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Original Article

Integration of Analytical and Computational Techniques for Bioactive Profiling of *Celtis timorensis* Span Bark

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INTRODUCTION

A wound occurs when there is damage to the body's tissue due to a puncture in the skin[1]. An injury is caused by a breakdown in the skin's barrier function, resulting in either a superficial or deep wound[2]. The healing process is complicated by chronic wounds, but acute wounds might go through the normal sequential stages of wound healing[3]. Particularly in hyperglycemic circumstances, chronic wound healing is hindered and imprisoned, usually during the inflammatory phase[4]. The wound's healing process stagnates and takes longer than expected. Chronic wounds are persistent because of a number of pathological factors, including poor blood circulation and bacterial infections in the wounds. These include diabetes mellitus and other chronic disorders[5].

At the molecular level, wound healing consists of a series of intricately linked biologic processes. They fall into three overlapping phases: remodelling, proliferative response, and inflammatory reaction[6]. In addition to vascular responses characterized by coagulation of blood and hemostasis, the inflammatory phase also involves cellular processes such as leukocyte infiltration, which plays a number of functions in antibacterial and cytokine manufacturing, that initiates the proliferation reaction for wound healing. During the proliferative phase, granulation tissue covers the wound surface and fills the wound area as the epithelium develops simultaneously. Granulation tissue is produced through the proliferation of fibroblasts, the deposition of collagen and other extracellular matrix, and the generation of newly blood vessels. The remodeling phase starts when the new tissue inside the wound forms, restoring the tissue's structural integrity and functional competency[7,8,9].

Plant extracts and natural medications have long been applied topically to promote wound healing[10]. The foundation of ancient medicine was the utilize of plants as a resource of medication[11]. Naturally occurring compounds called phytochemicals are found in plants[12]. They react with other biologic macromolecules or oxygen groups to initiate biological actions and fight diseases in humans[13]. Numerous studies conducted worldwide have demonstrated the potential significance of phytochemicals in the prevention and/or treatment of several fatal illnesses, including cancer and inflammatory conditions[14,15]. Phytochemicals may also offer therapeutic advantages for wound improvement and skin redevelopment[16].

The primary objectives of this study were to isolate, identify, and perform docking analysis on the lipid constituents from *Celtis timorensis* bark. The phytoconstituents were authenticated by GC-MS analysis, HPTLC fingerprinting[17,18] and HPLC analysis. By analyzing their interactions with target proteins through docking studies, the study was designed to understand the possible wound betterment property of the phytoconstituents in this plant.

MATERIALS AND METHODS

Collection of plant materials

A specimen of *Celtis timorensis* Span was collected from the Ranni Forest Division, Pathanamthitta District- Kerala, where the plant is widely available. Fresh leaves and bark were procured for further experimental procedures. The identification of the plant (Accession number: NMB 1125) was carried out by a botanist Dr. Saju Abraham, Head, Botany Department, Newman College, Thodupuzha, Idukki, Kerala.

Extraction

A 75 g sample of powdered Celtis timorensis bark was subjected to ethanol extraction (600 mL) via a Soxhlet device for 48 hours. Upon completion of the extraction, the solvent was evaporated under reduced pressure with a rotary evaporator, resulting in 3.2 g of ethanolic crude extract. The extract was dissolved in 50 mL of distilled water and subsequently partitioned with organic solvents of ascending polarity: hexane, chloroform, ethyl acetate, and acetone. Each fraction was filtered through Whatman No. 41 filter paper to remove any residues and concentrated to dryness under reduced pressure using the rotary evaporator. The respective solvent fractions obtained were: hexane (1.2 g), ethyl acetate (0.96 g), chloroform (0.12 g), acetone (0.26 g), and the remaining aqueous methanol fraction (1.02 g)[19,20]. Among these, the hexane extract was chosen for further investigations, as qualitative phytochemical screening revealed the presence of terpenoids and steroids as the major constituents.

Basic phytochemical profiling

Qualitative phytochemical analysis was used to assess the presence of various substances in the *Celtis timorensis* extract, including steroids, terpenoids, alkaloids, saponins, phenolic and flavonoid compounds, tannins, proteins and carbohydrates [21].

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Gas chromatography-mass spectrometry

GC-MS analysis was used to evaluate the hexane extract of *Celtis timorensis* bark. The instrument used was Shimadzu GC-MS (Model QP2020) with Column SH-Rxi-5Sil MS. After eight minutes of maintaining the oven temperature at 60°C, 1.0µl of sample was introduced for analysis. A 99.999% pure helium gas was utilized as both an eluent and a carrier gas. Helium gas flow rate was maintained at 1 mL/min. Throughout the experiment; the split ratio was 10 and the sample injector temperature was kept at 250 °C. 70eV was used for the ionization mass spectroscopy analysis. For about eight minutes, the mass spectra were captured for the mass range of 10–20 m/z. The compound was detected using a comparative analysis of their mass spectra. Upon elution through the column, the components separated and were monitored using electrical signals. Following their elution from the gas chromatographic column, individual compounds were subjected to an electron bombardment in the electron ionization detector, which caused them to fragment into smaller pieces. In reality, the fragments were mass-specific charged ions. The mass spectrum graph, also known as the molecule's fingerprint, was used to calibrate the m/z ratio that was obtained. The NIST 17 Library's mass spectra were used to identify the chemicals.

High-Performance TLC fingerprinting

HPTLC analysis of *Celtis timorensis* extract was conducted using the HPTLC CAMAG Linomat 5, model "Linomat 5_192444" with serial number 192444 (version 1.00.13).

