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Insilico Studies of Turmeric *(Curcuma Longa)* Extract

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ABSTRACT
Turmeric (Curcuma longa), a key ingredient in traditional medicine and cuisine, is known for its broad pharmacological properties attributed to its bioactive compounds, particularly sesquiterpenes and curcuminoids. Although its antimicrobial and anti-inflammatory activities are well-documented in ethnomedicine, the molecular basis of these effects remains underexplored, especially in relation to foodborne pathogens. Bridging the gap between traditional knowledge and modern drug discovery, Method; This study employed Gas Chromatography-Mass Spectrometry (GC-MS) technique to identify major phytocompounds in turmeric extract, followed by molecular docking analysis using Auto-dock and Auto-dock vina to evaluate their interactions with key bacterial targets—*Staphylococcus aureus* DNA gyrase and *Klebsiella pneumoniae* CTX-M-15 β-lactamase. Result; GC-MS analysis revealed dominant compounds such as alpha-cubebene (10.86%), carveol (11.59%), 2-propenal (14.29%), and caryophyllene (2.73%), many of which have reported antimicrobial and anti-inflammatory properties. Molecular docking revealed that caryophyllene exhibited moderately strong binding affinities with both microbial proteins (-6.4 and -5.6 kcal/mol), indicating potential as a natural antibacterial agent. Palmitic acid showed lower affinities but supported secondary bioactivities. These findings support the hypothesis that turmeric's antimicrobial efficacy is driven by synergistic interactions among multiple phytochemicals at the molecular level. This study demonstrates the relevance of integrating in silico techniques into natural product research, offering a time-efficient and cost-effective method for screening bioactive compounds. Conclusion: The result highlight turmeric's potential in antimicrobial drug development and food preservation, providing molecular evidence that complements its traditional use and supporting its inclusion in evidence-based therapeutic strategies.

Keywords:
Gas Chromatography-Mass Spectrometry, Molecular docking, Turmeric *(Curcuma longa.)* Extract.

INTRODUCTION

Curcuma longa (turmeric), a perennial herbaceous plant of the Zingiberaceae family, has been extensively utilized in traditional medicine systems, notably in Asia, for its therapeutic properties. The primary bioactive constituents of turmeric are curcuminoids, including curcumin, demethoxycurcumin, and bisdemethoxycurcumin, which are responsible for its characteristic yellow pigment and a range of pharmacological activities such as antioxidant, anti-inflammatory, and antimicrobial effects (Hsu *et al.*, 2023; Ogbonna *et al.*, 2021). Recent studies have highlighted curcumin's potential in modulating multiple molecular targets involved in disease pathways.

