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In-Silico and Phytochemical Evaluation of Neem Bark (Azadirachta indica): A Comprehensive Review

Omkar Balaji Kamble[1], Umme Roman Shaikh[2]

[1]Student, [2]Assistant Professor
[1,2]Department of Pharmacy, Sayali Charitable Trust's College of Pharmacy
Chhatrapati Sambhajinagar, Maharashtra, India

Abstract:
This research looked into the chemical makeup and healing properties of Neem bark (Azadirachta indica), combining lab tests with computer-based drug analysis. Because of its active natural compounds, Neem bark has long been part of traditional medicine. For this work, the bark was gathered fresh, washed thoroughly, left to dry in the open air, ground into powder, then soaked in solvent at room temperature. After extraction, the liquid underwent basic testing to detect key plant-derived chemicals. Tests showed the plant holds active substances like alkaloids, flavonoids, alongside glycosides. Among them, chemicals such as Nimbiol and Sugiol stood out during deeper examination. Tools like Molsoft and SwissADME helped assess how closely these fit typical medicine traits. Outcomes pointed toward solid structural features, along with suitable ratings for becoming drugs. Most results from Protox-II showed low risk across key toxic effects like liver harm, heart issues, DNA changes, cancer links, cell damage - pointing toward a generally safe profile. Alongside this, methods using computer models and network-based pharmacology helped explore how Neem bark chemicals might work in medicine. Evidence points to several active roles these natural substances could play in treatment strategies. What stands out is that science now backs long-standing uses of Neem bark in healing practices. Tools such as phytochemical checks paired with digital simulations prove helpful when studying plant-based remedies and their biological actions.

Keywords: Neem bark, Azadirachta indica, phytochemical screening, in-silico study, network pharmacology, drug-likeness analysis, Protox-II, SwissADME, phytoconstituents, computational pharmacology.

1. Introduction

For centuries, people have turned to healing herbs as a core part of folk medicine. What sets Neem apart - scientific name Azadirachta indica - is how deeply it contributes across many types of treatments. Part of the Meliaceae group, this tree earns the nickname "Village Pharmacy" thanks to its wide range of useful components.

From the hot zones of South Asia rises a leafy giant - neem - spreading across India, Bangladesh, Pakistan, Sri Lanka, and beyond into similar climates. Its presence isn't just shade; every piece plays a role. Leaves, bark, even the seeds tucked inside fruit, get drawn upon by age-old healing paths like Ayurveda, Siddha, and Unani. Roots dig deep, flowers bloom briefly, yet each part finds purpose. Across generations, these elements pass through hands shaped by practice, not theory. Not everything green is ignored here - the full plant matters.

For over two millennia, healers across India have turned to Neem when facing infections, swelling, imbalances in metabolism, or issues tied to the skin. Old Ayurvedic texts speak of it as having power against microbes, calming irritation, shielding cells from damage, helping regulate blood sugar, fighting

parasites, while also supporting tissue repair.

Among plant-based remedies, Neem stands out because it holds a range of active substances. Compounds like limonoids, flavonoids, and alkaloids give it its strength. Then there are tannins, glycosides, along with terpenoids and phenolics doing their part. From these, scientists have pulled specific agents - azadirachtin takes center stage. Others follow: nimbin, nimbidin, then nimbolide stepping in. Gedunin plays a role too, salannin joins, and quercetin rounds them out. Because of this mix, Neem works well in healing practices. From all sections of the Neem tree, it is the bark that stands out for healing, thanks to powerful traits like fighting germs, calming swelling, shielding cells, and speeding recovery. People have long turned to Neem bark to ease fevers, soothe sores, treat malaria, heal cuts, clear mouth issues, beat fungus, along with stomach troubles.

Because computers can now map how plant chemicals behave in the body, scientists are using new methods to study herbal treatments more closely. Instead of focusing on just one compound, researchers look at many active ingredients found in herbs, each affecting different parts inside cells. With tools that trace these complex interactions, it's easier to see how a single herb influences several processes at once. For plants like Neem, which affect various pathways, this kind of analysis reveals patterns traditional methods might miss.

Looking at neem bark, this review covers its plant chemicals first. Then comes how these substances act in the body, shown through lab studies. One part maps out connections between targets using network methods. Molecules get checked for medicine potential by computer models. Safety gets assessed through predicted toxic effects. Finally, treatment value is weighed using digital simulations.

1.1 Taxonomical Classification of Neem

Category	Classification
Kingdom	Plantae
Division	Magnoliophyte
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Azadirachta
Species	Azadirachta indica

1.2 Common Names of Neem

- English: Neem / Indian Lilac
- Hindi: Neem
- Marathi: Kadunimb

1.3 Morphology of Neem

Neem is a medium to large sized evergreen tree that generally grows up to 15–20 meters in height under favorable environmental conditions. The tree possesses a straight trunk with spreading branches forming a broad crown.

1.3.1 Stem and Bark

The bark of Neem is rough, hard, fissured, and grayish-brown in color. The inner bark possesses a reddish-brown appearance and bitter taste due to the presence of active phytoconstituents.

1.3.2 Leaves
Leaves are compound, alternate, pinnate, and dark green in color. Each leaf contains several serrated leaflets with characteristic bitter taste.

1.3.3 Flowers
Neem flowers are small, white, fragrant, and arranged in clusters. Flowering generally occurs during spring season.

1.3.4 Fruits
The fruit is a smooth olive-like drupe that changes from green to yellow upon maturation. Fruits contain one seed enclosed within a hard shell.

1.3.5 Seeds
Neem seeds are rich in oil and contain important limonoids such as azadirachtin.

1.4 Pharmacological Activity of Neem
Neem possesses a broad range of pharmacological activities due to the synergistic action of its phytoconstituents. Different parts of the plant exhibit significant medicinal properties and are widely used in traditional medicine systems.

Pharmacological Activities of Neem:

- Antimicrobial activity
- Anti-inflammatory activity
- Antioxidant activity
- Antidiabetic activity
- Anticancer activity
- Wound healing activity
- Antifungal activity
- Antiviral activity

The pharmacological activities of Neem are mainly associated with phytoconstituents such as flavonoids, tannins, alkaloids, glycosides, terpenoids, limonoids, and phenolic compounds.

