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Article

In Vitro and in Silico Evaluation of *Allium sativum* Extract as an Antimicrobial Strategy against Cariogenic Bacteria

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Abstract: Dental caries is a complex oral disorder resulting from the interaction of multiple contributing factors, with microbial activity playing a central role. It continues to represent a significant global health burden. The rising incidence of antibiotic resistance among cariogenic microorganisms has diminished the efficacy of traditional antimicrobial treatments, thereby emphasizing the urgent need for alternative therapeutic approaches. Molecular characterization of bacterial isolates was achieved through PCR amplification of species-specific gene sequences. The antibiotic sensitivity profile was determined using the standard Kirby–Bauer disk diffusion assay. Furthermore, the antimicrobial potential of garlic extract was investigated and evaluated in comparison with commonly utilized antibiotics. Molecular docking analysis was carried out using allicin, the principal bioactive compound of garlic, against essential bacterial enzymes, including DNA gyrase and topoisomerase, to elucidate protein–ligand interactions. The results revealed a polymicrobial profile of dental caries, with Streptococcus mutans and Lactobacillus acidophilus being the most prevalent species, followed by Porphyromonas gingivalis and Staphylococcus aureus. Antibiotic susceptibility testing demonstrated considerable resistance to amoxicillin, ampicillin, and erythromycin, whereas garlic extract exhibited notable antibacterial activity against most isolates. Molecular docking results showed strong binding affinities of allicin toward DNA gyrase and topoisomerase, supported by stable hydrogen bonding and hydrophobic interactions. In conclusion, the integration of molecular diagnostics, in vitro antimicrobial evaluation, and in silico analysis provides valuable insight into alternative strategies for managing dental caries and addressing antimicrobial resistance.

Keywords: Antibiotic Resistance, Dental Caries, Garlic Extract, Molecular Docking, Polymerase Chain Reaction (PCR), Topoisomerase

Introduction

The oral cavity is a complex, dynamic microbial environment that supports a diverse community of microorganisms, including bacteria, fungi, and viruses [1]. Maintaining a balanced relationship between commensal and pathogenic microbes is essential for oral health. However, disturbances in this equilibrium can lead to the onset of oral diseases, particularly dental caries [2]. Dental caries continues to be one of the most widespread chronic conditions globally, affecting people across all age groups and representing a major public health challenge, especially in developing regions [3], [4].

Dental caries is a complex condition arising from the interplay of multiple factors, including microbial activity, host susceptibility, lifestyle habits, diet, genetic predisposition, and environmental influences. Among these determinants, cariogenic microorganisms are critically involved in both the onset and progression of the disease by producing acids, forming biofilms, and promoting the demineralization of dental enamel. Streptococcus mutans is considered the principal causative organism of dental caries, largely due to its ability to adhere effectively to tooth surfaces, establish structured biofilms, and generate organic acids through the metabolism of fermentable carbohydrates [4], [5], [6]. In addition to *S. mutans*, other bacterial species such as *Lactobacillus acidophilus*, *Staphylococcus aureus*, and *Porphyromonas gingivalis* have been implicated in the progression of dental caries and associated periodontal complications, particularly in mixed infections. Traditionally, the identification of cariogenic bacteria has relied on culture-based microbiological methods. Although these techniques have provided valuable insights into the oral microbiota, they are limited by low sensitivity, prolonged processing time, and the inability to detect fastidious or difficult-to-culture organisms. Advances in molecular diagnostic techniques, particularly PCR, have significantly improved the detection and identification of oral pathogens by targeting species-specific genetic markers with high sensitivity and specificity[7], [8]. PCR-based assays allow rapid and accurate identification of cariogenic bacteria, facilitating timely detection and improved understanding of microbial diversity in dental caries [9], [10].

Despite advances in diagnostic and preventive strategies, the management of dental caries frequently involves the use of antimicrobial agents to control bacterial load and prevent disease progression [11]. However, the excessive and often inappropriate use of antibiotics has contributed to the emergence of antibiotic-resistant oral pathogens, complicating treatment outcomes and raising global health concerns. Increasing resistance among cariogenic bacteria to commonly prescribed antibiotics highlights the critical need for alternative or complementary antimicrobial approaches [12], [13]. In recent years, there has been growing interest in plant-derived natural products, particularly garlic (*Allium sativum*) extracts, as potential antimicrobial agents. Garlic is widely recognized for its antimicrobial and therapeutic properties against both Gram-positive and Gram-negative bacteria [14], [15]. Although several studies have reported the antimicrobial activity of garlic and its bioactive compounds against oral pathogens, most investigations have focused either on isolated laboratory strains [10], [16], [17] or solely on in vitro assays without integrating molecular diagnostics and mechanistic computational analysis[18].

