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Targeting IL-17-Mediated Inflammation in Periodontal Disease: Molecular Docking and Dynamics Study of Curcumin and Turmerone Compounds

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ABSTRACT: Interleukin-17 (IL-17) is a pro-inflammatory cytokine that plays a critical role in the pathogenesis of periodontitis. Curcumin and Turmerones, the major bioactive constituents of *Curcuma longa* (turmeric) are well known for their potent anti-inflammatory, anti-oxidant and immunomodulatory properties. The Aim of this study was to evaluate the molecular interaction of curcumin and major turmeric essential oil components—β-turmerone, ar-turmerone, and α-turmerone—with IL-17 using an in-silico approach. Molecular docking and dynamics simulations were done to investigate the interaction of curcumin, turmerone derivatives, and LY3509754 (IL-17A inhibitor 1) with IL-17 (PDB ID: 4HSA) using AutoDock Vina, aStability and conformational behaviour were analysed through RMSD, RMSF, Rg, SASA, and hydrogen bonding. Binding free energies were estimated using the MM-PBSA method. Docking analysis revealed that all compounds exhibited favourable binding affinities towards the IL-17 receptor complex indicating their potential to interfere with the IL-17 signalling pathways. Curcumin showed the highest binding energy (-7.2 kcal/mol), followed by β-turmerone (-6.9 kcal/mol). Key interactions with active site residues suggested stable ligand binding with minimal deviations in RMSD, RMSF, and radius of gyration. Curcumin demonstrated superior binding stability, while β-turmerone showed promising inhibitory potential. These findings highlight the

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therapeutic promise of turmeric derived compounds as natural host modulatory agents targeting IL-17 mediated inflammation in Periodontal disease.

1. INTRODUCTION

Periodontitis is defined as an inflammatory disease of the supporting tissues of the teeth caused by specific microorganisms or groups of specific microorganisms, resulting in progressive destruction of the periodontal ligament and alveolar bone with increased probing depth formation, recession, or both (Pihlstrom, Michalowicz and Johnson, 2005). The progression of periodontitis is largely driven by an exaggerated inflammatory response characterized by the release of cytokines, chemokines, and matrix-degrading enzymes that lead to connective tissue destruction and alveolar bone loss(Gaffen et al., 2006) .

Among multiple Pro-inflammatory cytokines studied in periodontal disease pathogenesis, Interleukin-17 (IL-17) has been emerging as a key mediator, which is mainly produced by T helper 17 (Th17) cells and plays an important role in neutrophil recruitment and in amplifying inflammatory responses. Reports revealed elevated levels of IL-17 in gingival tissues and gingival crevicular fluid of patients with periodontitis, where it was found to stimulate the production of pro-inflammatory mediators such as IL-6, TNF-α, and receptor activator of nuclear factor-ϰB ligand (RANKL) which contributed to the periodontal tissue destruction and bone resorption.(Kini et al., 2022)(Ikeuchi and Moutsopoulos, 2022). Recent studies have also revealed the dual role of the IL-17 pathway in periodontal disease, where it was found to participate in host defense against microbial pathogens, but under excess activation, promoted chronic inflammation and disease progression (Tang, Jin and Yang, 2025).

Recently, natural bioactive compounds have been studied extensively as potential therapeutic agents for modulating inflammatory pathways in periodontal disease. Curcuma longa (turmeric) is widely known for its anti-inflammatory and antioxidant properties, to suppress inflammatory signaling pathways and reduce cytokine production involved in periodontal inflammation (Hewlings and Kalman, 2017) . In addition to curcumin, turmeric essential oil contains multiple bioactive sesquiterpenes, known as turmerones, which include α-turmerone, β-turmerone, and ar-turmerone, which were known to demonstrate anti-inflammatory & immunomodulatory activities(Liju, Jeena and Kuttan, 2011).

In - silico techniques, such as Molecular docking and Molecular Dynamics simulations have aided with investigating ligand–protein interactions and identifying potential inhibitors of inflammatory mediators. These methods provide valuable insights into binding affinity, molecular interactions, and the stability of protein–ligand complexes, thereby leading to early drug discovery(Trott and Olson, 2010).

The main objective of this study is to evaluate the molecular interaction of curcumin and major turmeric essential oil components - β-turmerone, ar-turmerone, and α-turmerone with IL-17 using molecular docking and molecular dynamics simulations. The binding potential of these compounds was also compared with LY3509754, a known IL-17A inhibitor, to assess their potential as natural anti-inflammatory agents targeting IL-17-mediated periodontal inflammation.

2. MATERIALS AND METHODS

Molecular Docking

In this study, Molecular Docking was done to assess the binding affinities of Curcumin, β-turmerone, ar-turmerone, α-turmerone and LY3509754 against the IL17 protein [4HSA], with 3D structures which were converted using Open Babel (O'Boyle et al., 2011). Docking was performed using AutoDock Vina, which focused on the active site's catalytic pocket to analyze binding poses and interactions through PyMOL(Seeliger and de Groot, 2010) for insights into potential inhibitory activities of the Schiff base derivatives.

No	Protein targets	PDB ID	Resolution Å	Active site coordinates			Reference ligands
				X	Y	Z	
1	IL17	4HSA	3.15 Å	-60.808	64.692	-14.048	NAG

Table 1. List of target proteins, PDB IDs, active site coordinates, native ligands, and references.

