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EXPLORING THE WOUND HEALING EFFICACY OF SACCHARUM OFFICINARUM STEMS THROUGH COMPUTATIONAL DOCKING ANALYSIS

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ABSTRACT

The biological process of wound healing is intricate and includes collagen synthesis, tissue restoration, and microbial infection management. This work uses computational molecular docking and phytochemical analysis to assess the wound-healing potential of Saccharum officinarum (sugarcane) stem extract. Bioactive substances like flavonoids and phenolics, which may support tissue regeneration and antibacterial activity, are present in the extract. Strong binding interactions between plant chemicals and protein targets linked to wound healing were demonstrated by docking experiments, indicating possible therapeutic utility. Overall, the study suggests that sugarcane stems could be used to create plant-based compositions for wound healing.

KEYWORDS: Wound healing, Molecular docking, Phytochemicals, Antimicrobial activity, Plant-based therapeutics, Stem extract.

INTRODUCTION

Normal wound healing occurs in four stages: Haemostasis, Inflammation, growth, and Remodelling.[1] Acute wounds are resolved by normal wound healing processes in a timeframe appropriate to the severity of the wound. Healing is delayed in chronic wounds due to the persistent trauma, infection, or ischemia, as well as underlying conditions such as

vascular disease or diabetes.[2] Chronic wounds enjoy extended irritation that is characterized by an abundance of enzymes in the wound that is unregulated due to depressed levels of their inhibitors.[3] It's a article about the current state of material technologies for treating chronic wounds, which also covers what creates the ideal wound matrix and then presents a new synthetic scaffold made of nanotechnology, regarded as a new area of technology.

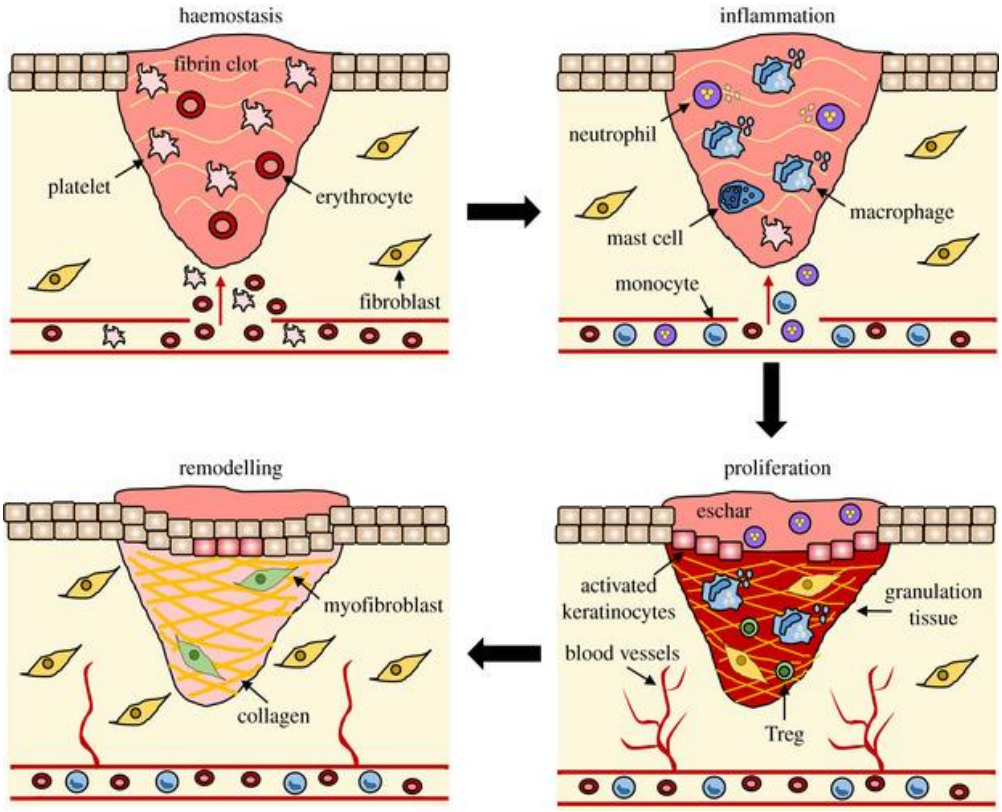


Fig. No. 01: Mechanism of wound healing.