Moreover, limited studies have evaluated garlic extract in comparison with conventional antibiotics using clinical isolates characterized by PCR-based identification. Therefore, the present study advances existing knowledge by combining molecular detection of cariogenic bacteria, phenotypic antimicrobial susceptibility profiling, and in silico docking analysis to provide a comprehensive evaluation of garlic-derived antimicrobial activity within a clinically relevant framework. Therefore, the present study aimed to (i) perform molecular identification of key cariogenic bacteria associated with dental caries using PCR-based techniques, (ii) evaluate their antimicrobial susceptibility profiles against commonly used antibiotics, (iii) assess the antibacterial potential of garlic extract in comparison with conventional antibiotics, and (iv) investigate the molecular interactions of garlic-derived bioactive compounds with essential bacterial enzymes using molecular docking analysis. This integrated diagnostic, experimental, and computational approach provides mechanistic and applied insights into alternative strategies for managing dental caries and combating antimicrobial resistance.

Materials and Methods

Study Design and Sample Collection

This investigation was designed as a cross-sectional study and carried out at the academic dental clinics affiliated with the College of Dentistry, Al-Muthanna University, Iraq. The study period extended from January to September 2025. Ethical clearance was granted by the Research Ethics Committee of Al-Muthanna University (Approval No.: MU-REC-2025-017). Prior to sample collection, all participants provided written informed consent in compliance with the principles outlined in the Declaration of Helsinki. A Study Design include collected 140 dental caries samples from individuals of different age groups and both sexes who attended the dental clinic during the study period (Figure 1). Samples were obtained from carious lesions under strict aseptic conditions with the assistance of a dentist. Dental plaque samples were collected by gently scraping the affected tooth surface using sterile dental instruments or swabs. Additional samples were collected during tooth extraction and transferred into sterile tubes containing 5 mL of brain heart infusion (BHI) broth as an enrichment medium due to its nutrient-rich composition, which supports the growth of fastidious oral bacteria, including *Streptococcus* and *Lactobacillus* species, thereby enhancing bacterial recovery and improving the sensitivity of subsequent culture and molecular analyses. In cases where multiple lesions were present, only one representative sample per patient was included in the final analysis to avoid biasing duplication. All samples were labelled with patient information, including age and sex, and transported immediately to the microbiology laboratory for further processing. When immediate processing was not possible, samples were incubated in BHI broth at 37C° for 24h. After incubation, bacterial cultures were examined for colony morphology. Distinct colonies were subculture on appropriate media to obtain pure isolates. Preliminary identification was performed using Gram staining and key biochemical tests, including catalase and oxidase tests, coagulase test, carbohydrate fermentation profiling, and haemolysis pattern on blood agar.

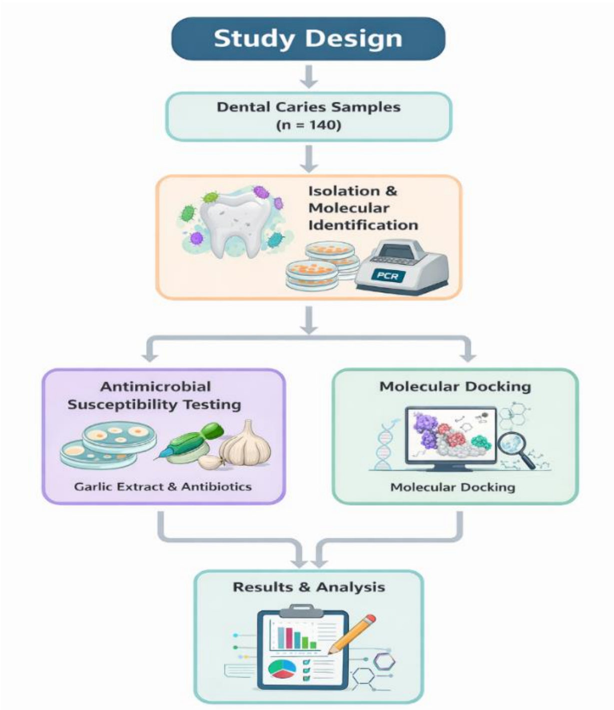


Figure 1. Schematic representation of the experimental design of the study, illustrating sample collection, bacterial isolation, PCR-based molecular identification, antimicrobial susceptibility testing, and molecular docking analysis.

Bacterial molecular identification

The DNA extracted from purified bacterial colonies by using a commercial Qiagen DNA extraction kit (Cat. No.: FAPGK 001) according to the manufacturer's instructions. The quality and concentration of extracted DNA were assessed using spectrophotometric analysis, and DNA samples were stored at −20 °C until further molecular analysis. PCR was performed to perform molecular identification of cariogenic bacterial species using species-specific primers targeting conserved genetic markers. The primer sequences, target genes, and expected amplicon sizes are listed in Table 1. Polymerase chain reaction amplification was carried out using a thermal cycler with an initial denaturation step at 95 °C for 5 minutes, followed by 35 amplification cycles consisting of denaturation, annealing, and extension phases under optimized conditions. The denaturation at 95 °C for 30 s, annealing at 55–60 °C (depending on primer melting temperature) for 30 s, and extension at 72 °C for 45 s, with a final extension step at 72 °C for 7 min. Amplified PCR products were analysed by agarose gel electrophoresis and visualized under ultraviolet illumination to confirm the presence of target genes.

Table 1. The target genes and primer sequences used for PCR-based identification of cariogenic bacteria.

