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Original Article

Antimicrobial Evaluation, LC-MS Characterization and Computational Molecular Study of Ethanol Extract of Marine Macro Algae *Sargassum tenerrimum* J. Agardh

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ABSTRACT

Objectives: The current research was aimed to assess the antimicrobial activity and LC-MS characterization, and computational molecular analysis of the ethanolic extract of marine macro algae *Sargassum tenerrimum* J. Agardh. **Materials and Methods:** Marine macro algae *S. tenerrimum* collected from the coastal sediment was shade-dried, ground into powder, extracted by soxhlation using ethanol as the solvent. The dried extract obtained underwent phytochemical assessment and evaluation of antimicrobial activity including Minimum Inhibitory Concentration (MIC). The active components in the extract were analyzed by Liquid Chromatography-Mass Spectrometry (LC-MS). Molecular docking study and Molecular Dynamic Simulations (MDS) on the docked complex were performed using PrankWeb and Desmond 2020.1, respectively. **Results:** Presence of Alkaloids, Glycosides, Phenolic compounds, Flavonoids, Saponins, Sterols, Tannins, Terpenoids, Carbohydrates, Proteins and amino acids were found in the phytochemical evaluation. In antimicrobial study, the Gram-positive bacteria such as *Enterococcus faecalis* and *Staphylococcus aureus* as well as the fungal pathogen *Candida albicans* were found to be inhibited. Some prominent compounds such as 3-Hexanone,2,5-dimethyl-; Pentadecanal; Cyclohexylethylamine; were identified in the LC-MS evaluation. In the docking and MDS evaluation, the compound, cyclohexylethylamine showed considerable structural and binding stability, and forms a thermodynamically stable complex. **Conclusion:** Outcome of this study indicated that Cyclohexylethylamine is a promising candidate, worthy for further biological or drug development studies.

Keywords: Antimicrobial activity, LC-MS study, Molecular dynamic simulations study, Preliminary phytochemical evaluation, *Sargassum tenerrimum* J. Agardh.

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INTRODUCTION

The biodiversity found in the Earth's most extensive habitat, the ocean, indicating a significant potential for discovering new bioactive compounds. Substances extracted from marine life exhibit unique structures and influence human disease targets through innovative mechanisms of action. The exploration of compounds derived from marine sources as potential medicinal agents has only commenced in recent times (Francesch *et al.*, 2024). It was not until the 1950s, with the emergence of scuba diving and advanced sampling technologies that researchers started to methodically explore the oceans for beneficial therapeutics. Numerous compounds of this nature lack terrestrial counterparts and possess distinct chemical structures and biological activities. Their potential applications as pharmaceuticals or as frameworks for medicinal chemistry render these products particularly intriguing for human use. Marine life, including sponges, tunicates, fish, soft corals, nudibranchs, sea hares, opisthobranch mollusks, echinoderms, bryozoans, prawns, shells, sea slugs, and marine microorganisms, provides a variety of bioactive compounds (Sahu *et al.*, 2022).

Marine macroalgae, commonly referred to as seaweeds, are regarded as significant sources of biomolecules within the marine ecosystem. They generate a diverse range of structurally distinct secondary metabolites that have numerous applications across various sectors, including the food and textile industries, biochemistry, and pharmacological uses in both human and veterinary medicine (Rizzo *et al.*, 2017; Vimala and Poonghuzhali, 2017). *Marine macroalgae* are recognized for their antimicrobial, antitumor, anti-inflammatory, anti-diabetic, antiprotozoal, antiviral, and antioxidant properties. The bioactive compounds they contain responsible for these properties.

The increasing emergence of antimicrobial-resistant pathogens, together with the limited structural diversity of existing

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antimicrobial drugs, necessitates the discovery of new antimicrobial agents. Marine organisms represent a particularly promising source because their enormous and relatively underexplored biodiversity provides access to chemically diverse and structurally unique secondary metabolites with potentially novel mechanisms of antimicrobial action (Newman and Cragg, 2020; Blunt *et al.*, 2018). In light of these considerations, it was decided that a study on *Marine macroalgae* would be conducted, aiming to establish a foundation for future research.