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Molecular dynamics:

The crystal structure of the protein-inhibitor complex was analyzed for its dynamic properties. The ligands chosen from the docking analysis included IL17-Protein Alone [IL17-APO], IL17-CUR [IL17-TOP1], IL17-BTUR [IL17-TOP2], and IL17-LY3 [IL17-STD]. The ligand topology was selected using the antichamber tool. Additionally, the pdb2gmx module of GROMACS (Malik et al., 2023) was employed to introduce hydrogens to the heavy atoms(Gnanaraj et al., 2022).

The prepared systems underwent vacuum minimization for 1500 steps using the steepest descent method. Following this, the structures were solvated within a cubic periodic box utilizing the simple point charge (SPCE) water model(Gangadharappa et al., 2020).To maintain the complex systems, an appropriate salt concentration of 0.15 M was achieved by introducing appropriate amounts of Na and Cl counter ions. The preparation of the system was based on methodologies outlined in previously published papers (Satapathy et al., 2022)(Kumar et al., 2022).

Each resulting structure from the NPT equilibration phase underwent a final production run in the NPT ensemble for a simulation duration of 300 ns. Subsequently, the simulation trajectory was analyzed using various tools available in the Gromacs software package, which included the protein root mean square deviation (RMSD), root mean square fluctuation (RMSF), radius of gyration (RG), solvent accessible surface area (SASA), and hydrogen bonding (H-Bond).

The Molecular Mechanics Poisson-Boltzmann Surface Area (MM-PBSA) method was utilized to investigate the binding free energy of IL17-APO, IL17-BTUR, IL17-CUR, and IL17-LY3 inhibitors with the protein throughout the simulation period. The GROMACS tool g_mmpbsa was used to calculate the Binding Free Energy for IL17-APO, IL17-BTUR, IL17-CUR, and IL17-LY3, which were analysed for the last 50 ns with dt 1000 frames.

3. RESULTS AND DISCUSSION

Molecular Docking

The Molecular Docking revealed varying binding affinities among the different complexes, which indicated the interaction strength between the ligand and the protein. 4HSA- CUR complex was found to exhibit a docking score of -7.2, highlighting its binding affinity.

These complexes were found to be engaging with a wide range of essential residues, such as ARG20, THR21, VAL22, MET23, VAL24, LEU26, LEU99, GLU102, SER106, PRO107, ASN108, PHE110, ARG111, and LEU112, showing a potentially stable and more effective binding mode.

The number of residues interacting within these complexes indicated the adoption of advantageous configuration by the ligand, which promoted the strong protein binding, leading to its low docking score.

On the other hand, the 4HSA-LY3 complex exhibits a strong binding affinity, exhibiting a docking score of -8.6. Although it engages with residues such as ARG20, THR21, VAL22, MET23, VAL24, LEU26, TYR62, LEU99, ASN108, SER109, PHE110, ARG111, and LEU112, this interaction appears notably more potent, likely resulting from an increased number of contacts or a superior binding orientation.

Protein-Ligand Complex	Docking score	Interactions
4HSA-CUR (Curcumin)	-7.2	ARG20, THR21, VAL22, MET23, VAL24, LEU26, LEU99, GLU102, SER106, PRO107, ASN108, PHE110, ARG111, LEU112,
4HSA-BTUR (beta-Turmerone)	-6.9	HIS15, TYR59, ALA96, LYS98, PRO117, ILE118, TYR119, LEU120, GLY121, TYR151, ILE155,
4HSA-ARTUR	-6.8	ARG20, THR21, VAL22, VAL24, LEU26, LEU99, PHE110, ARG111, LEU112,

(ar-Turmerone)		
4HSA-ATUR (alpha-Turmerone)	-6.3	THR21, VAL22, MET23, VAL24, LEU26, LEU99, ASN108, SER109, PHE110, ARG111, LEU112,
4HSA-LY3 (LY3509754)	-8.6	ARG20, THR21, VAL22, MET23, VAL24, LEU26, TYR62, LEU99, ASN108, SER109, PHE110, ARG111, LEU112,

