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

ISSN 2349-8870
Coden USA: EJBPBO
Volume: 13
Issue: 6
Year: 2026

IN SILICO MOLECULAR DOCKING ANALYSIS AND ADME PROFILING OF THE SIDDHA HERBAL FORMULATION GOWTHAMAR CHOORANAM AGAINST CHRONIC BRONCHITIS

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DOI: https://doi.org/10.5281/zenodo.20642068

How to cite this Article: R. Umabharathi*[1], K. Thangagomathi[2], K. Vignesh[3]. (2026). In Silico Molecular Docking Analysis And Adme Profiling of The Siddha Herbal Formulation Gowthamar Chooranam Against Chronic Bronchitis. European Journal of Biomedical and Pharmaceutical Sciences, 13(6), 453–461.

Article Received on 15/05/2026 **Article Revised on 05/06/2026** **Article Published on 10/06/2026**

ABSTRACT

Background and Objective: Chronic bronchitis is a chronic inflammatory respiratory disorder characterized by persistent cough, excessive sputum production, airway inflammation, and progressive obstruction of the bronchi. The disease significantly affects respiratory function and quality of life due to recurrent airway irritation and mucus accumulation. In Siddha medicine, conditions resembling chronic bronchitis are associated with derangement of Kabamm and Vaathamm, resulting in cough, phlegm accumulation, wheezing, and breathing difficulty. Although conventional therapies provide symptomatic relief, prolonged treatment is frequently associated with adverse effects, recurrence, and therapeutic resistance. Siddha herbal formulations have been traditionally used for respiratory disorders because of their anti-inflammatory, expectorant, broncho-dilatory, antioxidant, and immunomodulatory properties. Among them, Gowthamar Chooranam is a classical Siddha formulation traditionally indicated for chronic cough and respiratory ailments. However, its molecular mechanism and pharmacological potential against the disease remains scientifically unexplored. Therefore, the present study was designed to investigate the molecular docking interactions and ADME profiling of selected phytoconstituents of Gowthamar Chooranam against major inflammatory targets associated with chronic bronchitis using computational approaches. **Materials and Methods:** Preliminary molecular docking analysis was carried out using AutoDock tools to evaluate the interaction between selected phytoconstituents of Gowthamar Chooranam and inflammatory target proteins associated with chronic respiratory inflammation. The major phytocompounds were identified through literature review and phytochemical databases. ADME and drug-likeness profiling were performed using the SwissADME web server to evaluate pharmacokinetic properties, gastrointestinal absorption, cytochrome P450 inhibition, bioavailability, and medicinal chemistry parameters. **Results and Discussion:** The selected phytoconstituents exhibited significant binding affinity and stable molecular interactions with inflammatory target proteins involved in chronic bronchitis. ADME analysis demonstrated favorable pharmacokinetic properties, acceptable gastrointestinal absorption, and good drug-likeness profiles, indicating promising anti-inflammatory and bronchodilatory potential of the selected compounds. **Conclusion:** The present computational study suggests that Gowthamar Chooranam possesses significant therapeutic potential against airway inflammation through anti-inflammatory and immunomodulatory mechanisms. Further in vitro, in vivo, and clinical studies are required to validate the efficacy and safety of the formulation.

KEYWORDS: Siddha, Chronic bronchitis, Gowthamar Chooranam, Respiratory inflammation.

INTRODUCTION

Chronic bronchitis is a chronic inflammatory respiratory disorder characterized by persistent productive cough, excessive mucus secretion, airway obstruction, and progressive inflammation of the bronchial airways. It is one of the major respiratory diseases contributing to significant morbidity and reduction in the quality of life worldwide. The disease commonly develops due to prolonged exposure to cigarette smoke, environmental pollutants, allergens, occupational dust, and recurrent respiratory tract infections. Persistent inflammation of the bronchi leads to hypersecretion of mucus, edema of

the airway mucosa, impaired mucociliary clearance, and narrowing of the air passages, resulting in breathing difficulty, wheezing, chest congestion, and chronic cough.