MATERIALS AND METHODS

Sample Collection and Authentication

Marine macroalgae samples were handpicked from the ground sediment at a depth of 0-10 cm in the coastal area of Ramanathapuram, Tamil Nadu, India (latitude: 9.328077°, longitude: 78.330236°). Two distinct samples, designated as A1 and A2, were collected and washed with sterile water to eliminate impurities. The samples underwent shade drying until achieving a moisture content of 21.53±0.05% (wet basis) at a temperature of 26±2°C. Subsequently, the dried samples were sterilized by rinsing with dilute formic acid, followed by sterile water, and moisture was removed using cellulose filter paper. The sterilized samples were identified and authenticated by the Botanical Survey of India (BSI) in Kolkata. Sample A1 was identified as *Padina gymnospora* (Kuetz.) Sonder, while sample A2 was identified as *Sargassum tenerrimum* J. Agardh. (No.: CNH/Tech. II/2024/).

Powdering and extraction

The present study focused on sample A2, *S. tenerrimum*. The shade dried material of *S. tenerrimum* was ground into a powder using a mixer grinder. The resulting powder was stored in LDPE bags at a temperature of -20°C. The extraction of the powdered material was performed using the Soxhlet extraction method with ethanol as the solvent. Approximately 500 g of the powdered material was moistened with the solvent, placed in the Soxhlet extractor, and extracted with 500 mL of the solvent. The extract obtained was then filtered, and the solvent was distilled off to yield the dried extract. The percentage yield of the dried extract was subsequently calculated.

$$\text{Percentage yield} = \frac{\text{Weight of dry extract}}{\text{Weight of crude drug extracted}} \times 100$$

Preliminary phytochemical analysis

The prepared extract was assessed for the presence of phytochemicals including alkaloids, glycosides, phenolic compounds, tannins, flavanones, flavonoids, carbohydrates, proteins and amino acids, saponins, sterols, terpenoids as well as gum and mucilage. This evaluation was conducted following the procedures outlined in the published literature (Sebastin *et al.*, 2019; Anoob *et al.*, 2020).

In vitro antimicrobial activity

The assessment was conducted by agar well diffusion method in accordance with the methodology outlined in prior literature (Vimala and Poonghuzhali, 2017; Shama *et al.*, 2018; Avila-Romeroa *et al.*, 2023). Muller Hinton agar and Nutrient broth media were used in the antibacterial evaluation. Potato dextrose agar media was used in the antifungal evaluation. The bacterial and fungal culture were obtained from MTCC, Chandigarh, India, six pathogenic bacteria viz., Gram-positive organisms such as *Bacillus subtilis* (MTCC2394), *Enterococcus faecalis* (MTCC439), *Staphylococcus aureus* (MTCC3160), as well as Gram-negative organisms like *Escherichia coli* (MTCC1652), *Klebsiella pneumoniae* (MTCC109), *Proteus mirabilis* (MTCC3310), and *Pseudomonas aeruginosa* (MTCC4676) were screened in the antibacterial evaluation, while two fungal pathogens, viz., *Aspergillus niger* (MTCC282) and *Candida albicans* (MTCC3958), were screened in the antifungal evaluation. Cultures were adjusted to match the turbidity of a 0.5 McFarland standard, corresponding approximately to1.5 $\times 10^8$CFU/mL. Incubation temperature was 35±2°C. Incubation time were 18-24 hr and 24-48 hr for antibacterial assays and antifungal assays respectively. The Minimum Inhibitory Concentration (MIC) was established using the broth micro-dilution method using TTC as a viability indicator in accordance with CLSI guidelines (M07 for bacteria and CLSI M27 for *C. albicans* and CLSI M38 for *A. niger*).

