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Targeting Wound Pathogens with *Madhuca indica* Bioactive Compounds: An *In Silico* Perspective

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Abstract

Treating wound infections is increasingly challenging because of bacterial antibiotic resistance. Plants have recently emerged as a viable strategy for addressing antibiotic resistance and enhancing wound care. The antioxidant activity of Madhuca indica is essential for preventing oxidative stress by free radicals. In silico analysis of the bioactive compound was done by DPPH and the prominent phytochemicals were found in the extract after phytochemical screening. Phytochemical analysis of M. indica revealed that the plant contains flavonoids among many other bioactive compounds. M. indica exhibits concentration dependent radical scavenging activity, according to the DPPH test, where the percentage of radicals inhibited rises with concentrations as 10-50 µg/mL. The antimicrobial resistance patterns of bacterial targets were studied to elucidate the potential of M. indica compounds in combating these resistant strains. Multidrug resistance may be treated as the structural modification of the identified compounds, which may increase their efficiency and selectivity against the target microorganisms. Compounds from M. indica can also be added to already approved antibiotics; these combinations have synergistic effects that can help address the resistance issue. The activity indicated strong free radical scavenging activity that might help fight oxidative stress and aid in wound healing. The result of such computational predictions needs to be further studied in silico to validate the therapeutic application of several identified drugs. These possibilities suggest that novel antimicrobial agents derived from plants may be able to address the ongoing issue of multidrug resistance.

Keywords: *Antioxidant Activity, Bioactive Compounds, In Silico Analysis, Multidrug Resistant, Wound Pathogens.*

Introduction

Multidrug resistant organisms (MDROs) are considered problematic complications in various fields of medicine. Infections in the wound exacerbate chronic consequences, increase patient treatment costs and are aggravated by the presence of MDROs, such as *Pseudomonas aeruginosa and Acinetobacter baumannii* [1, 2]. The most important cause of injuries is burns. It affects the integrity of the skin and increases the risk of infection. Burn patients are susceptible to health related infections (HAI) which encompasses elements such as the disappearance of typical skin issues and

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necrotic tissue. As a result, many illnesses result in severe sickness and even death. Consequently, infections account for around 75% of burn patient deaths [3]. The wounds are difficult to treat with antibiotics for pathogens. Nevertheless, multidrug resistant (MDR) diseases have quickly emerged as a result of antibiotic abuse and overuse [4, 5], improving the effectiveness of antimicrobial agents and supporting wound healing. Plants are the most important medicinal properties for medical science [6]. India's plant heritage could be exploited in the post genomics era using computers and biochemical/biochemical, chemoinformatics, genomics and systems biology [7].

The discovery of the plants brings vital information about many medicinal uses including cancer. Collections may include species containing chemicals with known activity but not yet classified (e.g. traditional medicinal plants) or may include random taxa collected for large scale analysis [8]. Molecular biology has become the key to drug discovery in medicinal plants when suitable analytical techniques are used for the identification of physiologically relevant molecular targets. These three elements are grouped into one academic field, pharmacognosy [9].

Madhuca indica has been identified by several bioactive compounds that help to act against the MDR wound pathogen. Betulinic acid is also one of the worthy nutrients due to its uniqueness as antimicrobic and anti-inflammatory, for proceeding wound healing process and avoiding secondary infection. Lupeol was identified as playing roles in antibacterial activity and tissue healing which is traceable in wound healing. The flavonol quercetin complements its drawback with antioxidant and antimicrobial properties that promote cellular recuperation and protection from further oxidative damage to tissues [10]. Saponins are from *M. indica,* which has antimicrobial and antifungal activity effective for the treatment of wounds which is prone to infection. Gallic acid is appreciated for its antioxidant and antimicrobial implications that aid in the normal healing process by inhibiting bacterial growth. The compounds such as caffeic acid and vanillic acid represented significant antimicrobial and anti-inflammatory properties [11]. Caffeic acid is effective against pathogens that are usually resistant to other agents and vanillic acid decreases inflammation around the wounded area. Also, based on the current literature, Kaempferol possesses more or less antibacterial properties to all classes of bacteria and similarly, Ellagic acid has considered strong antioxidant and antimicrobial properties [12]. Tannins can be used in wound treatment by preventing new infections at the wound and drying area. Figure 1 shows the plant extract compounds for wound pathogens.

There are more than 800 plant species in the genus Madhuca [13]. Astringents and emollients processed from the bark, flower, fruit, leaves and seed can be used to treat fractures, burns, swelling, itching, snakebites, ulcers, pharyngitis and leprosy [14]. Various parts of *M. indica* are shown in Figure 2. The phytochemical analysis showed anti-inflammatory activity [15-17]. This study aims to identify *M. indica* compounds by *in silico* methods determine their suitability in the treatment of MDR wounds and determine successful candidates for the development of new antibiotics by considering the combination of target, functional linkage and drug pharmacokinetics.