The pathogenesis of chronic bronchitis involves activation of inflammatory mediators such as tumor necrosis factor-alpha (TNF-α), interleukin-6 (IL-6), interleukin-8 (IL-8), cyclooxygenase-2 (COX-2), and nuclear factor kappa-B (NF-κB), which play a major role in sustaining chronic airway inflammation. These inflammatory cytokines promote infiltration of neutrophils and macrophages into bronchial tissues, leading to oxidative stress, epithelial damage, mucus hypersecretion, and progressive airway obstruction. Current therapeutic approaches including bronchodilators, corticosteroids, antibiotics, and mucolytic agents mainly provide symptomatic relief and are often associated with adverse effects, recurrence, and therapeutic resistance during prolonged usage.

Siddha medicine, one of the oldest traditional systems of medicine practiced in South India, describes respiratory disorders under diseases caused by derangement of Kabamm and Vaathamm. Chronic bronchitis can be correlated with Irumal, Swasa kaasam, and other Kabamm Vaatham disorders characterized by persistent cough, excessive phlegm production, wheezing, chest tightness, and breathing difficulty. According to Siddha principles, imbalance of Mukkutram, particularly aggravated Kabamm, leads to obstruction of respiratory pathways and impairment of normal pulmonary function. Siddha formulations possessing anti-inflammatory, expectorant, bronchodilatory, antioxidant, and immunomodulatory activities have been traditionally used for the effective management of chronic respiratory disorders.

Among the classical Siddha formulations, Gowthamar Chooranam is traditionally indicated for various respiratory ailments including chronic cough, bronchial irritation, phlegm accumulation, and breathing difficulties. The herbal ingredients present in Gowthamar Chooranam are reported to possess significant therapeutic properties that may help suppress inflammatory mediators, reduce mucus accumulation, improve airway clearance, and enhance respiratory function. However, the molecular mechanism and pharmacological potential of Gowthamar Chooranam against chronic bronchitis remain insufficiently investigated.

Recent advancements in computational biology have enabled the application of molecular docking and ADME profiling techniques for evaluating the interaction between phytoconstituents and disease-associated target proteins. Molecular docking predicts the binding affinity and interaction pattern of bioactive compounds with inflammatory target proteins, while ADME analysis evaluates absorption, distribution, metabolism, excretion, and drug-likeness properties essential for drug discovery and development.

Therefore, the present study was designed to investigate the molecular docking interactions and ADME profiling of selected phytoconstituents present in Gowthamar Chooranam against important inflammatory target proteins associated with chronic bronchitis in order to scientifically validate its therapeutic potential.

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 Gowthamar Chooranam

Table 1: Ingredients of Gowthamar Chooranam.

Ingredients	Family	Active ingredients	
Terminalia chebula	Combretaceae	Chebulanin	Expectorant, anti-asthmatic, anti-inflammatory, reduces airway inflammation and cough
Piper longum	Piperaceae	Piperine	Bronchodilator, anti-asthmatic, mucolytic, improves respiratory function and relieves cough
Piper cubeba	Piperaceae	Cubebin	Expectorant, antimicrobial, relieves bronchial congestion and respiratory infections
Alpinia officinarum	Zingiberaceae	Galangin	Anti-inflammatory, anti-allergic, helps reduce airway inflammation and respiratory irritation
Myristica fragrans	Myristicaceae	Myristicin	Anti-inflammatory, expectorant, antimicrobial, supports relief from cough and cold

