WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 8, 395-403. Research Article ISSN 2277–7105

IN SILICO ASSESSMENT OF BURN HEALING PROPERTIES OF BIOACTIVE COMPOUNDS FROM *FICUS RELIGIOSA* LEAVES USING MOLECULAR DOCKING STUDIES

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Article Received on 15 March 2026,
Article Revised on 05 April 2026,
Article Published on 10 April 2026,

https://doi.org/10.5281/zenodo.19591785

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How to cite this Article: Lavanya V., Parvathi A., Selvamani R., Srikanth M., Aruna M.*, Manivannan R. (2026). In Silico Assessment of Burn Healing Properties of Bioactive Compounds From Ficus Religiosa Leaves Using Molecular Docking Studies. World Journal of Pharmaceutical Research, 15(8), 395–403.

ABSTRACT

Burn injuries represent a major public health issue worldwide and require effective therapeutic agents to accelerate wound healing and reduce inflammation. Medicinal plants have long been used in traditional medicine due to their rich phytochemical composition and therapeutic properties. *Ficus religiosa*, commonly known as the peepal tree, is widely used in Ayurvedic and Siddha medicine for treating various diseases including wounds, inflammation, and skin disorders. The present study aims to investigate the burn healing potential of bioactive compounds present in *Ficus religiosa* leaves using in silico molecular docking studies. The leaves were subjected to phytochemical screening to identify the presence of important bioactive constituents such as flavonoids, tannins, phenolic compounds, steroids, and triterpenoids. Selected phytoconstituents including β-sitosterol, lupeol, stigmasterol, and methyl oleanolate were chosen as ligands for molecular docking analysis. Docking studies were performed using PyRx software against important proteins involved in wound healing such as TNF-α, COX-2, VEGF, and TGF-β. The docking results demonstrated strong binding affinities between the selected phytoconstituents and target proteins, suggesting their potential role in anti-inflammatory and tissue regeneration mechanisms. The results of this study provide scientific evidence supporting the traditional medicinal use of *Ficus religiosa* in burn and wound

healing. Further in-vitro and in-vivo studies are required to validate these findings and explore its potential development into effective herbal therapeutics.

KEYWORDS: *Ficus religiosa*, Molecular Docking, Burn Healing, Phytochemicals, In Silico Studies, Wound Healing.

INTRODUCTION

Burn injuries are among the most severe forms of trauma affecting millions of people worldwide each year. They can cause extensive damage to skin tissues, resulting in inflammation, infection, and delayed wound healing. The wound healing process is complex and involves several biological stages including inflammation, tissue proliferation, and remodelling. During this process, various proteins and signalling molecules such as Tumor Necrosis Factor-alpha (TNF-α), Cyclooxygenase-2 (COX-2), Vascular Endothelial Growth Factor (VEGF), and Transforming Growth Factor-beta (TGF-β) play essential roles in regulating inflammation and tissue regeneration.

Medicinal plants have been widely used in traditional medicine for the treatment of wounds and burns. Plant-derived compounds are known to possess antimicrobial, anti-inflammatory, antioxidant, and wound healing properties. These natural compounds often exhibit fewer side effects compared to synthetic drugs.

Ficus religiosa, commonly known as the peepal tree, belongs to the Moraceae family and is widely distributed in tropical and subtropical regions. Various parts of this plant such as leaves, bark, and fruits are traditionally used to treat several ailments including diabetes, asthma, ulcers, skin diseases, and wounds. The leaves of *Ficus religiosa* contain numerous phytochemicals such as flavonoids, phenolic compounds, tannins, steroids, and triterpenoids which are responsible for its pharmacological activities.

In recent years, computational approaches such as in silico molecular docking have gained significant importance in drug discovery. Molecular docking helps predict the interaction between small molecules and biological targets, allowing researchers to understand the mechanism of action of potential therapeutic compounds.

The present study focuses on evaluating the burn healing potential of bioactive compounds from *Ficus religiosa* leaves through molecular docking studies against key proteins involved in inflammation and wound healing.

PLANT PROFILE

Botanical Description

Ficus religiosa is a large deciduous tree commonly found in India and Southeast Asia. It is widely known as the sacred fig or peepal tree and holds great medicinal and religious significance.

Taxonomical Classification

Classification	Description
Kingdom	Plantae
Class	Magnoliopsida
Order	Rosales
Family	Moraceae
Genus	Ficus
Species	Ficus religiosa

Common Names

- Peepal Tree
- Sacred Fig
- Bodhi Tree **Local Name** Arasamaram (Tamil) **Parts Used** Leaves

Phytochemicals Present

- Flavonoids
- Tannins
- Phenolic compounds
- Steroids
- Saponins
- Glycosides
- Terpenoids

These compounds are responsible for various pharmacological activities including antioxidant, antimicrobial, and anti-inflammatory effects.

MATERIALS AND METHODS

Collection of Plant Material

Leaves of *Ficus religiosa* were collected from Siddha Medicinal Plants Garden, Mettur Dam, Tamil Nadu. The plant material was authenticated and shade-dried.

