



**IN SILICO MOLECULAR DOCKING ANALYSIS AND ADME PROFILING OF THE
SIDDHA HERBAL PREPARATION- SENNAIURUVI PARPAM AGAINST GASTRIC
ULCER**

P. Dharani^{1*}, M. Santhiya², V. Manikandaprabu³, K. Vignesh⁴

^{1,2,3,4}Pg Scholar, Department of Noi Nadal, Government Siddha Medical College, Tirunelveli.



***Corresponding Author: P. Dharani**

Pg Scholar, Department of Noi Nadal, Government Siddha Medical College, Tirunelveli.

DOI: <https://doi.org/10.5281/zenodo.20524693>

How to cite this Article: P. Dharani^{1*}, M. Santhiya², V. Manikandaprabu³, K. Vignesh⁴ (2026). In Silico Molecular Docking Analysis And Adme Profiling Of The Siddha Herbal Preparation- Sennaiuruvi Parpam Against Gastric Ulcer. European Journal of Biomedical and Pharmaceutical Sciences, 13(6), 280–286.

This work is licensed under Creative Commons Attribution 4.0 International license.



Article Received on 05/05/2026

Article Revised on 25/05/2026

Article Published on 03/06/2026

ABSTRACT

Background and Objective: Siddha, one of the traditional systems of medicine practiced in India, is known for its unique approaches towards prevention, diagnosis as well as treatment of every disease. Ample literary evidence on medicinal formulations are found in Siddha literatures whose scientific validation is still partial. Gastric Ulcer is a common disease which is mentioned in Siddha as “Kunmam”, and is defined as a distinct breach in the mucosa of the gastrointestinal tract as a result of caustic effects of acid and pepsin in the lumen as defined by WHO. About 5 to 10 % of the world population are affected by Gastric ulcer. A strong scientific approach towards treatment perspectives are needed since the disease affects both physical and social-well being of the individuals. Many Siddha formulations for Kunmam are mentioned in literatures. One among them is the “Sennaiuruvi Parpam” mentioned in "Agathiyar 2000". A proper scientific validation of this formulation could pave the way for 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 and ADME profiling were done for Sennaiuruvi Parpam against Gastric Ulcer. The binding action of major phytoconstituents of the drugs in Sennaiuruvi Parpam against various targets were documented. **Results and Discussion:** Most of the phytochemicals present in the drugs of Sennaiuruvi Parpam shows significant binding capacities against the targets like Proton pump inhibitor and COX-2. Hence it may be considered for the treatment and management of Gastric Ulcer. **Conclusion:** The Siddha herbal preparation "Sennaiuruvi Parpam " posses inherent action against Gastric Ulcer by binding with various targets was concluded by the present study.

KEYWORDS: Siddha, Gastric Ulcer, Sennaiuruvi Parpam, Kunmam.

INTRODUCTION

Gastric Ulcer is one of the most common gastrointestinal disorders characterized by mucosal erosion occurring due to an imbalance between aggressive factors such as gastric acid, pepsin, reactive oxygen species, Helicobacter pylori infection, non-steroidal anti-inflammatory drugs (NSAIDs), and defensive mechanisms including mucus secretion, bicarbonate production, mucosal blood flow, and cellular regeneration. Gastric Ulcer continues to be a major health problem affecting millions of individuals

worldwide and significantly reducing quality of life. Clinical manifestations include epigastric pain, nausea, bloating, indigestion, anorexia, hematemesis, and melena. Persistent ulceration may further lead to serious complications such as perforation, hemorrhage, and gastric carcinoma.

The pathogenesis of gastric ulcer involves multiple molecular pathways including oxidative stress, inflammatory cytokine activation, apoptosis, and gastric acid hypersecretion. Pro-inflammatory mediators such as

tumor necrosis factor- α (TNF- α), interleukin-6 (IL-6), cyclooxygenase-2 (COX-2), nuclear factor kappa B (NF- κ B), and inducible nitric oxide synthase (iNOS) play significant roles in gastric mucosal injury and inflammation. Current therapeutic approaches mainly include proton pump inhibitors, H2 receptor antagonists, antibiotics, antacids, and cytoprotective agents. Although these therapies provide symptomatic relief, long-term use is associated with adverse effects including recurrence, drug resistance, nutrient malabsorption, renal complications, and altered gut microbiota. Therefore, identification of safer and multi-target therapeutic agents from traditional medicinal systems has gained considerable research interest.