Species	Target gene	sequences (5'-'3)	size	References
Streptococcus Mutans	gtfB	F - CTACACTTTCGGGTGGCTTG R -GAAGCTTTTCACCATTAGAAGCTG-3	261bp	[19
Staphylococcus aureus	Sa442	F -AATCTTTGTCGGTACACGATATTCTTCACG-3′ R-CGTAATGAGATTTCAGTAGATAATACAACA-3'	107bp	[20
Lactobacillus acidophilus	IDL22	F -CCACCTTCCTCCGGTTTGTCA3′ R - AACTATCGCTTACGCTACCACTTTGC3′	606bp	[21
Porphyromonas gingivalis	Pg	F - AGGCAGCTTGCCATACTGCG'3 R -ACTGTTAGCAACTACCGATGT '3	404bp	[22

Antibiotic Susceptibility Testing

Antibiotic testing was performed by using the Kirby Bauer disk diffusion method on Mueller Hinton agar supplemented with blood, following the guidelines of the Clinical and Laboratory Standards Institute (CLSI, 2023; M100, 33rd edition). The antibiotics tested included 10 µg amoxicillin, ampicillin (10 µg), erythromycin (15 µg), tetracycline (30 µg), ciprofloxacin (5 µg), clindamycin (2 µg), and vancomycin (30 µg). Fresh garlic (*Allium sativum*) cloves were obtained from a local market and taxonomically authenticated by a plant taxonomist at the Herbarium College of Pharmacy, Al-Muthanna University, under voucher specimen (Voucher No. MUPH017). The cloves were crushed under sterile conditions to obtain a crude garlic extract. A crude ethanolic garlic extract was prepared using a 1:10 (w/v) ratio by homogenizing 10 g of fresh garlic in 100 mL of 70% ethanol. The homogenate was filtered through sterile filter paper to remove particulate matter and stored at 4 °C until use. The antibacterial activity of garlic extract was evaluated using disc diffusion assays. Susceptibility was determined based on inhibition zone diameters and categorized as sensitive, intermediate, or resistant for comparative analysis with conventional antibiotics.

Molecular Docking Analysis

Allicin, the principal bioactive compound derived from garlic, was selected as the representative ligand. The three-dimensional structure of allicin was retrieved from public chemical databases and prepared for docking through energy minimization and optimization. Three-dimensional structures of essential bacterial target proteins, including topoisomerase and, DNA gyrase were retrieved from the Protein Data Bank (Table 2). Protein preparation involved removal of water molecules and co-crystallized ligands, followed by addition of polar hydrogens and assignment of appropriate charges. Docking simulations were performed using molecular docking software to predict binding affinities and interaction patterns between allicin and the selected target proteins. Docking results were evaluated based on binding energy values and interaction types. Protein–ligand complexes were visualized using molecular visualization tools to analyse binding orientation and interaction residues. AutoDock version 1.2.0 was used for Molecular docking. Two-dimensional interaction maps were generated using Discovery Studio Visualizer version 2021 to identify hydrogen bonds and hydrophobic interactions, and docking validation was conducted by re-docking native ligands into their respective binding sites, and root mean square deviation (RMSD) values were calculated to assess docking accuracy. The RMSD value of ≤ 2.0 Å was considered indicative of acceptable docking accuracy.

Table 2. Protein accession numbers and sequence lengths of DNA gyrase and topoisomerase retrieved for molecular docking analysis

Species	Gyrase		Topoisomerase	
	Accession No	Protein length	Accession No	Protein length
S.Mutans	A0A0D6A8N6	838	Q06AK7	700
S.aureus	P0A0K8	755	A0AAX1K4Q7	717
L.Acidophilus	Q5FN10	835	Q5FKE2	716
P.Gingivalis	A0AAE9XGM0	873	A0AAE9X5I4	702

Statistical Analysis

Data analysis was carried out using SPSS software (version 31.0.0.0). Descriptive statistical methods were applied to summarize the distribution of bacterial prevalence and patterns of antimicrobial susceptibility. Categorical data were presented as counts and percentages. Inferential comparisons were performed using either the Chi-square test or Fisher's exact test, depending on data suitability. A p-value below 0.05 was regarded as indicating statistical significance.

Results

Demographic Characteristics of the Study Population

Analysis of age distribution revealed that the highest number of samples (64/140) was obtained from individuals aged 20–40 years, representing the largest proportion of dental caries samples in this age group. Samples from individuals aged ≤20 years and ≥40 years accounted for 32/140 and 43/140, respectively (Figure 2). Regarding sex distribution, males represented 62% of the study population, while females accounted for 38%, reflecting a higher representation of dental caries among males. Analysis of oral hygiene practices showed that 67% of individuals reported brushing their teeth once daily, 24% brushed twice daily, and 9% reported irregular or no brushing habits.