PLANT PROFILE

Fig. No. 02: Saccharum officinarum stems.

Table 1: Taxonomy of The Selected Plant.

KINGDOM	Plantae
CLASS	Monocotyledon
SUBCLASS	Commelinid
SERIES	Glumaceae (sometimes included under Poales)
ORDER	Poales
FAMILY	Poaceae
GENUS	*Saccharum*
SPECIES	Saccharum officinarum

Table 2: Vernacular Names.

TAMIL	கரும்பு (*Karumbu*)
TELUGU	చెరుకు (*Cheruku*)
MALAYALAM	കരിമ്പ് (*Karumbu*)
HINDI	गन्ना (*Ganna*)
ENGLISH	Sugarcane

Saccharum officinarum stems are selected for wound healing because they contain bioactive compounds such as flavonoids and phenolics with antioxidant, anti-inflammatory, and antimicrobial properties. These constituents promote collagen synthesis, prevent infection, and accelerate tissue repair.

PROTEIN PROFILE

(FN1) –Fibronectin Gelatin-binding domain fragment

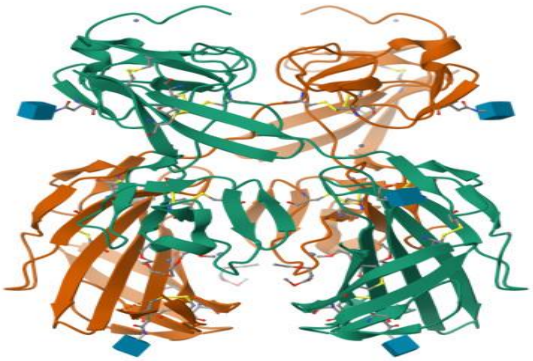
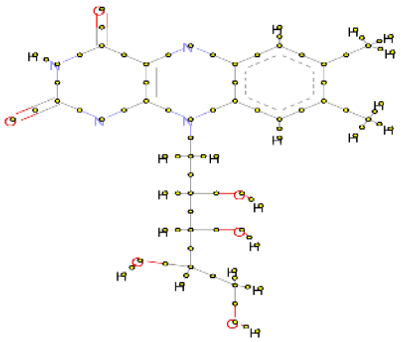


Fig. No. 03: (Protein ID: 3M7P).

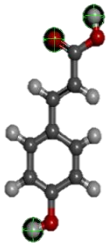
The Fibronectin gelatin-binding domain fragment (studied in 3M7P) is the collagen/gelatin-binding part of fibronectin, made of Fn I and Fn II modules. It connects fibronectin to the extracellular matrix by binding collagen, and its activity can be regulated by zinc. This makes it vital for cell adhesion, migration, and wound healing processes.

SELECTED LIGANDS

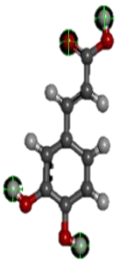
Riboflavin



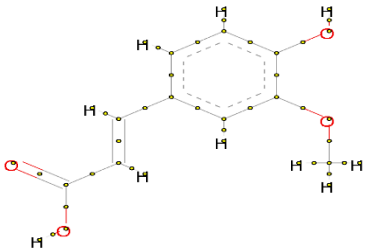
Flavylium



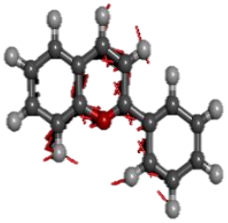
4- Hydroxycinnamic acid



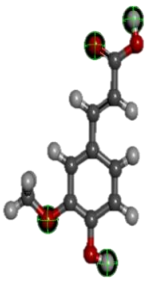
Caffeic acid



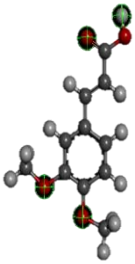
Ferulic acid



3,4-Dimethoxycinnamic acid



Nicotinic acid



MATERIALS AND METHODS

1. Phytochemical Database – IMPPAT

- The Indian Medicinal Plants, Phytochemistry and Therapeutics (IMPPAT) database was used to identify phytoconstituents present in the selected medicinal plant (*Saccharum officinarum* in this case, if relevant).
- Phytochemicals with reported biological activities related to wound healing were shortlisted for further study.