Omeprazole and Pantoprazole are commonly prescribed anti-ulcer medications; however, prolonged administration may result in headache, osteoporosis, rebound acid hypersecretion, and gastrointestinal infections. These limitations emphasize the necessity for alternative therapeutic interventions with improved safety and efficacy profiles.

Siddha Medicine is one of the oldest traditional systems of medicine practiced predominantly in South India and is well known for its holistic approach toward disease prevention and treatment. Numerous Siddha herbal and herbo-mineral formulations described in classical Siddha literature have been traditionally used for the management of gastrointestinal disorders including “Kunmam,” which can be correlated with gastric ulcer in modern medicine. Among these formulations, “Sennaiuruvi Parpam” is traditionally indicated for various digestive ailments and inflammatory disorders. Despite its long-standing therapeutic usage, the precise

molecular mechanism and pharmacological basis of this formulation remain scientifically unexplored.

Therefore, the present study was designed to investigate the therapeutic potential and molecular mechanisms of Siddha formulation Sennaiuruvi Parpam against gastric ulcer using network pharmacology and molecular docking approaches. The study aims to identify the active phytoconstituents, predict potential therapeutic targets, analyze protein–protein interaction networks and signaling pathways, and evaluate the binding interactions of selected bioactive compounds with ulcer-related target proteins. The findings of this study may provide scientific evidence supporting the traditional use of Sennaiuruvi Parpam and contribute toward the development of evidence-based Siddha therapeutics for gastric ulcer management.

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 phytochemicals, 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 Sennaiuruvi Parpam

Table 1: Ingredients of Sennaiuruvi Parpam.

Ingredients	Family	Active ingredients	
Achyranthes bidentata	Amaranthaceae	Stachydrine	Anti-inflammatory, reduces oxidative stress, protect gastric mucosa ^[3]
		Betaine	Cytoprotective effect, osmoprotectant, helps mucosal healing and reduces inflammation ^[4,5]
Piper nigrum	Piperaceae	Piperine	Anti-ulcer, Antioxidant, Anti-inflammatory activity ^[6,7]
Ferula asafoetida	Apiaceae	Umbelliferone	Anti-inflammatory, Anti-oxidant, Anti-microbial, Cytoprotective ^[8,9]

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

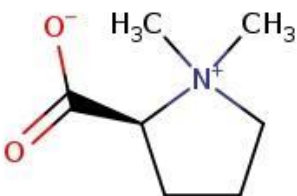
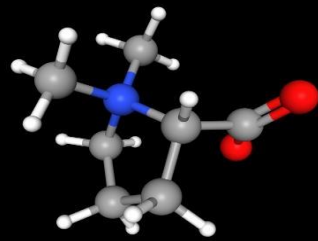
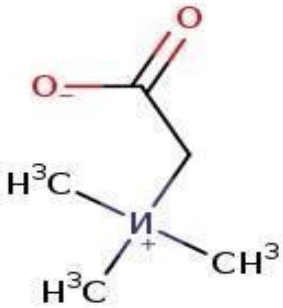
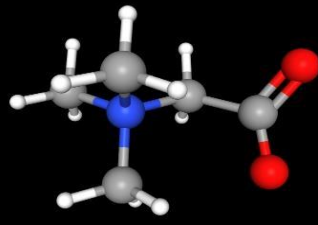
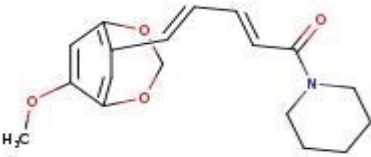
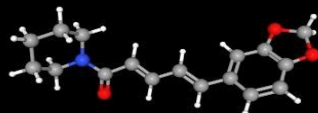
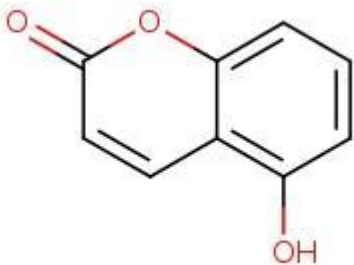
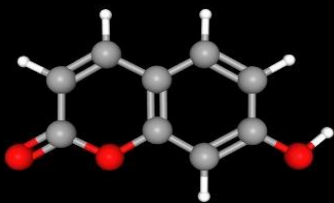
Table 2: Chemical properties of selected Ligands.