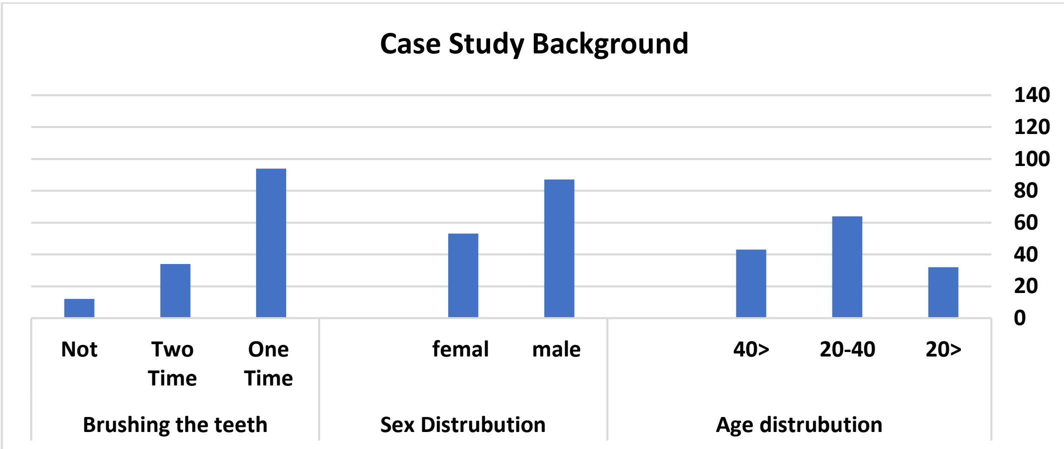


Figure 2. Background characteristics of dental caries patients included in the study, showing age distribution, sex distribution, and tooth-brushing habits.

Identification of Cariogenic Bacteria

PCR-based molecular analysis successfully identified multiple cariogenic bacterial species among the collected samples. *Streptococcus mutans* was detected in 87 out of 140 samples (62.14%), followed by Lactobacillus acidophilus, detected in 94 samples (67.14%). *Porphyromonas gingivalis* and *Staphylococcus aureus* were detected in 57 (40.71%) and 33 (23.57%) samples, respectively (Table 3). These results highlight the polymicrobial nature of dental caries and support the dominant role of S. mutans and *L. acidophilus* in the disease process.

Table 3. Prevalence of cariogenic bacteria detected by PCR using species-specific primers.

Primer Name	PCR product	TM	Total Sample	prevalence percentage
gtfB	261bp	59c	140	62.14%
Sa442	107bp	57c	140	40.71%
IDL22	606bp	57c	140	67.14%
Pg	404bp	59c	140	23.57%

A comparison between PCR and conventional culture-based identification methods revealed variability in detection rates among the studied bacterial species (Figure 3). While high concordance was observed for Streptococcus mutans and Lactobacillus acidophilus, notable discrepancies were found for Staphylococcus aureus and Porphyromonas gingivalis, where culture-based methods detected a higher number of isolates than PCR (Figure 4). These differences may reflect variations in bacterial viability, growth requirements, and sensitivity of the detection methods, emphasizing the advantage of PCR-based techniques in the accurate identification of cariogenic bacteria.

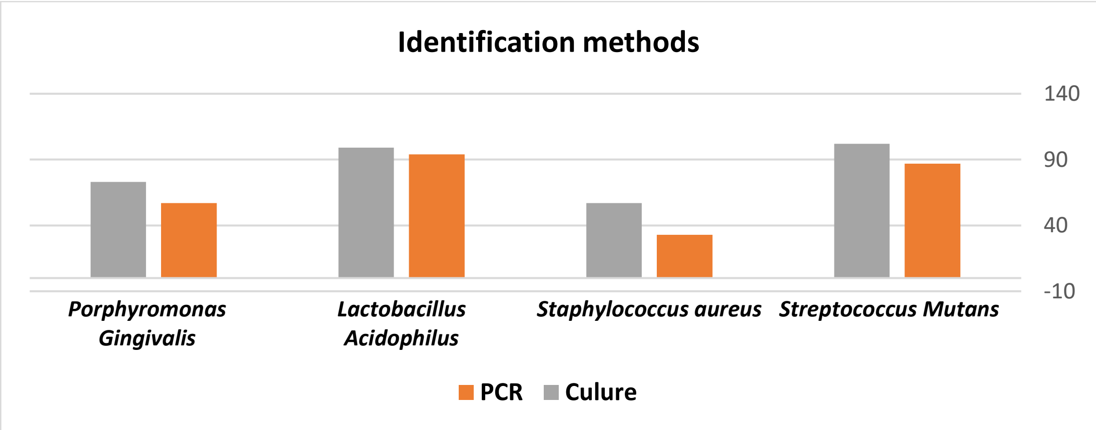


Figure 3. Comparative detection of cariogenic bacteria using PCR and conventional culture-based identification methods.