Preparation of Extract

The dried leaves were powdered using a mortar and pestle. The powdered sample was subjected to Soxhlet extraction using hydroalcoholic solvent for 4 hours.

Phytochemical Screening

Preliminary phytochemical analysis was carried out to detect the presence of:

- Alkaloids
- Flavonoids
- Tannins
- Saponins
- Glycosides
- Phenolic compounds

Molecular Docking Study

Selected phytoconstituents were docked against proteins involved in wound healing.

Target Proteins

- TNF-α
- COX-2
- VEGF
- TGF-β

Software Used

PyRx with AutoDock Vina.

Procedure

1. Protein structures were downloaded from Protein Data Bank (PDB).
2. Ligands were prepared and optimized.
3. Docking simulations were performed.
4. Binding energies were analyzed.

RESULTS

Phytochemical screening revealed the presence of flavonoids, tannins, phenols, steroids, and glycosides in the leaf extract of *Ficus religiosa*.

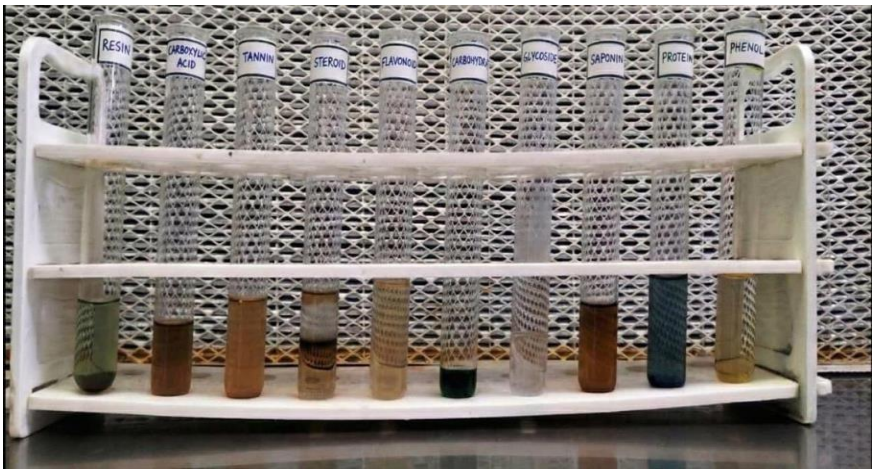
Molecular docking results showed that the selected phytochemicals exhibited strong binding

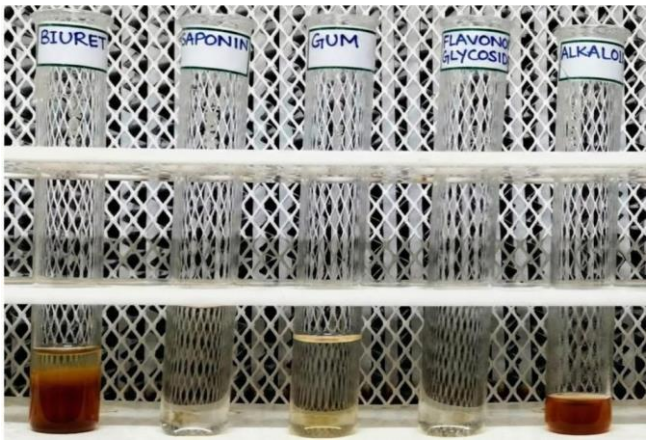
affinities with target proteins. Among the compounds studied, β-sitosterol and lupeol showed the highest binding affinity towards TNF-α and COX-2.

These interactions suggest potential anti-inflammatory and wound healing activity.

PRELIMINARY PHYTOCHEMICAL ANALYSIS OF *Ficus religiosa*

Table 1: Images showing Qualitative Phytochemical Screening Methods of FR,





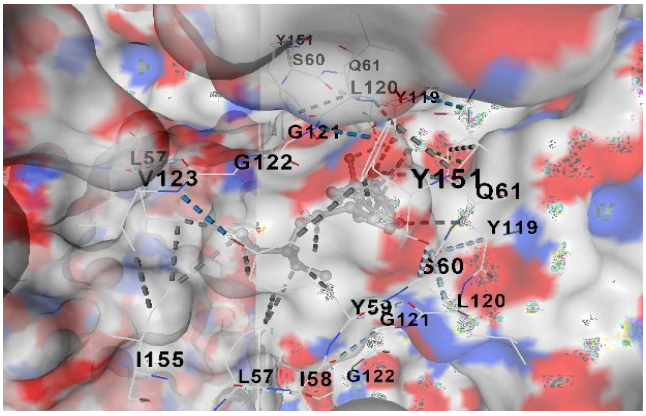
Results of Qualitative Phytochemical Screening Methods of FR

S. No	Name of Sample	Phytochemical Compound	Result
1	FR	Resins	+
2		Carboxylic Acid	+
3		Tannins	+
4		Steroids	+
5		Flavonoids	+
6		Carbohydrates	+
7		Glycosides	+
8		Saponification	+
9		Protein	-
10		Phenol	+
11		Biuret	-

