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IN SILICO MOLECULAR DOCKING ANALYSIS AND ADME PROFILING OF THE SIDDHA HERBAL FORMULATION- SATHURMUGA CHOORNAM AGAINST PALMOPLANTAR PSORIASIS

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ABSTRACT

Background and Objective: Palmoplantar psoriasis (PPP) is a chronic immune-mediated inflammatory skin disorder characterized by hyperkeratotic plaques, erythema, scaling, and sterile pustules affecting the palms and soles, significantly impairing the quality of life of affected individuals. The pathogenesis of PPP involves dysregulation of inflammatory cytokines such as interleukin-17A (IL-17A) and interleukin-36 gamma (IL-36γ), which contribute to keratinocyte hyperproliferation and chronic inflammatory responses through activation of NF-κB and MAPK signaling pathways. Although conventional therapies provide symptomatic relief, prolonged treatment is frequently associated with adverse effects, recurrence, and therapeutic resistance. Siddha medicine, one of the ancient traditional systems of medicine practiced in India, describes several herbal formulations with potent anti-inflammatory and immunomodulatory properties. Among them, Sathurmuga Choornam has been traditionally used for various dermatological disorders which includes psoriasis mentioned as Kalanjagapadai. However, its molecular mechanism and pharmacological potential against Palmoplantar psoriasis remain scientifically unexplored. Therefore, the present study was designed to investigate the Molecular Docking interactions and ADME profiling of the selected phytoconstituents of Sathurmuga Choornam against major inflammatory targets associated with Palmoplantar psoriasis using computational approaches. **Materials and Methods**: Preliminary Molecular Docking study through computational analysis were performed with the Auto Dock tool to study the efficacy and ADME profiling was performed for Sathurmuga Choornam against Palmoplantar psoriasis. The binding action of major phytoconstituents of the drugs in Sathurmuga Choornam against various targets was documented. **Results and Discussion**: The selected phytoconstituents exhibited significant binding affinity and stable interactions with IL-17A and IL-36γ proteins. ADME analysis demonstrated favorable pharmacokinetic properties, acceptable bioavailability, and drug-likeness profiles, indicating potential anti-inflammatory and immunomodulatory activity against Palmoplantar psoriasis. **Conclusion:** The study suggests that Sathurmuga Choornam possesses promising therapeutic potential against Palmoplantar psoriasis through significant molecular interactions with inflammatory targets.

KEYWORDS: Siddha, Palmoplantar psoriasis, Sathurmuga Choornam, Kalanjagapadai.

INTRODUCTION

Palmoplantar psoriasis (PPP) is a chronic, relapsing inflammatory skin disorder predominantly affecting the palms and soles, characterized by well-defined erythematous plaques with thick scaling, fissuring and hyperkeratosis. The disease considerably impairs the functional ability and quality of life of affected individuals due to pain, discomfort, and recurrent exacerbations. Although the exact etiology of PPP remains unclear, growing evidence suggests that immune dysregulation and abnormal keratinocyte proliferation play crucial roles in disease progression. Inflammatory cytokines including interleukin-17A (IL-17A), interleukin-36 gamma (IL-36γ), tumor necrosis factor-alpha (TNF-α), and various chemokines are considered

major mediators involved in the pathogenesis of Palmoplantar psoriasis.

The inflammatory cascade in PPP involves activation of T-helper 17 (Th17) cells and subsequent release of IL-17A, which stimulates keratinocytes to produce pro-inflammatory mediators through NF-κB and MAPK signaling pathways. Similarly, IL-36γ released from activated keratinocytes further amplifies inflammatory responses and neutrophilic infiltration, thereby contributing to chronic skin inflammation and epidermal hyperproliferation.

Current therapeutic approaches for Palmoplantar psoriasis include topical corticosteroids, retinoids, immunosuppressive agents, phototherapy, and biologics targeting inflammatory cytokines. However, prolonged treatment is often associated with adverse effects, recurrence, therapeutic resistance, and high economic burden. Therefore, identification of safer and effective alternative therapeutic agents from traditional medicinal systems has gained considerable research interest.