2. Compound Retrieval – PubChem

- The selected phytochemicals were retrieved from the PubChem database.

- Canonical SMILES, CID numbers, and 2D/3D SDF structures were obtained.

3. Structure Drawing – Chem Sketch

- When compounds were not directly available in PubChem, ACD/Chem Sketch software was used to draw 2D structures of the phytochemicals.
- The 2D structures were converted into 3D conformations and energy minimized before docking.

4. Protein Selection – Protein Data Bank (PDB)

- The target protein related to wound healing, such as Fibronectin (FN1) – Gelatin-binding domain fragment (PDB ID: 3M7P), was retrieved from the Protein Data Bank.
- The protein structure was downloaded in PDB format, and pre-processing (removal of water molecules, heteroatoms, and addition of polar hydrogens) was carried out.

5. Protein and Ligand Preparation – BIOVIA Discovery Studio

BIOVIA Discovery Studio Visualizer was used for:

- Cleaning and preparation of protein structure.
- Energy minimization of ligands.
- Conversion of files into docking-compatible formats (PDBQT).
- Visualization of hydrogen bonds, hydrophobic interactions, and active site pockets.

6. Molecular Docking – PyRx

- Docking studies were performed using PyRx (Python Prescription) software which integrates Auto Dock Vina.
- The binding pocket was defined around the active site residues of the target protein.
- Ligands were docked against the protein, and binding affinity (kcal/mol) values were obtained.
- The best conformations were selected based on lowest binding energy and number of interactions.

7. Visualization of Docking Results

- The docking poses were visualized using BIOVIA Discovery Studio to analyze molecular interactions (hydrogen bonds, van der Waals, electrostatic).
- The protein-ligand interaction diagrams were generated to interpret the docking results.

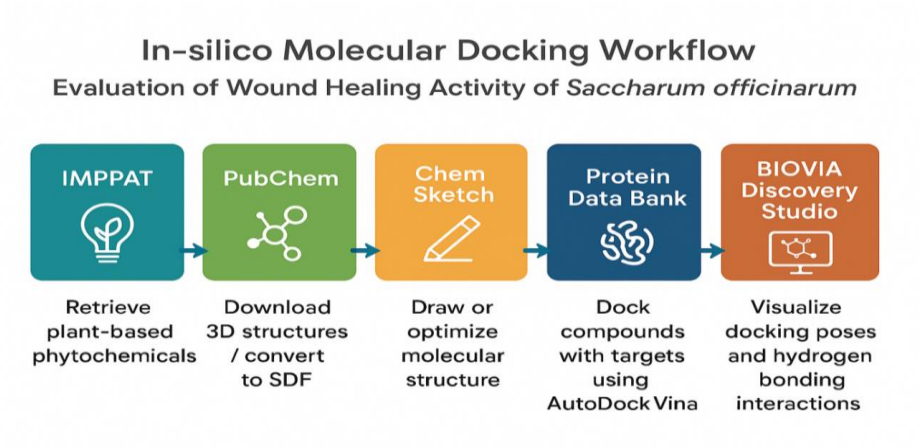


Fig. No. 04: Plan of work.

RESULTS

Docking was performed against wound-healing relevant protein target against Fibronectin (FN1) -gelatin-binding domain fragment. From S. officinarum stem who screened a library of commonly reported phytochemicals are:

1. Flavylium: -6.8 Kcal/mol
2. 4-Hydroycinnamic acid: -5.5 Kcal/mol
3. Caffeic acid: -6.0 Kcal/mol
4. Ferulic acid; -5.6 Kcal/mol
5. Stigma -3,5-dien-7-one-5.6 Kcal/mol
6. Nicotinic acid: -4.6 Kcal/mol
7. 3,4-Dimethoxycinnamic acid: -5.5 Kcal/mol
8. Riboflavin: -8.0 Kcal/mol

In our study, we docked the phytochemicals from Saccharum officinarum stem against the Fibronectin (FN1) – gelatin binding protein using Auto Dock VINA, selecting 8 ligands based on their binding affinities.