LC-MS analysis

Chromatographic separation was performed on a Shimadzu LCMS-8045 system using PDA detection at 340 nm and ESI-MS in positive mode. The samples were dissolved in methanol, filtered through a 0.22 µm membrane, and analysed using a gradient of acidified aqueous phase and methanol over 30 min. Mass spectra were acquired over m/z 150-1000, and major constituents were characterized based on retention time, UV spectra, and MS/MS fragmentation.

Molecular docking evaluation

The compounds selected based on structural diversity, presence of potentially interactive functional groups, reported biological relevance, and suitability for protein-ligand interaction analysis were subjected to docking evaluation. The evaluation was designed in reference with the reports of Lakshmisundaram *et al.*, 2025; Chigurupathi *et al.*, 2025. For docking, the 3D structure of three ligands, 3-Hexanone,2,5-dimethyl and pentadecanal and cyclohexylethylamine and the targets were retrieved from the PubChem database. The Crystallographic 3D structures of the target protein Thymidylate kinase (PDB ID: 5UIV) and Exo-B-(1,3)-glucanase (PDB ID: 1EQP) from *C. albicans* was retrieved from the Protein Data Bank. The ligands were then processed using UCSF Chimera to prepare it for molecular docking, and ensuring proper 3D conformation. Then the ligands were

geometrically optimized using the AMBER ff14SB force field. Gasteiger charges were assigned to the ligand for calculating the electrostatic interactions during the docking process. Energy minimization was carried out using the AMBER force field (specifically ff14SB). The active site of the protein was predicted using PrankWeb. The structure was analysed using P2Rank to generate and rank potential binding sites based on ligand ability scores.

Molecular Dynamics Simulation study

Based on the results obtained in the molecular docking evaluation, Cyclohexylethylamine was selected for the Molecular Dynamics Simulation study. In reference with previous literatures (Fathima *et al.*, 2024; Franco *et al.*, 2024; Kumari *et al.*, 2025; Yanuar *et al.*, 2018), using the Desmond 2020.1, MD simulations were done on docked complex of 1EQP-Cyclohexylethylamine. The MM-GBSA (Molecular Mechanics/Generalized Born Surface Area) binding free energy was calculated using the Python script thermal mmgbsa.py in the simulation trajectory with the VSGB solvation model and the OPLS5 force field over last 50 frames with a 1-step sampling size. The binding free energy of MM-GBSA (kcal/mol) was estimated using the principle of additivity. ΔG_{bind} is calculated by,

$$\Delta G_{bind} = \Delta G_{MM} + \Delta G_{Solv} - \Delta G_{SA}$$

ΔG_{bind} - the binding free energy; ΔG_{MM} - difference between the free energies of ligand-protein complexes and the total energies of protein and ligand in isolated form; ΔG_{Solv} - difference in the GSA solvation energies of the ligand-receptor complex and the sum of the solvation energies of the receptor and the ligand in the unbound state; ΔG_{SA} - the difference in the surface area energies for the protein and the ligand.

RESULTS

In the current research, the extraction of the sample material gave a percentage yield of 45%. The results of preliminary phytochemical evaluation of the ethanol extract of *S. tenerrimum* showed the presence of alkaloids, glycosides, phenolic compounds, flavonoids, saponins, sterols, tannins, terpenoids, carbohydrate, protein and amino acid.

In the evaluation of antibacterial activity, the results showed that the gram-positive species viz., *Enterococcus faecalis*, and *Staphylococcus aureus* were inhibited significantly by the extract. Particularly, the *S. aureus* was highly inhibited with 19 mm of zone of inhibition comparing with *E. faecalis* which showed 17 mm of zone of inhibition. Regarding with the minimum inhibitory concentration, both the *E. faecalis* and *S. aureus* showed 150 µg/mL as MIC. In the antifungal evaluation, one of the two tested organisms, *C. albicans* was effectively inhibited by test extract which showed 23 mm zone of inhibition with MIC of 125 µg/mL.