Siddha medicine, one of the oldest traditional systems of medicine practiced in India, contains numerous herbal formulations with potent anti-inflammatory, antioxidant, and immunomodulatory properties. Sathurmuga Choornam is a classical Siddha herbal formulation traditionally indicated for various inflammatory and dermatological disorders. Despite its extensive traditional usage, the molecular mechanism and pharmacological basis of this formulation against Palmoplantar psoriasis remain scientifically unexplored.

Recent advances in computational biology have enabled the application of Molecular Docking and ADME profiling for evaluating the interaction between phytoconstituents and disease-associated target proteins. Molecular Docking helps predict the binding affinity and interaction patterns of bioactive compounds with target proteins, while ADME analysis evaluates pharmacokinetic and drug-likeness properties essential for drug development.

Therefore, the present study was designed to investigate the Molecular Docking interactions and ADME profiling of selected phytoconstituents present in Sathurmuga Choornam against important inflammatory targets associated with Palmoplantar psoriasis, particularly IL-17A and IL-36γ.

MATERIALS AND METHODS

Recent advancements in computational biology have enabled the application of network pharmacology and Molecular Docking approaches to understand the multi-component and multi-target mechanisms of traditional medicines. Network pharmacology integrates systems biology, bioinformatics, and pharmacology to identify active phytocompounds, predict target proteins, and elucidate signaling pathways involved in disease modulation. Molecular Docking further helps in predicting the binding affinity and interaction pattern between bioactive compounds and target proteins at the molecular level. These computational strategies provide a cost-effective and efficient approach for preliminary drug discovery and scientific validation of traditional formulations.

Preparation of Ligand

Ingredients of Sathurmuga Choornam

The major phytoconstituents present in the ingredients of Sathurmuga Choornam were identified through a literature review and phytochemical databases.

Table 1: Ingredients of Sathurmuga Choornam.

Ingredients	Family	Active ingredients	
Pergularia daemia	Apocynaceae	Tylophorine	Anti-inflammatory, suppresses NF-κB signaling, reduces keratinocyte proliferation and inflammatory cytokine release
Curculigo orchioides	Hypoxidaceae	Lycorine	Immunomodulatory, inhibits inflammatory mediators such as IL-6 and TNF-α, reduces oxidative stress in psoriatic inflammation
Semecarpus anacardium	Anacardiaceae	Anacardic acid	Anti-psoriatic, inhibits pro-inflammatory cytokines, suppresses keratinocyte hyperproliferation and inflammatory pathways
Asparagus racemosus	Asparagaceae	Racemosol	Antioxidant, anti-inflammatory, helps reduce skin inflammation and immune-mediated responses associated with psoriasis

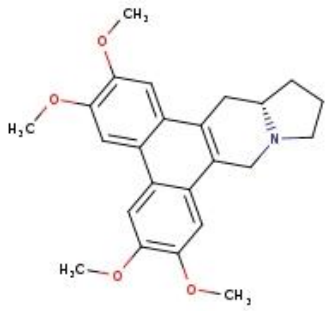
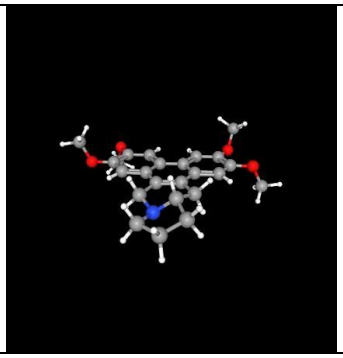
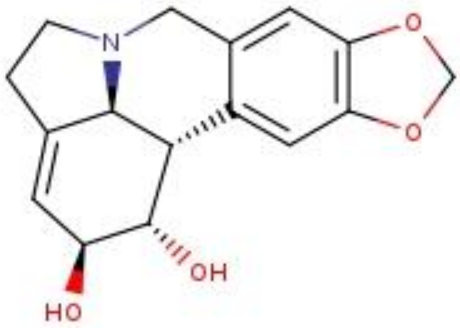
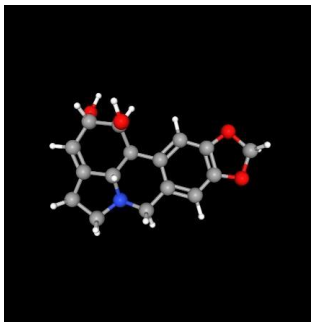
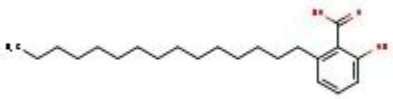
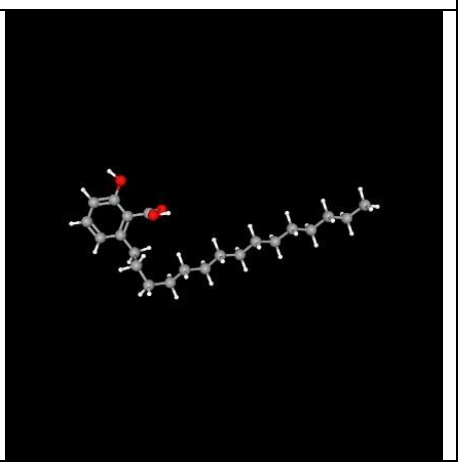
The identified phytochemicals along with their Molecular weight, Molecular formula, H-bond donor, H-bond acceptor, Rotatable bonds were listed in table 2.

