotyle javanica, it was observed that stigmasterol and its glucoside derivative have binding affinities ranging from −7.0 to −10.4 kcal/mol with *E. coli* DNA gyrase and β-lactamase, with the latter group of methoxy-substituted phenolics and heterocycles having reported binding energies of −6.1 to −6.3 kcal/mol against bacterial targets, primarily stabilized by conventional hydrogen bonding (Ali *et al.*, 2026). The precedents validate DNA gyrase B as a validated docking target for the 2,6-dimethoxyphenol present in the present *S. persica* GC–MS profile, and make the AutoDock Vina/ PubChem/ PDB/ Discovery Studio/ PyMOL toolset a literature-consistent tool-set for this class of analysis.

3. Methodology

3.1 Plant Material and Extraction

Stem parts from fresh *S. persica* were collected, identified, shade dried and ground to powder. For the powdered material, the solvent extraction (methanol extraction/Soxhlet apparatus) was performed to achieve crude extract that was further filtered, concentrated under reduced pressure (rotary evaporator) and stored at 4 °C in dark conditions before analysis (Shahid *et al.*, 2023).

3.2 GC–MS Phytochemical Profiling

The crude extract was subjected to GC–MS and analysed for volatiles and semi-volatiles bioactive component. Identification was carried out by matching the compound to the NIST/WILEY mass spectral library and by the retention time using the mass spectral fragmentation pattern and a similarity index above a certain threshold. The relative abundance was presented as a percentage peak area of the total ion chromatogram (Acevedo *et al.*, 2017). In the table 1, representative compounds identified are summarized, including the metabolite 2,6-dimethoxyphenol, which was chosen as the basis for further downstream computational screening due to its antibacterial precedent.

3.3 Ligand and Target Protein Retrieval
The 3D structure-data file (SDF) of 2,6-dimethoxyphenol (PubChem CID 68158) was downloaded from the PubChem database and converted to PDB/PDBQT. The RCSB Protein Data Bank (PDB) was used to obtain three-dimensional crystal structures of the following bacterial drug targets: DNA gyrase subunit B of *E. coli* (PDB ID: 1KZN) and DNA gyrase B of *S. aureus* (PDB ID: 3G7B). The co-crystallized water molecules, heteroatoms and the native ligand were removed from each receptor, followed by adding polar hydrogens and Kollman charges.

3.4 Molecular Docking (AutoDock Vina)
The molecular docking was carried out by employing AutoDock Vina software. The coordinates of the co-crystallized native ligand were used to define the ATP-binding pocket for cantering within ATP boxes to also ensure biologically relevant sampling, with the grid dimensions and spacing chosen according to the default parameter values (exhaustiveness = 8). The validity of the docking protocol was checked by re-docking the native co-crystallized ligand into the original binding site and calculating the root-mean-square deviation (RMSD) between the re-docked and the reference poses and the RMSD < 2.0 Å was accepted as the validity of the docking protocol. The best docking scores for each of the ligand-protein complexes were obtained for 2,6-Dimethoxyphenol, as shown in Table 2, the lowest (most negative) predicted binding energy (kcal/mol) for each docking pose.

3.5 Visualization and Interaction Analysis
The post-docking structural analysis and two-dimensional/three-dimensional visualization of the ligand–protein interactions were performed with BIOVIA Discovery Studio Visualizer and PyMOL. The interaction profile of 2,6-dimethoxyphenol with the active site residues of each of the target enzymes was mapped and compared with the interaction profile of the reference antibiotic to evaluate the plausibility of a common or complementary binding mode. For each complex, the active site residues within 4–5 Å of the docked ligand were identified and rendered images were created in PyMOL for figure preparation (Khan *et al.*, 2023).

3.6 Literature and Database Sources
All target validation, ligand bioactivity precedent and cross-referencing of docking targets were done following the standard procedure used in similar GC–MS guided in silico antibacterial screening studies reported in the past 5 years, using PubMed for literature retrieval and PubChem/RCSB PDB for chemical and structural data.