Table 2. Docking scores and interactions with the protein

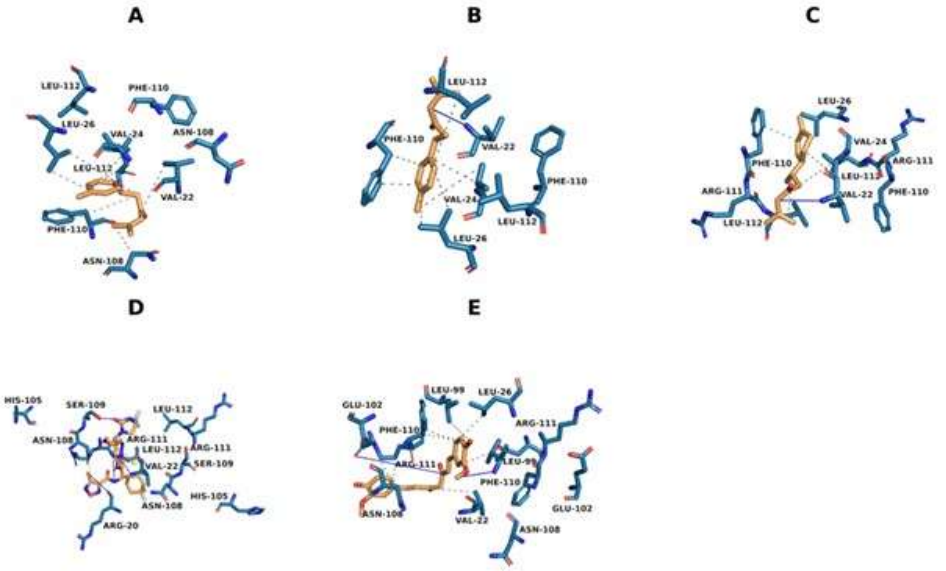


Figure 1: The 3D structures of the protein-ligand interaction of (A) 4HSA-ATUR, and (B) 4HSA- ARTUR, 4HSA-BTUR, 4HSA-LY3 and 4HSA-CUR complexes.

3.2 Molecular Dynamics

All-atom Molecular Dynamics (MD) simulation was done for investigation of structural behaviour of proteins and their corresponding ligand interactions. Molecular Dynamics has aided in computer-assisted drug discovery by facilitating a thorough examination of molecular systems at the atomic level. In this study, Molecular Dynamics simulations were done to evaluate the conformational shifts triggered by target protein binding. RMSD, RMSF, Rg, SASA, and Intermolecular Hydrogen bonding were assessed for both the isolated protein and the protein-ligand complex.

3.3 Root Mean Square Deviation (RMSD):

To examine the stability of the protein-ligand complex and understand system dynamics, Root Mean Square Deviation values were assessed (Figure 2). The findings demonstrated that both systems achieved equilibrium within 50 ns and uniform distribution was maintained for the rest of the simulation period. Furthermore, an evaluation of the RMSD values showed that the IL17-APO, IL17-BTUR, IL17-CUR, and IL17-LY3 complexes preserved their stability throughout the 300 ns duration, suggesting that the docked configurations remained stable over the course of the simulation. The average RMSD value for IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 was determined **to be 0.28 ± 0.03 nm, 0.29 ± 0.03 nm, 0.26 ± 0.04 nm** and 0.27 ± 0.02 nm. These findings suggest that IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 were stable systems that did not exhibit significant fluctuations during the simulation.

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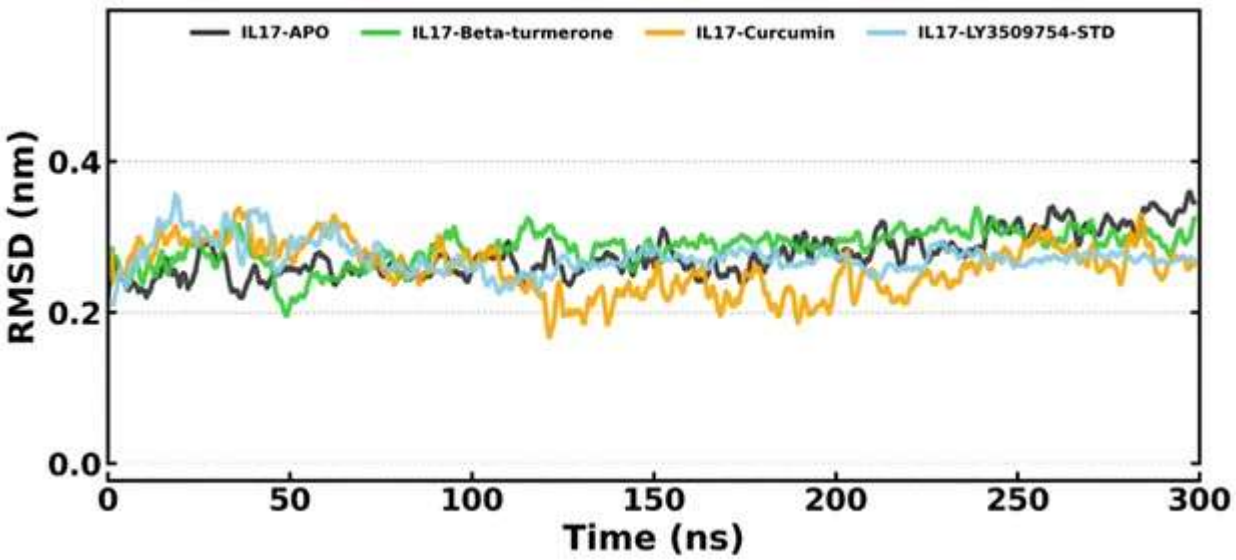


Figure 2: RMSD Conformational dynamics analysis of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3.

3.4 Root Mean Square Fluctuation (RMSF)

Root Mean Square Fluctuation was implemented for quantifying the mobility of individual residues and flexible segments within a protein throughout Molecular Dynamic simulations, thus helping with assessment of how ligand binding influences protein dynamics. Typically, rigid structural elements, including alpha-helices and beta-sheets, exhibit lower RMSF values, whereas disordered loop regions demonstrate higher degrees of flexibility. In this study, Root Mean Square Fluctuation (RMSF) values corresponding to each complex were determined and illustrated for every individual residue within the IL17-APO, IL17-BTUR, IL17-CUR, and IL17-LY3 system (Fig. 3) The average RMSF value for IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 was determined to be 0.12 ± 0.10 nm, 0.13 ± 0.10 nm, 0.14 ± 0.11 nm and 0.12 ± 0.09 nm. The results indicate that the IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 complex did not significantly alter the overall RMSF distribution.