Making the Test Solution: 10 mg of the *Celtis timorensis* extract, precisely weighed, were dissolved in 15 mL of methanol and sonicated for 10 minutes. The mixture was then filtered using standard qualitative filter paper (Whatman No. 1) after being diluted with methanol to a final amount of 20 mL (0.5 mg/mL).

TLC Analysis: Using an aluminium sheet support, a 30 × 10 cm TLC plate precoated by using silica gel 60 F254 (thickness: 0.2 mm). The spotting was done with a Linomat V Automatic Sample Spotter (CAMAG) using a 100 µL syringe. In a 20 × 10 cm CAMAG glass twin trough chamber, the developing process was carried out with a mobile phase consisting of Hexane: Ethyl acetate (8.5:1.5) formic acid. Saturated the chamber with the mobile phase for two hours. The plates were removed after the development of the chromatogram, dried at 105°C, and then UV-scanned at 254 and 366 nm using a CAMAG TLC Scanner 3 connected to WINCATS software.

High-performance liquid chromatography analysis

HPLC system and condition: The hexane extract of *Celtis timorensis* bark was analyzed through high-performance liquid chromatography using a Shimadzu (LC-20AD) Prominence UFLC system fitted with a photodiode array detector (SPD-M20A). Analyte separation was achieved on a C18 G column (dimensions 250 mm × 4.6 mm and a 5 µm particle size). An isocratic elution technique was followed, using a mobile phase consisting of acetonitrile and water in an 85:15 (v/v) ratio[22]. The mobile phase was passed through a 0.2 µm membrane filter and subjected to ultrasonic degassing to remove air bubbles and facilitate smooth flow. The flow rate was maintained at 2.0 mL/min under ambient temperature conditions. This method was optimized to accomplish efficient resolution and detection of the targeted phytochemical.

Chromatographic analysis: The reference compound, stigmasterol, was purchased from Yucca Enterprises, Mumbai, India. Individual stock solutions were formulated by dissolving the stigmasterol in methanol (1 mg/mL) and the test extract at a concentration of 5 mg/L. The mobile phases were acetonitrile and water in the ratio 85:15 v/v, and the chromatographic analysis was performed using an isocratic elution method. The flow rate was set at 1.0 mL/min under isothermal conditions at 25°C. The photodiode array detector was set at the wavelength of 202 nm, and the injection volume was 10 µl for every sample and reference standard.

Molecular docking

Using molecular docking studies, the phytoconstituents from *Celtis timorensis* bark discovered by GC-MS analysis were evaluated for their ability to heal wounds. The binding interactions between the phytoconstituents and target proteins linked to wound healing property were evaluated.

Preparation of ligand: In docking studies, the phytochemicals identified by GC-MS were selected as ligands. These ligands were initially prepared through ACD/Labs' ChemSketch software to design their chemical structures. OpenBabel, version 2.4.1, was subsequently employed to convert these structures into the PDB (Protein Data Bank) format, which is compatible with molecular docking tools. This conversion made it possible to precisely assess the ligands' potential for interacting with the target wound healing protein through docking simulation analysis.

Preparation of the proteins: The RCSB Protein Data Bank (https://www.rcsb.org/) provided the three-dimensional structures of the chosen matrix metalloproteinases (MMPs) in PDB format. MMP12 (PDB code: 2WO8) from Homo sapiens was utilized in this investigation[23]. This protein structure is complexed with a beta hydroxy carboxylic acid at a resolution of 2 Å. PyMOL DLP 3D (Checkboard) was used to process the PDB file that had been downloaded. Polar hydrogens were added to the target protein, while water molecules and heteroatoms were removed to purify the structure and the protein structure was saved in PDBQT format, which may be used for molecular docking studies to examine the interactions between the ligands and molecules.

Docking analysis: Conducted molecular docking studies using AutoDockTools-1.5.6rc3 to assess the potential wound healing activity of the identified phytocompounds, following the preparation of proteins and ligands. The process involved docking the ligands into the active sites of the target proteins, specifically focusing on those implicated in wound healing.

RESULTS

Basic phytochemical profiling

Terpenoids and steroids were found to be the major components in the initial phytochemical screening of *Celtis timorensis* bark. Other phytochemicals that may contribute to the plant's medicinal qualities, including as flavonoids, tannins, alkaloids and fixed oils were also found throughout the screening process.

GC-MS Analysis

The hexane extract of *Celtis timorensis* bark was subjected to GC-MS analysis to search for secondary metabolites (Figure 1, Figure 2). The chemical characterisation led to the identification of nineteen bioactive phytochemicals, as Table 1 illustrates. These substances include Hexadecanoic acid methyl ester, Estra-1,3,5(10)-trien-17á-ol, l-(+)-Ascorbic acid 2,6-dihexadecanoate, Eicosanoic acid, Pentadecanoic acid ethyl ester, Phthalic acid butyl tetradecyl ester, Diamyl phthalate, 9,12-Octadecadienoic acid ethyl ester, cis-Vaccenic acid, Hexadecanoic acid butyl ester, Isopropyl palmitate, 2-((3,5,5-Trimethylhexyloxy) carbonyl) benzoic acid, Diisooctyl adipate, Pentacosane, Tetratriacontane, Octacosane, Campesterol, Stigmasterol and Cholest-4-en-3-one. These substances might be significant because of their biological characteristics, which include the capacity to heal wounds.

