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IN SILICO NETWORK PHARMACOLOGY ANALYSIS AND MOLECULAR DOCKING STUDIES OF SIDDHA HERBAL PREPARATION- SANJEEVI THYLAM AGAINST URTICARIA

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ABSTRACT

Background and Objective: Siddha, one of the Traditional medicinal systems in India is undoubtedly known for its varied unique approach towards prevention, diagnosis as well as treatment of every disease. An ample of literary evidence on medicinal formulations are found in Siddha literatures whose scientific validation are still partial. Urticaria which is mentioned in Siddha as “Kaanakadi” is said to be a skin condition that is characterized by errythematous, edematous, itchy and transient plaques involving the mucous membrane of skin. 15 to 20 % of world population are affected by Urticarial diseases. A strong scientific approach towards treatment perspectives is needed since the disease affects both physical and social well being of the individuals. Many Siddha formulations for Kaanakadi are mentioned in literatures. One among them is the “Sanjeevi thylam” mentioned in "Chikicha rathna deepam". A proper scientific Validation of this formulation could pave way to Evidence based Medicine, which is the foundation of scientific community. **Materials and Methods:** Preliminary molecular docking study through computational analysis was done with the Auto Dock tool to study the efficacy of Sanjeevi Thylam against Urticaria. The binding action of major phytoconstituents of the drugs in Sanjeevi thylam against various targets were documented. **Results and Discussion:** Most of the phytochemicals of drugs present in Sanjeevi thylam showed significant binding capacities against the targets Histamine H1 receptor inhibitor and IL13. Hence it can be chosen for the treatment and management Urticaria. **Conclusion:** The Siddha herbal preparation "Sanjeevi thylam" has inherent action against Urticaria by binding with various targets was concluded by the present study.

KEYWORDS: Siddha, Urticaria, Sanjeevi thylam, Kaanakadi.

INTRODUCTION

Siddha, one of the Traditional medicinal systems in India is undoubtedly known for its varied unique approach towards prevention, diagnosis as well as treatment of every disease. An ample of literary evidence on medicinal formulations are found in Siddha literatures whose scientific validation are still partial. Urticaria which is mentioned in Siddha as “Kaanakadi” is said to be a skin condition that is characterized by errythematous, edematous, itchy and transient plaques involving the mucous membrane of skin. 15 to 20 % of world population are affected by this. A strong scientific approach towards treatment perspectives is needed since the disease affects both physical and social well being of the individuals. Many Siddha formulations for Kaanakadi are mentioned in literatures. One among them is the “Sanjeevi thylam” mentioned in "Chikicha rathna deepam". A proper scientific Validation of this formulation could pave way to Evidence based Medicine, which is the foundation of scientific community.

MATERIALS AND METHODS

Molecular modelling is the most important method for the investigation and reorganization of receptor protein and compound structure, potentially without giving more investment in research work and time. Structure

prediction of the target and the ligand is important for their interaction studies.

Preparation of Ligand

Ingredients of Sanjeevi thylam

Table 1: Ingredients of Sanjeevi thylam.

Ingredients	Family	Active ingredients
Coriandrum sativum	Apiaceae	Linalool
Cuminum cyminum	Apiaceae	Cuminaldehyde
Psoralea coryfolia	Fabaceae	Bakuchiol
Magnolia champaca	Magnoliaceae	Magnolol
Curcuma zedoaria	Zingiberaceae	Curcumin
Sesamum indicum	Pedaliaceae	Sesamin

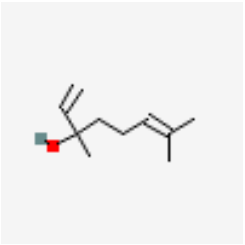
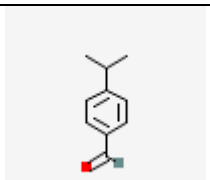
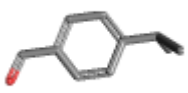
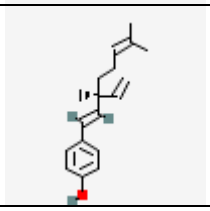
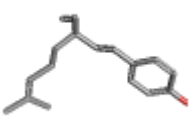
The phytochemical identified with its Molecular weight, Molecular formula, H-bond donor, H-bond acceptor, Rotatable bonds were listed in table 1.