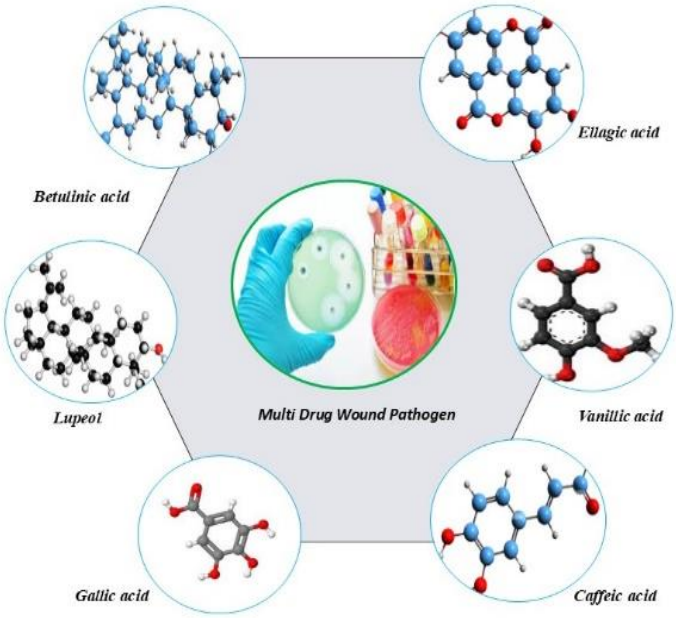


Figure 1. Bioactive Compounds in Plant Extracts

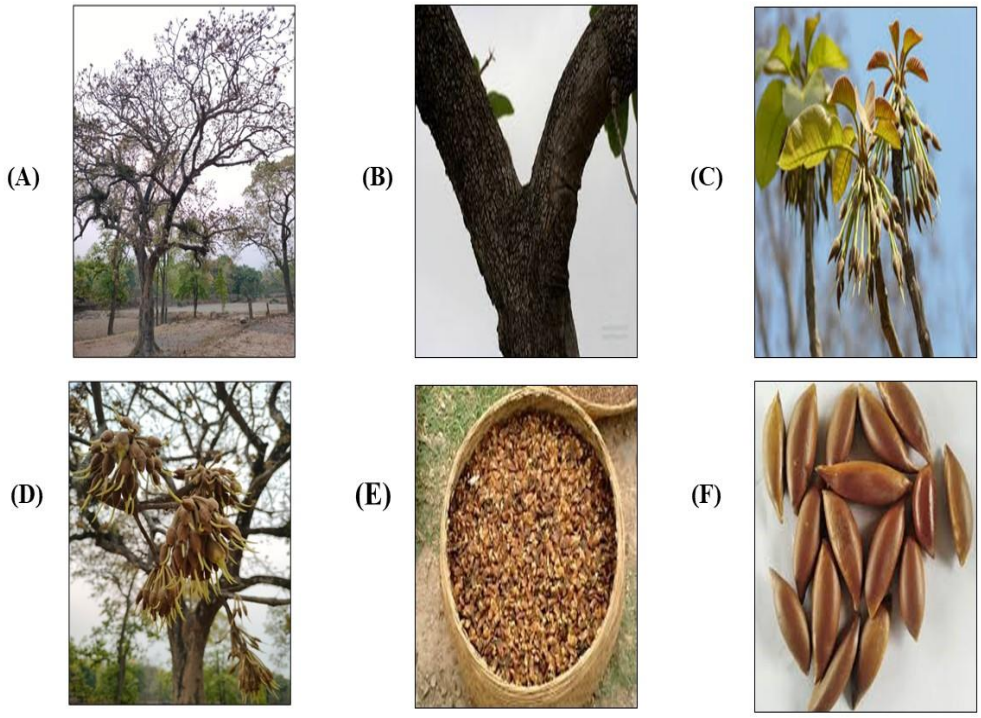


Figure 2. (A) Madhuca Indica Tree, (B) Grey Trunk, (C) Leaves, (D) Flowers, (E) Dried Flowers, (F) Seeds

Materials and Methods

In silico approaches, the study was designed to identify potential bioactive compounds from *M. indica* against MDR wound microorganisms. *In silico* screening, molecular docking and filter based discovery, along with ADMET (absorption, distribution, metabolism, excretion and toxicity) profiling were also performed to find potential antimicrobial agents. The compounds binding affinity and stability were determined to predict their ability to be effective against the resistant pathogens for further experimental determination.

Preparation of Aqueous Extract

M. indica plant belongs to the Sapotaceae family. *M. indica* has been endowed with antioxidant activity, which is essential for preventing oxidative stress brought on by free radicals. The damage caused by free radicals to chemicals, such as superoxide anion (Reactive Oxygen Species), makes other molecules unstable. *M. indica* flower collected from Mayurbhanj district, Odisha. The samples were verified by the Centre for Advanced Studies in Botany at the University of Madras, Chennai.

The preparation of *M. indica* powder, such as washing it with double distilled water to get rid of dust and solid particles and then letting it dry in the shade for three days. A mechanical grinder was used to powder the CAL once it had dried and a sieve was used to filter it. The resulting biosorbent was then preserved for use at a later time. To make the *M. indica* extract for the experiment, 100 mL of distilled water was combined with 25 g of dried *M. indica* powder and mixed. After being left overnight, the solution was boiled to 60°C for 20 min. The solution was cooled and any remaining particles were filtered out using Whatman No. 1 filter paper. The resulting liquid extract was then stored at 4°C for further future experiments [7].