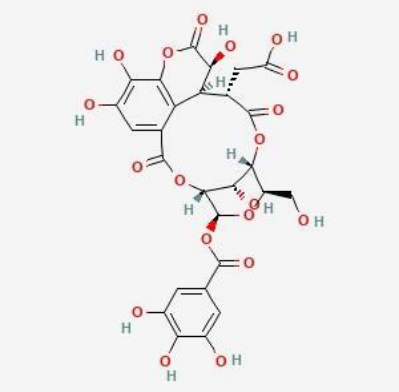
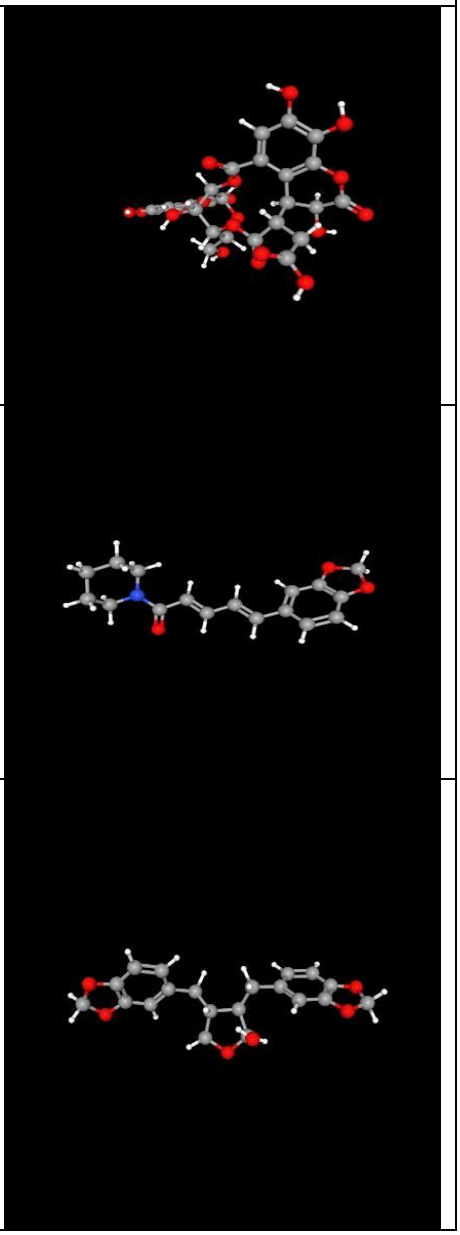
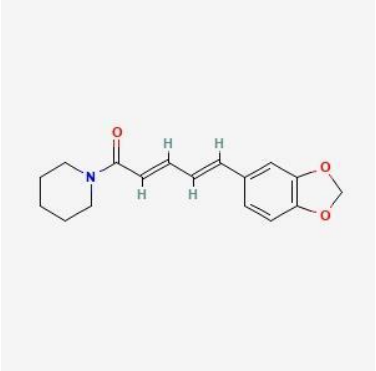
The identified phytochemicals along with their Molecular weight, Molecular formula, H-bond donor, H-bond acceptor, Rotatable bonds were listed in table 1.