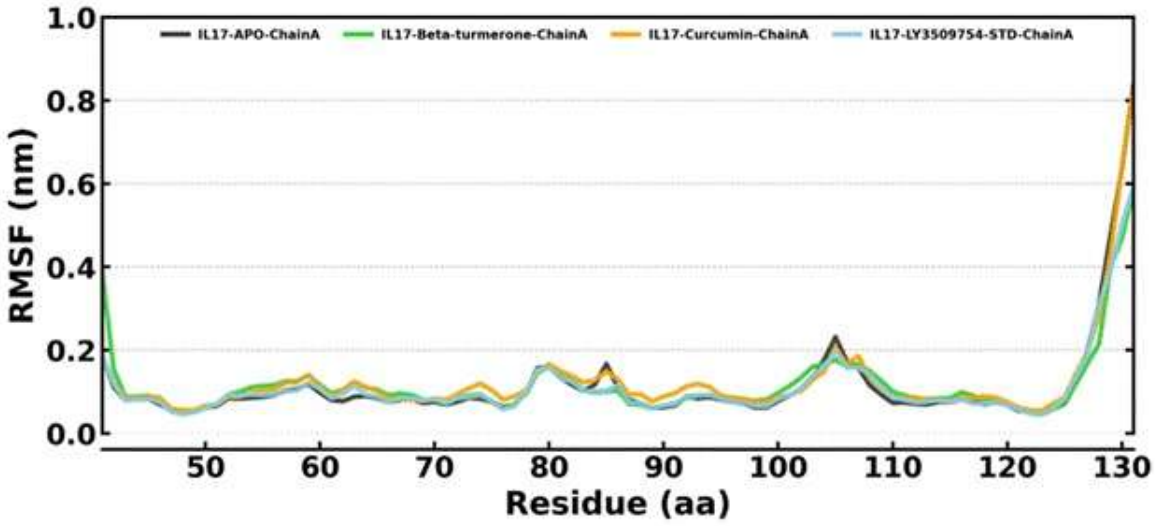


Figure 3: RMSF Conformational dynamics analysis of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 of Chain A.

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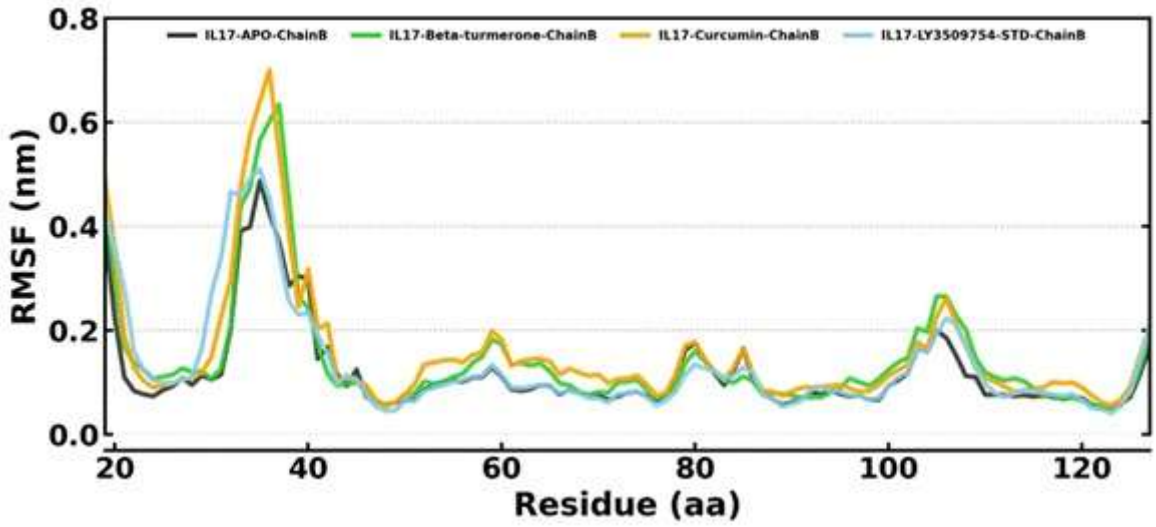


Figure 4: RMSF Conformational dynamics analysis of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 of Chain B.

Radius of gyration (Rg)

In order to evaluate the structural compactness and dynamic stability of the IL17-APO, IL17-BTUR, IL17-CUR, and IL17-LY3 complexes, the radius of gyration (Rg) values were calculated and plotted against time (Figure 5). The average Rg value for IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 was determined to be 1.97 ± 0.02 nm, 1.97 ± 0.02nm, 1.98 ± 0.01 nm and 1.99 ± 0.01 nm.