Fourier Transform Infrared Spectroscopy (FTIR)

FTIR is a widely used qualitative or semi quantitative approach for identifying bioactive chemicals in plants. It may detect functional groups and provide further structural information [18]. Using FTIR, *M. indica* was examined in the 4000-400 cm^{-1} region following the extraction procedure.

Gas Chromatography-Mass Spectrometry (GC-MS)

GC-MS data is used to identify the chemical profile of *M. indica,* which may be employed in virtual screening for wound pathogens, resistant to several drugs [19]. One millimetre of methanol solvent was used to dissolve 100 µL of an aqueous solution of *M. indica*. After 20 sec of vigorous agitation with a vortex stirrer, the solution was filtered through a 0.2 micron membrane filter. This transparent extract was then used for GC-MS analysis.

Phytochemical Analysis

The components of plant extracts are frequently examined using bioactivity and phytochemical screening, which also seeks to find the bioactive component that could be used in the creation of pharmaceuticals. Phytochemicals can bind with bacterial targets and compare their effectiveness with that of established antibiotics. This approach helps create effective therapeutic interventions for resistant infections and chronic wounds and infections due to MDR pathogens.

Foam test: In a graduated cylinder, 2 mL of plant extract was dissolved in 2 mL water and violently stirred for 15 min. The presence of saponins was indicated by foam formation.

Phenol Test: This is a Ferric chloride test. Three to four drops of a 6% ferric chloride solution are added to 2 mL of the extract. The presence of phenols and tannins is indicated by the production of deep blue, black and green colours.

Flavonoids Test: It is the Alkaline reagent test. A small quantity of sodium hydroxide solution is added to 2 mL of the extract. Flavonoids are indicated by the formation of a vivid yellow colour that goes colourless when diluted acid is added.

Legals test: 2 mL of pyridine with 1 mL of sodium nitroprusside solution is added to 2 mL of the extract. Additionally, a tiny quantity of NaOH solution is added. The presence of glycosides is shown by the colour changing from pink to red.

Steroids Test: Add 2 mL of the extract to 5 mL of chloroform, then add a few drops of pure H_2SO_4. The presence of steroids is

confirmed by a low chloroform layer that is red.

Amino Acid Test: Also known as Ninhydrin test, 2 mL of the extract and 2 mL of 0.25% ninhydrin reagent were added and allowed to stand in a water bath for some time. By generating a blue colour, one can determine the existence of amino acids. The presence of proteins is noted by a yellow tinge on fructose content with mononitrate. A colour that is close to pure blue between violet and pink or predominantly red is evidence of the amino acids.

Bontrager's test: 2 mL of the extract and 2 mL of chloroform were added and evaporated until completely dry and a few drops of concentrated H_2SO_4 were added and heated for 2 min. The presence of terpenoids is confirmed by a red or reddish brown colour.

Anthraquinone Glycoside Test: 2 mL of the extract and a small amount of nitric acid were carefully applied to the test tube's walls and the tube was then placed in a water bath for 10 to 15 min. The presence of anthraquinone glycoside is confirmed by the colour changing from yellow to orange [20].

Antioxidant Assay

It also described how to use the 2,2-diphenyl-1-picrylhydrazyl assay (DPPH) radical scavenging technique with an ascorbic acid standard to analyze the bioactive chemicals in *M. indica* in multidrug resistant bacteria *in silico*. The DPPH radical scavenging method is a simple technique that takes advantage of chemical decolourization. In this study, we examine the antioxidant activity of *M. indica*. The antioxidant reaction occurs when a purple coloured oxidized form of DPPH combines with an ethanolic solution, reducing DPPH and changing the background colour from dark purple to yellow. To create varied results, 1 mL of *M. indica* solution diluted with ethanol was mixed with 2 mL of DPPH standard solution (0.1 mM). The mixture was then mixed and allowed to come to room temperature in a dark atmosphere. Using a UV-visible spectrophotometer, the absorbance (A) of each medication at 517 nm was measured after 1 h of incubation to assess its free radical scavenging activity. Next, using the following formula, the per cent inhibition (I (%)) was determined [21].

Percentage of inhibition = (Absorbance of control) - (Absorbance of the sample)/ (Absorbance of control) × 100.

***In silico* Analysis**

In silico techniques provide effective approaches for screening and evaluating the bioactive properties of the compounds produced from medicinal plants, the potential interaction between these compounds and bacterial targets and their pharmacodynamics profiles. *In silico* is a bioinformatics tool that exploits molecular docking, pharmacophore models and ADMET profiling to assess the drug efficacy of plant born compounds as shown in Figure 3. Through molecular docking, it can estimate the interaction of the compound with the target proteins and evaluate the ADMET factors to shortlist the potential drug molecules. In genomics, computational tools identify genes and foresee protein properties necessary for the development of individual medications and studying of functions of genes. Furthermore, it simulates disease transmission, environmental contamination and gene editing impacts, which enable hypothesis testing and experiment optimization without expensive lab infrastructures The improved accuracy and shorter developmental time improve the effectiveness and efficiency. In this study, such computational methods are employed to screen out bioactive constituents of *M. indica* that could modulate key proteins in MDR pathogens causing wound infection.