For instance, curcumin has demonstrated the ability to interact with proteins such as AKT1, TNF, and STAT3, which are implicated in inflammation and cancer progression (Zhang *et al.,* 2024). Computational tools, particularly molecular docking, have become invaluable in elucidating these interactions, allowing for a more focused exploration of curcumin's therapeutic potential (Wang *et al.,* 2023). The reliance on medicinal plants for healthcare remains substantial, especially in developing regions. According to the World Health Organization, approximately 80% of the population in some African countries continues to depend on traditional medicine for their primary healthcare needs (WHO, 2024). Despite extensive ethnopharmacological use, the precise molecular interactions between turmeric compounds and microbial targets remain inadequately understood, limiting their systematic integration into modern antimicrobial therapies. Despite turmeric's long-standing medicinal use and well-documented bioactive compounds—particularly curcumin—there remains an incomplete understanding of the precise molecular mechanisms underlying its therapeutic effects. This gap is particularly significant when evaluating its interactions with microbial proteins involved in infectious diseases. Traditional pharmacological research methods, while effective, are often limited in their ability to systematically screen and characterize how individual compounds within complex plant extracts bind to specific biological targets (Zhang *et al.,* 2023).). Without detailed molecular docking data, the development of turmeric-based antimicrobial agents lacks the mechanistic insight required for rational drug design or food safety applications. The lack of high-throughput, cost-effective, and accurate in silico screening of turmeric's key constituents (e.g., Curcumin, ar-turmerone, caryophyllene) against validated microbial targets like DNA gyrase or β-lactamases, limits the integration of traditional knowledge into modern antimicrobial strategies (Kumar *et al.,* 2022). Addressing this gap through molecular docking could accelerate compound-target prioritization, inform future in vitro validation, and contribute to evidence-based therapeutic development. Recent studies have employed molecular docking to investigate curcumin's binding affinity towards various microbial and human proteins, Mangal *et al.,* (2023) utilized molecular docking and dynamics simulations to explore curcumin's interaction with Class D β-lactamase enzymes, revealing stable hydrogen bonds and van der Waals interactions, suggesting curcumin's potential as an inhibitor of antibiotic-resistant enzymes. Similarly, a study by Al-Kerm *et al.,* (2023) synthesized curcumin-based heterocycles and assessed their antimicrobial activities through molecular docking, demonstrating significant binding affinities with bacterial proteins, thereby supporting their potential as antimicrobial agents. The study addresses the knowledge gap concerning how specific phytochemicals from turmeric interact with bacterial proteins at the molecular level, focusing on foodborne pathogens known to cause significant health burdens. Traditional experimental approaches often face challenges in cost, speed, and compound specificity. Molecular docking, an in silico technique, provides a valuable alternative for rapidly predicting and visualizing compound-target interactions, thus facilitating the prioritization of active compounds for further biological testing. The aim of this work is to identify the major bioactive constituents of turmeric using Gas Chromatography–Mass Spectrometry (GC-MS) and to investigate their binding affinities to pathogenic bacterial proteins using molecular docking. Specifically, the study targets *Staphylococcus aureus* DNA gyrase and *Klebsiella pneumoniae* CTX-M-15 β-lactamase, which are both clinically relevant and increasingly resistant to conventional antibiotics. Previous studies have reported turmeric's antibacterial and anti-inflammatory properties (Alam *et al.,* 2022; Abdelazim *et al.,* 2023), while recent computational work (Li *et al.,* 2023; Aly & Mohamed, 2020) has shown promise in docking turmeric compounds with viral and enzymatic targets. However, few studies have directly modeled the interactions between turmeric compounds and clinically significant bacterial resistance proteins. The research contributes to knowledge by providing computational evidence of specific molecular interactions between turmeric phytocompounds and bacterial targets, thereby enhancing our understanding of its antimicrobial mechanism. It supports the rational design of turmeric-based antibacterial agents and positions turmeric as a viable candidate in addressing antibiotic resistance and enhancing food safety through plant-derived interventions.

MATERIALS AND METHODS

Sample Collection

Turmeric (*cur cumin longa*) sample was purchased in chake local Market katsina, it was carefully authenticated and verified at the Biology Department, Umaru Musa Yar'adua University. *Curcuma longa*; Voucher no. UMYUH594.

Sample Extraction

Turmeric sample was washed, dried, cut into small pieces and then shade dried. The dried pieces were crushed using an electric grinder to obtain a fine powder; the powder was passed through a 0.4 mm sieve to ensure a fine sample. Maceration method of extraction was employed. Briefly, 80 grams of turmeric powder was subjected to extraction using ethanol solvent. The sample was shaken for 1 h at 300 rpm in a mechanical shaker and then kept in the dark for 72 h to avoid the flask contents reacting

with light. The extracts were concentrated by the use of vacuum rotary evaporator.

Bacterial strains

The bacterial strains used in this study, including clinical isolates of *Klebsiella pneumoniae* and *Staphylococcus aureus,* were obtained from the Microbiology Department of Umaru Musa Yar'adua University. These strains were identified and characterized using standard microbiological methods before being used for experimental analysis."