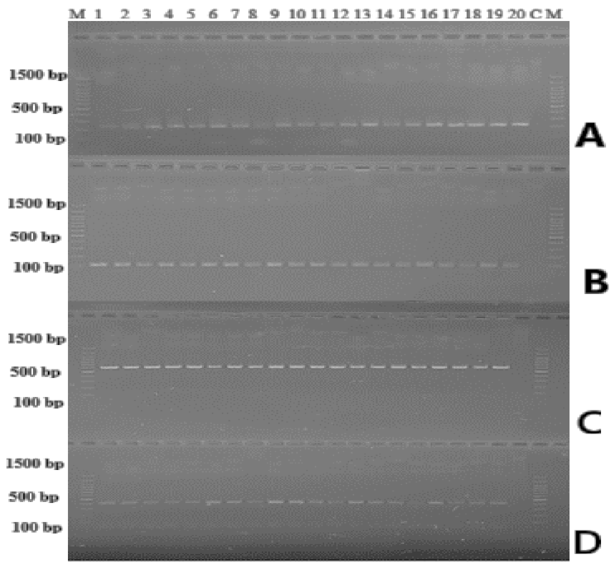


Figure 4. Agarose gel electrophoresis analysis of PCR-amplified target genes from cariogenic bacterial isolates. (A) gtfB gene specific for Streptococcus mutans (261 bp); (B) Sa442 gene specific for Staphylococcus aureus (107 bp); (C) IDL22 gene specific for Lactobacillus acidophilus (606 bp); and (D) Pg gene specific for Porphyromonas gingivalis (404 bp). M: DNA molecular weight marker (100 bp ladder); lanes 1–20 represent PCR-positive samples.

Antibiotic Susceptibility Profiles

Antibiotic testing was performed on bacterial isolates recovered from dental caries samples (Table 4). The results demonstrated variable susceptibility patterns among the tested antibiotics. High resistance rates were observed against erythromycin, ampicillin, and amoxicillin, while ciprofloxacin, clindamycin, and vancomycin exhibited relatively higher antibacterial activity. These findings indicate the presence of antibiotic-resistant cariogenic bacteria and highlight the limitations of conventional antibiotics in the management of dental caries-associated infections. The antibacterial activity of garlic extract was evaluated and compared with conventional antibiotics. Garlic extract demonstrated notable inhibitory activity against most tested bacterial isolates, with 77.6% of isolates showing susceptibility, exceeding the effectiveness of several commonly used antibiotics.

Table 4. Antimicrobial susceptibility profiles of cariogenic bacterial isolates against conventional antibiotics and garlic extract

Antimicrobial Agent	Sensitive n (%)	Intermediate n (%)	Resistant n (%)
Amoxicillin	71 (41.8%)	29 (17.1%)	70 (41.1%)
Ampicillin	66 (38.8%)	32 (18.8%)	72 (42.4%)
Erythromycin	60 (35.3%)	25 (14.7%)	85 (50.0%)
Tetracycline	79 (46.5%)	21 (12.4%)	70 (41.1%)
Ciprofloxacin	119 (70.0%)	17 (10.0%)	34 (20.0%)
Clindamycin	111 (65.3%)	23 (13.5%)	36 (21.2%)
Vancomycin	153 (90.0%)	10 (5.9%)	7 (4.1%)
Allicin (Garlic extract)	**132 (77.6%)**	**21 (12.4%)**	**17 (10.0%)**

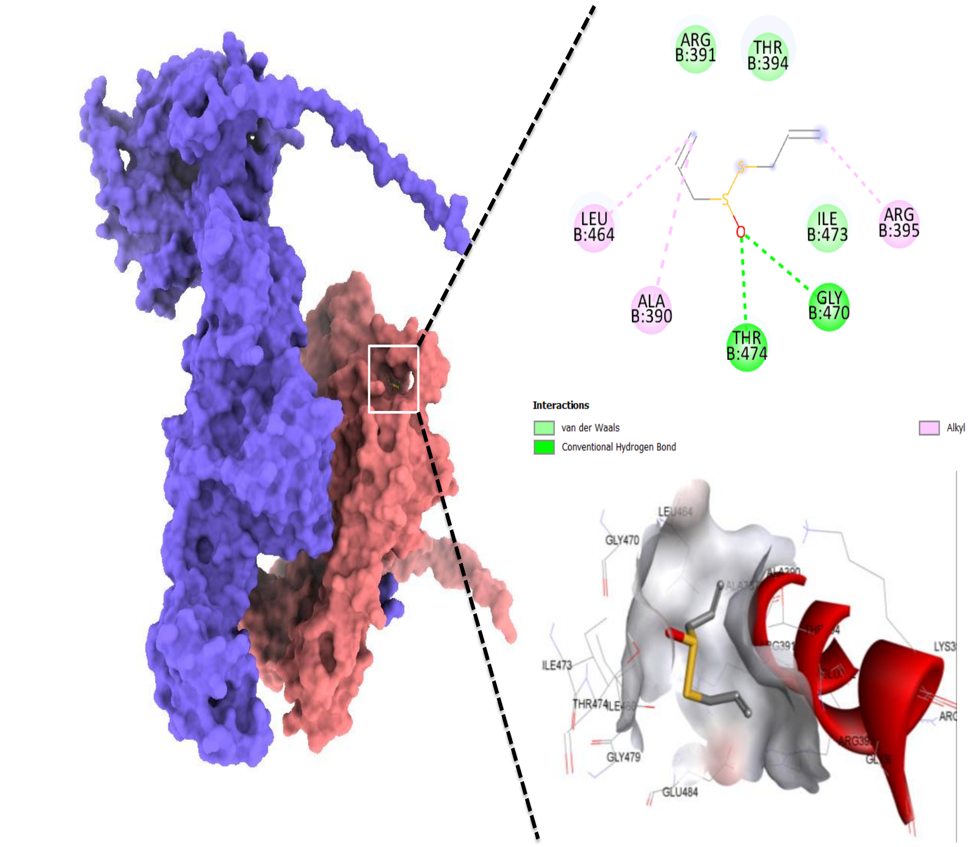
Molecular Docking Analysis

To elucidate the molecular basis of the observed antibacterial activity, molecular docking analysis was conducted using allicin, the principal bioactive compound derived from garlic (Table 5).