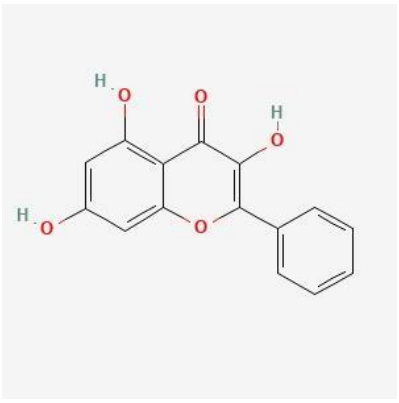
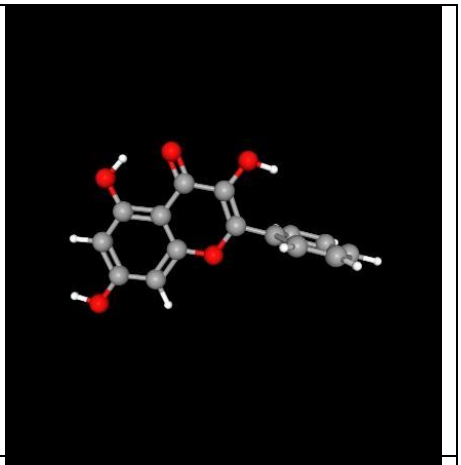
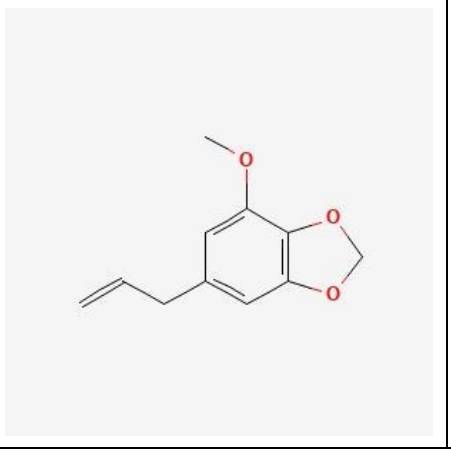
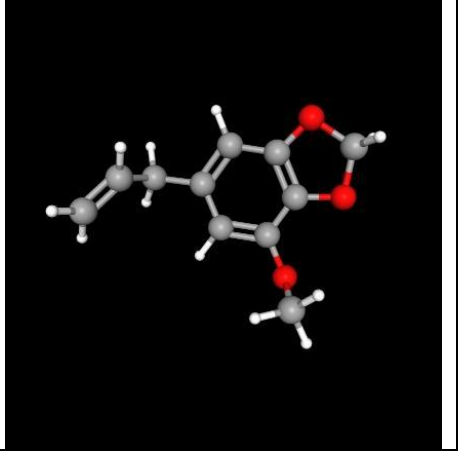
Table 2: Chemical properties of selected Ligands.

Compound	Molecular Weight g/mol	Molecular formula	H- bond donor	H- bond acceptor	Rotatable bonds
Chebulanin	625.5	C27H24O19	9	19	6
Piperine	285.34	C17H19NO3	0	3	3
Cubebin	315.36	C20H20O6	1	6	4
Galangin	270.24	C15H10O5	3	5	1
Myristicin	192.21	C11H12O3	0	3	3

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 structures of the ligands are shown in Table 3.

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

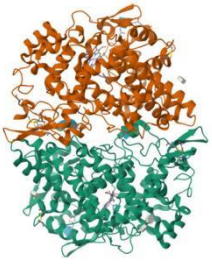
Compound	2D Structure	3D structure
Chebulanin		
Piperine		
Cubebin		

Galangin		
Myristicin		

Preparation of Target

The target proteins were selected based on SwissTargetPrediction (http://www.swisstargetprediction.ch/index.php). Also the target proteins TNF-α (PDB ID: 2AZ5) and COX-2 (PDB ID: 5IKR) were selected based on their established roles in chronic bronchitis pathogenesis and inflammatory signaling pathways reported in previous literature. The predicted target proteins were downloaded from RCSB PDB database (https://www.rcsb.org/) . The x-ray diffraction structures of the selected target proteins with a resolution below 2 Å 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 Chronic bronchitis
TNF-α	2AZ5		TNF-α is released from activated macrophages and epithelial cells following exposure to cigarette smoke and pollutants. It activates the NF-κB signaling pathway and stimulates the production of inflammatory cytokines such as IL-1β and IL-6.
COX-2	5IKR		COX-2 catalyzes the conversion of arachidonic acid into inflammatory prostaglandins, particularly PGE2, during airway inflammation. Its expression is increased in bronchial epithelial cells during chronic inflammatory conditions

Molecular Docking

Docking simulations were conducted using MGL AutoDock tools to evaluate the binding interactions between the target protein and each ligand. Molecular interaction analysis was performed using AutoDock 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 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.

