EUROPEAN JOURNAL OF BIOMEDICAL AND PHARMACEUTICAL SCIENCES
http://www.ejbps.com

ISSN 2349-8870
Volume: 12
Issue: 10
Year: 2025

IN SILICO NETWORK PHARMACOLOGY AND MOLECULAR DOCKING ANALYSIS OF SELECTIVE PHYTOCHEMICALS FROM *SARADAI KUDINEER* CHOORANAM FOR ANTI-INFLAMMATORY AND ANALGESIC ACTIVITY

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DOI: https://doi.org/10.5281/zenodo.17277469

Article Received on 23/08/2025 **Article Revised on 12/09/2025** **Article Accepted on 02/10/2025**

ABSTRACT
This study employs network pharmacology and molecular docking analysis to investigate the anti-inflammatory and analgesic potential of phytochemicals from Saradaikudineer Chooranam, a traditional Siddha formulation. By identifying bioactive compounds, predicting targets, and analyzing molecular interactions, this research aims to elucidate the mechanism of action and identify potential lead compounds for therapeutic development. The findings may provide insights into the integration of traditional knowledge and modern science, contributing to novel therapeutic discoveries for inflammation and pain management.

KEYWORDS: Trianthema decandra, Kudineer Chooranam, Siddha medicine, Phytoconstituents, Traditional formulations.

INTRODUCTION
Network pharmacology and molecular docking are powerful tools for investigating the complex interactions between phytochemicals and biological systems. This study focuses on Saradaikudineer Chooranam, a traditional Siddha formulation, and its potential anti-inflammatory and analgesic properties. Saradaikudineer Chooranam[2]*: A Siddha herbal formulation used to treat various ailments, including inflammation and pain. Plant-derived compounds with potential therapeutic benefits is approached to understanding the interactions between multiple compounds and biological targets through computational method for predicting the binding affinity between small molecules and proteins.

This research aims to determine the bioactive compounds present in Saradaikudineer Chooranam by using network pharmacology to predict the potential targets of these phytochemicals and analyze anti-inflammatory and analgesic effects of the phytochemicals using molecular docking analysis.[5]

MATERIALS AND METHODS
Molecular modeling is the most important method for the investigation and reorganization of receptor proteins and compound structures, potentially without requiring more investment in research work and time. Structure prediction of the target and the ligand is important for their interaction studies.

Table 1: Ingredients of Saradai kudineer chooranam.[1][2]

1	Saradai(Trianthema decandra)	1 part
2	Kadukkai(Terminalia chebula)	1 part
3	Chukku(Zingiber officinale)	1 part
4	Uppu(Salt)	Required amount

Preparation of Ligand
Trianthema decandra L. (Family: Aizoaceae), commonly known as horse purslane, is a creeping annual herb widely distributed in tropical regions and extensively used in traditional medicine. Phytochemical studies have revealed the presence of alkaloids, flavonoids, glycosides, triterpenes, saponins, and phenolic compounds, which are responsible for its wide range of biological activities. The plant is well known for its hepatoprotective effect, being traditionally prescribed for jaundice, hepatitis, and other liver ailments. It also demonstrates significant anti-inflammatory, analgesic, diuretic, antioxidant, anthelmintic, and antimicrobial activities, supporting its use in rheumatism, painful inflammatory conditions, edema, urinary disorders, intestinal worms, and skin infections. Leaf juice is commonly administered as a liver tonic and digestive aid, while decoctions and poultices are employed for their diuretic, anti-inflammatory, and pain-relieving properties. Collectively, these findings highlight the therapeutic potential of T. decandra, particularly as a natural hepatoprotective, anti-

inflammatory, and analgesic agent, meriting further pharmacological exploration.

Fig no.1: Trianthema decandral.

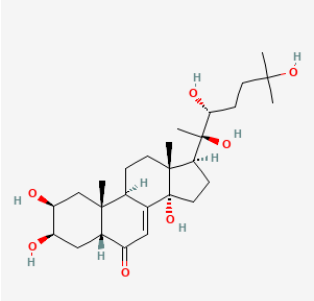
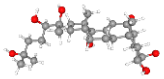
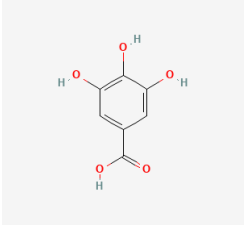
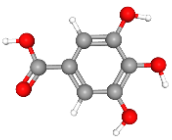
The phytochemicals identified with their Molecular weight, Molecular formula, H-bond donor, H-bond acceptor, and Rotatable bonds were listed in Table 2.[5][6][7]

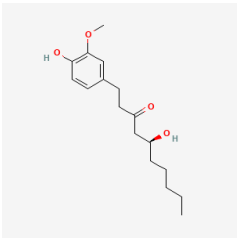
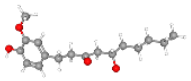
Table 2: Chemical properties of selected Ligands.