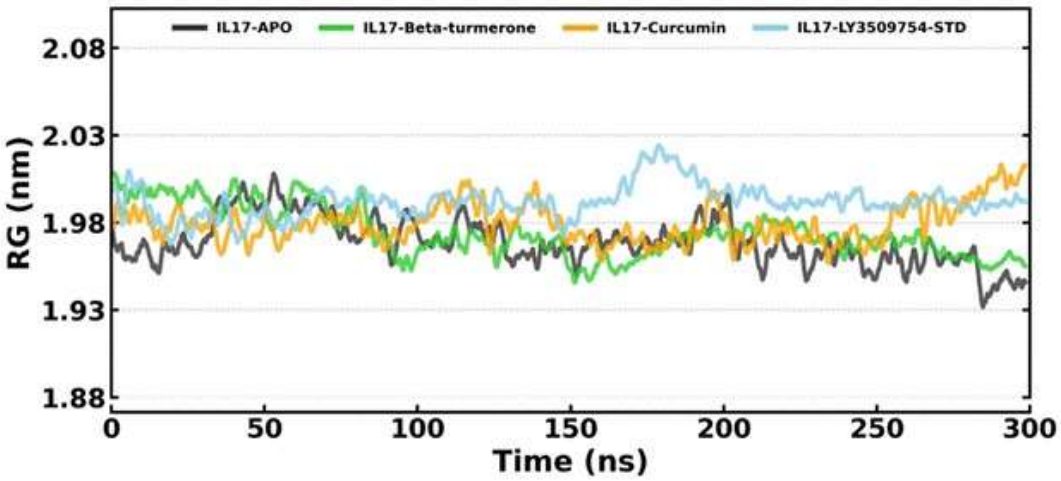


Figure 5: Rg Conformational dynamics analysis of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 complex.

Solvent accessible surface area (SASA)

Solvent Accessible Surface Area aids in assessment of the accessibility of a protein molecule within a solvent medium. In this study, SASA values were calculated and illustrated to demonstrate how the binding of IL17-APO, IL17-BTUR, IL17-CUR, and IL17-LY3 influenced the solvent accessibility of the target protein (Fig. 6). The plot revealed a similar pattern in the SASA values of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3. The average SASA value for IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 was determined to be 118.57 ± 3.11 nm, 116.07 ± 5.21 nm, 124.20 ± 3.25 nm and 114.65 ± 4.50 nm. The SASA values show fair equilibration without significant fluctuations throughout the simulation.

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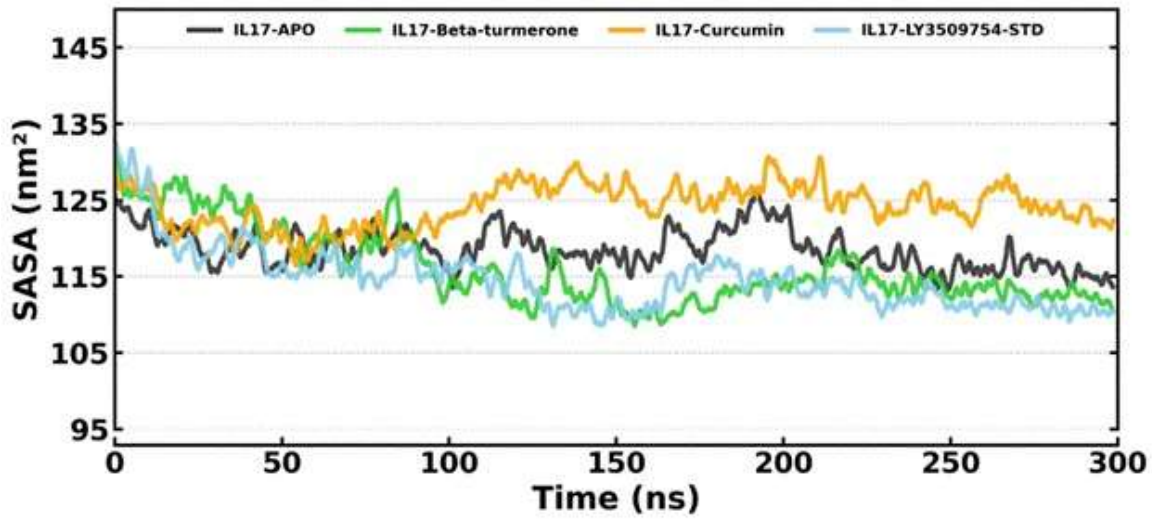


Figure 6: SASA Conformational dynamics analysis of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3complex.

Intra and Inter Hydrogen Bond

The Intra and Intermolecular hydrogen bond evaluation is essential to evaluate the stability of the isolated protein interactions (IL17-APO, IL17-BTUR, IL17-CUR, and IL17-LY3). In this study, Intra and Intermolecular hydrogen bonds were examined for temporal evolution within these IL17 complexes, with the corresponding data (Figure 7). The average Intra H-Bond value for Complex was determined to be 150.45 ± 6.27 nm, 149.88 ± 6.31 nm, 146.91 ± 6.57 nm and 151.26 ± 7.62 nm.