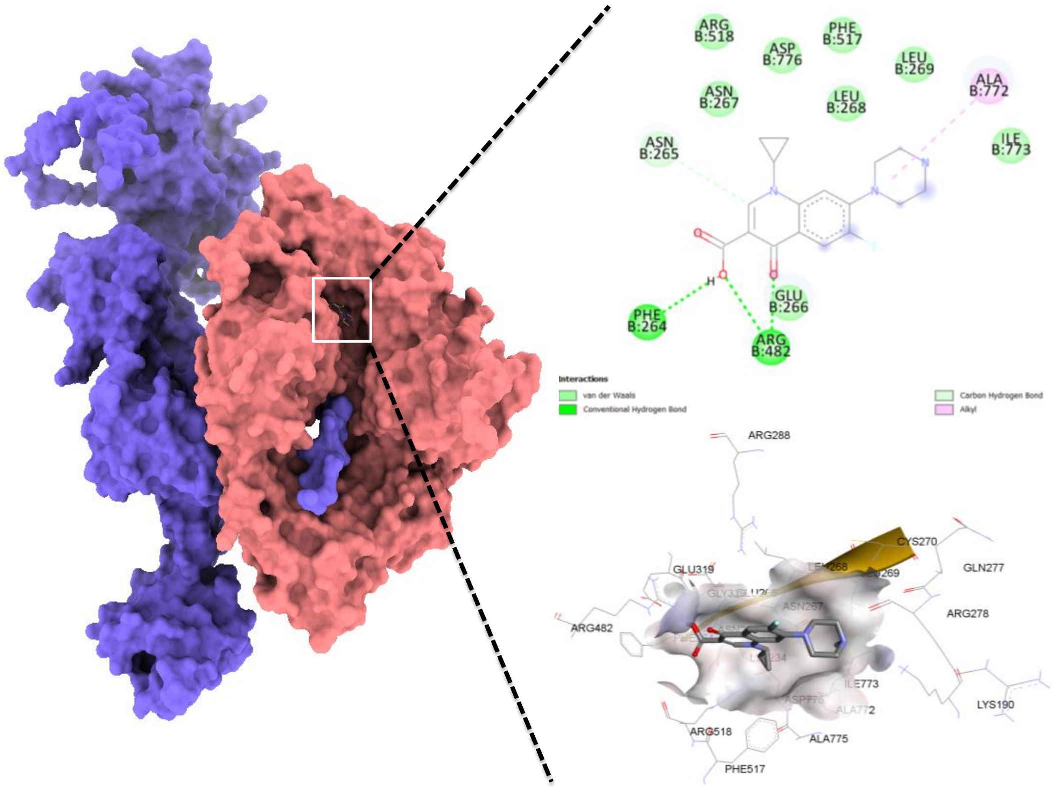
Table 5. Binding free energy components (kcal/mol) of amoxicillin and allicin interactions with DNA gyrase and topoisomerase

Energies (kcal/mol)	Gyrase+ Amoxicillin	Topoisomerase + Amoxicillin	Gyrase+ Allicin	Topoisomerase +Allicin
ΔG_{bind}	-15.59±2.63	-14.75±2.99	-27.53±4.1	-25.15±1.13
ΔG_{bind}Lipo	-13.96±1.03	-11.50±3.1	-18.83±2.3	-13.43±1.6
ΔG_{bind}vdW	-11.10±2.0	-10.63±2.63	-12.68±2.17	-14.160±3.0
ΔG_{bind}Coulomb	-8.12±1.99	-13.66±2.88	-2.14±1.01	-6.22±0.99
$\Delta G_{bind}H_{bond}$	-0.41±0.22	-1.87±0.5	-0.06±0.01	-0.62±0.16
ΔG_{bind}SolvGB	15.5±1.09	61.54±2.8	14.65±2.27	22.2±1.7
ΔG_{bind}Covalent	1.56±1.2	4.22±1.07	0.85±0.5	2.66±1.12

Docking simulations revealed strong binding affinities of allicin toward essential bacterial enzymes, including DNA gyrase and topoisomerase. Allicin demonstrated lower binding energy values compared with ciprofloxacin, indicating more stable protein–ligand complexes. Interaction analysis showed that allicin formed hydrogen bonds and hydrophobic interactions with conserved catalytic residues within the active sites of the target proteins (Figure 5).