Fig.No.1.1 Neem

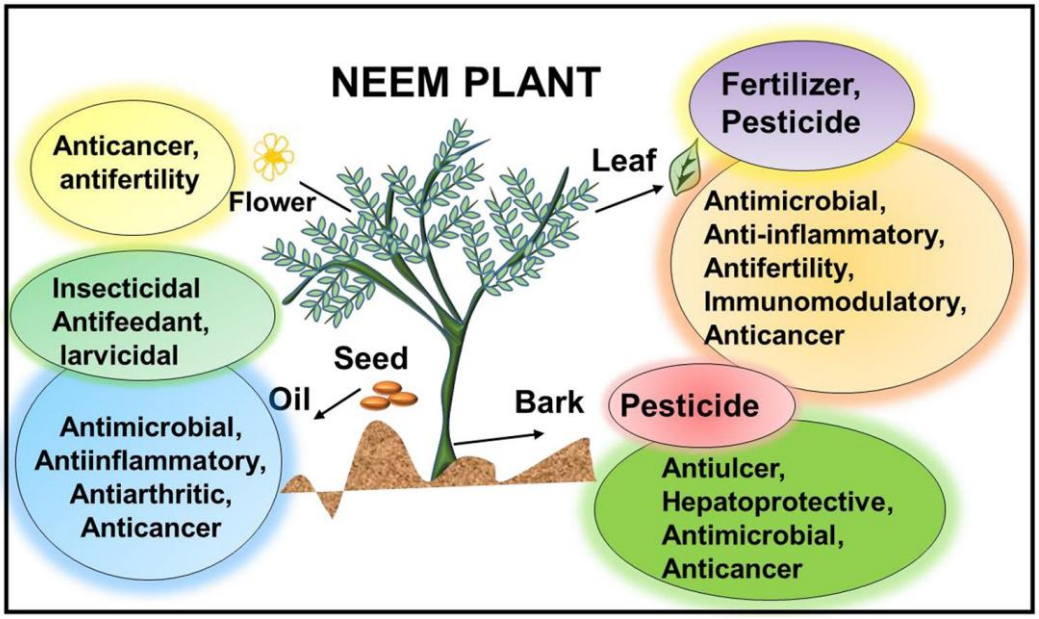


Fig.No.1.2 Pharmacological Activities

1.5 Introduction to Neem Bark

Deep inside the trunk of the Azadirachta indica tree, neem bark holds a quiet strength. Though often overlooked, its role in ancient healing practices runs deep across generations. Because it interacts powerfully with biological processes, people have turned to it again and again when facing infections or swelling. Skin troubles, too, find resistance within its layers. Hidden compounds - limonoids leading the way - act together like threads in a web. Flavonoids join them, supported by sharp-tasting tannins and complex alkaloids. Even glycosides weave through, backed by aromatic terpenoids that shape much of its potency.

For ages, neem bark found its place in Ayurveda thanks to sharp bitterness, drying effects, germ-fighting strength, and power to mend tissues. People once turned to it when dealing with high temperatures, sores, injuries, rashes on the skin, bouts of malaria, sugar imbalances, plus stomach troubles.

Out here, the bark feels coarse under your fingers. Its outside shows deep grayish-brown shades, while inside it warms into reddish tones. Bitterness hits first when tasted - no mistaking that sharp punch. This comes from natural plant compounds at work within. Nimbidin plays a role, just like nimbin does. Nimbolide joins in too, along with gedunin shaping how things unfold.

It turns out Neem bark holds a mix of active substances, each playing a role in how the body responds biologically. Because these elements hit more than one target inside cells, they shift how molecules communicate. That behavior opens doors for digital modeling in drug research, where patterns matter more than single effects. Scientists now see this plant layer not just as raw material but as a web of interactions worth mapping closely.

1.5.1 Botanical Description of Neem Bark

From the tree known as Azadirachta indica comes neem bark, part of the Meliaceae group. Tough and cracked, its outer layer feels rough under hand. Inside, tones shift toward red-brown, unlike the dull gray-brown seen on the surface. A close look reveals fibers when broken, showing how dense yet layered it truly is. Besides holding many natural compounds that affect living systems, the bark shows up often in plant-based drug studies due to its healing value. While researchers examine its chemical makeup, they also track how it behaves in traditional medicine practices across regions.

1.5.2 Traditional Use of Neem Bark

Neem bark has been used in Ayurvedic medicine for centuries because of its bitter, astringent, antimicrobial, and healing properties. Traditionally, Neem bark has been utilized for the management of:

- Fever

- Ulcers
- Wounds
- Skin infections
- Malaria
- Diabetes
- Gastrointestinal disorders

The traditional medicinal importance of Neem bark is associated with its broad spectrum therapeutic activities and phytochemical composition.

1.5.3 Characteristics of Neem Bark

Rough under the fingers, neem bark wraps itself in a coat of grayish brown outside. Inside, it reveals a shade closer to reddish brown when split open. Bitterness hits the tongue fast - that sharp note comes straight from compounds like nimbidin, nimbin. Nimbolide plays its part too, working behind the flavor alongside gedunin. Each element adds up without warning.

Besides holding key plant chemicals, the bark teams up flavonoids with tannins. Alkaloids join glycosides inside it, playing roles in healing uses. Terpenoids mix in, tied to how the body reacts. Phenolic compounds appear too, shaping its medical effects. Each part links to actions seen in treatments**.**

Fig.No.1.3 Neem Bark

1.6 Introduction to Network Pharmacology

Starting off differently each time, here goes: Picture a mix of drug science meeting computer-driven data work, tied together through living system insights. Instead of just one path, it links how medicines hit multiple spots in cells - genes, proteins, even whole networks. Rather than isolating pieces, it maps tangled connections across biological layers. Think molecules talking to disease circuits using math-backed models. It pulls lab knowledge into digital landscapes where effects unfold on many fronts at once. From roots in chemistry to outcomes in health, it tracks ripple patterns instead of straight lines.

Most old-style medicine sticks to a single-drug, single-target, single-illness idea. Yet when it comes to herbs, that mindset falls short - plants pack many natural compounds. These substances work across several body systems at once, not just one path. So, looking through a narrow lens misses much of what happens inside.