DOCKING SCORE

S.NO	LIGAND NAME	PUBCHEM ID	BINDING AFFINITY
1.	Flavylium	145858	-6.8 Kcal/mol
2.	4-Hydroycinnamic acid	637542	-5.5 Kcal/mol
3.	Caffeic acid	689043	-6.0 Kcal/mol
4.	Ferulic acid	445858	-5.6 Kcal/mol
5.	Stigma-3,5-dien-7-one	12444466	-5.6 Kcal/mol
6.	Nicotinic acid	938	-4.6 Kcal/mol
7.	3,4-Dimethoxycinnamic acid	717531	-5.5 Kcal/mol
8.	Riboflavin	493570	-8.0 Kcal/mol

SWISS ADME

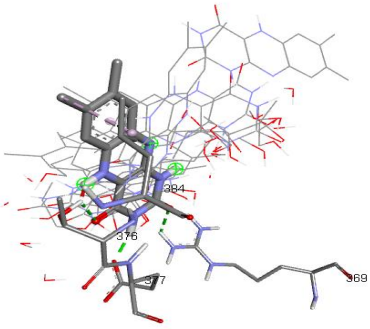
S.No.	Name of Compound	Molecular weight	H acceptor	H donar	TPSA	Violation	Log P
1	Riboflavin	376.36 g/mol	8	5	161.56 Å²	0	1.63
2	Flavylium	207.25 g/mol	0	1	13.14 Å²	0	0.76
3	3,4-Dimethoxycinnamic acid	208.21 g/mol	4	1	55.76 Å²	0	2.01
4	Cholecalciferol	384.64 g/mol	1	1	20.23 Å²	2	2.34
5	Swertiajaponin	462.40 g/mol	11	7	190.28 Å²	2	2.18
6	Orientin	448.38 g/mol	11	8	201.28 Å²	2	1.00
7	Pantothenic acid	219.23 g/mol	5	4	106.86 Å²	0	0.95
8	Nicotinic acid	123.11 g/mol	3	1	50.19 Å²	0	0.86
9	Inositol	84.16 g/mol	0	0	0	0	2.10
10	Swertism	446.40 g/mol	10	6	170.05 Å²	1	2.50
11	Stigmasta-3,5-dien-7-one	410.67 g/mol	1	0	17.07 Å²	1	4.86
12	5,7-dihydroxy-2-(4-hydroxyphenyl)-6-[(2R,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-8-[(2S,3S,4S,5S)-3,4,5-trihydroxyoxan-2-yl]chromen-4-one	564.49 g/mol	14	10	250.97 Å²	3	1.35
13	Orientin 7,3-dimethyl ether	476.43 g/mol	11	6	179.28 Å²	2	2.44
14	Neoisoschaftoside	564.49 g/mol	14	10	250.97 Å²	3	1.68
15	Isoschaftoside	564.49 g/mol	14	10	250.97 Å²	3	1.68
16	Ferulic acid	194.18 g/mol	4	2	66.76 Å²	0	1.62
17	Caffeic acid	180.16 g/mol	4	3	77.76 Å²	0	0.97
18	4-Hydroxycinnamic acid	78.11 g/mol	0	0	0	0	1.58
19	Vicenin-2	594.52 g/mol	15	11	271.20 Å²	3	1.73
20	5-hydroxy-2-(4-hydroxy-3,5-dimethy0xyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	492.43 g/mol	12	6	188.51 Å²	2	2.69
21	Neocarlinoside	580.49 g/mol	15	11	271.20 Å²	3	1.58

PROTOX

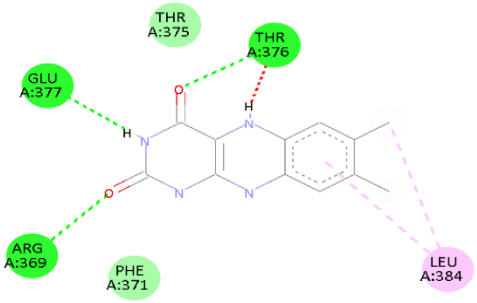
S.No.	Phyto constituents	Hepatotoxicity	Immunotoxicity	Cytotoxicity	Carcinogenecity	Mutagenecity
1	Riboflavin	Inactive	Inactive	Inactive	Inactive	Inactive
2	Flavylium	Inactive	Inactive	Inactive	Active	Active
3	4-Hydroycinnamic acid	Active	Inactive	Active	Inactive	Inactive
4	Caffeic acid	Inactive	Inactive	Inactive	Active	Inactive
5	Ferulic acid	Inactive	Active	Inactive	Inactive	Inactive
6	Stigma-3,5-dien-7-one	Inactive	Inactive	Inactive	Inactive	Inactive
7	Nicotinic acid	Active	Inactive	Inactive	Inactive	Inactive
8	3,4-Dimethoxycinnamic acid	Inactive	Inactive	Active	Inactive	Inactive