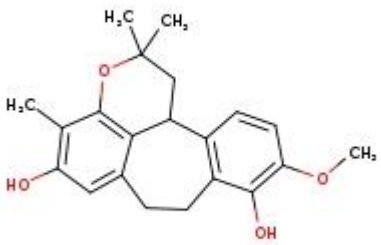
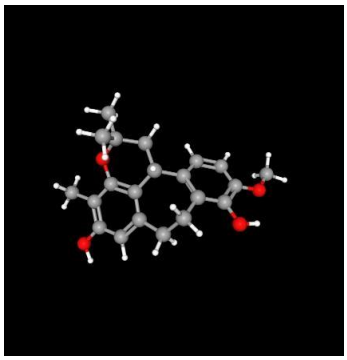
Table 2: Chemical properties of selected Ligands.

Compound	Molecular Weight g/mol	Molecular formula	H- bond donor	H- bond acceptor	Rotatable bonds
Tylophorine	393.5	$C_{24}H_{27}NO_4$	0	5	4
Lycorine	287.31	$C_{16}H_{17}NO_4$	2	5	0
Anacardic acid	348.5	$C_{22}H_{36}O_3$	2	3	15
Racemosol	340.4	$C_{21}H_{24}O_4$	2	4	1

Each selected phytochemical was prepared for docking by obtaining its 2D and 3D structures from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/) in SDF format and converted to PDB format, followed by energy minimization to ensure stable conformations and reduced steric hindrance. Each ligand was then parameterized with appropriate partial charges and rotatable bonds to enable flexible interactions with the target protein. The structures of the ligands are shown in Table 3.

Table 3: 2D and 3D structure of the selected Ligands.

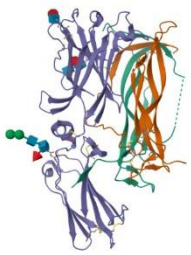
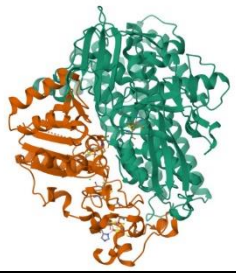
Compound	2D Structure	3D structure
Tylophorine		
Lycorine		
Anacardic acid		

Racemosol		

Preparation of Target

The target proteins were selected based on Swiss Target Prediction (http://www.swisstargetprediction.ch/index.php). The predicted target proteins were downloaded from RCSB PDB database (https://www.rcsb.org/). The x-ray diffraction structures of the different target proteins under study having resolution not less than 2 A^0 were used for the study (Table 3). Co-factors, ligands, water molecules, etc., were removed and converted into PDB format.

Table 4: Selected targets and their action.

Target protein	PDB ID	Structure	Role in Palmoplantar psoriasis
IL-17A	4HSA		IL-17A binds to IL-17 receptor on keratinocytes and activates NF-κB and MAPK signaling pathways, leading to the release of pro-inflammatory cytokines and chemokines such as IL-6, TNF-α, CXCL1, and IL-8. This promotes neutrophil recruitment and keratinocyte hyperproliferation in Palmoplantar lesions.
IL-36 ϒ	5MDJ		IL-36γ released from activated keratinocytes binds to IL-36 receptor and stimulates NF-κB and MAPK pathways, inducing IL-8, TNF-α, and IL-23 production. This enhances neutrophilic infiltration and amplifies chronic inflammatory signaling in Palmoplantar psoriasis.