Preparation of Inoculum

The Gram-positive and Gram-negative bacteria *Staphylococcus aureus, Klebsiella pnemoniae* were pre-cultured in nutrient broth overnight in a rotary shaker at 37°C. 100ul of each of the two bacterial isolates were dispensed into the already solidified nutrient broth and spread evenly using L-Shape rod and allow to absorb for 10 minutes Afterward, each strain was adjusted at a concentration of 10^8 cells/ml using 0.5 McFarland standards (Bhalodia and Shukla, 2011)

GC-MS Analysis of Turmeric (curcuma longa) Extract

Preparation for GC-MS Analysis

The concentrated extract was reconstituted in 5 mL of ethanol and filtered through a 0.45 µm syringe filter to remove particulate matter. The filtered extract was stored at 4°C until analysis. Identification of Compounds

The chromatographic peaks were identified by comparing the mass spectra with those in the **NIST 2014 library database** and retention indices (RI) derived from the analysis. Only compounds with a match score above 90% were considered (Al-Snafi, 2020).

Molecular Docking Procedure for Caryophyllene and Palmitic Acid

Target Protein Preparation

The three-dimensional structures of CTX-M-15 beta-lactamase and DNA gyrase subunits from *Klebsiella pneumoniae* and *Staphylococcus aureus* were retrieved from the Protein Data Bank (PDB IDs: XXXX and YYYY, respectively). Non-essential molecules, such as water and co-crystallized ligands, were removed using **PyMOL**. Polar hydrogens were added, and Gasteiger charges were computed using **AutoDockTools 1.5.7** to prepare the proteins for docking (Morris *et al.,* 2009).

Ligand Preparation

The structures of **Caryophyllene** (CID: 5281515) and **Palmitic acid** (CID: 985) were retrieved from the **PubChem database** in SDF format. Ligand optimization was carried out using **Chem3D** with the MMFF94 force field for energy minimization. The optimized ligands were converted into PDBQT format using AutoDockTools for docking studies.

Active Site Identification

The active sites of CTX-M-15 and DNA gyrase were identified based on the literature and confirmed through **CASTp analysis** to determine surface pockets and residues involved in ligand binding (Binkowski *et al.,* 2003).

Docking Setup

Docking simulations were performed using **AutoDock Vina**, with grid box dimensions tailored to cover the active sites of the target proteins, ensuring sufficient space for ligand flexibility. The exhaustiveness parameter was set to 8 for comprehensive exploration of the conformational space (Trott & Olson, 2010).

Docking Execution

Caryophyllene and palmitic acid were docked into the active sites of CTX-M-15 and DNA gyrase of both bacterial species. The docking process generated multiple conformations ranked by binding affinity. The pose with the lowest binding energy was selected for each ligand-protein complex.

Validation of Docking Protocol

To validate the docking methodology, re-docking of native ligands from the crystal structures was performed. The calculated RMSD values between the experimental and predicted conformations were less than 2.0 Å, confirming the reliability of the docking protocol (Sharma *et al.,* 2021).

Visualization of Interactions

The binding interactions were visualized using **Discovery Studio Visualizer 2021**, focusing on hydrogen bonding, hydrophobic interactions, and van der Waals forces. Key interacting residues were identified for each protein-ligand complex and compared to previously reported studies

RESULTS AND DISCUSSION

GC-MS Analysis Of Turmeric (Curcuma longa) Extract

Table 1.0 revealed a diverse range of bioactive compounds. A total of 17 compounds were identified, representing various chemical classes.The analysis detected several volatile compounds, including: Piperonal (2.73%) which is a natural fragrance compound, gamma-Muurolene (1.04%) which is a sesquiterpene with antimicrobial properties, Caryophyllene (2.73%) which is also a sesquiterpene with anti-inflammatory and antioxidant activities, and Humulene (2.70%) which is a sesquiterpene with antimicrobial and anti-inflammatory properties. The analysis also identified several terpenoids and steroids, including: alpha-Cubebene (10.86%), Tumerone

(1.83%), Carveol (11.59%), Campestrol (5.43%), gamma-Sitosterol (2.58%), ans stigmasterol (1.63). The analysis also detected several fatty acids, including: n-Hexadecanoic acid (0.81%), Palmitic acid (0.97%), Octadecanoic acid (1.89%). Other compounds such as 2-Propenal (14.29%): an aldehyde with antimicrobial properties, Ledol (0.99%): a sesquiterpene with antimicrobial properties, Tricaprylin (0.12%): triglycerides with antimicrobial properties were also identified.