Results:
The methanolic extract of *S. persica* was analysed using the gas chromatography–mass spectrometry (GC–MS) technique, which led to the identification of various bioactive metabolites with different classes and relative abundance (Table 1). The identified compounds were highest for benzyl isothiocyanate (18.4%), 2,6-dimethoxyphenol (12.6%), stigmastane (6.1%), stigmasterol (5.5%), hexadecanoic acid methyl ester (4.9%) and 2-(2-methylvinyl) thiophene (5.8%). The phenol, sulfur containing, steroidal, fatty-acid-derived, and heterocyclic metabolites detected reveal the chemical diversity of the extract. 2,6-dimethoxyphenol was chosen for further molecular docking analysis, as it was found at a relatively high abundance in the GC–MS profile and has antibacterial relevance.

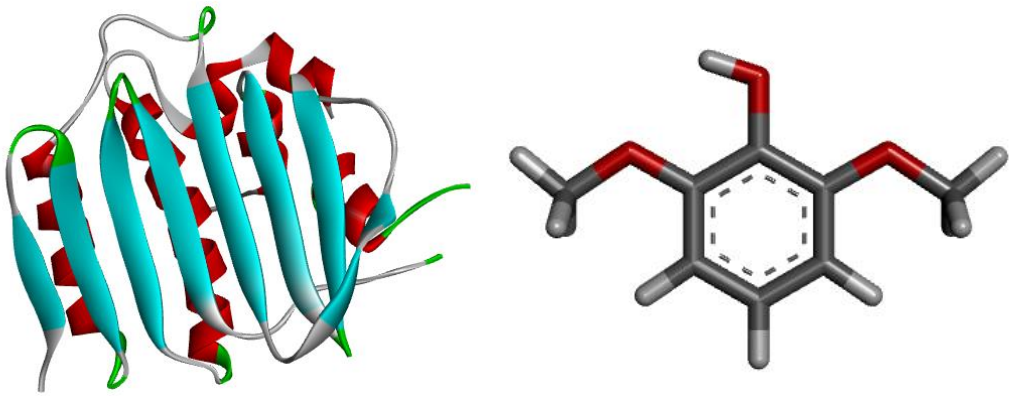
Table 1: Representative bioactive metabolites identified by GC–MS in the *S. persica* extract.

S. No.	RT (min)	Compound Name	Molecular Formula	Mol. Wt. (g/mol)	Peak Area (%)	PubChem CID
1	6.42	2-(2-Methylvinyl) thiophene	C_7H_8S	124.20	5.8	638623
2	9.15	Benzyl isothiocyanate	C_8H7NS	149.21	18.4	17368
3	14.27	Stigmastane	$C_{29}H_{52}$	404.72	6.1	5352578
4	16.03	2,6-Dimethoxyphenol	$C_8H_{10}O_3$	154.16	12.6	68158
5	18.44	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	270.45	4.9	8181
6	23.87	Stigmasterol	$C_{29}H_{48}O$	412.69	5.5	5280794

The docking of 2,6-dimethoxyphenol with the DNA gyrase B of *E. coli* (PDB ID: 1KZN) and DNA gyrase B of *S. aureus* (PDB ID: 3G7B) was then performed to examine the binding ability of the compound toward DNA gyrase B (Table 2). The compound exhibited predicted binding energies of −5.3 kcal/mol to the GyrB of *E. coli* and −4.3 kcal/mol to the GyrB of *S. aureus*. The negative binding energies shown represent energetically favourable ligand–protein interactions within the specified ATP bindings sites, and a higher binding affinity is expected for the *E. coli* target under the given docking conditions. Results provide preliminary structural basis for a possible interaction between 2,6-dimethoxyphenol and bacterial DNA gyrase B and further investigations are warranted using interaction-residue analysis and experimental antibacterial validation. Important: these values for docking should be viewed as computational values, not as direct evidence for antibacterial activity.

Table 2: Predicted binding energies of 2,6-dimethoxyphenol against bacterial DNA gyrase B targets

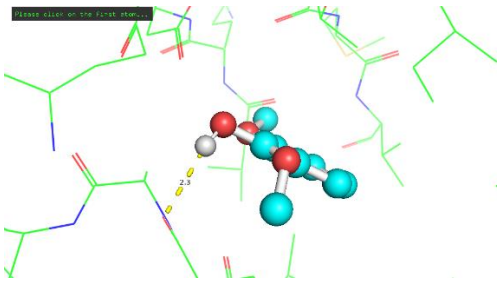
Target Protein (PDB ID)	Organism	Ligand	Binding Energy (kcal/mol)
DNA Gyrase B (1KZN)	*E. coli*	2,6-Dimethoxyphenol	−5.3
DNA Gyrase B (3G7B)	*S. aureus*	2,6-Dimethoxyphenol	−4.3