The LC-MS analysis of the extract identified the presence of some prominent compounds (Table 1).

Results of molecular docking analysis of selected compounds against the target protein Thymidylate kinase and Exo-B-(1,3)-glucanase from *C. albicans* is shown in Table 2. Comparing with other tested compounds, pentadecanal exhibited the strongest binding affinity against the target protein Thymidylate kinase with a binding energy of -5.70kcal/mol (Figure 1) which clearly indicated that pentadecanal appears to be the most promising candidate among the three tested compounds against the target protein Thymidylate kinase.

In case of docking against the target protein Exo-B-(1,3)-Glucanase, comparing with other tested compounds, cyclohexylethylamine exhibited the strongest binding affinity with a binding energy of -8.06kcal/mol, (Figure 2), which suggested a highly favourable and stable interaction with the active site. Thus, cyclohexylethylamine, the promising lead compound was selected for the MDS study.

In the molecular dynamic simulation analysis of cyclohexylethylamine, the convergence of RMSD values suggested that no significant unfolding or ligand dissociation occurred, reflecting a stable and consistent binding interaction. The dynamic equilibrium observed in the final 100 ns, underscores that the 1EQP-Cyclohexylethylamine complex is conformationally stable. The RMSF plot of MDS confirmed that the 1EQP maintains structural stability upon ligand binding, with flexible regions limited to peripheral loops or termini, while the binding site remains structurally restrained-reinforcing the potential for a stable and functionally relevant complex formation. The Rg plot revealed that there are no sharp spikes or drastic drops in Rg that suggested transient unfolding, aggregation, or significant tertiary structure reorganization. It also strongly supported that the 1EQP retains its structural compactness and integrity upon binding with cyclohexylethylamine, validating the thermodynamic favorability and stability of the complex. The hydrogen bond analysis confirmed that the 1EQP-Cyclohexylethylamine complex is dynamically stable, potentially viable in downstream biological or pharmacological studies. The MM/GBSA results indicated a highly stable complex between the ligand and the protein.

Table 1: Some prominent compounds found in the LC-MS analysis of ethanol extract of *S. tenerrimum*.

Sl. No.	Compound name	Mol. Weight
1.	3-Hexanone,2,5-dimethyl-	128.3
2.	Pentadecanal	225.5
3.	Cyclohexylethylamine	127.3
4.	1-*O*-butyl 2-*O*-(6-ethyloctan-3-yl) benzene-1,2-dicarboxylate	363.4
5.	Propane, 1,3-bis(octadecyloxy)-	582.0

Overall, the negative ΔG_{bind} demonstrates that the complex is energetically favorable and stable, primarily due to van der Waals, electrostatic, and lipophilic interactions. These findings indicated that the ligand is well-accommodated in the binding site, and its strong interaction profile could be further optimized by enhancing hydrogen bonding or mitigating desolvation costs to develop even more potent analogs (Table 3 and Figure 3).

DISCUSSION

Marine macroalgae are rich in structurally diverse phytochemicals (Yu *et al.*, 2018; Mateos *et al.*, 2020; Hannan *et al.*, 2020; Afzal *et al.*, 2023; Kim *et al.*, 2018). The results of phytochemical analysis of this study is in accordance with the previous literature. The present study demonstrated antimicrobial activity in the ethanol extract of the *S. tenerrimum*, indicating the presence of biologically active metabolites capable of interfering with microbial growth. The antimicrobial potential of *S. tenerrimum* is consistent with previous investigations in which different solvent extracts of this species exhibited activity against both bacterial and fungal microorganisms (Manivannan *et al.*, 2011). These findings support the potential of *S. tenerrimum* as a source of antimicrobial constituents.

The LC-MS investigation of the present study notably identified the presence of three compounds 3-Hexanone, 2,5-dimethyl-, Pentadecanal and Cyclohexylethylamine. The occurrence of these compounds in *S. tenerrimum* is also supported by an independent study carried out by Kalasariya and Patel 2011.