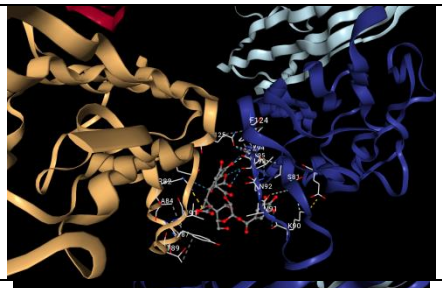
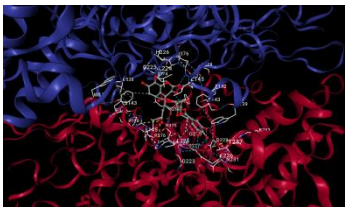
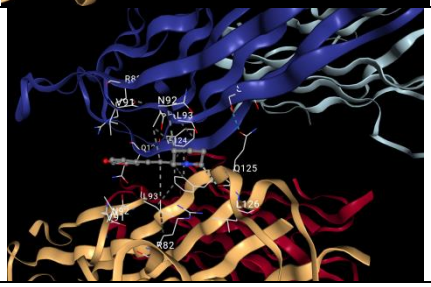
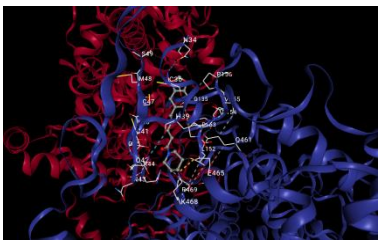
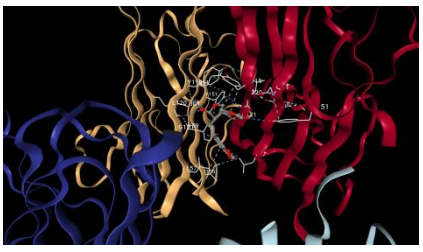
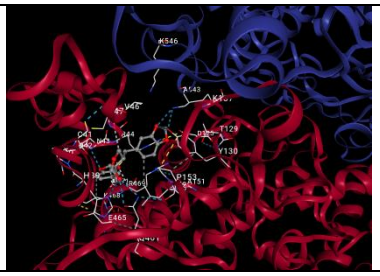
RESULTS AND DISCUSSION

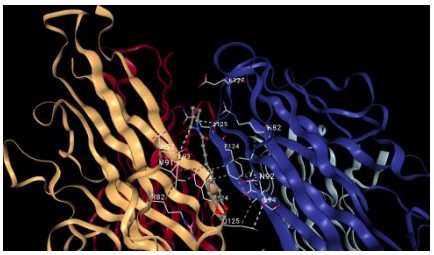
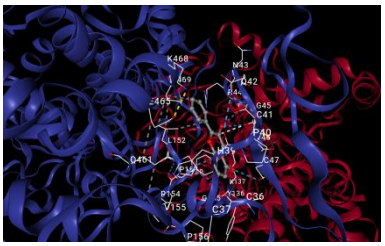
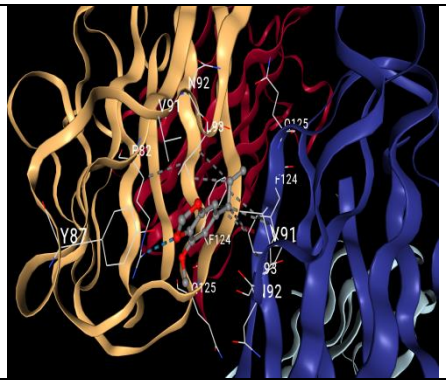
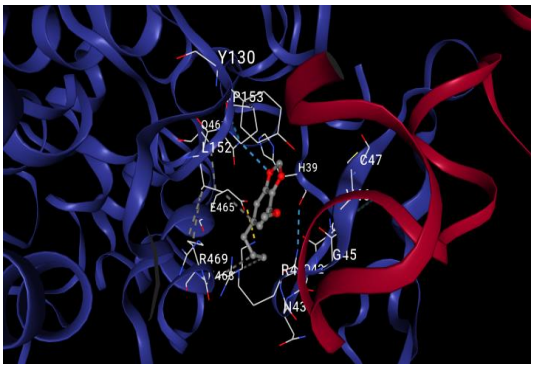
The molecular docking analysis performed in the present study demonstrated significant binding interactions between the selected phytoconstituents of Gowthamar Chooranam and the inflammatory target proteins TNF-α (PDB ID: 2AZ5) and COX-2 (PDB ID: 5IKR), which play a major role in the pathogenesis of chronic bronchitis.