Table 1. GC-MS Profiling of Hexane Extract from *Celtis timorensis* Bark

No:	Compound Name	Retention Time	Probability	Percentage Area (%)	SI	RSI
1.	Hexadecanoic acid, methyl ester	16.48	65.27	0.83	898	904
2.	Estra-1,3,5(10)-trien-17á-ol	17	15.13	0.64	806	806
3.	l-(+)-Ascorbic acid 2,6-dihexadecanoate	17.18	40.42	4.62	846	846
4.	Eicosanoic acid	17.12	3.41	4.22	708	741
5.	Pentadecanoic acid, ethyl ester	17.24	5.05	4.02	793	793
6.	Phthalic acid, butyl tetradecyl ester	17.90	5.97	0.7	768	768
7.	Diamyl phthalate	18.11	3.49	1.12	829	829
8.	9,12-Octadecadienoic acid, ethyl ester	18.94	5.64	0.91	804	859
9.	cis-Vaccenic acid	19.06	4.61	0.69	799	821
10.	Hexadecanoic acid, butyl ester	19.19	71.76	2.20	901	906
11.	Isopropyl palmitate	19.19	3.23	2.20	795	810
12.	2-((3,5,5-Trimethylhexyloxy) carbonyl) benzoic acid	20.55	16.79	2.91	820	864
13.	Diisooctyl adipate	21.18	3.69	1.32	628	721
14.	Pentacosane	24.51	6.29	1.3	722	763
15.	Tetratriacontane	25.27	8.37	1.22	842	887
16.	Octacosane	26.94	5.96	1.43	777	876
17.	Campesterol	28.57	57.20	0.78	855	885
18.	Stigmasterol	28.95	25.92	0.75	793	842
19.	Cholest-4-en-3-one	30.42	9.14	0.90	757	800

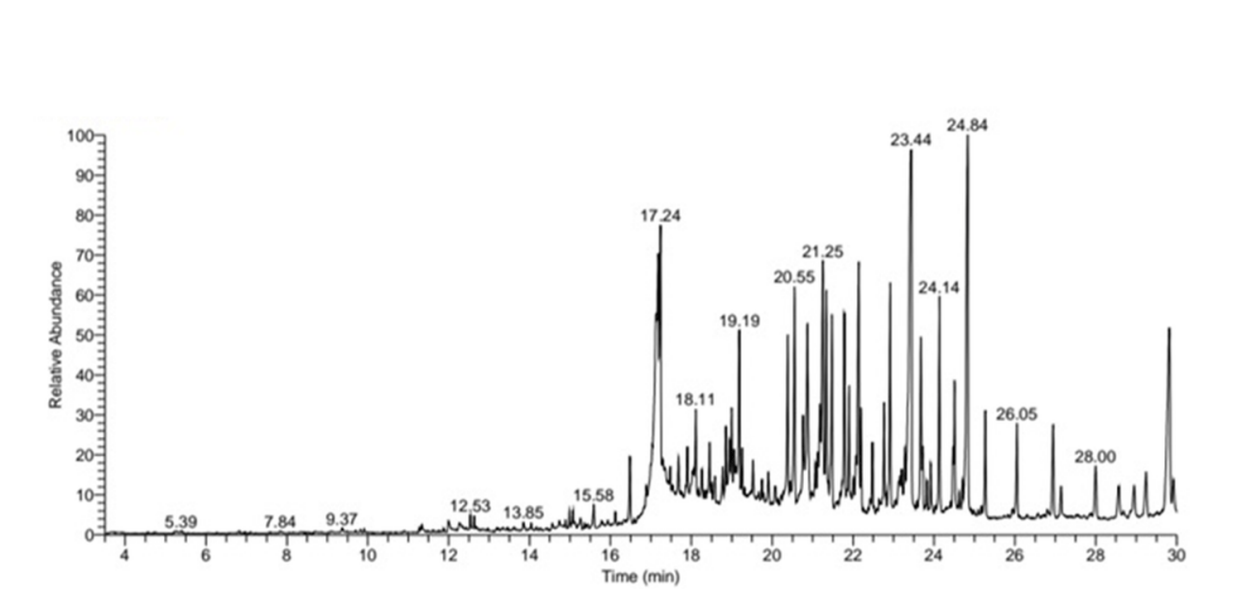


Figure 1. GC-MS chromatogram of *Celtis timorensis* bark extract

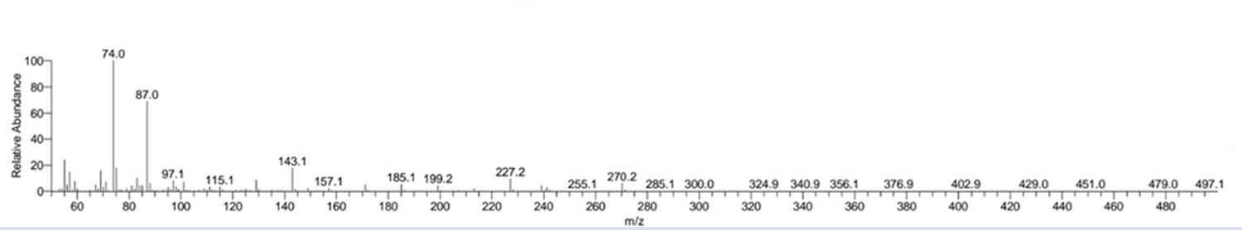


Figure 2. Mass Spectrum of *Celtis timorensis* bark extract

High-Performance TLC Fingerprinting for Terpenoids

High Performance Thin-Layer Chromatography (HPTLC) fingerprint of the hexane extract of *Celtis timorensis* bark were carried out at two different wavelengths 254 nm and 366 nm. There were bright terpenoid chemicals present as the bands fluoresced at 254 nm (Figure 3). Multiple terpenoid compounds were present in the sample, as seen by white or light-colored bands at 366 nm (Figure 4). Eight separate bands with final Rf values of 0.14, 0.17, 0.23, 0.35, 0.40, 0.52, 0.64, 1.00, and 1.06 were identified at 254 nm (Table 2) of the HPTLC study, while two bands with final Rf values of 0.14 and 0.18 were observed at 366 nm (Table 3). These values indicate the terpenoid compounds relative mobility on the chromatographic plate when Hexane: Ethyl acetate (8.5:1.5) formic acid is employed as the mobile phase.