Molecular Docking

Docking simulations were conducted using MGL Auto Dock tools to evaluate the binding interactions between the target protein and each ligand. Molecular interaction analysis was performed using Auto Dock 1.5.7 Morris et al.(2009) by following steps: Gasteiger partial charges were added to the ligand atoms. Nonpolar hydrogen atoms were merged, and rotatable bonds were defined. A grid box was centered on key active site residues to confine docking to relevant regions. Parameters, including binding affinity (ΔG), inhibition constant (Ki) and interaction surface, were calculated for each ligand. Docking was repeated using the SwissDock Vina platform.

ADME and Drug-Likeness Prediction

The pharmacokinetic properties of the selected phytocompounds were evaluated using the SwissADME web server to determine their drug-likeness, absorption, distribution, metabolism, and excretion characteristics. Parameters including gastrointestinal absorption, blood–brain barrier permeability, cytochrome P450 inhibition, P-glycoprotein interaction, skin permeation, Lipinski's rule of five, bioavailability score, and medicinal chemistry properties were analyzed.

RESULTS AND DISCUSSION

The molecular docking analysis performed in the present study demonstrated significant binding interactions between the selected phytoconstituents of Sathurmuga Choornam and the inflammatory target proteins IL-17A (PDB ID: 4HSA) and IL-36γ (PDB ID: 5MDJ), which

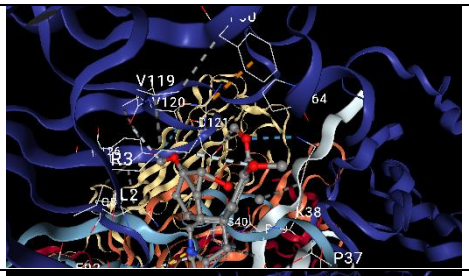
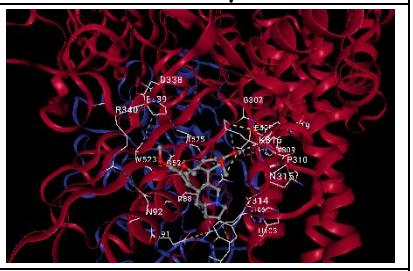
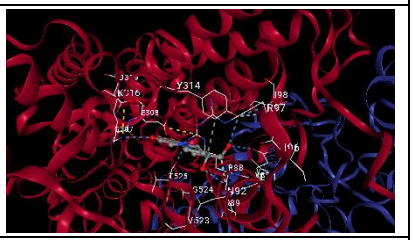
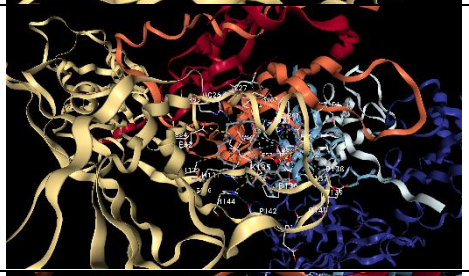
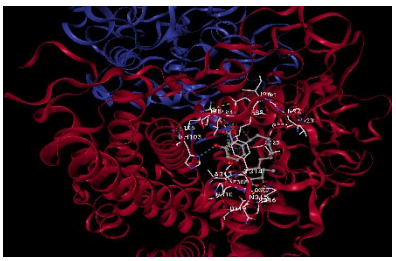
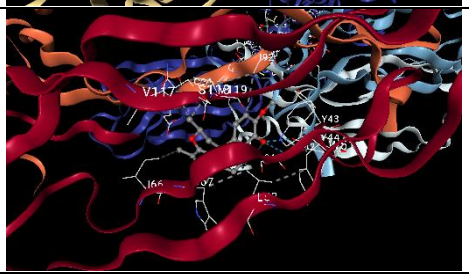
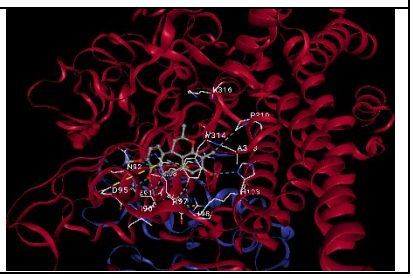
are critically involved in the pathogenesis of Palmoplantar psoriasis.