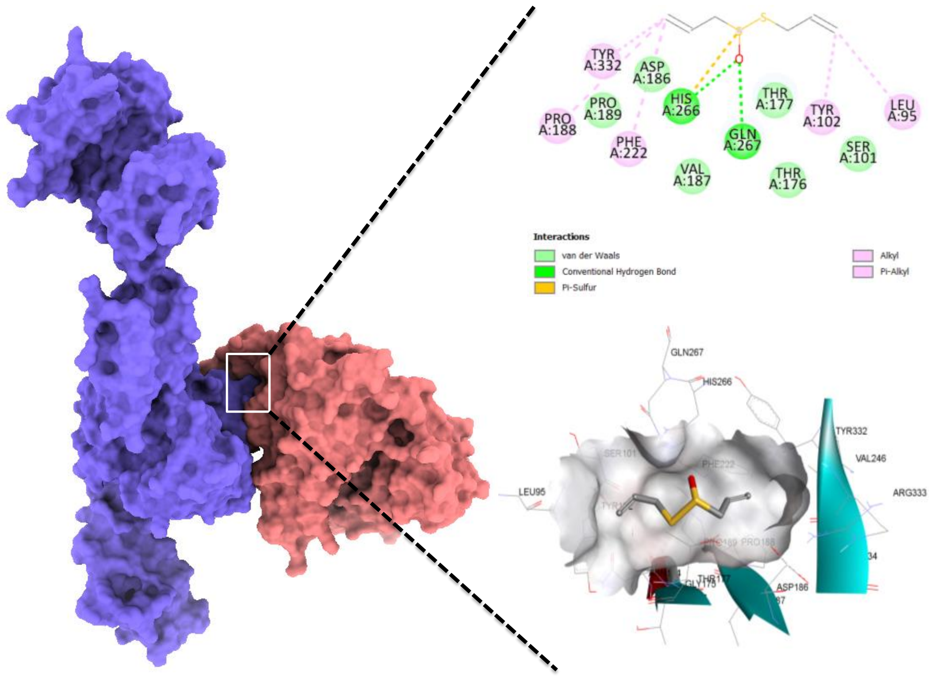


Gyrase+Allicin

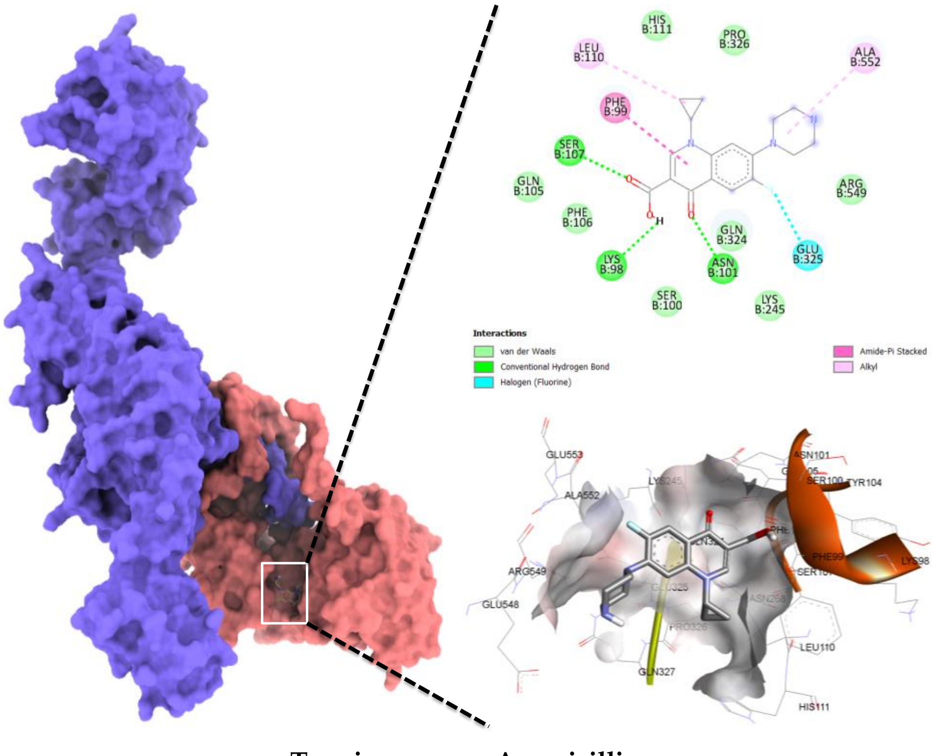


Gyrase+ Amoxicillin

A



Topoisomerase+Allicin



Topoisomerase+ Amoxicillin

B

Figure 5. (A) Surface visualization of the binding pocket highlighting the interaction residues involved in Allicin binding to DNA gyrase and topoisomerase 4. Amino acid residues forming hydrogen bonds with allicin are indicated by yellow dotted lines, while the corresponding 2D protein–ligand interaction diagrams illustrate the interactions of DNA gyrase and topoisomerase with allicin, respectively. Interacting residues are shown in green. **(B)** Surface representation of the binding pocket showing the interacting residues associated with amoxicillin binding to DNA gyrase and topoisomerase 4. Hydrogen bond interactions with amoxicillin are depicted using yellow dotted lines, and the corresponding 2D protein-ligand interaction diagrams present the interactions of DNA gyrase and topoisomerase with amoxicillin, respectively. Interacting residues are highlighted in green.