High-performance liquid chromatography analysis

HPLC analysis of the hexane extract derived from the bark of *Celtis timorensis* confirmed the presence of stigmasterol, a phytosterol. Identified with its anti-inflammatory and wound-healing effects. The concentration of the stigmasterol was to be 0.09% w/w, which is a significant amount for an extract. This result supports the traditional healing practices of Celtis timorensis and underscores its value as a natural source of bioactive sterols. The resulting HPLC chromatogram (Figure: 5, Figure: 6) of the standard stigmasterol and plant extract sample was recorded and presented below (Table 4).

Molecular docking

Phytochemicals from *Celtis timorensis* were investigated for their interactions with important proteins involved in wound healing using molecular docking analysis. The specifics of the simulations provided a closer look at how these chemicals interact to the target proteins (Table 5). These results provide important information for future studies into the phytochemicals' potential therapeutic applications for wound healing.

The study found that stigmasterol had the strongest binding affinity for the target protein 2WO8, with a docking score of -13.4. This high score indicates a robust and stable interaction with the protein's active site, suggesting stigmasterol could be highly effective for wound healing. It chiefly forms hydrogen bonds and hydrophobic interactions with the residues PHE C:237, LYS C:233, VAL C:243, PHE C:248, ALA C:234, and HIS C:218. These interactions, which are displayed in the 2D interaction plot, demonstrate stigmasterol's potential as a key molecule in the development of treatments for wound healing (Figure 7).

Campesterol likewise exhibited strong binding, with a docking score of -12.3. It mostly interacted with hydrophobic residues, including TYR C:240, LYS C:241, HIS C:218; PHE C:237; VAL C:235; and LEU C:214. On the basis of interactions, campesterol seems as a promising therapeutic candidate for the treatment of wounds (Figure 8).

The docking score for eicosanoic acid was -12.1. It suggests a robust interaction with the hydrophobic residues in the 2WO8 active site, VAL C:243, PHE C:248, and TYR C:240. These interactions suggest that eicosanoic acid may contribute a vital role in healing of wounds (Figure 9). In contrast, diisooctyl adipate displayed the lowest binding affinity of all the compounds, with a docking score of -6.1, indicating a far less potential for therapeutic effects.

DISCUSSION AND CONCLUSION

According to preliminary phytochemical screening, terpenoids and steroids were found to be the most common class of chemicals in *Celtis timorensis* bark. This is an important discovery because these phytoconstituents are recognized for a wide range of biological actions, such as their ability to reduce inflammation and promote healing of wound[24].