Compound	Molecular Weight g/mol	Molecular formula	H- bond donar	H- bond acceptor	Rotatable bonds
Ecdysterone (Saradai)	480.6	$C_{27}H_{44}O_7$	6	7	5
Gallic acid (Kadukkai)	170.12	$C_7H_6O_5$	4	5	1
Gingerol (Chukku)	294.4	$C_{17}H_{26}O_4$	2	4	10

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.[3][4]

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

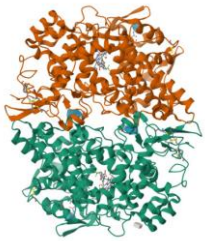
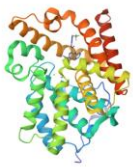
Compound	2D Structure	3D structure
Ecdysterone		
Gallic acid		

Gingerol		

PREPARATION OF TARGET

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

Table: Selected targets and their action.[3][4]

Target protein	PDB ID	Structure	Action
COX2 Inhibitor	3NTG		1. Anti inflammatory 2. Anti analgesic 3. Anti pyertic
IL6	5SFK		1.Anti inflammatory 2.Anti analgesic

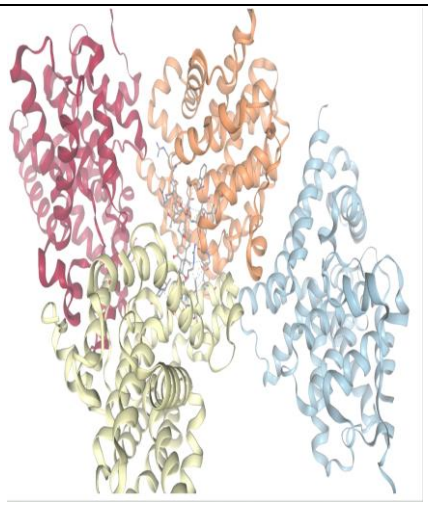
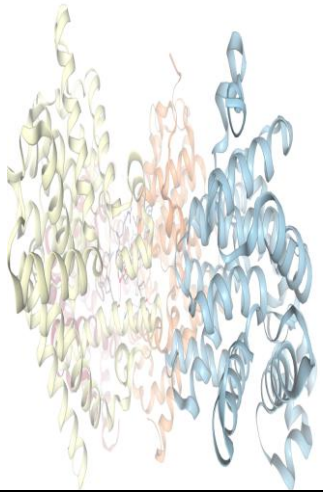
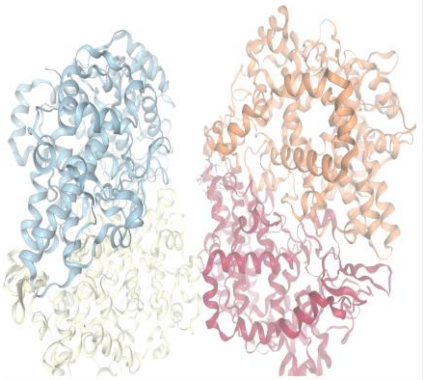
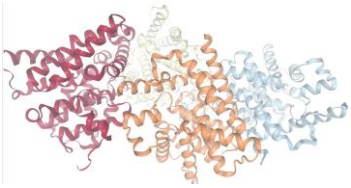
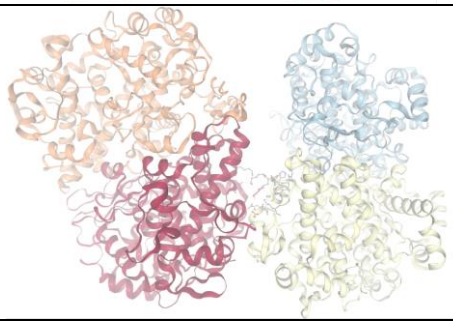
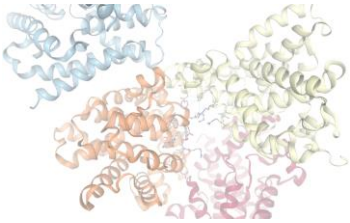
MOLECULAR DOCKING

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 done by using Auto Dock 1.5.7, Morris et al. (2009), by following the 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 Swissdock vina page.[1,2]

RESULTS AND DISCUSSION

A total of 3 bioactive lead compounds were retrieved from the herbal ingredients. From the reported data of the herbal preparation, the phytochemicals like Ecdysterone, Gallic acid, and Gingerol present in the siddha formulation Saradai kudineer reveal a maximum of 20 interactions with the core active amino acid residues present on the target protein COX2 inhibitor and IL-6, which in turn exhibits analgesic and anti-inflammatory activity.[3][4]

Compounds	COX2 INHIBITOR		Il-6	
	No. Of Interactions	Highest Binding Free energy Kcal/ mol (COX 2 Inhibitors)	No. Of Interactions	Highest Binding Free energy Kcal/ mol (IL6)
Ecdysterone	20	-4.475	13	-6.070
Gallic acid	20	-3.335	20	-3.719
Gingerol	20	-4.228	20	4.628

Compound	COX2 INHIBITOR	Il-6
Ecdysterone		
Gallic acid		
Gingerol		

CONCLUSION

Based on the results of the computational analysis, it was concluded that the bioactive compounds like Ecdysterone, Gallic acid, and Gingerol present in the siddha formulation Saradai kudineer possess significant binding against the target COX2 Inhibitors and IL6, interacting with active amino acids present on the active site. thereby it was concluded that these compounds may exert promising anti-inflammatory and analgesic activity. Thereby, phytocomponents that inhibit the target COX2 inhibitors and IL6 may act as a potential therapeutic agent for the management of Cervical spondylosis, Osteoarthritis, Ankylosing spondylitis, Rheumatoid arthritis, Acute and chronic pain.

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