3-Hexanone, 2,5-dimethyl- is a low-molecular-weight aliphatic ketone with a carbonyl functional group. Although direct experimental evidence for antimicrobial activity of the purified 2,5-dimethyl-3-hexanone molecule is limited, structurally related aliphatic ketones have shown antimicrobial or antifungal effects. Therefore, its presence in the ethanol extract may contribute to the observed bioactivity (Saitkulova *et al.*, 1989). The presence of a carbonyl group in 3-Hexanone, 2,5-dimethyl- provides a potential site for hydrogen-bonding interactions with amino-acid residues in microbial proteins. Therefore, its detection in the

Table 2: Binding interactions between ligand and target proteins in molecular docking analysis.

Sl. No.	Target	Compound Name	Binding Energy
1.	Thymidylate kinase (PDB ID: 5UIV)	3-Hexanone,2,5-dimethyl-	-5.13
2.		Cyclohexylethylamine	-4.20
3.		Pentadecanal	-5.70
4.	Exo-B-(1,3)-Glucanase (PDB ID: 1EQP)	3-Hexanone,2,5-dimethyl-	-4.00
5.		Cyclohexylethylamine	-8.06
6.		Pentadecanal	-4.74

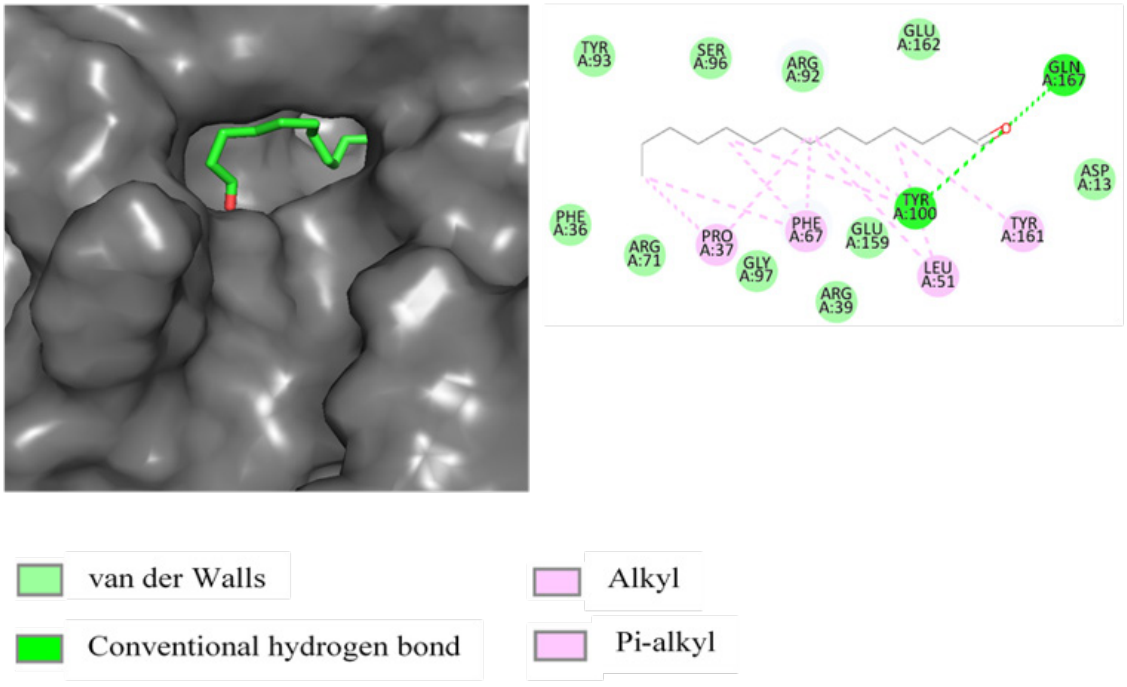

Figure 1: Thymidylate kinase complex with Pentadecanal. (Image generation: Prank Web).