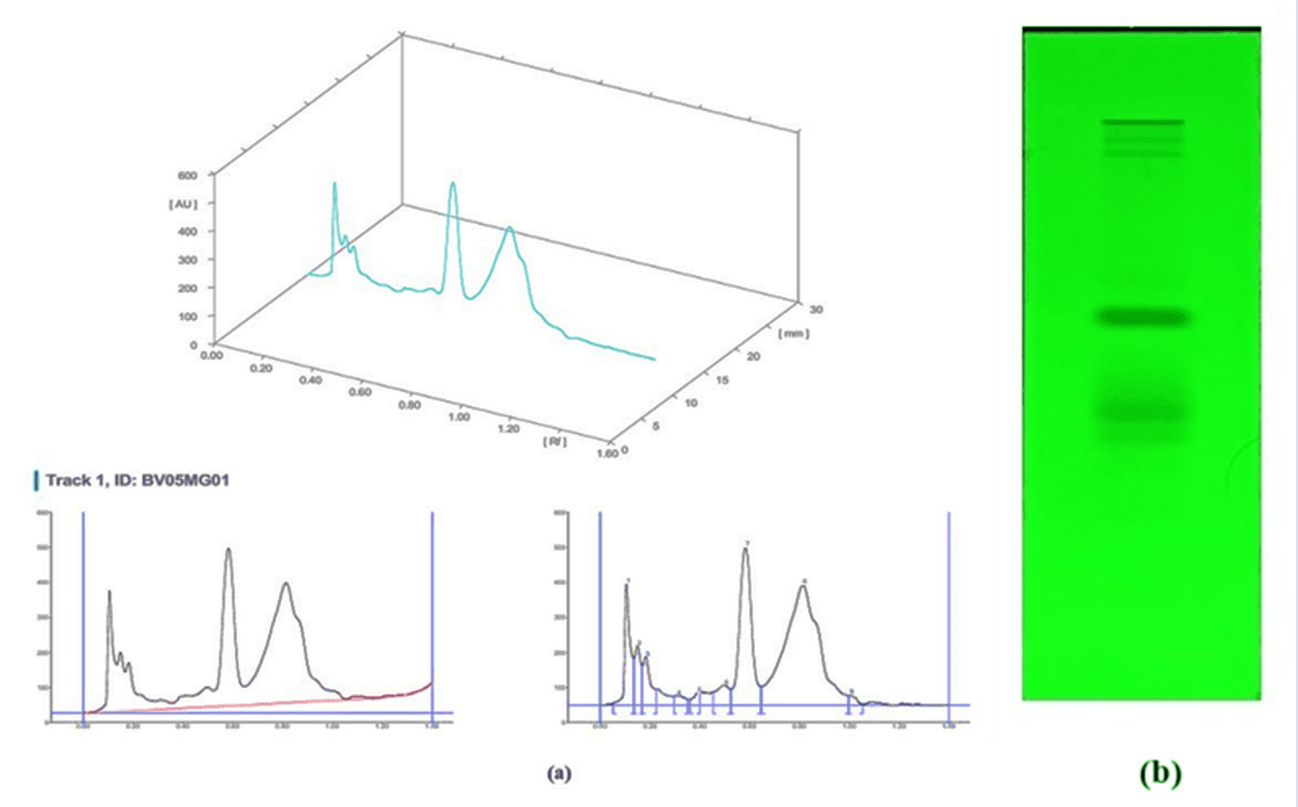


Figure 3. (a) HPTLC study of *Celtis timorensis* bark under visible light at 254 nm. (b) TLC Plate Visualization at 254 nm

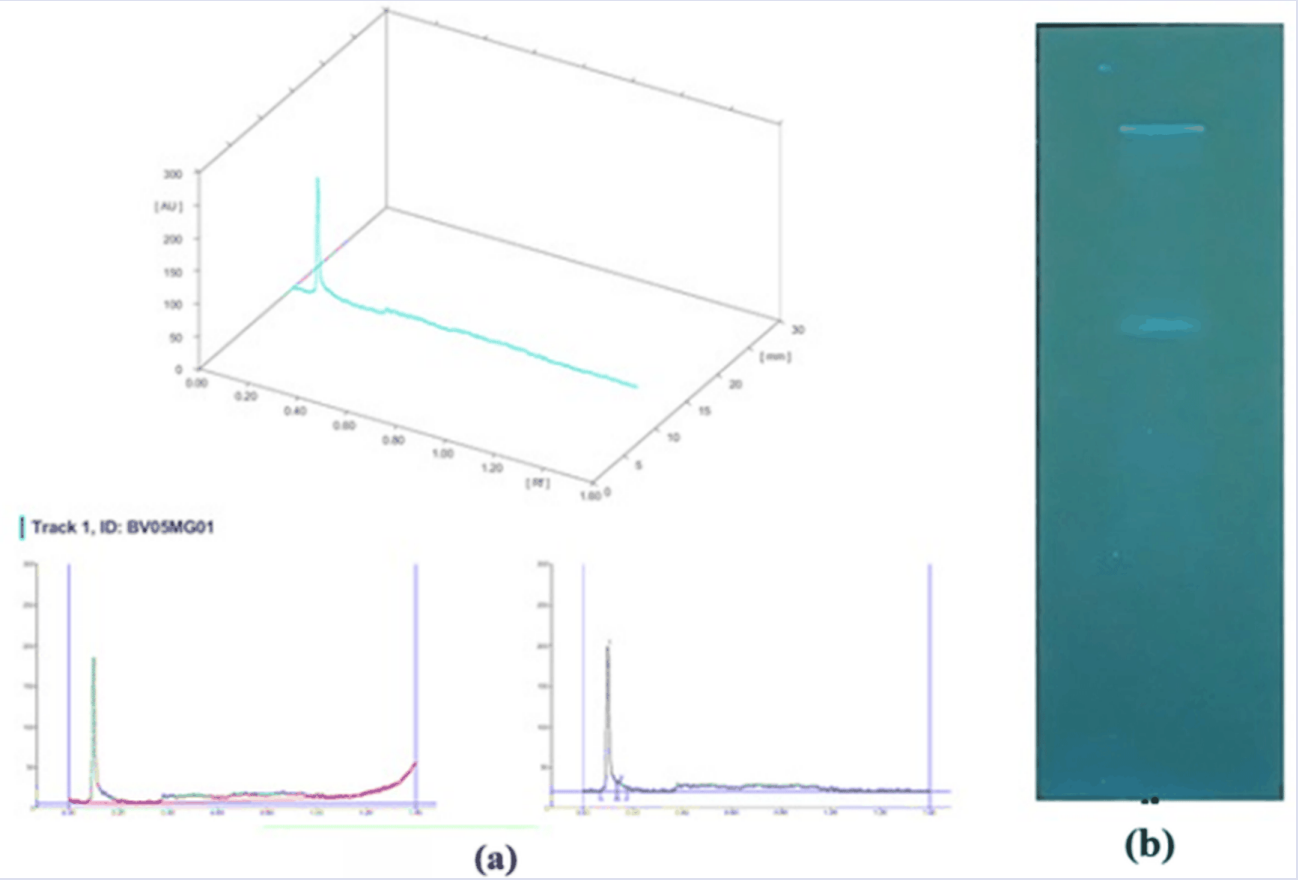


Figure 4. (a) HPTLC study of *Celtis timorensis* bark under UV light at 366 nm. (b) TLC Plate