Table 5: Binding energies of different compounds.

Compounds	TNF-α		COX-2	
	No. of Interactions	Highest Binding Free Energy (Kcal/ mol)	No. of Interactions	Highest Binding Free Energy Kcal/ mol
Chebulanin	16	-9.2	11	-5.1
Piperine	20	-7.7	20	-8.7
Cubebin	20	-7.8	20	-10.5
Galangin	19	-7.6	18	-8.8
Myristicin	20	-6.1	19	-6.6

Table 6: Docking interactions of Different compounds.

Compound	TNF-α	COX-2
Chebulanin		
Piperine		
Cubebin		

Galangin		
Myristicin		

A total of five major bioactive compounds, namely Chebulanin, Piperine, Cubebin, Galangin, and Myristicin, were selected for docking analysis based on their reported pharmacological activities and phytochemical significance. The docking results revealed favorable binding affinity and stable ligand–protein interactions with both target proteins. Among the selected compounds, Chebulanin exhibited strong binding affinity against TNF-α with a binding energy of −9.2 kcal/mol, indicating stable interaction with the active site residues of the protein. Similarly, Cubebin demonstrated the highest binding affinity against COX-2 with a binding energy of −10.5 kcal/mol and 20 molecular interactions, suggesting possible anti-inflammatory activity.

Piperine also exhibited significant binding interactions with both TNF-α and COX-2 targets. Piperine showed strong binding affinity against COX-2 with a binding energy of −8.7 kcal/mol and 20 molecular interactions, indicating its potential bronchodilatory and anti-inflammatory activity. Galangin demonstrated stable molecular interactions with TNF-α and COX-2 with binding energies of −7.6 kcal/mol and −8.8 kcal/mol respectively, suggesting its possible role in suppression of inflammatory mediators associated with chronic airway inflammation. Myristicin also exhibited moderate but significant binding affinity against both target proteins, indicating supportive anti-inflammatory and expectorant activity.

The observed molecular interactions suggest that the selected phytoconstituents may inhibit inflammatory signaling pathways associated with chronic bronchitis by interacting with cytokine-mediated inflammatory targets. TNF-α is an important pro-inflammatory cytokine released from activated macrophages and bronchial epithelial cells following exposure to cigarette smoke, allergens, and environmental pollutants. Activation of TNF-α stimulates NF-κB signaling pathways and promotes the release of inflammatory mediators such as IL-1β, IL-6, and IL-8, which contribute to chronic airway inflammation, mucus hypersecretion, and bronchial obstruction.

Similarly, COX-2 is a major inflammatory enzyme involved in the conversion of arachidonic acid into inflammatory prostaglandins during airway inflammation. Increased expression of COX-2 in bronchial epithelial cells contributes to edema, bronchial irritation, oxidative stress, and progression of chronic inflammatory respiratory conditions. Therefore, effective inhibition of TNF-α and COX-2 may help reduce airway inflammation, mucus accumulation, bronchial irritation, and respiratory discomfort associated with chronic bronchitis.

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)
Chebulanin	Low	No	No	No	Yes	No	No	No	-11. 47
Piperine	High	Yes	Yes	Yes	No	Yes	Yes	Yes	-5. 58
Cubebin	High	Yes	No	No	No	No	No	Yes	-6. 07
Galangin	High	No	No	Yes	Yes	Yes	No	Yes	-6. 32
Myristicin	High	Yes	Yes	Yes	Yes	Yes	Yes	Yes	-5. 39

Drug-likeness

Table 8: Drug-likeness of the compounds.

Compounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability
Chebulanin	No 3 violations	No 3 violations	No 1 violation	No 1 violation	No 4 violations	0.11
Piperine	Yes 0 violations	Yes	Yes	Yes	Yes	0.55
Cubebin	Yes 0 violations	Yes	Yes	Yes	Yes	0.55
Galangin	Yes 0 violations	Yes	Yes	Yes	Yes	0.55
Myristicin	Yes 0 violations	Yes	Yes	Yes	No 1 violation	0.55

Among the investigated compounds, Piperine, Cubebin, Galangin, and Myristicin exhibited high gastrointestinal (GI) absorption, suggesting favorable oral bioavailability and efficient intestinal uptake following administration. In contrast, Chebulanin demonstrated low GI absorption, which may be attributed to its high molecular weight and multiple hydrogen-bonding groups that limit passive membrane permeability.

Blood-brain barrier (BBB) permeability analysis revealed that Piperine, Cubebin, and Myristicin possess the ability to cross biological membranes effectively, whereas Chebulanin and Galangin were predicted to be non-BBB permeant. Although BBB penetration is not essential for the treatment of chronic bronchitis, the results indicate good membrane permeability characteristics for these compounds.

P-glycoprotein (P-gp) substrate analysis showed that Piperine and Myristicin may interact with efflux transport systems. Such interactions could influence drug absorption and tissue distribution, potentially enhancing intracellular retention of co-administered compounds. The remaining phytoconstituents were predicted to be non-substrates of P-gp, suggesting reduced transporter-mediated elimination.

Cytochrome P450 inhibition analysis demonstrated that Piperine and Myristicin inhibit multiple CYP isoforms, including CYP1A2, CYP2C9, CYP2D6, and CYP3A4. This property may contribute to prolonged systemic exposure of bioactive compounds by reducing metabolic degradation. Cubebin exhibited minimal CYP inhibition except for CYP3A4, indicating a comparatively lower risk of metabolic interactions. Galangin showed moderate inhibition of CYP1A2, CYP2C19, CYP2C9, and CYP3A4, whereas Chebulanin exhibited limited CYP inhibition.

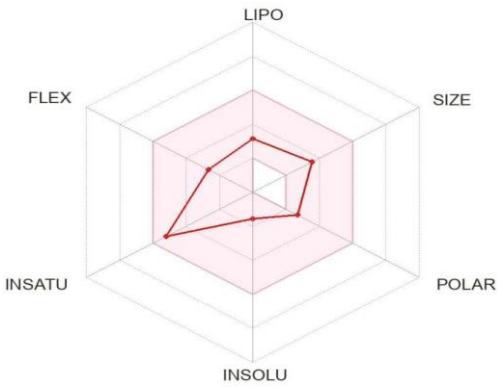
Skin permeation values (Log Kp) ranged from -5.39 to -11.47 cm/s. Myristicin and Piperine exhibited comparatively better membrane permeability, whereas Chebulanin showed the lowest permeability due to its large molecular structure and high polarity.

Drug-likeness assessment revealed that Piperine, Cubebin, and Galangin fully satisfied Lipinski's Rule of Five, Ghose, Veber, Egan, and Muegge criteria without any violations, indicating favorable oral drug-like characteristics. Myristicin also demonstrated acceptable drug-likeness with only one Muegge violation. In contrast, Chebulanin exhibited multiple violations owing to its high molecular weight, elevated polarity, and excessive hydrogen bond donor and acceptor counts.