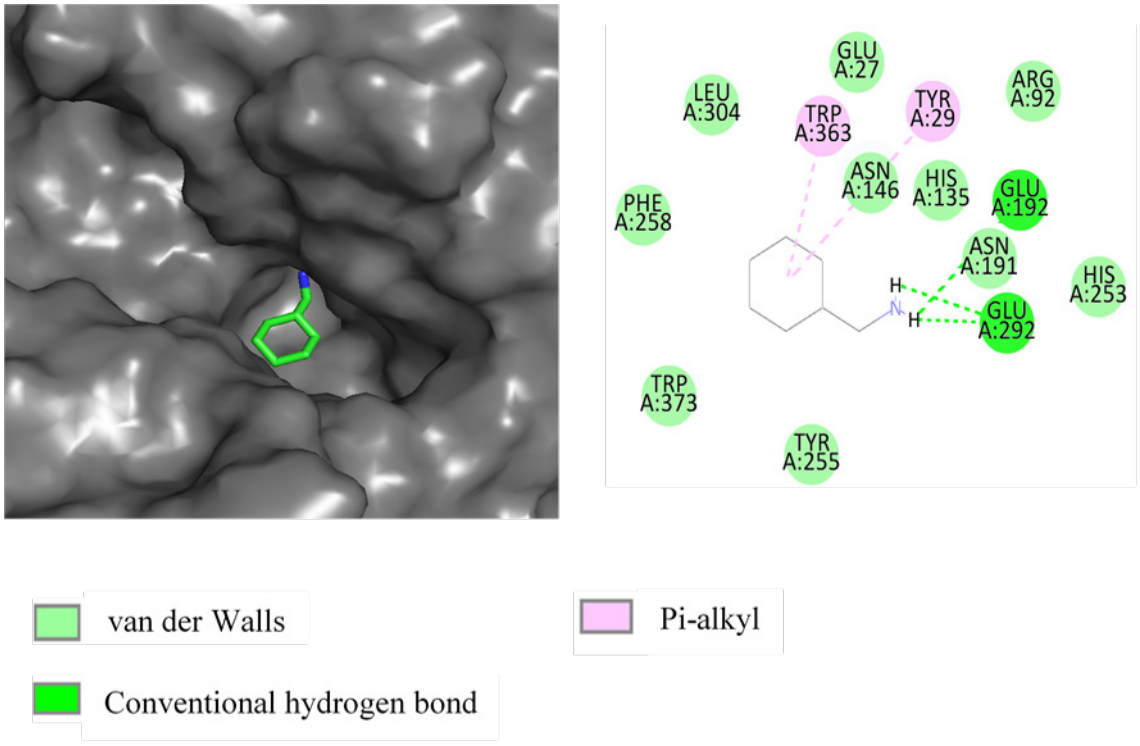

Figure 2: Exo-B-(1,3)-glucanase complex with Cyclohexylethylamine. (Image generation: Prank Web).

Table 3: Binding free energy calculations for 1EQP and Cyclohexylethylamine by MMGBSA analysis.

Energies (kcal/mol)	1EQP and Cyclohexylethylamine
ΔG_{bind} (total binding free energy)	-47.76
ΔG_{bind}Lipo (lipophilic contribution)	-6.15
ΔG_{bind}vdW (van der Waals)	-20.12
ΔG_{bind}Coulomb (electrostatic interactions)	-14.51
$\Delta G_{bind}H_{bond}$ (hydrogen bonding)	-0.64
ΔG_{bind}SolvGB (generalized born solvation energy	22.14
ΔG_{bind}Covalent (covalent interactions)	0.22
ΔG_{bind}Packing (Packing energy)	-0.69

Negative values favour binding.

ethanol extract may be relevant to the overall antimicrobial potential (Kalasariya and Patel 2011).