Lower binding energy values indicate stronger ligand–protein interaction and greater binding stability. Against both target proteins with binding energies of −8.5 kcal/mol and −8.6 kcal/mol respectively, suggesting its potential anti-inflammatory activity through stable receptor binding. Anacardic acid demonstrated moderate but significant binding affinities against IL-17A (−7.5 kcal/mol) and IL-36γ (−7.3 kcal/mol) with 20 molecular interactions against each target protein.

The observed binding interactions suggest that the selected phytoconstituents may inhibit inflammatory signaling pathways associated with Palmoplantar psoriasis by interacting with cytokine-mediated targets involved in keratinocyte proliferation and chronic skin inflammation. IL-17A is a major pro-inflammatory cytokine involved in activation of NF-κB and MAPK signaling pathways, resulting in the release of inflammatory mediators such as IL-6, TNF-α, CXCL1, and IL-8, which contribute to keratinocyte hyperproliferation and neutrophilic infiltration in psoriatic lesions.

Similarly, IL-36γ released from activated keratinocytes stimulates inflammatory signaling pathways and amplifies chronic inflammation by inducing IL-8, TNF-α, and IL-23 production. Effective inhibition of IL-36γ signaling may therefore reduce inflammatory cell recruitment and epidermal damage associated with Palmoplantar psoriasis.

Table 6: Molecular interactions of selected phytoconstituents with target proteins.

Compound	IL-17A	IL-36γ
Tylophorine		
Lycorine		
Anacardic acid		
Racemosol		

ADME PROPERTIES

Table 7: ADME properties of Different compounds.

Compounds	GI absorption	BBB permeant	P-gp	CYP1A2 inhibitors	CYP2C19 inhibitors	CYP2C9 inhibitors	CYP2D6 inhibitors	CYP3A4 inhibitors	Log Kp (cm/s)
Tylophorine	High	Yes	Yes	No	Yes	Yes	Yes	Yes	-5.34
Lycorine	High	No	Yes	No	No	No	Yes	No	-8.07
Anacardic acid	High	No	No	Yes	Yes	No	No	No	-1.84
Racemosol	High	Yes	Yes	Yes	No	Yes	Yes	Yes	-5.34

ADME profiling of the selected phytoconstituents demonstrated favorable pharmacokinetic properties for most compounds. Tylophorine, Lycorine, Anacardic acid, and Racemosol exhibited high gastrointestinal absorption, indicating good oral bioavailability potential. Tylophorine and Racemosol showed blood–brain barrier permeability and P-glycoprotein interaction, whereas Lycorine and Anacardic acid were found to be non-BBB permeant. The CYP450 inhibition profile revealed that some compounds may interact with metabolic enzymes, particularly CYP2C19, CYP2C9, CYP2D6, and CYP3A4.

Drug-likeness

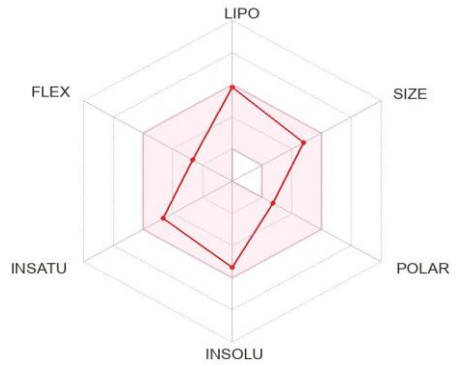
Table 8: Drug likeness of the compounds.

Compounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability
Tylophorine	Yes 0 violation	Yes	Yes	Yes	Yes	0.55
Lycorine	Yes 0 violation	Yes	Yes	Yes	Yes	0.55
Anacardic acid	Yes 1 violation	No 1 violation	No 1 violation	No 1 violation	No 1 violation	0.85
Racemosol	Yes 0 violation	Yes	Yes	Yes	Yes	0.55

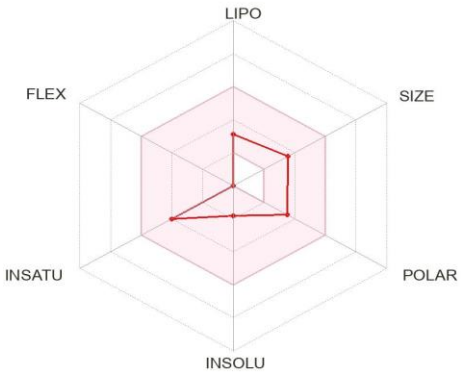
Drug-likeness evaluation based on Lipinski, Ghose, Veber, Egan, and Muegge filters indicated that Tylophorine, Lycorine, and Racemosol satisfied most of the drug-likeness criteria without significant violations, with a bioavailability score of 0.55. Anacardic acid showed one violation in multiple parameters but demonstrated a comparatively higher bioavailability score of 0.85. These findings indicate that the selected phytoconstituents possess acceptable pharmacokinetic and medicinal chemistry properties suitable for further therapeutic investigation.

Overall, the present computational study suggests that the phytoconstituents present in Sathurmuga Choornam possess promising anti-inflammatory and immunomodulatory activity against Palmoplantar psoriasis through significant molecular interactions with IL-17A and IL-36γ target proteins. The synergistic action of these bioactive compounds may contribute to suppression of inflammatory cytokine signaling and keratinocyte hyperproliferation associated with psoriatic lesions. However, further in vitro, in vivo, and clinical investigations are necessary to validate the therapeutic efficacy and safety of the formulation.

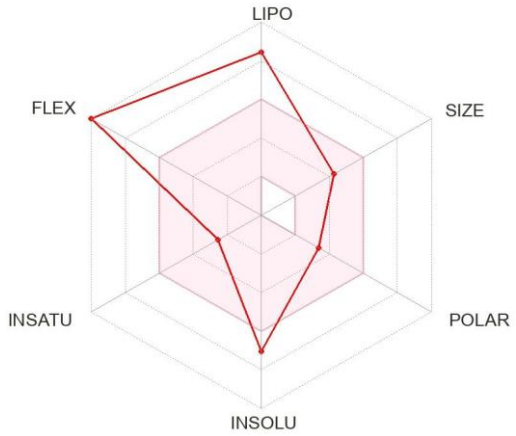
Tylophorine



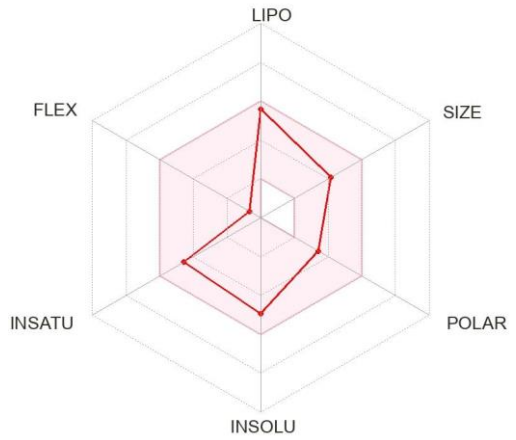
Lycorine



Anacardic Acid



Racemosol



CONCLUSION

The present molecular docking study demonstrated that the phytoconstituents present in the Siddha herbal formulation Sathurmuga Choornam exhibited significant binding affinity against the inflammatory target proteins IL-17A and IL-36γ involved in Palmoplantar psoriasis. The selected compounds demonstrated stable molecular interactions with the target proteins, suggesting potential anti-inflammatory and immunomodulatory activity against Palmoplantar psoriasis. ADME and drug-likeness analysis also revealed favorable pharmacokinetic properties, good gastrointestinal absorption, and acceptable bioavailability for most of the selected phytocompounds. These findings indicate that Sathurmuga Choornam may serve as a promising therapeutic formulation for the management of Palmoplantar psoriasis. However, further in vitro, in vivo, and clinical studies are required to validate the therapeutic efficacy and safety of the formulation.

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