Instead of narrow views, network pharmacology brings broader insight into how treatments work across whole biological systems. By mapping complex relationships, it reveals which molecules interact and what paths they follow during therapy. First proposed by Andrew L. Hopkins, this approach shifted how

scientists explore drugs and their effects. Through connections rather than isolated parts, it reshapes the search for new medicines.

1.6.1 Principle of Network Pharmacology

The basic principle of network pharmacology is based on the concept that complex diseases require multi-target therapeutic approaches rather than single-target therapy. Medicinal plants contain several phytochemicals that act together on multiple proteins and pathways to produce therapeutic effects.

The Principle Involves:

1. Identification of active compounds
2. Prediction of molecular targets
3. Construction of interaction networks
4. Pathway enrichment analysis
5. Biological interpretation of therapeutic mechanisms

This systems-based approach helps in understanding the overall pharmacological behavior of medicinal plants and their phytoconstituents.

1.6.2 Advantages of Network Pharmacology

Advantages

- Multi-target therapeutic analysis
- Systems-level understanding
- Improved drug discovery process
- Better understanding of herbal medicines
- Reduced cost and time
- High-throughput computational screening
- Integration of bioinformatics and pharmacology
- Identification of molecular pathways
- Prediction of therapeutic mechanisms

Network pharmacology provides a scientific platform for understanding the therapeutic actions of Neem bark phytoconstituents and supports modern herbal drug discovery research.

1.6.3 Role of Computational Tools in Network Pharmacology

Various computational databases and software tools are used in network pharmacology studies for molecular analysis, pharmacokinetic evaluation, toxicity prediction, and therapeutic assessment of medicinal plant compounds.

Commonly Used Computational Tools:

Software/Database	Applications
IMPPAT	Phytochemical identification
Dr. Duke's Database	Ethnobotanical and phytochemical data
SwissADME	ADME prediction
Protox-II	Toxicity prediction
Molsoft	Drug-likeness prediction

These computational tools help researchers perform computational analysis efficiently and accurately. The integration of these tools provides a scientific basis for evaluating the therapeutic potential of Neem bark compounds.

1.7 Introduction of Software Used in Study

These days, scientists often turn to digital tools when studying plant-based medicines. Not just lab work but computer methods help uncover how natural compounds might treat illness. One such approach uses large data sets to spot active ingredients in plants. Instead of testing everything by hand, researchers simulate outcomes using programs on machines. For this particular project, specialists examined substances found in Neem tree bark. They leaned on several online repositories and analytical platforms during their process. Some steps involved checking if molecules behave like known drugs. Others focused on possible harmful effects these extracts could trigger. How the body absorbs or removes them was also part of the exploration. Each stage relied heavily on virtual models rather than physical experiments.

1.7.1 Dr. Duke's Phytochemical and Ethnobotanical Database

Inside a quiet corner of the internet sits Dr. Duke's collection - free for anyone who looks. Put together by USDA minds, it quietly holds plant stories tied to healing. Each entry breathes out details on natural compounds found in green life. Instead of just listing facts, it maps how substances behave inside living systems. Rooted in tradition, it also records how people across cultures have used these plants through time.

Plants hold natural compounds that scientists often trace using this database. One-way researchers explore healing traits is by checking plant ingredients here. Healing uses of herbs get studied through data stored inside. This tool helps spot active parts found in traditional remedies. Information gathered supports understanding how certain plants work. What grows in nature sometimes reveals medical potential through analysis.

In the present study, Dr. Duke's Database was used for:

- Identification of Neem bark phytoconstituents
- Collection of phytochemical information
- Biological activity analysis
- Literature-supported medicinal data

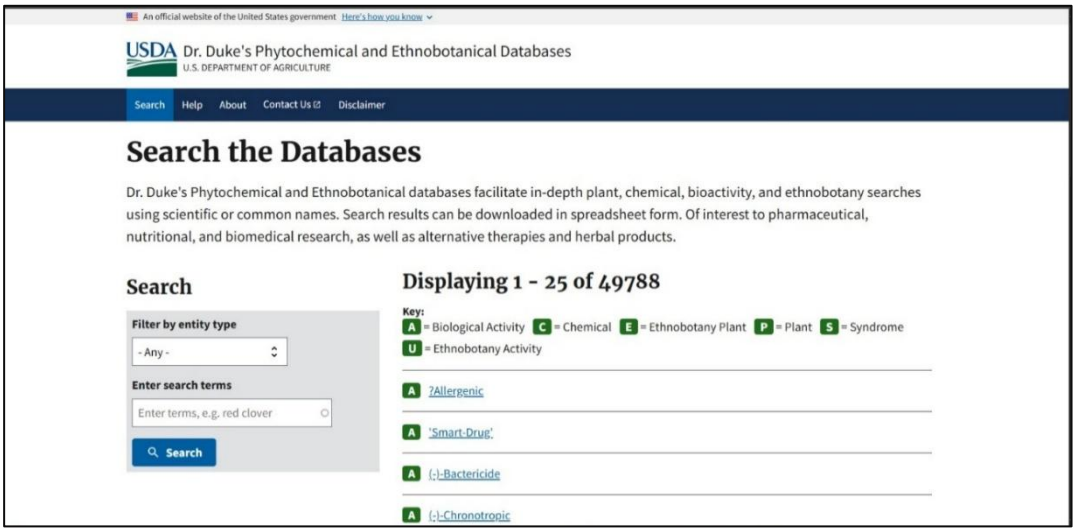


Fig.No.1.4 Dr Dukes Software Homepage

1.7.2 IMPPAT Database

IMPPAT stands for Indian Medicinal Plants, Phytochemistry and Therapeutics Database. It is a curated database specifically designed for Indian medicinal plants and their phytochemical constituents.

The database contains information regarding:

- Medicinal plants
- Phytochemical compounds

- Chemical structures
- Therapeutic uses
- Drug-likeness properties

IMPPAT is considered an important database in computational pharmacology research.