Pentadecanal represents a particularly interesting candidate because experimental evidence exists for its antibacterial and anti-biofilm properties. Pentadecanal is a long-chain fatty aldehyde, and its aldehyde functionality together with its hydrophobic hydrocarbon chain may facilitate interaction with microbial cell-associated components. Experimental studies of (Venuti *et al.*, 2022). Demonstrated that purified pentadecanal inhibited the growth of *Listeria monocytogenes*, with a reported MIC of 0.6 mg/mL. In another study, pentadecanal displayed anti-biofilm activity against *Staphylococcus epidermidis* (Casillo *et al.*, 2017).

Cyclohexylethylamine represents a nitrogen-containing aliphatic amine in the extract. Its primary amine functional group and a hydrophobic cyclohexyl moiety, providing two chemically different features that may contribute to ligand-protein interactions. The amine group can participate in hydrogen bonding and, depending on the protonation state and microenvironment, electrostatic interactions with acidic residues within a protein binding site. The cyclohexyl group can additionally contribute hydrophobic interactions. Thus, this compound provides a structurally distinct candidate compared with the oxygen-containing ketone and aldehyde metabolites. The biological relevance of cyclohexylethylamine is supported by an investigation in which the cyanobacteria and green algae reported (S)-(+)-1-cyclohexylethylamine as the major GC-MS component of a *Microcystis aeruginosa* extract, representing approximately 91.9% of the detected profile, in a study in which algal extracts demonstrated activity against human pathogenic microorganisms. However, the study did not establish that purified cyclohexylethylamine itself was responsible for the antimicrobial activity (Al-Wathnani *et al.*, 2012).