(A) (B)

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-5.3	0.000	0.000
2	-5.3	0.272	3.884
3	-4.8	3.137	5.181
4	-4.6	2.003	2.700
5	-4.6	2.007	4.559
6	-4.6	1.628	4.358
7	-4.4	2.329	5.034
8	-4.1	1.519	2.294
9	-4.0	2.380	3.908

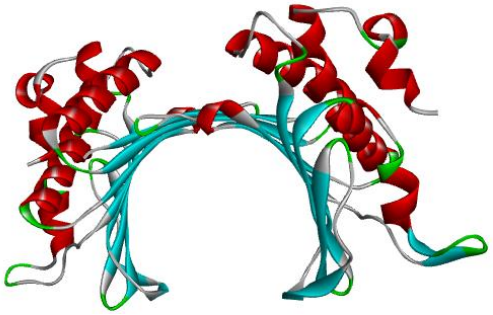
(C)



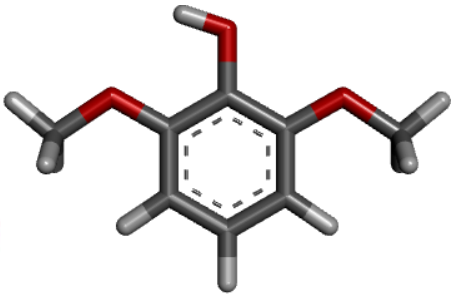
(D)

Figure 1: Molecular docking analysis of 2,6-dimethoxyphenol with DNA gyrase B (PDB: 1KZN) from *Escherichia coli*. (A) Three-dimensional structure of the DNA gyrase B protein; (B) 2,6-dimethoxyphenol ligand structure; (C) predicted docking poses and binding affinities generated using AutoDock Vina, with the best binding energy of −5.3 kcal/mol; and (D) three-dimensional visualization of the ligand positioned within the predicted binding pocket of DNA gyrase B.

The docking analysis showed that 2,6-dimethoxyphenol formed a favourable interaction with the DNA gyrase B protein (PDB: 1KZN). The best docking pose showed a binding affinity of −5.3 kcal/mol, with additional poses displaying comparable affinities. The ligand was positioned within the predicted binding pocket of 1KZN, supporting its potential to interact with the bacterial target. These findings provide preliminary computational evidence for the antibacterial potential of 2,6-dimethoxyphenol against *E. coli*.



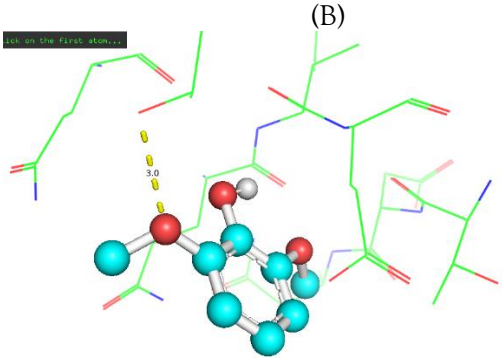
(A)



(B)

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-4.3	0.000	0.000
2	-4.3	15.379	17.413
3	-4.3	15.374	17.658
4	-4.2	18.272	19.646
5	-4.2	18.148	19.489
6	-4.0	1.936	4.306
7	-4.0	12.682	14.243
8	-3.9	17.498	18.819
9	-3.9	1.818	2.735

(C)



(D)

Figure 2: Molecular docking analysis of 2,6-dimethoxyphenol with DNA gyrase B (PDB: 3G7B) from Staphylococcus aureus. (A) Three-dimensional structure of the DNA gyrase B protein; (B) chemical structure of 2,6-dimethoxyphenol; (C) predicted docking poses and binding affinities generated using AutoDock Vina, with the best binding energy of −4.3 kcal/mol; and (D) three-dimensional representation of the docked ligand within the predicted binding region of DNA gyrase B.

The docking analysis showed that 2,6-dimethoxyphenol exhibited a favourable interaction with DNA gyrase B of *S. aureus* (PDB: 3G7B). The best docking pose demonstrated a binding affinity of −4.3 kcal/mol, with the ligand positioned within the predicted binding region of the target protein. The

interaction profile and docking pose support the potential of 2,6-dimethoxyphenol to interact with *S. aureus* DNA gyrase B. These findings provide preliminary computational evidence for its possible antibacterial activity against *S. aureus*.