12		Saponin	+
13		Gum	+
14		Flavanoglycosides	+
15		Alkaloids	+

Molecular docking interactions of phytoconstituents with TNF-α

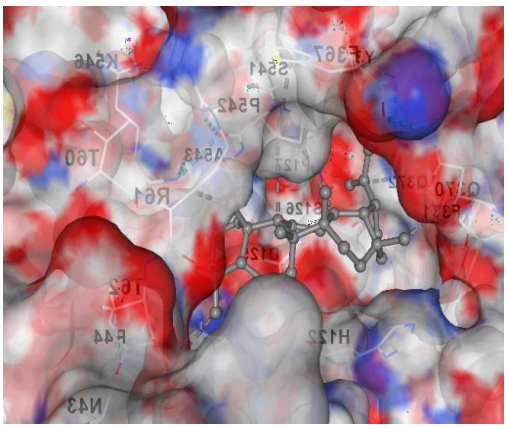
Ligand	Target Protein	PDB ID	Binding Energy (kcal/mol)
Lupeol	TNF-α	2AZ5	-8.6
β-Sitosterol			-8.7
Stigmasterol			-8.4
Lanosterol			-8.0



β-Sitosterol

Ligands and their Target Binding Scores Molecular docking interactions of phytoconstituents with COX-2

Ligand	Target Protein	PDB ID	Binding Energy (kcal/mol)
Lupeol	COX-2	5IKR	-9.1
β-Sitosterol			-8.9
Stigmasterol			-8.6
Methyl oleanolate			-8.7

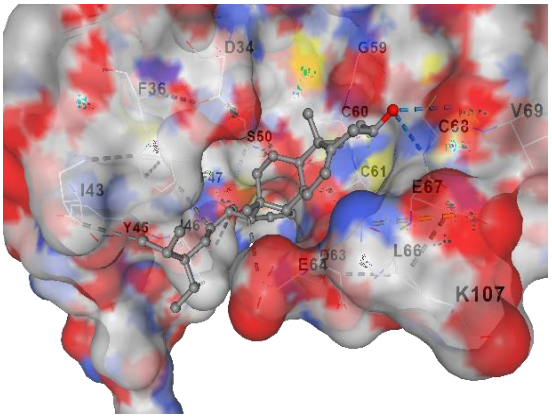


Lupeol

Ligands and their Target Binding Scores

Molecular docking interactions of phytoconstituents with VEGF

Ligand	Target Protein	PDB ID	Binding Energy (kcal/mol)
Stigmasterol	VEGF	1VPF	-8.5
Lupeol			-8.4
β-Sitosterol			-8.2
Methyl oleanolate			-8.2

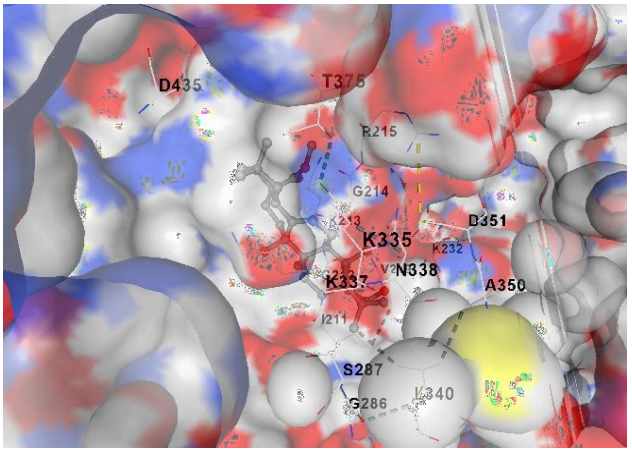


Stigmasterol

Ligands and their Target Binding Scores

Molecular docking interactions of phytoconstituents with TGF-β

Ligand	Target Protein	PDB ID	Binding Energy (kcal/mol)
Methyl oleanolate	TGF-β	1VJY	-8.8
Lupeol			-8.3



Methyl oleanolate

Ligands and their Target Binding Scores

DISCUSSION

The results obtained from the molecular docking study suggest that the bioactive compounds present in *Ficus religiosa* leaves interact effectively with proteins involved in wound healing

mechanisms.

Proteins such as TNF-α and COX-2 are responsible for inflammation during wound healing. Inhibition of these proteins helps reduce inflammation and accelerate tissue repair. Compounds like β-sitosterol and lupeol showed strong binding interactions with these proteins, indicating their potential therapeutic role.

Additionally, interactions with VEGF and TGF-β suggest the ability of these compounds to promote angiogenesis and collagen formation, which are essential for tissue regeneration.

Thus, the phytochemicals present in *Ficus religiosa* may contribute significantly to burn wound healing.

CONCLUSION

The present study demonstrates that *Ficus religiosa* leaves contain several bioactive compounds with potential burn healing properties. Molecular docking studies revealed strong interactions between selected phytochemicals and proteins involved in inflammation and tissue regeneration.

These findings support the traditional use of *Ficus religiosa* in wound and burn treatment. However, further experimental studies including in-vitro and in-vivo investigations are necessary to confirm the therapeutic potential of these compounds.

Future Directions

Future studies should focus on:

- Isolation and characterization of active compounds
- In-vitro wound healing assays
- In-vivo burn wound models
- Clinical evaluation of herbal formulations

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