Compound	Molecular Weight g/mol	Molecular formula	H- bond donor	H- bond acceptor	Rotatable bonds
Stachydrine	143.18	C ₇ H ₁₃ NO ₂	0	2	1
Betaine	117.15	C ₅ H ₁₁ NO ₂	0	2	1
Piperine	315.36	C ₁₈ H ₂₁ NO ₄	0	4	5
Umbelliferone	162.14	C ₉ H ₆ O ₃	1	3	0

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 structure of the ligands are shown in Table 2

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


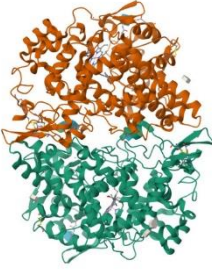
Compound	2D Structure	3D structure
Stachydrine		
Betaine		
Piperine		
Umbelliferone		

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 structure of the different target proteins under study having resolution not less than 2 Å⁰ 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 Gastric Ulcer
H ⁺ /K ⁺ ATP ase	5YLU		The proton pump exchanges intracellular H ⁺ ions with extracellular K ⁺ ions in parietal cells using ATP hydrolysis. Excess activation increases gastric acid secretion, lowers gastric pH, disrupts the mucosal barrier, and promotes autodigestion of gastric epithelium, resulting in ulcer formation.
COX-2	5IKR		Gastric mucosal damage stimulates inflammatory cytokines and arachidonic acid metabolism, leading to increased COX-2 expression. Elevated COX-2 produces excess prostaglandins such as PGE ₂ , resulting in inflammation, edema, leukocyte infiltration, oxidative stress, and mucosal erosion. Persistent activation aggravates ulcer progression and delays healing.

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 (K_i) 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.

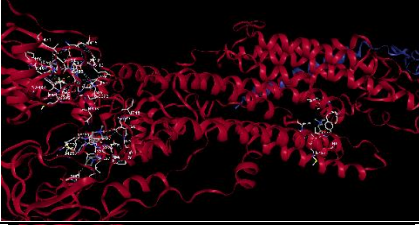
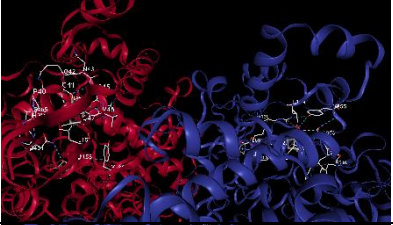
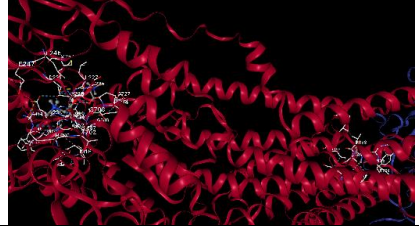
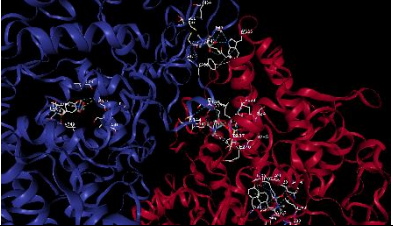
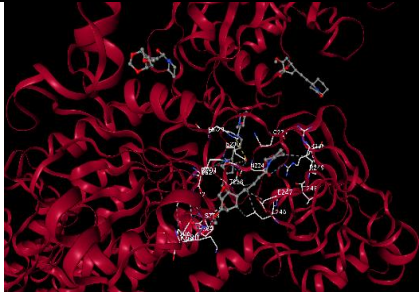
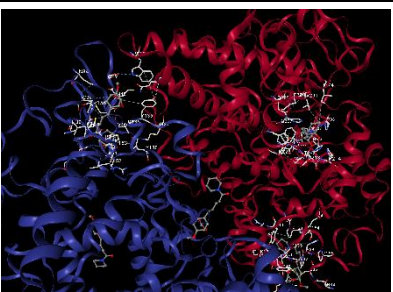
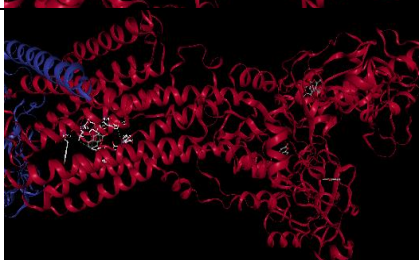
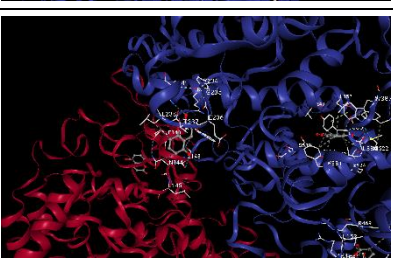
RESULTS AND DISCUSSION