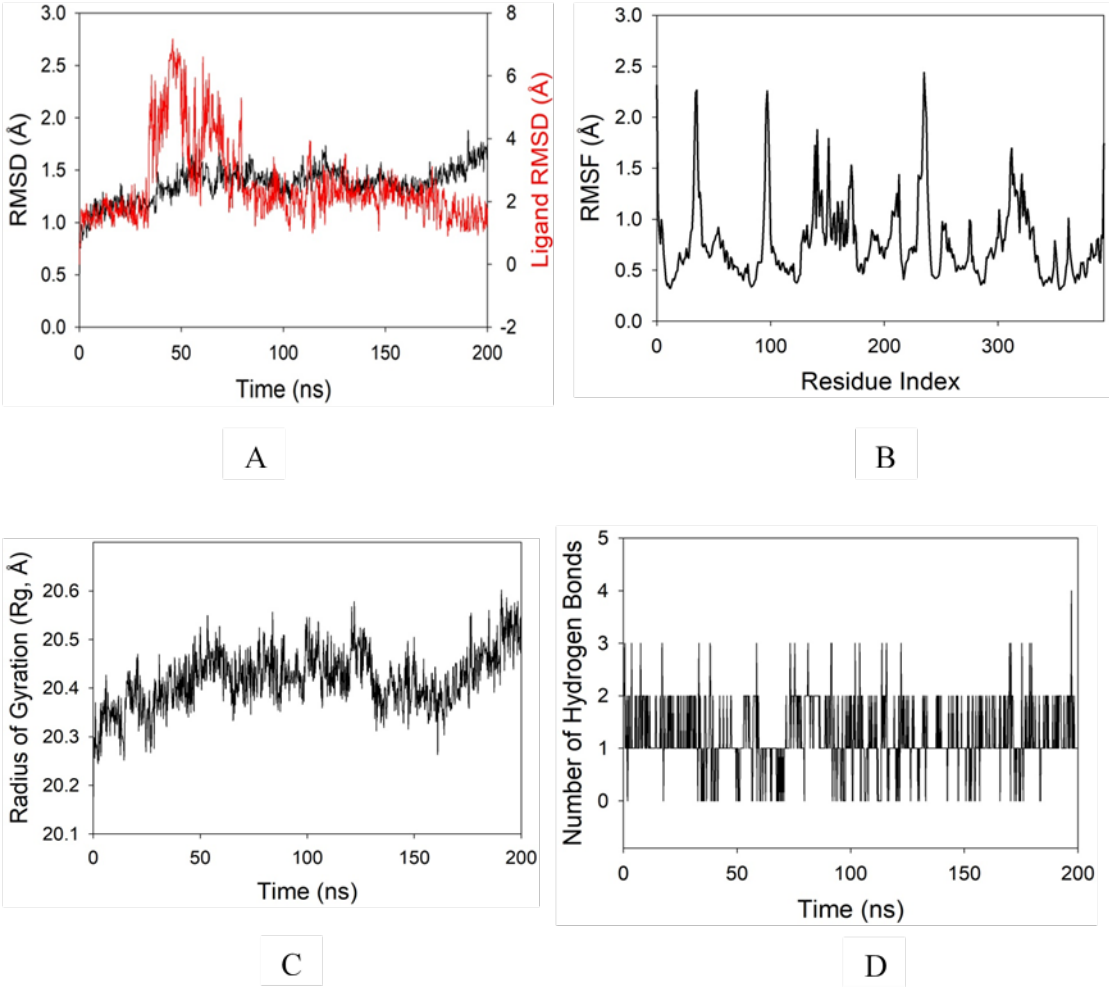

Figure 3: Molecular dynamic simulation analysis of 1EQP-Cyclohexylethylamine complex. A-RMSD plot of the IEQP-Cyclohexylethylamine complex over 200 ns MD simulation (The black line represents the backbone RMSD of the protein, while the red line indicates the RMSD of the ligand relative to its initial bound conformation). B- RMSF plot of the 1EQP-Cyclohexylethylamine complex depicting residue-wise atomic fluctuations over the simulation period (Peaks indicate flexible loop or terminal regions, while lower RMSF values reflect stable residues, particularly within the ligand-binding site). C- Radius of gyration (Rg) plot of the IEQP-Cyclohexylethylamine complex over 200 ns MD simulation (Consistent protein compactness and structural stability with minor fluctuations throughout the trajectory was found). D- Number of hydrogen bonds formed between 1EQP and Cyclohexylethylamine over 200 ns MD simulation (The plot indicates consistent formation of 1-2 hydrogen bonds, supporting stable and sustained protein-ligand interactions throughout the trajectory).

CONCLUSION

The current investigation on *S. tenerrimum* initially concentrated on the extraction of powdered material through soxhlation, utilizing ethanol as the solvent. The preliminary phytochemical assessment of the extract revealed the presence of Alkaloids, Glycosides, Phenolic compounds, Flavonoids, Saponins, Sterols, Tannins, Terpenoids, Carbohydrates, as well as Proteins and amino acids. The antimicrobial assessment of the extract demonstrated notable efficacy against Gram-positive bacteria, including *S. aureus* and *E. faecalis*, as well as the fungal pathogen *C. albicans*. LC-MS characterization of ethanol extract revealed the presence of some prominent compounds, among them, Cyclohexylethylamine was found as the potential candidate by docking and molecular dynamics simulation analyses. Of course, it points out the necessity of further *in vitro* and *in vivo* validation of this candidate.

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ABBREVIATIONS

CFU: Colony-Forming Unit; **CLSI:** Clinical and Laboratory Standards Institute; **LC-MS:** Liquid Chromatography-Mass Spectrometry; **MDS:** Molecular Dynamics Simulations; **MIC:** Minimum Inhibitory Concentration; **MM-GBSA:** Molecular Mechanics-Generalized Born Surface Area; **MTCC:** Microbial Type Culture Collection and Gene Bank; **PDA:** Photodiode Array; **PDB:** Protein Data Bank; **Rg:** Radius of Gyration; **RMSD:** Root Mean Square Deviation; **RMSF:** Root Mean Square Fluctuation; **TTC:** Triphenyl Tetrazolium Chloride.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

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