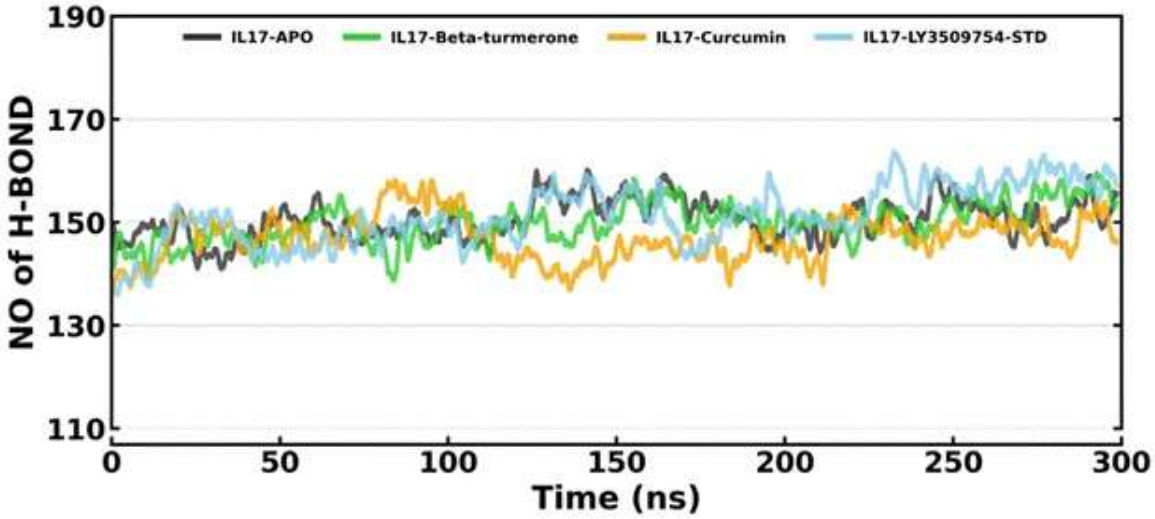


Figure 7: Intramolecular hydrogen bonds of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 during the simulation time.

The formation of hydrogen bonds is necessary for evaluation of the stability of protein-ligand complexes. This study assessed the temporal evolution of hydrogen bonding within the IL17-BTUR, IL17-CUR, and IL17-LY3 systems (Figure 8). The analysis indicated that the docked complex remained stable during the simulation, maintained by at least 0 to 5 hydrogen bonds with the IL17-BTUR , IL17-CUR, and IL17-LY3.

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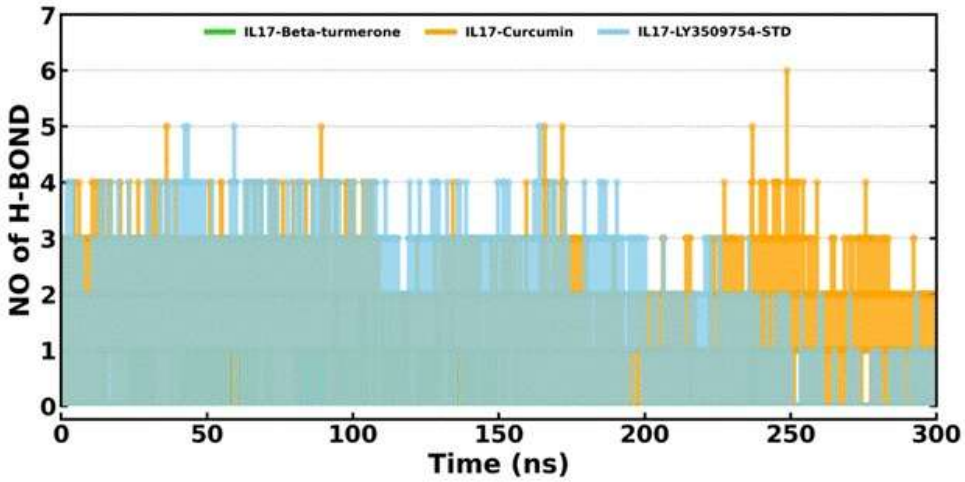


Figure 8: Intermolecular hydrogen bonds between protein-ligand during the simulation time.

Principal Component Analysis (PCA)

Principal component analysis (PCA) was performed to investigate the concerted motions within the IL17-APO, IL17-BTUR, IL17-CUR, and IL17-LY3 systems. Given that the primary Eigenvectors (EVs) are used in determination of the global dynamics of protein molecules and are used to analyze the conformational behavior of these complexes throughout the simulation period (Fig. 9). The plot showed that the IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 complexes occupied almost all the conformational motions and overlapped. In general, the lower amount of movements were observed in the IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 suggesting that IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 didn't significantly affect the target conformation and dynamics, thus aiding in the stability of the complex.