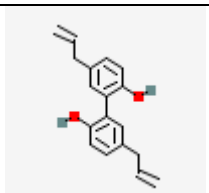
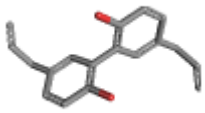
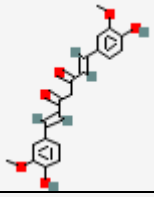
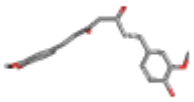
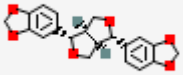
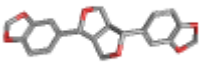
Table 2: Chemical properties of selected Ligands.

Compound	Molecular Weight g/mol	Molecular formula	H- bond donar	H- bond acceptor	Rotatable bonds
Linalool	154.25	$C_{10}H_{18}O$	1	1	4
Cuminaldehyde	148.20	$C_{10}H_{12}O$	0	1	2
Bakuchiol	256.4	$C_{18}H_{24}O$	1	1	6
Magnolol	266.3	$C_{18}H_{18}O_2$	2	2	5
Curcumin	368.4	$C_{21}H_{20}O_6$	2	6	8
Sesamin	354.4	$C_{20}H_{18}O_6$	0	6	2

Each selected phytochemical was prepared for docking by obtaining its 2D and 3D structures from 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 structured of ligands are shown in Table 2.

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

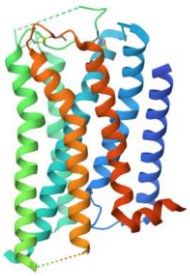
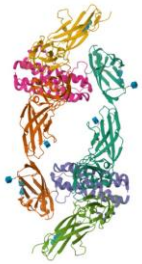
Compound	2D Structure	3D structure
Linalool		
Cuminaldehyde		
Bakuchiol		

Magnolol		
Curcumin		
Sesamin		

Preparation of Target

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

Table 3: Selected targets and their action.

Target protein	PDB ID	Structure	Role in Urticaria
Histamine H1 receptor Inhibitor	8X5X		By binding to H1R on endothelial cells and sensory nerves, these drugs inhibit the Gq/11 protein signaling pathway. This prevents the release of intracellular calcium, effectively stopping vasodilation and vascular permeability that cause urticarial wheals.
IL-13	8DPS		An critical type 2 cytokine that contributes to the persistence of inflammation and the sensation of itching.

Molecular Docking

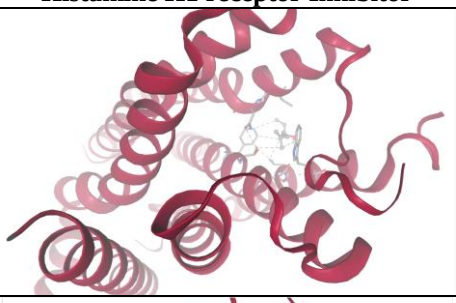
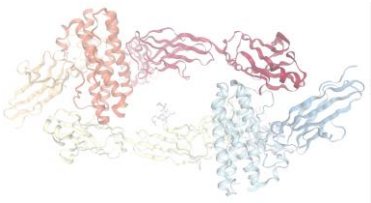
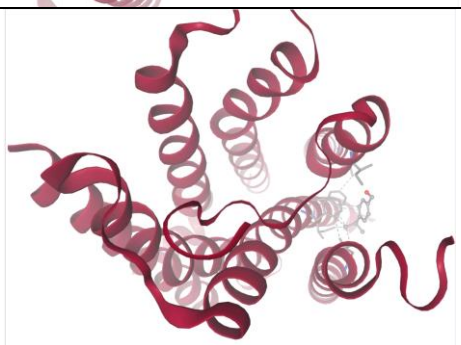
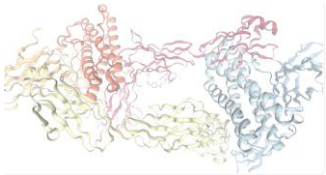
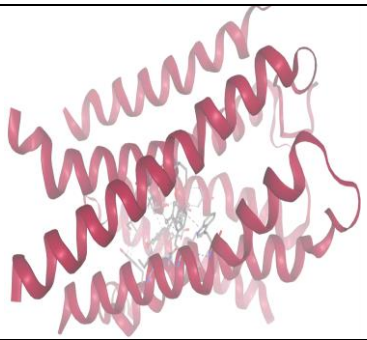
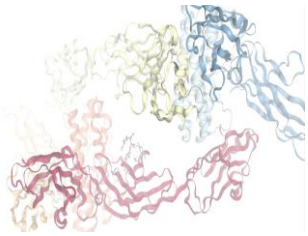
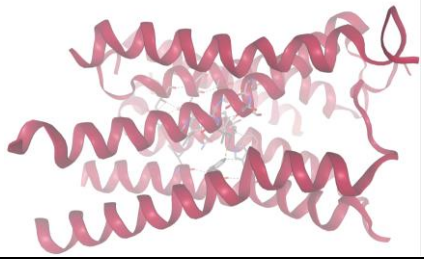
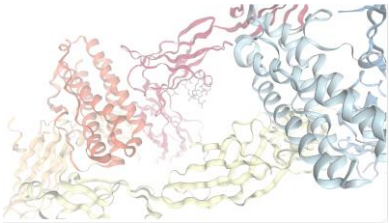
Docking simulations were conducted using MGL Auto Dock tools to evaluate the binding interactions between the target protein and each ligand. Molecular interaction analysis done by using Auto Dock 1.5.7 Morris et al.(2009) by following steps: Gasteiger partial charges were added to the ligand atoms. 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 were repeated using Swissdock vina page.