In the present study, IMPPAT was used for:

- Identification of phytoconstituents present in Neem bark
- Structural analysis of compounds
- Collection of molecular information
- Drug-likeness evaluation support

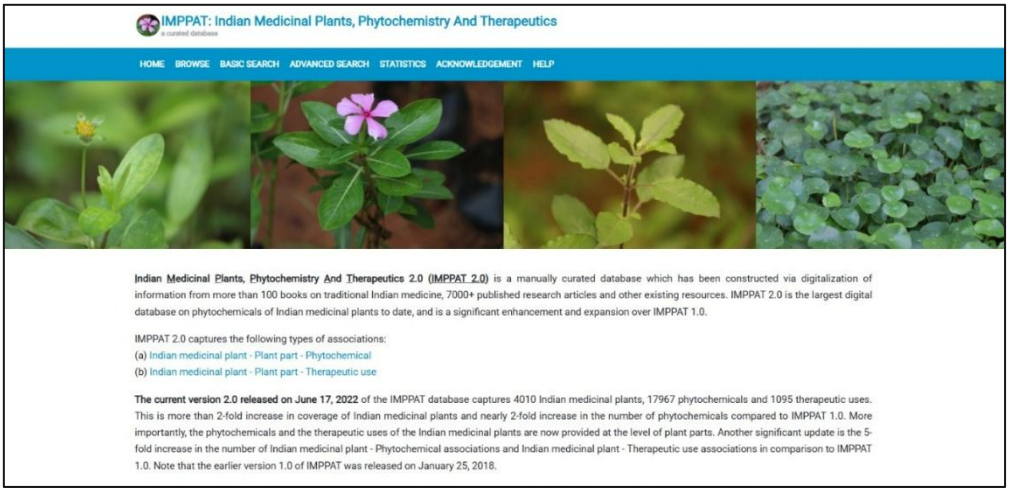


Fig.No.1.5 IMPPAT Software Homepage

1.7.3 Molsoft

Molsoft is a computational cheminformatics software platform used for molecular property analysis and drug-likeness prediction. It helps researchers evaluate the pharmaceutical suitability of chemical compounds.

In the present study, Molsoft was used for:

- Drug-likeness prediction
- Molecular property analysis
- Evaluation of phytoconstituent suitability

In herbal and pharmaceutical research, Molsoft is widely used for evaluation of compounds based on drug discovery parameters.

1.7.4 Protox-II

Protox-II is an online toxicity prediction platform used for prediction of toxicity profiles of chemical compounds. It is one of the most commonly used computational tools for toxicity analysis in pharmaceutical research.

Protox-II utilizes machine learning and molecular similarity approaches for toxicity prediction.

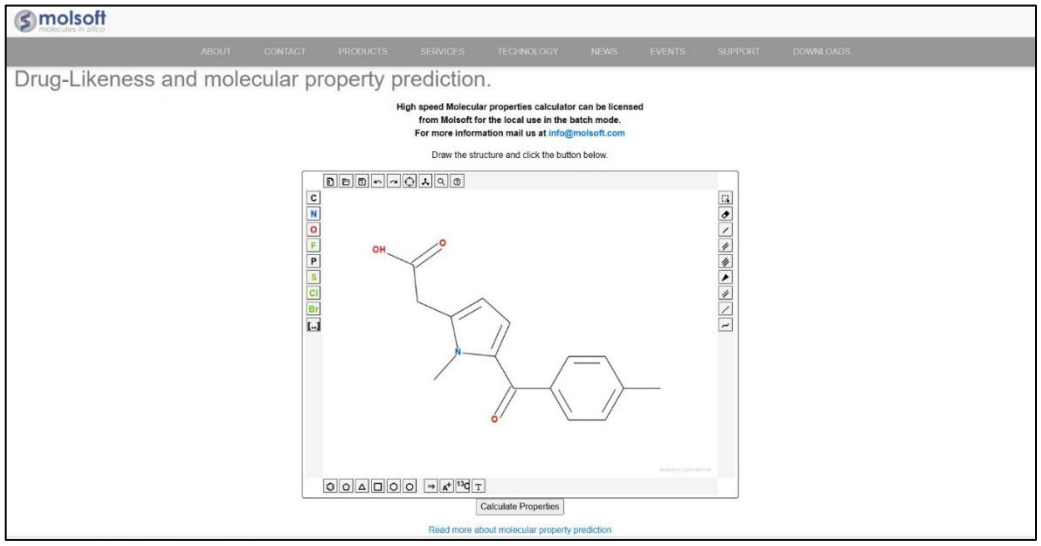


Fig.No.1.6 Molesoft Software Homepage

In the present study, Protox-II was used for:

- Toxicity prediction of Neem bark phytoconstituents
- Safety profile analysis
- Evaluation of toxicological class

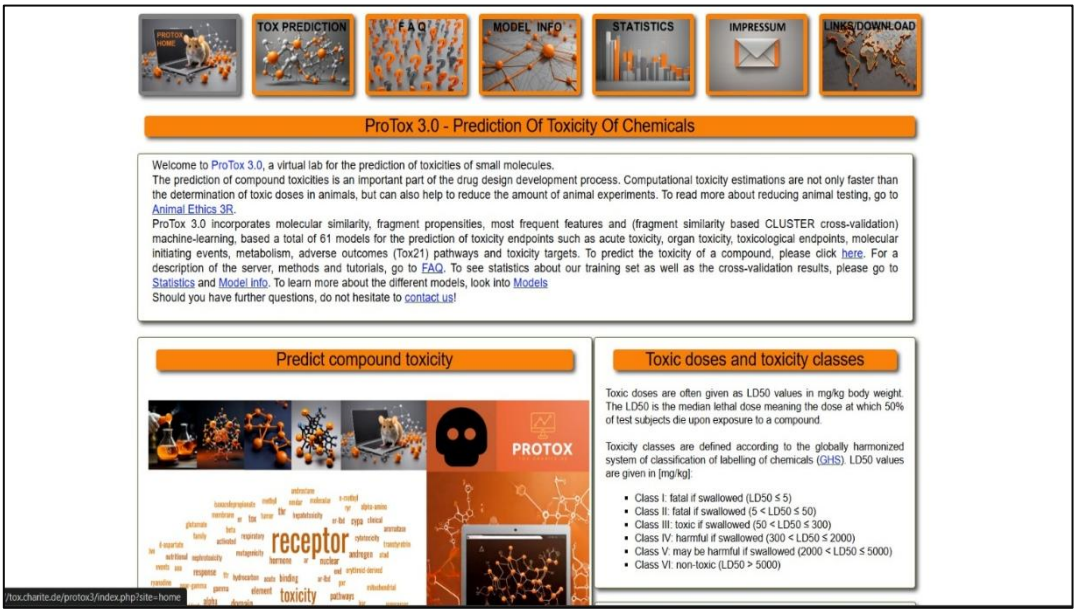


Fig.No.1.7 Protox II Software Homepage

1.7.5 SwissADME

SwissADME is a free web-based computational tool used for prediction of pharmacokinetic properties, drug-likeness, and medicinal chemistry parameters of compounds.