Discussion:

The GC–MS analytical data showed that the phytochemical profile of *S. persica* is highly diverse in terms of potentially bioactive metabolites, mainly phenolic compounds, sulfur-containing metabolites, fatty acid derivatives and sterols. The following compounds were identified, of which 2,6-dimethoxyphenol was the most abundant (12.6% peak area). The antibacterial relevance from previously published reports and presence in GC–MS profile of the extract were a justification for its consideration in molecular docking. Molecular docking analysis showed that 2,6-dimethoxyphenol could bind with both bacterial targets in an attractive manner. The compound showed a predicted binding energy of −5.3 kcal/mol with *E. coli* GyrB (1KZN) and −4.3 kcal/mol with *S. aureus* GyrB (3G7B). Comparatively more favorable ligand–protein interactions under the applied docking conditions is indicated by the stronger predicted affinity to the *E. coli* target. The computational results, however, should be considered as preliminary evidence and not direct proof of antibacterial activity. The overall findings support the possible mechanistic action of 2,6-dimethoxyphenol in *S. persica* antibacterial activity. DNA gyrase B is an important bacterial target, and its inhibition could potentially interfere with bacterial DNA replication and growth. The docking results thus suggest a structural hypothesis between the identified metabolite in the GC–MS and the antibacterial activity against *E. coli* and *S. aureus*. This proposed mechanism needs further experimental studies, such as in vitro antibacterial assays and biochemical validation of DNA gyrase inhibition.

Conclusion:

In the present study, 2,6-dimethoxyphenol of *S. persica* was evaluated as a potential antibacterial lead using GC–MS guided computational approach against *E. coli* & *S. aureus*. The compound contributed 12.6% to GC–MS peak area and had a favorable predicted interaction with DNA gyrase B with binding energies of −5.3 kcal/mol (1KZN) and −4.3 kcal/mol (3G7B), respectively. The results obtained here offer a structural basis for the exploration of 2,6-dimethoxyphenol as a natural product-derived antibacterial agent and emphasize the importance of combination of phytochemical profiling with molecular docking for mechanism-oriented screening. However, the docking results are still predictive and need to be validated with MIC/MBC assays, DNA gyrase inhibition assays and other biochemical assays before the definitive antibacterial activity or target engagement is determined.

Conflict of Interest

The authors declare that there are no conflicts of interest associated with this study.

REFERENCES:

Acevedo, F., P. Torres, B.D. Oomah, S.M. de Alencar, A.P. Massarioli, R. Martín-Venegas, V. Albarral-Ávila, C. Burgos-Díaz, R. Ferrer, and M. Rubilar. 2017. Volatile and non-volatile/semi-volatile compounds and in vitro bioactive properties of Chilean Ulmo (Eucryphia cordifolia Cav.) honey. *Food Research International*. 94:20-28.

Afzal, S., A. Shahid, M. Iii, K. Islam, and F. Rasool. 2024. The tole of microbiomes in animal health and disease: Current insights and future directions. *Afirican Journal of Biological*. 6:10394-10408.

Ali, A.S., Y.A. Nageye, and K.E. Bello. 2026. Antioxidant and Antibacterial Activities of Secondary Metabolites Produced by Streptomyces Isolates Against Extended-Spectrum β-Lactamase-Producing Bacteria. *MicrobiologyOpen*. 15:e70282.

Aliaño-González, M.J., J. Gabaston, V. Ortiz-Somovilla, and E. Cantos-Villar. 2022. Wood waste from fruit trees: Biomolecules and their applications in agri-food industry. *Biomolecules*. 12:238.

Ayoub, N., N. Badr, S.S. Al-Ghamdi, A. Alzahrani, R. Alsulaimani, A. Nassar, R. Qadi, I.K. Afifi, and N. Swilam. 2021. GC/MS profiling and ex vivo antibacterial activity of Salvadora persica (siwak) against Enterococcus faecalis as intracanal medicament. *Evidence-Based Complementary and Alternative Medicine*. 2021:6333867.