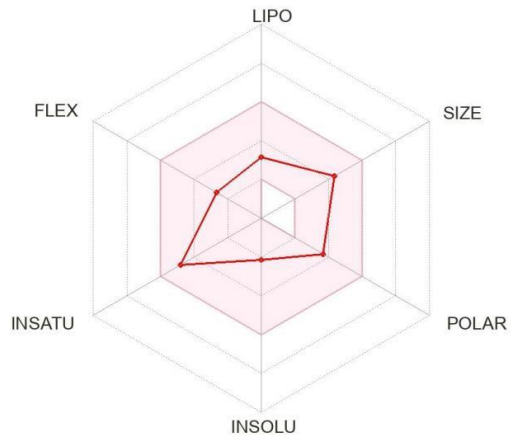
The bioavailability score further supported these findings. Piperine, Cubebin, Galangin, and Myristicin demonstrated a bioavailability score of 0.55, suggesting favorable systemic exposure following oral administration, whereas Chebulanin showed a comparatively low score of 0.11.

Overall, the ADME analysis indicates that Piperine, Cubebin, Galangin, and Myristicin possess favorable pharmacokinetic and drug-likeness characteristics that support their potential development as bioactive agents against chronic bronchitis. Among them, Cubebin appears particularly promising because of its excellent docking affinity toward COX-2 combined with favorable ADME properties, while Piperine demonstrated balanced molecular interactions and pharmacokinetic behavior. These findings provide additional evidence supporting the therapeutic potential of Gowthamar Chooranam in the management of chronic inflammatory respiratory disorders.

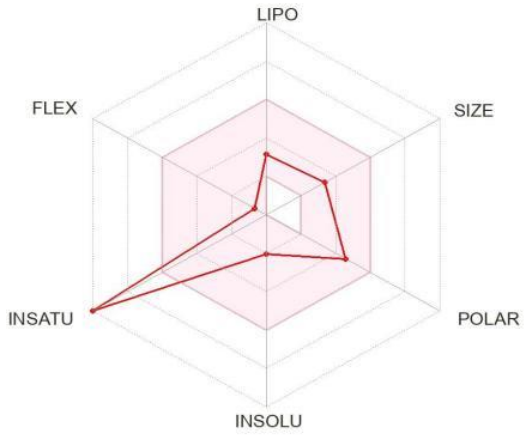
Chebulanin



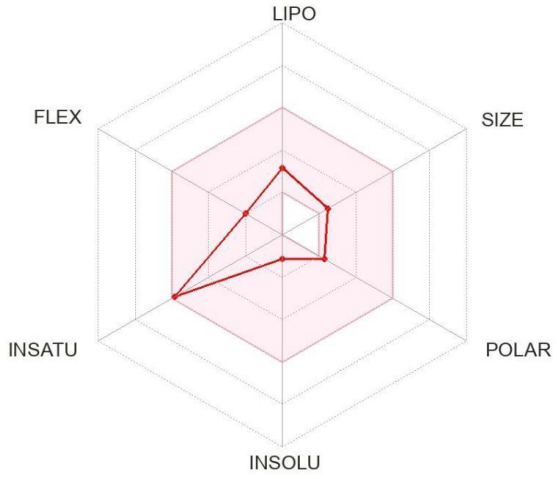
Piperine



Cubebin



Galangin
Myristicin



CONCLUSION

The present molecular docking study demonstrated that the phytoconstituents present in the Siddha herbal formulation Gowthamar Chooranam exhibited significant binding affinity against the inflammatory target proteins TNF-α and COX-2 associated with chronic bronchitis. The selected bioactive compounds showed stable molecular interactions with the active site residues of the target proteins, suggesting potential anti-inflammatory and bronchodilatory activity. The synergistic action of the phytoconstituents may help reduce airway inflammation, mucus hypersecretion, and respiratory obstruction associated with chronic bronchitis. Therefore, the present computational study scientifically supports the traditional Siddha use of Gowthamar Chooranam in the management of chronic respiratory disorders. However, further in vitro, in vivo, and clinical studies are necessary to validate the efficacy and safety of the formulation.

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