PROTEIN AND LIGAND INTERACTION

1. Riboflavin

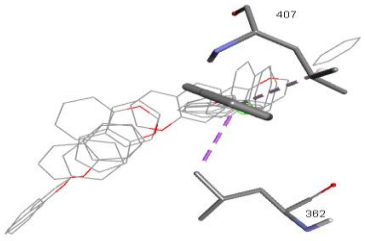


a) 3D structure

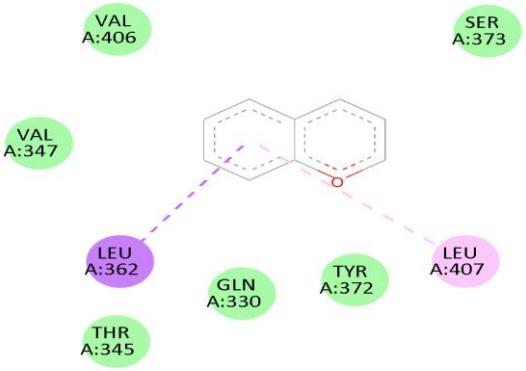


b) 2D structure

2. Flavyllium

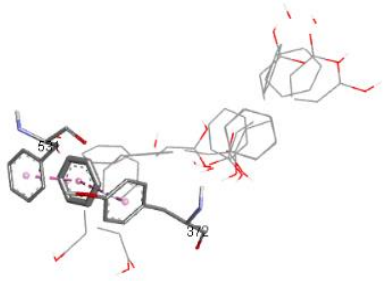


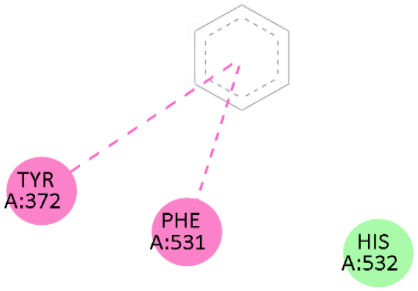
a) 3D structure



b) 2D structure

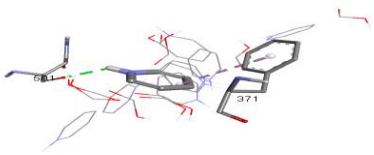
3. 4-Hydroycinnamic acid

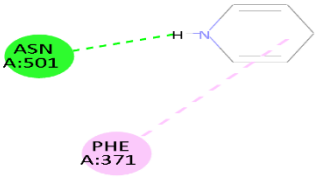




a) 3D structure **b) 2D structure**

4. Nicotinic acid





a) 3D structure **b) 2D structure**

DISCUSSION

The molecular docking study of selected phytoconstituents from Saccharum officinarum stems against wound-healing associated protein targets demonstrated variable binding affinities. Among the tested compounds, Riboflavin (−8.0 kcal/mol) and Stigma-3,5-dien-7-one (−7.7 kcal/mol) exhibited the strongest interactions, suggesting significant potential to modulate wound-healing pathways. Flavylium (−6.8 kcal/mol) and Caffeic acid (−6.0 kcal/mol) also showed moderate binding, indicating possible supportive activity in tissue repair through antioxidant and anti-inflammatory mechanisms. In contrast, Nicotinic acid (−4.6 kcal/mol) and 4-hydroxycinnamic acid (−5.5 kcal/mol) displayed comparatively weaker affinities, implying a limited direct role in protein modulation.

CONCLUSION

Overall, these results suggest that Saccharum officinarum stems contains bioactive compounds, particularly Riboflavin and Stigma-3,5-dien-7-one, that may contribute to wound-healing by stabilizing protein targets involved in extracellular matrix remodelling,

angiogenesis, and tissue regeneration. However, in addition experimental validation via in vitro and in vivo wound-healing models is essential to confirm these computational predictions and to establish their therapeutic relevance.

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