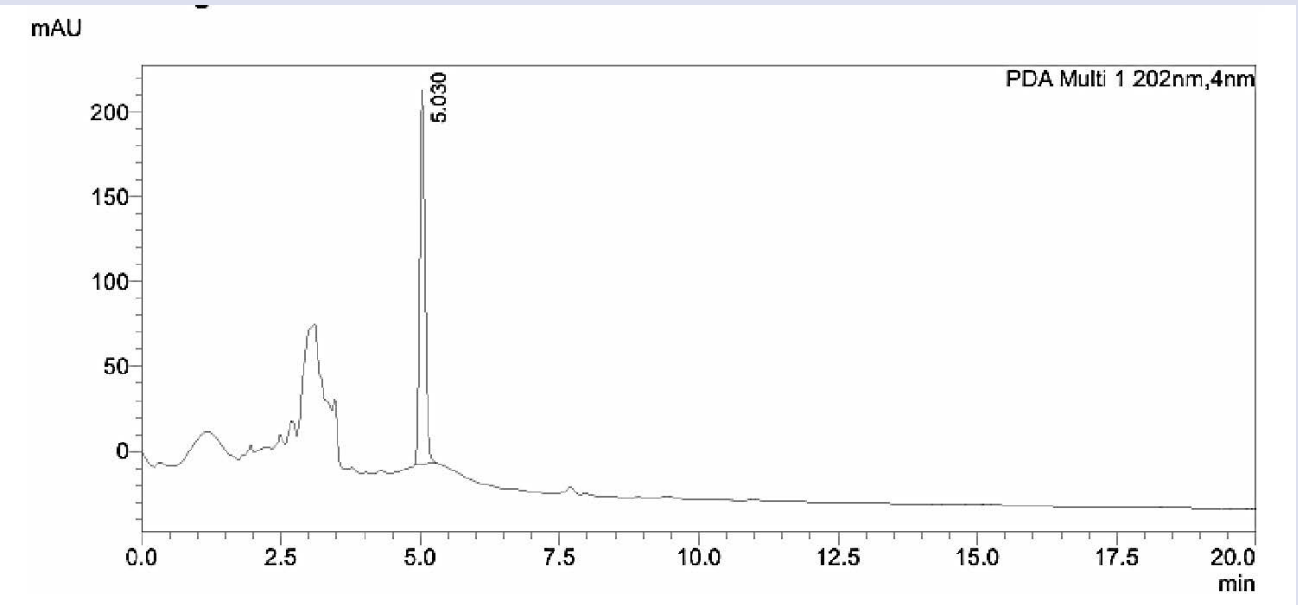


Figure 5. HPLC Chromatogram of Stigmasterol

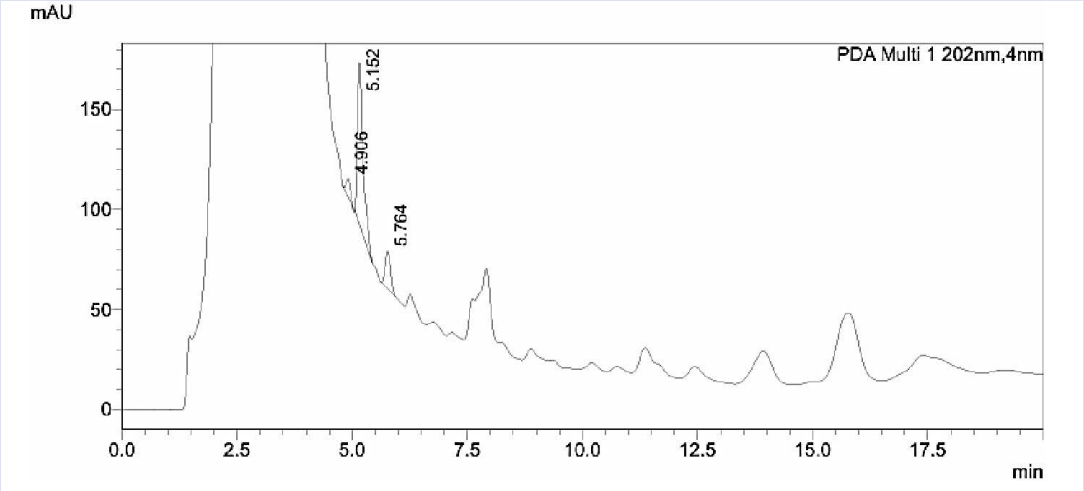


Figure 6. HPLC Chromatogram of *Celtis timorensis* extract

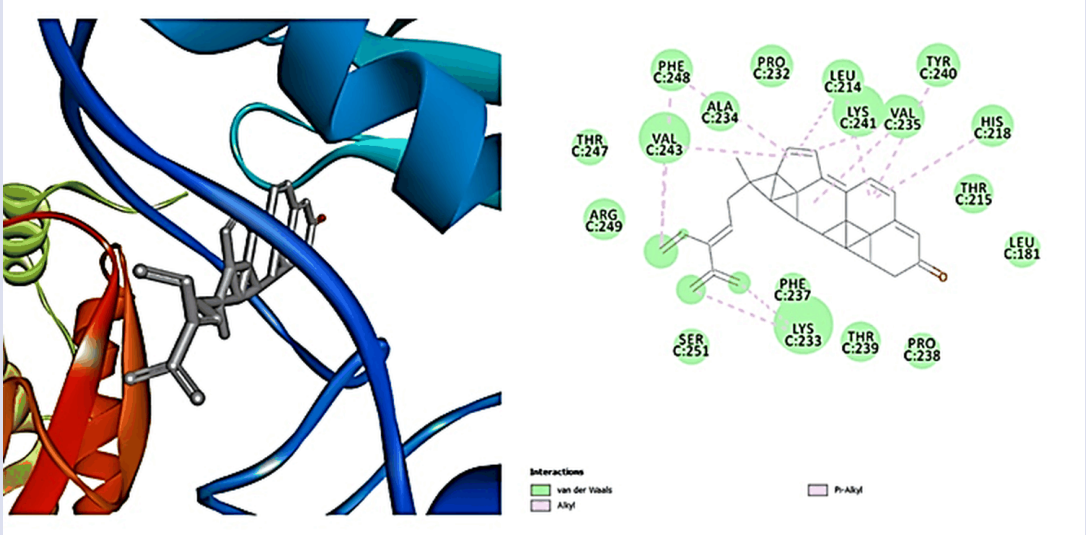


Figure 7. Docking structure and 2D interaction of stigmasterol

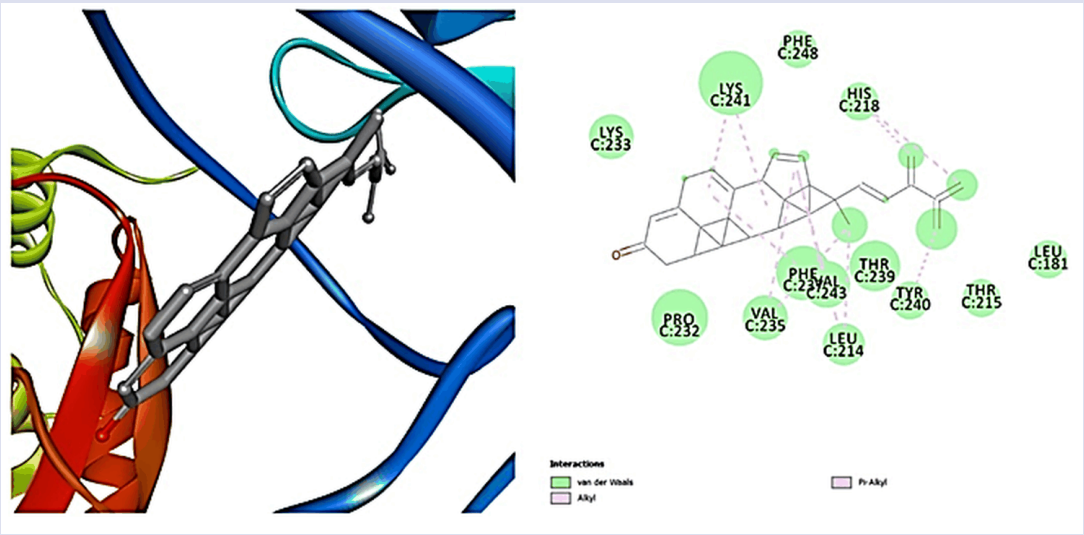


Figure 8. Docking structure and 2D interaction of campesterol

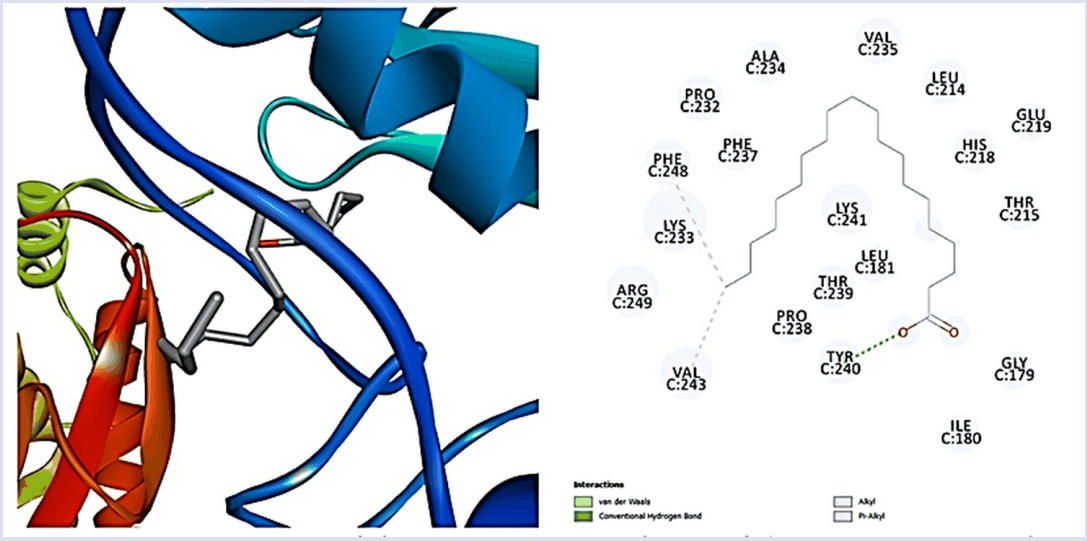


Figure 9. Docking structure and 2D interaction of eicosanoic acid

Table 2. **HPTLC profiling with Rf values at 254 nm**

Peak	Starting Rf	Starting Height	Maximum Rf	Maximum Height	Maximum %	Final Rf	Final Height	Area	% Area
1	0.05	4.9	0.11	346.7	21.77	0.14	134.0	22608.0	8.66
2	0.14	134.03	0.15	168.9	10.60	0.17	112.9	11934.1	4.57
3	0.17	113.0	0.18	137.7	8.64	0.23	45.6	12290.1	4.71
4	0.30	25.0	0.31	27.4	1.72	0.35	16.4	3339.7	1.28
5	0.36	16.7	0.39	34.7	2.18	0.40	33.8	2668.0	1.02
6	0.45	36.5	0.50	56.5	3.55	0.52	45.8	8498.7	3.25
7	0.52	45.8	0.58	450.0	28.25	0.64	53.6	62699.9	24.01
8	0.65	53.5	0.81	343.1	21.54	1.00	27.3	134660.0	51.57
9	1.00	27.3	1.00	27.8	1.74	1.06	2.0	2414.6	0.92