The software is extensively used in modern drug discovery and in-silico pharmacology research.

The software provides graphical and tabulated analysis of compounds based on pharmacokinetic parameters.

In the present study, SwissADME was used for:

- ADME analysis of Neem bark phytoconstituents

- Evaluation of pharmacokinetic properties
- Drug-likeness prediction
- Lipinski rule evaluation

Importance of Software

The software and databases used in the present study play an important role in computational analysis and network pharmacology investigation of Neem bark phytoconstituents.

These tools collectively help in:

- Identification of phytochemicals
- Molecular analysis
- Drug-likeness prediction
- Toxicity assessment
- Pharmacokinetic evaluation
- Computational therapeutic analysis

The integration of these computational tools provides a scientific basis for evaluating the therapeutic potential of Neem bark compounds

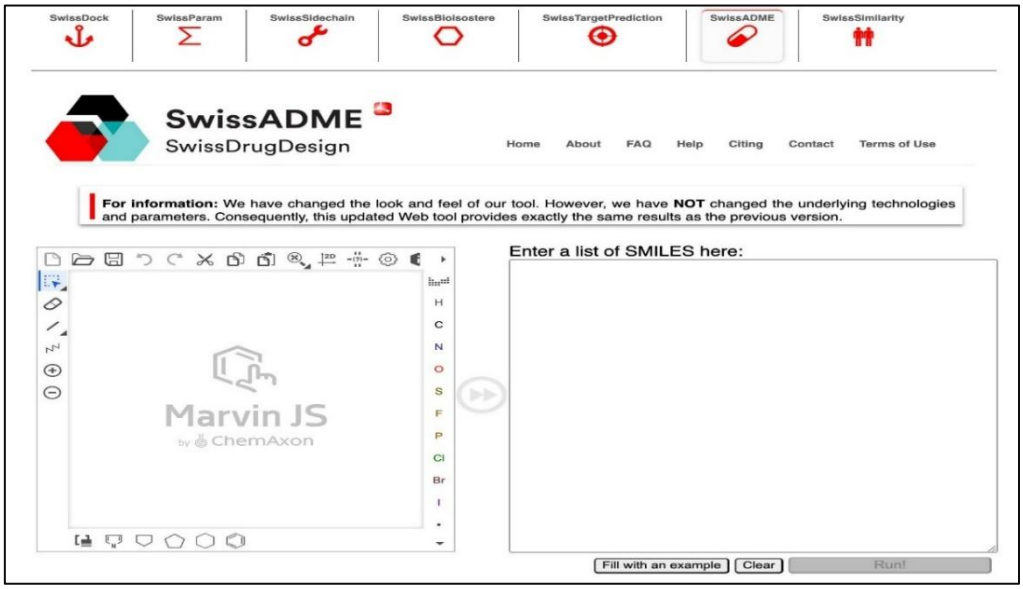


Fig.No.1.8 SwissADME

6. Literature Review

Some scientists looked into neem's plant chemicals, healing effects, and computer-based treatment possibilities. Studies show neem holds many naturally working substances behind its wide medical uses. New tools in digital drug research plus connection mapping added deeper insight on how these natural parts may act inside the body.

Kavey M.R.H., Hossain M.A., Shohag M.S.R., Ansari I.A., et al. (2025)

Looking at Neem compounds, Kavey MRH and team in 2025 explored how they might work on multiple fronts against Alzheimer's. Through network analysis, docking studies, and simulations, they mapped out key genes tied to the disease - like ESR1, HSP90AA1, SRC, HIF1A, and EP300. These plant-based substances showed strong binding behavior with proteins, holding steady during testing phases. Instead of just one pathway, their effect spread across several critical points linked to illness control. While results are early, stability in interaction patterns suggests a layered influence worth further attention.

Jadar P.G., Haritha M.M. (2024)
A fresh look at Neem's natural compounds began by pulling data from the IMPPAT library. With Molsoft's digital tools, their behavior inside the body took shape on screen. Instead of lab tests, simulations shaped insights into how these plant chemicals might act like medicines.
Among Neem-based compounds, traits like size, fat solubility, ability to form hydrogen bonds, alongside compliance with Lipinski's criteria appeared in the analysis. It turned out many active parts from Neem met key benchmarks tied to how drugs behave inside the body.
Computational screening might just be a quiet game changer in finding new herbal medicines, one overlooked compound at a time. Discovery gets a nudge forward when algorithms dig through plant data faster than traditional methods ever could. Instead of endless lab trials, computers spot promising candidates early. This shift opens doors without loud announcements or grand claims. Potential leads emerge not from chance but from pattern recognition buried in complexity. Pharmaceutical research gains depth simply by listening to what data quietly suggests.
Surprisingly, Neem's plant compounds show traits similar to those of potential medicines. These features make them fit well into computer-based drug studies. Instead of lab tests, researchers can explore their actions through digital models. Networks mapping how they interact with biological systems also benefit. Their behavior aligns closely with what such analyses require.

Andrew L. Hopkins (2008)
Among those exploring new paths in medicine, Hopkins AL made strides in 2008 by framing network pharmacology as a way to rethink how drugs are found. Instead of focusing on single molecules, the work looked at how entire networks within cells respond. Herbal remedies, it turns out, often carry many working parts rather than just one. These components may hit several biological spots at once. Because of this, their effects can arise from teamwork across various pathways. Seeing these connections helps make sense of why plant-based treatments sometimes succeed where others fail.