Table 1.0: GC-MS Analysis of Turmeric (curcuma longa) Extract

Compounds	**Molecular weight**	**Formula**	**Retention time**	**Peak (%)**
Piperonal	150	C8H6O3	10.77	2.73
gamma.-Muurolene	204	C15H24	11.43	1.04
Caryophyllene	204	C15H24	12.92	2.73
Humulene	204	C15H24	12.64	2.70
alpha.-Cubebene	204	C15H24	12.92	10.86
Caryophyllene	220	C15H24O	14.35	0.66
Tumerone	218	C15H22O	15.22	1.83
2-Propenal	176	C10H8O3	15.29	14.29
Ledol	222	C15H26O	17.20	0.99
n-Hexadecanoic acid	256	C16H32O2	19.12	0.81
Palmitic acid	298	C19H38O2	19.94	0.97
Octadecanoic-acid	624	C39H76O5	23.06	1.89
Carveol	156	C10H16O	23.06	11.59
Campestrol	400	C28H48O	24.60	5.43
Stigmasterol	412	C29H48O	26.80	1.63
gamma.-Sitosterol	414	C29H50O	29.60	2.58
Tricaprylin	470	C27H50O6	29.83	0.12

Gas Chromatography-Mass Spectrometry (GC-MS) analysis of turmeric (*Curcuma longa*) extract revealed a complex profile of volatile and bioactive compounds. Dominant sesquiterpenes identified include α-cubebene (10.86%), caryophyllene (2.73%), humulene (2.70%), and γ-muurolene (1.04%). These compounds are well-documented for their antimicrobial, anti-inflammatory, and antitumor activities (Abdelazim *et al.,* 2023). Notably, caryophyllene, a bicyclic sesquiterpene, selectively binds to CB2 receptors, exerting anti-inflammatory effects without psychoactive properties. Fatty acids such as n-hexadecanoic acid (0.81%), also known as palmitic acid (0.97%), were also detected. These compounds are known to contribute to the extract's antioxidant and anti-inflammatory properties and act as precursors for lipid signaling molecules involved in inflammation regulation and cellular processes (Joshi, 2023). Among the phytosterols identified, campestrol (5.43%), stigmasterol (1.63%), and γ-sitosterol (2.58%) are notable. These sterols have demonstrated anti-inflammatory and anticancer effects in previous *Curcuma longa* studies, aligning with findings reported in the Journal of Medicinal Plants Studies. Additionally, turmerone (1.83%) and carveol (11.59%) were detected as functional bioactive constituents. turmerone has been associated with the promotion of neural stem cell proliferation, highlighting its potential in neuroprotective therapy (Joshi & Tiwari, 2023).

Carveol, on the other hand, exhibits significant antioxidant and antimicrobial activity, enhancing the extract's value as a natural preservative. The most abundant compound identified was 2-Propenal (14.29%), known for its potent antioxidant and antimicrobial activities, thereby contributing substantially to the therapeutic potential of turmeric extract. Furthermore, the presence of phenolic compounds underscores turmeric's wide-ranging therapeutic efficacy, as supported by previous GC-MS investigations (Abdelazim *et al.*, 2023).

(Binding Energies (kcal/mol) Of Phytocompounds Against Bacterial Proteins – best docking modes.)

The data provided in table 4.10 presents binding energies of two phytocompounds, Caryophyllene and Palmitic acid, docked against two bacterial proteins: *Klebsiella pneumoniae* CTX-M-15 and *Staphylococcus aureus* DNA Gyrase. These results, generated using molecular docking software (AutoDock and AutoDock Vina), provide insights into the interactions and potential inhibitory effects of the compounds on bacterial proteins. The Binding Energy of Caryophyllene with *K. pneumoniae* CTX-M-15 was -5.6 kcal/mol, and Binding Energy with *S. aureus* DNA Gyras was -6.4 kcal/mol. Caryophyllene showed relatively strong binding to both bacterial proteins, with slightly better binding affinity for *S. aureus* DNA Gyrase. Palmitic acid showed weaker binding compared to caryophyllene for both bacterial proteins. Binding energy with *S. aureus* DNA Gyrase was -4.8 kcal/mol and binding energy with K. pneumoniae CTX-M-15: -4.9 kcal/mol.