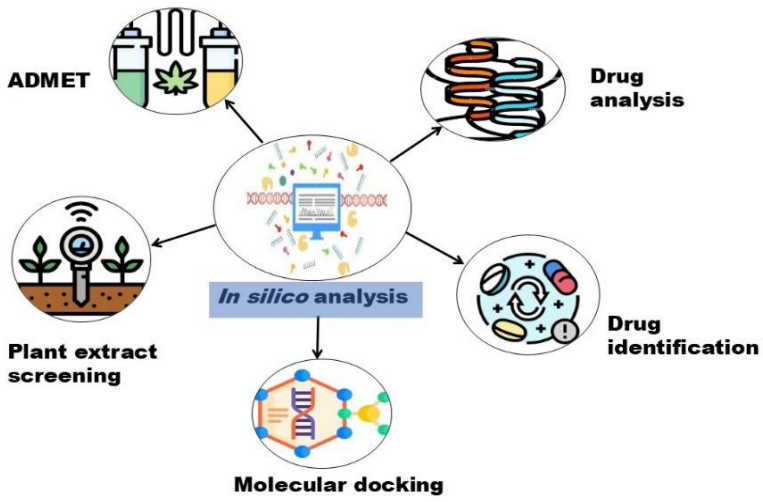


Figure 3. *In Silico* Approach of Plant Extract on Multidrug Resistant

The protein structures were acquired from RCSB PDB and verified using a repair/ build/check model to confirm their integrity. Auto Dock Tools were used to prepare the pdbqt files. The ligands obtained from PubChem were subjected to optimization using Avogadro software and subsequently converted for docking. AutoDock4 performed molecular docking using a refined grid and then used cluster analysis to identify the most favourable binding positions. Analyzing binding interactions and affinities was conducted using Biovia Discovery Studio. Swiss ADME was used to conduct *in silico* ADME research, which involved evaluating drug likeness according to Lipinski's rule of five and predicting therapeutic efficacy and safety by examining interactions with biological components. Figure 4 shows an *in silico* investigation of *M. indica* flower extracts against multidrug resistant wound pathogens.

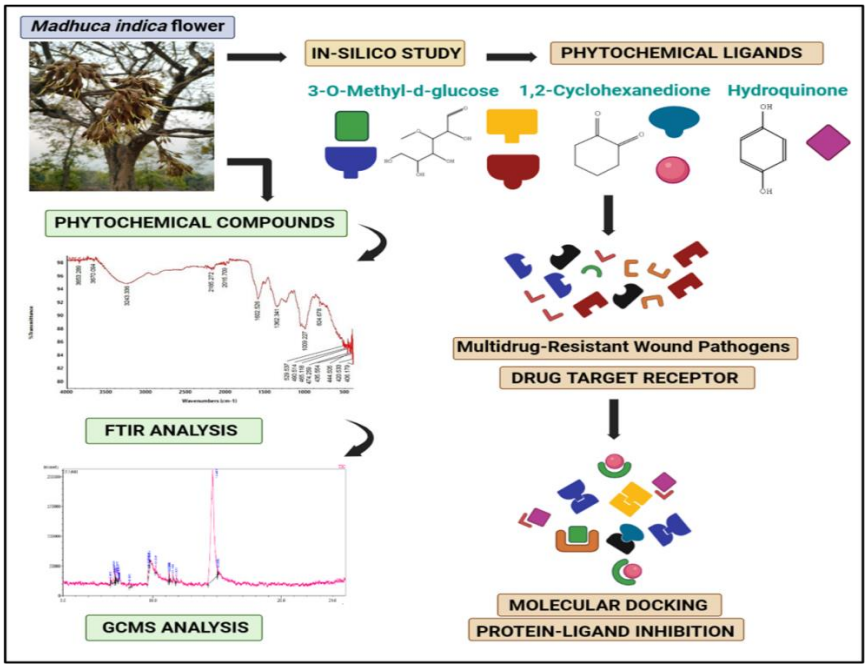


Figure 4. *In Silico* Investigation of *Madhuca indica* Flower Extracts Against Multidrug Resistant Wound Pathogen Through Phytochemical Analysis, FTIR, GC-MS, Molecular Docking and Protein-Ligand Inhibition

Results and Discussion

The identification of functional groups, specific molecules with strong antioxidant activity and antimicrobial phytochemicals indicated the bioactive substances of *M. indica* based on FTIR, GC-MS, DPPH and phytochemical assays. These outcomes indicate *M. indica's* effectiveness against MDR wound infections.

Fourier Transform Infrared Spectroscopy

Characterization of the substance was done using functional group infrared absorption by FTIR spectroscopy. In the use of FTIR for the determination of bioactive compounds in plant systems it has grown to be used qualitatively or semi quantitatively to identify the functional groups and obtain more structural information. Following the extraction process, the *M. indica* was characterized using FTIR sacrifice in the range of 4000-400 $cm^{-1,}$ as shown in Figure 5. This study proved well in establishing the several functional groups in *M. indica.* The compounds present in the *M. indica* exhibited peaks at 3285 cm^{-1}, 2933 cm^{-1}, 1624 cm^{-1}, 1403 cm^{-1}, 1226 cm^{-1} and 1033 cm^{-1} for hydroxyl, alkane, aromatic and ether functional groups that may be responsible for its antibacterial action against multidrug pathogens.