Pandey G., Verma K.K., Singh M. (2014)
Looking into neem bark extracts, researchers checked their chemical makeup alongside ability to fight bacteria and oxidative damage. Tests showed clear signs of key natural compounds like flavonoids, tannins, alkaloids, glycosides, terpenoids. While examining plant-based substances, scientists found several active ingredients present. These components often linked to biological effects turned up consistently across samples tested. Among findings were molecules known for influencing health-related processes within living systems.
From behind lab benches came results showing Neem bark fights harmful microbes effectively. Not far into the analysis emerged proof of its ability to neutralize unstable molecules - pointing toward protective chemical behavior within the plant's tissue.
One reason behind Neem bark's effects might lie in its dense mix of plant compounds. Not surprisingly, researchers point to its role as a key resource in developing medicines from herbs. What stands out is how often such natural extracts appear in studies looking for new treatments. Though less talked about, the bark has shown consistent results across different lab tests. Its value comes through not just in tradition but also in repeatable experiments. Few plants offer quite the range seen here when it comes to chemical variety.
Surprising results show Neem bark's plant chemicals matter more than thought - opening doors for computer-driven drug research built on solid data. Hidden patterns in the compounds point toward smarter ways to map how natural substances interact inside biological networks.

7. Aim And Objectives of Work

3.1 Aim of The Study

The aim of the present study was to investigate the phytochemical constituents and therapeutic potential of Neem bark (*Azadirachta indica*) using phytochemical screening, network pharmacology, and in-silico pharmacological approaches**.**

3.2 Objectives of the Study

Primary Objectives:

- To collect and authenticate Neem bark for research study.
- To prepare Neem bark extract using cold maceration method.
- To perform phytochemical screening of Neem bark extract.
- To identify phytoconstituents present in Neem bark.

Secondary Objectives:

- To evaluate drug-likeness properties using Molsoft software.
- To predict toxicity profile using Protox-II software.
- To analyze pharmacokinetic properties using SwissADME.
- To study therapeutic potential using computational pharmacology approaches.

8. Plan of Work

The present work was systematically designed to evaluate the phytochemical and computational pharmacological properties of Neem bark using experimental and in-silico approaches. The study was carried out through a sequence of organized steps to ensure proper phytochemical analysis and computational evaluation of selected phytoconstituents.

Collection of Neem Bark
↓
Authentication of Plant Material
↓
Cleaning and Shade Drying
↓
Preparation of Coarse Powder
↓
Extraction by Cold Maceration
↓
Preliminary Phytochemical Screening
↓
Identification of Phytoconstituents
↓
Drug-Likeness Prediction (Molsoft)
↓
ADME Analysis (SwissADME)
↓
Toxicity Prediction (Protox-II)
↓
Results and Discussion
↓
Conclusion

9. Methodology

To explore what chemicals live inside neem bark (Azadirachta indica), this study set up a clear plan. Plant bits were gathered step by step, then soaked slowly in solvent to pull out compounds. After that, basic tests helped spot key natural substances through trusted lab steps. Everything done in the lab follows the approach laid out here next.

5.1 Collection of Neem Bark

Fresh bark of Neem (Azadirachta indica) was collected from healthy and mature Neem trees. The collected bark was carefully selected to avoid contamination, fungal growth, and damaged portions. The plant material was procured for phytochemical and computational pharmacology studies.

5.2 Authentication of Plant Material

The collected neem bark was authenticated based on its morphological characteristics such as color, texture, odor, and appearance. Authentication of the plant material was carried out to ensure that the selected crude drug was genuine and suitable for further experimental studies.

5.3 Cleaning and Drying

Starting with a rinse, the collected bark got cleaned well using pure water to wash away dirt, grime, and foreign matter. Once it looked clean, workers sliced it into tiny chunks before leaving it out of direct sun to dry slowly near normal indoor conditions for about two weeks. Keeping it cools during drying helped keep delicate natural compounds intact without breaking them down.

5.4 Preparation of Powder

Once fully dry, the neem bark went into a grinder, turning it into rough powder. After grinding, a sieve sorted the particles by size - keeping them even. Stored away afterward, the powder stayed sealed tight, safe from damp air and sun rays waiting for its next step.

5.5 Preparation of Extract by Cold Maceration Method

Principle:

Cold maceration is a simple extraction technique in which powdered plant material is soaked in a suitable solvent for a specified period at room temperature. During this process, the solvent penetrates the plant tissues and dissolves the active phytochemical constituents present in the crude drug.

Materials Required:

1. Neem bark powder
2. Ethanol (70%)
3. Conical flask with stopper
4. Muslin cloth
5. Whatman filter paper
6. Measuring cylinder
7. Glass rod
8. Water bath

Procedure:

1. Approximately 100 g of dried neem bark powder was accurately weighed and transferred into a clean conical flask.
2. About 500 mL of 70% ethanol was added to the flask containing the powdered drug.
3. The flask was tightly closed with a stopper to prevent evaporation of the solvent.
4. The mixture was allowed to stand for 72 hours at room temperature.
5. During the maceration period, the flask was shaken intermittently to facilitate proper extraction of phytoconstituents.
6. After completion of extraction, the mixture was filtered first through muslin cloth and then through Whatman filter paper to remove solid plant residues.
7. The obtained filtrate was concentrated on a water bath at controlled temperature to obtain a semisolid crude extract.
8. The prepared extract was stored in an airtight container for further phytochemical screening.

5.6 Preliminary Phytochemical Screening

The Neem bark extract was subjected to preliminary phytochemical screening for identification of different phytoconstituents.

5.6.1 Phytochemical Tests Performed:

Sr. No	Phytochemical	Test Performed
1.	Alkaloids	Mayer's Test
2.	Flavonoids	Alkaline Reagent Test
3.	Glycosides	Keller-Killiani Test
4.	Tannins	Ferric Chloride Test
5.	Saponins	Foam Test
6.	Terpenoids	Salkowski Test
7.	Phenols	Ferric Chloride Test
8.	Carbohydrates	Molisch Test

5.7 Test Procedures

Sr. No.	Test	Procedure	Observation	Inference
1	Mayer's Test (Alkaloids)	Few drops of Mayer's reagent were added to the extract.	Cream colored precipitate formed.	Presence of Alkaloids
2	Alkaline Reagent Test (Flavonoids)	Sodium hydroxide solution was added to the extract.	Yellow coloration appeared.	Presence of Flavonoids
3	Keller-Killiani Test (Glycosides)	Glacial acetic acid, ferric chloride and conc. H_2SO_4 were added to the extract.	Brown ring formed.	Presence of Glycosides
4	Ferric Chloride Test (Tannins)	Ferric chloride solution was added to the extract.	Blue-black or green coloration appeared.	Presence of Tannins
5	Foam Test (Saponins)	The extract was shaken vigorously with water.	Stable foam was formed.	Presence of Saponins
6	Salkowski Test (Terpenoids)	Chloroform and conc. H_2SO_4 were added to the extract.	Reddish-brown coloration appeared.	Presence of Terpenoids
7	Ferric Chloride Test (Phenols)	Ferric chloride solution was added to the extract.	Dark blue coloration appeared.	Presence of Phenolic compounds
8	Molisch Test (Carbohydrates)	Molisch reagent and conc. H_2SO_4 were added to the extract.	Violet ring was formed.	Presence of Carbohydrates