A total of four bioactive lead compounds were retrieved from the herbal ingredients. From the reported data of the herbal preparation, the phytochemicals present in the Siddha formulation Sennaiuruvi Parpam revealed a maximum of 20 interactions with the core active amino acid residues present on the target protein Proton pump inhibitors and COX-2 which in turn exhibit anti-ulcer and anti-inflammatory activity.

Table 5: Binding energies of different compounds.

Compounds	H ⁺ /K ⁺ ATP ase		COX-2	
	No. of Interactions	Highest Binding Free Energy (Kcal/ mol)	No. of Interactions	Highest Binding Free Energy (Kcal/ mol)
Stachydrine	5	-3	10	-5.1
Betaine	5	-3.7	20	-4.1
Piperine	14	-8.3	20	-2.690
Umbelliferone	12	-6.6	18	-9.0

Table 6: Docking interactions of Different compounds.

Compound	H ⁺ /K ⁺ ATP ase	COX-2
Stachydrine		
Betaine		
Piperine		
Umbelliferone		

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)
Stachydrine	Low	No	No	No	No	No	No	No	-6.89
Betaine	Low	No	Yes	No	No	No	No	No	-7.11
Piperine	High	Yes	No	Yes	No	Yes	No	No	-6.04
Umbelliferone	High	Yes	No	Yes	No	No	No	No	-6.19

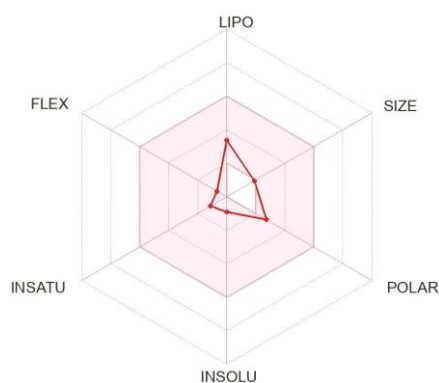
Among the selected phytoconstituents, Piperine and Umbelliferone demonstrated favorable pharmacokinetic profiles with high gastrointestinal absorption and acceptable drug-likeness properties. Piperine exhibited good membrane permeability due to its lipophilic nature, whereas Umbelliferone showed balanced absorption characteristics with minimal rule violations. Stachydrine and Betaine displayed comparatively low GI absorption owing to their polar nature; however, their cytoprotective and anti-inflammatory activities may still contribute synergistically to the therapeutic efficacy of the formulation. None of the compounds exhibited significant CYP450 inhibition except Piperine, suggesting relatively lower risk of metabolic interactions.

Drug-likeness

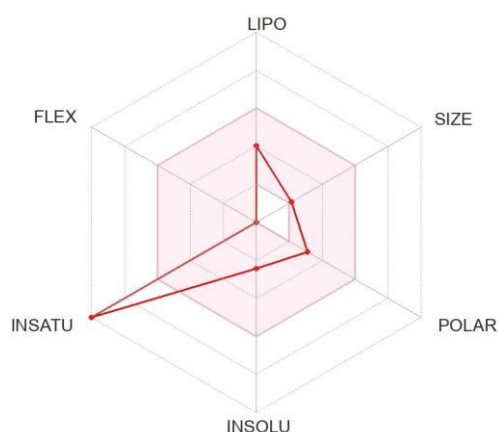
Table 8: Drug-likeness of the compounds.

Compounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability
Stachydrine	Yes 0 violations	No 2 violations	Yes	Yes	No 1 violation	0.55
Betaine	Yes 0 violations	No 4 violations	Yes	Yes	No 1 violation	0.55
Piperine	Yes 0 violation	Yes	Yes	Yes	Yes	0.55
Umbelliferone	Yes 0 violation	No 1 violation	Yes	Yes	No	0.55