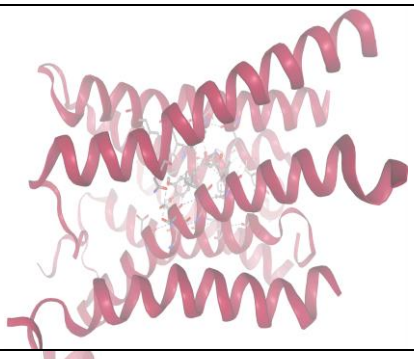
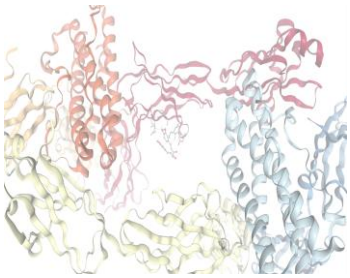
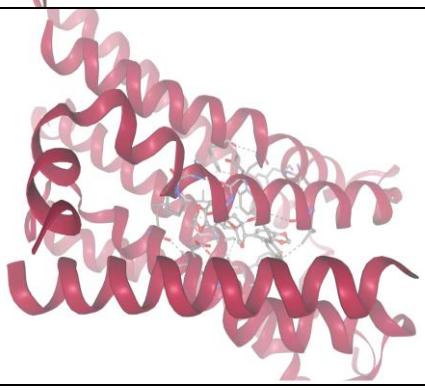
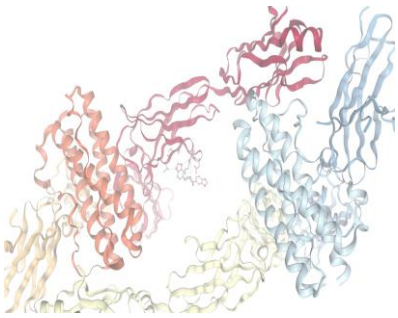
RESULTS AND DISCUSSION

Total of 6 bioactive lead compounds were retrieved from the herbal ingredients, From the reported data of the herbal preparation, the phytochemical present in the

siddha formulation Sanjeevi thylam reveals maximum of 20 interactions with the core active amino acid residues present on the target protein Histamine H1 receptor inhibitor and Il 13 which in turn exhibits anti-histamine and anti-inflammatory activity.

Compounds	Histamine H1 receptor Inhibitor		Il-13	
	No. Of Interactions	Highest Binding Free energy Kcal/ mol	No. Of Interactions	Highest Binding Free energy Kcal/ mol
Linalool	20	-3.434	19	-1.934
Cuminaldehyde	20	-3.392	20	-1.489
Bakuchiol	7	-3.022	19	-2.690
Magnolol	12	--3.002	19	-2.900
Curcumin	8	-4.065	20	-3.266
Sesamin	7	-0.949	20	-3.101

Compound	Histamine H1 receptor Inhibitor	Il-13
Linalool		
Cuminaldehyde		
Bakuchiol		
Magnolol		

Curcumin		
Sesamin		

CONCLUSION

Based on the results of the computational analysis it was concluded that the bio-active compound's present in the siddha formulation Sanjeevi thylam possess significant binding against the target histamine H1 receptor Inhibitors and IL13 interacting with active amino acid present on the active site thereby it was concluded that these compounds may exerts promising anti-inflammatory and anti-histamine activity. Thereby phytocomponents which inhibit the target may act as a potential therapeutic agent for management of Urticaria.

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