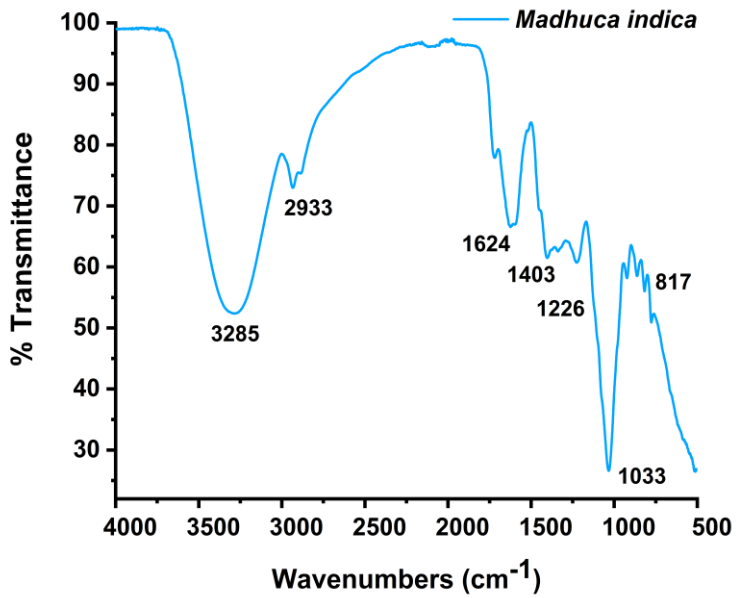


Figure 5. The Functional Groups of the Bioactive Compounds Present in *Madhuca indica* Extract are Identified from its FTIR Spectrum

Gas Chromatography-Mass Spectrometry

Gas Chromatography analysis of liquids, gasses or solids is done using mass spectrometry. Typically, the sample is put straight into the GC for gases and liquids. Solids are analyzed by pyrolysis, solvent extraction or desorption. The presence of many bioactive components in *M. indica* is suggested by the GC-MS spectra, which show multiple notable peaks at various RTs, as shown in Figure 6. The high intensity seen at 14.662 min suggests a high concentration of a chemical that may be investigated further for its potential application in the treatment of wound bacteria that are resistant to many drugs.

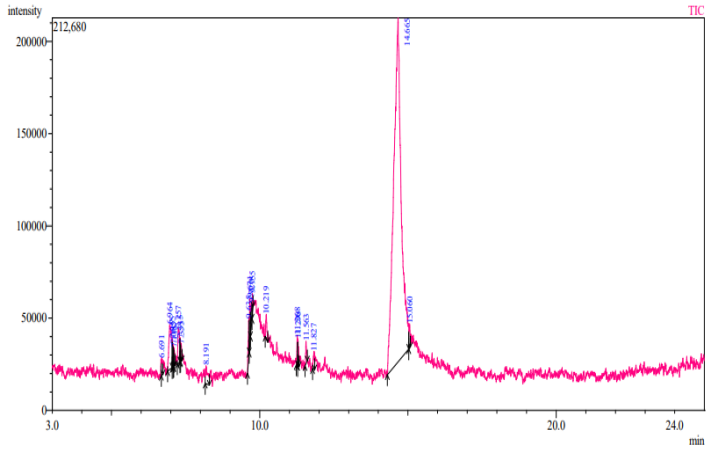


Figure 6. Bioactive Compounds Present in *Madhuca indica* Extract are Identified from its Gas Chromatography Mass Spectrometry

Antioxidant Activity

The *in silico* approach that can be used to assess the antioxidant potential is to estimate the efficiency of compounds in scavenging the free radicals and the effects of oxidative stress. These approaches apply molecular docking and molecular dynamics (MD) simulations to evaluate the binding of bioactive compounds and targets. Thus, the effective way to predict the activity of natural or synthetic compounds is the simulation of their interactions. In this way, the testing of the antioxidant activity can be carried out before experimental work. This method reduces the time needed for drug discovery; it can be used for the identification of lead molecules; it can also be as used in the advancement of therapies that are based on the application of antioxidants, especially for diseases and processes that are associated with oxidative stress such as inflammation and ageing.

DPPH

Based on ascorbic acid, the DPPH free radical scavenging method was employed to perform an *in silico* study on the bioactive molecule of MI for MDR wound microorganisms. The decolorization process might be applied to assessing the DPPH radical scavenging method which is a simple and basic operation. A chemical change takes place and the DPPH radical is converted from deep violet colour form to yellow colour when ethanolic solutions containing oxidized molecules of DPPH with deep violet colour are reacted with antioxidant molecules, dilute 1 mL of *M. indica* with ethanol at varying concentrations (30-60 µg/mL) was stirred with 2 mL of a standard solution of DPPH (0.1 mM). At the end of this period, the results are mixed and stored in the same dark place at 37 ^{0}C. The DPPH radical scavenging method is a simple process involving chemical decolourization. DPPH exists in its oxidized state distinguished by with purple color and reacts with a compound to be tested by forming a non purple product at the background which turns yellow. For different concentrations of *M. indica* (within a range of 30 to 60 µg/mL), 1 mL of *M. indica* in ethanol solution was combined with 2 mL of DPPH standard solution at a concentration of 0.1 mM, as shown in Figure 7. The cloudy solution is then stirred for 10 min and then allowed to stand at room temperature in a covered beaker. 1 h after the eggs were infected, the effects of the drug on free *M. indica* exhibit concentration dependent radical scavenging activity, according to the DPPH test, where the percentage of radicals inhibited rises with concentrations as 10-50 µg/mL. The activity is close to the benchmark, indicating strong free radical scavenging activity that

might help fight oxidative stress and aid in wound healing.