Figure 5.1: Test Procedures for Preliminary Phytochemical Screening

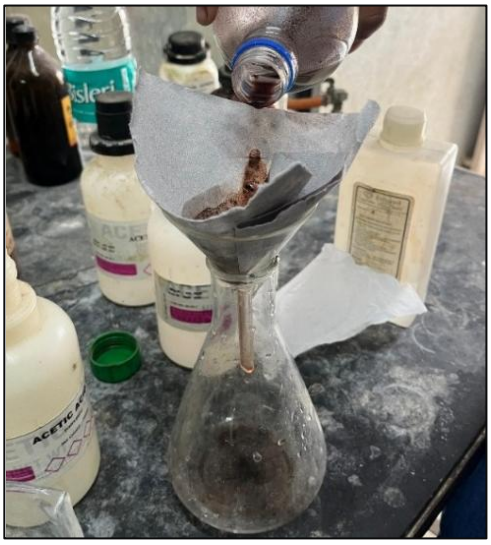


Fig.No.5.2 Filtration

Fig.No.5.3 Test Performed

6. Result And Discussion

6.1 Phytoconstituent Analysis of neem bark

Chemical Name	Activity Count	Plant Part	Molecular Weight	HBD	HBA	Drug Likeness Score
1-TIGLOYL-3-ACETYL-11-METHOXY-AZADIRACHTININ	0	BARK	734.7 g/mol	2	16 (> 10)	-0.61
6-DESACETYLNIMBINENE	0	BARK	440.22	1	6	-0.19
NIMBINENE	0	BARK	482.23	0	7	-0.29
NIMBIOL	0	BARK	272.4 g/mol	1	2	0.37
SUGIOL	1	BARK	300.4 g/mol	1	2	0.46

6.2 Drug-Likeness Analysis

1) 1-Tigloyl-3-Acetyl-11-Methoxy-Azadirachtinin

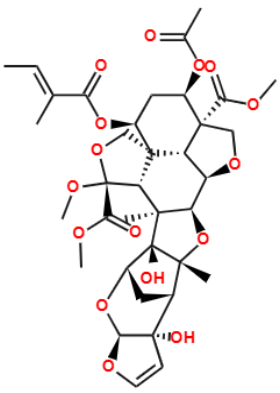
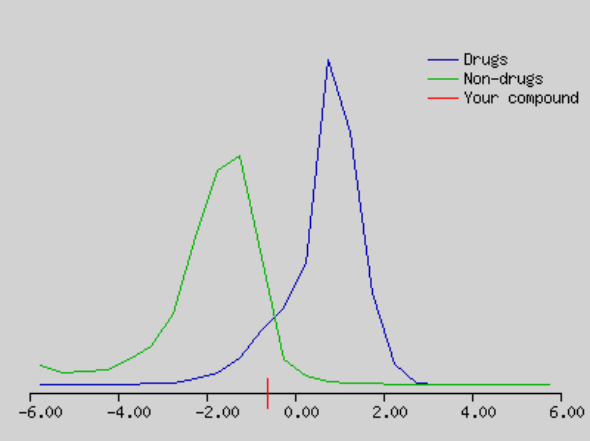


Fig.No.6.2.1 Molecular Structure

Drug-likeness model score: -0.61



2) 6-Desacetylnimbinene

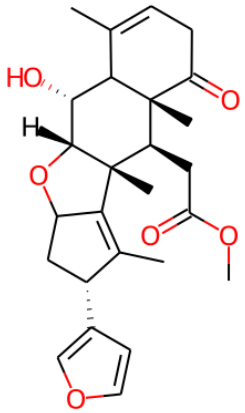
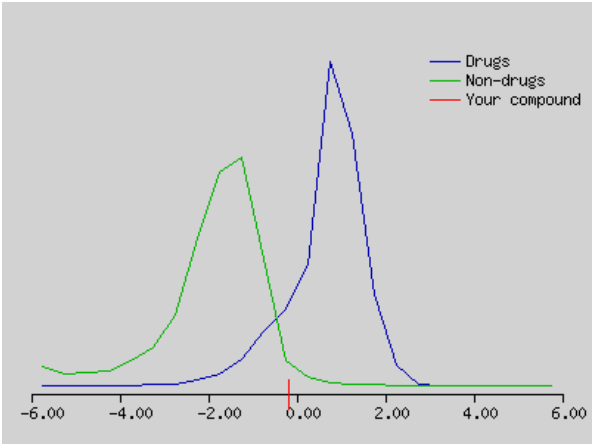


Fig.No.6.2.2 Molecular Structure

Drug-likeness model score: -0.19



3) Nimbinene

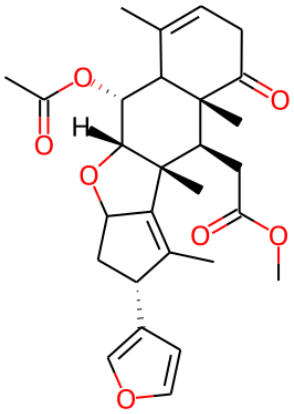
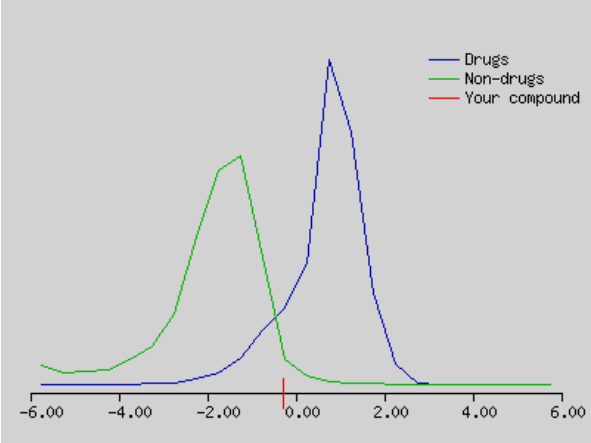