Discussion

Dental caries remains a complex and multifactorial disease in which microbial factors play a central role in disease initiation and progression [2], [5]. The present study provides an integrated analysis of demographic characteristics, molecular identification of cariogenic bacteria, antimicrobial susceptibility patterns, and the potential role of garlic-derived compounds as alternative antimicrobial agents. By combining molecular diagnostics with experimental and computational approaches, this study provides a comprehensive perspective on both the detection and control of cariogenic bacteria. The demographic analysis revealed that individuals aged 20–40 years represented the largest proportion of dental caries cases. This finding is consistent with previous reports suggesting that lifestyle factors, dietary habits, and oral hygiene practices during early adulthood may contribute significantly to caries development [23], [24]. The higher prevalence of dental caries observed among males compared to females may be attributed to differences in oral hygiene behaviours, dietary patterns, and healthcare-seeking behaviour. Furthermore, the predominance of once-daily brushing among the study population underscores the importance of oral hygiene practices as a key modifiable risk factor for dental caries [25].

Molecular identification using PCR confirmed the polymicrobial nature of dental caries. *Streptococcus mutans* and *Lactobacillus acidophilus* were the most frequently detected species, supporting their well-established role in enamel demineralization, acid production, and disease progression [26]. The detection of *Staphylococcus aureus* and *Porphyromonas gingivalis* in a subset of samples suggests that these bacteria may contribute to disease severity, secondary infections, or periodontal complications, particularly in mixed infections[27]. The observed discrepancies between PCR and culture-based identification, especially for fastidious organisms, highlight the comparatively sensitivity and specificity of molecular methods in detecting cariogenic bacteria [28]. Antibiotic susceptibility testing revealed considerable resistance among the isolated cariogenic bacteria to commonly prescribed antibiotics such as amoxicillin, ampicillin, and erythromycin. These findings align with growing global concerns regarding antimicrobial resistance and emphasize the limitations of relying solely on conventional antibiotics for managing dental caries–associated infections [13]. In contrast, higher susceptibility rates were observed for ciprofloxacin, clindamycin, and vancomycin; however, their use may be limited by cost, adverse effects, and the risk of further resistance development. In this context, the evaluation of garlic extract as a natural antimicrobial agent becomes relevant. Garlic extract demonstrated notable antibacterial activity against a large proportion of the tested isolates, surpassing several conventional antibiotics [29], [30]. This finding supports previous studies reporting the broad-spectrum antimicrobial properties of garlic and highlights its potential as an alternative or adjunctive agent in oral infection management. The effectiveness of garlic extract against antibiotic-resistant isolates further underscores its clinical relevance, particularly in settings where antibiotic resistance is prevalent[31], [32].

To further elucidate the molecular basis of the observed antibacterial activity, molecular docking analysis was employed using allicin, the principal bioactive compound derived from garlic. The docking results demonstrated strong binding affinities of allicin toward essential bacterial enzymes, including DNA gyrase and topoisomerase [18]. These enzymes play critical roles in bacterial DNA replication and cell survival, making them key antimicrobial targets. The formation of stable hydrogen bonds and hydrophobic interactions with conserved catalytic residues support a mechanistic explanation for the inhibitory effects observed *in vitro*. Importantly, the integration of *in vitro* antimicrobial susceptibility data with *in silico* docking analysis strengthens the biological plausibility of the findings [33]. While antibiotic susceptibility testing reflects phenotypic responses, molecular docking offers insight into the underlying molecular interactions that may drive these responses. The ability of allicin to interact with multiple bacterial targets suggests a multi-target mode of action, which may reduce the likelihood of resistance development compared to single-target antibiotics.

Overall, this study highlights the value of combining molecular diagnostics, antimicrobial susceptibility testing, and computational modelling to better understand and manage dental caries. The findings support the potential use of garlic-derived compounds as complementary antimicrobial agents and encourage further investigation into their clinical applicability, safety, and efficacy.

Conclusion

This study provides a comprehensive evaluation of the antimicrobial potential of *Allium sativum* extract against cariogenic bacteria, integrating molecular diagnostics, in vitro susceptibility testing, and in silico molecular docking analysis. The findings confirmed the polymicrobial nature of dental caries, with *Streptococcus mutans* and *Lactobacillus acidophilus* as the predominant species and highlighted a concerning level of resistance to commonly prescribed antibiotics such as amoxicillin, ampicillin, and erythromycin. Notably, garlic extract exhibited substantial antibacterial activity, with most isolates showing sensitivity, supported by strong molecular interactions of allicin with essential bacterial enzymes including DNA gyrase and topoisomerase. Collectively, these results underscore the potential of garlic-derived compounds as alternative or complementary agents in the management of dental caries. Future scope: Further research is warranted to validate these findings in vivo, explore optimized formulations of garlic-based oral therapeutics, and assess clinical safety and efficacy. Expanding such studies could contribute to the development of sustainable, plant-based strategies to combat antimicrobial resistance in oral infections.

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