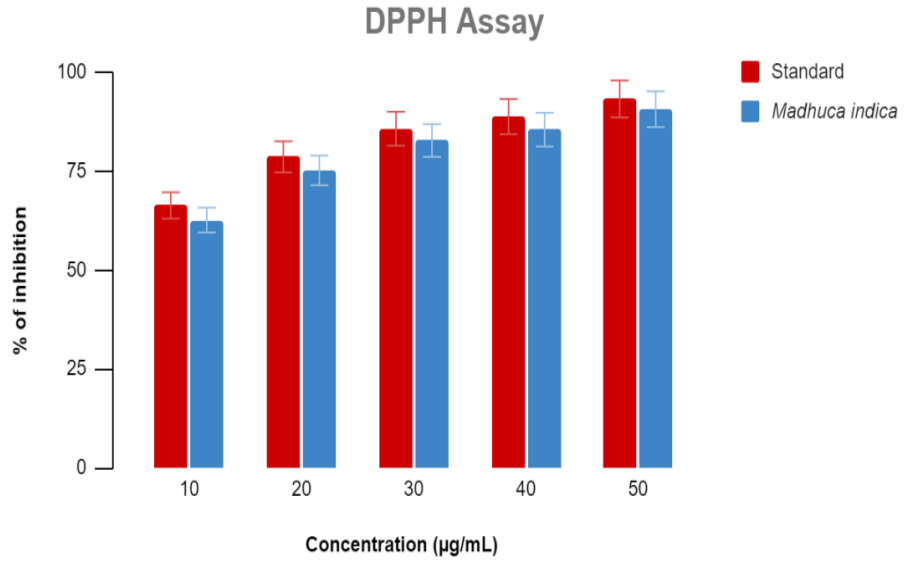


Figure 7. 2,2-Diphenyl-1-Picrylhydrazyl Assay of *Madhuca indica*

Phytochemical Analysis

M. indica's dry powder was gathered and the aqueous extract was kept for further examination at 4°C. Prominent phytochemicals were found in all three extracts after phytochemical screening. Several bioactive phytochemicals of *M. indica* were demonstrated which show therapeutic activities against multidrug resistance problematic wound pathogens. The highest concentration is found in flavonoids (+++), antioxidant and antimicrobial substances that could be responsible for infection control and inflammation. There is a high potential for alkaloids, tannins, terpenoids and saponins due to their antimicrobial, anti-inflammatory properties that can heal the damaged tissue. Protein condition is ++ and carbohydrates ++ contribute to tissue building. The presence of phenols (+) and fatty acid (++) compliments the plant's ability to combat oxidative stress and treat resistant infections for healing. Table 1 shows a phytochemical analysis of *M. indica* revealing that the plant contains flavonoids among many other bioactive compounds. These compounds; Terpenoids flavonoids and tannins possess anti-bacterial properties that enhance the efficiency of the plant in fighting antibiotic resistant diseases.

Table 1. Phytochemical Analysis of *Madhuca indica*

Phytochemicals	***Madhuca indica***
Alkaloid	++
Carbohydrates	++
Tannins	++
Glycoside	-
Proteins	++
Flavonoid	+++
Terpenoids	++
Phenol	+
Fatty acids	++
Saponin	++

Molecular Docking Analysis

Molecular docking involves the coming together of two or more molecular structures or for instance medications, enzymes or proteins. The model that works for bringing together projections of two molecular structures mainly of proteins (enzymes) relates to tiny molecules (ligands) the docking. To alter the amenities of proteins and their functional capacity, proteins and nucleic acids need to recognize small molecules that allow them to constitute supramolecular assemblies. Molecular docking gives an understanding of how small molecules act in a target protein's active site. The techniques employed are the identification of the position of the ligand in the protein binding site and the prediction of the interactions between the ligand and proteins. From Table 2, *M. indica* shows strong and multiple hydrogen interactions with essential amino acid residues and moderate binding energy thus it may be able to tie pathogen proteins reacted to several drugs. Table 3 shows *M. indica* protein interactions including 3-O-Methyl-d-glucose and hydroquinone bind with the target proteins through stable 3D and 2D. These interactions have demonstrated binding potential that may imply their possible efficacy against infections that are not easily killed by several drugs.