Fig.No.6.2.3 Molecular Structure

Drug-likeness model score: -0.29



4) Nimbiol

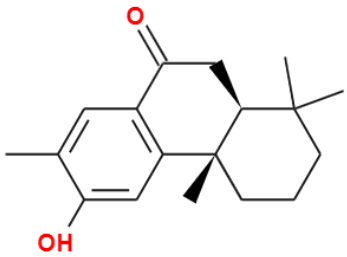
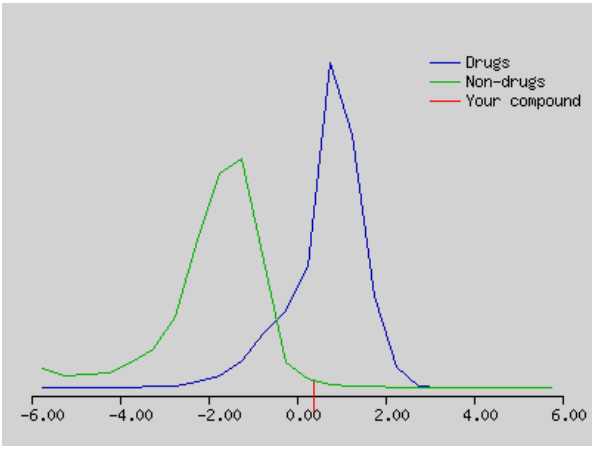


Fig.No.6.2.4 Molecular Structure

Drug-likeness model score: 0.37



5) **Sugiol**

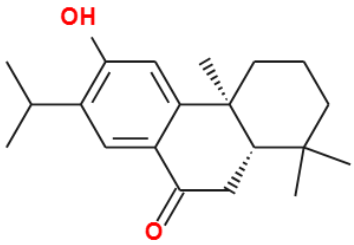
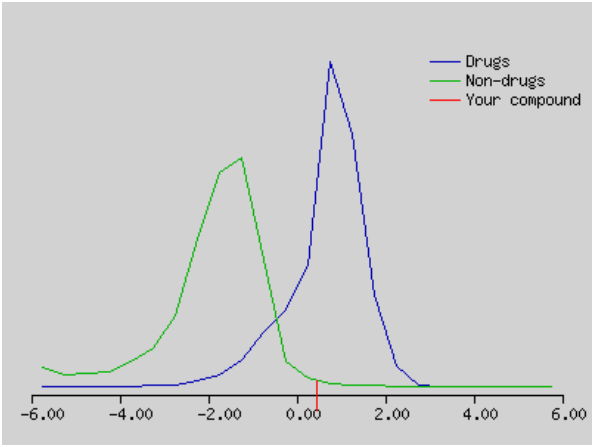


Fig.No.6.2.5 Molecular Structure

Drug-likeness model score: 0.46



6.3 Protox-II Toxicity Prediction (Nimbiol)

Toxicity Parameter	Prediction	Probability
Hepatotoxicity	Inactive	0.71
Neurotoxicity	Inactive	0.54
Nephrotoxicity	Inactive	0.89
Respiratory Toxicity	Inactive	0.56
Cardiotoxicity	Inactive	0.64
Carcinogenicity	Inactive	0.73
Immunotoxicity	Inactive	0.98
Mutagenicity	Inactive	0.92
Cytotoxicity	Inactive	0.87
BBB Barrier	Active	0.90
Ecotoxicity	Active	0.65

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BBB Barrier	Active	0.90
Ecotoxicity	Active	0.65

6.5 Discussion and Interpretation

This study aimed to examine the phytochemical composition and therapeutic potential of Neem bark through phytochemical screening and computational pharmacology methods.

Initial screening confirmed the presence of key bioactive compounds in the Neem bark extract, including alkaloids, flavonoids, glycosides, tannins, saponins, terpenoids, phenols, and carbohydrates—substances widely recognized for their medicinal and pharmacological effects.

Further analysis highlighted two notable constituents, Nimbiol and Sugiol. Evaluation of drug-like properties showed that both compounds exhibit suitable molecular characteristics and acceptable drug-likeness profiles, with Sugiol scoring higher, suggesting greater potential for pharmacological application.

Toxicity predictions using the ProTox-II tool indicated low risk across major categories such as hepatotoxicity, cardiotoxicity, mutagenicity, carcinogenicity, and cytotoxicity, pointing to a favorable safety profile for these compounds.

Structural analysis and computational modeling suggest that Nimbiol and Sugiol may hold considerable therapeutic value and could be of significant medicinal interest.
In conclusion, the findings reinforce the pharmacological relevance of Neem bark and highlight the effectiveness of computational techniques—including network pharmacology, drug-likeness assessment, and toxicity prediction—in assessing plant-derived compounds.

7. Conclusion

This study successfully assessed the phytochemical composition and therapeutic potential of Neem bark using phytochemical analysis and computational pharmacology methods.
Initial screening revealed the presence of key bioactive compounds in the Neem bark extract, including alkaloids, flavonoids, glycosides, tannins, saponins, terpenoids, phenols, and carbohydrates. These constituents are associated with a range of medicinal properties, underlining the pharmacological significance of Neem bark.
Further analysis identified specific compounds such as Nimbiol and Sugiol. Evaluation of their drug-like properties indicated favorable molecular characteristics and acceptable drug-likeness scores, suggesting they are suitable candidates for further investigation in drug development.
Examination of molecular structures highlighted functional groups linked to biological activity. Toxicity predictions using Protox-II showed predominantly non-toxic outcomes across major parameters—such as hepatotoxicity, cardiotoxicity, mutagenicity, carcinogenicity, and cytotoxicity—indicating a generally safe profile for these compounds.
The findings suggest that Neem bark contains bioactive substances with significant therapeutic potential. The study also confirms the effectiveness of computational tools like SwissADME, Molsoft, and Protox-II in analyzing plant-derived compounds.
In conclusion, the results provide scientific validation for the traditional use of Neem bark and point to its promising role in future research on herbal medicines, computational drug discovery, and therapeutic development.

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