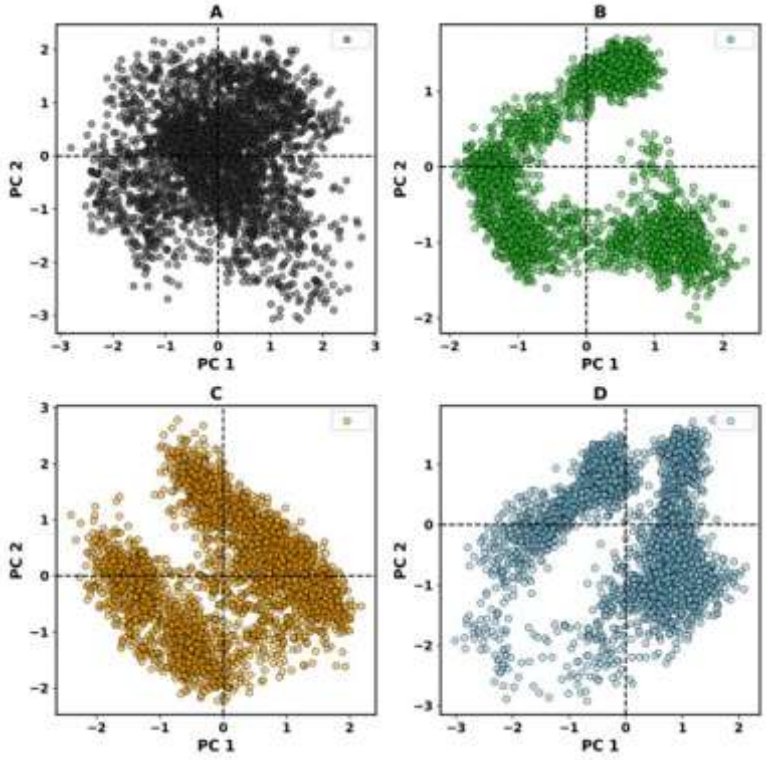


Fig 9: Principal component analysis 2D projection plot shows the conformation sampling of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 on PC1 and PC2.

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Free Energy Landscapes (FELs) :

The protein folding mechanisms and overall stability were assessed using Free Energy Landscapes (FELs). FEL plots provide a representation of the most stable conformational ensembles for a protein structure.The FEL plots for PC1 and PC2 were tabulated (Fig. 10), where deeper blue regions indicated a more stable protein conformation with lower energy. The plots indicated energy values ranging 0 to 16 kJ/mol throughout the simulation of IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3, revealing that the IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 complex displayed a single global minimum, which was confined to a large local basin. These findings suggest that IL17-APO, IL17-BTUR , IL17-CUR, and IL17-LY3 did not cause any significant conformational changes in the target structure, thus aiding in stabilization (Fig. 10).

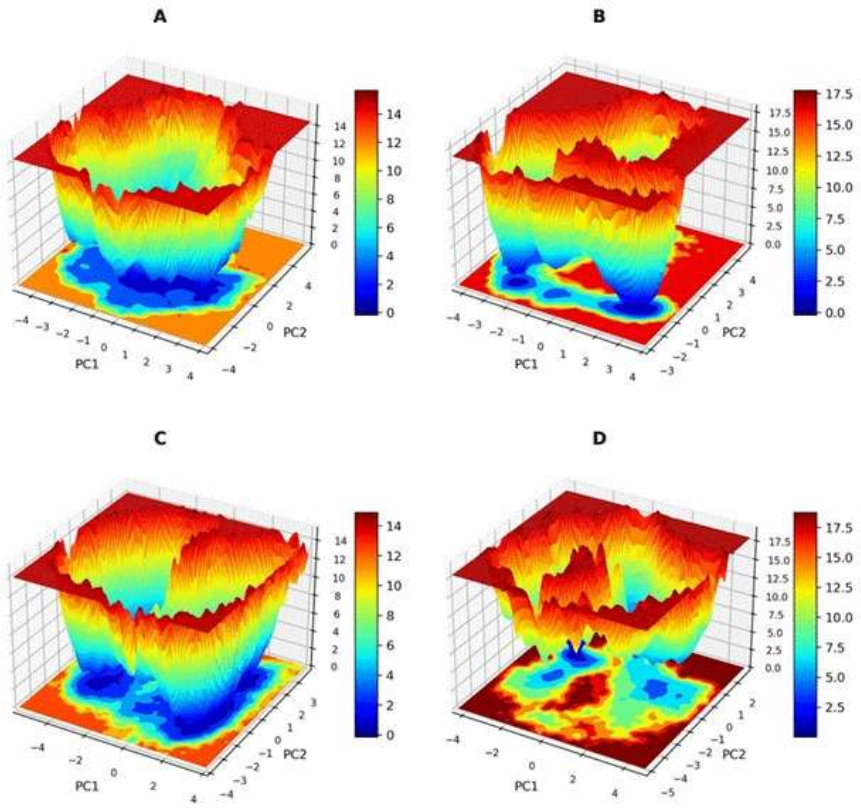


Figure 10: The free energy landscape plots for (A) IL17-APO, (B) IL17-BTUR , (C) IL17-CUR, and (D) IL17-LY3.

MM - PBSA

The relative binding strength within the protein of summary energy was evaluated to determine the binding affinity of IL17-BTUR , IL17-CUR, and IL17-LY3 . The binding strength of IL17-BTUR , IL17-CUR, and IL17-LY3 concerning inhibitors computed and compared (Table 3) using the MM-PBSA method. Across a stable simulation trajectory, we calculate residue-level contributions to the interaction energy.