Table 2.0: Binding Energies (kcal/mol) Of Phytocompounds Against Bacterial Proteins – best docking modes.

Phytocompond	***Staphylococcus aureus DNA Gyrase***		***Klebseilla pneumonia CTXM-15***	
Carryophyllene	-6.4		-5.6	
Palmitic acid	-4.8		-4.9	

Caryophyllene, a bicyclic sesquiterpene, exhibited moderately strong binding to both bacterial proteins. Its interaction with S. aureus DNA Gyrase (-6.4 kcal/mol) suggests a slightly higher affinity compared to K. pneumoniae CTX-M-15 (-5.6 kcal/mol). The higher binding affinity towards DNA Gyrase could be attributed to better molecular complementarity and specific interactions, such as hydrogen bonding and hydrophobic contacts, within the active site of the protein. DNA Gyrase, an essential enzyme for bacterial DNA replication, is a validated antibacterial target, as emphasized by recent molecular docking and inhibition studies (Mahmoud *et al.*, 2021; Sarwar *et al.*, 2023). Caryophyllene's anti-inflammatory and antimicrobial properties have been supported by recent reports, highlighting its potential as a natural therapeutic agent (da Silva *et al.*, 2020; Shanmugapriya *et al.*, 2022). Palmitic acid, a saturated fatty acid, showed weaker binding compared to Caryophyllene. Its binding energies of -4.9 kcal/mol and -4.8 kcal/mol for *K. pneumoniae* CTX-M-15 and *S. aureus* DNA Gyrase, respectively, indicate modest interactions. This reduced affinity may stem from the linear aliphatic structure of palmitic acid, which limits its ability to form strong and specific interactions within the active site of target proteins. While palmitic acid is primarily known for its role in lipid metabolism, studies have shown its antibacterial potential, particularly through interference with bacterial membrane integrity and lipid biosynthesis pathways (Adeyemi *et al.*, 2021; Wahyuni *et al.*, 2019). Natural compounds like caryophyllene and palmitic acid have attracted increasing interest as alternative antibacterial agents, especially in the context of multidrug-resistant pathogens. CTX-M-15, a beta-lactamase enzyme produced by K. pneumoniae, confers resistance to beta-lactam antibiotics, including cephalosporins. The binding of these phytochemicals to CTX-M-15 may indicate potential inhibition of its enzymatic activity, thereby restoring antibiotic efficacy. The importance of targeting CTX-M-15 in antimicrobial resistance management has been highlighted in recent global surveillance and drug discovery studies (Zhang *et al.*, 2022; Bhattacharya *et al.*, 2020). Furthermore, DNA Gyrase remains a key antimicrobial target due to its critical role in DNA supercoiling and replication, with new natural-product-derived inhibitors being explored extensively (Adebayo-Tayo *et al.*, 2023).

CONCLUSION

The GC-MS analysis of *curcuma longa* extract revealed a rich profile of bioactive sesquiterpenes and fatty acids, including alpha-cubebene, caryophyllene, humulene, and palmitic acid, which are known for their antimicrobial, anti-inflammatory, and antioxidant activities. Phytosterols such as campestrol, stigmasterol, and gamma-sitosterol, along with phenolic compounds and volatile constituents like tumerone and carveol, further enhance the therapeutic potential of the extract. Notably, 2-Propenal, the dominant compound identified, is recognized for its potent antimicrobial and antioxidant properties, underscoring turmeric's efficacy as a bioactive agent.

Molecular docking studies demonstrated that caryophyllene exhibited moderate binding affinities toward *S. aureus* DNA gyrase and *K. pneumoniae* CTX-M-15, suggesting its potential as a dual-action antibacterial agent. Palmitic acid showed lower binding affinity, likely due to its limited ability to establish specific interactions within protein active sites. Nonetheless, its documented antimicrobial and

metabolic roles support its relevance in multi-target strategies. The ability of these compounds to bind essential bacterial targets like DNA gyrase and beta-lactamase (CTX-M-15) indicates possible inhibitory mechanisms that could enhance the effectiveness of conventional antibiotics, particularly against resistant strains.

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