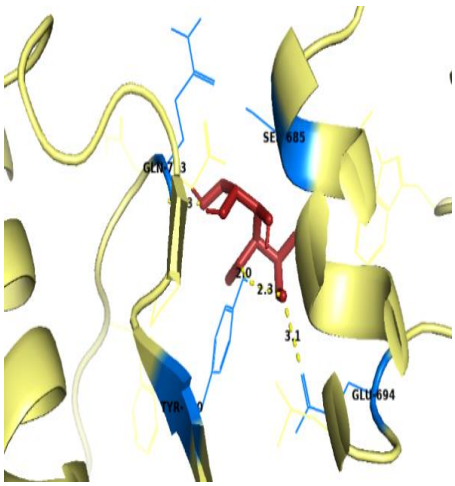
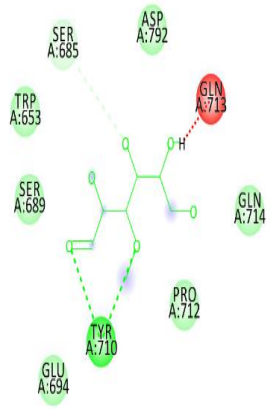
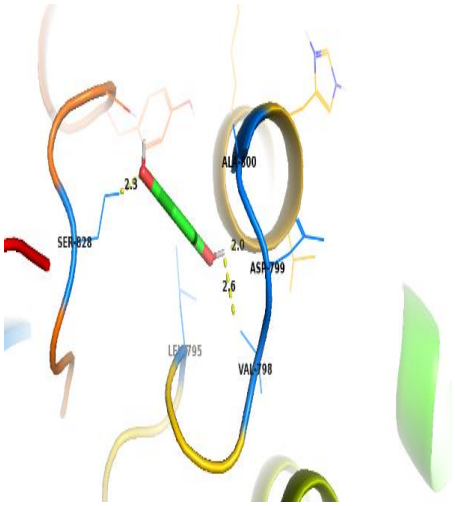
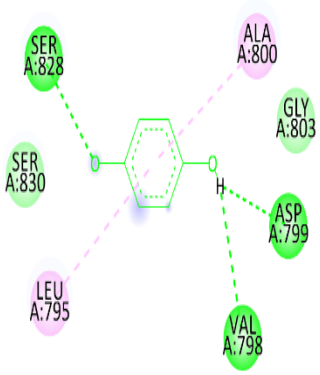
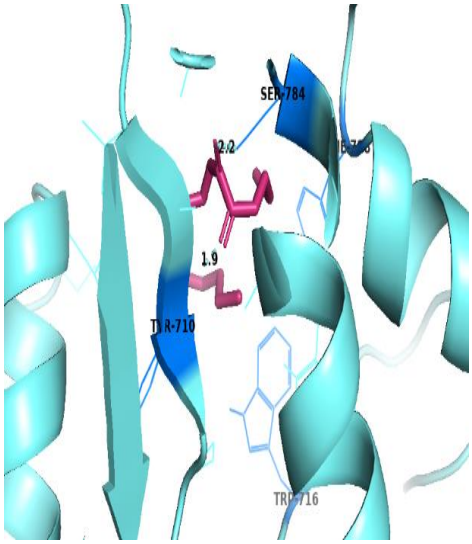
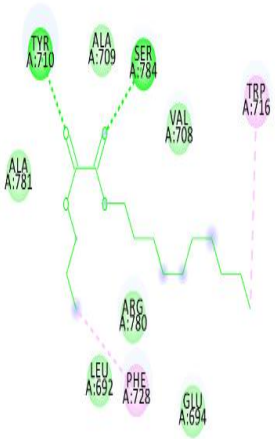
Table 2. Analysis Of Molecular Docking

Ligand	**Binding Affinity**	**Distance**	**Hydrogen Interaction**	**Amino acid residues**
3-O-Methyl-d-glucose	**-4.3**	3.1 (GLU 694) 2.3 (TYR 710) 2.3 (GLN 713) 2.5 (SER 685) 2.0 (TYR 710)	1. Conventional Hydrogen Bond 3. Carbon hydrogen bond 2. Van der Waal	1. GLU A:694, PRO A;712, GLN A:714, ASP A:792, TRP A:653, SER A:689 2. SER A:685
Hydroquinone	**-4.2**	2.0 (ASP 799) 2.6(VAL 798) 2.3(SER 828)	1. Van der Waals 2. Conventional Hydrogen Bond 3. Carbon hydrogen bond	1. SER A:830, GLY A:803 2. SER A:828, VAL A:798, ASP A: 799 3. LEU A:795, ALA A;800
Oxalic acid, decyl propyl ester	**-4.1**	2.2 (SER 784) 1.9 (TYR 710)	1. Carbon hydrogen bond 2. Van der Waals 3. Conventional Hydrogen Bond	1. ALA A:781, LEU A:692, ARG A:780, GLU A:694, ALA A:709 2. TYR A:710, SER A:784 3. TRP A: 716, PHE A:728

Absorption, Distribution, Metabolism and Elimination Properties of Drug (ADME)

The hardest and most demanding aspect drug improvement process is frequently optimizing a therapeutic molecule's ADME characteristics. Drug effectiveness may also be significantly impacted by the ADME profile. By concentrating primarily on promising ones, *in silico* ADME studies could enhance analysis and assessment and lower the risk of ambiguity in the latter phases of drug development. To this end, various *in silico* methods have been developed to predict ADME properties based on chemical models, such as data driven methods for structural analysis based on ligand protein docking (e.g., QSAR), similarity studies and 3D QSAR and pharmacophore modelling, as shown in Figure 8.