System	van der Waal energy	Electrostatic energy	Polar solvation energy	SASA Energy	Binding energy
IL17-BTUR	-173.335 +/- 8.585 kJ/mol	-27.228 +/- 13.050 kJ/mol	118.569 +/- 15.487 kJ/mol	-17.281 +/- 0.689 kJ/mol	-99.275 +/- 10.755 kJ/mol

IL17-CUR	-216.417 +/- 15.880 kJ/mol	-77.307 +/- 17.720 kJ/mol	188.004 +/- 25.985 kJ/mol	-23.618 +/- 0.669 kJ/mol	-129.338 +/- 21.860 kJ/mol
IL17-LY3	-148.862 +/- 11.119 kJ/mol	-22.769 +/- 6.111 kJ/mol	112.416 +/- 16.197 kJ/mol	-16.468 +/- 0.573 kJ/mol	-75.683 +/- 11.268 kJ/mol

4. DISCUSSION:

The results of this in-silico study provide a molecular basis for the potential therapeutic efficacy of Curcuma longa derivatives in management of periodontitis. Periodontitis is caused by dysregulation of host immune response where Interleukin-17 (IL-17) acts as a recruiter of neutrophils and resorption of alveolar bone via the RANKL pathway (Pihlstrom, Michalowicz and Johnson, 2005)(Gaffen et al., 2006). By targeting the IL-17 receptor complex (PDB ID: 4HSA), this study shows that natural polyphenols have the potential for the interruption of this inflammatory cascade.

Molecular docking analysis revealed that, β-Turmerone showed competitive potential of -6.9 kcal/mol, and Curcumin showed significant competitive potential with a score of -7.2 kcal/mol. In MM-PBSA analysis, provides a more rigorous estimation of binding free energy—indicated that β-Turmerone (-99.275 kJ/mol) actually showed good inhibitory potential , comparative to the standard inhibitor LY3509754 (-75.683 kJ/mol) in terms of total binding energy over the simulation trajectory. The superior performance of β-Turmerone can be attributed to its high van der Waals and electrostatic energy contributions. As shown in the docking results, Among the tested compounds, Curcumin demonstrated a docking score of -7.2 kcal/mol, while ß-turmerone showed a docking score of -6.9 kcal/mol. Although the standard inhibitor LY3509754 exhibited a stronger docking score (-8.6 kcal/mol), Curcumin and B-turmerone interacted with several critical amino acid residues including ARG20, THR21, VAL22, LEU99, ASN108, PHE110, ARG111, and LEU112, indicating favorable occupancy of the IL-17 binding pocket and sterical hindrance of the cytokine's ability to bind to its cognate receptor (IL-17RA), thereby dampening downstream pro-inflammatory signaling (Hobani, Jerah and Bidwai, 2017).

The Molecular Dynamics (MD) simulations over 300 ns confirmed that the binding of turmeric compounds does not compromise the structural integrity of the IL-17 protein. The RMSD values for all complexes examined remained below 0.3 nm, which indicated achievement of stable equilibrium by the systems. The Radius of Gyration (Rg) and SASA values were found to be consistent among all systems, indicating that the protein-ligand complexes remained in a condensed, stable state throughout the simulation. The RMSF graphs for both Chain A and Chain B, revealed the binding of Curcumin and Turmerones did not induce abnormal fluctuations in the protein backbone. This slight reduction in motion was observed in the Principal Component Analysis (PCA) further proving the stabilizing effect of these ligands on the structure of IL-17 .

While Curcumin is well-documented for its anti-inflammatory properties in dental literature, turmerones (the sesquiterpene components of turmeric oil) are less explored in the context of periodontitis, revealing the dual efficacy of both Turmeron(Mohd Asngari et al., 2026). Our findings suggest that β-turmerone possesses a stable binding profile and favorable MM-PBSA energy (-99.275 kJ/mol), making it a viable candidate for "host modulatory therapy" (HMT).

Host modulation therapy (HMT) has emerged as an important adjunctive approach in periodontal therapy, which aims to reduce tissue destruction by regulation of the host inflammatory response rather than directly targeting periodontal pathogens(Balta et al., 2021). By inhibiting IL-17, these compounds could theoretically reduce the production of IL-6 and TNF-α in the gingival microenvironment,ultimately protecting the alveolar bone from osteoclast-mediated resorption. The favorable binding affinity, stability, and free-energy profiles demonstrated by β-turmerone and curcumin in the present study, suggest that these phytochemicals may function as natural host-modulating agents. .which could potentially attenuate periodontal tissue destruction, while minimizing the adverse effects associated with long term pharmacological immunosuppression. This aligns with the shift in periodontal therapy toward modulating the host response rather than solely focusing on microbial elimination.

CONCLUSION:

This in-silico study demonstrated that Curcumin and β-turmerone from Curcuma longa exhibit favorable interactions with IL-17, a pivotal cytokine involved in periodontal inflammation and alveolar bone destruction. However, the findings of the present study are limited to In- silico methods and requires further In-vitro, In-vivo, and clinical trials to validate the inhibitory effects of β-turmerone and other turmerones on IL-17 signaling and to establish their efficacy, safety, and bioavailability in periodontal therapy.

Declarations:

AUTHOR CONTRIBUTIONS

Dr Manthra Prathoshni.S, Dr. Divya Kumar, Dr. Vamsi Lavu: Conceptualization, Investigation & writing

Dr. Dhanadivya Krishnakumar , Dr. Deepak Moses Ravindran , Dr.S.K. Balaji : Writing—Review & Editing.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ETHICS STATEMENT

Ethical approval was not required for this study.

DATA AVAILABILITY STATEMENT

Data supporting the findings of this study are available from the corresponding author upon reasonable request.

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