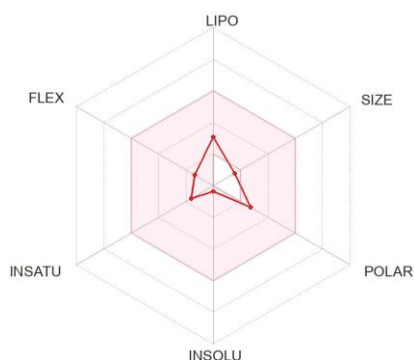
Stachydrine



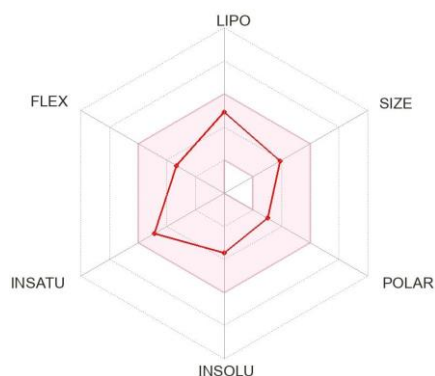
Umbelliferone



Betaine



Piperine



CONCLUSION

Based on the results of the computational analysis it was concluded that the bio-active compounds present in the siddha formulation Sennaiuruvi parpam possess significant binding against the target Proton pump inhibitors and COX-2 interacting with active amino acid residues present at the active site thereby suggesting that these compounds may exert promising anti-inflammatory and anti-ulcer activity. The phytochemicals which inhibit the target may act as a potential therapeutic agent for management of Gastric ulcer. However, further in vitro, in vivo, and clinical investigations are required to validate the computational findings and establish the therapeutic safety profile of Sennaiuruvi Parpam.

REFERENCES

1. Agathiyar, 2000.
2. Dr. K. S. Uthamarayan, Dr. K. N. Kuppasamy Mudhaliyar, Siddha vaithiya thirattu, First Publication - 1998, Second Publication - 2009. Sagadevi thylam, Pg. No. 278, 279.
3. C.Kannusamy Pillai, Chikitcha Rathna Deepam. Nethiranjanam, Pg. No. 286.
4. He Y, Wang X, Li S, Zhang Y, Chen L. Phytochemistry and pharmacological activities of *Achyranthes bidentata*: a review. *J Pharm Pharmacol*, 2024; 76(8): 930-948.
5. Jin W, Zhang Y, Li Q, et al. Chemical constituents and biological activities of *Achyranthes bidentata* Blume. *Arch Pharm Res*, 2021; 44(3): 241-257.

6. Tang W, Eisenbrand G. Chinese Drugs of Plant Origin: Chemistry, Pharmacology, and Use in Traditional and Modern Medicine. Berlin: Springer, 1992; p. 83-88.
7. Craig SA. Betaine in human nutrition. *Am J Clin Nutr*, 2004; 80(3): 539-549.
8. Srinivasan K. Black pepper and its pungent principle-piperine: a review of diverse physiological effects. *Crit Rev Food Sci Nutr*, 2007; 47(8): 735-748
9. Meghwal M, Goswami TK. Piper nigrum and piperine: an update. *Phytother Res*, 2013; 27(8): 1121-1130.
10. Mahendra P, Bisht S. Ferula asafoetida: traditional uses and pharmacological activity. *Pharmacogn Rev*, 2012; 6(12): 141-146.
11. Iranshahy M, Iranshahi M. Traditional uses, phytochemistry and pharmacology of asafoetida (*Ferula asafoetida* oleo-gum-resin)—A review. *J Ethnopharmacol*, 2011; 134(1): 1-10.
12. Bugnon M, Röhrig UF, Goullieux M, Perez MAS, Daina A, Michielin O, Zoete V. SwissDock 2024: major enhancements for small-molecule docking with Attracting Cavities and AutoDock Vina. *Nucleic Acids Res*, 2024.
13. Eberhardt J, Santos-Martins D, Tillack AF, Forli S. AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings. *J. Chem. Inf. Model.*, 2021.
14. Daniel Elieh-Ali-Komi, Martin Metz, Pavel Kolkhir, Emek Kocatürk, Jörg Scheffel, Stefan Frischbutter, Dorothea Terhorst-Molawi, Lena Fox, Marcus Maurer.
15. Hopkins AL. Network pharmacology: the next paradigm in drug discovery. *Nat Chem Biol*, 2008; 4(11): 682-690.
16. Veber DF, Johnson SR, Cheng HY, Smith BR, Ward KW, Kopple KD. Molecular properties that influence the oral bioavailability of drug candidates. *J Med Chem*, 2002; 45(12): 2615-2623.