Balaji, V., and G. Mahalingam. 2026. GC-MS profiling, in vitro antioxidant and toxicity evaluation, and in silico pharmacokinetic and molecular docking prediction of the phytocompounds of Rungia repens (L.) Nees targeting SarA of Staphylococcus aureus. *Frontiers in Chemistry*. 14:1778720.

Balto, H., M.S. Bekhit, S.H. Auda, A. Elansary, R.S. Bhat, N. Marraiki, and S. Al-Hadlaq. 2024. Synergistic effect of Salvadora persica and chitosan nanoparticles against oropharyngeal microorganisms. *Scientific Reports*. 14:12997.

Bhatia, R. 2026. New Antibiotics: Needs, Challenges, and Status. *Drug-Resistant Infections: Global Burden, Antimicrobial Stewardship, Prevention, and One Health Approaches*:281-293.

Birlutiu, V., and R.-M. Birlutiu. 2025. An overview of the epidemiology of multidrug resistance and bacterial resistance mechanisms: what solutions are available? A comprehensive review. *Microorganisms*. 13:2194.

Elsaman, T., M.A. Mohamed, M.S. Mohamed, E.M. Eltayib, and A.E. Abdalla. 2025. Microbial-based natural products as potential inhibitors targeting DNA gyrase B of Mycobacterium tuberculosis: An in silico study. *Frontiers in Chemistry*. 13:1524607.

Islam, M.A., and T.S. Pillay. 2020. Identification of promising anti-DNA gyrase antibacterial compounds using de novo design, molecular docking and molecular dynamics studies. *Journal of Biomolecular Structure and Dynamics*. 38:1798-1809.

Khan, A., S. Pradeep, and S.G. Dastager. 2023. In vitro anticancer evaluation of Enceleamycin A and its underlying mechanism. *RSC advances*. 13:34183-34193.

Kouteu, P.A.N., A.G. Kemegne, M.M. Pahane, A.S.Y. Fanta, A.K. Membangmi, D.V.T. Tchamaleu, G.A. Agbor, and M.R. Mouangue. 2024. Face-Centered Central Composite Design for the Optimization of the Extraction of Phenolic Compounds from Kernels and Shells of Raphia farinifera and Evaluation of the Antioxidant, Antimicrobial, and Anti-Inflammatory Activities. *Journal of Food Processing and Preservation*. 2024:8849005.

Lebkiri, N., Y. Abbas, H. Assila, I. Maroui, O. El-guourrami, D. Iraqi, R. Abdelwahd, and G. Diria. 2026. Computational investigation of the antibacterial and antioxidant potential of Rosa damascena essential oil from Morocco: Molecular docking and ADMET analysis of fourteen volatile compounds. *Industrial Crops and Products*. 251:124117.

Pardeshi, S., V. Jadhav, S. Disale, H. Suryavanshi, V.A. Adole, and B. Sapkal. 2026. Indole-functionalized 1, 2, 3-triazole derivatives: Synthesis, antimicrobial activity, molecular docking, DFT and ADME studies. *Journal of Molecular Structure*:146282.

Shahid, A., A. Arif, U. Ejaz, Z.S. Amin, S. Mansoor, H.M. Usman, and M. Naeem. 2023a. Therapeutic effects of Salvadora persica extracts against Sarcoptes scabiei var. hominis and their secondary infections.

Shahid, A., A. Arif, M. Rehman, S. Arshad, A. Akram, and H. Samar. 2022. Therapeutic Effect of Salvadora persica on multiple skin diseases. *J Plant Biochem Physiol*. 10:1-7.

Shahid, A., M. Fatima, M.S.I. Khan, U. Ali, S.Z. Fareed, and M.A. Qureshi. 2023b. From microbes to immunity: a comprehensive review of microbiome modulation. *Journal of Health and Rehabilitation Research*. 3:801-807.

Tang, K.W.K., B.C. Millar, and J.E. Moore. 2023. Antimicrobial resistance (AMR). *British journal of biomedical science*. 80:11387.

Tariq, F., T. Sultan, Z. Fatima, A. Rahat, A. Shahid, and A. Ahmad. 2026. Meropenem in the Management of Severe Multidrug-Resistant Bacterial Infections. *Pakistan Journal of Medical & Cardiological Review*. 5:1139-1155.

Yuan, C., and X. Hao. 2023. Antibacterial mechanism of action and in silico molecular docking studies of Cupressus funebris essential oil against drug resistant bacterial strains. *Heliyon*. 9.