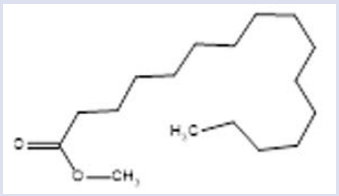
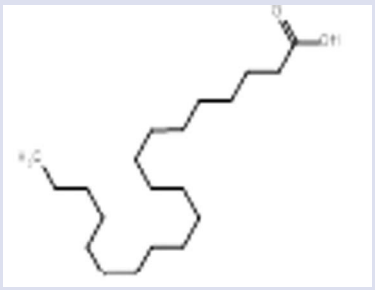
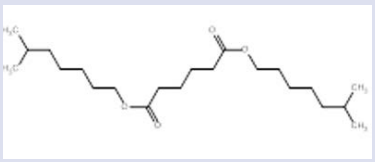
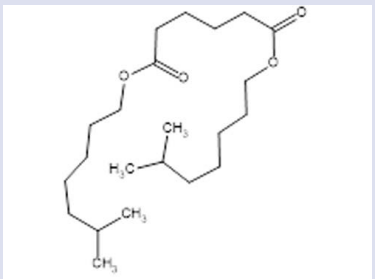
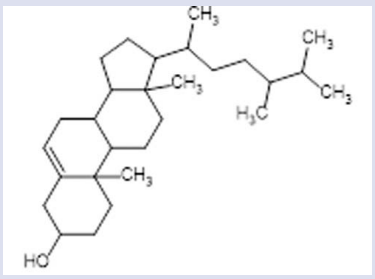
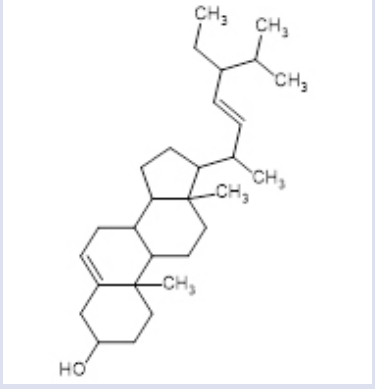
Table 3. **HPTLC profiling with Rf values at 366 nm**

Peak	Starting Rf	Starting Height	Maximum Rf	Maximum Height	Maximum %	Final Rf	Final Height	Area	% Area
1	0.07	0.8	0.10	179.0	93.22	0.14	11.5	1629.3	87.45
2	0.14	11.5	0.15	13.0	6.78	0.18	4.6	233.8	12.55

Table 4. **Comparison of Retention Time and Peak Area for Standard Stigmasterol and *Celtis timorensis* Extract**

Sl No:	Peak ID	Retention time	Area	Concentration
	Stigmasterol (Reference)	5.030	1506076	10 µg/mL
	Celtis timorensis extract	5.152	682331	50 µg/mL

Table 5. Binding Dynamics and Affinity of Ligands with Protein 2WO8

Protein Used	Phytochemicals	Structure	Affinity (kcal/mol)	Interacting Residue	Number of H bonds
2WO8	Hexadecanoic acid, methyl ester		-6.5	PHE C:237 ALA C:182	02
	Eicosanoic acid		-12.1	VAL C:243 PHE C:248 TYR C:240	03
	cis-Vaccenic acid		-6.2	HIS C:218 TYR C:240	02
	Diisooctyl adipate		-6.1	LYS C:241 PHE C:237 VAL C:235 LEU C:181 THR C:215	05
	Campesterol		-12.3	LYS C:241 HIS C:218 TYR C:240 LEU C:214 VAL C:243 PHE C:237 VAL C:235	07
	Stigmasterol		-13.4	PHE C:237 LYS C:233 VAL C:243 PHE C:248 ALA C:234 LEU C:214 LYS C:241 VAL C:235 TYR C:240 HIS C:218	10

Nineteen bioactive phytochemicals were identified in the hexane extract of *Celtis timorensis* using GC-MS analysis. Among these substances with proven biological activity are stigmasterol, hexadecanoic acid methyl ester and eicosanoic acid. It has been observed that stigmasterol and hexadecenoic acid possesses anti-inflammatory properties, which may help to heal wounds by lowering inflammation and promoting tissue regeneration[25,26]. In a similar way, long-chain fatty acid eicosanoic acid is well-known for its contribution to the preservation of skin barrier function[24], which is essential for efficient wound healing[27].

The HPTLC fingerprinting of *Celtis timorensis* bark extract revealed a diverse range of terpenoid compounds, as evidenced by distinct bands at 254 nm and 366 nm, each with unique Rf values, highlighting the relative mobilities of the compounds. These findings demonstrate the richness and variety of terpenoids contained in the extract.

High-performance liquid chromatography (HPLC) of the hexane extract derived from the bark of Celtis timorensis confirmed the presence of stigmasterol—a notable phytosterol associated with various therapeutic properties, especially its role in reducing inflammation[28] and enhancing wound repair. Detected at a concentration of 0.09% w/w, stigmasterol appears in a meaningful amount, implying its involvement in the medicinal effects traditionally attributed to the plant. This outcome not only supports the long-standing use of *Celtis timorensis* in traditional healing practices but also emphasizes its potential as a natural source of pharmacologically active sterols.

Based on docking data, stigmasterol is a promising candidate for wound healing. It has a high binding affinity of -13.4. Campesterol and eicosanoic acid additionally have close ranks, with scores of -12.3 and -12.1, respectively. The strong therapeutic potential of these compounds is indicated by notable affinities and interactions between campesterol, eicosanoic acid and stigmasterol with key residues inside the protein's active site (2WO8). The potential value of Diisooctyl adipate is lower and it showed a decreased binding affinity. These findings highlights the potential for stigmasterol, campesterol, and eicosanoic acid to aid in wound healing therapies, indicating a need for more research and development.

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