Table 3. 3d and 2d Interaction of *Madhuca indica* Substances (3-o-Methyl-d-Glucose and Hydroquinone)

Name of the Ligands	**3D Interaction**	**2D Interaction**
3-O-Methyl-d-glucose		
Hydroquinone		
Oxalic acid, decyl propyl ester		

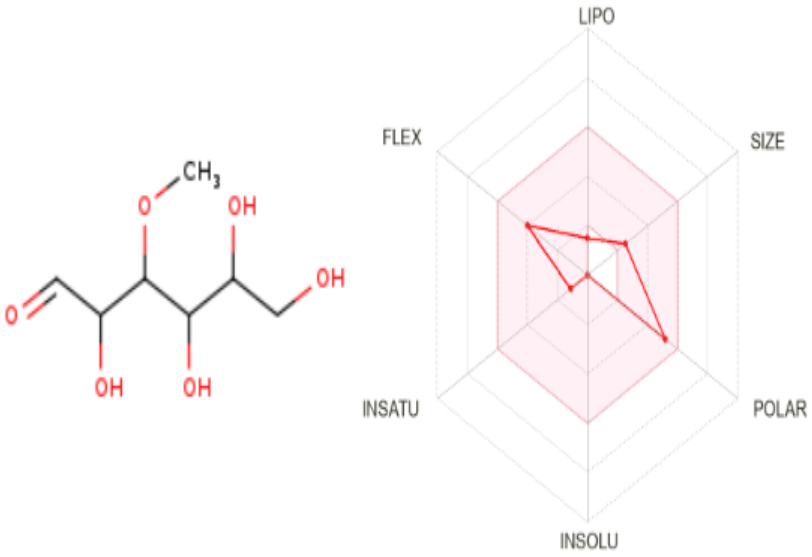


Figure 8. ADME Properties of the Drug in *Madhuca indica*

Table 4 shows **the** Physicochemical characteristics of the *M. indica* compounds molecular weight (194.18 g/mol), predicting high drug likeness and water solubility with no Lipinski violations. It should be recognized that systemic delivery might be hindered by inadequate GI absorption and an inability to enter the CNS across the BBB.

Table 4. Physiochemical Properties of *Madhuca indica* on Drug Activity

PHYSIOCHEMICAL PROPERTIES	
Formula	$C_7H_{14}O_6$
TPSA	107.22 Å²
Canonical smiles	OCC(C(C(C(C=O) O) OC) O) O
BBB permeant	No
GI absorption	Low
Mol wt (g/mol)	194.18 g/ mol
Water solubility	Highly soluble
Canonical smiles	OCC(C(C(C(C=O) O) OC) O) O
Bioavailability Score	0.55
Synthetic Accessibility	3.52
Lipinski violations	Yes; 0 violation

Discussion

In silico methods in the discovery of bioactive chemicals for the management of antibiotic resistant diseases and the prospect of *M. indica* as a source of new antimicrobial compounds. To confirm the therapeutic use of various discovered medications, the outcome

of such computational predictions has to be further investigated *in vitro*, *vivo* and *silico* as a study conducted [22]. Some medicinal plants that are used in folk medicine, such as *M. indica* are known to contain various phytochemicals that have been said to possess many therapeutic values. The compounds cited in the past works include triterpenoids, flavonoids and phenolic acids, some of which have anti-inflammatory, antioxidant and antimicrobial properties [23]. This work was able to show high antioxidant capacity through the significant DPPH, ABTS and phosphomolybdate radical scavenging activity. Through this *in silico* study, authors were able to parse through various structural features of these compounds and predict their biological functionalities. Specifically, molecular docking predicts Target interaction. The GC-MS and FTIR methods were used to investigate bioactive compounds in samples of different edible plants. These analyses established constant halogens, aliphatic amines, primary and secondary amines, esters, ethers, aromatics, lipids, triglycerides and nitro composites. The present compounds, therefore, held better, anticancer and anti-inflammatory characteristics than studies reported previous studies [24]. These functional groups and structures point to ORED8 the possible therapeutic value of these plant sections to warrant investigation in the biomedical field [25-27]. Such interactions are important because bacterial growth and survival may be prevented and hence reduce infection incidences, particularly in wound healing processes. The *in silico* strategy to study the anti-wound microbial molecules of *M. indica a*gainst MDR pathogens is somewhat constrained, firstly due to the model based predictions of the cellular effects that might not demonstrate the real biological implications. To support these findings further and to evaluate efficiencies and safety some further studies should be conducted in laboratory and clinic settings. Combining *in vitro* and *vivo* approaches could augment the application of the treatment methods.

Conclusion

Treating wound infections is made more difficult by bacterial pathogens resistance to antibiotics. However, the fast evolution of multidrug resistant wound infections has been facilitated by the abuse and overuse of antibiotics. Since pharmacologically significant chemicals have long been used in medical systems, plants are a great source of them. Focused study on natural chemicals for the drug development process might be facilitated by the ancient wisdom derived from medicinal plants. Because medicinal plants have several benefits over synthetic chemicals, they are more significant sources for drug development, particularly lead molecules. The current need cannot be met by traditional screening methods for therapeutic plants since, in the post genomic age, the molecular targets for the majority of illnesses are known. The study aims to analyze the potent candidates for forming new antimicrobial drugs with severe consideration of the compound target interactions, binding activities and pharmacokinetics. *In silico* methods in the discovery of bioactive chemicals for the management of antibiotic resistant diseases and the prospect of *M. indica* as a source of new antimicrobial compounds. The result of such computational predictions needs to be further studied *in silico* to validate the therapeutic application of several identified drugs.

Conflict of Interest

The authors declare that they have no conflict of interest.

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